

## **Supporting Information**

### **Quantum Tunneling in Reactions Modulated by External Electric Fields: Reactivity and Selectivity**

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## 1. Computational details and additional analysis

### 1.1. Computational details

All geometry optimization (using a verytight keyword), frequency and energy-evaluation calculations except DLPNO-CCSD(T1) method were conducted using Gaussian16 program.<sup>1</sup> Applied EEF was computed using a keyword of “Field=M+N” (<https://gaussian.com/field/>), where M and N represent the direction and magnitude (1 au =  $5.14 \times 10^{11}$  V/m). All calculations for non-tunneling and tunneling reaction rates were carried out by Polyrate17<sup>2</sup> with Gaussrate17<sup>3</sup> interface to Gaussian16. The non-tunneling rate constants ( $k_{\text{CVT}}$ ) were computed by canonical variational transition state theory (CVT).<sup>4</sup> while the transmission coefficient ( $\kappa_{\text{SCT}}$ ) was calculated by the multidimensional small curvature tunneling (SCT)<sup>5-6</sup> approximation method to give tunneling-involving rate constant ( $k_{\text{SCT}} = \kappa_{\text{SCT}} \times k_{\text{CVT}}$ ). The overall rate constants,  $k_{\text{CVT+SCT}} = k_{\text{CVT}} + k_{\text{SCT}}$ , were obtained. The quantized reactant state tunneling (QRST)<sup>7-8</sup> with full states was applied for the reactions of hydroxycarbenes (R-C-OH; R=H, OH, CH<sub>3</sub>, CN) (Scheme S3a)<sup>9-12</sup> at low temperature. 200 quantized reactant states were included in the tunneling calculations (variable STATES in QRST keyword) for the arene molecule bearing two hydroxycarbene groups (Scheme S3d, S3e).

On the basis of our benchmark study using high-level DLPNO-CCSD(T1)/aug-cc-pVTZ<sup>13-15</sup> method (implemented in ORCA5.0 and using tightPNO)<sup>16</sup> in the absence of EEF, several common and reliable DFT functionals and basis sets were tested and selected. Compared to the previous work using highly accurate focal-point analysis (FPA)//AE-CCSD(T)/cc-pCVQZ method (Table S2),<sup>9</sup> the  $\omega$ B97X-D/6-31G(d,p)<sup>18-20,23</sup> method was found to give the most reliable barrier in terms of enthalpy (the error of about 0.1~0.6 kcal/mol). In addition, the energy barrier ( $\Delta E^\ddagger$ ) for S<sub>N</sub>2 reaction under no-EEF by M06-2X/6-31+G(d)<sup>17-22</sup> method gives the most similar energy barrier to the DLPNO-CCSD(T1)/aug-cc-pVTZ (~0.2 kcal/mol difference, Table S111). For the di- $\pi$ -methane (DPM) rearrangement of benzobarrelene, the  $\omega$ B97X-D/6-31G(d) method almost reproduces the energy barrier by the DLPNO-CCSD(T1)/aug-cc-pVTZ method (~0.02 kcal/mol difference, Table S122) for the first step (**TS1**). Therefore,  $\omega$ B97X-D and M06-2X functionals combined with 6-31G(d,p) basis sets were used to compute the hydroxycarbenes.<sup>9-12</sup> Whereas, M06-2X/6-31+G(d) with PCM model (water

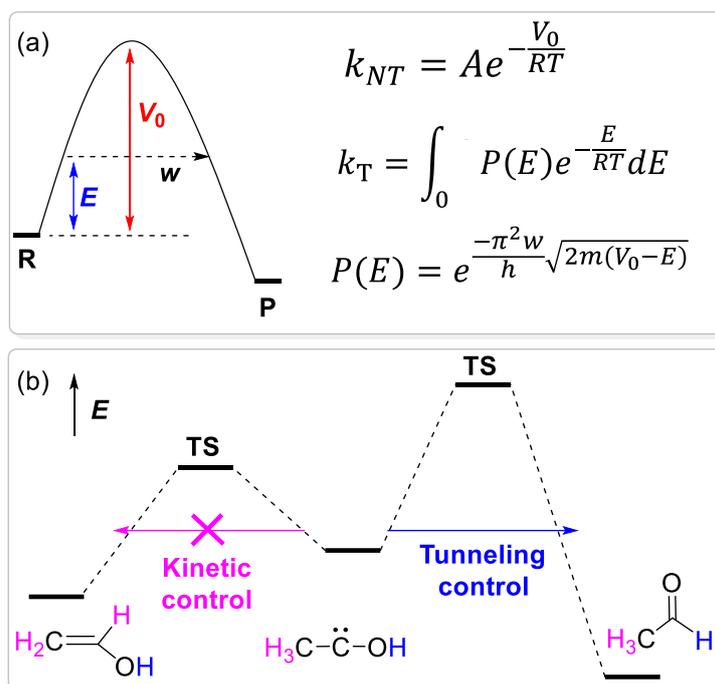
solution) was used to compute S<sub>N</sub>2 reaction,<sup>24</sup> and ωB97X-D/6-31G(d) was selected to further study the DPM rearrangement of benzobarrelene.<sup>25-27</sup>

The crossover temperature ( $T_c$ ) was calculated by following equation:<sup>28</sup>

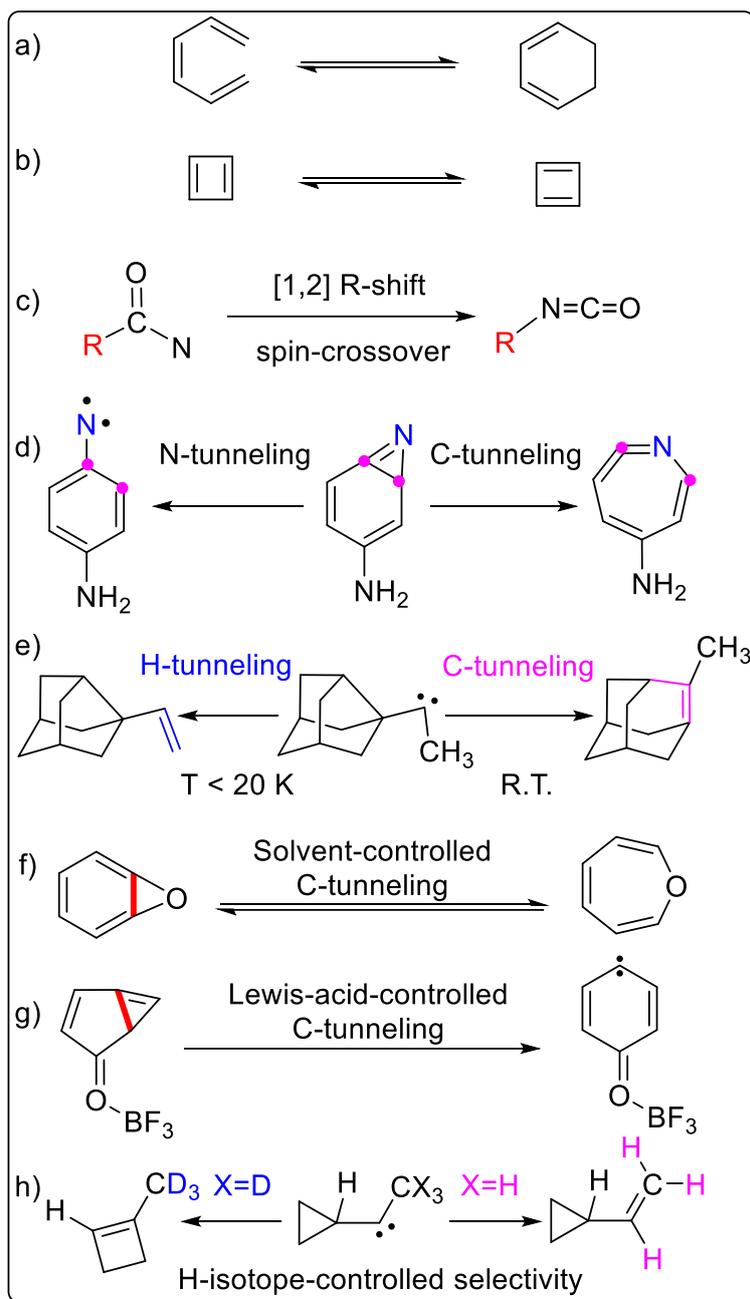
$$T_c = \frac{\hbar\Omega}{2\pi k_B},$$

where the  $\Omega$  is the absolute value of the imaginary frequency corresponding to the transition state mode, and  $k_B$  is a Boltzmann's constant.

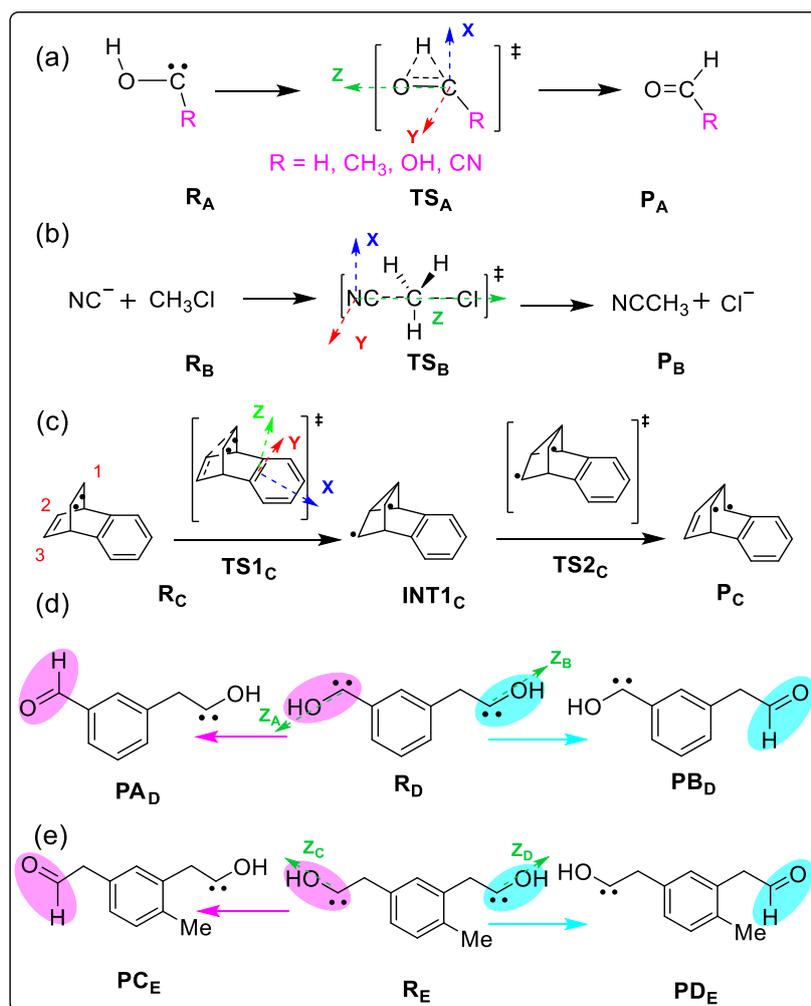
## 1.2 Previous works and our present work



**Scheme S1.** (a) Key features of QT in a reaction ( $k_{NT}$  and  $k_T$  are the reaction rate constants without tunneling and with tunneling contributions, respectively;  $P(E)$  is the transmission probability of tunneling at energy ( $E$ )). (b) Kinetic- and tunneling-controlled 1,2-H migration.



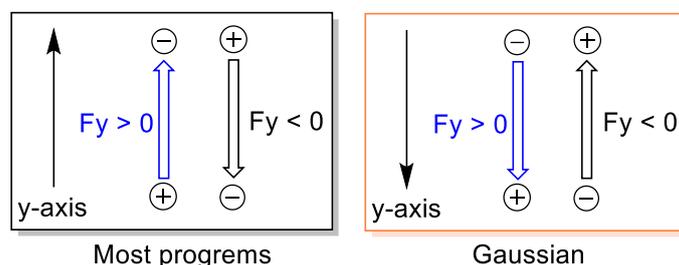
**Scheme S2.** Selected examples involving heavy-atom-tunneling reactions.



**Scheme S3.** (a) 1,2-H migration of four hydroxycarbenes ( $\text{R}-\text{C}-\text{OH}$ ;  $\text{R} = \text{H}, \text{OH}, \text{CH}_3, \text{CN}$ ). (b)  $\text{S}_\text{N}2$  reaction. (c) Triplet di- $\pi$ -methane (DPM) rearrangement of benzobarrelene. (d) Chemo- and (e) site-selectivity of the 1,2-H migration of one arene molecule bearing two hydroxycarbene groups with similar/same reactivity. The direction of EEF is indicated by the colored arrows.

**Table S1.** Comparison of summarizing the various focus between the work by Kozuch (*Chem. Sci.* 2021, 12, 3179-3187) and our work under the EEF.

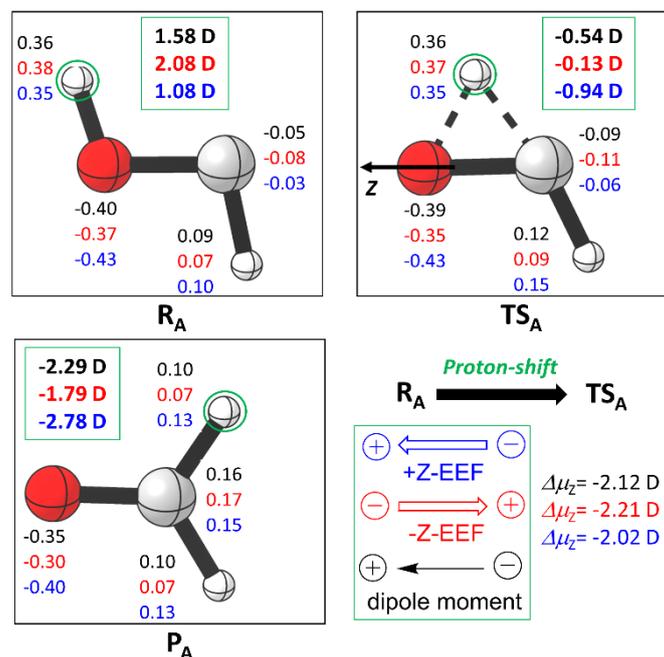
	Work by Kozuch	Our present work
<b>Systems</b>	Ground state carbon-tunneling	Excited-state carbon tunneling
	Neutral system	H-tunneling Charged or neutral system
<b>Properties</b>	Overall reaction rate constant	Overall, non-tunneling, and tunneling-involving rate constants
		Quantum tunneling contribution ratio, crossover temperature and transmission coefficient decrease, when the barrier is reduced and becomes narrower under EEF
		Selectivity controlled by EEF
<b>Reaction condition</b>	at cryogenic condition	< 400K



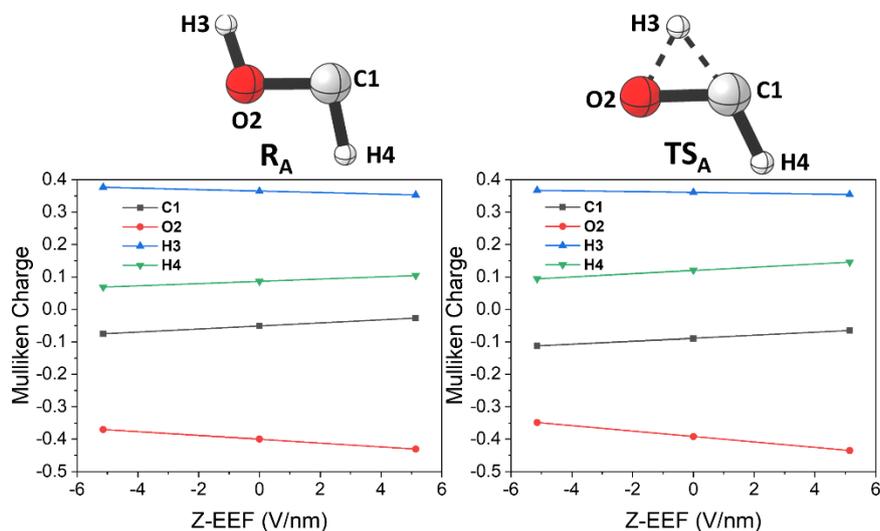
**Scheme S4.** Conventions for field vectors in different programs.

Considering an EEF along the y-axis, most programs use the convention originating in physics, wherein the direction of the EEF vector is from positive to negative. However, the convention in Gaussian is opposite (Scheme S4). To avoid confusion, here we uniformly use the Gaussian convention in this work.

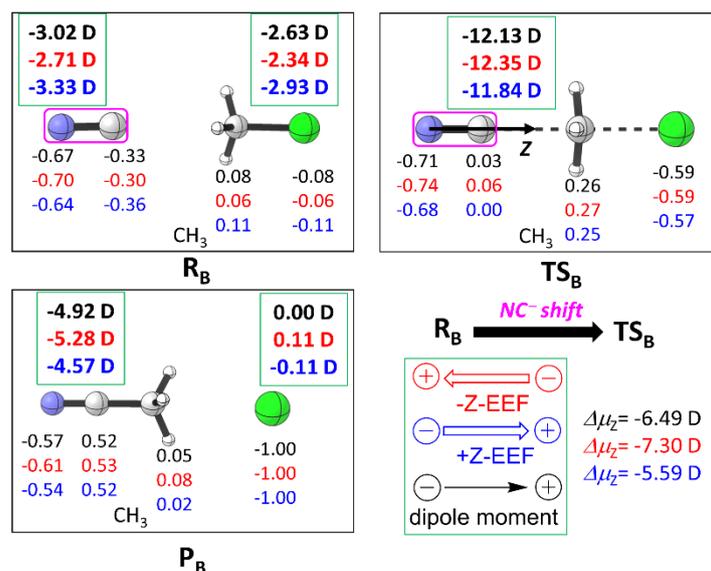
### 1.3 Electronic structures in the EEF



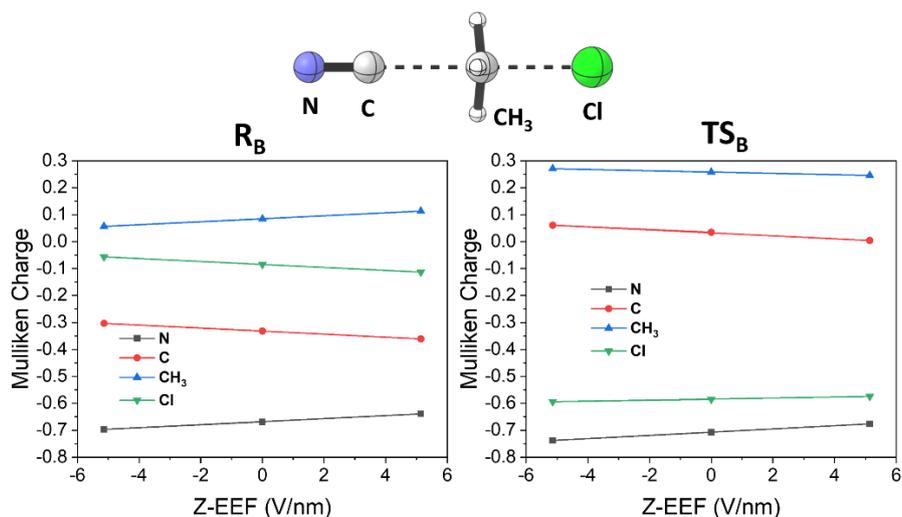
**Figure S1.** Mulliken atomic charges and Z-axis dipole moments (Debye) for reactant ( $R_A$ ), transition state ( $TSA$ ) and product ( $P_A$ ) under the Z-EEF ( $\pm 5.14$  V/nm) and no field (0 V/nm). The charge and dipole values are color-coded: no field (in black), for Z-EEF =  $-5.14$  V/nm (in red) and for Z-EEF =  $+5.14$  V/nm (in blue).



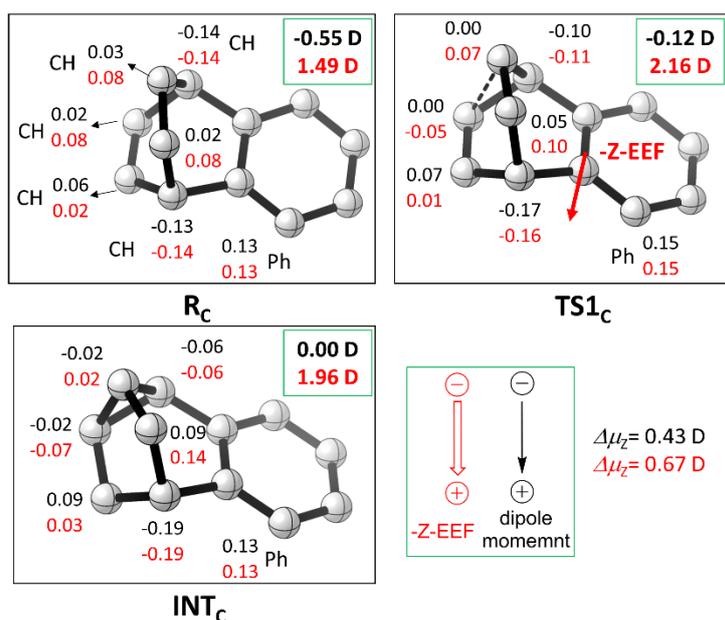
**Figure S2.** Changes of Mulliken atomic charges for reactant ( $R_A$ ), transition state ( $TSA$ ) under the Z-EEF ( $\pm 5.14$  V/nm) and no field (0 V/nm).



**Figure S3.** Mulliken atomic charges and Z-axis dipole moments (Debye, D) for isolated reactant ( $R_B$ ), transition state ( $TS_B$ ) and isolated product ( $P_B$ ) under the Z-EEF (-1.54 or 1.54 V/nm) and no field (0 V/nm). The charge and dipole values are color-coded: no field (in black), Z-EEF = -1.54 V/nm (in red) and Z-EEF = +1.54 V/nm (in blue).



**Figure S4.** Changes of Mulliken atomic charges for reactant ( $R_B$ ), transition state ( $TS_B$ ) under the Z-EEF (-1.54 or 1.54 V/nm) and no field (0 V/nm).



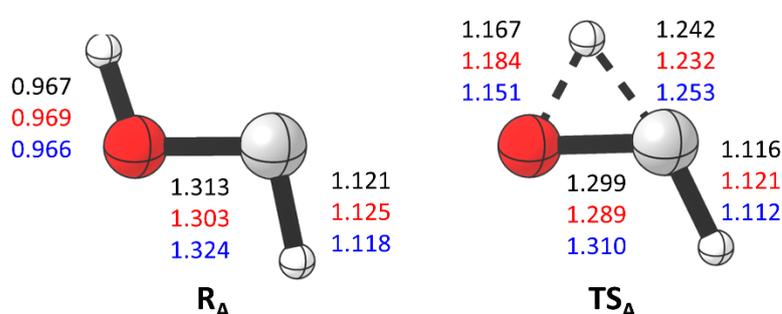
**Figure S5.** Mulliken atom charges and Z-axis dipole moments (Debye, D) for reactant ( $R_c$ ), transition state ( $TS1_c$ ) and intermediate ( $INT_c$ ) under the Z-EEF ( $-5.14$  V/nm) and no field ( $0$  V/nm). The charge and dipole values are color-coded: no field (in black) and Z-EEF =  $-5.14$  V/nm (in red).

To understand the EEF effect on the three reactions, the atomic charges of these reactions in the EEF and no field were summarized (Figures S1-S5). When the EEF was applied, the EEF promotes H/proton migration from the reactants to the corresponding transition states in the 1,2-H migration reaction. The H/proton (positively-charged) migrate from the left side to the right side in this reaction. Under the positive Z-EEF, such H/proton approaches the negative direction of the Z-EEF, which increases the Z-axis dipole moment by  $0.10$  Debye compared with no-field (Figure S1). Therefore, the transition states should gain large electrostatic stabilization than the reactants and, thus, lower the barriers.

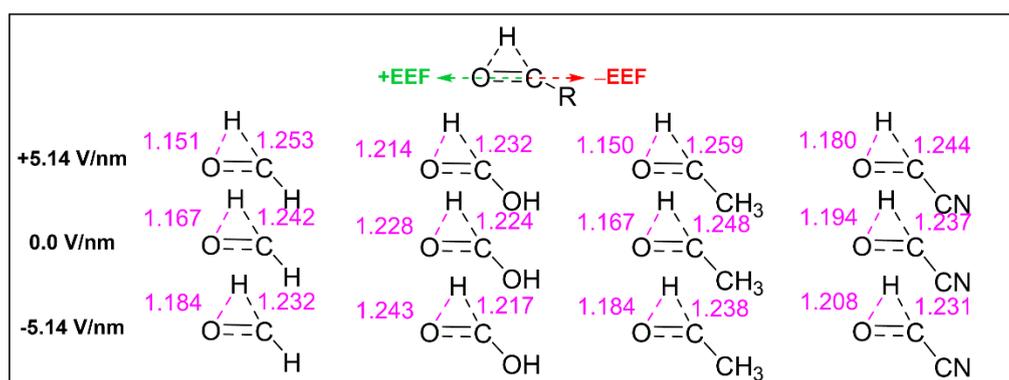
In the same manner, for the  $S_N2$  reaction, the CN anion on the left side attacks the alkyl carbon, accompanied by dissociation of the Cl anion on the right side. Overall, the formal negative charge is shifted from the left side to the right side. Therefore, under the positive Z-EEF, such negative-charge shifting approaches and is parallel to the positive direction of the Z-EEF, which should gain large electrostatic stabilization in the transition states (relative to the reactants) and, thus, lower the barrier. Some polarization in the transition states further enhances such preferential electrostatic

stabilization. Therefore, a larger change in the Z-axis dipole moment (0.89 D) from the reactant to the transition state by the positive Z-EEF was found, compared with no-field case (Figure S3). A similar trend (but smaller effect) can be observed in the EEF for the DPM system (Figure S5). As suggested by Kozuch (*Chem. Sci.* **2020**, *12*, 3179-3187), such electrostatic stabilization by EEF should also increase thermodynamically driving force, which results in earlier transition states and, thus, narrower barrier width, according to Hammond postulate.

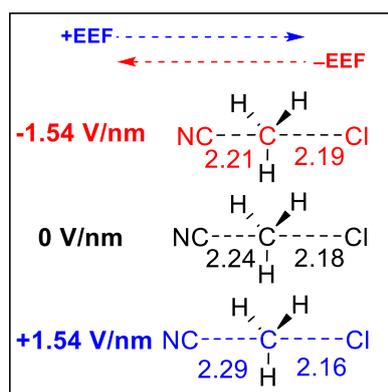
#### 1.4 Geometrical structures in the EEF



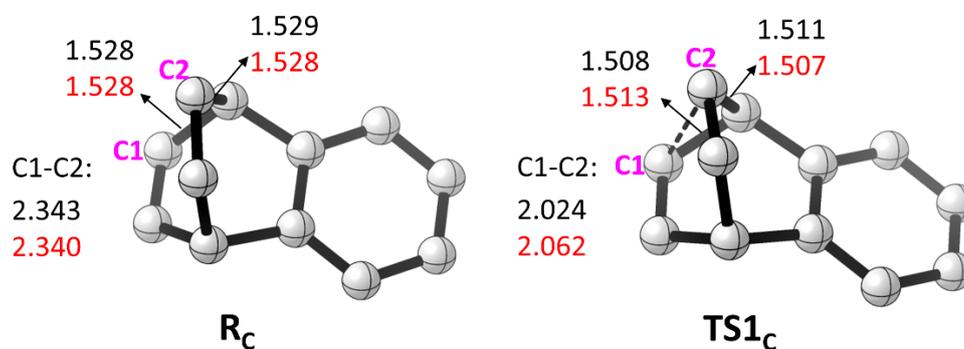
**Figure S6.** The computed O-H bond length (in Angstrom) of the 1,2-H migration for reactant ( $\mathbf{R}_A$ ) and transition state ( $\mathbf{TS}_A$ ) for hydroxycarbenes (H-C-OH) under the Z-EEF ( $\pm 5.14$  V/nm) and no field (0 V/nm). The bond length values are color-coded: no field (in black), for Z-EEF =  $-5.14$  V/nm (in red) and for Z-EEF =  $+5.14$  V/nm (in blue).



**Figure S7.** The computed O-H bond length (in Angstrom) of the 1,2-H migration transition state ( $\mathbf{TS}_A$ ) for various hydroxycarbenes (R-C-OH; R = H, OH, CH<sub>3</sub>, CN) under the Z-EEF ( $\pm 5.14$  V/nm) and no field (0 V/nm).



**Figure S8.** The computed key bond length (in Angstrom) of the  $S_N2$  transition state (**TS<sub>B</sub>**) under the Z-EEF (V/nm).



**Figure S9.** Change in the key bond length (in Angstrom) of triplet DPM rearrangement for reactant (**R<sub>c</sub>**) transition state (**TS1<sub>c</sub>**) under the Z-EEF (-5.14 V/nm and 0 V/nm). The bond length values are color-coded: no field (in black) and Z-EEF = -5.14 V/nm (in red).

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### 3. Figures and Tables

#### 3.1 The 1,2-H Migration of Hydroxycarbenes using the $\omega$ B97X-D method

**Table S2.** Computed barrier in terms of enthalpies ( $\Delta H$  in kcal/mol) for the H-migration reaction of different hydroxycarbenes (R-C-OH; R = H, OH, CH<sub>3</sub>, CN) using different DFT methods in gas phase. The values in parentheses are the computed barrier error ( $\Delta\Delta H$ ) relative to the highest-level computational results using the focal-point analysis (FPA)//AE-CCSD(T)/cc-pCVQZ method by the Schreiner group (ref. S9)

Methods	R = H( $\Delta\Delta H$ )	R = CH <sub>3</sub> ( $\Delta\Delta H$ )	R = CN( $\Delta\Delta H$ )	R = OH( $\Delta\Delta H$ )
FPA//AE-CCSD(T)	<b>29.7 (0.0)</b>	<b>28.0 (0.0)</b>	<b>33.3 (0.0)</b>	<b>34.1 (0.0)</b>
B3LYP-D3/6-31G(d,p)	29.3 (0.4)	27.1 (0.9)	32.7 (0.6)	32.6 (1.5)
PBE0-D3/6-31G(d,p)	28.5 (1.2)	26.4 (1.6)	32.1 (1.2)	32.1 (2.0)
$\omega$ B97X-D/6-31G(d,p)	30.1 (0.4)	28.1 (0.1)	33.9 (0.6)	34.2 (0.1)
M06-2X/6-31G(d,p)	31.0 (1.3)	28.9 (0.9)	34.6 (1.3)	35.7 (1.6)

**Table S3.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) for the H-migration in H-C-OH using different DFT methods in gas phase. The values in parentheses are computed barrier error ( $\Delta\Delta E$ ) relative to the high-level results by the DLPNO-CCSD(T1)/aug-cc-pVTZ//M06-2X/6-31G(d,p) method.

Methods	$\Delta E(\Delta\Delta E)$
DLPNO-CCSD(T1)	<b>34.4 (0.0)</b>
M06-2X/6-31+G(d)	37.0 (2.4)
M06-2X/6-31G(d,p)	34.7 (0.3)
M06-2X/6-31+G(d,p)	35.6 (1.2)
M06-2X/cc-pVTZ	35.3 (0.9)
B3LYP-D3/6-31G(d,p)	33.0 (1.4)
PBE0-D3/6-31G(d,p)	32.2 (2.2)
$\omega$ B97X-D/6-31G(d,p)	33.8 (0.6)

**Table S4.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) for the H-migration reaction of different hydroxycarbenes (R-C-OH; R = H, OH, CH<sub>3</sub>, CN) by the M06-2X/6-31G(d,p) method, compared to the high-level computational results by the DLPNO-CCSD(T1)/aug-cc-pVTZ//M06-2X/6-31G(d,p) method in gas phase.

	Methods	$\Delta E(\Delta\Delta E)$
<b>H-C-OH</b>	DLPNO-CCSD(T1)	34.4 (0.0)
	M06-2X/6-31G(d,p)	34.7 (0.3)
<b>H<sub>3</sub>C-C-OH</b>	DLPNO-CCSD(T1)	32.2 (0.0)
	M06-2X/6-31G(d,p)	32.3 (0.1)
<b>NC-C-OH</b>	DLPNO-CCSD(T1)	37.3 (0.0)
	M06-2X/6-31G(d,p)	38.2 (0.9)
<b>HO-C-OH</b>	DLPNO-CCSD(T1)	38.5 (0.0)
	M06-2X/6-31G(d,p)	39.4 (0.9)

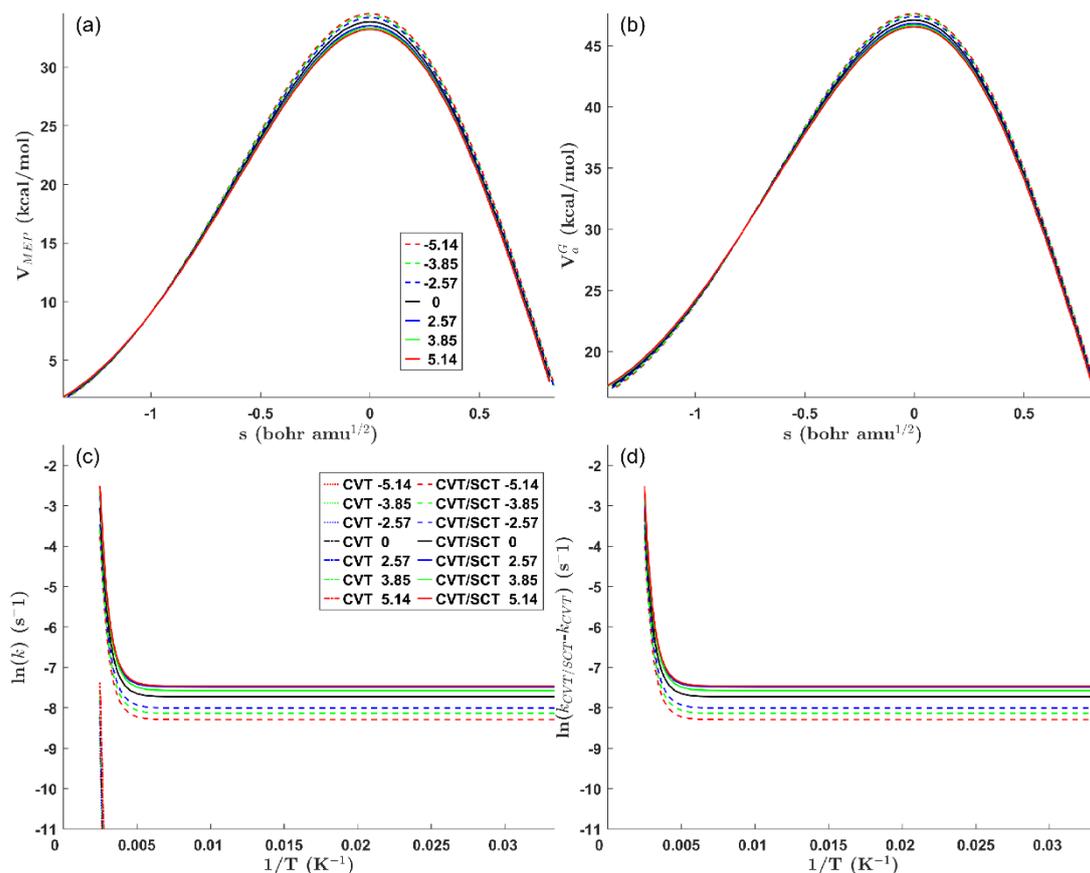
**Table S5.** Mulliken atomic charge of C, O, H in the hydroxycarbenes reactant (R-C-OH; R = H, OH, CH<sub>3</sub>, CN) using the  $\omega$ B97X-D method in gas phase.

	<b>R = H</b>	<b>R = CH<sub>3</sub></b>	<b>R = CN</b>	<b>R = OH</b>
C	-0.05	0.08	0.12	0.16
O	-0.40	-0.42	-0.38	-0.43
H	0.36	0.36	0.38	0.35

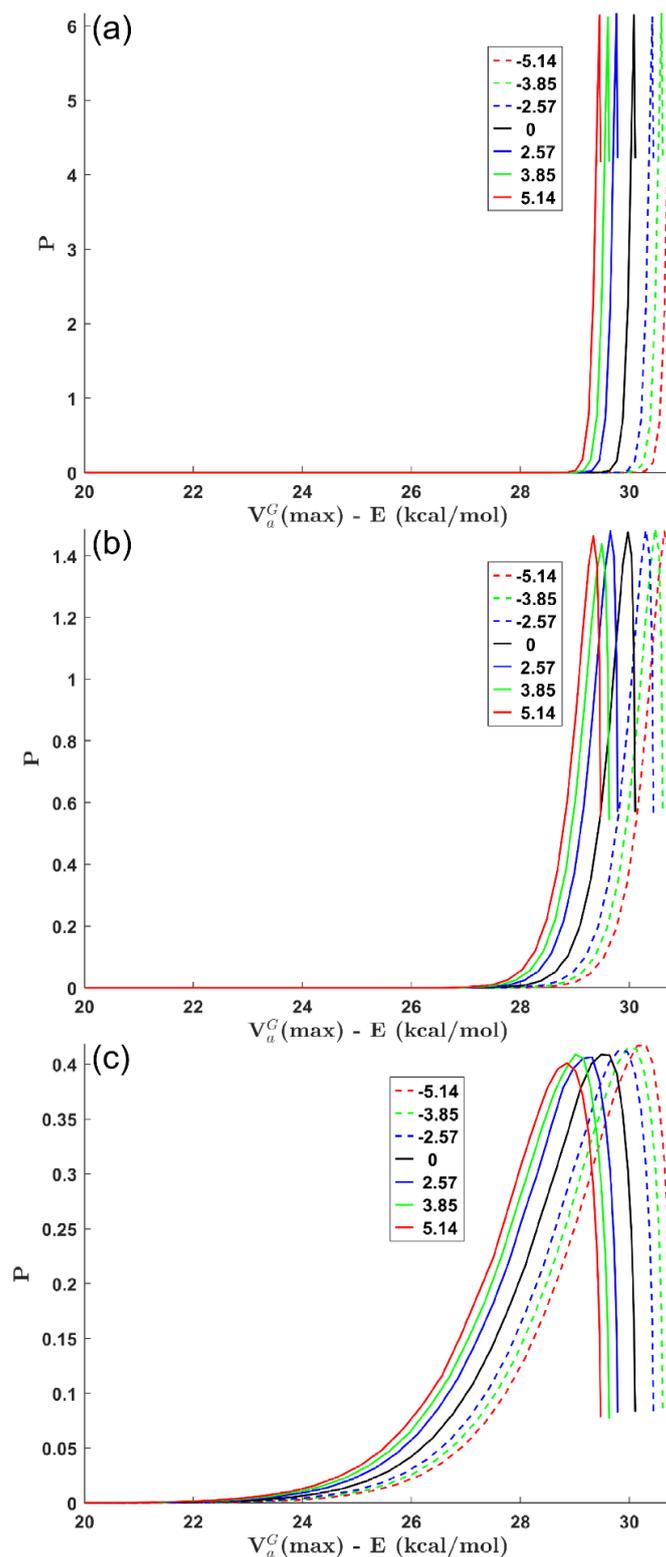
## H-C-OH

**Table S6.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) for the H-migration of H-C-OH using the  $\omega$ B97X-D method under different EEF strengths (in V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

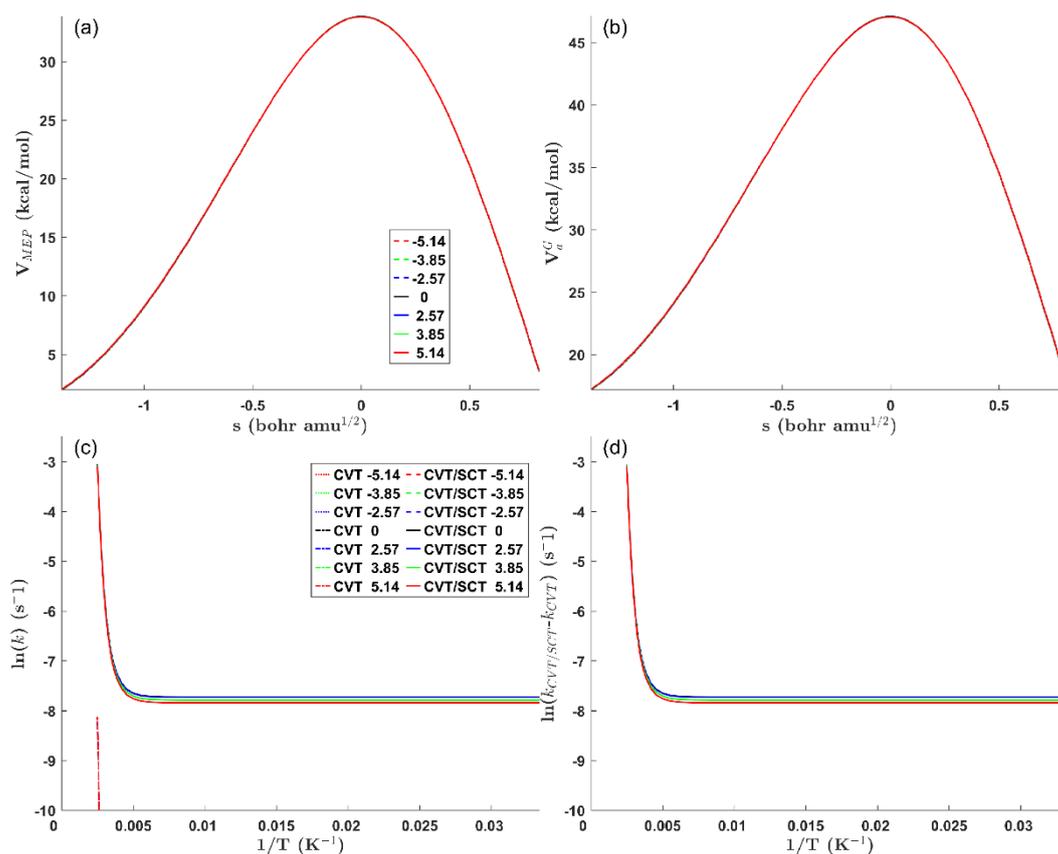
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	34.58	34.40	34.22	33.88	33.54	33.37	33.21
$\Delta V_a^G(\max)$	47.64	47.51	47.38	47.11	46.83	46.69	46.56
$\Omega$	2146	2143	2139	2132	2123	2119	2114
$T_c$	491	491	490	488	486	485	484
<b>Y-EEF Direction</b>							
$\Delta E$	33.84	33.86	33.87	33.88	33.87	33.86	33.84
$\Delta V_a^G(\max)$	47.07	47.08	47.09	47.11	47.09	47.08	47.07
$\Omega$	2129	2130	2131	2132	2131	2130	2129
$T_c$	488	488	488	488	488	488	488
<b>Z-EEF Direction</b>							
$\Delta E$	39.24	37.87	36.53	33.88	31.28	30.01	28.75
$\Delta V_a^G(\max)$	52.39	51.05	49.73	47.11	44.54	43.27	42.03
$\Omega$	2146	2144	2141	2132	2117	2106	2094
$T_c$	491	491	490	488	485	482	479



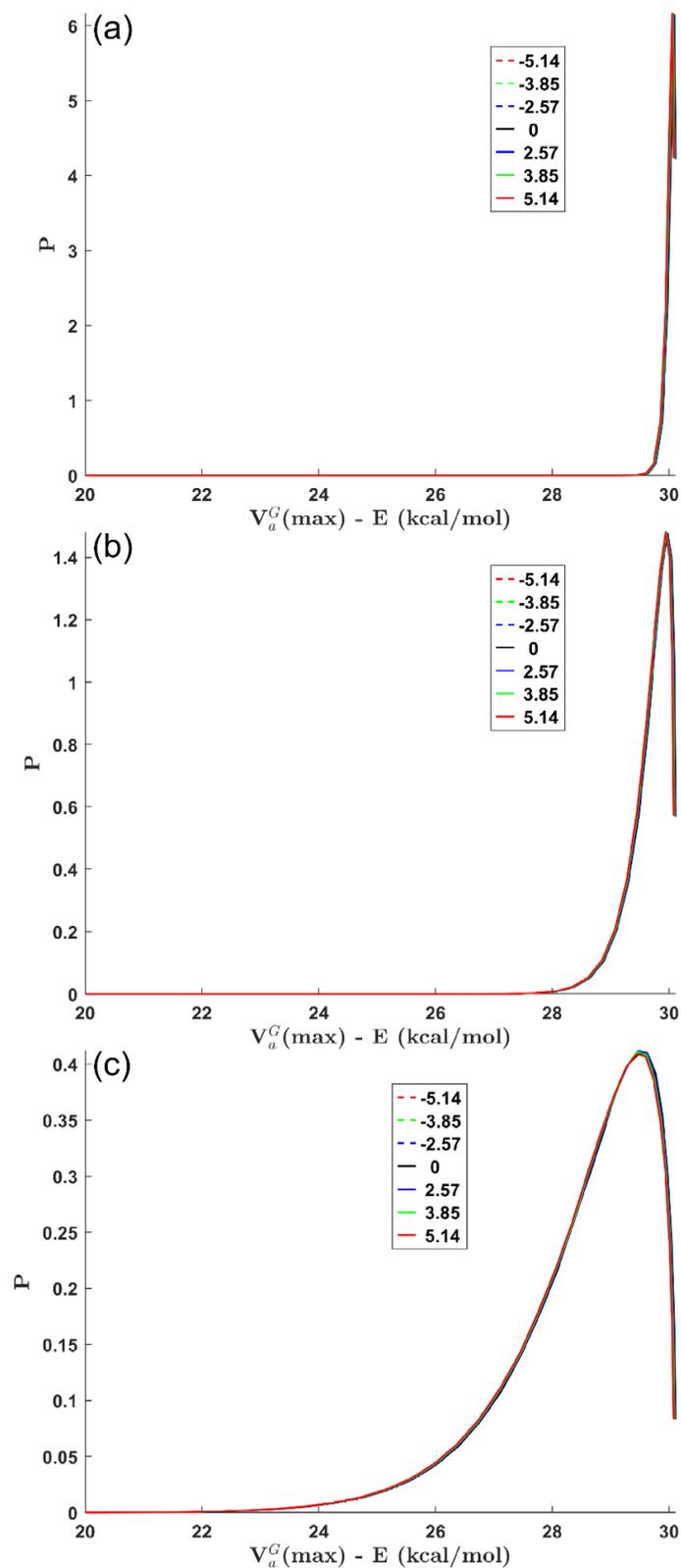
**Figure S10.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration in H-C-OH using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



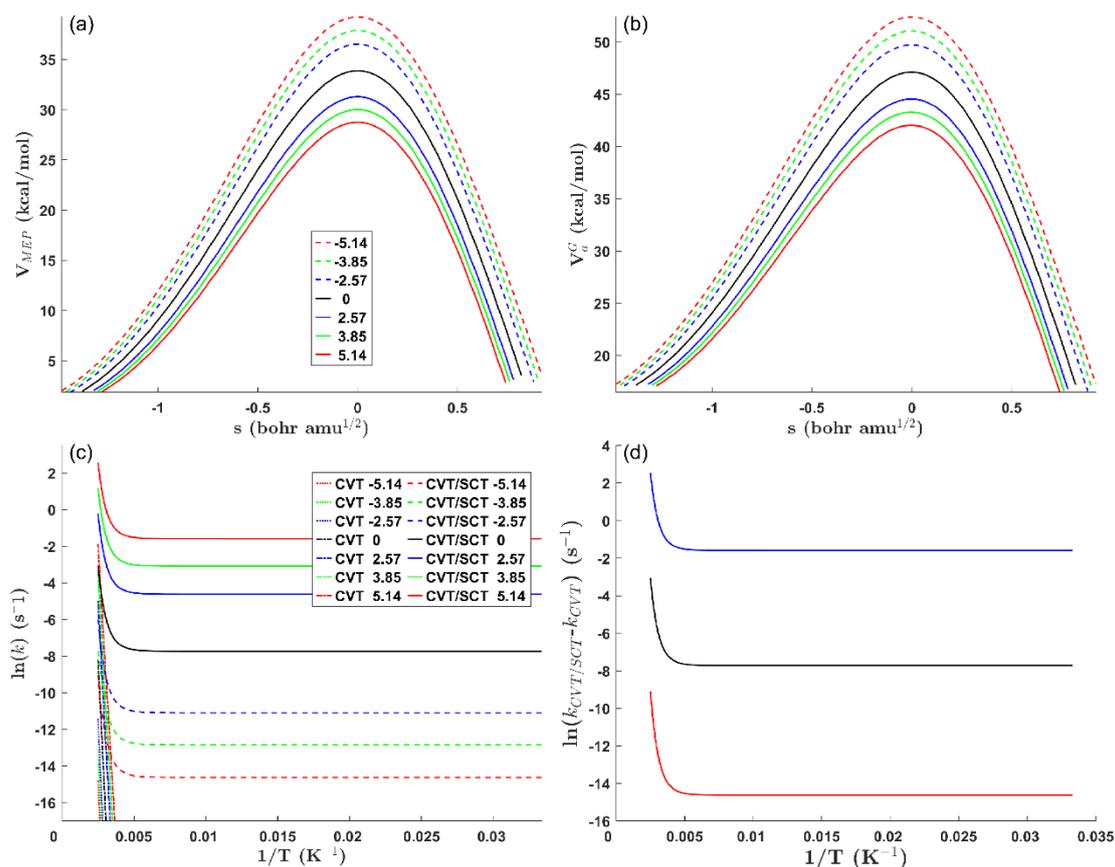
**Figure S11.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of H-C-OH at (a) 30K, (b) 100K and (c) 200K, by the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



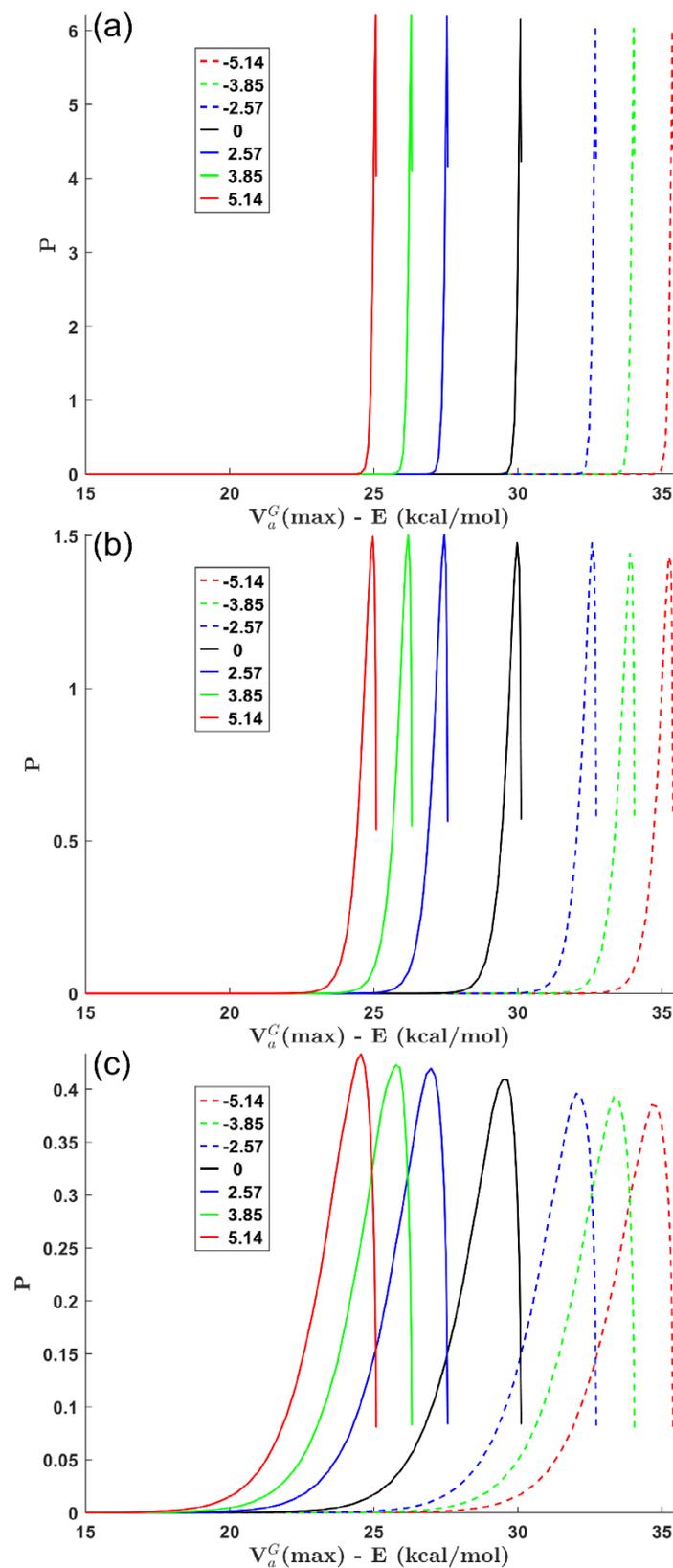
**Figure S12.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration in H-C-OH using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



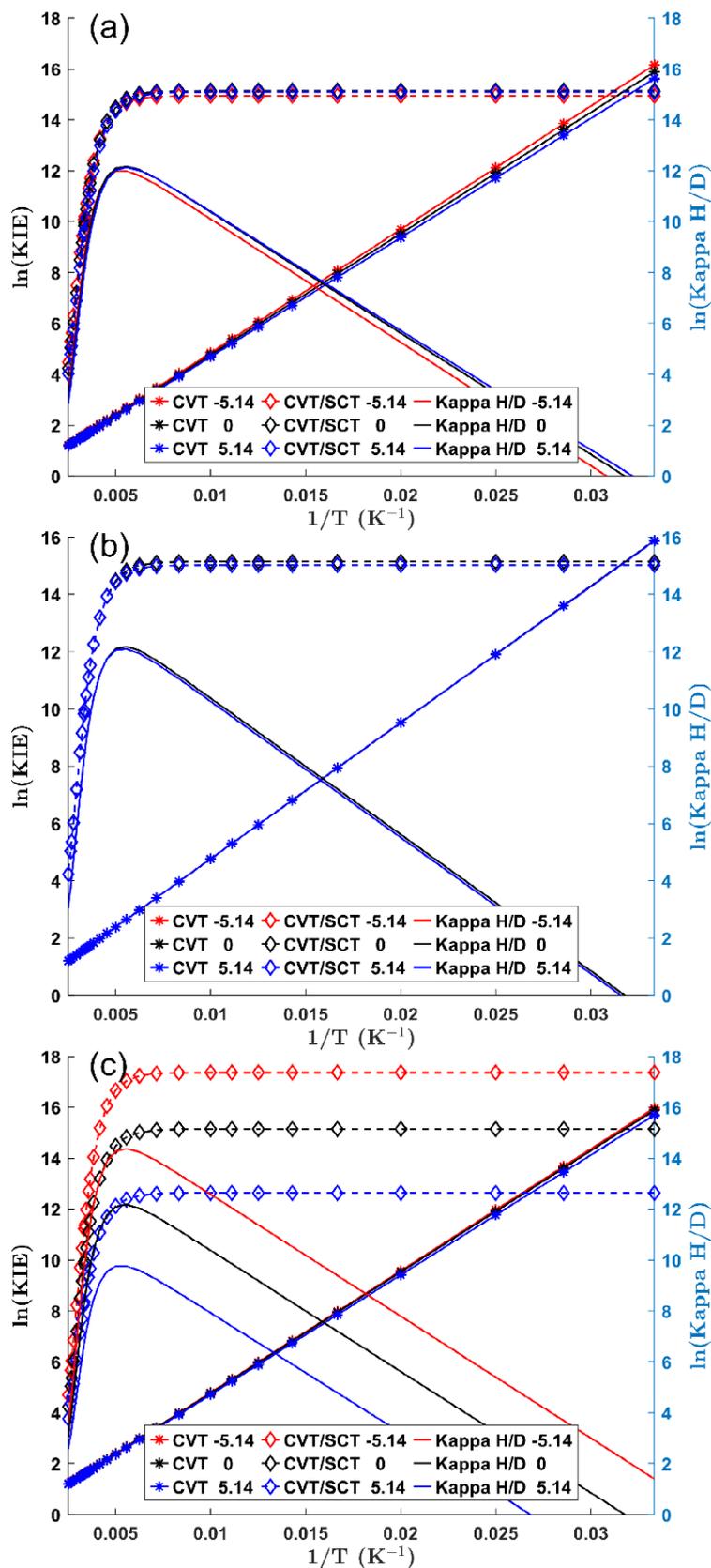
**Figure S13.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of H-C-OH at (a) 30K, (b) 100K and (c) 200K using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S14.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H-C-OH using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S15.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of H-C-OH at (a) 30K, (b) 100K and (c) 200K, using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S16.** Arrhenius plots of  $\ln(H/D \text{ KIE})$  and  $\ln(\kappa(H)/\kappa(D))$  versus  $1/T$  for the H-migration of H-C-OH using the  $\omega$ B97X-D method along various directions (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S7.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T, in K), negative direction of X-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of X-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	3.08E-213	5.46E-212	9.36E-211	2.47E-208	5.56E-206	7.81E-205	1.05E-203
35	3.94E-181	4.63E-180	5.29E-179	6.28E-177	6.53E-175	6.29E-174	5.82E-173
40	4.82E-157	4.16E-156	3.51E-155	2.29E-153	1.33E-151	9.67E-151	6.78E-150
50	2.64E-123	1.48E-122	8.15E-122	2.31E-120	5.96E-119	2.91E-118	1.38E-117
60	8.49E-101	3.57E-100	1.48E-99	2.40E-98	3.60E-97	1.35E-96	4.94E-96
70	1.04E-84	3.55E-84	1.20E-83	1.31E-82	1.33E-81	4.13E-81	1.26E-80
80	1.23E-72	3.60E-72	1.04E-71	8.43E-71	6.43E-70	1.73E-69	4.59E-69
90	3.05E-63	7.95E-63	2.05E-62	1.31E-61	7.98E-61	1.93E-60	4.57E-60
100	1.01E-55	2.40E-55	5.63E-55	2.99E-54	1.52E-53	3.36E-53	7.32E-53
120	1.99E-44	4.08E-44	8.31E-44	3.34E-43	1.29E-42	2.51E-42	4.79E-42
140	2.38E-36	4.40E-36	8.09E-36	2.66E-35	8.51E-35	1.50E-34	2.61E-34
160	2.77E-30	4.74E-30	8.07E-30	2.29E-29	6.33E-29	1.04E-28	1.69E-28
180	1.47E-25	2.36E-25	3.80E-25	9.58E-25	2.37E-24	3.67E-24	5.66E-24
200	8.92E-22	1.37E-21	2.10E-21	4.83E-21	1.09E-20	1.62E-20	2.39E-20
220	1.12E-18	1.66E-18	2.45E-18	5.22E-18	1.09E-17	1.57E-17	2.23E-17
240	4.35E-16	6.23E-16	8.88E-16	1.78E-15	3.50E-15	4.87E-15	6.73E-15
260	6.78E-14	9.44E-14	1.31E-13	2.48E-13	4.64E-13	6.30E-13	8.50E-13
273.15	1.26E-12	1.72E-12	2.35E-12	4.32E-12	7.85E-12	1.05E-11	1.39E-11
280	5.17E-12	7.02E-12	9.52E-12	1.72E-11	3.08E-11	4.09E-11	5.40E-11
290	3.61E-11	4.86E-11	6.52E-11	1.16E-10	2.03E-10	2.66E-10	3.48E-10
298.15	1.60E-10	2.14E-10	2.84E-10	4.96E-10	8.58E-10	1.12E-09	1.45E-09
300	2.22E-10	2.96E-10	3.93E-10	6.83E-10	1.18E-09	1.53E-09	1.99E-09
310	1.22E-09	1.61E-09	2.11E-09	3.61E-09	6.11E-09	7.89E-09	1.01E-08
320	6.00E-09	7.85E-09	1.02E-08	1.72E-08	2.86E-08	3.67E-08	4.68E-08
340	1.10E-07	1.42E-07	1.82E-07	2.97E-07	4.80E-07	6.06E-07	7.62E-07
360	1.47E-06	1.87E-06	2.37E-06	3.76E-06	5.91E-06	7.36E-06	9.14E-06
373.15	6.98E-06	8.78E-06	1.10E-05	1.72E-05	2.66E-05	3.29E-05	4.06E-05
380	1.50E-05	1.88E-05	2.36E-05	3.65E-05	5.60E-05	6.90E-05	8.47E-05
400	1.22E-04	1.51E-04	1.87E-04	2.83E-04	4.25E-04	5.18E-04	6.30E-04

**Table S8.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T, in K), negative direction of X-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of X-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
35	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
40	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
50	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
60	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
70	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
80	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
90	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
100	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.62E-04	5.15E-04	5.77E-04
120	2.50E-04	2.94E-04	3.34E-04	4.42E-04	5.63E-04	5.15E-04	5.77E-04
140	2.51E-04	2.95E-04	3.35E-04	4.43E-04	5.64E-04	5.17E-04	5.78E-04
160	2.53E-04	2.97E-04	3.37E-04	4.47E-04	5.69E-04	5.21E-04	5.83E-04
180	2.58E-04	3.03E-04	3.44E-04	4.56E-04	5.81E-04	5.33E-04	5.97E-04
200	2.68E-04	3.16E-04	3.60E-04	4.77E-04	6.07E-04	5.60E-04	6.26E-04
220	2.89E-04	3.41E-04	3.89E-04	5.16E-04	6.58E-04	6.11E-04	6.82E-04
240	3.27E-04	3.85E-04	4.41E-04	5.86E-04	7.50E-04	7.03E-04	7.84E-04
260	3.92E-04	4.63E-04	5.32E-04	7.09E-04	9.13E-04	8.68E-04	9.66E-04
273.15	4.61E-04	5.44E-04	6.28E-04	8.39E-04	1.08E-03	1.04E-03	1.16E-03
280	5.09E-04	6.01E-04	6.95E-04	9.30E-04	1.21E-03	1.17E-03	1.30E-03
290	6.00E-04	7.09E-04	8.21E-04	1.10E-03	1.44E-03	1.40E-03	1.56E-03
298.15	6.99E-04	8.26E-04	9.59E-04	1.29E-03	1.69E-03	1.67E-03	1.86E-03
300	7.25E-04	8.57E-04	9.96E-04	1.34E-03	1.76E-03	1.74E-03	1.94E-03
310	9.01E-04	1.07E-03	1.24E-03	1.68E-03	2.21E-03	2.21E-03	2.47E-03
320	1.15E-03	1.36E-03	1.59E-03	2.16E-03	2.86E-03	2.90E-03	3.25E-03
340	2.06E-03	2.44E-03	2.87E-03	3.94E-03	5.27E-03	5.47E-03	6.16E-03
360	4.16E-03	4.95E-03	5.85E-03	8.12E-03	1.09E-02	1.16E-02	1.32E-02
373.15	7.03E-03	8.39E-03	9.94E-03	1.39E-02	1.88E-02	2.03E-02	2.31E-02
380	9.41E-03	1.12E-02	1.33E-02	1.87E-02	2.53E-02	2.76E-02	3.15E-02
400	2.34E-02	2.80E-02	3.34E-02	4.71E-02	6.41E-02	7.13E-02	8.19E-02

**Table S9.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T, in K), negative direction of Y-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of Y-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.36E-208	3.51E-208	2.94E-208	2.47E-208	2.94E-208	3.51E-208	4.36E-208
35	1.02E-176	8.50E-177	7.30E-177	6.28E-177	7.30E-177	8.50E-177	1.02E-176
40	3.52E-153	2.99E-153	2.62E-153	2.29E-153	2.62E-153	2.99E-153	3.52E-153
50	3.25E-120	2.85E-120	2.56E-120	2.31E-120	2.56E-120	2.85E-120	3.25E-120
60	3.19E-98	2.86E-98	2.62E-98	2.40E-98	2.62E-98	2.86E-98	3.19E-98
70	1.67E-82	1.52E-82	1.41E-82	1.31E-82	1.41E-82	1.52E-82	1.67E-82
80	1.05E-70	9.64E-71	9.02E-71	8.43E-71	9.02E-71	9.64E-71	1.05E-70
90	1.59E-61	1.48E-61	1.39E-61	1.31E-61	1.39E-61	1.48E-61	1.59E-61
100	3.55E-54	3.33E-54	3.16E-54	2.99E-54	3.16E-54	3.33E-54	3.55E-54
120	3.86E-43	3.65E-43	3.49E-43	3.34E-43	3.49E-43	3.65E-43	3.86E-43
140	3.01E-35	2.88E-35	2.77E-35	2.66E-35	2.77E-35	2.88E-35	3.01E-35
160	2.55E-29	2.45E-29	2.37E-29	2.29E-29	2.37E-29	2.45E-29	2.55E-29
180	1.06E-24	1.02E-24	9.89E-25	9.58E-25	9.89E-25	1.02E-24	1.06E-24
200	5.27E-21	5.11E-21	4.97E-21	4.83E-21	4.97E-21	5.11E-21	5.27E-21
220	5.66E-18	5.49E-18	5.36E-18	5.22E-18	5.36E-18	5.49E-18	5.66E-18
240	1.91E-15	1.86E-15	1.82E-15	1.78E-15	1.82E-15	1.86E-15	1.91E-15
260	2.66E-13	2.59E-13	2.54E-13	2.48E-13	2.54E-13	2.59E-13	2.66E-13
273.15	4.62E-12	4.51E-12	4.42E-12	4.32E-12	4.42E-12	4.51E-12	4.62E-12
280	1.84E-11	1.80E-11	1.76E-11	1.72E-11	1.76E-11	1.80E-11	1.84E-11
290	1.23E-10	1.20E-10	1.18E-10	1.16E-10	1.18E-10	1.20E-10	1.23E-10
298.15	5.27E-10	5.16E-10	5.07E-10	4.96E-10	5.07E-10	5.16E-10	5.27E-10
300	7.26E-10	7.10E-10	6.98E-10	6.83E-10	6.98E-10	7.10E-10	7.26E-10
310	3.83E-09	3.75E-09	3.68E-09	3.61E-09	3.68E-09	3.75E-09	3.83E-09
320	1.82E-08	1.78E-08	1.75E-08	1.72E-08	1.75E-08	1.78E-08	1.82E-08
340	3.14E-07	3.08E-07	3.03E-07	2.97E-07	3.03E-07	3.08E-07	3.14E-07
360	3.95E-06	3.88E-06	3.82E-06	3.76E-06	3.82E-06	3.88E-06	3.95E-06
373.15	1.81E-05	1.78E-05	1.75E-05	1.72E-05	1.75E-05	1.78E-05	1.81E-05
380	3.83E-05	3.76E-05	3.71E-05	3.65E-05	3.71E-05	3.76E-05	3.83E-05
400	2.96E-04	2.91E-04	2.87E-04	2.83E-04	2.87E-04	2.91E-04	2.96E-04

**Table S10.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T, in K), negative direction of Y-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of Y-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
35	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
40	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
50	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
60	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
70	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
80	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
90	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
100	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
120	3.94E-04	4.16E-04	4.39E-04	4.42E-04	4.39E-04	4.16E-04	3.94E-04
140	3.95E-04	4.17E-04	4.40E-04	4.43E-04	4.40E-04	4.17E-04	3.95E-04
160	3.98E-04	4.20E-04	4.43E-04	4.47E-04	4.43E-04	4.20E-04	3.98E-04
180	4.07E-04	4.29E-04	4.53E-04	4.56E-04	4.53E-04	4.29E-04	4.07E-04
200	4.26E-04	4.49E-04	4.73E-04	4.77E-04	4.73E-04	4.49E-04	4.26E-04
220	4.61E-04	4.86E-04	5.12E-04	5.16E-04	5.12E-04	4.86E-04	4.61E-04
240	5.25E-04	5.53E-04	5.82E-04	5.86E-04	5.82E-04	5.53E-04	5.25E-04
260	6.38E-04	6.71E-04	7.05E-04	7.09E-04	7.05E-04	6.71E-04	6.38E-04
273.15	7.58E-04	7.95E-04	8.35E-04	8.39E-04	8.35E-04	7.95E-04	7.58E-04
280	8.41E-04	8.82E-04	9.25E-04	9.30E-04	9.25E-04	8.82E-04	8.41E-04
290	1.00E-03	1.05E-03	1.10E-03	1.10E-03	1.10E-03	1.05E-03	1.00E-03
298.15	1.18E-03	1.23E-03	1.29E-03	1.29E-03	1.29E-03	1.23E-03	1.18E-03
300	1.22E-03	1.28E-03	1.34E-03	1.34E-03	1.34E-03	1.28E-03	1.22E-03
310	1.54E-03	1.61E-03	1.67E-03	1.68E-03	1.67E-03	1.61E-03	1.54E-03
320	1.99E-03	2.08E-03	2.16E-03	2.16E-03	2.16E-03	2.08E-03	1.99E-03
340	3.67E-03	3.81E-03	3.94E-03	3.94E-03	3.94E-03	3.81E-03	3.67E-03
360	7.66E-03	7.90E-03	8.13E-03	8.12E-03	8.13E-03	7.90E-03	7.66E-03
373.15	1.32E-02	1.36E-02	1.39E-02	1.39E-02	1.39E-02	1.36E-02	1.32E-02
380	1.78E-02	1.83E-02	1.87E-02	1.87E-02	1.87E-02	1.83E-02	1.78E-02
400	4.54E-02	4.64E-02	4.71E-02	4.71E-02	4.71E-02	4.64E-02	4.54E-02

**Table S11.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T, in K), negative direction of Z-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of Z-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	9.10E-247	5.40E-237	2.49E-227	2.47E-208	8.49E-190	1.05E-180	9.85E-172
35	7.18E-210	1.71E-201	3.29E-193	6.28E-177	4.86E-161	3.01E-153	1.48E-145
40	3.44E-182	7.35E-175	1.30E-167	2.29E-153	1.83E-139	1.20E-132	6.46E-126
50	2.02E-143	1.47E-137	9.27E-132	2.31E-120	3.05E-109	8.69E-104	2.10E-98
60	1.46E-117	1.13E-112	7.65E-108	2.40E-98	4.44E-89	1.56E-84	4.77E-80
70	4.44E-99	6.85E-95	9.48E-91	1.31E-82	1.15E-74	9.02E-71	6.31E-67
80	3.29E-85	1.52E-81	6.38E-78	8.43E-71	7.52E-64	1.93E-60	4.46E-57
90	2.04E-74	3.69E-71	6.14E-68	1.31E-61	1.98E-55	2.12E-52	2.07E-49
100	8.91E-66	7.60E-63	6.02E-60	2.99E-54	1.09E-48	5.79E-46	2.84E-43
120	8.31E-53	2.30E-50	5.99E-48	3.34E-43	1.43E-38	2.68E-36	4.69E-34
140	1.56E-43	1.94E-41	2.28E-39	2.66E-35	2.49E-31	2.21E-29	1.84E-27
160	1.44E-36	9.76E-35	6.32E-33	2.29E-29	6.83E-26	3.45E-24	1.66E-22
180	3.81E-31	1.62E-29	6.58E-28	9.58E-25	1.17E-21	3.84E-20	1.20E-18
200	8.40E-27	2.45E-25	6.88E-24	4.83E-21	2.91E-18	6.70E-17	1.48E-15
220	3.04E-23	6.51E-22	1.35E-20	5.22E-18	1.76E-15	3.04E-14	5.08E-13
240	2.83E-20	4.69E-19	7.56E-18	1.78E-15	3.68E-13	5.02E-12	6.62E-11
260	9.25E-18	1.24E-16	1.61E-15	2.48E-13	3.41E-11	3.80E-10	4.11E-09
273.15	2.64E-16	3.11E-15	3.57E-14	4.32E-12	4.68E-10	4.65E-09	4.49E-08
280	1.33E-15	1.48E-14	1.60E-13	1.72E-11	1.66E-09	1.56E-08	1.43E-07
290	1.24E-14	1.27E-13	1.26E-12	1.16E-10	9.53E-09	8.28E-08	7.00E-07
298.15	6.85E-14	6.57E-13	6.14E-12	4.96E-10	3.63E-08	2.97E-07	2.37E-06
300	9.96E-14	9.42E-13	8.69E-12	6.83E-10	4.86E-08	3.93E-07	3.10E-06
310	7.00E-13	6.16E-12	5.29E-11	3.61E-09	2.24E-07	1.69E-06	1.24E-05
320	4.36E-12	3.58E-11	2.88E-10	1.72E-08	9.37E-07	6.64E-06	4.60E-05
340	1.23E-10	8.92E-10	6.33E-09	2.97E-07	1.28E-05	8.08E-05	4.99E-04
360	2.40E-09	1.56E-08	9.92E-08	3.76E-06	1.31E-04	7.47E-04	4.17E-03
373.15	1.43E-08	8.67E-08	5.16E-07	1.72E-05	5.29E-04	2.84E-03	1.49E-02
380	3.44E-08	2.02E-07	1.17E-06	3.65E-05	1.05E-03	5.48E-03	2.79E-02
400	3.78E-07	2.04E-06	1.08E-05	2.83E-04	6.91E-03	3.31E-02	1.55E-01

**Table S12.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of for the H-migration of H-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T, in K), negative direction of Z-EEF ( $-5.14 \sim -2.57$  V/nm); positive direction of Z-EEF ( $2.57 \sim 5.14$  V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
35	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
40	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
50	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
60	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
70	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
80	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
90	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.04E-01
100	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.05E-01
120	4.47E-07	2.63E-06	1.52E-05	4.42E-04	9.87E-03	4.58E-02	2.05E-01
140	4.48E-07	2.64E-06	1.53E-05	4.43E-04	9.89E-03	4.59E-02	2.05E-01
160	4.52E-07	2.66E-06	1.54E-05	4.47E-04	9.97E-03	4.63E-02	2.07E-01
180	4.63E-07	2.72E-06	1.58E-05	4.56E-04	1.02E-02	4.72E-02	2.10E-01
200	4.87E-07	2.86E-06	1.65E-05	4.77E-04	1.06E-02	4.91E-02	2.19E-01
220	5.35E-07	3.13E-06	1.79E-05	5.16E-04	1.14E-02	5.28E-02	2.35E-01
240	6.23E-07	3.64E-06	2.06E-05	5.86E-04	1.29E-02	5.94E-02	2.63E-01
260	7.84E-07	4.55E-06	2.53E-05	7.09E-04	1.54E-02	7.09E-02	3.13E-01
273.15	9.61E-07	5.54E-06	3.03E-05	8.39E-04	1.80E-02	8.28E-02	3.64E-01
280	1.09E-06	6.24E-06	3.39E-05	9.30E-04	1.99E-02	9.10E-02	3.99E-01
290	1.34E-06	7.62E-06	4.09E-05	1.10E-03	2.33E-02	1.07E-01	4.65E-01
298.15	1.62E-06	9.16E-06	4.86E-05	1.29E-03	2.71E-02	1.23E-01	5.36E-01
300	1.69E-06	9.58E-06	5.06E-05	1.34E-03	2.81E-02	1.28E-01	5.55E-01
310	2.22E-06	1.24E-05	6.47E-05	1.68E-03	3.47E-02	1.57E-01	6.79E-01
320	3.01E-06	1.67E-05	8.55E-05	2.16E-03	4.42E-02	1.98E-01	8.52E-01
340	6.17E-06	3.32E-05	1.65E-04	3.94E-03	7.80E-02	3.43E-01	1.45E+00
360	1.45E-05	7.53E-05	3.63E-04	8.12E-03	1.54E-01	6.64E-01	2.76E+00
373.15	2.72E-05	1.38E-04	6.51E-04	1.39E-02	2.56E-01	1.08E+00	4.43E+00
380	3.85E-05	1.92E-04	8.98E-04	1.87E-02	3.38E-01	1.42E+00	5.75E+00
400	1.13E-04	5.40E-04	2.45E-03	4.71E-02	8.01E-01	3.26E+00	1.29E+01

**Table S13.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T, in K), negative direction of X-EEF ( $-5.14$  V/nm); positive direction of X-EEF ( $5.14$  V/nm); no field ( $0.0$  V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	2.97E-220	3.13E-215	1.73E-210
35	3.81E-187	7.70E-183	8.93E-179
40	2.63E-162	1.54E-158	5.54E-155
50	1.63E-127	1.68E-124	1.17E-121
60	2.63E-104	8.51E-102	2.00E-99
70	1.02E-87	1.44E-85	1.55E-83
80	2.86E-75	2.18E-73	1.31E-71
90	1.39E-65	6.57E-64	2.50E-62
100	7.94E-58	2.54E-56	6.72E-55
120	3.50E-46	6.28E-45	9.62E-44
140	7.44E-38	8.83E-37	9.16E-36
160	1.33E-31	1.16E-30	8.99E-30
180	9.90E-27	6.78E-26	4.18E-25
200	7.89E-23	4.45E-22	2.29E-21
220	1.24E-19	5.98E-19	2.65E-18
240	5.77E-17	2.44E-16	9.52E-16
260	1.05E-14	3.97E-14	1.39E-13
273.15	2.13E-13	7.54E-13	2.50E-12
280	9.14E-13	3.14E-12	1.01E-11
290	6.78E-12	2.23E-11	6.88E-11
298.15	3.15E-11	1.00E-10	3.00E-10
300	4.41E-11	1.39E-10	4.14E-10
310	2.54E-10	7.73E-10	2.22E-09
320	1.31E-09	3.86E-09	1.07E-08
340	2.64E-08	7.27E-08	1.90E-07
360	3.81E-07	9.92E-07	2.45E-06
373.15	1.89E-06	4.75E-06	1.14E-05
380	4.16E-06	1.03E-05	2.43E-05
400	3.59E-05	8.48E-05	1.92E-04

**Table S14.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the  $\omega$ B97X-D method along the X-EEF direction with various strengths at different temperatures (T, in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	8.06E-11	1.17E-10	1.61E-10
35	8.06E-11	1.17E-10	1.61E-10
40	8.06E-11	1.17E-10	1.61E-10
50	8.06E-11	1.17E-10	1.61E-10
60	8.06E-11	1.17E-10	1.61E-10
70	8.06E-11	1.17E-10	1.61E-10
80	8.06E-11	1.17E-10	1.61E-10
90	8.06E-11	1.17E-10	1.61E-10
100	8.07E-11	1.17E-10	1.61E-10
120	8.12E-11	1.18E-10	1.63E-10
140	8.35E-11	1.22E-10	1.69E-10
160	9.06E-11	1.34E-10	1.88E-10
180	1.08E-10	1.66E-10	2.38E-10
200	1.51E-10	2.46E-10	3.62E-10
220	2.57E-10	4.56E-10	7.00E-10
240	5.64E-10	1.09E-09	1.78E-09
260	1.63E-09	3.39E-09	6.03E-09
273.15	3.80E-09	8.32E-09	1.55E-08
280	6.20E-09	1.39E-08	2.65E-08
290	1.33E-08	3.07E-08	6.05E-08
298.15	2.59E-08	6.12E-08	1.23E-07
300	3.02E-08	7.18E-08	1.45E-07
310	7.20E-08	1.75E-07	3.60E-07
320	1.78E-07	4.41E-07	9.20E-07
340	1.15E-06	2.94E-06	6.25E-06
360	7.57E-06	1.95E-05	4.18E-05
373.15	2.54E-05	6.53E-05	1.41E-04
380	4.70E-05	1.21E-04	2.61E-04
400	2.66E-04	6.82E-04	1.47E-03

**Table S15.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T, in K), negative direction of Y-EEF ( $-5.14$  V/nm); positive direction of Y-EEF ( $5.14$  V/nm); no field ( $0.0$  V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	5.61E-215	3.13E-215	5.61E-215
35	1.27E-182	7.70E-183	1.27E-182
40	2.38E-158	1.54E-158	2.38E-158
50	2.38E-124	1.68E-124	2.38E-124
60	1.14E-101	8.51E-102	1.14E-101
70	1.85E-85	1.44E-85	1.85E-85
80	2.72E-73	2.18E-73	2.72E-73
90	7.98E-64	6.57E-64	7.98E-64
100	3.03E-56	2.54E-56	3.03E-56
120	7.28E-45	6.28E-45	7.28E-45
140	1.00E-36	8.83E-37	1.00E-36
160	1.30E-30	1.16E-30	1.30E-30
180	7.48E-26	6.78E-26	7.48E-26
200	4.87E-22	4.45E-22	4.87E-22
220	6.49E-19	5.98E-19	6.49E-19
240	2.63E-16	2.44E-16	2.63E-16
260	4.25E-14	3.97E-14	4.25E-14
273.15	8.06E-13	7.54E-13	8.06E-13
280	3.35E-12	3.14E-12	3.35E-12
290	2.37E-11	2.23E-11	2.37E-11
298.15	1.06E-10	1.00E-10	1.06E-10
300	1.48E-10	1.39E-10	1.48E-10
310	8.20E-10	7.73E-10	8.20E-10
320	4.09E-09	3.86E-09	4.09E-09
340	7.68E-08	7.27E-08	7.68E-08
360	1.04E-06	9.92E-07	1.04E-06
373.15	4.99E-06	4.75E-06	4.99E-06
380	1.08E-05	1.03E-05	1.08E-05
400	8.88E-05	8.48E-05	8.88E-05

**Table S16.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths at different temperatures (T, in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	1.17E-10	1.17E-10	1.17E-10
35	1.17E-10	1.17E-10	1.17E-10
40	1.17E-10	1.17E-10	1.17E-10
50	1.17E-10	1.17E-10	1.17E-10
60	1.17E-10	1.17E-10	1.17E-10
70	1.17E-10	1.17E-10	1.17E-10
80	1.17E-10	1.17E-10	1.17E-10
90	1.17E-10	1.17E-10	1.17E-10
100	1.17E-10	1.17E-10	1.17E-10
120	1.18E-10	1.18E-10	1.18E-10
140	1.22E-10	1.22E-10	1.22E-10
160	1.33E-10	1.34E-10	1.33E-10
180	1.61E-10	1.66E-10	1.61E-10
200	2.30E-10	2.46E-10	2.30E-10
220	4.12E-10	4.56E-10	4.12E-10
240	9.66E-10	1.09E-09	9.66E-10
260	3.02E-09	3.39E-09	3.02E-09
273.15	7.49E-09	8.32E-09	7.49E-09
280	1.26E-08	1.39E-08	1.26E-08
290	2.81E-08	3.07E-08	2.81E-08
298.15	5.63E-08	6.12E-08	5.63E-08
300	6.62E-08	7.18E-08	6.62E-08
310	1.63E-07	1.75E-07	1.63E-07
320	4.12E-07	4.41E-07	4.12E-07
340	2.78E-06	2.94E-06	2.78E-06
360	1.86E-05	1.95E-05	1.86E-05
373.15	6.27E-05	6.53E-05	6.27E-05
380	1.16E-04	1.21E-04	1.16E-04
400	6.60E-04	6.82E-04	6.60E-04

**Table S17.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T, in K), negative direction of Z-EEF ( $-5.14$  V/nm); positive direction of Z-EEF ( $5.14$  V/nm); no field ( $0.0$  V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.06E-253	3.13E-215	1.51E-178
35	8.21E-216	7.70E-183	2.13E-151
40	2.17E-187	1.54E-158	5.00E-131
50	1.40E-147	1.68E-124	1.71E-102
60	5.00E-121	8.51E-102	1.86E-83
70	4.74E-102	1.44E-85	7.56E-70
80	8.25E-88	2.18E-73	1.24E-59
90	9.96E-77	6.57E-64	1.10E-51
100	7.39E-68	2.54E-56	2.56E-45
120	1.53E-54	6.28E-45	9.24E-36
140	5.10E-45	8.83E-37	6.36E-29
160	7.20E-38	1.16E-30	8.71E-24
180	2.66E-32	6.78E-26	8.73E-20
200	7.65E-28	4.45E-22	1.40E-16
220	3.44E-24	5.98E-19	5.95E-14
240	3.84E-21	2.44E-16	9.28E-12
260	1.47E-18	3.97E-14	6.70E-10
273.15	4.56E-17	7.54E-13	7.97E-09
280	2.41E-16	3.14E-12	2.64E-08
290	2.37E-15	2.23E-11	1.37E-07
298.15	1.37E-14	1.00E-10	4.85E-07
300	2.01E-14	1.39E-10	6.41E-07
310	1.49E-13	7.73E-10	2.71E-06
320	9.72E-13	3.86E-09	1.05E-05
340	2.99E-11	7.27E-08	1.24E-04
360	6.29E-10	9.92E-07	1.11E-03
373.15	3.91E-09	4.75E-06	4.16E-03
380	9.64E-09	1.03E-05	7.97E-03
400	1.13E-07	8.48E-05	4.70E-02

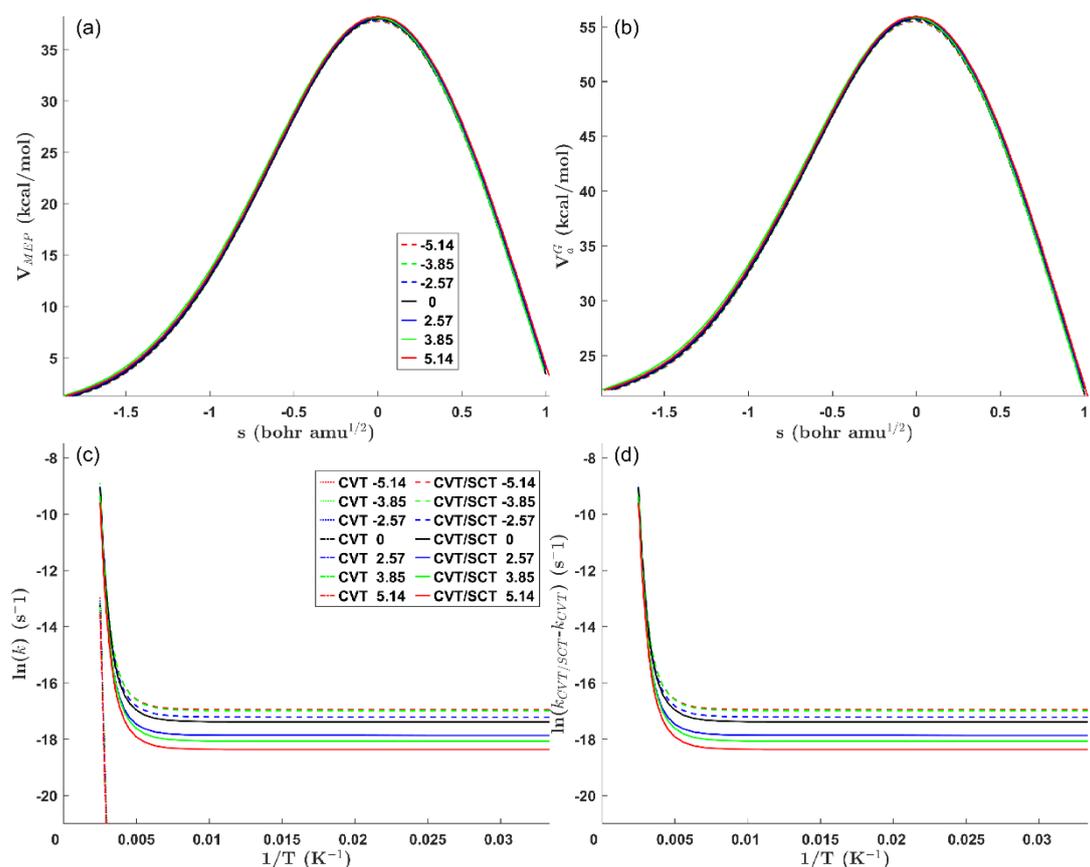
**Table S18.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths at different temperatures (T, in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.28E-14	1.17E-10	6.68E-07
35	1.28E-14	1.17E-10	6.68E-07
40	1.28E-14	1.17E-10	6.68E-07
50	1.28E-14	1.17E-10	6.68E-07
60	1.28E-14	1.17E-10	6.68E-07
70	1.28E-14	1.17E-10	6.68E-07
80	1.28E-14	1.17E-10	6.68E-07
90	1.28E-14	1.17E-10	6.68E-07
100	1.28E-14	1.17E-10	6.68E-07
120	1.29E-14	1.18E-10	6.72E-07
140	1.34E-14	1.22E-10	6.90E-07
160	1.48E-14	1.34E-10	7.45E-07
180	1.85E-14	1.66E-10	8.81E-07
200	2.83E-14	2.46E-10	1.20E-06
220	5.68E-14	4.56E-10	1.96E-06
240	1.58E-13	1.09E-09	4.04E-06
260	6.23E-13	3.39E-09	1.06E-05
273.15	1.82E-12	8.32E-09	2.30E-05
280	3.32E-12	1.39E-08	3.58E-05
290	8.42E-12	3.07E-08	7.10E-05
298.15	1.87E-11	6.12E-08	1.28E-04
300	2.25E-11	7.18E-08	1.47E-04
310	6.31E-11	1.75E-07	3.14E-04
320	1.83E-10	4.41E-07	6.88E-04
340	1.66E-09	2.94E-06	3.37E-03
360	1.53E-08	1.95E-05	1.62E-02
373.15	6.40E-08	6.53E-05	4.38E-02
380	1.33E-07	1.21E-04	7.27E-02
400	1.03E-06	6.82E-04	3.00E-01

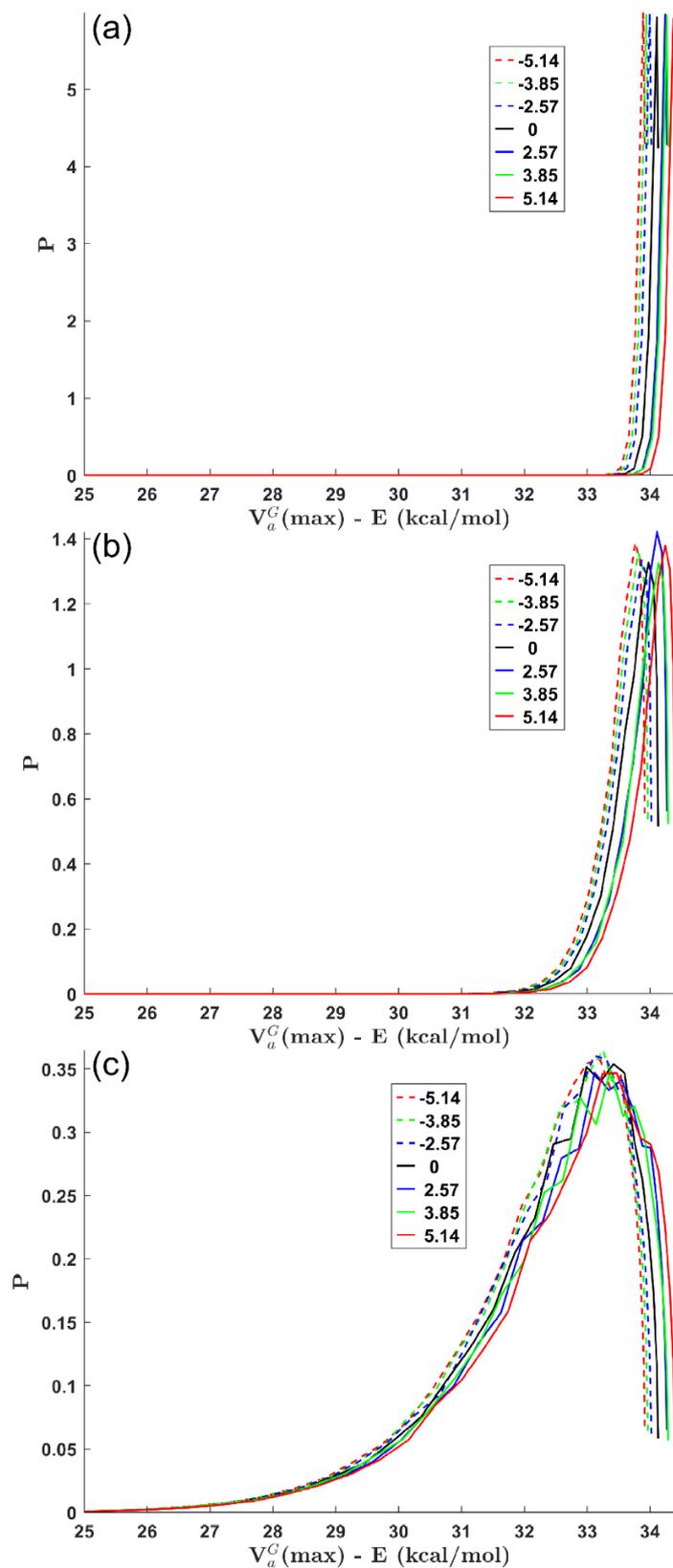
## HO-C-OH

**Table S19.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) for the H-migration of HO-C-OH using the  $\omega$ B97X-D method under different EEF strengths (V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

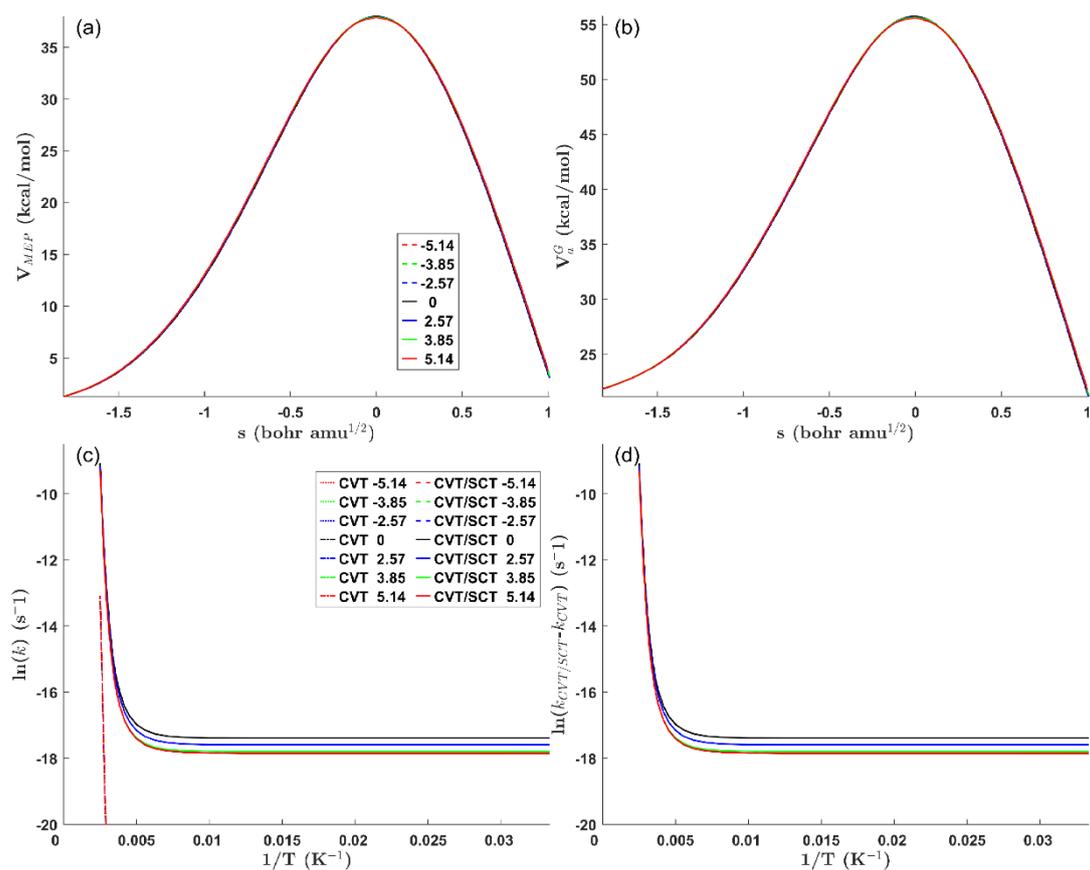
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	37.77	37.82	37.87	37.98	38.10	38.11	38.24
$\Delta V_a^G(\max)$	55.51	55.57	55.63	55.74	55.85	55.86	55.96
$\Omega$	1975	1973	1971	1966	1960	1959	1954
$T_c$	452	452	451	450	449	449	447
<b>Y-EEF Direction</b>							
$\Delta E$	37.88	37.93	37.96	37.98	37.96	37.93	37.88
$\Delta V_a^G(\max)$	55.62	55.67	55.71	55.74	55.71	55.67	55.62
$\Omega$	1965	1966	1966	1966	1966	1966	1965
$T_c$	450	450	450	450	450	450	450
<b>Z-EEF Direction</b>							
$\Delta E$	43.06	41.77	40.50	37.98	35.51	34.28	33.08
$\Delta V_a^G(\max)$	60.69	59.45	58.21	55.74	53.31	52.10	50.90
$\Omega$	1968	1967	1967	1966	1965	1963	1962
$T_c$	451	451	450	450	450	450	449



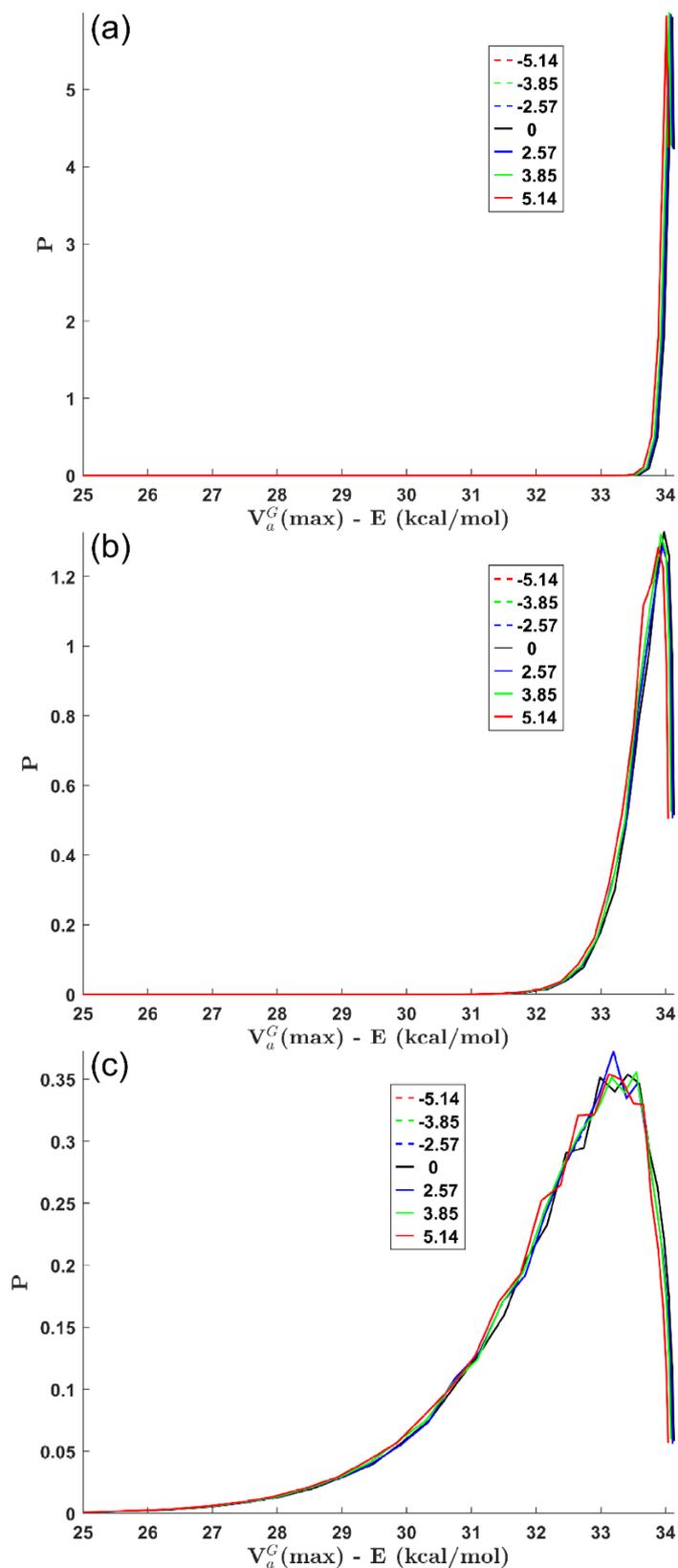
**Figure S17.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of HO-C-OH using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



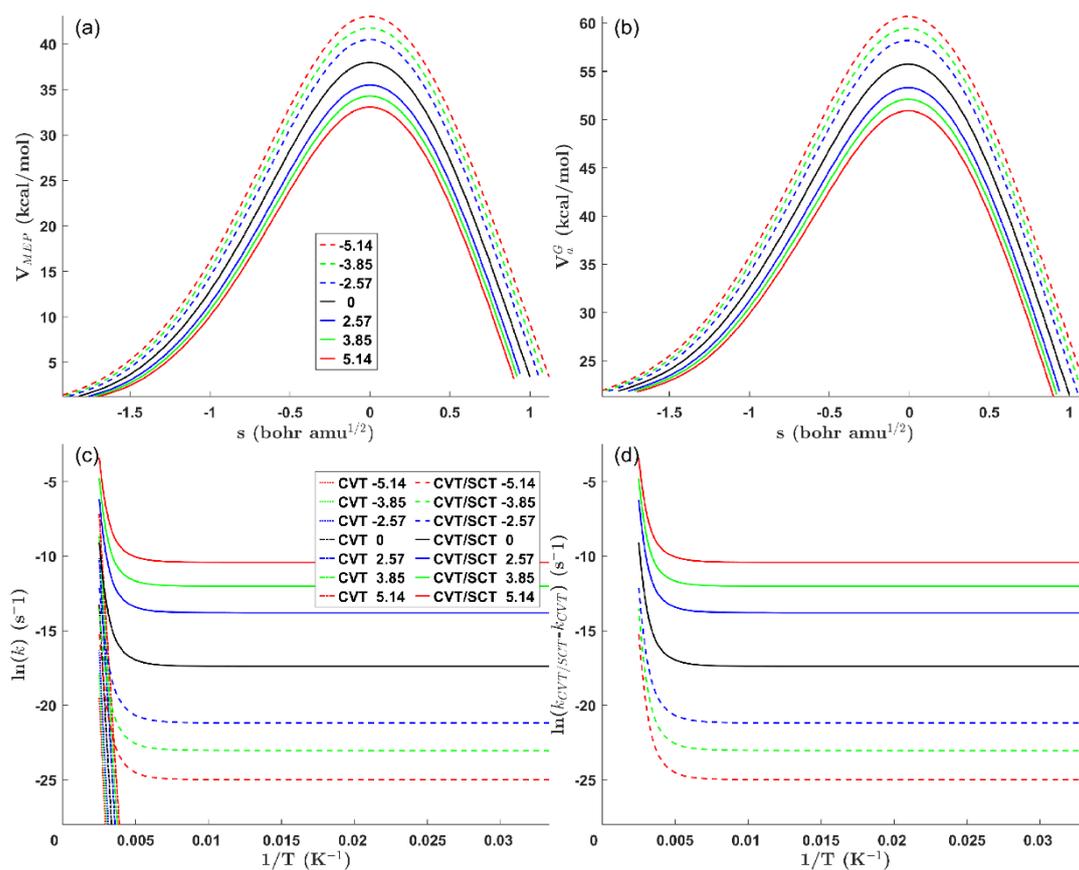
**Figure S18.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of HO-C-OH at (a) 30K, (b) 100K and (c) 200K, using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



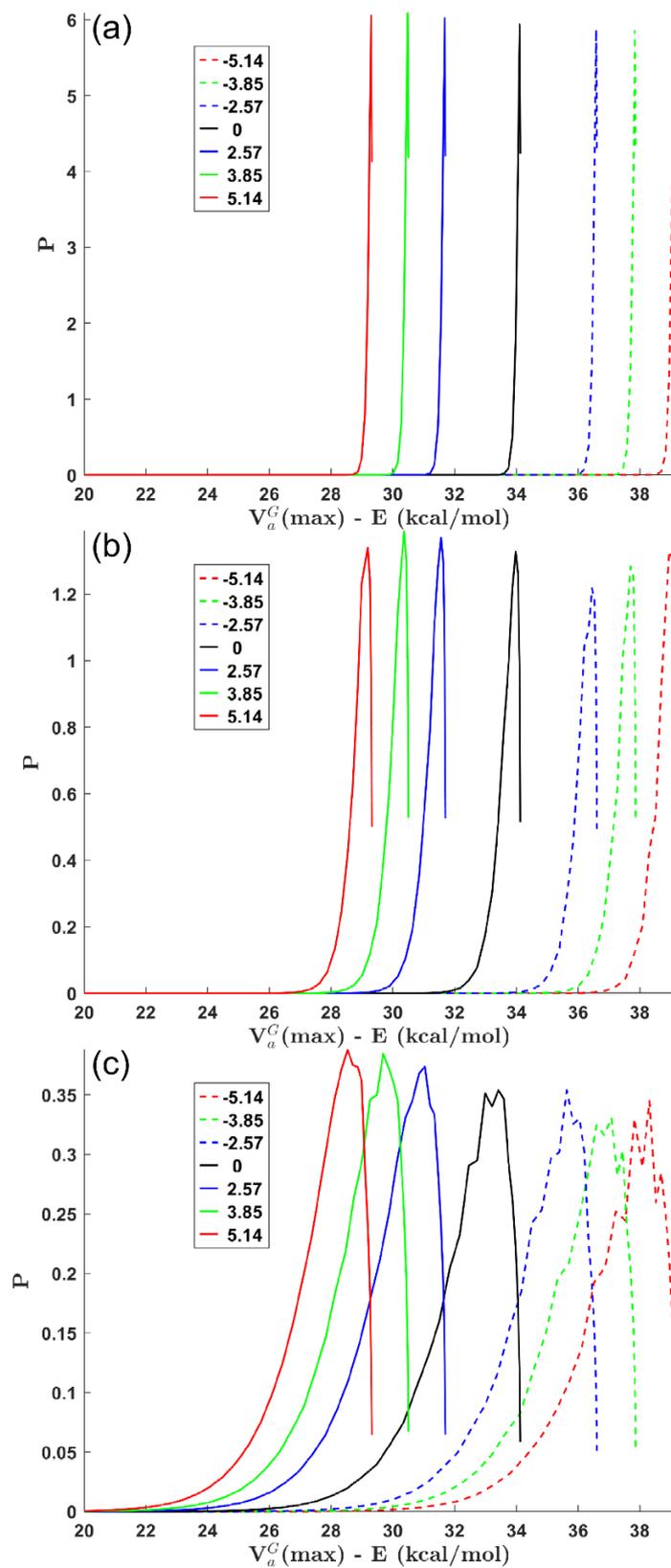
**Figure S19.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of HO-C-OH using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



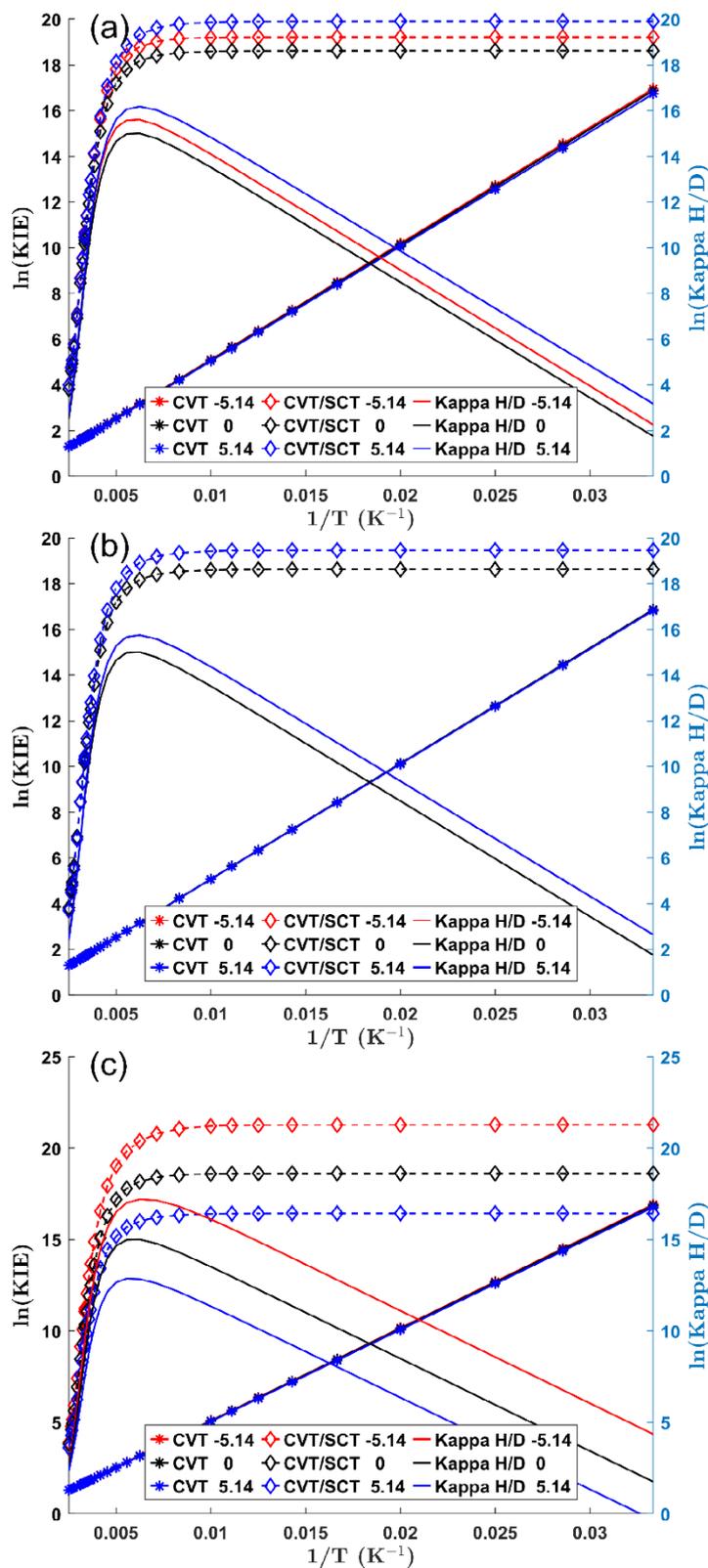
**Figure S20.** Tunneling contributions/probability (P) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of HO-C-OH at (a) 30K, (b) 100K and (c) 200K using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S21.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of HO-C-OH using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S22.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of HO-C-OH at (a) 30K, (b) 100K and (c) 200K, using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S23.** Arrhenius plots of  $\ln(\text{H/D KIE})$  and  $\ln(\kappa(\text{H})/\kappa(\text{D}))$  versus  $1/T$  for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along various directions (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S20.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.25E-236	1.80E-236	7.35E-237	1.13E-237	1.23E-238	8.70E-239	1.39E-239
35	9.88E-201	4.73E-201	2.20E-201	4.40E-202	6.58E-203	4.96E-203	1.02E-203
40	3.37E-174	1.77E-174	9.03E-175	2.21E-175	4.20E-176	3.31E-176	8.20E-177
50	4.88E-137	2.92E-137	1.70E-137	5.50E-138	1.46E-138	1.23E-138	3.96E-139
60	3.00E-112	1.95E-112	1.25E-112	4.85E-113	1.61E-113	1.42E-113	5.43E-114
70	1.56E-94	1.08E-94	7.37E-95	3.27E-95	1.28E-95	1.15E-95	5.02E-96
80	3.09E-81	2.24E-81	1.60E-81	7.83E-82	3.45E-82	3.19E-82	1.52E-82
90	6.86E-71	5.15E-71	3.82E-71	2.02E-71	9.78E-72	9.22E-72	4.74E-72
100	1.31E-62	1.02E-62	7.77E-63	4.37E-63	2.28E-63	2.18E-63	1.19E-63
120	3.58E-50	2.89E-50	2.31E-50	1.43E-50	8.32E-51	8.13E-51	4.84E-51
140	2.80E-41	2.33E-41	1.92E-41	1.27E-41	8.04E-42	7.98E-42	5.06E-42
160	1.34E-34	1.14E-34	9.64E-35	6.70E-35	4.51E-35	4.53E-35	3.01E-35
180	2.13E-29	1.85E-29	1.59E-29	1.15E-29	8.14E-30	8.25E-30	5.70E-30
200	3.13E-25	2.76E-25	2.42E-25	1.81E-25	1.32E-25	1.35E-25	9.65E-26
220	8.15E-22	7.27E-22	6.45E-22	4.95E-22	3.75E-22	3.85E-22	2.81E-22
240	5.77E-19	5.20E-19	4.67E-19	3.66E-19	2.84E-19	2.94E-19	2.19E-19
260	1.50E-16	1.37E-16	1.24E-16	9.88E-17	7.86E-17	8.15E-17	6.20E-17
273.15	3.75E-15	3.43E-15	3.12E-15	2.52E-15	2.03E-15	2.11E-15	1.62E-15
280	1.78E-14	1.63E-14	1.49E-14	1.21E-14	9.82E-15	1.02E-14	7.88E-15
290	1.52E-13	1.39E-13	1.28E-13	1.04E-13	8.56E-14	8.90E-14	6.93E-14
298.15	7.83E-13	7.21E-13	6.62E-13	5.44E-13	4.50E-13	4.68E-13	3.66E-13
300	1.12E-12	1.03E-12	9.50E-13	7.82E-13	6.47E-13	6.74E-13	5.28E-13
310	7.31E-12	6.75E-12	6.22E-12	5.16E-12	4.30E-12	4.48E-12	3.53E-12
320	4.24E-11	3.93E-11	3.63E-11	3.03E-11	2.54E-11	2.65E-11	2.10E-11
340	1.05E-09	9.76E-10	9.07E-10	7.65E-10	6.50E-10	6.81E-10	5.45E-10
360	1.82E-08	1.71E-08	1.59E-08	1.35E-08	1.16E-08	1.22E-08	9.89E-09
373.15	1.01E-07	9.48E-08	8.87E-08	7.59E-08	6.57E-08	6.91E-08	5.62E-08
380	2.35E-07	2.21E-07	2.07E-07	1.78E-07	1.55E-07	1.63E-07	1.33E-07
400	2.36E-06	2.22E-06	2.09E-06	1.81E-06	1.59E-06	1.67E-06	1.38E-06

**Table S21.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.33E-08	4.14E-08	3.33E-08	2.81E-08	1.74E-08	1.41E-08	1.05E-08
35	4.34E-08	4.14E-08	3.33E-08	2.81E-08	1.74E-08	1.41E-08	1.05E-08
40	4.34E-08	4.15E-08	3.34E-08	2.81E-08	1.74E-08	1.41E-08	1.05E-08
50	4.34E-08	4.15E-08	3.34E-08	2.81E-08	1.75E-08	1.41E-08	1.05E-08
60	4.35E-08	4.15E-08	3.34E-08	2.81E-08	1.75E-08	1.41E-08	1.05E-08
70	4.35E-08	4.16E-08	3.34E-08	2.81E-08	1.75E-08	1.41E-08	1.05E-08
80	4.35E-08	4.16E-08	3.35E-08	2.81E-08	1.75E-08	1.42E-08	1.05E-08
90	4.36E-08	4.17E-08	3.35E-08	2.82E-08	1.75E-08	1.42E-08	1.05E-08
100	4.37E-08	4.18E-08	3.36E-08	2.82E-08	1.76E-08	1.42E-08	1.06E-08
120	4.43E-08	4.24E-08	3.41E-08	2.87E-08	1.78E-08	1.45E-08	1.08E-08
140	4.57E-08	4.38E-08	3.53E-08	2.98E-08	1.85E-08	1.51E-08	1.12E-08
160	4.86E-08	4.68E-08	3.77E-08	3.20E-08	1.97E-08	1.63E-08	1.21E-08
180	5.38E-08	5.21E-08	4.21E-08	3.59E-08	2.20E-08	1.85E-08	1.37E-08
200	6.25E-08	6.11E-08	4.94E-08	4.26E-08	2.58E-08	2.22E-08	1.65E-08
220	7.70E-08	7.62E-08	6.19E-08	5.39E-08	3.24E-08	2.85E-08	2.12E-08
240	1.02E-07	1.03E-07	8.39E-08	7.39E-08	4.41E-08	4.00E-08	2.99E-08
260	1.50E-07	1.52E-07	1.26E-07	1.13E-07	6.71E-08	6.26E-08	4.72E-08
273.15	2.07E-07	2.11E-07	1.76E-07	1.59E-07	9.55E-08	9.04E-08	6.86E-08
280	2.50E-07	2.56E-07	2.14E-07	1.95E-07	1.18E-07	1.12E-07	8.55E-08
290	3.42E-07	3.52E-07	2.96E-07	2.72E-07	1.65E-07	1.60E-07	1.22E-07
298.15	4.56E-07	4.69E-07	3.97E-07	3.67E-07	2.25E-07	2.19E-07	1.69E-07
300	4.88E-07	5.03E-07	4.27E-07	3.94E-07	2.42E-07	2.37E-07	1.82E-07
310	7.26E-07	7.51E-07	6.41E-07	5.97E-07	3.71E-07	3.66E-07	2.84E-07
320	1.13E-06	1.17E-06	1.01E-06	9.42E-07	5.95E-07	5.91E-07	4.60E-07
340	3.09E-06	3.21E-06	2.79E-06	2.64E-06	1.72E-06	1.73E-06	1.36E-06
360	9.81E-06	1.01E-05	8.91E-06	8.46E-06	5.69E-06	5.81E-06	4.58E-06
373.15	2.23E-05	2.29E-05	2.03E-05	1.93E-05	1.33E-05	1.36E-05	1.08E-05
380	3.48E-05	3.57E-05	3.17E-05	3.01E-05	2.09E-05	2.16E-05	1.71E-05
400	1.33E-04	1.35E-04	1.21E-04	1.15E-04	8.26E-05	8.59E-05	6.86E-05

**Table S22.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	5.36E-237	2.60E-237	1.64E-237	1.13E-237	1.64E-237	2.60E-237	5.37E-237
35	1.68E-201	9.01E-202	6.08E-202	4.40E-202	6.08E-202	9.01E-202	1.68E-201
40	7.13E-175	4.14E-175	2.94E-175	2.21E-175	2.94E-175	4.14E-175	7.14E-175
50	1.41E-137	9.14E-138	6.93E-138	5.50E-138	6.93E-138	9.14E-138	1.41E-137
60	1.07E-112	7.43E-113	5.90E-113	4.85E-113	5.90E-113	7.43E-113	1.07E-112
70	6.44E-95	4.72E-95	3.88E-95	3.27E-95	3.88E-95	4.72E-95	6.45E-95
80	1.42E-81	1.08E-81	9.11E-82	7.83E-82	9.12E-82	1.08E-81	1.42E-81
90	3.45E-71	2.71E-71	2.32E-71	2.02E-71	2.32E-71	2.71E-71	3.45E-71
100	7.08E-63	5.69E-63	4.96E-63	4.37E-63	4.96E-63	5.69E-63	7.08E-63
120	2.14E-50	1.78E-50	1.59E-50	1.43E-50	1.59E-50	1.78E-50	2.14E-50
140	1.80E-41	1.54E-41	1.40E-41	1.27E-41	1.40E-41	1.54E-41	1.80E-41
160	9.12E-35	7.96E-35	7.30E-35	6.70E-35	7.30E-35	7.96E-35	9.12E-35
180	1.52E-29	1.35E-29	1.25E-29	1.15E-29	1.25E-29	1.35E-29	1.52E-29
200	2.32E-25	2.08E-25	1.94E-25	1.81E-25	1.94E-25	2.08E-25	2.32E-25
220	6.23E-22	5.64E-22	5.29E-22	4.95E-22	5.29E-22	5.64E-22	6.23E-22
240	4.52E-19	4.13E-19	3.90E-19	3.66E-19	3.90E-19	4.13E-19	4.52E-19
260	1.20E-16	1.11E-16	1.05E-16	9.88E-17	1.05E-16	1.11E-16	1.20E-16
273.15	3.04E-15	2.81E-15	2.67E-15	2.52E-15	2.67E-15	2.81E-15	3.04E-15
280	1.45E-14	1.34E-14	1.28E-14	1.21E-14	1.28E-14	1.34E-14	1.45E-14
290	1.25E-13	1.16E-13	1.10E-13	1.04E-13	1.10E-13	1.16E-13	1.25E-13
298.15	6.49E-13	6.03E-13	5.76E-13	5.44E-13	5.76E-13	6.03E-13	6.49E-13
300	9.31E-13	8.66E-13	8.27E-13	7.82E-13	8.27E-13	8.66E-13	9.31E-13
310	6.11E-12	5.69E-12	5.45E-12	5.16E-12	5.45E-12	5.69E-12	6.11E-12
320	3.57E-11	3.33E-11	3.19E-11	3.03E-11	3.19E-11	3.33E-11	3.57E-11
340	8.94E-10	8.38E-10	8.05E-10	7.65E-10	8.05E-10	8.38E-10	8.94E-10
360	1.57E-08	1.48E-08	1.42E-08	1.35E-08	1.42E-08	1.48E-08	1.57E-08
373.15	8.77E-08	8.27E-08	7.97E-08	7.59E-08	7.97E-08	8.27E-08	8.77E-08
380	2.05E-07	1.94E-07	1.87E-07	1.78E-07	1.87E-07	1.94E-07	2.05E-07
400	2.07E-06	1.96E-06	1.90E-06	1.81E-06	1.90E-06	1.96E-06	2.07E-06

**Table S23.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.78E-08	1.86E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
35	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
40	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
50	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
60	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
70	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
80	1.78E-08	1.87E-08	2.30E-08	2.81E-08	2.30E-08	1.87E-08	1.78E-08
90	1.79E-08	1.87E-08	2.31E-08	2.82E-08	2.31E-08	1.88E-08	1.79E-08
100	1.79E-08	1.88E-08	2.31E-08	2.82E-08	2.31E-08	1.88E-08	1.79E-08
120	1.82E-08	1.91E-08	2.35E-08	2.87E-08	2.35E-08	1.91E-08	1.82E-08
140	1.89E-08	1.98E-08	2.45E-08	2.98E-08	2.45E-08	1.98E-08	1.90E-08
160	2.04E-08	2.13E-08	2.63E-08	3.20E-08	2.63E-08	2.13E-08	2.04E-08
180	2.30E-08	2.39E-08	2.97E-08	3.59E-08	2.97E-08	2.39E-08	2.31E-08
200	2.75E-08	2.83E-08	3.54E-08	4.26E-08	3.54E-08	2.83E-08	2.75E-08
220	3.51E-08	3.57E-08	4.51E-08	5.39E-08	4.51E-08	3.57E-08	3.51E-08
240	4.85E-08	4.89E-08	6.22E-08	7.39E-08	6.22E-08	4.89E-08	4.85E-08
260	7.43E-08	7.44E-08	9.51E-08	1.13E-07	9.51E-08	7.44E-08	7.43E-08
273.15	1.05E-07	1.05E-07	1.35E-07	1.59E-07	1.35E-07	1.05E-07	1.05E-07
280	1.30E-07	1.29E-07	1.65E-07	1.95E-07	1.65E-07	1.29E-07	1.30E-07
290	1.81E-07	1.80E-07	2.31E-07	2.72E-07	2.31E-07	1.80E-07	1.81E-07
298.15	2.46E-07	2.44E-07	3.12E-07	3.67E-07	3.12E-07	2.44E-07	2.46E-07
300	2.65E-07	2.63E-07	3.35E-07	3.94E-07	3.35E-07	2.63E-07	2.65E-07
310	4.04E-07	4.01E-07	5.09E-07	5.97E-07	5.09E-07	4.01E-07	4.04E-07
320	6.44E-07	6.38E-07	8.05E-07	9.42E-07	8.05E-07	6.38E-07	6.44E-07
340	1.86E-06	1.83E-06	2.27E-06	2.64E-06	2.27E-06	1.83E-06	1.86E-06
360	6.21E-06	6.10E-06	7.39E-06	8.46E-06	7.39E-06	6.10E-06	6.21E-06
373.15	1.46E-05	1.43E-05	1.70E-05	1.93E-05	1.70E-05	1.43E-05	1.46E-05
380	2.32E-05	2.27E-05	2.68E-05	3.01E-05	2.68E-05	2.27E-05	2.32E-05
400	9.33E-05	9.06E-05	1.04E-04	1.15E-04	1.04E-04	9.06E-05	9.33E-05

**Table S24.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.15E-274	6.66E-265	9.05E-256	1.13E-237	5.61E-220	3.05E-211	1.31E-202
35	2.60E-233	2.02E-225	1.36E-217	4.40E-202	6.50E-187	1.99E-179	5.01E-172
40	1.05E-202	8.38E-196	5.94E-189	2.21E-175	4.15E-162	1.48E-155	4.41E-149
50	7.62E-160	2.54E-154	7.68E-149	5.50E-138	2.30E-127	4.00E-122	6.06E-117
60	2.96E-131	1.19E-126	4.38E-122	4.85E-113	3.45E-104	8.04E-100	1.67E-95
70	8.01E-111	7.06E-107	5.80E-103	3.27E-95	1.27E-87	7.03E-84	3.52E-80
80	1.72E-95	4.87E-92	1.30E-88	7.83E-82	3.43E-75	6.47E-72	1.12E-68
90	1.47E-83	1.72E-80	1.90E-77	2.02E-71	1.62E-65	1.32E-62	9.99E-60
100	5.20E-74	3.00E-71	1.65E-68	4.37E-63	9.03E-58	3.77E-55	1.47E-52
120	1.13E-59	2.26E-57	4.33E-55	1.43E-50	3.84E-46	5.86E-44	8.44E-42
140	2.02E-49	1.89E-47	1.71E-45	1.27E-41	7.99E-38	5.94E-36	4.21E-34
160	1.01E-41	5.35E-40	2.76E-38	6.70E-35	1.41E-31	6.13E-30	2.55E-28
180	9.99E-36	3.41E-34	1.13E-32	1.15E-29	1.04E-26	2.97E-25	8.14E-24
200	6.36E-31	1.52E-29	3.56E-28	1.81E-25	8.25E-23	1.68E-21	3.31E-20
220	5.49E-27	9.83E-26	1.72E-24	4.95E-22	1.29E-19	2.00E-18	3.01E-17
240	1.06E-23	1.49E-22	2.05E-21	3.66E-19	6.02E-17	7.41E-16	8.86E-15
260	6.42E-21	7.36E-20	8.28E-19	9.88E-17	1.10E-14	1.11E-13	1.10E-12
273.15	2.61E-19	2.66E-18	2.66E-17	2.52E-15	2.23E-13	2.02E-12	1.78E-11
280	1.57E-18	1.51E-17	1.43E-16	1.21E-14	9.57E-13	8.21E-12	6.88E-11
290	1.86E-17	1.65E-16	1.44E-15	1.04E-13	7.11E-12	5.66E-11	4.40E-10
298.15	1.23E-16	1.03E-15	8.47E-15	5.44E-13	3.30E-11	2.48E-10	1.82E-09
300	1.86E-16	1.54E-15	1.25E-14	7.82E-13	4.63E-11	3.44E-10	2.49E-09
310	1.61E-15	1.24E-14	9.43E-14	5.16E-12	2.67E-10	1.86E-09	1.27E-08
320	1.22E-14	8.82E-14	6.28E-13	3.03E-11	1.38E-09	9.06E-09	5.81E-08
340	4.91E-13	3.16E-12	2.00E-11	7.65E-10	2.79E-08	1.63E-07	9.37E-07
360	1.32E-11	7.62E-11	4.36E-10	1.35E-08	4.04E-07	2.14E-06	1.11E-05
373.15	9.47E-11	5.15E-10	2.76E-09	7.59E-08	2.01E-06	1.00E-05	4.92E-05
380	2.51E-10	1.32E-09	6.88E-09	1.78E-07	4.43E-06	2.15E-05	1.02E-04
400	3.57E-09	1.73E-08	8.27E-08	1.81E-06	3.84E-05	1.72E-04	7.56E-04

**Table S25.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.38E-11	9.82E-11	6.29E-10	2.81E-08	1.02E-06	6.01E-06	3.02E-05
35	1.38E-11	9.83E-11	6.30E-10	2.81E-08	1.02E-06	6.01E-06	3.02E-05
40	1.38E-11	9.83E-11	6.30E-10	2.81E-08	1.02E-06	6.00E-06	3.02E-05
50	1.38E-11	9.84E-11	6.30E-10	2.81E-08	1.02E-06	6.00E-06	3.02E-05
60	1.38E-11	9.85E-11	6.30E-10	2.81E-08	1.02E-06	6.00E-06	3.02E-05
70	1.38E-11	9.85E-11	6.31E-10	2.81E-08	1.02E-06	6.00E-06	3.02E-05
80	1.38E-11	9.86E-11	6.31E-10	2.81E-08	1.02E-06	6.00E-06	3.02E-05
90	1.39E-11	9.88E-11	6.32E-10	2.82E-08	1.03E-06	6.01E-06	3.02E-05
100	1.39E-11	9.91E-11	6.34E-10	2.82E-08	1.03E-06	6.02E-06	3.03E-05
120	1.42E-11	1.01E-10	6.46E-10	2.87E-08	1.04E-06	6.09E-06	3.06E-05
140	1.48E-11	1.05E-10	6.76E-10	2.98E-08	1.08E-06	6.28E-06	3.16E-05
160	1.61E-11	1.14E-10	7.36E-10	3.20E-08	1.14E-06	6.66E-06	3.35E-05
180	1.84E-11	1.29E-10	8.45E-10	3.59E-08	1.26E-06	7.33E-06	3.69E-05
200	2.24E-11	1.56E-10	1.03E-09	4.26E-08	1.47E-06	8.44E-06	4.25E-05
220	2.97E-11	2.03E-10	1.36E-09	5.39E-08	1.81E-06	1.03E-05	5.18E-05
240	4.36E-11	2.92E-10	1.97E-09	7.39E-08	2.40E-06	1.34E-05	6.76E-05
260	7.32E-11	4.79E-10	3.18E-09	1.13E-07	3.49E-06	1.91E-05	9.59E-05
273.15	1.12E-10	7.20E-10	4.71E-09	1.59E-07	4.75E-06	2.56E-05	1.28E-04
280	1.45E-10	9.18E-10	5.93E-09	1.95E-07	5.71E-06	3.05E-05	1.51E-04
290	2.18E-10	1.36E-09	8.61E-09	2.72E-07	7.71E-06	4.04E-05	1.99E-04
298.15	3.15E-10	1.94E-09	1.20E-08	3.67E-07	1.01E-05	5.23E-05	2.55E-04
300	3.45E-10	2.11E-09	1.30E-08	3.94E-07	1.08E-05	5.56E-05	2.71E-04
310	5.71E-10	3.43E-09	2.07E-08	5.97E-07	1.58E-05	7.94E-05	3.83E-04
320	9.90E-10	5.81E-09	3.41E-08	9.42E-07	2.39E-05	1.18E-04	5.60E-04
340	3.37E-09	1.89E-08	1.04E-07	2.64E-06	6.16E-05	2.91E-04	1.33E-03
360	1.32E-08	7.02E-08	3.67E-07	8.46E-06	1.81E-04	8.17E-04	3.59E-03
373.15	3.46E-08	1.77E-07	8.90E-07	1.93E-05	3.90E-04	1.70E-03	7.27E-03
380	5.81E-08	2.92E-07	1.43E-06	3.01E-05	5.90E-04	2.53E-03	1.06E-02
400	2.77E-07	1.31E-06	6.03E-06	1.15E-04	2.05E-03	8.37E-03	3.33E-02

**Table S26.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	1.83E-243	5.31E-245	7.49E-247
35	4.77E-207	2.29E-208	5.96E-210
40	9.98E-180	6.99E-181	2.87E-182
50	1.83E-141	2.18E-142	1.70E-143
60	6.13E-116	1.03E-116	1.24E-117
70	1.07E-97	2.32E-98	3.78E-99
80	5.23E-84	1.37E-84	2.81E-85
90	2.36E-73	7.16E-74	1.76E-74
100	7.95E-65	2.72E-65	7.70E-66
120	5.06E-52	2.06E-52	7.27E-53
140	7.27E-43	3.37E-43	1.39E-43
160	5.49E-36	2.80E-36	1.30E-36
180	1.25E-30	6.87E-31	3.49E-31
200	2.44E-26	1.43E-26	7.82E-27
220	8.01E-23	4.92E-23	2.87E-23
240	6.88E-20	4.41E-20	2.70E-20
260	2.11E-17	1.40E-17	8.94E-18
273.15	5.77E-16	3.91E-16	2.56E-16
280	2.87E-15	1.96E-15	1.30E-15
290	2.60E-14	1.80E-14	1.22E-14
298.15	1.40E-13	9.84E-14	6.73E-14
300	2.03E-13	1.43E-13	9.79E-14
310	1.40E-12	9.92E-13	6.90E-13
320	8.52E-12	6.12E-12	4.31E-12
340	2.31E-10	1.69E-10	1.22E-10
360	4.34E-09	3.24E-09	2.39E-09
373.15	2.52E-08	1.90E-08	1.42E-08
380	6.02E-08	4.56E-08	3.44E-08
400	6.42E-07	4.94E-07	3.79E-07

**Table S27.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	1.95E-16	2.28E-16	2.36E-17
35	1.95E-16	2.28E-16	2.36E-17
40	1.95E-16	2.28E-16	2.36E-17
50	1.95E-16	2.28E-16	2.36E-17
60	1.95E-16	2.29E-16	2.37E-17
70	1.96E-16	2.29E-16	2.37E-17
80	1.96E-16	2.30E-16	2.39E-17
90	1.97E-16	2.32E-16	2.42E-17
100	2.00E-16	2.36E-16	2.48E-17
120	2.14E-16	2.55E-16	2.75E-17
140	2.50E-16	3.01E-16	3.38E-17
160	3.32E-16	4.06E-16	4.89E-17
180	5.40E-16	6.66E-16	8.89E-17
200	1.16E-15	1.45E-15	2.21E-16
220	3.60E-15	4.49E-15	8.04E-16
240	1.66E-14	2.07E-14	4.35E-15
260	1.14E-13	1.40E-13	3.42E-14
273.15	4.89E-13	5.83E-13	1.60E-13
280	1.10E-12	1.29E-12	3.76E-13
290	3.78E-12	4.29E-12	1.38E-12
298.15	1.07E-11	1.19E-11	4.09E-12
300	1.37E-11	1.50E-11	5.26E-12
310	5.08E-11	5.42E-11	2.05E-11
320	1.90E-10	1.98E-10	8.02E-11
340	2.54E-09	2.58E-09	1.15E-09
360	2.98E-08	3.01E-08	1.42E-08
373.15	1.37E-07	1.39E-07	6.75E-08
380	2.94E-07	3.00E-07	1.47E-07
400	2.43E-06	2.52E-06	1.27E-06

**Table S28.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	2.64E-244	5.31E-245	2.65E-244
35	9.08E-208	2.29E-208	9.13E-208
40	2.34E-180	6.99E-181	2.35E-180
50	5.74E-142	2.18E-142	5.76E-142
60	2.33E-116	1.03E-116	2.34E-116
70	4.67E-98	2.32E-98	4.68E-98
80	2.53E-84	1.37E-84	2.54E-84
90	1.24E-73	7.16E-74	1.24E-73
100	4.46E-65	2.72E-65	4.47E-65
120	3.13E-52	2.06E-52	3.14E-52
140	4.84E-43	3.37E-43	4.84E-43
160	3.85E-36	2.80E-36	3.86E-36
180	9.14E-31	6.87E-31	9.15E-31
200	1.85E-26	1.43E-26	1.85E-26
220	6.24E-23	4.92E-23	6.25E-23
240	5.49E-20	4.41E-20	5.50E-20
260	1.72E-17	1.40E-17	1.72E-17
273.15	4.75E-16	3.91E-16	4.76E-16
280	2.37E-15	1.96E-15	2.38E-15
290	2.17E-14	1.80E-14	2.17E-14
298.15	1.18E-13	9.84E-14	1.18E-13
300	1.71E-13	1.43E-13	1.71E-13
310	1.18E-12	9.92E-13	1.18E-12
320	7.26E-12	6.12E-12	7.26E-12
340	1.99E-10	1.69E-10	1.99E-10
360	3.78E-09	3.24E-09	3.78E-09
373.15	2.21E-08	1.90E-08	2.21E-08
380	5.28E-08	4.56E-08	5.29E-08
400	5.69E-07	4.94E-07	5.69E-07

**Table S29.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	6.22E-17	2.28E-16	6.23E-17
35	6.22E-17	2.28E-16	6.23E-17
40	6.22E-17	2.28E-16	6.23E-17
50	6.23E-17	2.28E-16	6.23E-17
60	6.23E-17	2.29E-16	6.24E-17
70	6.24E-17	2.29E-16	6.25E-17
80	6.27E-17	2.30E-16	6.28E-17
90	6.35E-17	2.32E-16	6.35E-17
100	6.49E-17	2.36E-16	6.49E-17
120	7.15E-17	2.55E-16	7.15E-17
140	8.74E-17	3.01E-16	8.74E-17
160	1.24E-16	4.06E-16	1.24E-16
180	2.17E-16	6.66E-16	2.17E-16
200	5.06E-16	1.45E-15	5.06E-16
220	1.70E-15	4.49E-15	1.70E-15
240	8.55E-15	2.07E-14	8.56E-15
260	6.39E-14	1.40E-13	6.39E-14
273.15	2.90E-13	5.83E-13	2.90E-13
280	6.70E-13	1.29E-12	6.71E-13
290	2.41E-12	4.29E-12	2.41E-12
298.15	7.11E-12	1.19E-11	7.11E-12
300	9.12E-12	1.50E-11	9.12E-12
310	3.55E-11	5.42E-11	3.55E-11
320	1.39E-10	1.98E-10	1.39E-10
340	2.01E-09	2.58E-09	2.01E-09
360	2.52E-08	3.01E-08	2.52E-08
373.15	1.21E-07	1.39E-07	1.20E-07
380	2.64E-07	3.00E-07	2.63E-07
400	2.29E-06	2.52E-06	2.29E-06

**Table S30.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.85E-281	5.31E-245	6.85E-210
35	1.29E-239	2.29E-208	2.86E-178
40	3.18E-208	6.99E-181	1.51E-154
50	2.92E-164	2.18E-142	2.56E-121
60	6.16E-135	1.03E-116	3.76E-99
70	5.56E-114	2.32E-98	2.62E-83
80	2.95E-98	1.37E-84	2.04E-71
90	5.10E-86	7.16E-74	3.67E-62
100	3.18E-76	2.72E-65	9.41E-55
120	1.61E-61	2.06E-52	1.26E-43
140	5.29E-51	3.37E-43	1.14E-35
160	4.18E-43	2.80E-36	1.08E-29
180	5.91E-37	6.87E-31	4.92E-25
200	5.00E-32	1.43E-26	2.65E-21
220	5.44E-28	4.92E-23	3.03E-18
240	1.27E-24	4.41E-20	1.08E-15
260	9.05E-22	1.40E-17	1.57E-13
273.15	4.04E-20	3.91E-16	2.79E-12
280	2.54E-19	1.96E-15	1.13E-11
290	3.19E-18	1.80E-14	7.66E-11
298.15	2.21E-17	9.84E-14	3.33E-10
300	3.39E-17	1.43E-13	4.59E-10
310	3.09E-16	9.92E-13	2.46E-09
320	2.46E-15	6.12E-12	1.18E-08
340	1.08E-13	1.69E-10	2.09E-07
360	3.14E-12	3.24E-09	2.68E-06
373.15	2.37E-11	1.90E-08	1.24E-05
380	6.41E-11	4.56E-08	2.64E-05
400	9.70E-10	4.94E-07	2.08E-04

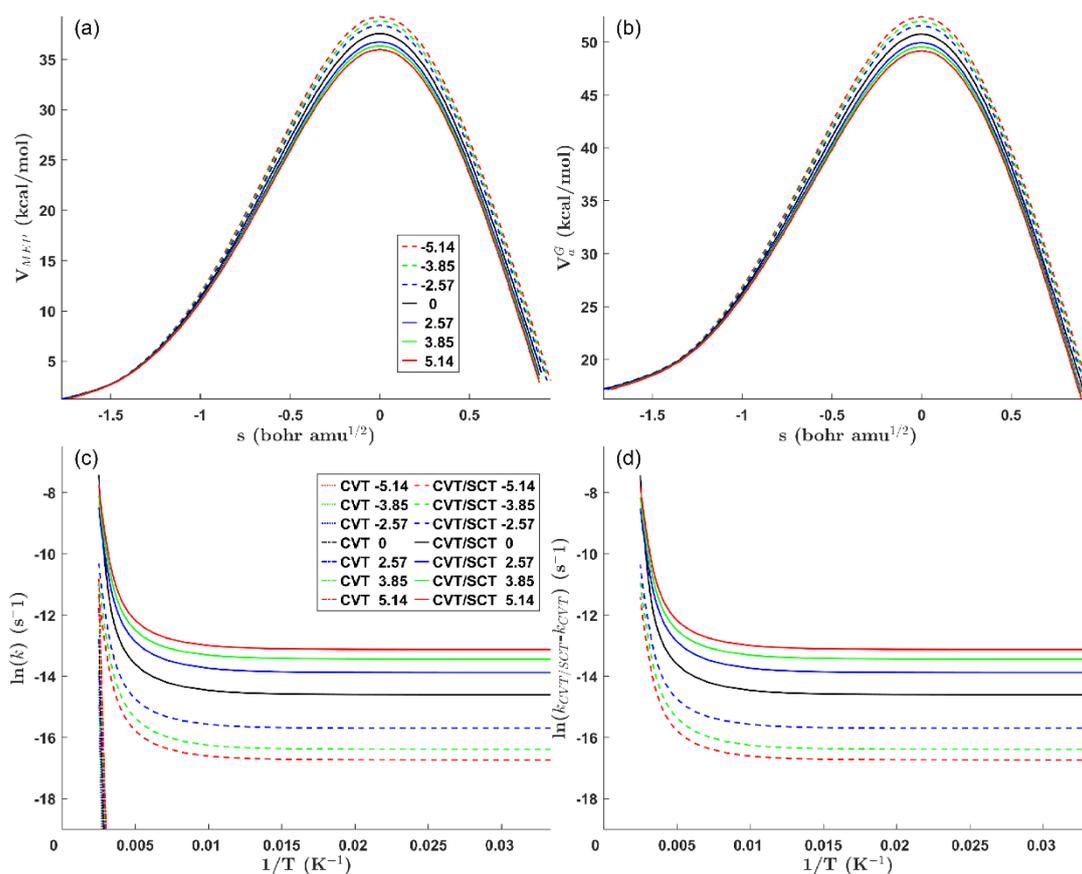
**Table S31.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	7.84E-21	2.28E-16	2.21E-12
35	7.86E-21	2.28E-16	2.20E-12
40	7.87E-21	2.28E-16	2.20E-12
50	7.90E-21	2.28E-16	2.20E-12
60	7.92E-21	2.29E-16	2.20E-12
70	7.95E-21	2.29E-16	2.20E-12
80	8.02E-21	2.30E-16	2.21E-12
90	8.19E-21	2.32E-16	2.23E-12
100	8.53E-21	2.36E-16	2.27E-12
120	1.01E-20	2.55E-16	2.45E-12
140	1.38E-20	3.01E-16	2.86E-12
160	2.24E-20	4.06E-16	3.73E-12
180	4.45E-20	6.66E-16	5.69E-12
200	1.19E-19	1.45E-15	1.08E-11
220	4.71E-19	4.49E-15	2.74E-11
240	2.81E-18	2.07E-14	9.97E-11
260	2.51E-17	1.40E-13	5.18E-10
273.15	1.29E-16	5.83E-13	1.80E-09
280	3.20E-16	1.29E-12	3.60E-09
290	1.28E-15	4.29E-12	1.03E-08
298.15	4.12E-15	1.19E-11	2.49E-08
300	5.40E-15	1.50E-11	3.06E-08
310	2.37E-14	5.42E-11	9.28E-08
320	1.06E-13	1.98E-10	2.83E-07
340	2.04E-12	2.58E-09	2.55E-06
360	3.46E-11	3.01E-08	2.07E-05
373.15	2.01E-10	1.39E-07	7.60E-05
380	4.86E-10	3.00E-07	1.46E-04
400	5.60E-09	2.52E-06	8.94E-04

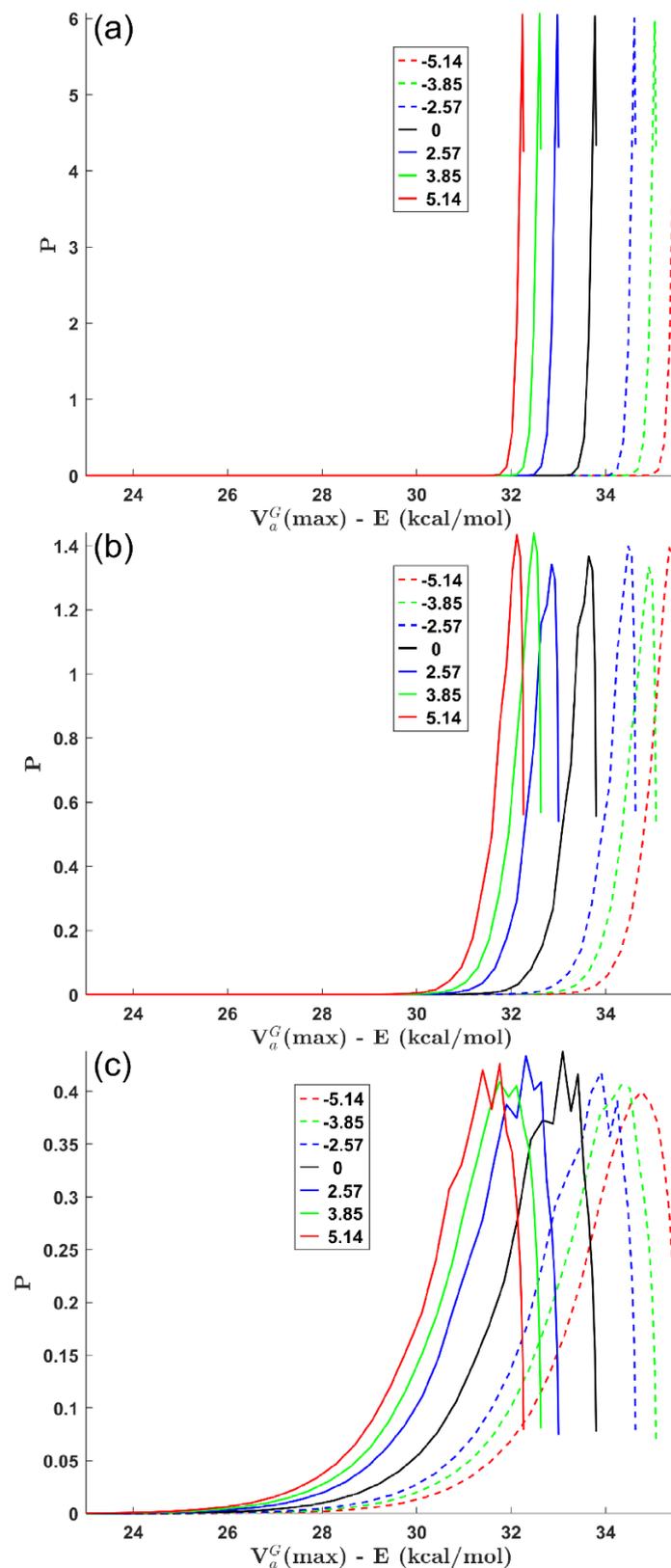
## NC-C-OH

**Table S32.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) for the H-migration of NC-C-OH using the  $\omega$ B97X-D method under different EEF strengths (V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

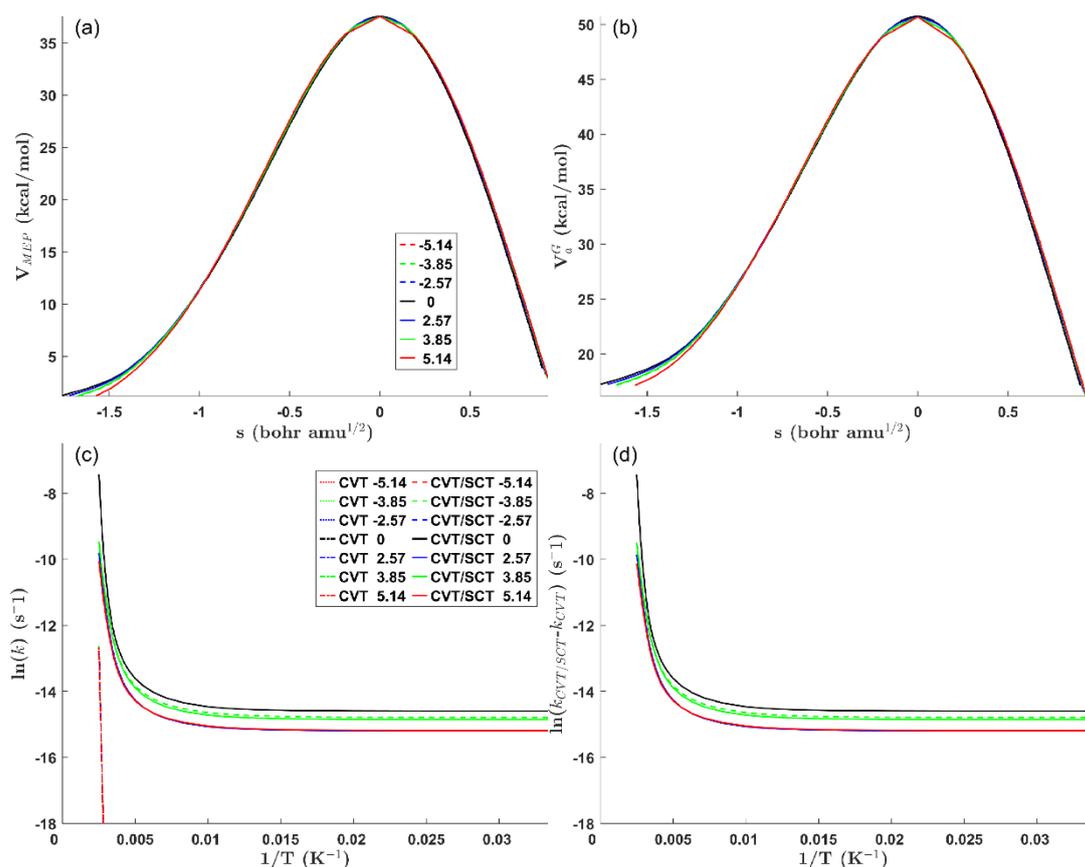
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	39.26	38.83	38.39	37.55	36.74	36.35	35.98
$\Delta V_a^G(\max)$	52.41	51.98	51.56	50.73	49.94	49.55	49.18
$\Omega$	2144	2141	2138	2131	2123	2118	2114
$T_c$	491	490	490	488	486	485	484
<b>Y-EEF Direction</b>							
$\Delta E$	37.54	37.50	37.55	37.55	37.55	37.55	37.54
$\Delta V_a^G(\max)$	50.67	50.62	50.70	50.73	50.70	50.67	50.67
$\Omega$	2136	2130	2131	2131	2131	2130	2136
$T_c$	489	488	488	488	488	488	489
<b>Z-EEF Direction</b>							
$\Delta E$	41.94	40.89	39.78	37.55	35.31	34.19	33.08
$\Delta V_a^G(\max)$	55.05	54.02	52.92	50.73	48.54	47.46	46.40
$\Omega$	2138	2138	2136	2131	2123	2117	2111
$T_c$	490	489	489	488	486	485	483



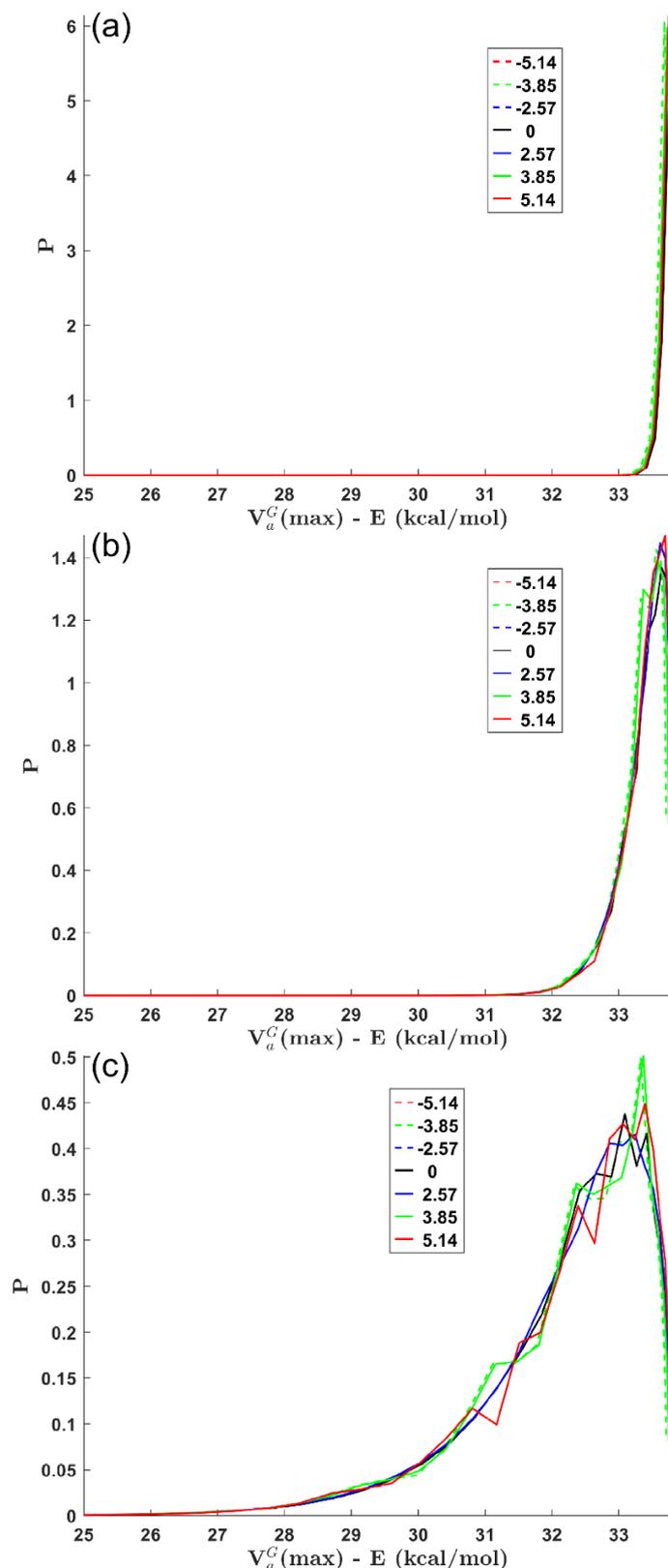
**Figure S24.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of NC-C-OH using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



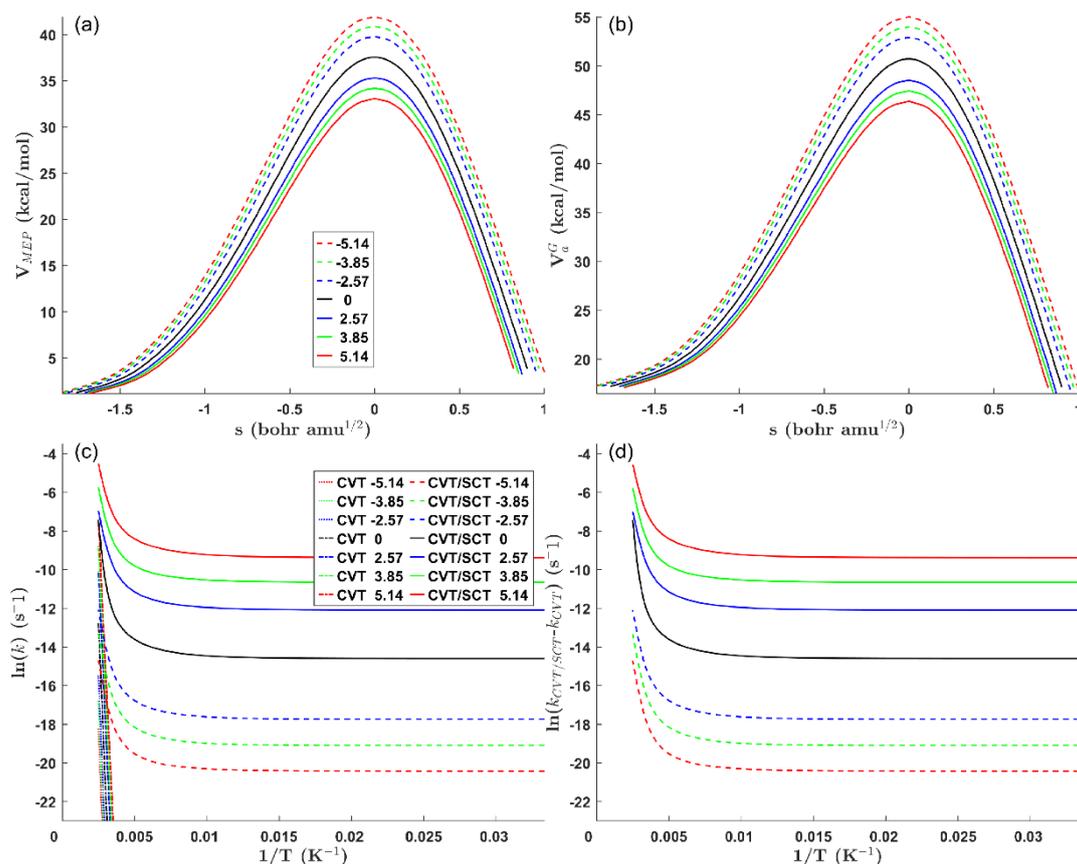
**Figure S25.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of NC-C-OH at (a) 30K, (b) 100K and (c) 200K, using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



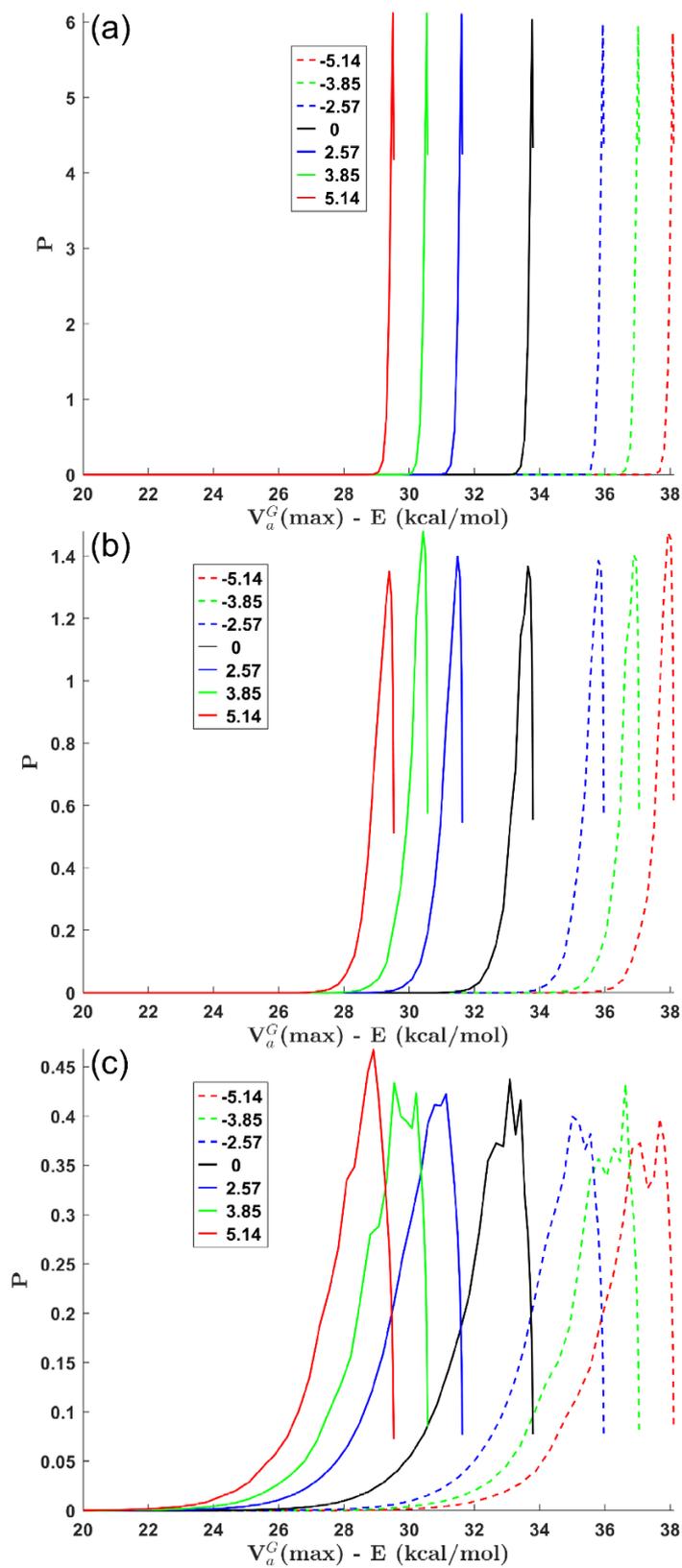
**Figure S26.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of NC-C-OH using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



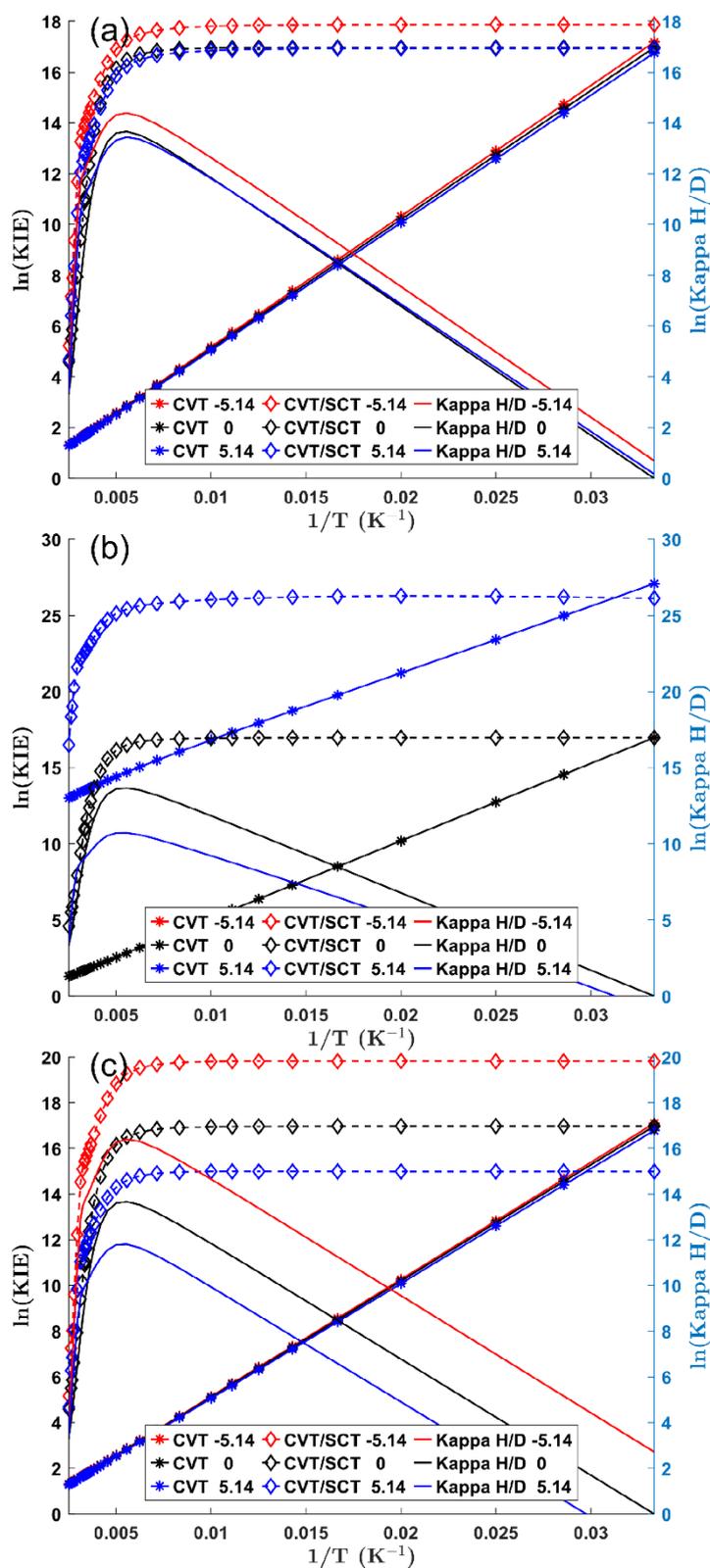
**Figure S27.** Tunneling contributions/probability (P) to the SCT transmission coefficient ( $\kappa_{SCT}$ ) for the H-migration of NC-C-OH at (a) 30K, (b) 100K and (c) 200K using the  $\omega$ B97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S28.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of NC-C-OH using the  $\omega$ B97X-Dmethod along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S29.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of NC-C-OH at (a) 30K, (b) 100K and (c) 200K, using the  $\omega$ B97X-D method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S30.** Arrhenius plots of  $\ln H/D$  (KIE) and  $\ln(\kappa(H)/\kappa(D))$  versus  $1/T$  for the H-migration of NC-C-OH using the  $\omega$ B97X-D method along the direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S33.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.13E-247	1.85E-244	2.63E-241	3.28E-235	1.92E-229	1.07E-226	4.60E-224
35	1.19E-210	6.75E-208	3.40E-205	5.71E-200	5.02E-195	1.13E-192	2.05E-190
40	7.10E-183	1.82E-180	4.21E-178	1.57E-173	3.32E-169	3.80E-167	3.58E-165
50	5.64E-144	4.76E-142	3.71E-140	1.68E-136	4.84E-133	2.15E-131	8.16E-130
60	5.01E-118	2.02E-116	7.60E-115	8.45E-112	6.45E-109	1.52E-107	3.15E-106
70	1.76E-99	4.18E-98	9.36E-97	3.82E-94	1.13E-91	1.69E-90	2.27E-89
80	1.45E-85	2.32E-84	3.53E-83	6.79E-81	9.85E-79	1.05E-77	1.02E-76
90	9.85E-75	1.16E-73	1.30E-72	1.39E-70	1.16E-68	9.53E-68	7.18E-67
100	4.61E-66	4.23E-65	3.72E-64	2.50E-62	1.34E-60	8.92E-60	5.49E-59
120	4.78E-53	3.03E-52	1.86E-51	6.20E-50	1.71E-48	8.31E-48	3.78E-47
140	9.72E-44	4.74E-43	2.25E-42	4.54E-41	7.81E-40	3.02E-39	1.11E-38
160	9.49E-37	3.80E-36	1.49E-35	2.07E-34	2.49E-33	8.15E-33	2.54E-32
180	2.63E-31	9.06E-31	3.04E-30	3.17E-29	2.90E-28	8.31E-28	2.28E-27
200	6.04E-27	1.84E-26	5.48E-26	4.51E-25	3.32E-24	8.56E-24	2.13E-23
220	2.25E-23	6.21E-23	1.68E-22	1.14E-21	7.02E-21	1.66E-20	3.80E-20
240	2.16E-20	5.47E-20	1.36E-19	7.92E-19	4.18E-18	9.23E-18	1.97E-17
260	7.23E-18	1.71E-17	3.97E-17	2.02E-16	9.41E-16	1.95E-15	3.93E-15
273.15	2.09E-16	4.74E-16	1.06E-15	4.99E-15	2.16E-14	4.33E-14	8.42E-14
280	1.06E-15	2.37E-15	5.19E-15	2.35E-14	9.82E-14	1.94E-13	3.71E-13
290	9.98E-15	2.16E-14	4.62E-14	1.99E-13	7.91E-13	1.52E-12	2.86E-12
298.15	5.54E-14	1.18E-13	2.46E-13	1.02E-12	3.91E-12	7.40E-12	1.36E-11
300	8.08E-14	1.71E-13	3.56E-13	1.46E-12	5.55E-12	1.05E-11	1.92E-11
310	5.72E-13	1.18E-12	2.40E-12	9.45E-12	3.44E-11	6.36E-11	1.14E-10
320	3.59E-12	7.25E-12	1.44E-11	5.45E-11	1.90E-10	3.45E-10	6.10E-10
340	1.03E-10	1.99E-10	3.81E-10	1.33E-09	4.33E-09	7.58E-09	1.30E-08
360	2.03E-09	3.79E-09	7.02E-09	2.29E-08	6.98E-08	1.18E-07	1.97E-07
373.15	1.21E-08	2.22E-08	4.02E-08	1.26E-07	3.70E-07	6.16E-07	1.00E-06
380	2.93E-08	5.32E-08	9.53E-08	2.93E-07	8.42E-07	1.39E-06	2.25E-06
400	3.26E-07	5.74E-07	1.00E-06	2.91E-06	7.94E-06	1.28E-05	2.02E-05

**Table S34.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	5.39E-08	7.61E-08	1.52E-07	4.57E-07	9.41E-07	1.46E-06	2.00E-06
35	5.39E-08	7.61E-08	1.52E-07	4.57E-07	9.41E-07	1.46E-06	2.00E-06
40	5.40E-08	7.62E-08	1.52E-07	4.57E-07	9.42E-07	1.46E-06	2.00E-06
50	5.42E-08	7.64E-08	1.52E-07	4.59E-07	9.45E-07	1.47E-06	2.01E-06
60	5.46E-08	7.72E-08	1.54E-07	4.63E-07	9.54E-07	1.48E-06	2.03E-06
70	5.55E-08	7.85E-08	1.56E-07	4.71E-07	9.71E-07	1.50E-06	2.06E-06
80	5.69E-08	8.06E-08	1.60E-07	4.83E-07	9.97E-07	1.54E-06	2.11E-06
90	5.88E-08	8.36E-08	1.65E-07	5.01E-07	1.03E-06	1.59E-06	2.18E-06
100	6.13E-08	8.76E-08	1.73E-07	5.24E-07	1.08E-06	1.66E-06	2.27E-06
120	6.83E-08	9.86E-08	1.93E-07	5.88E-07	1.22E-06	1.85E-06	2.53E-06
140	7.84E-08	1.15E-07	2.21E-07	6.81E-07	1.41E-06	2.12E-06	2.90E-06
160	9.25E-08	1.37E-07	2.61E-07	8.08E-07	1.68E-06	2.49E-06	3.42E-06
180	1.12E-07	1.68E-07	3.16E-07	9.84E-07	2.05E-06	3.01E-06	4.14E-06
200	1.40E-07	2.12E-07	3.94E-07	1.23E-06	2.57E-06	3.74E-06	5.15E-06
220	1.80E-07	2.76E-07	5.08E-07	1.58E-06	3.32E-06	4.81E-06	6.63E-06
240	2.42E-07	3.76E-07	6.82E-07	2.12E-06	4.46E-06	6.45E-06	8.91E-06
260	3.42E-07	5.38E-07	9.63E-07	3.01E-06	6.29E-06	9.09E-06	1.26E-05
273.15	4.44E-07	7.02E-07	1.25E-06	3.93E-06	8.13E-06	1.18E-05	1.63E-05
280	5.13E-07	8.15E-07	1.44E-06	4.58E-06	9.39E-06	1.36E-05	1.89E-05
290	6.42E-07	1.03E-06	1.81E-06	5.85E-06	1.17E-05	1.70E-05	2.36E-05
298.15	7.78E-07	1.25E-06	2.19E-06	7.28E-06	1.42E-05	2.06E-05	2.86E-05
300	8.14E-07	1.31E-06	2.29E-06	7.68E-06	1.48E-05	2.15E-05	2.99E-05
310	1.04E-06	1.69E-06	2.95E-06	1.04E-05	1.90E-05	2.76E-05	3.84E-05
320	1.35E-06	2.20E-06	3.82E-06	1.45E-05	2.45E-05	3.56E-05	4.97E-05
340	2.31E-06	3.79E-06	6.54E-06	3.09E-05	4.17E-05	6.07E-05	8.47E-05
360	3.96E-06	6.57E-06	1.13E-05	7.49E-05	7.15E-05	1.04E-04	1.45E-04
373.15	5.63E-06	9.40E-06	1.61E-05	1.42E-04	1.02E-04	1.48E-04	2.07E-04
380	6.76E-06	1.13E-05	1.93E-05	2.02E-04	1.22E-04	1.78E-04	2.48E-04
400	1.15E-05	1.93E-05	3.29E-05	5.96E-04	2.08E-04	3.03E-04	4.24E-04

**Table S35.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	5.14E-235	1.40E-234	5.06E-235	3.28E-235	5.06E-235	7.52E-235	5.14E-235
35	8.40E-200	1.98E-199	8.29E-200	5.71E-200	8.29E-200	1.16E-199	8.40E-200
40	2.20E-173	4.66E-173	2.17E-173	1.57E-173	2.17E-173	2.93E-173	2.20E-173
50	2.21E-136	4.01E-136	2.18E-136	1.68E-136	2.18E-136	2.77E-136	2.21E-136
60	1.06E-111	1.75E-111	1.05E-111	8.45E-112	1.05E-111	1.29E-111	1.06E-111
70	4.67E-94	7.13E-94	4.63E-94	3.82E-94	4.63E-94	5.50E-94	4.67E-94
80	8.13E-81	1.17E-80	8.05E-81	6.79E-81	8.05E-81	9.39E-81	8.13E-81
90	1.64E-70	2.27E-70	1.63E-70	1.39E-70	1.63E-70	1.87E-70	1.64E-70
100	2.91E-62	3.89E-62	2.89E-62	2.50E-62	2.89E-62	3.28E-62	2.91E-62
120	7.09E-50	8.98E-50	7.04E-50	6.20E-50	7.04E-50	7.85E-50	7.09E-50
140	5.13E-41	6.25E-41	5.10E-41	4.54E-41	5.10E-41	5.61E-41	5.13E-41
160	2.31E-34	2.74E-34	2.30E-34	2.07E-34	2.30E-34	2.51E-34	2.31E-34
180	3.51E-29	4.07E-29	3.50E-29	3.17E-29	3.50E-29	3.80E-29	3.51E-29
200	4.98E-25	5.66E-25	4.97E-25	4.51E-25	4.97E-25	5.36E-25	4.98E-25
220	1.26E-21	1.41E-21	1.26E-21	1.14E-21	1.26E-21	1.35E-21	1.26E-21
240	8.67E-19	9.59E-19	8.68E-19	7.92E-19	8.68E-19	9.27E-19	8.68E-19
260	2.21E-16	2.41E-16	2.21E-16	2.02E-16	2.21E-16	2.35E-16	2.21E-16
273.15	5.44E-15	5.91E-15	5.44E-15	4.99E-15	5.44E-15	5.79E-15	5.44E-15
280	2.56E-14	2.78E-14	2.57E-14	2.35E-14	2.57E-14	2.73E-14	2.56E-14
290	2.17E-13	2.33E-13	2.17E-13	1.99E-13	2.17E-13	2.30E-13	2.17E-13
298.15	1.11E-12	1.19E-12	1.11E-12	1.02E-12	1.11E-12	1.18E-12	1.11E-12
300	1.59E-12	1.71E-12	1.59E-12	1.46E-12	1.59E-12	1.69E-12	1.59E-12
310	1.03E-11	1.10E-11	1.03E-11	9.45E-12	1.03E-11	1.09E-11	1.03E-11
320	5.91E-11	6.30E-11	5.92E-11	5.45E-11	5.92E-11	6.26E-11	5.91E-11
340	1.44E-09	1.53E-09	1.45E-09	1.33E-09	1.45E-09	1.53E-09	1.44E-09
360	2.48E-08	2.61E-08	2.48E-08	2.29E-08	2.48E-08	2.62E-08	2.48E-08
373.15	1.36E-07	1.43E-07	1.37E-07	1.26E-07	1.37E-07	1.44E-07	1.36E-07
380	3.16E-07	3.31E-07	3.17E-07	2.93E-07	3.17E-07	3.34E-07	3.16E-07
400	3.14E-06	3.27E-06	3.15E-06	2.91E-06	3.15E-06	3.31E-06	3.14E-06

**Table S36.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.53E-07	3.78E-07	2.52E-07	4.57E-07	2.52E-07	3.54E-07	2.53E-07
35	2.54E-07	3.78E-07	2.52E-07	4.57E-07	2.52E-07	3.55E-07	2.54E-07
40	2.54E-07	3.79E-07	2.52E-07	4.57E-07	2.52E-07	3.55E-07	2.54E-07
50	2.55E-07	3.81E-07	2.53E-07	4.59E-07	2.53E-07	3.57E-07	2.55E-07
60	2.58E-07	3.85E-07	2.55E-07	4.63E-07	2.55E-07	3.61E-07	2.58E-07
70	2.63E-07	3.93E-07	2.59E-07	4.71E-07	2.59E-07	3.67E-07	2.63E-07
80	2.70E-07	4.04E-07	2.66E-07	4.83E-07	2.66E-07	3.77E-07	2.70E-07
90	2.80E-07	4.19E-07	2.75E-07	5.01E-07	2.75E-07	3.90E-07	2.80E-07
100	2.92E-07	4.37E-07	2.87E-07	5.24E-07	2.87E-07	4.07E-07	2.92E-07
120	3.25E-07	4.89E-07	3.19E-07	5.88E-07	3.19E-07	4.53E-07	3.25E-07
140	3.70E-07	5.60E-07	3.65E-07	6.81E-07	3.65E-07	5.20E-07	3.70E-07
160	4.30E-07	6.58E-07	4.28E-07	8.08E-07	4.28E-07	6.13E-07	4.30E-07
180	5.12E-07	7.92E-07	5.15E-07	9.84E-07	5.15E-07	7.42E-07	5.12E-07
200	6.26E-07	9.80E-07	6.39E-07	1.23E-06	6.39E-07	9.25E-07	6.26E-07
220	7.91E-07	1.25E-06	8.21E-07	1.58E-06	8.21E-07	1.19E-06	7.91E-07
240	1.04E-06	1.67E-06	1.10E-06	2.12E-06	1.10E-06	1.61E-06	1.04E-06
260	1.45E-06	2.34E-06	1.56E-06	3.01E-06	1.56E-06	2.28E-06	1.45E-06
273.15	1.87E-06	3.01E-06	2.02E-06	3.93E-06	2.02E-06	2.97E-06	1.87E-06
280	2.15E-06	3.47E-06	2.34E-06	4.58E-06	2.34E-06	3.44E-06	2.15E-06
290	2.67E-06	4.31E-06	2.94E-06	5.85E-06	2.94E-06	4.32E-06	2.67E-06
298.15	3.22E-06	5.20E-06	3.57E-06	7.28E-06	3.57E-06	5.24E-06	3.22E-06
300	3.36E-06	5.42E-06	3.74E-06	7.68E-06	3.74E-06	5.48E-06	3.37E-06
310	4.28E-06	6.89E-06	4.82E-06	1.04E-05	4.82E-06	7.05E-06	4.28E-06
320	5.49E-06	8.82E-06	6.26E-06	1.45E-05	6.26E-06	9.14E-06	5.49E-06
340	9.14E-06	1.46E-05	1.08E-05	3.09E-05	1.08E-05	1.56E-05	9.14E-06
360	1.53E-05	2.43E-05	1.86E-05	7.49E-05	1.86E-05	2.68E-05	1.53E-05
373.15	2.14E-05	3.39E-05	2.66E-05	1.42E-04	2.66E-05	3.81E-05	2.14E-05
380	2.54E-05	4.02E-05	3.20E-05	2.02E-04	3.20E-05	4.57E-05	2.54E-05
400	4.28E-05	6.65E-05	5.54E-05	5.96E-04	5.54E-05	7.80E-05	4.28E-05

**Table S37.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.18E-266	6.02E-259	5.14E-251	3.28E-235	1.92E-219	1.14E-211	4.19E-204
35	6.34E-227	2.57E-220	1.62E-213	5.71E-200	1.87E-186	8.61E-180	2.63E-173
40	4.06E-197	2.46E-191	2.19E-185	1.57E-173	1.05E-161	7.11E-156	3.37E-150
50	2.25E-155	9.58E-151	5.51E-146	1.68E-136	4.86E-127	2.25E-122	7.79E-118
60	1.58E-127	1.14E-123	1.05E-119	8.45E-112	6.49E-104	5.00E-100	3.04E-96
70	1.25E-107	2.55E-104	6.41E-101	3.82E-94	2.19E-87	4.70E-84	8.23E-81
80	1.08E-92	8.48E-90	8.01E-87	6.79E-81	5.56E-75	4.57E-72	3.14E-69
90	4.50E-81	1.70E-78	7.50E-76	1.39E-70	2.51E-65	9.77E-63	3.25E-60
100	9.05E-72	1.89E-69	4.54E-67	2.50E-62	1.34E-57	2.88E-55	5.34E-53
120	8.38E-58	7.25E-56	6.97E-54	6.20E-50	5.39E-46	4.71E-44	3.64E-42
140	8.17E-48	3.77E-46	1.88E-44	4.54E-41	1.07E-37	4.93E-36	2.04E-34
160	2.59E-40	7.45E-39	2.28E-37	2.07E-34	1.84E-31	5.20E-30	1.34E-28
180	1.80E-34	3.58E-33	7.49E-32	3.17E-29	1.31E-26	2.56E-25	4.57E-24
200	8.60E-30	1.28E-28	1.97E-27	4.51E-25	1.02E-22	1.46E-21	1.95E-20
220	5.86E-26	6.86E-25	8.22E-24	1.14E-21	1.56E-19	1.76E-18	1.84E-17
240	9.27E-23	8.89E-22	8.65E-21	7.92E-19	7.14E-17	6.53E-16	5.58E-15
260	4.76E-20	3.86E-19	3.14E-18	2.02E-16	1.28E-14	9.83E-14	7.07E-13
273.15	1.76E-18	1.29E-17	9.51E-17	4.99E-15	2.58E-13	1.79E-12	1.16E-11
280	1.01E-17	7.08E-17	4.95E-16	2.35E-14	1.10E-12	7.27E-12	4.52E-11
290	1.12E-16	7.34E-16	4.80E-15	1.99E-13	8.13E-12	5.02E-11	2.92E-10
298.15	7.04E-16	4.40E-15	2.73E-14	1.02E-12	3.76E-11	2.20E-10	1.22E-09
300	1.05E-15	6.52E-15	4.00E-14	1.46E-12	5.26E-11	3.05E-10	1.67E-09
310	8.62E-15	5.04E-14	2.91E-13	9.45E-12	3.02E-10	1.65E-09	8.51E-09
320	6.19E-14	3.43E-13	1.88E-12	5.45E-11	1.56E-09	8.05E-09	3.93E-08
340	2.26E-12	1.14E-11	5.62E-11	1.33E-09	3.10E-08	1.45E-07	6.41E-07
360	5.56E-11	2.57E-10	1.16E-09	2.29E-08	4.45E-07	1.90E-06	7.70E-06
373.15	3.79E-10	1.66E-09	7.11E-09	1.26E-07	2.20E-06	8.91E-06	3.42E-05
380	9.79E-10	4.18E-09	1.74E-08	2.93E-07	4.84E-06	1.91E-05	7.14E-05
400	1.30E-08	5.17E-08	2.00E-07	2.91E-06	4.16E-05	1.53E-04	5.31E-04

**Table S38.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of NC-C-OH using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.36E-09	5.09E-09	1.97E-08	4.57E-07	5.62E-06	2.37E-05	8.46E-05
35	1.36E-09	5.09E-09	1.97E-08	4.57E-07	5.62E-06	2.37E-05	8.47E-05
40	1.36E-09	5.10E-09	1.97E-08	4.57E-07	5.63E-06	2.37E-05	8.48E-05
50	1.37E-09	5.11E-09	1.97E-08	4.59E-07	5.65E-06	2.38E-05	8.52E-05
60	1.37E-09	5.15E-09	1.99E-08	4.63E-07	5.70E-06	2.40E-05	8.62E-05
70	1.39E-09	5.22E-09	2.02E-08	4.71E-07	5.79E-06	2.44E-05	8.79E-05
80	1.42E-09	5.33E-09	2.07E-08	4.83E-07	5.94E-06	2.49E-05	9.05E-05
90	1.46E-09	5.49E-09	2.14E-08	5.01E-07	6.14E-06	2.57E-05	9.40E-05
100	1.51E-09	5.71E-09	2.23E-08	5.24E-07	6.41E-06	2.66E-05	9.85E-05
120	1.66E-09	6.33E-09	2.49E-08	5.88E-07	7.14E-06	2.92E-05	1.11E-04
140	1.88E-09	7.25E-09	2.86E-08	6.81E-07	8.18E-06	3.30E-05	1.28E-04
160	2.20E-09	8.55E-09	3.38E-08	8.08E-07	9.62E-06	3.81E-05	1.51E-04
180	2.65E-09	1.04E-08	4.12E-08	9.84E-07	1.16E-05	4.52E-05	1.81E-04
200	3.31E-09	1.30E-08	5.18E-08	1.23E-06	1.44E-05	5.52E-05	2.23E-04
220	4.31E-09	1.70E-08	6.75E-08	1.58E-06	1.84E-05	6.95E-05	2.82E-04
240	5.90E-09	2.32E-08	9.19E-08	2.12E-06	2.44E-05	9.10E-05	3.70E-04
260	8.62E-09	3.37E-08	1.32E-07	3.01E-06	3.41E-05	1.25E-04	5.04E-04
273.15	1.15E-08	4.47E-08	1.74E-07	3.93E-06	4.36E-05	1.58E-04	6.35E-04
280	1.35E-08	5.24E-08	2.04E-07	4.58E-06	5.01E-05	1.81E-04	7.21E-04
290	1.74E-08	6.72E-08	2.59E-07	5.85E-06	6.20E-05	2.22E-04	8.78E-04
298.15	2.16E-08	8.33E-08	3.19E-07	7.28E-06	7.44E-05	2.65E-04	1.04E-03
300	2.27E-08	8.76E-08	3.34E-07	7.68E-06	7.77E-05	2.76E-04	1.08E-03
310	3.01E-08	1.16E-07	4.37E-07	1.04E-05	9.83E-05	3.47E-04	1.34E-03
320	4.02E-08	1.55E-07	5.77E-07	1.45E-05	1.26E-04	4.40E-04	1.68E-03
340	7.28E-08	2.81E-07	1.03E-06	3.09E-05	2.08E-04	7.17E-04	2.68E-03
360	1.32E-07	5.16E-07	1.84E-06	7.49E-05	3.48E-04	1.18E-03	4.32E-03
373.15	1.94E-07	7.64E-07	2.68E-06	1.42E-04	4.86E-04	1.63E-03	5.90E-03
380	2.36E-07	9.34E-07	3.26E-06	2.02E-04	5.79E-04	1.94E-03	6.94E-03
400	4.18E-07	1.68E-06	5.74E-06	5.96E-04	9.64E-04	3.19E-03	1.12E-02

**Table S39.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	3.87E-255	1.39E-242	2.41E-231
35	4.73E-217	2.73E-206	1.17E-196
40	1.77E-188	4.60E-179	1.23E-170
50	1.85E-148	6.27E-141	3.46E-134
60	9.12E-122	1.72E-115	7.12E-110
70	1.09E-102	2.61E-97	1.70E-92
80	2.26E-88	1.15E-83	1.87E-79
90	3.14E-77	4.78E-73	2.65E-69
100	2.60E-68	1.51E-64	3.55E-61
120	6.39E-55	8.78E-52	5.64E-49
140	2.41E-45	1.18E-42	3.02E-40
160	3.74E-38	8.48E-36	1.09E-33
180	1.49E-32	1.85E-30	1.39E-28
200	4.55E-28	3.52E-26	1.71E-24
220	2.15E-24	1.12E-22	3.84E-21
240	2.51E-21	9.45E-20	2.41E-18
260	9.92E-19	2.84E-17	5.64E-16
273.15	3.15E-17	7.69E-16	1.32E-14
280	1.68E-16	3.80E-15	6.10E-14
290	1.68E-15	3.42E-14	4.99E-13
298.15	9.80E-15	1.84E-13	2.49E-12
300	1.44E-14	2.66E-13	3.55E-12
310	1.08E-13	1.81E-12	2.23E-11
320	7.14E-13	1.10E-11	1.25E-10
340	2.24E-11	2.94E-10	2.90E-09
360	4.80E-10	5.48E-09	4.76E-08
373.15	3.01E-09	3.16E-08	2.55E-07
380	7.47E-09	7.52E-08	5.83E-07
400	8.86E-08	7.96E-07	5.57E-06

**Table S40.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	9.27E-16	1.94E-14	8.83E-14
35	9.27E-16	1.94E-14	8.83E-14
40	9.28E-16	1.94E-14	8.84E-14
50	9.33E-16	1.95E-14	8.89E-14
60	9.45E-16	1.97E-14	9.01E-14
70	9.68E-16	2.01E-14	9.24E-14
80	1.00E-15	2.07E-14	9.62E-14
90	1.06E-15	2.17E-14	1.01E-13
100	1.13E-15	2.29E-14	1.09E-13
120	1.34E-15	2.67E-14	1.30E-13
140	1.70E-15	3.31E-14	1.67E-13
160	2.32E-15	4.44E-14	2.33E-13
180	3.55E-15	6.68E-14	3.67E-13
200	6.37E-15	1.19E-13	6.79E-13
220	1.39E-14	2.68E-13	1.52E-12
240	3.60E-14	8.21E-13	4.00E-12
260	1.02E-13	3.48E-12	1.13E-11
273.15	2.01E-13	1.06E-11	2.23E-11
280	2.85E-13	1.97E-11	3.15E-11
290	4.69E-13	5.15E-11	5.18E-11
298.15	7.00E-13	1.17E-10	7.75E-11
300	7.66E-13	1.41E-10	8.51E-11
310	1.27E-12	4.06E-10	1.45E-10
320	2.35E-12	1.20E-09	2.87E-10
340	1.94E-11	1.10E-08	2.45E-09
360	3.38E-10	9.97E-08	3.40E-08
373.15	2.10E-09	4.05E-07	1.79E-07
380	5.19E-09	8.26E-07	4.11E-07
400	6.20E-08	6.06E-06	3.95E-06

**Table S41.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	8.85E-247	1.39E-242	8.85E-247
35	1.20E-210	2.73E-206	1.20E-210
40	1.50E-183	4.60E-179	1.50E-183
50	1.34E-145	6.27E-141	1.34E-145
60	2.76E-120	1.72E-115	2.76E-120
70	3.43E-102	2.61E-97	3.43E-102
80	1.31E-88	1.15E-83	1.31E-88
90	4.93E-78	4.78E-73	4.93E-78
100	1.45E-69	1.51E-64	1.45E-69
120	7.60E-57	8.78E-52	7.60E-57
140	9.67E-48	1.18E-42	9.67E-48
160	6.74E-41	8.48E-36	6.74E-41
180	1.45E-35	1.85E-30	1.45E-35
200	2.74E-31	3.52E-26	2.74E-31
220	8.78E-28	1.12E-22	8.78E-28
240	7.42E-25	9.45E-20	7.42E-25
260	2.25E-22	2.84E-17	2.25E-22
273.15	6.15E-21	7.69E-16	6.15E-21
280	3.05E-20	3.80E-15	3.05E-20
290	2.76E-19	3.42E-14	2.76E-19
298.15	1.49E-18	1.84E-13	1.49E-18
300	2.16E-18	2.66E-13	2.16E-18
310	1.49E-17	1.81E-12	1.49E-17
320	9.06E-17	1.10E-11	9.06E-17
340	2.46E-15	2.94E-10	2.46E-15
360	4.66E-14	5.48E-09	4.66E-14
373.15	2.72E-13	3.16E-08	2.72E-13
380	6.49E-13	7.52E-08	6.49E-13
400	6.98E-12	7.96E-07	6.98E-12

**Table S42.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	1.14E-18	1.94E-14	1.14E-18
35	1.04E-18	1.94E-14	1.04E-18
40	9.94E-19	1.94E-14	9.94E-19
50	9.78E-19	1.95E-14	9.78E-19
60	1.02E-18	1.97E-14	1.02E-18
70	1.09E-18	2.01E-14	1.09E-18
80	1.19E-18	2.07E-14	1.19E-18
90	1.31E-18	2.17E-14	1.31E-18
100	1.45E-18	2.29E-14	1.45E-18
120	1.81E-18	2.67E-14	1.81E-18
140	2.33E-18	3.31E-14	2.33E-18
160	3.16E-18	4.44E-14	3.16E-18
180	4.65E-18	6.68E-14	4.65E-18
200	7.66E-18	1.19E-13	7.66E-18
220	1.46E-17	2.68E-13	1.46E-17
240	3.25E-17	8.21E-13	3.25E-17
260	8.17E-17	3.48E-12	8.17E-17
273.15	1.53E-16	1.06E-11	1.53E-16
280	2.13E-16	1.97E-11	2.13E-16
290	3.41E-16	5.15E-11	3.41E-16
298.15	4.97E-16	1.17E-10	4.97E-16
300	5.40E-16	1.41E-10	5.40E-16
310	8.46E-16	4.06E-10	8.46E-16
320	1.32E-15	1.20E-09	1.32E-15
340	3.80E-15	1.10E-08	3.80E-15
360	2.41E-14	9.97E-08	2.41E-14
373.15	1.17E-13	4.05E-07	1.17E-13
380	2.73E-13	8.26E-07	2.73E-13
400	2.91E-12	6.06E-06	2.91E-12

**Table S43.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	4.42E-274	1.39E-242	2.14E-211
35	2.73E-233	2.73E-206	1.47E-179
40	1.09E-202	4.60E-179	1.13E-155
50	7.81E-160	6.27E-141	3.25E-122
60	3.01E-131	1.72E-115	6.77E-100
70	8.11E-111	2.61E-97	6.07E-84
80	1.74E-95	1.15E-83	5.69E-72
90	1.48E-83	4.78E-73	1.18E-62
100	5.27E-74	1.51E-64	3.40E-55
120	1.15E-59	8.78E-52	5.38E-44
140	2.06E-49	1.18E-42	5.51E-36
160	1.03E-41	8.48E-36	5.70E-30
180	1.03E-35	1.85E-30	2.76E-25
200	6.53E-31	3.52E-26	1.56E-21
220	5.62E-27	1.12E-22	1.85E-18
240	1.08E-23	9.45E-20	6.82E-16
260	6.53E-21	2.84E-17	1.02E-13
273.15	2.65E-19	7.69E-16	1.84E-12
280	1.59E-18	3.80E-15	7.45E-12
290	1.87E-17	3.42E-14	5.12E-11
298.15	1.24E-16	1.84E-13	2.24E-10
300	1.87E-16	2.66E-13	3.10E-10
310	1.62E-15	1.81E-12	1.67E-09
320	1.22E-14	1.10E-11	8.10E-09
340	4.88E-13	2.94E-10	1.45E-07
360	1.30E-11	5.48E-09	1.88E-06
373.15	9.30E-11	3.16E-08	8.77E-06
380	2.46E-10	7.52E-08	1.88E-05
400	3.47E-09	7.96E-07	1.49E-04

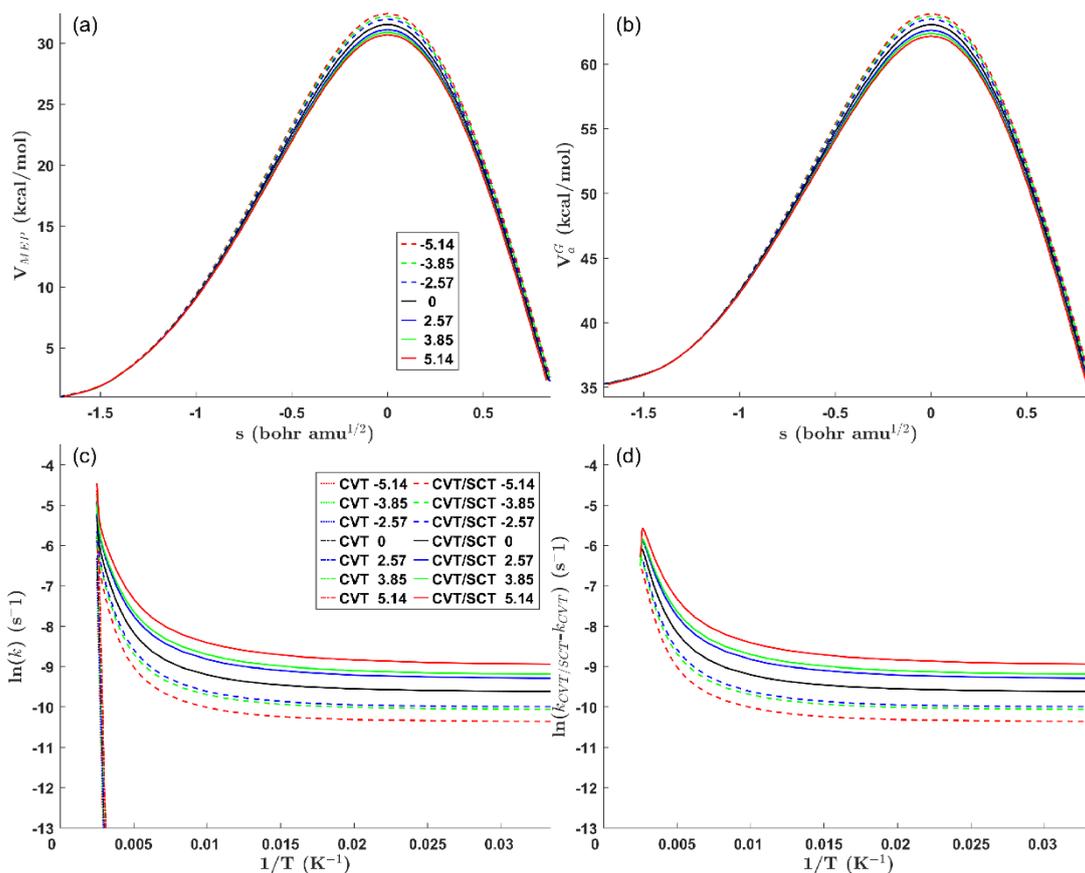
**Table S44.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of NC-C-OD using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	3.37E-18	1.94E-14	2.62E-11
35	3.37E-18	1.94E-14	2.62E-11
40	3.36E-18	1.94E-14	2.63E-11
50	3.37E-18	1.95E-14	2.64E-11
60	3.39E-18	1.97E-14	2.66E-11
70	3.44E-18	2.01E-14	2.71E-11
80	3.52E-18	2.07E-14	2.79E-11
90	3.64E-18	2.17E-14	2.89E-11
100	3.80E-18	2.29E-14	3.04E-11
120	4.35E-18	2.67E-14	3.50E-11
140	5.35E-18	3.31E-14	4.27E-11
160	7.26E-18	4.44E-14	5.62E-11
180	1.14E-17	6.68E-14	8.20E-11
200	2.18E-17	1.19E-13	1.37E-10
220	5.36E-17	2.68E-13	2.72E-10
240	1.60E-16	8.21E-13	6.24E-10
260	5.09E-16	3.48E-12	1.55E-09
273.15	1.08E-15	1.06E-11	2.85E-09
280	1.57E-15	1.97E-11	3.91E-09
290	2.69E-15	5.15E-11	6.13E-09
298.15	4.15E-15	1.17E-10	8.85E-09
300	4.59E-15	1.41E-10	9.62E-09
310	8.35E-15	4.06E-10	1.54E-08
320	1.97E-14	1.20E-09	2.68E-08
340	3.55E-13	1.10E-08	1.43E-07
360	8.87E-12	9.97E-08	1.38E-06
373.15	6.36E-11	4.05E-07	6.16E-06
380	1.68E-10	8.26E-07	1.31E-05
400	2.40E-09	6.06E-06	1.04E-04

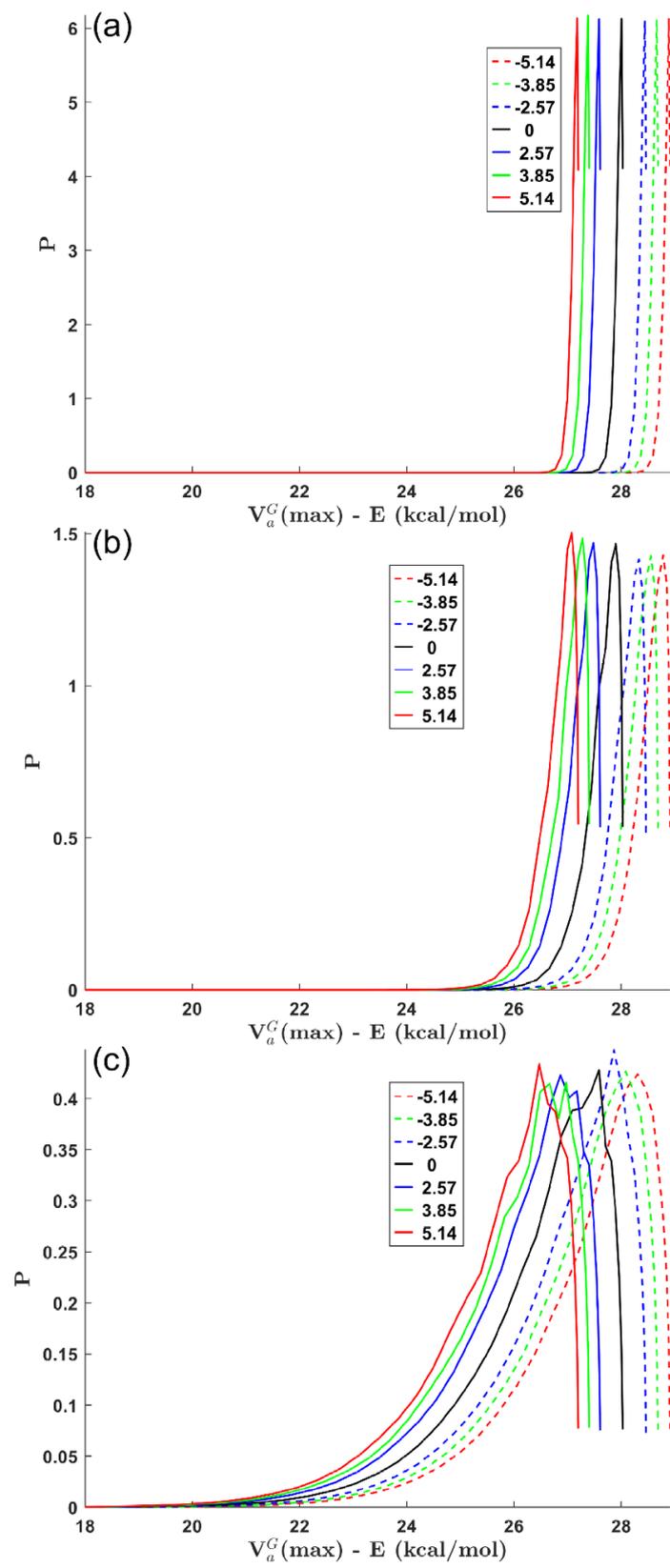
### H<sub>3</sub>C-C-OH

**Table S45.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) for the H-migration of H<sub>3</sub>C-C-OH using the  $\omega$ B97X-D method under different EEF strengths (V/nm). The  $\Omega$  (in cm<sup>-1</sup>) is the magnitude of the imaginary frequency for the transition state, and T<sub>c</sub> is the crossover temperature (in K).

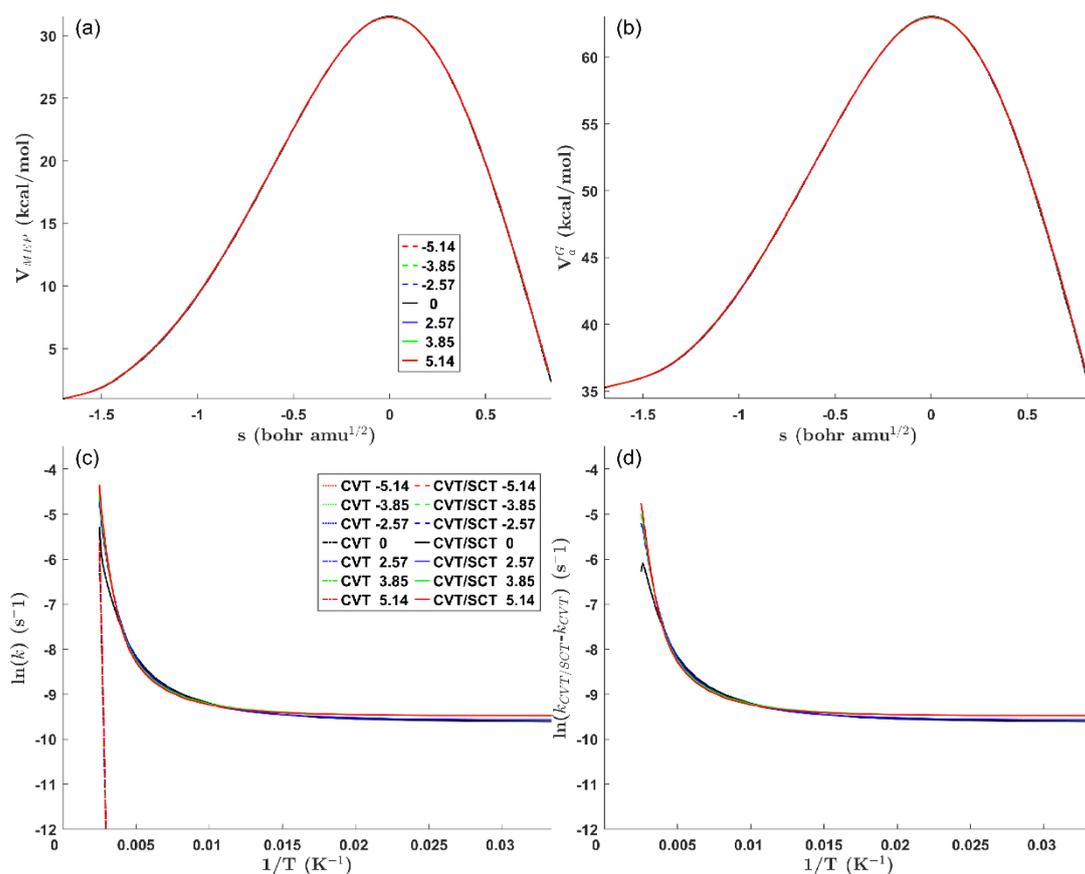
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	32.45	32.22	31.99	31.55	31.12	30.91	30.71
$\Delta V_a^G(\max)$	63.92	63.70	63.49	63.05	62.61	62.39	62.16
$\Omega$	2061	2058	2054	2046	2037	2033	2028
T <sub>c</sub>	472	471	470	468	466	465	464
<b>Y-EEF Direction</b>							
$\Delta E$	31.50	31.53	31.54	31.55	31.54	31.53	31.50
$\Delta V_a^G(\max)$	63.00	63.04	63.06	63.05	63.06	63.04	63.00
$\Omega$	2044	2045	2046	2046	2046	2045	2044
T <sub>c</sub>	468	468	468	468	468	468	468
<b>Z-EEF Direction</b>							
$\Delta E$	36.94	35.57	34.21	31.55	28.94	27.66	26.39
$\Delta V_a^G(\max)$	68.40	67.05	65.71	63.05	60.44	59.15	57.86
$\Omega$	2065	2062	2058	2046	2027	2014	1999
T <sub>c</sub>	473	472	471	468	464	461	458



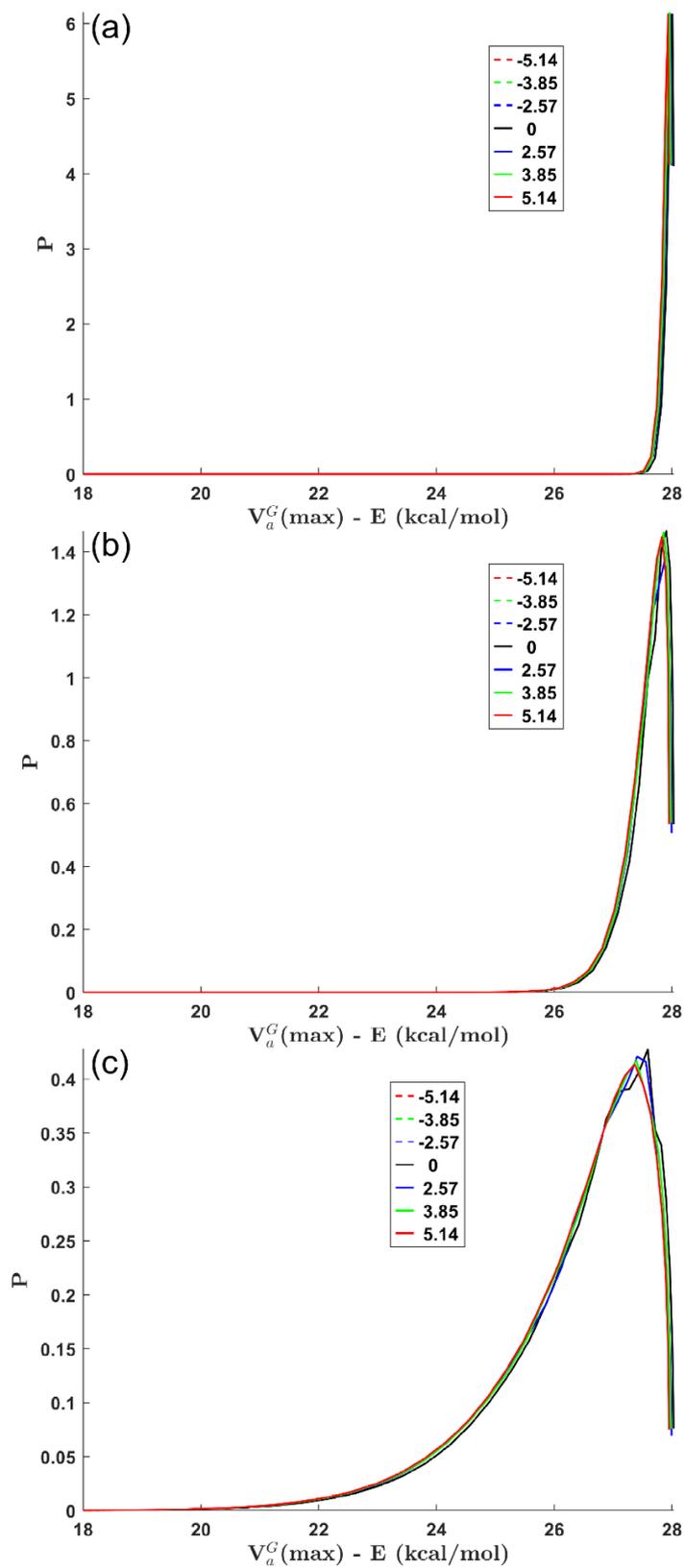
**Figure S31.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H<sub>3</sub>C-C-OH using the  $\omega$ B97X-D method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



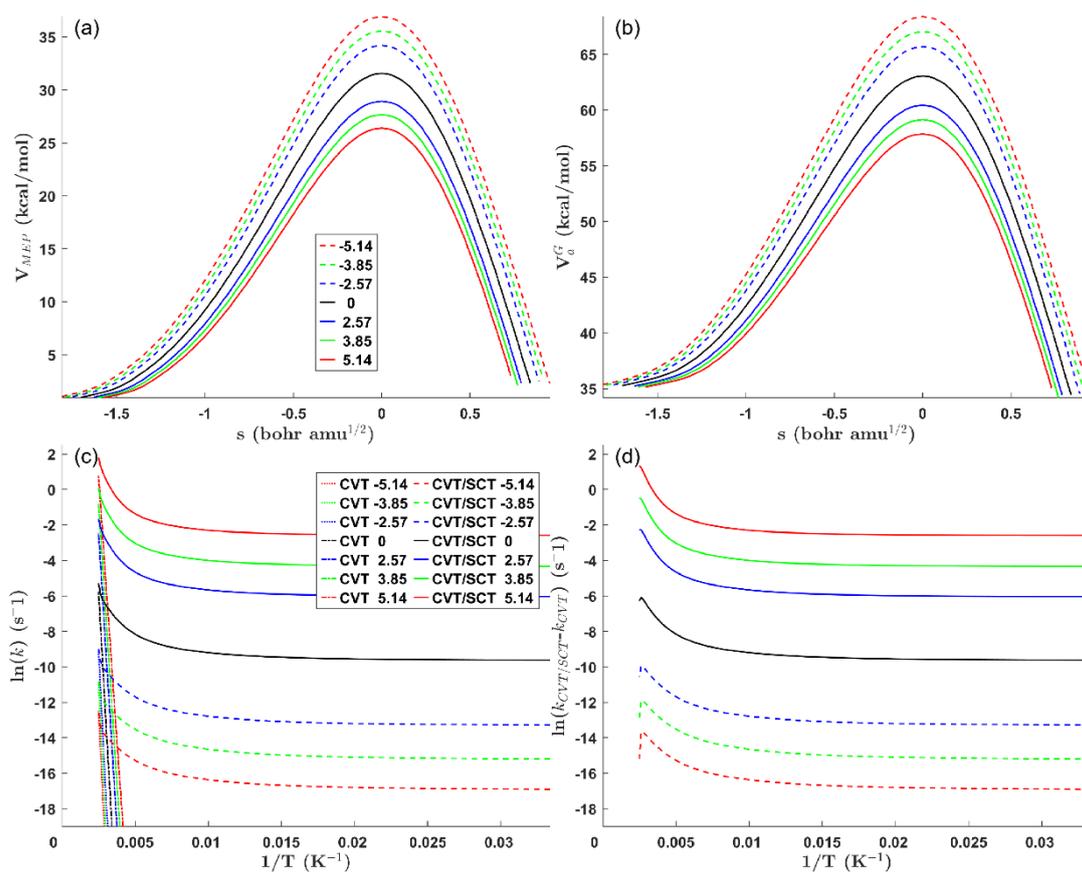
**Figure S32.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  at (a) 30K, (b) 100K and (c) 200K, using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



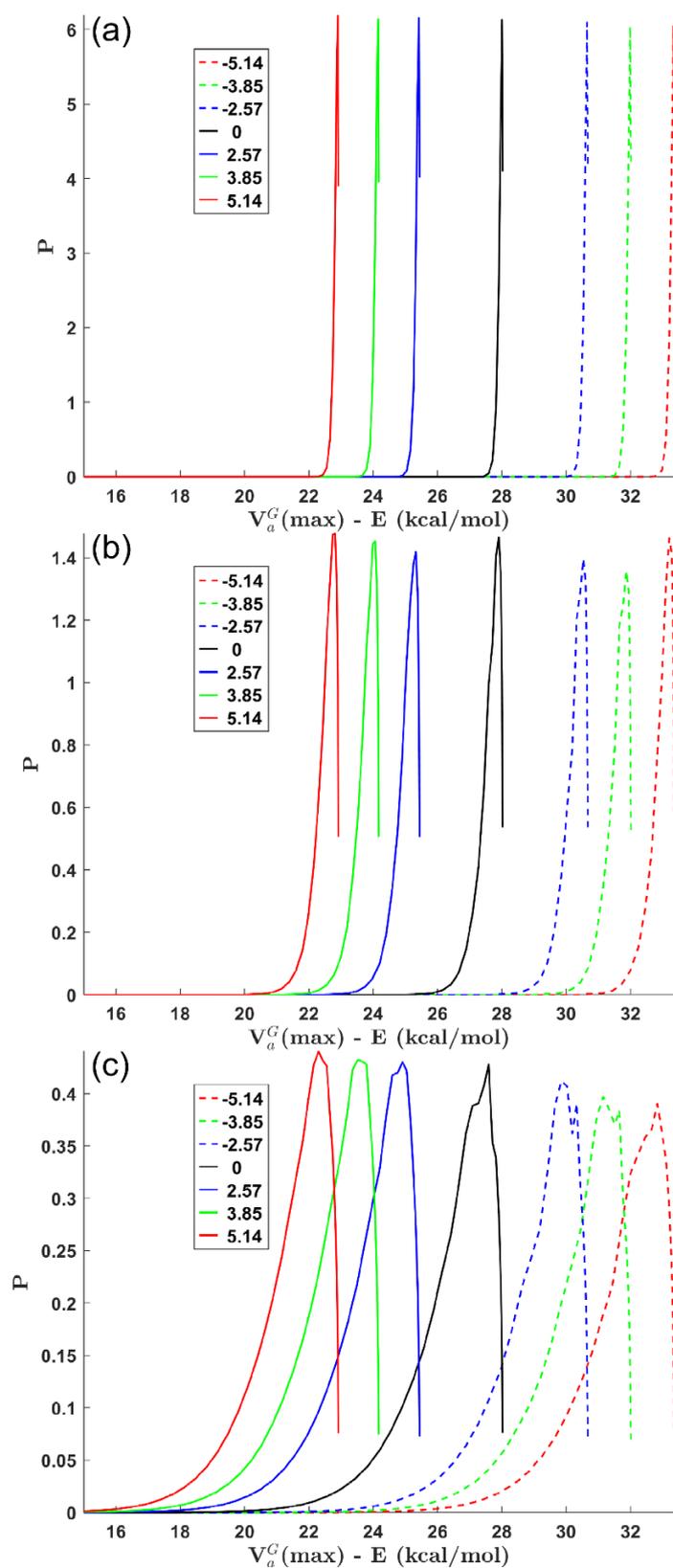
**Figure S33.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H<sub>3</sub>C-C-OH using the ωB97X-D method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



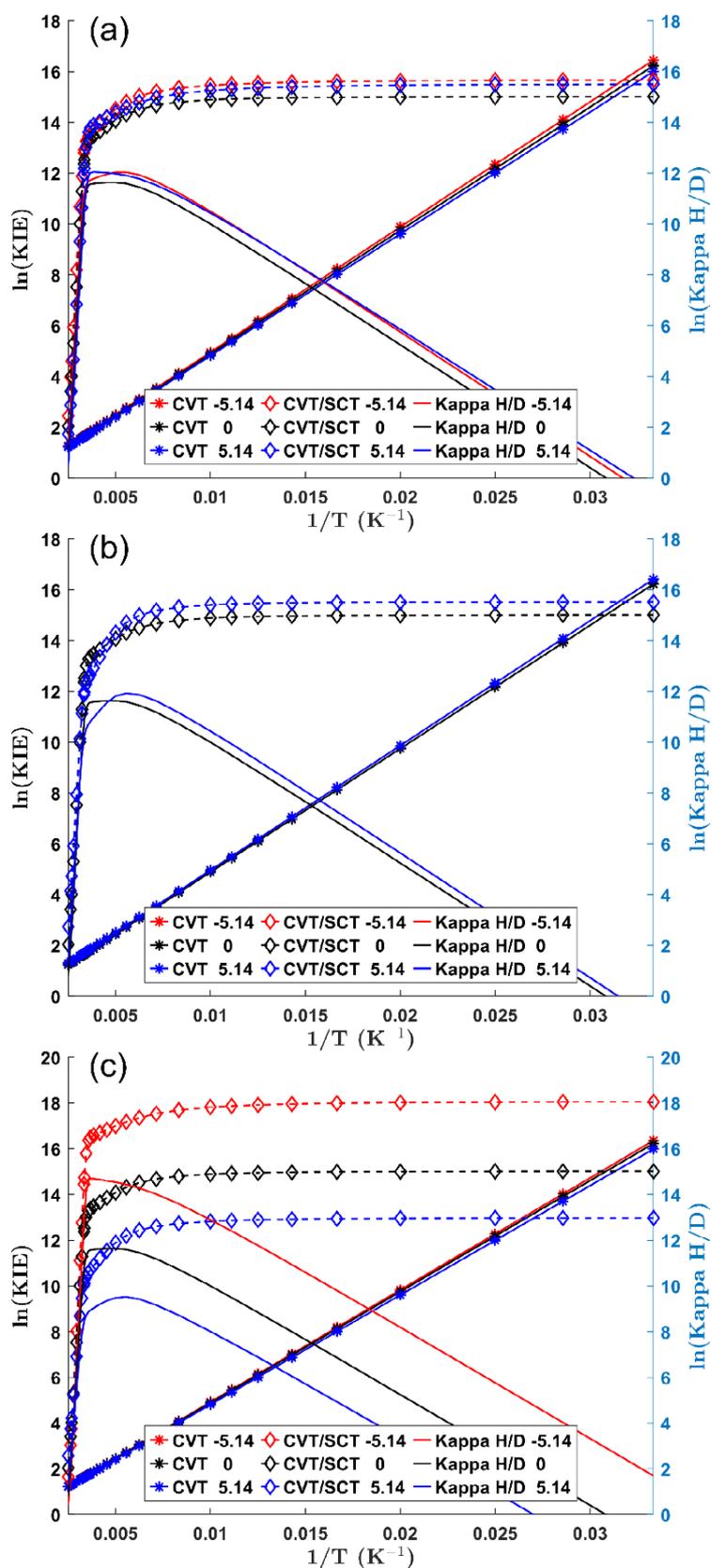
**Figure S34.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  at (a) 30K, (b) 100K and (c) 200K using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S35.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of  $H_3C-C-OH$  using the  $\omega B97X-D$  method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S36.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  at (a) 30K, (b) 100K and (c) 200K, using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S37.** Arrhenius plots of  $\ln(H/D \text{ KIE})$  and  $\ln(\kappa(H)/\kappa(D))$  versus  $1/T$  for the H-migration of  $H_3C-C-OH$  using the  $\omega B97X-D$  method along the direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red:  $-5.14 \text{ V/nm}$ ; blue:  $5.14 \text{ V/nm}$  and black: no field ( $0.0 \text{ V/nm}$ )).

**Table S46.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.21E-199	5.58E-198	2.38E-196	3.50E-193	3.97E-190	1.24E-188	3.71E-187
35	1.75E-169	4.67E-168	1.16E-166	6.02E-164	2.50E-161	4.76E-160	8.80E-159
40	7.42E-147	1.31E-145	2.19E-144	5.17E-142	1.01E-139	1.33E-138	1.71E-137
50	3.65E-115	3.63E-114	3.44E-113	2.72E-111	1.84E-109	1.45E-108	1.12E-107
60	5.04E-94	3.41E-93	2.22E-92	8.45E-91	2.83E-89	1.59E-88	8.76E-88
70	6.48E-79	3.33E-78	1.66E-77	3.75E-76	7.60E-75	3.33E-74	1.45E-73
80	1.41E-67	5.92E-67	2.41E-66	3.68E-65	5.12E-64	1.87E-63	6.79E-63
90	9.44E-59	3.37E-58	1.17E-57	1.32E-56	1.37E-55	4.34E-55	1.37E-54
100	1.09E-51	3.43E-51	1.05E-50	9.29E-50	7.65E-49	2.16E-48	6.11E-48
120	4.41E-41	1.14E-40	2.90E-40	1.78E-39	1.03E-38	2.46E-38	5.89E-38
140	1.70E-33	3.84E-33	8.53E-33	4.03E-32	1.82E-31	3.85E-31	8.17E-31
160	8.46E-28	1.72E-27	3.47E-27	1.35E-26	5.05E-26	9.74E-26	1.89E-25
180	2.32E-23	4.36E-23	8.11E-23	2.71E-22	8.78E-22	1.58E-21	2.87E-21
200	8.33E-20	1.47E-19	2.57E-19	7.60E-19	2.19E-18	3.73E-18	6.41E-18
220	6.82E-17	1.14E-16	1.90E-16	5.09E-16	1.34E-15	2.17E-15	3.56E-15
240	1.84E-14	2.96E-14	4.71E-14	1.16E-13	2.82E-13	4.41E-13	6.97E-13
260	2.12E-12	3.28E-12	5.04E-12	1.16E-11	2.63E-11	3.98E-11	6.10E-11
273.15	3.30E-11	5.00E-11	7.52E-11	1.66E-10	3.63E-10	5.39E-10	8.11E-10
280	1.25E-10	1.87E-10	2.78E-10	6.03E-10	1.29E-09	1.90E-09	2.84E-09
290	7.76E-10	1.15E-09	1.68E-09	3.56E-09	7.42E-09	1.08E-08	1.59E-08
298.15	3.15E-09	4.61E-09	6.69E-09	1.38E-08	2.83E-08	4.08E-08	5.95E-08
300	4.28E-09	6.25E-09	9.05E-09	1.86E-08	3.80E-08	5.46E-08	7.95E-08
310	2.12E-08	3.05E-08	4.37E-08	8.79E-08	1.75E-07	2.49E-07	3.59E-07
320	9.49E-08	1.35E-07	1.91E-07	3.77E-07	7.35E-07	1.03E-06	1.48E-06
340	1.47E-06	2.05E-06	2.84E-06	5.37E-06	1.01E-05	1.39E-05	1.95E-05
360	1.68E-05	2.30E-05	3.13E-05	5.71E-05	1.04E-04	1.41E-04	1.94E-04
373.15	7.24E-05	9.81E-05	1.32E-04	2.36E-04	4.19E-04	5.64E-04	7.71E-04
380	1.49E-04	2.01E-04	2.69E-04	4.75E-04	8.36E-04	1.12E-03	1.52E-03
400	1.07E-03	1.41E-03	1.87E-03	3.21E-03	5.49E-03	7.26E-03	9.74E-03

**Table S47.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	3.19E-05	4.29E-05	4.57E-05	6.72E-05	9.31E-05	1.03E-04	1.32E-04
35	3.21E-05	4.32E-05	4.60E-05	6.78E-05	9.42E-05	1.04E-04	1.34E-04
40	3.24E-05	4.36E-05	4.65E-05	6.87E-05	9.59E-05	1.06E-04	1.37E-04
50	3.33E-05	4.50E-05	4.80E-05	7.13E-05	1.00E-04	1.12E-04	1.46E-04
60	3.46E-05	4.70E-05	5.03E-05	7.51E-05	1.07E-04	1.19E-04	1.56E-04
70	3.65E-05	4.97E-05	5.34E-05	7.99E-05	1.15E-04	1.29E-04	1.70E-04
80	3.88E-05	5.30E-05	5.71E-05	8.58E-05	1.24E-04	1.39E-04	1.85E-04
90	4.16E-05	5.69E-05	6.16E-05	9.27E-05	1.35E-04	1.52E-04	2.03E-04
100	4.48E-05	6.16E-05	6.68E-05	1.01E-04	1.48E-04	1.67E-04	2.23E-04
120	5.29E-05	7.29E-05	7.98E-05	1.20E-04	1.79E-04	2.02E-04	2.72E-04
140	6.34E-05	8.78E-05	9.67E-05	1.46E-04	2.19E-04	2.47E-04	3.35E-04
160	7.74E-05	1.07E-04	1.19E-04	1.80E-04	2.72E-04	3.06E-04	4.16E-04
180	9.61E-05	1.34E-04	1.49E-04	2.26E-04	3.41E-04	3.83E-04	5.23E-04
200	1.22E-04	1.69E-04	1.89E-04	2.86E-04	4.32E-04	4.84E-04	6.61E-04
220	1.57E-04	2.18E-04	2.45E-04	3.68E-04	5.52E-04	6.15E-04	8.39E-04
240	2.07E-04	2.86E-04	3.20E-04	4.76E-04	7.05E-04	7.82E-04	1.06E-03
260	2.75E-04	3.78E-04	4.21E-04	6.16E-04	9.00E-04	9.89E-04	1.34E-03
273.15	3.32E-04	4.54E-04	5.05E-04	7.29E-04	1.05E-03	1.15E-03	1.55E-03
280	3.67E-04	5.00E-04	5.54E-04	7.95E-04	1.14E-03	1.24E-03	1.67E-03
290	4.24E-04	5.75E-04	6.35E-04	9.01E-04	1.28E-03	1.39E-03	1.86E-03
298.15	4.77E-04	6.44E-04	7.08E-04	9.95E-04	1.40E-03	1.51E-03	2.03E-03
300	4.90E-04	6.60E-04	7.26E-04	1.02E-03	1.43E-03	1.54E-03	2.07E-03
310	5.64E-04	7.56E-04	8.28E-04	1.15E-03	1.59E-03	1.71E-03	2.29E-03
320	6.48E-04	8.65E-04	9.42E-04	1.29E-03	1.77E-03	1.90E-03	2.53E-03
340	8.51E-04	1.12E-03	1.21E-03	1.62E-03	2.18E-03	2.31E-03	3.06E-03
360	1.11E-03	1.45E-03	1.55E-03	2.03E-03	2.69E-03	2.85E-03	3.76E-03
373.15	1.34E-03	1.73E-03	1.86E-03	2.43E-03	3.23E-03	3.46E-03	4.56E-03
380	1.50E-03	1.94E-03	2.09E-03	2.75E-03	3.69E-03	4.02E-03	5.30E-03
400	2.48E-03	3.19E-03	3.61E-03	5.09E-03	7.41E-03	8.75E-03	1.16E-02

**Table S48.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.24E-192	7.60E-193	6.11E-193	3.50E-193	6.11E-193	7.60E-193	1.24E-192
35	1.80E-163	1.18E-163	9.78E-164	6.02E-164	9.78E-164	1.18E-163	1.80E-163
40	1.36E-141	9.38E-142	7.96E-142	5.17E-142	7.96E-142	9.38E-142	1.36E-141
50	5.99E-111	4.46E-111	3.90E-111	2.72E-111	3.91E-111	4.46E-111	5.99E-111
60	1.67E-90	1.30E-90	1.17E-90	8.45E-91	1.17E-90	1.30E-90	1.67E-90
70	6.87E-76	5.55E-76	5.03E-76	3.75E-76	5.03E-76	5.55E-76	6.87E-76
80	6.39E-65	5.29E-65	4.85E-65	3.68E-65	4.85E-65	5.29E-65	6.39E-65
90	2.20E-56	1.86E-56	1.72E-56	1.32E-56	1.72E-56	1.86E-56	2.20E-56
100	1.51E-49	1.29E-49	1.20E-49	9.29E-50	1.20E-49	1.29E-49	1.51E-49
120	2.77E-39	2.43E-39	2.27E-39	1.78E-39	2.27E-39	2.43E-39	2.77E-39
140	6.08E-32	5.42E-32	5.11E-32	4.03E-32	5.11E-32	5.42E-32	6.08E-32
160	1.99E-26	1.80E-26	1.70E-26	1.35E-26	1.70E-26	1.80E-26	1.99E-26
180	3.95E-22	3.59E-22	3.41E-22	2.71E-22	3.41E-22	3.59E-22	3.95E-22
200	1.09E-18	1.00E-18	9.55E-19	7.60E-19	9.55E-19	1.00E-18	1.09E-18
220	7.26E-16	6.69E-16	6.38E-16	5.09E-16	6.38E-16	6.69E-16	7.26E-16
240	1.65E-13	1.52E-13	1.46E-13	1.16E-13	1.46E-13	1.52E-13	1.65E-13
260	1.63E-11	1.52E-11	1.45E-11	1.16E-11	1.45E-11	1.52E-11	1.63E-11
273.15	2.33E-10	2.17E-10	2.08E-10	1.66E-10	2.08E-10	2.17E-10	2.33E-10
280	8.44E-10	7.88E-10	7.54E-10	6.03E-10	7.54E-10	7.88E-10	8.44E-10
290	4.96E-09	4.64E-09	4.44E-09	3.56E-09	4.44E-09	4.64E-09	4.96E-09
298.15	1.93E-08	1.80E-08	1.73E-08	1.38E-08	1.73E-08	1.80E-08	1.93E-08
300	2.59E-08	2.43E-08	2.33E-08	1.86E-08	2.33E-08	2.43E-08	2.59E-08
310	1.22E-07	1.14E-07	1.10E-07	8.79E-08	1.10E-07	1.14E-07	1.22E-07
320	5.22E-07	4.90E-07	4.70E-07	3.77E-07	4.70E-07	4.90E-07	5.22E-07
340	7.41E-06	6.97E-06	6.69E-06	5.37E-06	6.69E-06	6.97E-06	7.41E-06
360	7.86E-05	7.41E-05	7.12E-05	5.71E-05	7.12E-05	7.41E-05	7.86E-05
373.15	3.24E-04	3.06E-04	2.94E-04	2.36E-04	2.94E-04	3.06E-04	3.24E-04
380	6.52E-04	6.16E-04	5.92E-04	4.75E-04	5.92E-04	6.16E-04	6.52E-04
400	4.39E-03	4.15E-03	3.99E-03	3.21E-03	3.99E-03	4.15E-03	4.39E-03

**Table S49.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	7.68E-05	7.65E-05	7.01E-05	6.72E-05	7.01E-05	7.65E-05	7.68E-05
35	7.69E-05	7.67E-05	7.04E-05	6.78E-05	7.04E-05	7.67E-05	7.69E-05
40	7.71E-05	7.70E-05	7.09E-05	6.87E-05	7.09E-05	7.70E-05	7.71E-05
50	7.82E-05	7.83E-05	7.27E-05	7.13E-05	7.27E-05	7.83E-05	7.82E-05
60	8.01E-05	8.06E-05	7.56E-05	7.51E-05	7.56E-05	8.06E-05	8.01E-05
70	8.29E-05	8.38E-05	7.96E-05	7.99E-05	7.96E-05	8.38E-05	8.29E-05
80	8.67E-05	8.80E-05	8.47E-05	8.58E-05	8.47E-05	8.80E-05	8.67E-05
90	9.16E-05	9.32E-05	9.09E-05	9.27E-05	9.09E-05	9.32E-05	9.16E-05
100	9.74E-05	9.95E-05	9.81E-05	1.01E-04	9.81E-05	9.95E-05	9.74E-05
120	1.12E-04	1.15E-04	1.16E-04	1.20E-04	1.16E-04	1.15E-04	1.12E-04
140	1.33E-04	1.37E-04	1.40E-04	1.46E-04	1.40E-04	1.37E-04	1.33E-04
160	1.60E-04	1.65E-04	1.72E-04	1.80E-04	1.73E-04	1.65E-04	1.60E-04
180	1.98E-04	2.05E-04	2.16E-04	2.26E-04	2.16E-04	2.05E-04	1.98E-04
200	2.51E-04	2.60E-04	2.77E-04	2.86E-04	2.77E-04	2.60E-04	2.51E-04
220	3.29E-04	3.42E-04	3.66E-04	3.68E-04	3.66E-04	3.42E-04	3.29E-04
240	4.50E-04	4.65E-04	4.96E-04	4.76E-04	4.96E-04	4.65E-04	4.50E-04
260	6.39E-04	6.53E-04	6.88E-04	6.16E-04	6.88E-04	6.53E-04	6.39E-04
273.15	8.20E-04	8.28E-04	8.61E-04	7.29E-04	8.61E-04	8.28E-04	8.20E-04
280	9.38E-04	9.40E-04	9.70E-04	7.95E-04	9.70E-04	9.40E-04	9.38E-04
290	1.15E-03	1.13E-03	1.15E-03	9.01E-04	1.15E-03	1.13E-03	1.15E-03
298.15	1.36E-03	1.32E-03	1.33E-03	9.95E-04	1.33E-03	1.32E-03	1.36E-03
300	1.41E-03	1.37E-03	1.37E-03	1.02E-03	1.37E-03	1.37E-03	1.41E-03
310	1.73E-03	1.66E-03	1.64E-03	1.15E-03	1.64E-03	1.66E-03	1.73E-03
320	2.13E-03	2.01E-03	1.94E-03	1.29E-03	1.94E-03	2.01E-03	2.13E-03
340	3.22E-03	2.93E-03	2.72E-03	1.62E-03	2.72E-03	2.92E-03	3.22E-03
360	4.83E-03	4.24E-03	3.80E-03	2.03E-03	3.80E-03	4.24E-03	4.83E-03
373.15	6.36E-03	5.47E-03	4.80E-03	2.43E-03	4.80E-03	5.47E-03	6.36E-03
380	7.42E-03	6.32E-03	5.49E-03	2.75E-03	5.49E-03	6.32E-03	7.42E-03
400	1.30E-02	1.10E-02	9.50E-03	5.09E-03	9.50E-03	1.10E-02	1.30E-02

**Table S50.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.97E-232	3.12E-222	1.88E-212	3.50E-193	2.45E-174	4.42E-165	6.21E-156
35	3.01E-197	7.51E-189	1.82E-180	6.02E-164	8.59E-148	7.40E-140	5.13E-132
40	3.74E-171	8.29E-164	1.80E-156	5.17E-142	7.08E-128	6.22E-121	4.52E-114
50	1.31E-134	9.77E-129	7.27E-123	2.72E-111	5.59E-100	2.01E-94	6.22E-89
60	3.10E-110	2.42E-105	1.90E-100	8.45E-91	2.28E-81	9.77E-77	3.68E-72
70	8.15E-93	1.26E-88	1.99E-84	3.75E-76	4.59E-68	4.29E-64	3.60E-60
80	9.61E-80	4.43E-76	2.09E-72	3.68E-65	4.42E-58	1.32E-54	3.59E-51
90	1.43E-69	2.56E-66	4.74E-63	1.32E-56	2.61E-50	3.22E-47	3.64E-44
100	1.99E-61	1.67E-58	1.46E-55	9.29E-50	4.35E-44	2.64E-41	1.48E-38
120	3.33E-49	9.04E-47	2.56E-44	1.78E-39	9.56E-35	2.00E-32	3.93E-30
140	1.84E-40	2.22E-38	2.82E-36	4.03E-32	4.61E-28	4.52E-26	4.18E-24
160	6.76E-34	4.44E-32	3.09E-30	1.35E-26	4.84E-23	2.68E-21	1.41E-19
180	8.77E-29	3.59E-27	1.56E-25	2.71E-22	3.95E-19	1.40E-17	4.77E-16
200	1.09E-24	3.07E-23	9.16E-22	7.60E-19	5.38E-16	1.34E-14	3.22E-13
220	2.49E-21	5.11E-20	1.12E-18	5.09E-16	2.00E-13	3.73E-12	6.70E-11
240	1.57E-18	2.50E-17	4.24E-16	1.16E-13	2.79E-11	4.09E-10	5.78E-09
260	3.71E-16	4.74E-15	6.48E-14	1.16E-11	1.83E-09	2.19E-08	2.53E-07
273.15	8.75E-15	9.85E-14	1.19E-12	1.66E-10	2.07E-08	2.19E-07	2.25E-06
280	4.04E-14	4.28E-13	4.86E-12	6.03E-10	6.67E-08	6.69E-07	6.50E-06
290	3.32E-13	3.23E-12	3.37E-11	3.56E-09	3.35E-07	3.10E-06	2.79E-05
298.15	1.66E-12	1.52E-11	1.49E-10	1.38E-08	1.15E-06	1.01E-05	8.52E-05
300	2.37E-12	2.13E-11	2.06E-10	1.86E-08	1.51E-06	1.30E-05	1.09E-04
310	1.49E-11	1.25E-10	1.12E-09	8.79E-08	6.20E-06	4.98E-05	3.89E-04
320	8.38E-11	6.54E-10	5.49E-09	3.77E-07	2.33E-05	1.76E-04	1.29E-03
340	1.96E-09	1.35E-08	1.00E-07	5.37E-06	2.61E-04	1.75E-03	1.14E-02
360	3.24E-08	1.99E-07	1.32E-06	5.71E-05	2.25E-03	1.36E-02	7.98E-02
373.15	1.74E-07	1.00E-06	6.22E-06	2.36E-04	8.17E-03	4.63E-02	2.56E-01
380	3.99E-07	2.22E-06	1.34E-05	4.75E-04	1.55E-02	8.50E-02	4.56E-01
400	3.84E-06	1.96E-05	1.08E-04	3.21E-03	8.79E-02	4.44E-01	2.19E+00

**Table S51.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of  $\text{H}_3\text{C-C-OH}$  using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.54E-08	2.51E-07	1.71E-06	6.72E-05	2.41E-03	1.32E-02	7.53E-02
35	4.63E-08	2.55E-07	1.74E-06	6.78E-05	2.42E-03	1.33E-02	7.55E-02
40	4.74E-08	2.61E-07	1.77E-06	6.87E-05	2.45E-03	1.34E-02	7.59E-02
50	5.04E-08	2.77E-07	1.86E-06	7.13E-05	2.52E-03	1.37E-02	7.75E-02
60	5.43E-08	2.98E-07	1.99E-06	7.51E-05	2.64E-03	1.43E-02	8.01E-02
70	5.89E-08	3.25E-07	2.14E-06	7.99E-05	2.79E-03	1.50E-02	8.37E-02
80	6.44E-08	3.56E-07	2.32E-06	8.58E-05	2.98E-03	1.59E-02	8.83E-02
90	7.06E-08	3.92E-07	2.54E-06	9.27E-05	3.20E-03	1.70E-02	9.39E-02
100	7.77E-08	4.33E-07	2.79E-06	1.01E-04	3.46E-03	1.83E-02	1.00E-01
120	9.49E-08	5.35E-07	3.40E-06	1.20E-04	4.10E-03	2.15E-02	1.17E-01
140	1.17E-07	6.67E-07	4.20E-06	1.46E-04	4.93E-03	2.57E-02	1.38E-01
160	1.46E-07	8.39E-07	5.24E-06	1.80E-04	6.02E-03	3.11E-02	1.66E-01
180	1.84E-07	1.06E-06	6.61E-06	2.26E-04	7.49E-03	3.84E-02	2.03E-01
200	2.32E-07	1.35E-06	8.39E-06	2.86E-04	9.48E-03	4.84E-02	2.55E-01
220	2.92E-07	1.70E-06	1.07E-05	3.68E-04	1.22E-02	6.22E-02	3.26E-01
240	3.67E-07	2.14E-06	1.35E-05	4.76E-04	1.60E-02	8.16E-02	4.29E-01
260	4.56E-07	2.66E-06	1.70E-05	6.16E-04	2.12E-02	1.09E-01	5.74E-01
273.15	5.23E-07	3.05E-06	1.97E-05	7.29E-04	2.56E-02	1.32E-01	7.02E-01
280	5.61E-07	3.27E-06	2.12E-05	7.95E-04	2.83E-02	1.47E-01	7.80E-01
290	6.20E-07	3.62E-06	2.36E-05	9.01E-04	3.26E-02	1.70E-01	9.12E-01
298.15	6.70E-07	3.91E-06	2.56E-05	9.95E-04	3.66E-02	1.92E-01	1.04E+00
300	6.82E-07	3.98E-06	2.61E-05	1.02E-03	3.76E-02	1.98E-01	1.07E+00
310	7.49E-07	4.36E-06	2.89E-05	1.15E-03	4.32E-02	2.30E-01	1.25E+00
320	8.19E-07	4.77E-06	3.18E-05	1.29E-03	4.96E-02	2.66E-01	1.46E+00
340	9.72E-07	5.66E-06	3.83E-05	1.62E-03	6.50E-02	3.55E-01	1.99E+00
360	1.16E-06	6.74E-06	4.62E-05	2.03E-03	8.50E-02	4.75E-01	2.71E+00
373.15	1.37E-06	7.95E-06	5.46E-05	2.43E-03	1.03E-01	5.85E-01	3.37E+00
380	1.58E-06	9.13E-06	6.21E-05	2.75E-03	1.17E-01	6.62E-01	3.82E+00
400	4.09E-06	2.19E-05	1.34E-04	5.09E-03	1.93E-01	1.07E+00	6.06E+00

**Table S52.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	8.65E-207	3.13E-200	4.15E-194
35	1.31E-175	5.45E-170	9.64E-165
40	3.21E-152	2.65E-147	1.04E-142
50	1.86E-119	1.58E-115	7.49E-112
60	1.32E-97	2.49E-94	2.89E-91
70	5.50E-82	3.51E-79	1.49E-76
80	2.89E-70	8.19E-68	1.65E-65
90	3.83E-61	5.77E-59	6.49E-57
100	7.67E-54	6.99E-52	4.93E-50
120	7.04E-43	3.01E-41	1.06E-39
140	4.89E-35	1.22E-33	2.61E-32
160	3.79E-29	6.32E-28	9.32E-27
180	1.46E-24	1.78E-23	1.97E-22
200	6.94E-21	6.57E-20	5.77E-19
220	7.12E-18	5.50E-17	3.99E-16
240	2.32E-15	1.51E-14	9.37E-14
260	3.13E-13	1.76E-12	9.57E-12
273.15	5.34E-12	2.76E-11	1.39E-10
280	2.11E-11	1.05E-10	5.07E-10
290	1.39E-10	6.55E-10	3.01E-09
298.15	5.92E-10	2.67E-09	1.18E-08
300	8.13E-10	3.63E-09	1.59E-08
310	4.24E-09	1.80E-08	7.55E-08
320	1.99E-08	8.10E-08	3.26E-07
340	3.37E-07	1.26E-06	4.69E-06
360	4.17E-06	1.45E-05	5.03E-05
373.15	1.88E-05	6.25E-05	2.09E-04
380	3.97E-05	1.29E-04	4.22E-04
400	3.02E-04	9.24E-04	2.86E-03

**Table S53.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	5.03E-12	2.02E-11	2.43E-11
35	5.08E-12	2.04E-11	2.49E-11
40	5.15E-12	2.08E-11	2.57E-11
50	5.39E-12	2.18E-11	2.79E-11
60	5.76E-12	2.32E-11	3.09E-11
70	6.25E-12	2.51E-11	3.48E-11
80	6.89E-12	2.76E-11	3.96E-11
90	7.68E-12	3.06E-11	4.55E-11
100	8.65E-12	3.43E-11	5.28E-11
120	1.13E-11	4.48E-11	7.30E-11
140	1.56E-11	6.14E-11	1.05E-10
160	2.28E-11	8.94E-11	1.57E-10
180	3.59E-11	1.37E-10	2.41E-10
200	6.02E-11	2.19E-10	3.73E-10
220	1.05E-10	3.52E-10	5.69E-10
240	1.82E-10	5.58E-10	8.47E-10
260	3.10E-10	8.64E-10	1.23E-09
273.15	4.35E-10	1.15E-09	1.62E-09
280	5.23E-10	1.36E-09	2.05E-09
290	7.36E-10	2.00E-09	4.05E-09
298.15	1.17E-09	3.60E-09	1.03E-08
300	1.35E-09	4.30E-09	1.32E-08
310	3.87E-09	1.44E-08	5.46E-08
320	1.48E-08	5.78E-08	2.28E-07
340	2.35E-07	8.71E-07	3.28E-06
360	2.92E-06	1.01E-05	3.56E-05
373.15	1.33E-05	4.38E-05	1.49E-04
380	2.80E-05	9.06E-05	3.01E-04
400	2.15E-04	6.56E-04	2.06E-03

**Table S54.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	9.14E-200	3.13E-200	9.14E-200
35	1.37E-169	5.45E-170	1.37E-169
40	6.00E-147	2.65E-147	6.00E-147
50	3.09E-115	1.58E-115	3.09E-115
60	4.43E-94	2.49E-94	4.43E-94
70	5.86E-79	3.51E-79	5.86E-79
80	1.31E-67	8.19E-68	1.31E-67
90	8.92E-59	5.77E-59	8.92E-59
100	1.05E-51	6.99E-52	1.05E-51
120	4.37E-41	3.01E-41	4.37E-41
140	1.72E-33	1.22E-33	1.72E-33
160	8.76E-28	6.32E-28	8.76E-28
180	2.44E-23	1.78E-23	2.44E-23
200	8.89E-20	6.57E-20	8.89E-20
220	7.37E-17	5.50E-17	7.37E-17
240	2.01E-14	1.51E-14	2.01E-14
260	2.33E-12	1.76E-12	2.33E-12
273.15	3.64E-11	2.76E-11	3.64E-11
280	1.38E-10	1.05E-10	1.38E-10
290	8.59E-10	6.55E-10	8.59E-10
298.15	3.49E-09	2.67E-09	3.49E-09
300	4.75E-09	3.63E-09	4.75E-09
310	2.35E-08	1.80E-08	2.35E-08
320	1.05E-07	8.10E-08	1.05E-07
340	1.63E-06	1.26E-06	1.63E-06
360	1.87E-05	1.45E-05	1.87E-05
373.15	8.07E-05	6.25E-05	8.07E-05
380	1.66E-04	1.29E-04	1.66E-04
400	1.19E-03	9.24E-04	1.19E-03

**Table S55.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	1.39E-11	2.02E-11	1.39E-11
35	1.40E-11	2.04E-11	1.40E-11
40	1.41E-11	2.08E-11	1.41E-11
50	1.43E-11	2.18E-11	1.43E-11
60	1.48E-11	2.32E-11	1.48E-11
70	1.56E-11	2.51E-11	1.56E-11
80	1.66E-11	2.76E-11	1.66E-11
90	1.80E-11	3.06E-11	1.80E-11
100	1.98E-11	3.43E-11	1.98E-11
120	2.50E-11	4.48E-11	2.50E-11
140	3.36E-11	6.14E-11	3.36E-11
160	4.92E-11	8.94E-11	4.92E-11
180	8.07E-11	1.37E-10	8.07E-11
200	1.51E-10	2.19E-10	1.51E-10
220	3.18E-10	3.52E-10	3.18E-10
240	7.07E-10	5.58E-10	7.07E-10
260	1.56E-09	8.64E-10	1.56E-09
273.15	2.60E-09	1.15E-09	2.60E-09
280	3.41E-09	1.36E-09	3.41E-09
290	5.30E-09	2.00E-09	5.30E-09
298.15	8.57E-09	3.60E-09	8.57E-09
300	9.81E-09	4.30E-09	9.81E-09
310	2.50E-08	1.44E-08	2.50E-08
320	8.39E-08	5.78E-08	8.39E-08
340	1.14E-06	8.71E-07	1.14E-06
360	1.30E-05	1.01E-05	1.30E-05
373.15	5.63E-05	4.38E-05	5.63E-05
380	1.16E-04	9.06E-05	1.16E-04
400	8.40E-04	6.56E-04	8.40E-04

**Table S56.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	3.90E-239	3.13E-200	7.08E-163
35	2.44E-203	5.45E-170	5.72E-138
40	1.74E-176	2.65E-147	2.79E-119
50	7.04E-139	1.58E-115	4.19E-93
60	8.55E-114	2.49E-94	1.22E-75
70	7.23E-96	3.51E-79	3.74E-63
80	2.05E-82	8.19E-68	8.79E-54
90	6.02E-72	5.77E-59	1.73E-46
100	1.44E-63	6.99E-52	1.20E-40
120	5.49E-51	3.01E-41	7.07E-32
140	5.45E-42	1.22E-33	1.33E-25
160	3.11E-35	6.32E-28	6.93E-21
180	5.70E-30	1.78E-23	3.27E-17
200	9.36E-26	6.57E-20	2.88E-14
220	2.66E-22	5.50E-17	7.47E-12
240	2.03E-19	1.51E-14	7.73E-10
260	5.60E-17	1.76E-12	3.95E-08
273.15	1.45E-15	2.76E-11	3.84E-07
280	6.98E-15	1.05E-10	1.16E-06
290	6.08E-14	6.55E-10	5.26E-06
298.15	3.19E-13	2.67E-09	1.68E-05
300	4.59E-13	3.63E-09	2.16E-05
310	3.05E-12	1.80E-08	8.14E-05
320	1.80E-11	8.10E-08	2.82E-04
340	4.59E-10	1.26E-06	2.73E-03
360	8.19E-09	1.45E-05	2.06E-02
373.15	4.61E-08	6.25E-05	6.91E-02
380	1.08E-07	1.29E-04	1.26E-01
400	1.11E-06	9.24E-04	6.42E-01

**Table S57.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of  $\text{H}_3\text{C-C-OD}$  using the  $\omega\text{B97X-D}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	6.52E-16	2.02E-11	1.75E-07
35	6.69E-16	2.04E-11	1.76E-07
40	6.91E-16	2.08E-11	1.77E-07
50	7.50E-16	2.18E-11	1.83E-07
60	8.30E-16	2.32E-11	1.92E-07
70	9.33E-16	2.51E-11	2.05E-07
80	1.06E-15	2.76E-11	2.21E-07
90	1.22E-15	3.06E-11	2.43E-07
100	1.41E-15	3.43E-11	2.70E-07
120	1.96E-15	4.48E-11	3.44E-07
140	2.83E-15	6.14E-11	4.61E-07
160	4.22E-15	8.94E-11	6.59E-07
180	6.39E-15	1.37E-10	1.02E-06
200	9.64E-15	2.19E-10	1.74E-06
220	1.43E-14	3.52E-10	3.14E-06
240	2.05E-14	5.58E-10	5.80E-06
260	2.87E-14	8.64E-10	1.07E-05
273.15	3.60E-14	1.15E-09	1.58E-05
280	4.34E-14	1.36E-09	1.96E-05
290	8.53E-14	2.00E-09	2.82E-05
298.15	2.64E-13	3.60E-09	4.19E-05
300	3.60E-13	4.30E-09	4.67E-05
310	2.12E-12	1.44E-08	9.67E-05
320	1.23E-11	5.78E-08	2.46E-04
340	3.16E-10	8.71E-07	1.98E-03
360	5.70E-09	1.01E-05	1.46E-02
373.15	3.23E-08	4.38E-05	4.91E-02
380	7.61E-08	9.06E-05	8.95E-02
400	7.86E-07	6.56E-04	4.61E-01

**Table S58.** Computed half-life (h) for the H-migration of the hydroxycarbenes (R-C-OH: R = H, CH<sub>3</sub>, OH, CN) using the ωB97X-D method along the X-, Y- and Z-EEF directions with various strengths (0.0 ~ 5.14 V/nm) at low temperature of 30 K

	Various EEF strengths (V/nm)						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>R = H</b>							
<b>X-EEF</b>	0.77	0.65	0.58	0.44	0.34	0.37	0.33
<b>Y-EEF</b>	0.49	0.46	0.44	0.44	0.44	0.46	0.49
<b>Z-EEF</b>	430.65	73.19	12.66	0.44	0.02	0.00	0.00
<b>R = CH<sub>3</sub></b>							
<b>X-EEF</b>	6.03	4.49	4.21	2.86	2.07	1.87	1.46
<b>Y-EEF</b>	2.51	2.52	2.75	2.86	2.75	2.52	2.51
<b>Z-EEF</b>	4240.09	766.93	112.57	2.86	0.08	0.01	0.00
<b>R = OH</b>							
<b>X-EEF</b>	4445.7	4649.8	5780.8	6850.5	11063.2	13652.5	18333.3
<b>Y-EEF</b>	10814.6	10349.5	8369.6	6850.5	8369.6	10294.1	10814.6
<b>Z-EEF</b>	13949275.4	1960285.1	306041.3	6850.5	188.7	32.0	6.4
<b>R = CN</b>							
<b>X-EEF</b>	3571.4	2529.6	1266.4	421.2	204.6	131.8	96.3
<b>Y-EEF</b>	760.9	509.3	763.9	421.2	763.9	543.8	760.9
<b>Z-EEF</b>	141544.1	37819.3	9771.6	421.2	34.3	8.1	2.3

## 2.2 The 1,2-H Migration of Hydroxycarbenes using the M06-2X method

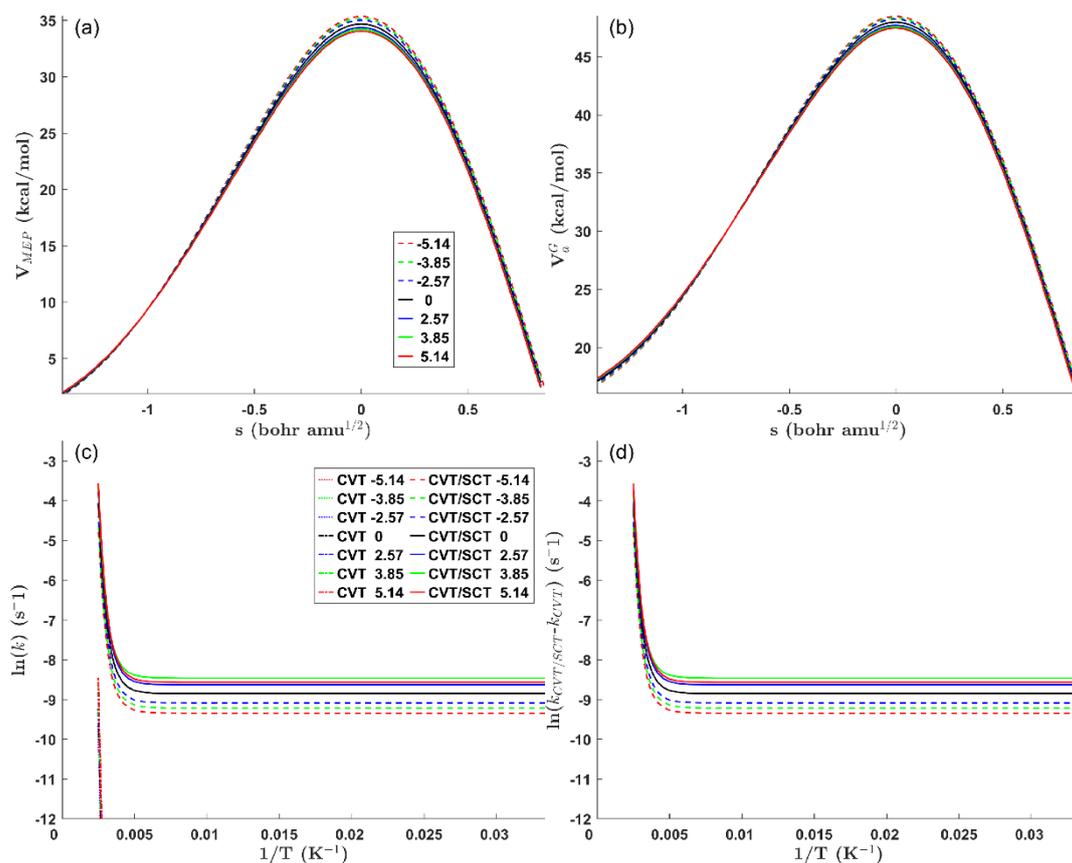
**Table S59.** Mulliken atomic charge of C, O, H in the hydroxycarbene reactants (R-C-OH: R = H, OH, CH<sub>3</sub>, CN) using the M06-2X method under the no-EEF (0.0 V/nm).

	R = H	R = CH <sub>3</sub>	R = CN	R = OH
C	-0.03	0.10	0.15	-0.03
O	-0.42	-0.44	-0.39	-0.42
H	0.37	0.36	0.39	0.37

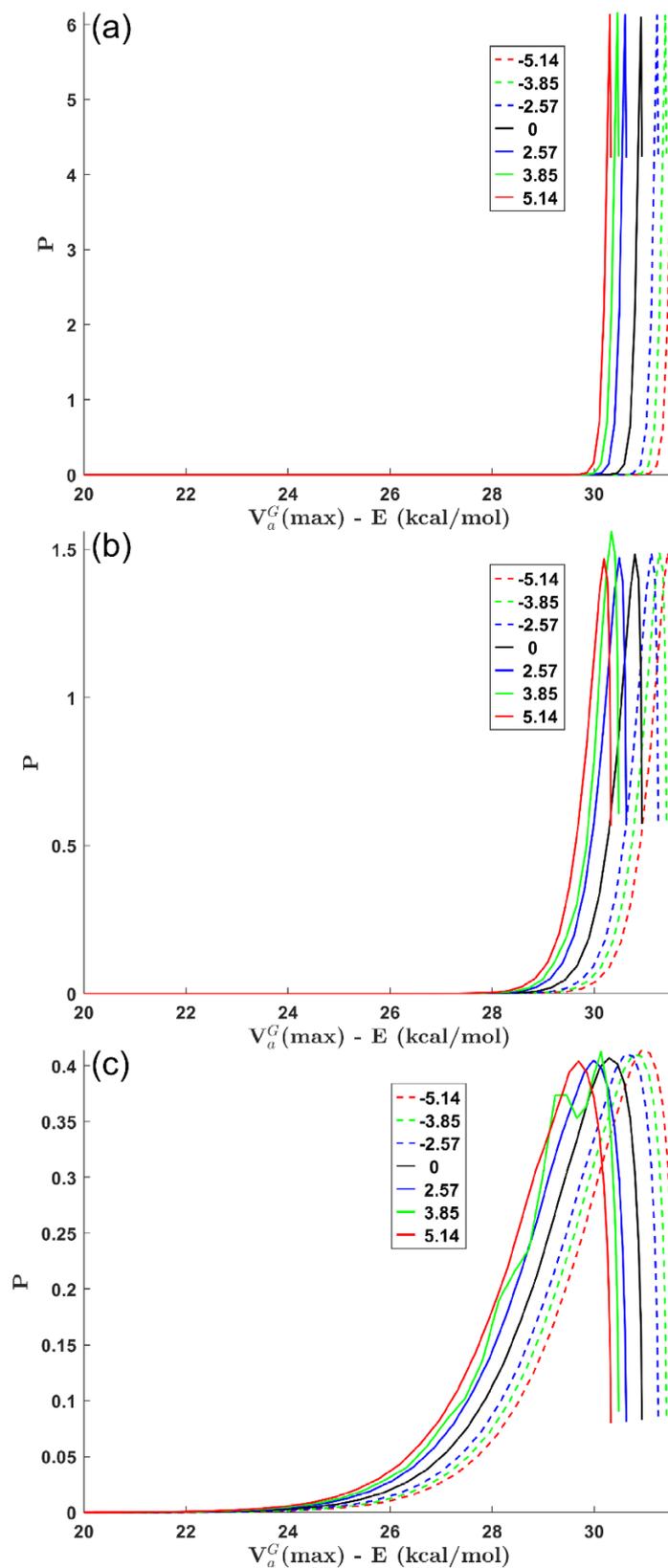
### H-C-OH

**Table S60.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of H-C-OH using the M06-2X/6-31G(d,p) method under different EEF strengths (V/nm). The  $\Omega$  (in cm<sup>-1</sup>) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

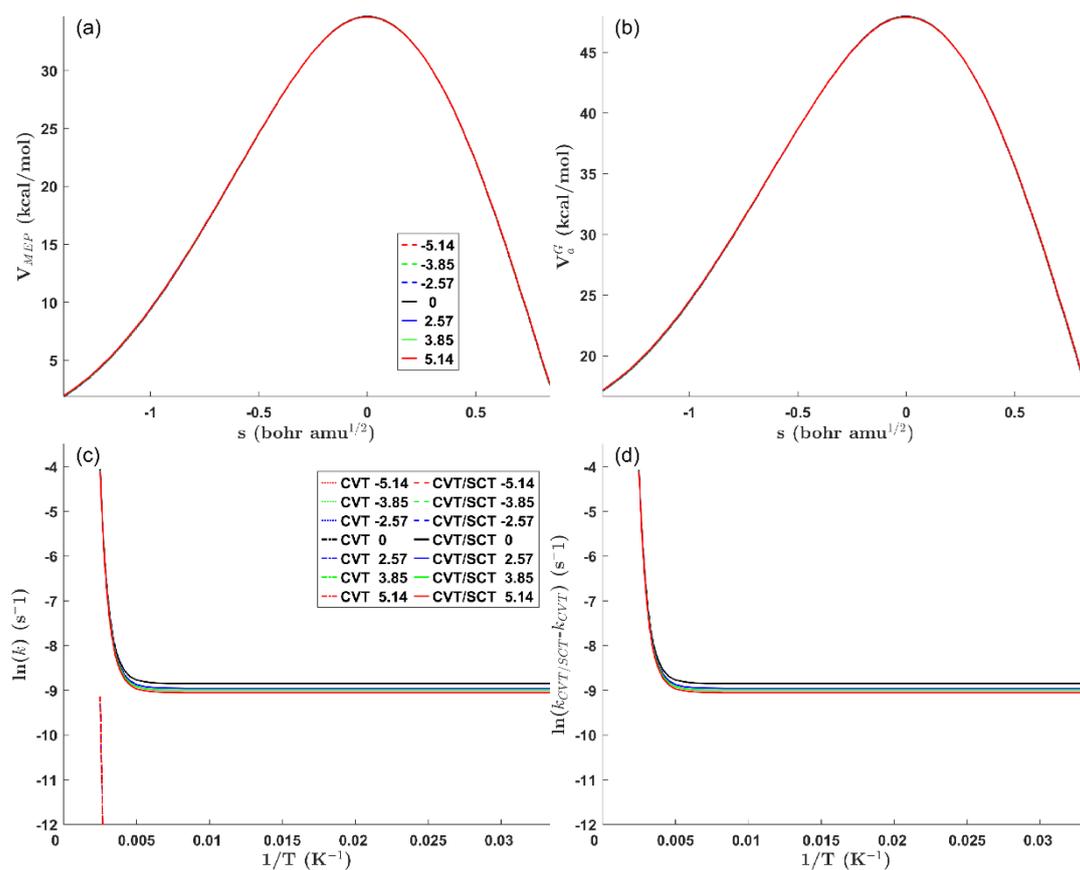
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	35.36	35.19	35.02	34.68	34.36	34.20	34.04
$\Delta V_a^G(\max)$	48.46	48.34	48.22	47.96	47.70	47.57	47.44
$\Omega$	2136	2134	2131	2125	2118	2114	2110
$T_c$	489	489	488	487	485	484	483
<b>Y-EEF Direction</b>							
$\Delta E$	34.63	34.66	34.67	34.68	34.67	34.66	34.63
$\Delta V_a^G(\max)$	47.90	47.92	47.94	47.96	47.94	47.92	47.90
$\Omega$	2120	2122	2124	2125	2124	2122	2120
$T_c$	486	486	486	487	486	486	486
<b>Z-EEF Direction</b>							
$\Delta E$	40.00	38.65	37.31	34.68	32.12	30.86	29.61
$\Delta V_a^G(\max)$	53.21	51.88	50.56	47.96	45.42	44.17	42.93
$\Omega$	2126	2127	2128	2125	2116	2109	2102
$T_c$	487	487	487	487	484	483	481



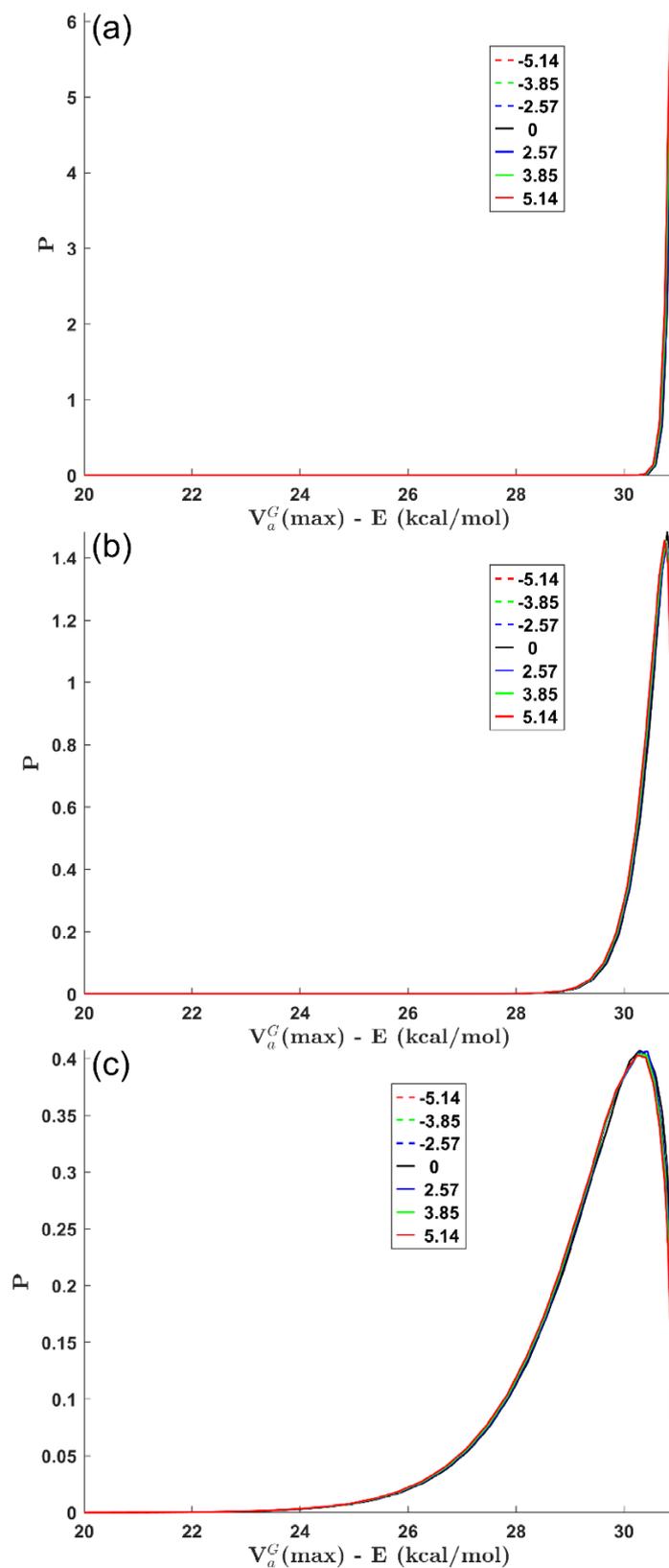
**Figure S38.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H-C-OH using the M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



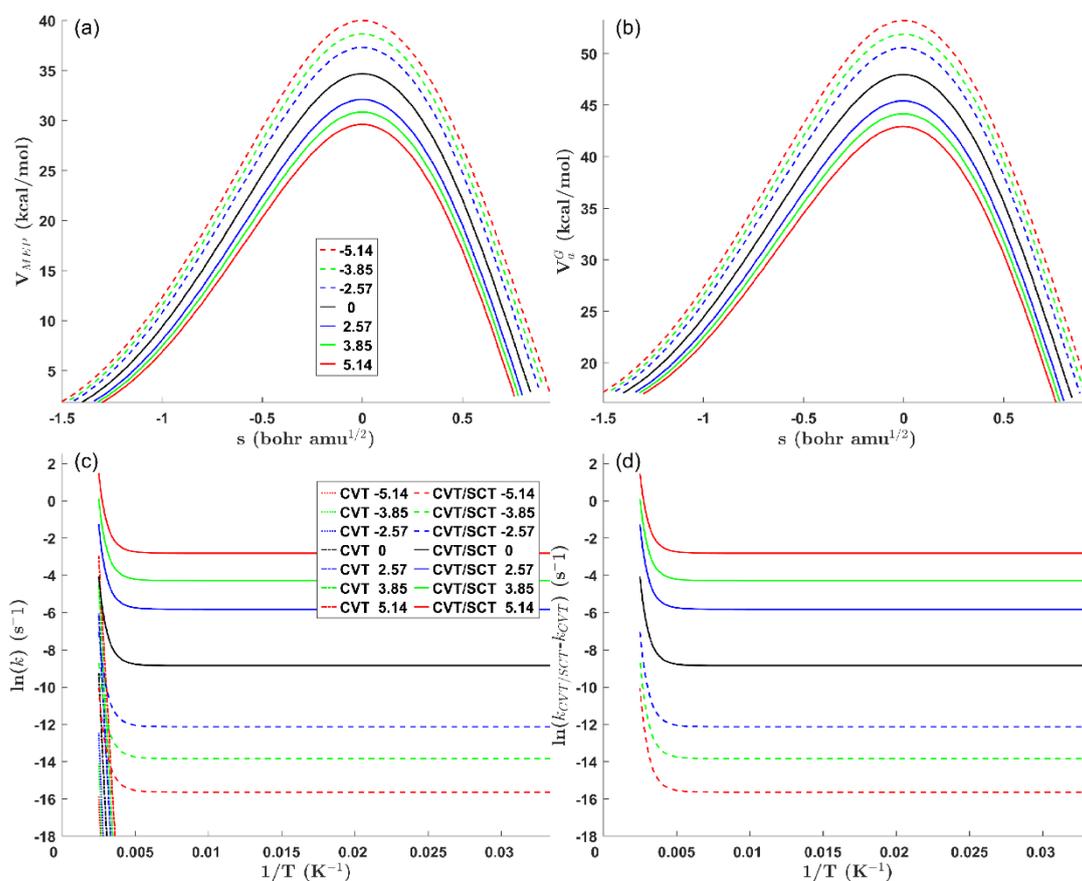
**Figure S39.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of H-C-OH at (a) 30K, (b) 100K and (c) 200K, using the M06-2X method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



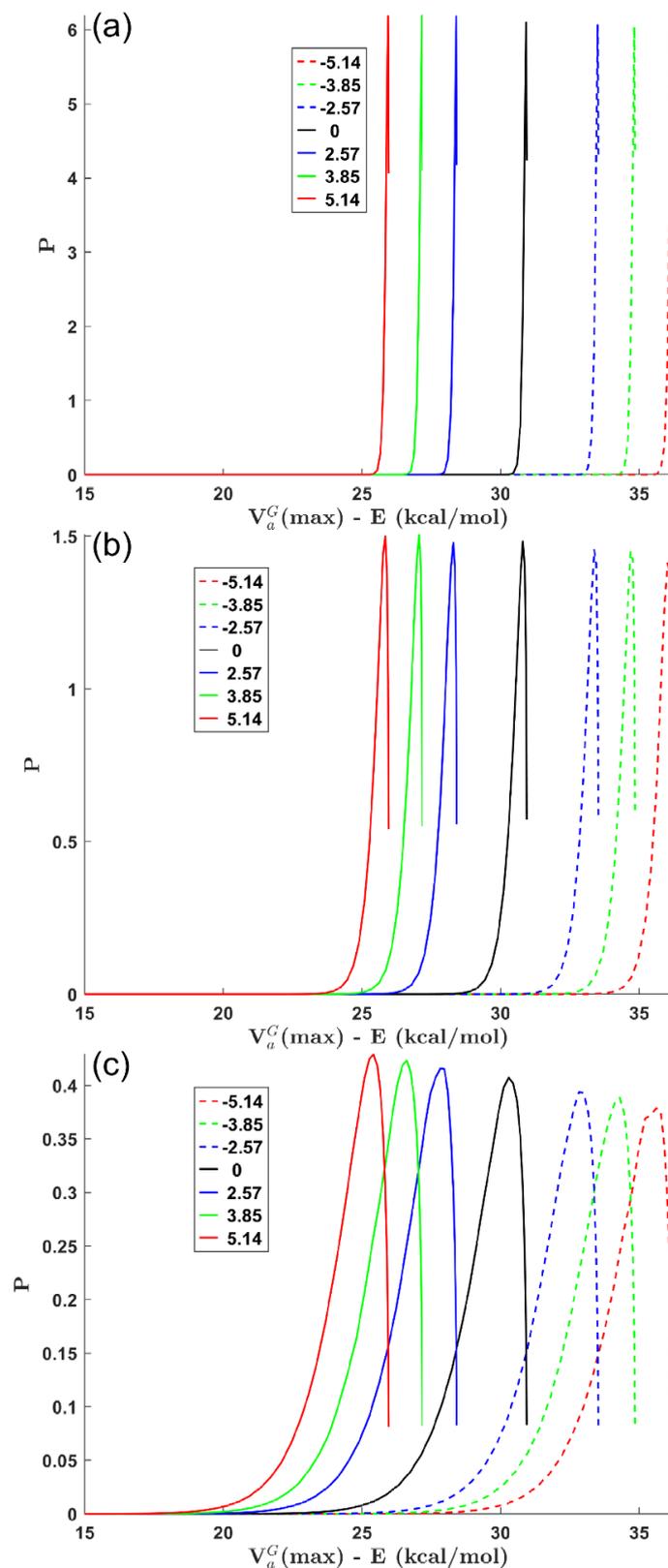
**Figure S40.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H-C-OH using the M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm))



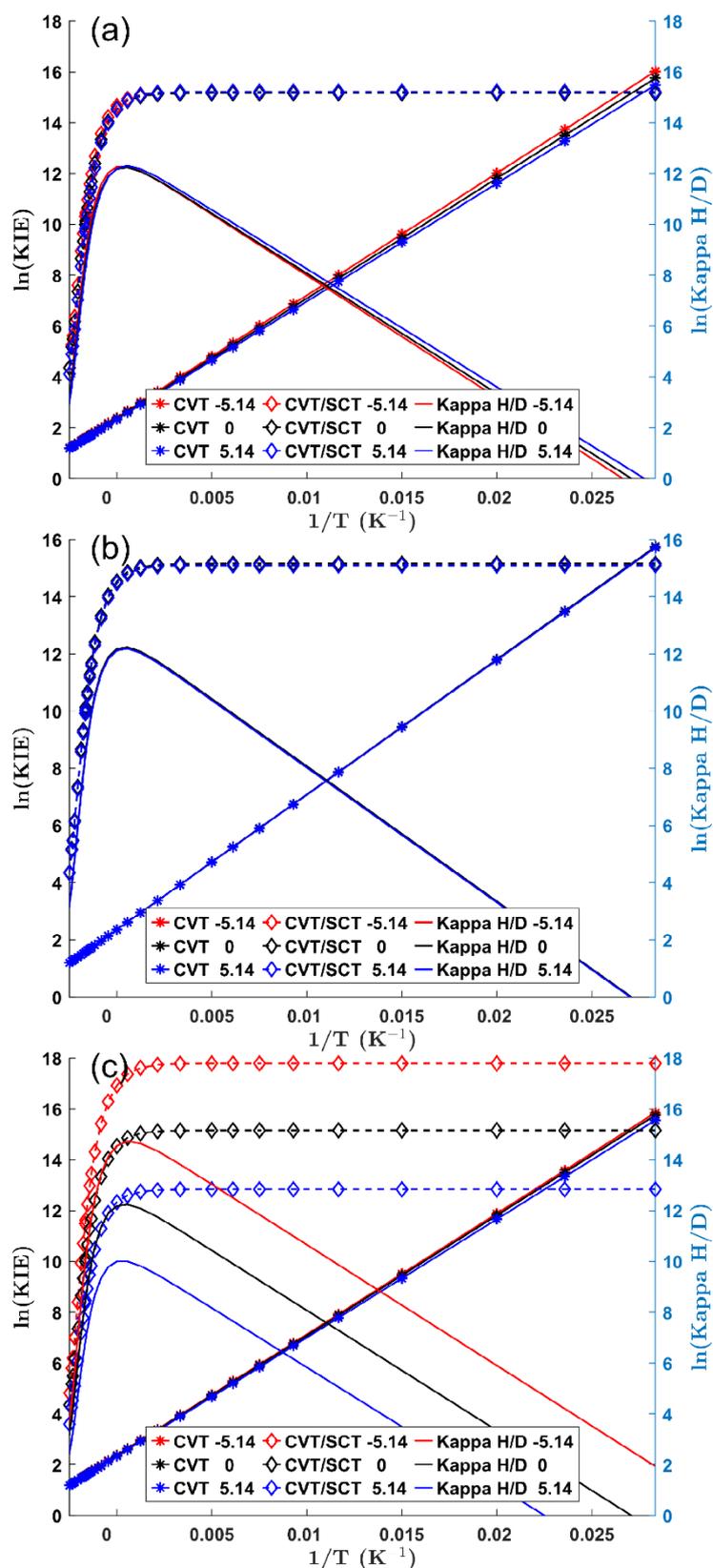
**Figure S41.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of H-C-OH at (a) 30K, (b) 100K and (c) 200K using the M06-2X method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S42.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $\text{s}^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of H-C-OH using the M06-2X method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S43.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of H-C-OH at (a) 30K, (b) 100K and (c) 200K, using the M06-2X method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S44.** Arrhenius plots of  $\ln H/D$  (KIE) and  $\ln(\kappa(H)/\kappa(D))$  versus  $1/T$  for the H-migration of H-C-OH using the M06-2X method along the direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S61.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	4.58E-219	7.11E-218	1.07E-216	2.24E-214	4.01E-212	5.05E-211	6.09E-210
35	3.98E-186	4.17E-185	4.28E-184	4.17E-182	3.55E-180	3.11E-179	2.63E-178
40	2.05E-161	1.60E-160	1.23E-159	6.75E-158	3.30E-156	2.20E-155	1.43E-154
50	8.41E-127	4.36E-126	2.22E-125	5.47E-124	1.23E-122	5.61E-122	2.50E-121
60	1.03E-103	4.07E-103	1.58E-102	2.28E-101	3.05E-100	1.08E-99	3.76E-99
70	3.29E-87	1.07E-86	3.41E-86	3.36E-85	3.10E-84	9.18E-84	2.67E-83
80	7.99E-75	2.23E-74	6.18E-74	4.57E-73	3.20E-72	8.26E-72	2.10E-71
90	3.48E-65	8.67E-65	2.14E-64	1.27E-63	7.15E-63	1.66E-62	3.81E-62
100	1.81E-57	4.11E-57	9.29E-57	4.61E-56	2.18E-55	4.66E-55	9.83E-55
120	6.95E-46	1.38E-45	2.72E-45	1.03E-44	3.77E-44	7.09E-44	1.32E-43
140	1.34E-37	2.41E-37	4.31E-37	1.35E-36	4.10E-36	7.06E-36	1.20E-35
160	2.23E-31	3.73E-31	6.20E-31	1.69E-30	4.46E-30	7.16E-30	1.14E-29
180	1.56E-26	2.47E-26	3.88E-26	9.44E-26	2.24E-25	3.41E-25	5.16E-25
200	1.19E-22	1.80E-22	2.70E-22	6.00E-22	1.31E-21	1.91E-21	2.77E-21
220	1.80E-19	2.62E-19	3.79E-19	7.85E-19	1.59E-18	2.25E-18	3.15E-18
240	8.13E-17	1.15E-16	1.61E-16	3.13E-16	5.98E-16	8.20E-16	1.12E-15
260	1.44E-14	1.98E-14	2.70E-14	5.00E-14	9.09E-14	1.22E-13	1.62E-13
273.15	2.88E-13	3.89E-13	5.24E-13	9.42E-13	1.66E-12	2.20E-12	2.88E-12
280	1.23E-12	1.65E-12	2.20E-12	3.90E-12	6.79E-12	8.90E-12	1.16E-11
290	9.03E-12	1.20E-11	1.59E-11	2.75E-11	4.70E-11	6.11E-11	7.90E-11
298.15	4.16E-11	5.48E-11	7.20E-11	1.23E-10	2.07E-10	2.67E-10	3.43E-10
300	5.82E-11	7.65E-11	1.00E-10	1.71E-10	2.87E-10	3.69E-10	4.74E-10
310	3.33E-10	4.34E-10	5.64E-10	9.44E-10	1.56E-09	1.99E-09	2.53E-09
320	1.71E-09	2.21E-09	2.85E-09	4.69E-09	7.63E-09	9.67E-09	1.22E-08
340	3.39E-08	4.31E-08	5.48E-08	8.77E-08	1.38E-07	1.73E-07	2.15E-07
360	4.84E-07	6.08E-07	7.62E-07	1.19E-06	1.83E-06	2.26E-06	2.78E-06
373.15	2.38E-06	2.97E-06	3.69E-06	5.67E-06	8.59E-06	1.05E-05	1.29E-05
380	5.24E-06	6.50E-06	8.05E-06	1.23E-05	1.84E-05	2.25E-05	2.74E-05
400	4.48E-05	5.50E-05	6.74E-05	1.01E-04	1.48E-04	1.79E-04	2.16E-04

**Table S62.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the H-migration of H-C-OH using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
35	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
40	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
50	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
60	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
70	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
80	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
90	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
100	8.79E-05	1.00E-04	1.13E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
120	8.80E-05	1.00E-04	1.14E-04	1.44E-04	1.79E-04	2.12E-04	1.91E-04
140	8.82E-05	1.00E-04	1.14E-04	1.44E-04	1.80E-04	2.13E-04	1.92E-04
160	8.88E-05	1.01E-04	1.15E-04	1.45E-04	1.81E-04	2.15E-04	1.93E-04
180	9.06E-05	1.03E-04	1.17E-04	1.49E-04	1.85E-04	2.19E-04	1.98E-04
200	9.44E-05	1.08E-04	1.22E-04	1.55E-04	1.94E-04	2.28E-04	2.07E-04
220	1.02E-04	1.16E-04	1.32E-04	1.68E-04	2.11E-04	2.46E-04	2.26E-04
240	1.15E-04	1.32E-04	1.50E-04	1.92E-04	2.41E-04	2.78E-04	2.60E-04
260	1.38E-04	1.59E-04	1.81E-04	2.34E-04	2.95E-04	3.36E-04	3.20E-04
273.15	1.63E-04	1.87E-04	2.15E-04	2.78E-04	3.53E-04	3.97E-04	3.84E-04
280	1.80E-04	2.07E-04	2.38E-04	3.10E-04	3.93E-04	4.40E-04	4.29E-04
290	2.13E-04	2.46E-04	2.82E-04	3.69E-04	4.70E-04	5.22E-04	5.15E-04
298.15	2.49E-04	2.87E-04	3.31E-04	4.34E-04	5.55E-04	6.13E-04	6.11E-04
300	2.59E-04	2.99E-04	3.44E-04	4.52E-04	5.78E-04	6.37E-04	6.37E-04
310	3.23E-04	3.73E-04	4.31E-04	5.69E-04	7.31E-04	8.02E-04	8.11E-04
320	4.14E-04	4.80E-04	5.56E-04	7.39E-04	9.53E-04	1.04E-03	1.07E-03
340	7.50E-04	8.73E-04	1.01E-03	1.37E-03	1.78E-03	1.94E-03	2.03E-03
360	1.53E-03	1.79E-03	2.09E-03	2.86E-03	3.76E-03	4.12E-03	4.40E-03
373.15	2.62E-03	3.07E-03	3.60E-03	4.95E-03	6.54E-03	7.22E-03	7.80E-03
380	3.53E-03	4.14E-03	4.85E-03	6.71E-03	8.89E-03	9.85E-03	1.07E-02
400	9.02E-03	1.05E-02	1.24E-02	1.73E-02	2.30E-02	2.58E-02	2.85E-02

**Table S63.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	5.39E-214	3.85E-214	2.93E-214	2.24E-214	2.93E-214	3.85E-214	5.39E-214
35	8.83E-182	6.61E-182	5.24E-182	4.17E-182	5.24E-182	6.61E-182	8.83E-182
40	1.30E-157	1.01E-157	8.25E-158	6.75E-158	8.25E-158	1.01E-157	1.30E-157
50	9.26E-124	7.56E-124	6.43E-124	5.47E-124	6.43E-124	7.56E-124	9.26E-124
60	3.54E-101	2.99E-101	2.61E-101	2.28E-101	2.61E-101	2.99E-101	3.54E-101
70	4.90E-85	4.24E-85	3.77E-85	3.36E-85	3.77E-85	4.24E-85	4.90E-85
80	6.36E-73	5.60E-73	5.06E-73	4.57E-73	5.06E-73	5.60E-73	6.36E-73
90	1.70E-63	1.52E-63	1.39E-63	1.27E-63	1.39E-63	1.52E-63	1.70E-63
100	5.99E-56	5.42E-56	4.99E-56	4.61E-56	4.99E-56	5.42E-56	5.99E-56
120	1.28E-44	1.18E-44	1.10E-44	1.03E-44	1.10E-44	1.18E-44	1.28E-44
140	1.63E-36	1.52E-36	1.43E-36	1.35E-36	1.43E-36	1.52E-36	1.63E-36
160	1.99E-30	1.87E-30	1.77E-30	1.69E-30	1.77E-30	1.87E-30	1.99E-30
180	1.09E-25	1.03E-25	9.87E-26	9.44E-26	9.87E-26	1.03E-25	1.09E-25
200	6.85E-22	6.51E-22	6.25E-22	6.00E-22	6.25E-22	6.51E-22	6.85E-22
220	8.85E-19	8.45E-19	8.14E-19	7.85E-19	8.14E-19	8.45E-19	8.85E-19
240	3.49E-16	3.35E-16	3.24E-16	3.13E-16	3.24E-16	3.35E-16	3.49E-16
260	5.54E-14	5.33E-14	5.16E-14	5.00E-14	5.16E-14	5.33E-14	5.54E-14
273.15	1.04E-12	1.00E-12	9.70E-13	9.42E-13	9.70E-13	1.00E-12	1.04E-12
280	4.29E-12	4.13E-12	4.01E-12	3.90E-12	4.01E-12	4.13E-12	4.29E-12
290	3.02E-11	2.91E-11	2.83E-11	2.75E-11	2.83E-11	2.91E-11	3.02E-11
298.15	1.35E-10	1.30E-10	1.26E-10	1.23E-10	1.26E-10	1.30E-10	1.35E-10
300	1.87E-10	1.81E-10	1.76E-10	1.71E-10	1.76E-10	1.81E-10	1.87E-10
310	1.03E-09	9.96E-10	9.70E-10	9.44E-10	9.70E-10	9.96E-10	1.03E-09
320	5.10E-09	4.94E-09	4.82E-09	4.69E-09	4.82E-09	4.94E-09	5.10E-09
340	9.49E-08	9.20E-08	8.98E-08	8.77E-08	8.98E-08	9.20E-08	9.49E-08
360	1.28E-06	1.24E-06	1.21E-06	1.19E-06	1.21E-06	1.24E-06	1.28E-06
373.15	6.09E-06	5.92E-06	5.79E-06	5.67E-06	5.79E-06	5.92E-06	6.09E-06
380	1.32E-05	1.28E-05	1.25E-05	1.23E-05	1.25E-05	1.28E-05	1.32E-05
400	1.08E-04	1.05E-04	1.03E-04	1.01E-04	1.03E-04	1.05E-04	1.08E-04

**Table S64.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the H-migration of H-C-OH using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
35	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
40	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
50	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
60	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
70	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
80	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
90	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
100	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
120	1.17E-04	1.24E-04	1.29E-04	1.44E-04	1.29E-04	1.24E-04	1.17E-04
140	1.18E-04	1.24E-04	1.30E-04	1.44E-04	1.30E-04	1.24E-04	1.18E-04
160	1.19E-04	1.25E-04	1.31E-04	1.45E-04	1.31E-04	1.25E-04	1.19E-04
180	1.22E-04	1.28E-04	1.34E-04	1.49E-04	1.34E-04	1.28E-04	1.22E-04
200	1.27E-04	1.34E-04	1.40E-04	1.55E-04	1.40E-04	1.34E-04	1.27E-04
220	1.39E-04	1.46E-04	1.52E-04	1.68E-04	1.52E-04	1.46E-04	1.39E-04
240	1.59E-04	1.67E-04	1.75E-04	1.92E-04	1.75E-04	1.67E-04	1.59E-04
260	1.96E-04	2.06E-04	2.14E-04	2.34E-04	2.14E-04	2.06E-04	1.96E-04
273.15	2.35E-04	2.46E-04	2.57E-04	2.78E-04	2.57E-04	2.46E-04	2.35E-04
280	2.62E-04	2.75E-04	2.86E-04	3.10E-04	2.86E-04	2.75E-04	2.62E-04
290	3.15E-04	3.30E-04	3.43E-04	3.69E-04	3.43E-04	3.30E-04	3.15E-04
298.15	3.73E-04	3.90E-04	4.06E-04	4.34E-04	4.06E-04	3.90E-04	3.73E-04
300	3.89E-04	4.07E-04	4.23E-04	4.52E-04	4.23E-04	4.07E-04	3.89E-04
310	4.94E-04	5.16E-04	5.36E-04	5.69E-04	5.36E-04	5.16E-04	4.94E-04
320	6.48E-04	6.75E-04	7.00E-04	7.39E-04	7.00E-04	6.75E-04	6.48E-04
340	1.22E-03	1.27E-03	1.31E-03	1.37E-03	1.31E-03	1.27E-03	1.22E-03
360	2.62E-03	2.70E-03	2.77E-03	2.86E-03	2.77E-03	2.70E-03	2.62E-03
373.15	4.60E-03	4.72E-03	4.83E-03	4.95E-03	4.83E-03	4.72E-03	4.60E-03
380	6.27E-03	6.43E-03	6.57E-03	6.71E-03	6.57E-03	6.43E-03	6.27E-03
400	1.64E-02	1.67E-02	1.70E-02	1.73E-02	1.70E-02	1.67E-02	1.64E-02

**Table S65.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of H-C-OH using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.52E-252	8.11E-243	3.25E-233	2.24E-214	5.20E-196	5.34E-187	4.23E-178
35	8.02E-215	1.74E-206	2.96E-198	4.17E-182	2.30E-166	1.22E-158	5.16E-151
40	1.60E-186	3.15E-179	5.01E-172	6.75E-158	4.00E-144	2.30E-137	1.08E-130
50	6.90E-147	4.72E-141	2.72E-135	5.47E-124	5.70E-113	1.46E-107	3.18E-102
60	1.89E-120	1.38E-115	8.71E-111	2.28E-101	3.47E-92	1.11E-87	3.12E-83
70	1.48E-101	2.18E-97	2.84E-93	3.36E-85	2.49E-77	1.81E-73	1.18E-69
80	2.24E-87	9.93E-84	3.95E-80	4.57E-73	3.51E-66	8.41E-63	1.82E-59
90	2.42E-76	4.22E-73	6.69E-70	1.27E-63	1.67E-57	1.69E-54	1.56E-51
100	1.64E-67	1.36E-64	1.03E-61	4.61E-56	1.48E-50	7.48E-48	3.49E-45
120	2.98E-54	8.04E-52	2.02E-49	1.03E-44	4.01E-40	7.16E-38	1.20E-35
140	9.03E-45	1.09E-42	1.25E-40	1.35E-36	1.16E-32	9.88E-31	7.96E-29
160	1.19E-37	7.89E-36	4.97E-34	1.69E-30	4.66E-27	2.28E-25	1.06E-23
180	4.15E-32	1.73E-30	6.87E-29	9.44E-26	1.08E-22	3.43E-21	1.04E-19
200	1.14E-27	3.28E-26	9.01E-25	6.00E-22	3.40E-19	7.62E-18	1.64E-16
220	4.95E-24	1.05E-22	2.13E-21	7.85E-19	2.49E-16	4.21E-15	6.87E-14
240	5.36E-21	8.79E-20	1.39E-18	3.13E-16	6.15E-14	8.21E-13	1.06E-11
260	2.00E-18	2.64E-17	3.37E-16	5.00E-14	6.54E-12	7.15E-11	7.59E-10
273.15	6.13E-17	7.15E-16	8.08E-15	9.42E-13	9.73E-11	9.48E-10	8.98E-09
280	3.21E-16	3.53E-15	3.76E-14	3.90E-12	3.60E-10	3.31E-09	2.97E-08
290	3.14E-15	3.18E-14	3.12E-13	2.75E-11	2.17E-09	1.85E-08	1.54E-07
298.15	1.80E-14	1.71E-13	1.58E-12	1.23E-10	8.61E-09	6.93E-08	5.43E-07
300	2.64E-14	2.47E-13	2.25E-12	1.71E-10	1.17E-08	9.25E-08	7.16E-07
310	1.94E-13	1.69E-12	1.43E-11	9.44E-10	5.62E-08	4.17E-07	3.02E-06
320	1.26E-12	1.02E-11	8.10E-11	4.69E-09	2.46E-07	1.71E-06	1.17E-05
340	3.82E-11	2.74E-10	1.92E-09	8.77E-08	3.63E-06	2.26E-05	1.37E-04
360	7.96E-10	5.13E-09	3.22E-08	1.19E-06	4.00E-05	2.24E-04	1.23E-03
373.15	4.92E-09	2.97E-08	1.75E-07	5.67E-06	1.68E-04	8.89E-04	4.60E-03
380	1.21E-08	7.06E-08	4.03E-07	1.23E-05	3.43E-04	1.76E-03	8.82E-03
400	1.40E-07	7.50E-07	3.92E-06	1.01E-04	2.38E-03	1.12E-02	5.19E-02

**Table S66.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) o for the H-migration of H-C-OH using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.62E-07	9.82E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
35	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
40	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
50	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
60	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
70	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
80	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
90	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
100	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.98E-03	1.38E-02	6.02E-02
120	1.62E-07	9.83E-07	5.40E-06	1.44E-04	2.99E-03	1.39E-02	6.02E-02
140	1.63E-07	9.86E-07	5.42E-06	1.44E-04	2.99E-03	1.39E-02	6.04E-02
160	1.64E-07	9.95E-07	5.47E-06	1.45E-04	3.02E-03	1.40E-02	6.08E-02
180	1.69E-07	1.02E-06	5.59E-06	1.49E-04	3.08E-03	1.43E-02	6.21E-02
200	1.77E-07	1.07E-06	5.87E-06	1.55E-04	3.21E-03	1.49E-02	6.47E-02
220	1.95E-07	1.17E-06	6.40E-06	1.68E-04	3.46E-03	1.61E-02	6.96E-02
240	2.27E-07	1.35E-06	7.37E-06	1.92E-04	3.91E-03	1.81E-02	7.84E-02
260	2.86E-07	1.68E-06	9.12E-06	2.34E-04	4.70E-03	2.17E-02	9.36E-02
273.15	3.51E-07	2.04E-06	1.10E-05	2.78E-04	5.53E-03	2.54E-02	1.09E-01
280	3.98E-07	2.29E-06	1.23E-05	3.10E-04	6.10E-03	2.80E-02	1.20E-01
290	4.91E-07	2.78E-06	1.49E-05	3.69E-04	7.20E-03	3.29E-02	1.41E-01
298.15	5.95E-07	3.33E-06	1.78E-05	4.34E-04	8.39E-03	3.82E-02	1.63E-01
300	6.24E-07	3.48E-06	1.86E-05	4.52E-04	8.71E-03	3.96E-02	1.69E-01
310	8.20E-07	4.50E-06	2.39E-05	5.69E-04	1.08E-02	4.89E-02	2.07E-01
320	1.12E-06	6.01E-06	3.16E-05	7.39E-04	1.38E-02	6.21E-02	2.62E-01
340	2.30E-06	1.19E-05	6.15E-05	1.37E-03	2.48E-02	1.09E-01	4.56E-01
360	5.42E-06	2.70E-05	1.36E-04	2.86E-03	5.02E-02	2.16E-01	8.87E-01
373.15	1.02E-05	4.97E-05	2.45E-04	4.95E-03	8.49E-02	3.58E-01	1.45E+00
380	1.45E-05	6.98E-05	3.40E-04	6.71E-03	1.14E-01	4.73E-01	1.91E+00
400	4.32E-05	2.00E-04	9.37E-04	1.73E-02	2.81E-01	1.13E+00	4.44E+00

**Table S67.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	5.06E-226	3.24E-221	1.15E-216
35	4.33E-192	5.71E-188	4.52E-184
40	1.24E-166	5.00E-163	1.29E-159
50	5.62E-131	4.30E-128	2.30E-125
60	3.43E-107	8.67E-105	1.63E-102
70	3.43E-90	3.93E-88	3.49E-86
80	1.96E-77	1.24E-75	6.30E-74
90	1.66E-67	6.65E-66	2.18E-64
100	1.48E-59	4.08E-58	9.41E-57
120	1.26E-47	2.01E-46	2.74E-45
140	4.32E-39	4.62E-38	4.34E-37
160	1.11E-32	8.79E-32	6.24E-31
180	1.08E-27	6.83E-27	3.90E-26
200	1.08E-23	5.65E-23	2.71E-22
220	2.03E-20	9.16E-20	3.80E-19
240	1.10E-17	4.37E-17	1.61E-16
260	2.27E-15	8.13E-15	2.71E-14
273.15	4.97E-14	1.67E-13	5.24E-13
280	2.21E-13	7.21E-13	2.20E-12
290	1.72E-12	5.39E-12	1.58E-11
298.15	8.31E-12	2.52E-11	7.18E-11
300	1.17E-11	3.53E-11	1.00E-10
310	7.06E-11	2.05E-10	5.62E-10
320	3.81E-10	1.07E-09	2.84E-09
340	8.23E-09	2.17E-08	5.44E-08
360	1.27E-07	3.17E-07	7.54E-07
373.15	6.54E-07	1.58E-06	3.65E-06
380	1.47E-06	3.50E-06	7.95E-06
400	1.34E-05	3.05E-05	6.64E-05

**Table S68.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	2.20E-11	3.75E-11	4.69E-11
35	2.20E-11	3.75E-11	4.69E-11
40	2.20E-11	3.75E-11	4.69E-11
50	2.20E-11	3.75E-11	4.69E-11
60	2.20E-11	3.75E-11	4.69E-11
70	2.20E-11	3.75E-11	4.69E-11
80	2.20E-11	3.75E-11	4.69E-11
90	2.20E-11	3.75E-11	4.69E-11
100	2.20E-11	3.76E-11	4.70E-11
120	2.21E-11	3.78E-11	4.74E-11
140	2.28E-11	3.90E-11	4.91E-11
160	2.47E-11	4.27E-11	5.43E-11
180	2.94E-11	5.21E-11	6.80E-11
200	4.05E-11	7.49E-11	1.02E-10
220	6.81E-11	1.34E-10	1.92E-10
240	1.47E-10	3.11E-10	4.74E-10
260	4.28E-10	9.60E-10	1.57E-09
273.15	1.02E-09	2.35E-09	4.05E-09
280	1.67E-09	3.92E-09	6.93E-09
290	3.66E-09	8.72E-09	1.60E-08
298.15	7.26E-09	1.74E-08	3.28E-08
300	8.52E-09	2.05E-08	3.87E-08
310	2.08E-08	5.04E-08	9.78E-08
320	5.30E-08	1.28E-07	2.54E-07
340	3.71E-07	8.77E-07	1.79E-06
360	2.67E-06	5.98E-06	1.24E-05
373.15	9.55E-06	2.04E-05	4.29E-05
380	1.83E-05	3.81E-05	8.04E-05
400	1.14E-04	2.21E-04	4.67E-04

**Table S69.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	8.06E-221	3.24E-221	8.06E-221
35	1.25E-187	5.71E-188	1.25E-187
40	9.89E-163	5.00E-163	9.89E-163
50	7.42E-128	4.30E-128	7.42E-128
60	1.37E-104	8.67E-105	1.37E-104
70	5.80E-88	3.93E-88	5.80E-88
80	1.75E-75	1.24E-75	1.75E-75
90	9.00E-66	6.65E-66	9.00E-66
100	5.35E-58	4.08E-58	5.35E-58
120	2.52E-46	2.01E-46	2.52E-46
140	5.61E-38	4.62E-38	5.61E-38
160	1.04E-31	8.79E-32	1.04E-31
180	7.95E-27	6.83E-27	7.95E-27
200	6.48E-23	5.65E-23	6.48E-23
220	1.04E-19	9.16E-20	1.04E-19
240	4.90E-17	4.37E-17	4.90E-17
260	9.03E-15	8.13E-15	9.03E-15
273.15	1.85E-13	1.67E-13	1.85E-13
280	7.95E-13	7.21E-13	7.95E-13
290	5.93E-12	5.39E-12	5.93E-12
298.15	2.76E-11	2.52E-11	2.76E-11
300	3.87E-11	3.53E-11	3.87E-11
310	2.24E-10	2.05E-10	2.24E-10
320	1.17E-09	1.07E-09	1.17E-09
340	2.36E-08	2.17E-08	2.36E-08
360	3.43E-07	3.17E-07	3.43E-07
373.15	1.71E-06	1.58E-06	1.71E-06
380	3.77E-06	3.50E-06	3.77E-06
400	3.27E-05	3.05E-05	3.27E-05

**Table S70.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	3.25E-11	3.75E-11	3.25E-11
35	3.25E-11	3.75E-11	3.25E-11
40	3.25E-11	3.75E-11	3.25E-11
50	3.25E-11	3.75E-11	3.25E-11
60	3.25E-11	3.75E-11	3.25E-11
70	3.25E-11	3.75E-11	3.25E-11
80	3.25E-11	3.75E-11	3.25E-11
90	3.25E-11	3.75E-11	3.25E-11
100	3.25E-11	3.76E-11	3.25E-11
120	3.27E-11	3.78E-11	3.27E-11
140	3.38E-11	3.90E-11	3.38E-11
160	3.70E-11	4.27E-11	3.70E-11
180	4.53E-11	5.21E-11	4.53E-11
200	6.56E-11	7.49E-11	6.56E-11
220	1.19E-10	1.34E-10	1.19E-10
240	2.80E-10	3.11E-10	2.80E-10
260	8.78E-10	9.60E-10	8.78E-10
273.15	2.16E-09	2.35E-09	2.16E-09
280	3.62E-09	3.92E-09	3.62E-09
290	8.09E-09	8.72E-09	8.09E-09
298.15	1.62E-08	1.74E-08	1.62E-08
300	1.91E-08	2.05E-08	1.91E-08
310	4.72E-08	5.04E-08	4.72E-08
320	1.21E-07	1.28E-07	1.21E-07
340	8.32E-07	8.77E-07	8.32E-07
360	5.73E-06	5.98E-06	5.73E-06
373.15	1.97E-05	2.04E-05	1.97E-05
380	3.68E-05	3.81E-05	3.68E-05
400	2.14E-04	2.21E-04	2.14E-04

**Table S71.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.99E-259	3.24E-221	7.43E-185
35	1.01E-220	5.71E-188	8.36E-157
40	1.10E-191	5.00E-163	9.29E-136
50	5.10E-151	4.30E-128	2.80E-106
60	6.82E-124	8.67E-105	1.30E-86
70	1.66E-104	3.93E-88	1.49E-72
80	5.85E-90	1.24E-75	5.32E-62
90	1.22E-78	6.65E-66	8.70E-54
100	1.41E-69	4.08E-58	3.27E-47
120	5.65E-56	2.01E-46	2.45E-37
140	3.02E-46	4.62E-38	2.83E-30
160	6.06E-39	8.79E-32	5.71E-25
180	2.95E-33	6.83E-27	7.76E-21
200	1.06E-28	5.65E-23	1.59E-17
220	5.70E-25	9.16E-20	8.22E-15
240	7.40E-22	4.37E-17	1.51E-12
260	3.21E-19	8.13E-15	1.26E-10
273.15	1.07E-17	1.67E-13	1.62E-09
280	5.88E-17	7.21E-13	5.59E-09
290	6.09E-16	5.39E-12	3.07E-08
298.15	3.65E-15	2.52E-11	1.13E-07
300	5.41E-15	3.53E-11	1.50E-07
310	4.17E-14	2.05E-10	6.67E-07
320	2.84E-13	1.07E-09	2.69E-06
340	9.39E-12	2.17E-08	3.45E-05
360	2.11E-10	3.17E-07	3.34E-04
373.15	1.37E-09	1.58E-06	1.30E-03
380	3.43E-09	3.50E-06	2.55E-03
400	4.23E-08	3.05E-05	1.59E-02

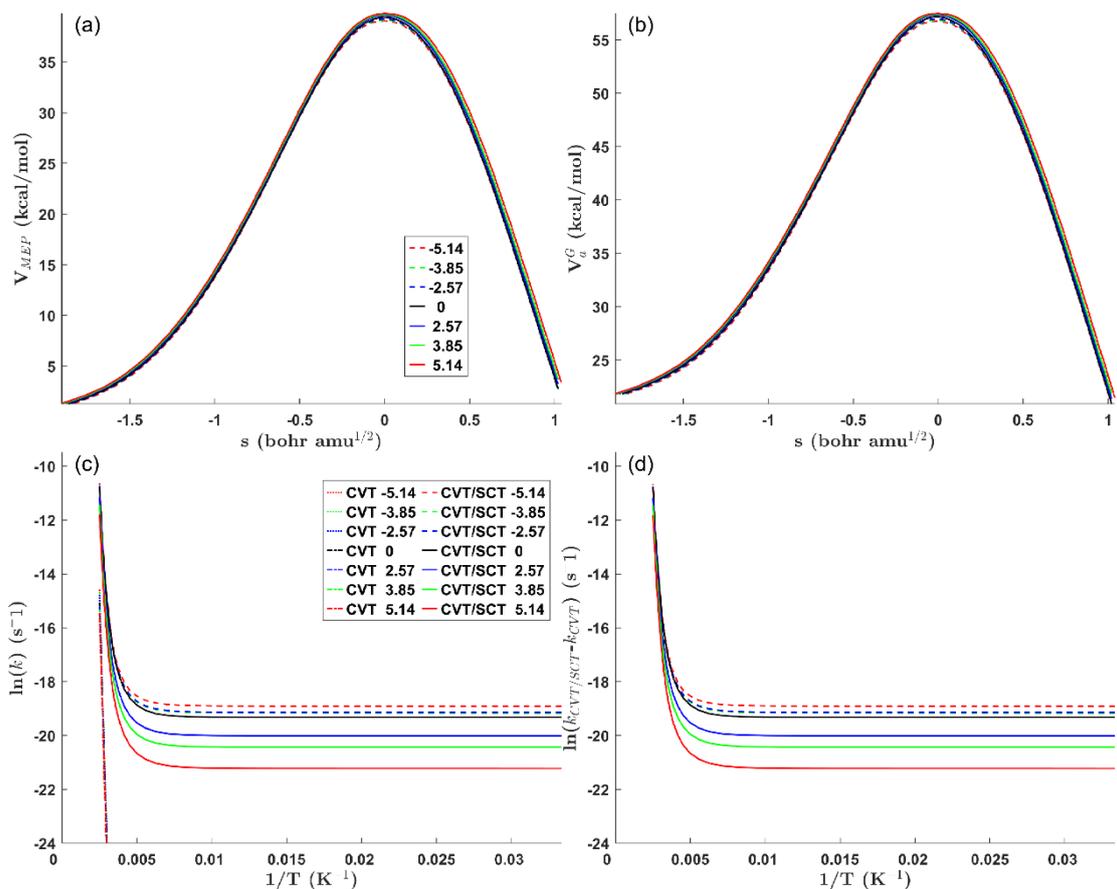
**Table S72.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) for the D-migration of H-C-OD using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	3.04E-15	3.75E-11	1.60E-07
35	3.04E-15	3.75E-11	1.60E-07
40	3.04E-15	3.75E-11	1.60E-07
50	3.04E-15	3.75E-11	1.60E-07
60	3.04E-15	3.75E-11	1.60E-07
70	3.04E-15	3.75E-11	1.60E-07
80	3.04E-15	3.75E-11	1.60E-07
90	3.04E-15	3.75E-11	1.60E-07
100	3.04E-15	3.76E-11	1.60E-07
120	3.07E-15	3.78E-11	1.61E-07
140	3.22E-15	3.90E-11	1.65E-07
160	3.66E-15	4.27E-11	1.78E-07
180	4.84E-15	5.21E-11	2.10E-07
200	7.87E-15	7.49E-11	2.85E-07
220	1.64E-14	1.34E-10	4.69E-07
240	4.58E-14	3.11E-10	9.81E-07
260	1.75E-13	9.60E-10	2.65E-06
273.15	5.04E-13	2.35E-09	5.86E-06
280	9.20E-13	3.92E-09	9.21E-06
290	2.35E-12	8.72E-09	1.86E-05
298.15	5.30E-12	1.74E-08	3.42E-05
300	6.40E-12	2.05E-08	3.95E-05
310	1.83E-11	5.04E-08	8.67E-05
320	5.43E-11	1.28E-07	1.96E-04
340	5.13E-10	8.77E-07	1.03E-03
360	4.90E-09	5.98E-06	5.43E-03
373.15	2.09E-08	2.04E-05	1.57E-02
380	4.37E-08	3.81E-05	2.69E-02
400	3.49E-07	2.21E-04	1.22E-01

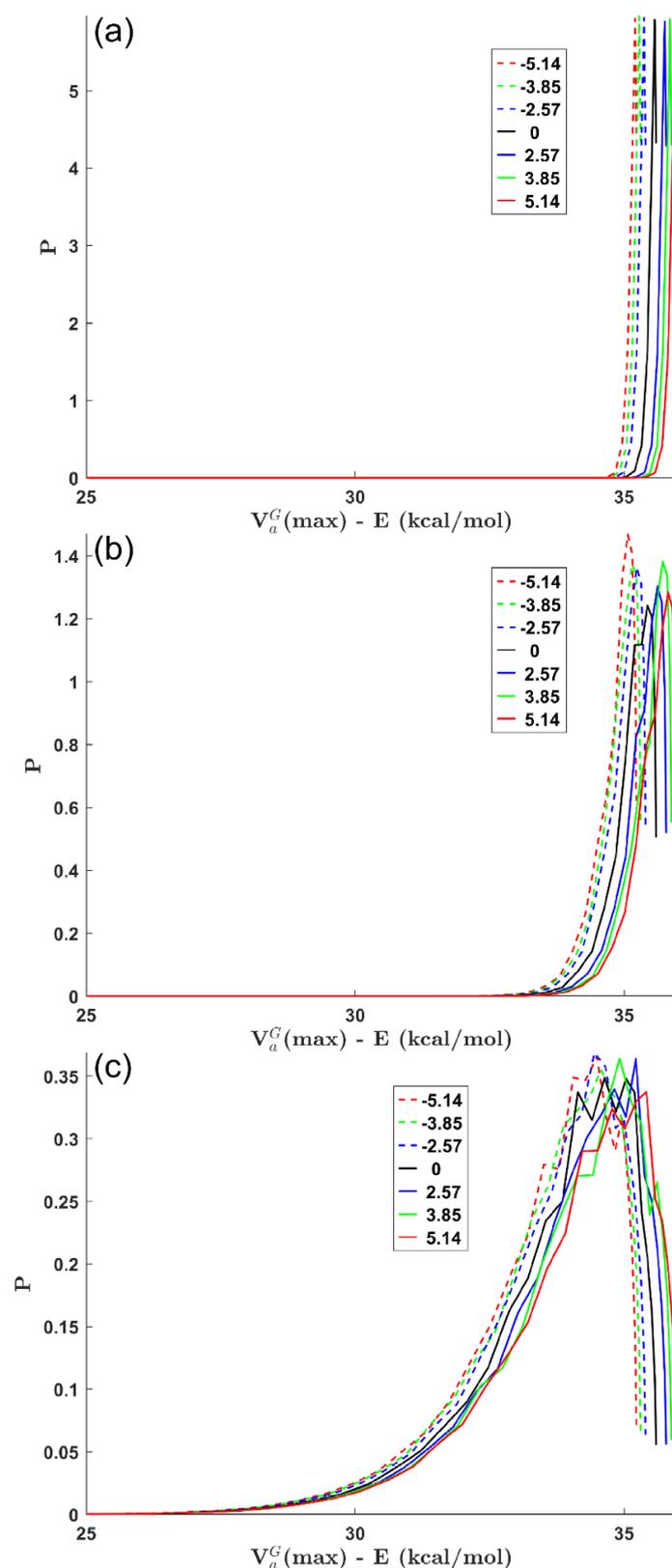
## HO-C-OH

**Table S73.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) for the H-migration of HO-C-OH using the M06-2X method under different EEF strengths (in V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

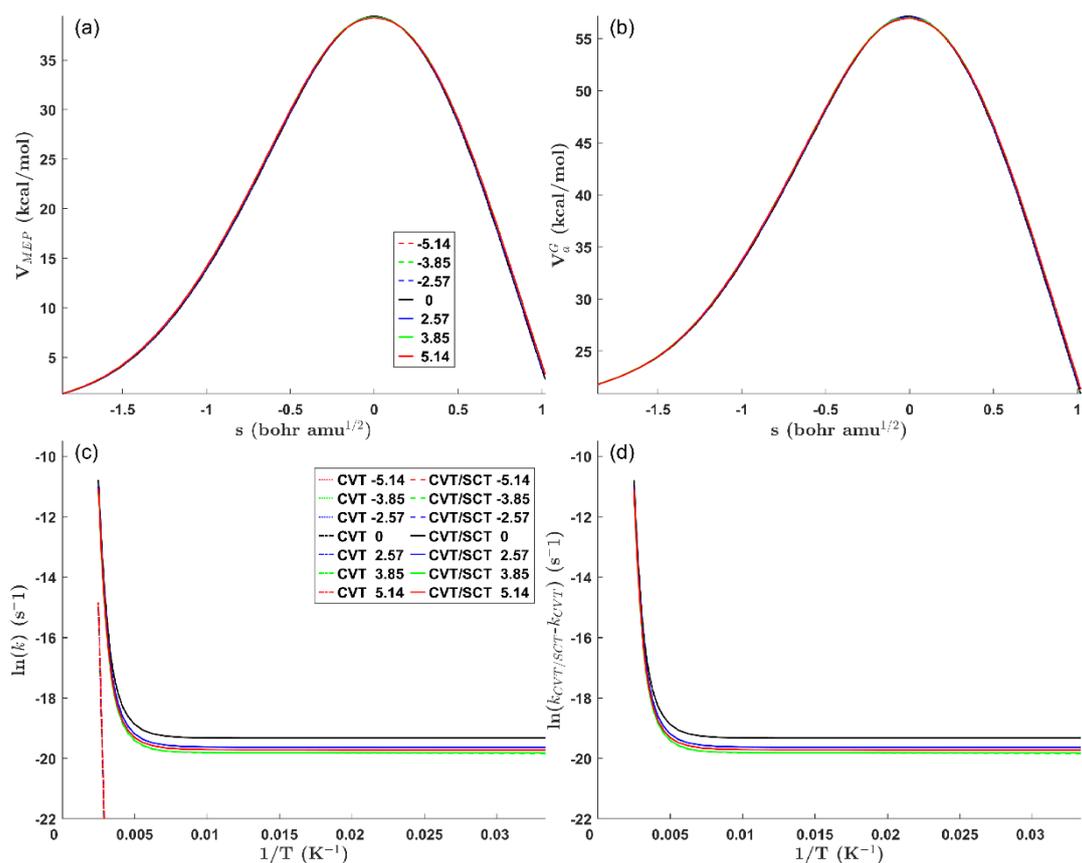
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	39.09	39.16	39.24	39.41	39.60	39.70	39.80
$\Delta V_a^G(\max)$	56.78	56.87	56.96	57.15	57.32	57.40	57.48
$\Omega$	1935	1934	1934	1932	1930	1929	1927
$T_c$	443	443	443	442	442	442	441
<b>Y-EEF Direction</b>							
$\Delta E$	39.31	39.35	39.39	39.41	39.39	39.35	39.31
$\Delta V_a^G(\max)$	57.00	57.06	57.11	57.15	57.11	57.06	57.00
$\Omega$	1931	1932	1932	1932	1932	1932	1931
$T_c$	442	442	442	442	442	442	442
<b>Z-EEF Direction</b>							
$\Delta E$	44.47	43.19	41.92	39.41	36.95	35.73	34.53
$\Delta V_a^G(\max)$	62.06	60.82	59.59	57.15	54.73	53.53	52.34
$\Omega$	1939	1938	1936	1932	1927	1925	1922
$T_c$	444	444	443	442	441	441	440



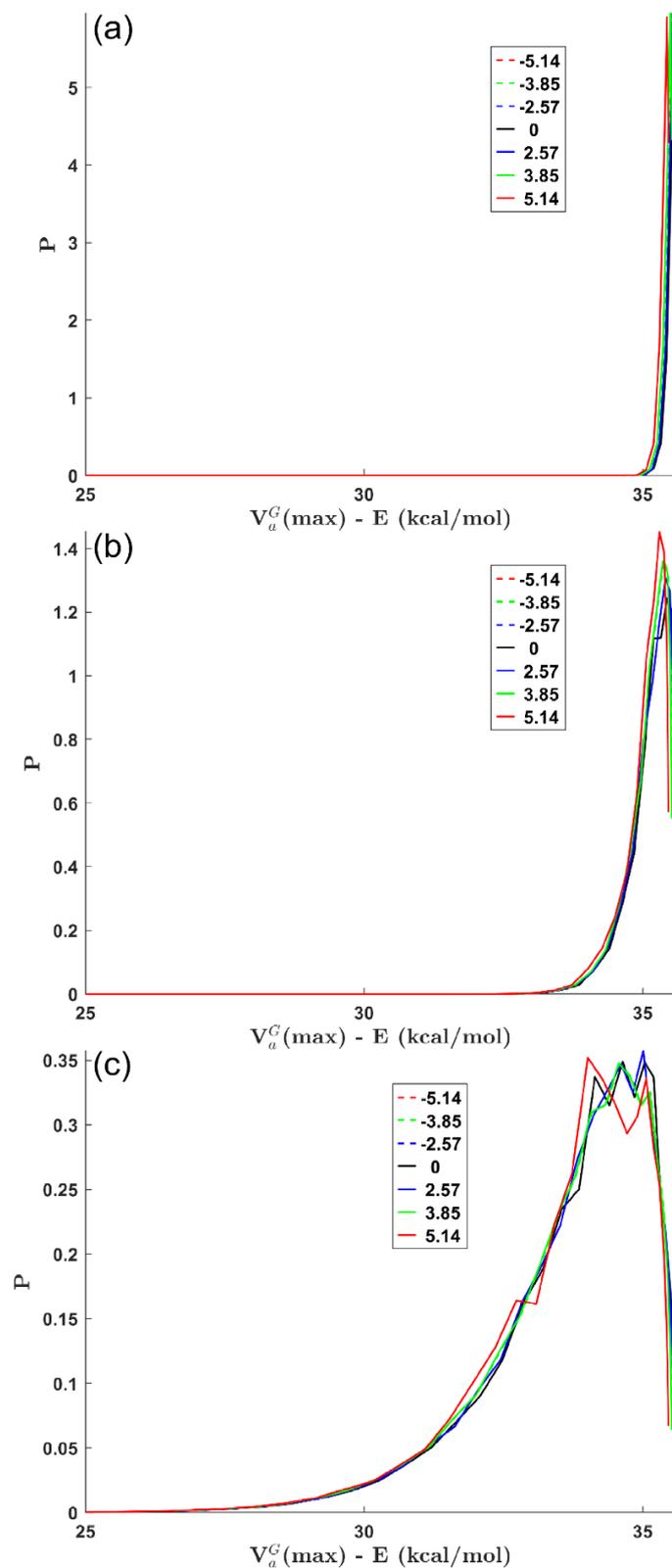
**Figure S45.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of HO-C-OH using the M06-2X method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



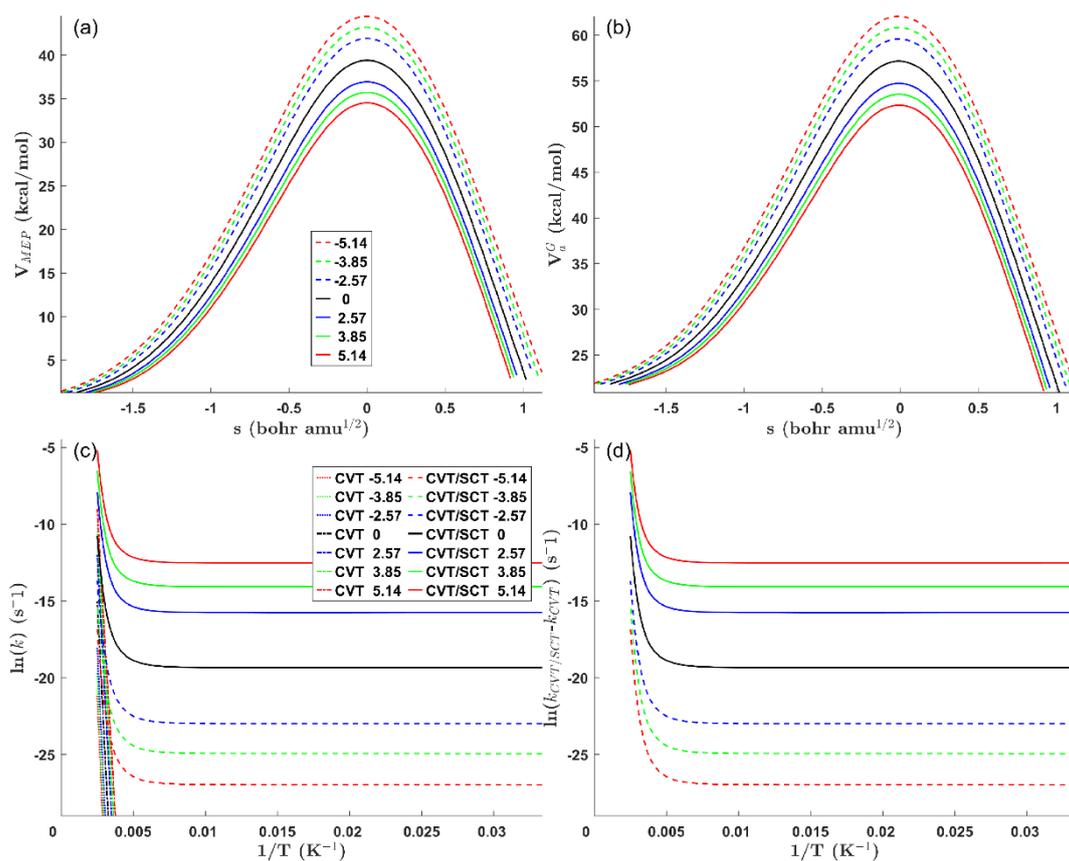
**Figure S46.** Tunneling contributions/probability (P) to the SCT transmission coefficient ( $\kappa_{SCT}$ ) for the H-migration of HO-C-OH at (a) 30K, (b) 100K and (c) 200K, using the M06-2X method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



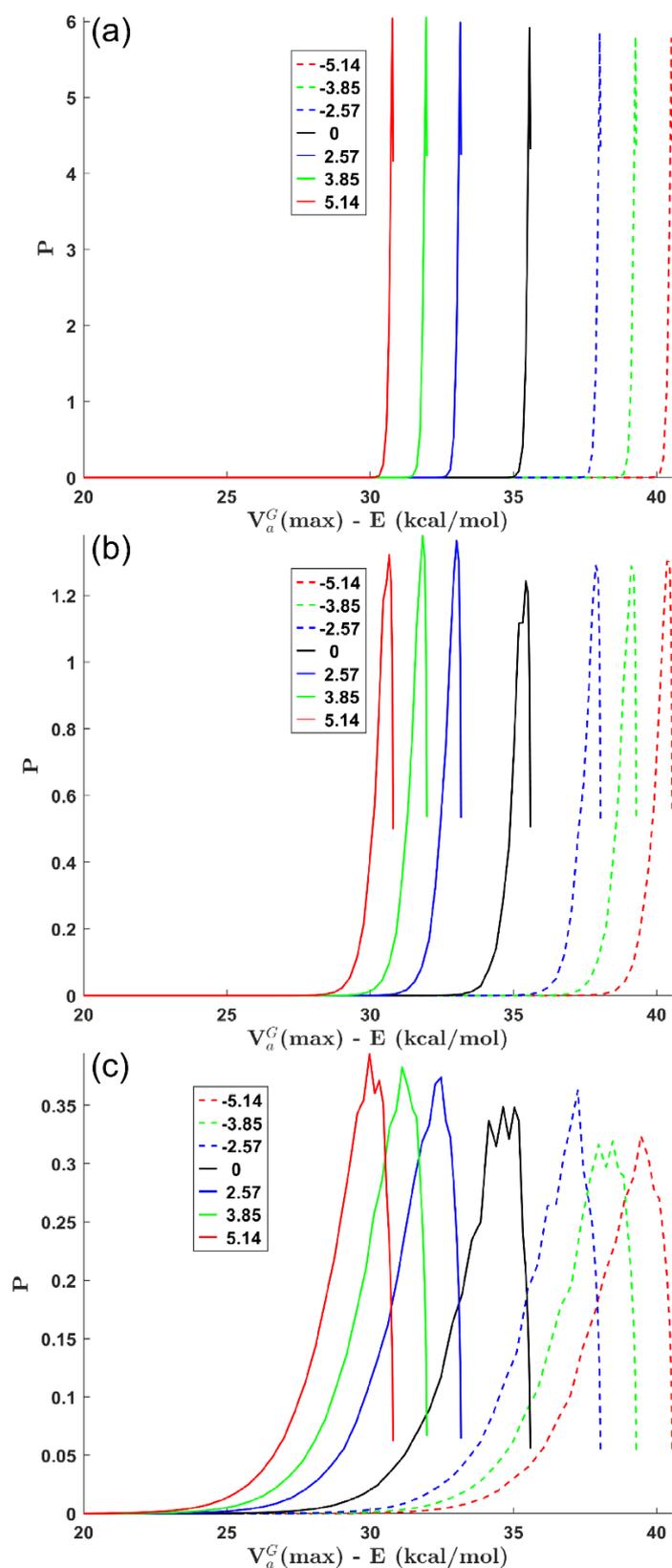
**Figure S47.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



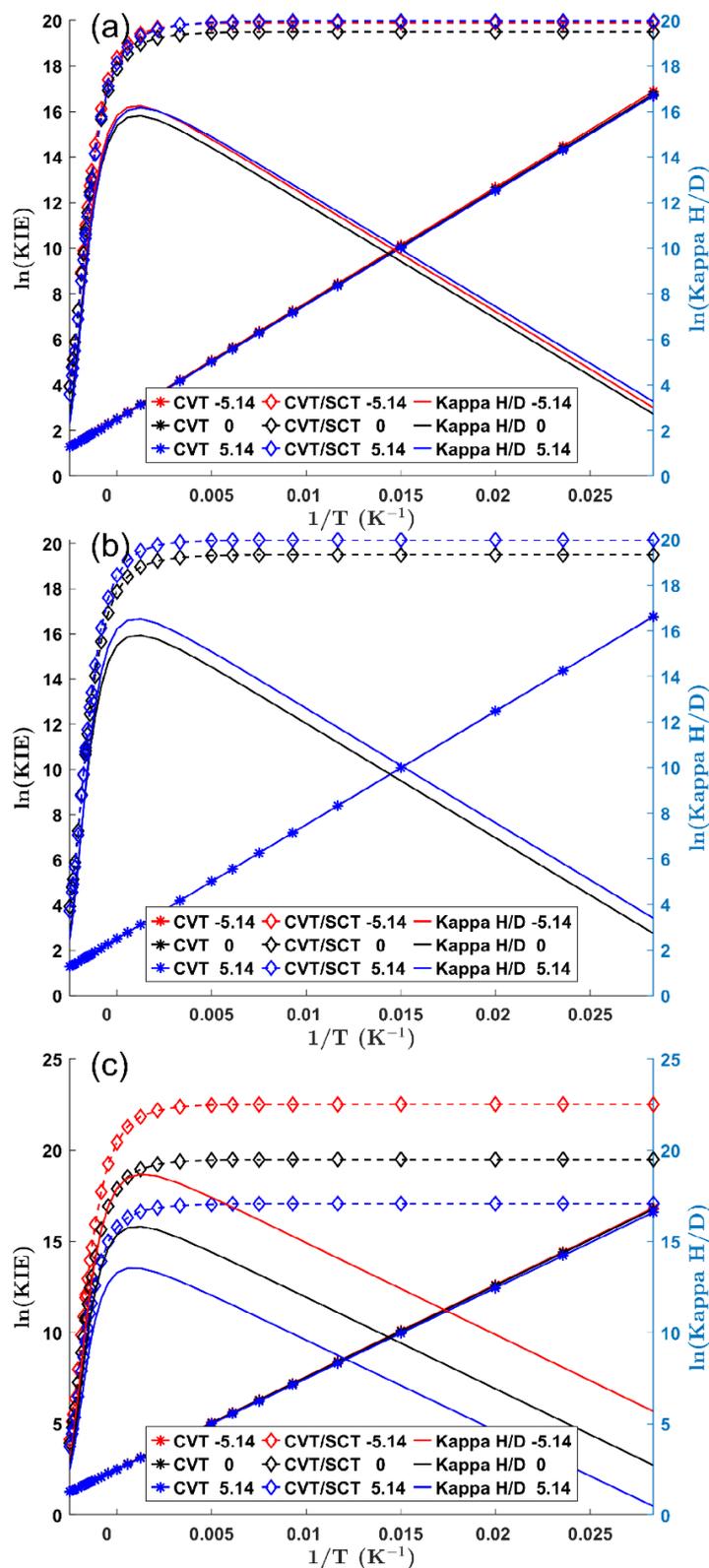
**Figure S48.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration HO-C-OH at (a) 30K, (b) 100K and (c) 200K using the M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S49.** (a) Potential energy surface along the minimum energy path ( $V_{\text{MEP}}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^{\text{G}}$ ), (c) Arrhenius plots of the non-tunneling ( $k_{\text{CVT}}$ ) and overall ( $k_{\text{CVT+SCT}}$ ) rate constants (in  $\text{s}^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{\text{CVT+SCT}} - k_{\text{CVT}}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S50.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) for the H-migration of HO-C-OH at (a) 30K, (b) 100K and (c) 200K, using the M06-2X method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S51.** Arrhenius plots of  $\ln H/D$  (KIE) and  $\ln(\kappa(H)/\kappa(D))$  versus  $1/T$  for the H-migration of HO-C-OH using M06-2X/6-31G(d,p) method along direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S74.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.11E-245	2.93E-246	6.83E-247	2.47E-248	1.08E-249	2.00E-250	3.86E-251
35	6.05E-209	1.92E-209	5.53E-210	3.21E-211	2.19E-212	5.18E-213	1.26E-213
40	2.19E-181	8.04E-182	2.70E-182	2.23E-183	2.14E-184	6.04E-185	1.76E-185
50	8.68E-143	3.89E-143	1.63E-143	2.21E-144	3.39E-145	1.23E-145	4.60E-146
60	4.84E-117	2.48E-117	1.20E-117	2.27E-118	4.77E-119	2.05E-119	9.02E-120
70	1.22E-98	6.88E-99	3.69E-99	8.85E-100	2.32E-100	1.13E-100	5.57E-101
80	7.84E-85	4.75E-85	2.76E-85	7.89E-86	2.45E-86	1.30E-86	7.04E-87
90	4.37E-74	2.80E-74	1.73E-74	5.68E-75	2.01E-75	1.15E-75	6.63E-76
100	1.75E-65	1.17E-65	7.57E-66	2.78E-66	1.10E-66	6.61E-67	4.04E-67
120	1.43E-52	1.03E-52	7.15E-53	3.10E-53	1.43E-53	9.42E-54	6.26E-54
140	2.47E-43	1.86E-43	1.36E-43	6.66E-44	3.45E-44	2.41E-44	1.70E-44
160	2.13E-36	1.66E-36	1.27E-36	6.80E-37	3.83E-37	2.81E-37	2.08E-37
180	5.40E-31	4.33E-31	3.41E-31	1.96E-31	1.18E-31	8.98E-32	6.88E-32
200	1.15E-26	9.44E-27	7.62E-27	4.63E-27	2.95E-27	2.31E-27	1.82E-27
220	4.05E-23	3.39E-23	2.79E-23	1.78E-23	1.19E-23	9.52E-24	7.68E-24
240	3.70E-20	3.15E-20	2.63E-20	1.75E-20	1.21E-20	9.90E-21	8.15E-21
260	1.19E-17	1.03E-17	8.74E-18	5.99E-18	4.28E-18	3.57E-18	2.99E-18
273.15	3.37E-16	2.93E-16	2.51E-16	1.75E-16	1.28E-16	1.07E-16	9.09E-17
280	1.70E-15	1.48E-15	1.28E-15	8.99E-16	6.61E-16	5.59E-16	4.75E-16
290	1.57E-14	1.38E-14	1.19E-14	8.52E-15	6.35E-15	5.40E-15	4.62E-15
298.15	8.66E-14	7.62E-14	6.62E-14	4.77E-14	3.59E-14	3.07E-14	2.64E-14
300	1.26E-13	1.11E-13	9.64E-14	6.96E-14	5.25E-14	4.49E-14	3.87E-14
310	8.81E-13	7.80E-13	6.82E-13	4.97E-13	3.79E-13	3.26E-13	2.82E-13
320	5.47E-12	4.86E-12	4.27E-12	3.15E-12	2.42E-12	2.10E-12	1.83E-12
340	1.53E-10	1.37E-10	1.21E-10	9.13E-11	7.16E-11	6.26E-11	5.50E-11
360	2.97E-09	2.68E-09	2.39E-09	1.83E-09	1.46E-09	1.29E-09	1.14E-09
373.15	1.76E-08	1.60E-08	1.43E-08	1.10E-08	8.89E-09	7.89E-09	7.03E-09
380	4.24E-08	3.85E-08	3.46E-08	2.68E-08	2.17E-08	1.93E-08	1.72E-08
400	4.65E-07	4.24E-07	3.83E-07	3.01E-07	2.47E-07	2.22E-07	1.99E-07

**Table S75.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	6.13E-09	4.75E-09	4.86E-09	4.04E-09	2.04E-09	1.34E-09	6.07E-10
35	6.14E-09	4.76E-09	4.87E-09	4.04E-09	2.04E-09	1.34E-09	6.08E-10
40	6.14E-09	4.77E-09	4.87E-09	4.04E-09	2.04E-09	1.34E-09	6.08E-10
50	6.15E-09	4.78E-09	4.88E-09	4.04E-09	2.04E-09	1.34E-09	6.08E-10
60	6.16E-09	4.79E-09	4.88E-09	4.04E-09	2.04E-09	1.34E-09	6.09E-10
70	6.16E-09	4.80E-09	4.89E-09	4.04E-09	2.04E-09	1.34E-09	6.09E-10
80	6.17E-09	4.80E-09	4.89E-09	4.04E-09	2.04E-09	1.34E-09	6.10E-10
90	6.17E-09	4.81E-09	4.90E-09	4.05E-09	2.05E-09	1.34E-09	6.12E-10
100	6.19E-09	4.83E-09	4.92E-09	4.06E-09	2.06E-09	1.35E-09	6.16E-10
120	6.28E-09	4.90E-09	4.99E-09	4.13E-09	2.10E-09	1.37E-09	6.32E-10
140	6.48E-09	5.07E-09	5.18E-09	4.31E-09	2.19E-09	1.44E-09	6.68E-10
160	6.89E-09	5.42E-09	5.55E-09	4.65E-09	2.38E-09	1.56E-09	7.36E-10
180	7.62E-09	6.04E-09	6.20E-09	5.27E-09	2.72E-09	1.78E-09	8.55E-10
200	8.86E-09	7.09E-09	7.32E-09	6.34E-09	3.29E-09	2.15E-09	1.06E-09
220	1.09E-08	8.88E-09	9.23E-09	8.16E-09	4.27E-09	2.79E-09	1.41E-09
240	1.46E-08	1.21E-08	1.26E-08	1.14E-08	6.05E-09	3.95E-09	2.06E-09
260	2.18E-08	1.82E-08	1.92E-08	1.78E-08	9.52E-09	6.23E-09	3.36E-09
273.15	3.03E-08	2.56E-08	2.71E-08	2.55E-08	1.38E-08	9.05E-09	5.01E-09
280	3.70E-08	3.14E-08	3.33E-08	3.15E-08	1.71E-08	1.13E-08	6.34E-09
290	5.12E-08	4.36E-08	4.65E-08	4.43E-08	2.44E-08	1.61E-08	9.26E-09
298.15	6.89E-08	5.90E-08	6.29E-08	6.03E-08	3.35E-08	2.23E-08	1.30E-08
300	7.39E-08	6.34E-08	6.77E-08	6.49E-08	3.61E-08	2.41E-08	1.41E-08
310	1.12E-07	9.62E-08	1.03E-07	9.92E-08	5.58E-08	3.77E-08	2.25E-08
320	1.76E-07	1.53E-07	1.63E-07	1.58E-07	9.02E-08	6.16E-08	3.75E-08
340	4.97E-07	4.34E-07	4.61E-07	4.49E-07	2.65E-07	1.86E-07	1.18E-07
360	1.62E-06	1.43E-06	1.51E-06	1.46E-06	8.99E-07	6.51E-07	4.25E-07
373.15	3.78E-06	3.35E-06	3.50E-06	3.38E-06	2.14E-06	1.58E-06	1.06E-06
380	5.98E-06	5.31E-06	5.52E-06	5.32E-06	3.43E-06	2.55E-06	1.72E-06
400	2.39E-05	2.14E-05	2.19E-05	2.09E-05	1.42E-05	1.08E-05	7.57E-06

**Table S76.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.31E-247	6.50E-248	3.89E-248	2.47E-248	3.89E-248	8.15E-248	2.31E-247
35	2.18E-210	7.36E-211	4.74E-211	3.21E-211	4.73E-211	8.93E-211	2.18E-210
40	1.20E-182	4.62E-183	3.14E-183	2.23E-183	3.14E-183	5.48E-183	1.20E-182
50	8.49E-144	3.96E-144	2.91E-144	2.21E-144	2.91E-144	4.54E-144	8.49E-144
60	6.98E-118	3.70E-118	2.86E-118	2.27E-118	2.86E-118	4.14E-118	6.98E-118
70	2.32E-99	1.34E-99	1.08E-99	8.85E-100	1.08E-99	1.48E-99	2.32E-99
80	1.84E-85	1.14E-85	9.40E-86	7.89E-86	9.40E-86	1.24E-85	1.84E-85
90	1.20E-74	7.87E-75	6.64E-75	5.68E-75	6.64E-75	8.50E-75	1.20E-74
100	5.48E-66	3.74E-66	3.21E-66	2.78E-66	3.21E-66	4.00E-66	5.48E-66
120	5.47E-53	3.97E-53	3.50E-53	3.10E-53	3.50E-53	4.21E-53	5.47E-53
140	1.08E-43	8.23E-44	7.39E-44	6.66E-44	7.39E-44	8.67E-44	1.08E-43
160	1.04E-36	8.17E-37	7.45E-37	6.80E-37	7.45E-37	8.57E-37	1.04E-36
180	2.87E-31	2.30E-31	2.13E-31	1.96E-31	2.13E-31	2.41E-31	2.87E-31
200	6.54E-27	5.36E-27	4.99E-27	4.63E-27	4.99E-27	5.59E-27	6.54E-27
220	2.44E-23	2.03E-23	1.91E-23	1.78E-23	1.91E-23	2.11E-23	2.44E-23
240	2.33E-20	1.96E-20	1.86E-20	1.75E-20	1.86E-20	2.04E-20	2.33E-20
260	7.83E-18	6.67E-18	6.35E-18	5.99E-18	6.35E-18	6.93E-18	7.83E-18
273.15	2.26E-16	1.94E-16	1.85E-16	1.75E-16	1.85E-16	2.02E-16	2.26E-16
280	1.15E-15	9.92E-16	9.50E-16	8.99E-16	9.50E-16	1.03E-15	1.15E-15
290	1.09E-14	9.36E-15	8.99E-15	8.52E-15	8.99E-15	9.73E-15	1.09E-14
298.15	6.04E-14	5.23E-14	5.02E-14	4.77E-14	5.02E-14	5.43E-14	6.04E-14
300	8.80E-14	7.62E-14	7.33E-14	6.96E-14	7.33E-14	7.92E-14	8.80E-14
310	6.24E-13	5.43E-13	5.23E-13	4.97E-13	5.23E-13	5.64E-13	6.24E-13
320	3.93E-12	3.42E-12	3.30E-12	3.15E-12	3.30E-12	3.55E-12	3.93E-12
340	1.13E-10	9.86E-11	9.56E-11	9.13E-11	9.56E-11	1.02E-10	1.13E-10
360	2.23E-09	1.96E-09	1.91E-09	1.83E-09	1.91E-09	2.04E-09	2.23E-09
373.15	1.34E-08	1.18E-08	1.15E-08	1.10E-08	1.15E-08	1.23E-08	1.34E-08
380	3.24E-08	2.87E-08	2.80E-08	2.68E-08	2.80E-08	2.98E-08	3.24E-08
400	3.61E-07	3.21E-07	3.14E-07	3.01E-07	3.14E-07	3.33E-07	3.61E-07

**Table S77.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.75E-09	2.43E-09	2.98E-09	4.04E-09	2.98E-09	2.47E-09	2.75E-09
35	2.75E-09	2.44E-09	2.98E-09	4.04E-09	2.98E-09	2.47E-09	2.75E-09
40	2.75E-09	2.45E-09	2.99E-09	4.04E-09	2.99E-09	2.47E-09	2.75E-09
50	2.75E-09	2.45E-09	2.99E-09	4.04E-09	2.99E-09	2.48E-09	2.75E-09
60	2.76E-09	2.46E-09	2.99E-09	4.04E-09	2.99E-09	2.48E-09	2.76E-09
70	2.76E-09	2.46E-09	2.99E-09	4.04E-09	2.99E-09	2.48E-09	2.76E-09
80	2.76E-09	2.47E-09	2.99E-09	4.04E-09	2.99E-09	2.48E-09	2.76E-09
90	2.77E-09	2.47E-09	3.00E-09	4.05E-09	3.00E-09	2.49E-09	2.77E-09
100	2.78E-09	2.48E-09	3.01E-09	4.06E-09	3.01E-09	2.50E-09	2.78E-09
120	2.82E-09	2.52E-09	3.06E-09	4.13E-09	3.06E-09	2.54E-09	2.82E-09
140	2.92E-09	2.61E-09	3.19E-09	4.31E-09	3.19E-09	2.64E-09	2.92E-09
160	3.13E-09	2.80E-09	3.44E-09	4.65E-09	3.44E-09	2.83E-09	3.13E-09
180	3.49E-09	3.13E-09	3.88E-09	5.27E-09	3.88E-09	3.17E-09	3.49E-09
200	4.10E-09	3.70E-09	4.63E-09	6.34E-09	4.63E-09	3.75E-09	4.10E-09
220	5.17E-09	4.68E-09	5.92E-09	8.16E-09	5.92E-09	4.75E-09	5.17E-09
240	7.09E-09	6.44E-09	8.22E-09	1.14E-08	8.22E-09	6.54E-09	7.09E-09
260	1.08E-08	9.86E-09	1.27E-08	1.78E-08	1.27E-08	1.00E-08	1.08E-08
273.15	1.54E-08	1.40E-08	1.82E-08	2.55E-08	1.82E-08	1.43E-08	1.54E-08
280	1.90E-08	1.73E-08	2.25E-08	3.15E-08	2.25E-08	1.76E-08	1.90E-08
290	2.68E-08	2.44E-08	3.16E-08	4.43E-08	3.16E-08	2.48E-08	2.68E-08
298.15	3.66E-08	3.32E-08	4.32E-08	6.03E-08	4.31E-08	3.39E-08	3.66E-08
300	3.94E-08	3.58E-08	4.65E-08	6.49E-08	4.65E-08	3.65E-08	3.94E-08
310	6.07E-08	5.50E-08	7.13E-08	9.92E-08	7.13E-08	5.62E-08	6.06E-08
320	9.75E-08	8.84E-08	1.14E-07	1.58E-07	1.14E-07	9.04E-08	9.75E-08
340	2.86E-07	2.59E-07	3.30E-07	4.49E-07	3.30E-07	2.65E-07	2.86E-07
360	9.77E-07	8.84E-07	1.10E-06	1.46E-06	1.10E-06	9.06E-07	9.77E-07
373.15	2.35E-06	2.12E-06	2.61E-06	3.38E-06	2.61E-06	2.18E-06	2.35E-06
380	3.77E-06	3.40E-06	4.14E-06	5.32E-06	4.14E-06	3.49E-06	3.77E-06
400	1.58E-05	1.42E-05	1.68E-05	2.09E-05	1.68E-05	1.46E-05	1.58E-05

**Table S78.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.16E-284	2.90E-275	3.37E-266	2.47E-248	1.16E-230	5.30E-222	1.94E-213
35	3.97E-242	2.65E-234	1.56E-226	3.21E-211	4.49E-196	1.19E-188	2.61E-181
40	2.02E-210	1.42E-203	8.93E-197	2.23E-183	4.00E-170	1.26E-163	3.32E-157
50	5.13E-166	1.54E-160	4.24E-155	2.21E-144	8.88E-134	1.40E-128	1.92E-123
60	2.13E-136	7.81E-132	2.66E-127	2.27E-118	1.56E-109	3.34E-105	6.40E-101
70	3.12E-115	2.55E-111	1.96E-107	8.85E-100	3.32E-92	1.71E-88	8.01E-85
80	2.38E-99	6.31E-96	1.58E-92	7.89E-86	3.36E-79	5.94E-76	9.67E-73
90	5.45E-87	6.01E-84	6.33E-81	5.68E-75	4.43E-69	3.42E-66	2.44E-63
100	4.26E-77	2.33E-74	1.22E-71	2.78E-66	5.60E-61	2.22E-58	8.23E-56
120	3.02E-62	5.79E-60	1.07E-57	3.10E-53	8.16E-49	1.19E-46	1.65E-44
140	1.26E-51	1.14E-49	9.98E-48	6.66E-44	4.09E-40	2.94E-38	2.01E-36
160	1.20E-43	6.14E-42	3.07E-40	6.80E-37	1.40E-33	5.90E-32	2.37E-30
180	1.95E-37	6.46E-36	2.09E-34	1.96E-31	1.73E-28	4.79E-27	1.28E-25
200	1.85E-32	4.31E-31	9.83E-30	4.63E-27	2.07E-24	4.12E-23	7.90E-22
220	2.22E-28	3.87E-27	6.63E-26	1.78E-23	4.56E-21	6.90E-20	1.01E-18
240	5.62E-25	7.71E-24	1.04E-22	1.75E-20	2.81E-18	3.39E-17	3.97E-16
260	4.30E-22	4.82E-21	5.31E-20	5.99E-18	6.51E-16	6.47E-15	6.26E-14
273.15	2.00E-20	2.00E-19	1.96E-18	1.75E-16	1.52E-14	1.35E-13	1.17E-12
280	1.29E-19	1.21E-18	1.12E-17	8.99E-16	6.97E-14	5.87E-13	4.83E-12
290	1.66E-18	1.44E-17	1.24E-16	8.52E-15	5.68E-13	4.44E-12	3.40E-11
298.15	1.18E-17	9.65E-17	7.80E-16	4.77E-14	2.83E-12	2.09E-11	1.51E-10
300	1.81E-17	1.46E-16	1.17E-15	6.96E-14	4.03E-12	2.94E-11	2.10E-10
310	1.70E-16	1.28E-15	9.54E-15	4.97E-13	2.52E-11	1.73E-10	1.16E-09
320	1.38E-15	9.79E-15	6.85E-14	3.15E-12	1.41E-10	9.08E-10	5.72E-09
340	6.37E-14	4.01E-13	2.50E-12	9.13E-11	3.27E-09	1.88E-08	1.06E-07
360	1.92E-12	1.09E-11	6.14E-11	1.83E-09	5.35E-08	2.79E-07	1.43E-06
373.15	1.49E-11	7.92E-11	4.19E-10	1.10E-08	2.86E-07	1.41E-06	6.79E-06
380	4.08E-11	2.11E-10	1.08E-09	2.68E-08	6.55E-07	3.13E-06	1.47E-05
400	6.38E-10	3.03E-09	1.43E-08	3.01E-07	6.26E-06	2.76E-05	1.20E-04

**Table S79.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the H-migration of HO-C-OH using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.93E-12	1.48E-11	1.04E-10	4.04E-09	1.44E-07	7.77E-07	3.63E-06
35	1.94E-12	1.48E-11	1.04E-10	4.04E-09	1.44E-07	7.76E-07	3.62E-06
40	1.94E-12	1.49E-11	1.04E-10	4.04E-09	1.44E-07	7.76E-07	3.62E-06
50	1.94E-12	1.49E-11	1.04E-10	4.04E-09	1.43E-07	7.76E-07	3.62E-06
60	1.94E-12	1.49E-11	1.04E-10	4.04E-09	1.43E-07	7.75E-07	3.62E-06
70	1.94E-12	1.49E-11	1.04E-10	4.04E-09	1.43E-07	7.75E-07	3.62E-06
80	1.95E-12	1.49E-11	1.04E-10	4.04E-09	1.44E-07	7.75E-07	3.62E-06
90	1.95E-12	1.50E-11	1.04E-10	4.05E-09	1.44E-07	7.76E-07	3.62E-06
100	1.96E-12	1.50E-11	1.05E-10	4.06E-09	1.44E-07	7.78E-07	3.63E-06
120	2.01E-12	1.53E-11	1.07E-10	4.13E-09	1.46E-07	7.89E-07	3.68E-06
140	2.11E-12	1.61E-11	1.12E-10	4.31E-09	1.51E-07	8.15E-07	3.81E-06
160	2.30E-12	1.75E-11	1.22E-10	4.65E-09	1.62E-07	8.68E-07	4.06E-06
180	2.66E-12	2.01E-11	1.39E-10	5.27E-09	1.80E-07	9.59E-07	4.50E-06
200	3.28E-12	2.47E-11	1.69E-10	6.34E-09	2.10E-07	1.11E-06	5.23E-06
220	4.39E-12	3.29E-11	2.22E-10	8.16E-09	2.61E-07	1.37E-06	6.43E-06
240	6.55E-12	4.83E-11	3.20E-10	1.14E-08	3.49E-07	1.80E-06	8.48E-06
260	1.12E-11	8.03E-11	5.18E-10	1.78E-08	5.15E-07	2.61E-06	1.22E-05
273.15	1.73E-11	1.22E-10	7.69E-10	2.55E-08	7.10E-07	3.52E-06	1.65E-05
280	2.25E-11	1.56E-10	9.72E-10	3.15E-08	8.58E-07	4.22E-06	1.96E-05
290	3.43E-11	2.32E-10	1.42E-09	4.43E-08	1.17E-06	5.65E-06	2.61E-05
298.15	5.02E-11	3.31E-10	1.99E-09	6.03E-08	1.55E-06	7.38E-06	3.39E-05
300	5.49E-11	3.61E-10	2.16E-09	6.49E-08	1.65E-06	7.87E-06	3.61E-05
310	9.23E-11	5.89E-10	3.44E-09	9.92E-08	2.44E-06	1.14E-05	5.17E-05
320	1.63E-10	1.01E-09	5.72E-09	1.58E-07	3.75E-06	1.72E-05	7.68E-05
340	5.69E-10	3.32E-09	1.79E-08	4.49E-07	9.91E-06	4.38E-05	1.90E-04
360	2.30E-09	1.26E-08	6.40E-08	1.46E-06	3.00E-05	1.28E-04	5.36E-04
373.15	6.13E-09	3.22E-08	1.58E-07	3.38E-06	6.59E-05	2.74E-04	1.12E-03
380	1.04E-08	5.36E-08	2.57E-07	5.32E-06	1.01E-04	4.15E-04	1.68E-03
400	5.15E-08	2.49E-07	1.13E-06	2.09E-05	3.63E-04	1.45E-03	5.60E-03

**Table S80.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	5.19E-253	1.30E-255	2.20E-258
35	3.13E-215	1.84E-217	7.78E-220
40	6.89E-187	7.69E-189	6.44E-191
50	3.42E-147	9.36E-149	2.05E-150
60	1.03E-120	5.13E-122	2.12E-123
70	8.64E-102	6.59E-103	4.31E-104
80	1.37E-87	1.44E-88	1.33E-89
90	1.54E-76	2.09E-77	2.52E-78
100	1.08E-67	1.79E-68	2.68E-69
120	2.08E-54	4.64E-55	9.60E-56
140	6.56E-45	1.82E-45	4.76E-46
160	8.94E-38	2.92E-38	9.13E-39
180	3.22E-32	1.20E-32	4.29E-33
200	9.12E-28	3.75E-28	1.50E-28
220	4.05E-24	1.81E-24	7.96E-25
240	4.49E-21	2.15E-21	1.02E-21
260	1.70E-18	8.66E-19	4.38E-19
273.15	5.28E-17	2.78E-17	1.46E-17
280	2.78E-16	1.49E-16	7.95E-17
290	2.74E-15	1.50E-15	8.21E-16
298.15	1.58E-14	8.79E-15	4.91E-15
300	2.32E-14	1.30E-14	7.26E-15
310	1.71E-13	9.76E-14	5.59E-14
320	1.12E-12	6.48E-13	3.79E-13
340	3.42E-11	2.06E-11	1.25E-11
360	7.19E-10	4.45E-10	2.79E-10
373.15	4.46E-09	2.81E-09	1.80E-09
380	1.10E-08	6.99E-09	4.51E-09
400	1.28E-07	8.35E-08	5.53E-08

**Table S81.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	1.41E-17	1.38E-17	1.30E-18
35	1.41E-17	1.38E-17	1.30E-18
40	1.41E-17	1.38E-17	1.30E-18
50	1.41E-17	1.38E-17	1.30E-18
60	1.41E-17	1.38E-17	1.30E-18
70	1.41E-17	1.38E-17	1.31E-18
80	1.42E-17	1.39E-17	1.32E-18
90	1.43E-17	1.41E-17	1.35E-18
100	1.46E-17	1.44E-17	1.39E-18
120	1.57E-17	1.58E-17	1.59E-18
140	1.87E-17	1.92E-17	2.04E-18
160	2.56E-17	2.71E-17	3.07E-18
180	4.29E-17	4.72E-17	5.73E-18
200	9.52E-17	1.09E-16	1.43E-17
220	3.04E-16	3.63E-16	5.25E-17
240	1.47E-15	1.80E-15	2.94E-16
260	1.05E-14	1.28E-14	2.43E-15
273.15	4.66E-14	5.50E-14	1.17E-14
280	1.07E-13	1.23E-13	2.78E-14
290	3.83E-13	4.22E-13	1.05E-13
298.15	1.13E-12	1.19E-12	3.21E-13
300	1.45E-12	1.52E-12	4.16E-13
310	5.69E-12	5.69E-12	1.71E-12
320	2.26E-11	2.17E-11	7.15E-12
340	3.43E-10	3.12E-10	1.20E-10
360	4.54E-09	4.02E-09	1.74E-09
373.15	2.25E-08	1.98E-08	9.13E-09
380	5.02E-08	4.41E-08	2.09E-08
400	4.60E-07	4.06E-07	2.07E-07

**Table S82.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	1.21E-254	1.30E-255	1.21E-254
35	1.25E-216	1.84E-217	1.25E-216
40	4.11E-188	7.69E-189	4.11E-188
50	3.59E-148	9.36E-149	3.59E-148
60	1.57E-121	5.13E-122	1.57E-121
70	1.73E-102	6.59E-103	1.73E-102
80	3.36E-88	1.44E-88	3.36E-88
90	4.42E-77	2.09E-77	4.42E-77
100	3.53E-68	1.79E-68	3.53E-68
120	8.17E-55	4.64E-55	8.17E-55
140	2.96E-45	1.82E-45	2.96E-45
160	4.48E-38	2.92E-38	4.48E-38
180	1.75E-32	1.20E-32	1.75E-32
200	5.30E-28	3.75E-28	5.30E-28
220	2.48E-24	1.81E-24	2.48E-24
240	2.87E-21	2.15E-21	2.87E-21
260	1.13E-18	8.66E-19	1.13E-18
273.15	3.59E-17	2.78E-17	3.59E-17
280	1.91E-16	1.49E-16	1.91E-16
290	1.91E-15	1.50E-15	1.91E-15
298.15	1.11E-14	8.79E-15	1.11E-14
300	1.64E-14	1.30E-14	1.64E-14
310	1.23E-13	9.76E-14	1.23E-13
320	8.09E-13	6.48E-13	8.09E-13
340	2.53E-11	2.06E-11	2.53E-11
360	5.43E-10	4.45E-10	5.43E-10
373.15	3.41E-09	2.81E-09	3.41E-09
380	8.45E-09	6.99E-09	8.45E-09
400	1.00E-07	8.35E-08	1.00E-07

**Table S83.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	4.81E-18	1.38E-17	4.81E-18
35	4.81E-18	1.38E-17	4.81E-18
40	4.82E-18	1.38E-17	4.82E-18
50	4.82E-18	1.38E-17	4.82E-18
60	4.83E-18	1.38E-17	4.83E-18
70	4.84E-18	1.38E-17	4.84E-18
80	4.86E-18	1.39E-17	4.86E-18
90	4.91E-18	1.41E-17	4.91E-18
100	5.02E-18	1.44E-17	5.02E-18
120	5.47E-18	1.58E-17	5.47E-18
140	6.54E-18	1.92E-17	6.54E-18
160	8.99E-18	2.71E-17	8.99E-18
180	1.52E-17	4.72E-17	1.52E-17
200	3.45E-17	1.09E-16	3.45E-17
220	1.17E-16	3.63E-16	1.17E-16
240	6.19E-16	1.80E-15	6.19E-16
260	4.91E-15	1.28E-14	4.91E-15
273.15	2.32E-14	5.50E-14	2.32E-14
280	5.52E-14	1.23E-13	5.52E-14
290	2.07E-13	4.22E-13	2.07E-13
298.15	6.37E-13	1.19E-12	6.37E-13
300	8.25E-13	1.52E-12	8.25E-13
310	3.40E-12	5.69E-12	3.40E-12
320	1.42E-11	2.17E-11	1.42E-11
340	2.35E-10	3.12E-10	2.35E-10
360	3.32E-09	4.02E-09	3.32E-09
373.15	1.71E-08	1.98E-08	1.71E-08
380	3.88E-08	4.41E-08	3.88E-08
400	3.72E-07	4.06E-07	3.72E-07

**Table S84.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.06E-291	1.30E-255	1.21E-220
35	2.15E-248	1.84E-217	1.74E-187
40	6.61E-216	7.69E-189	1.30E-162
50	2.08E-170	9.36E-149	9.02E-128
60	4.64E-140	5.13E-122	1.57E-104
70	2.26E-118	6.59E-103	6.44E-88
80	4.25E-102	1.44E-88	1.89E-75
90	1.96E-89	2.09E-77	9.53E-66
100	2.69E-79	1.79E-68	5.58E-58
120	4.45E-64	4.64E-55	2.57E-46
140	3.41E-53	1.82E-45	5.68E-38
160	5.09E-45	2.92E-38	1.05E-31
180	1.18E-38	1.20E-32	8.01E-27
200	1.49E-33	3.75E-28	6.54E-23
220	2.25E-29	1.81E-24	1.05E-19
240	6.89E-26	2.15E-21	4.97E-17
260	6.20E-23	8.66E-19	9.20E-15
273.15	3.17E-21	2.78E-17	1.88E-13
280	2.12E-20	1.49E-16	8.12E-13
290	2.91E-19	1.50E-15	6.06E-12
298.15	2.17E-18	8.79E-15	2.83E-11
300	3.36E-18	1.30E-14	3.96E-11
310	3.32E-17	9.76E-14	2.30E-10
320	2.84E-16	6.48E-13	1.19E-09
340	1.43E-14	2.06E-11	2.42E-08
360	4.67E-13	4.45E-10	3.52E-07
373.15	3.77E-12	2.81E-09	1.75E-06
380	1.06E-11	6.99E-09	3.87E-06
400	1.76E-10	8.35E-08	3.36E-05

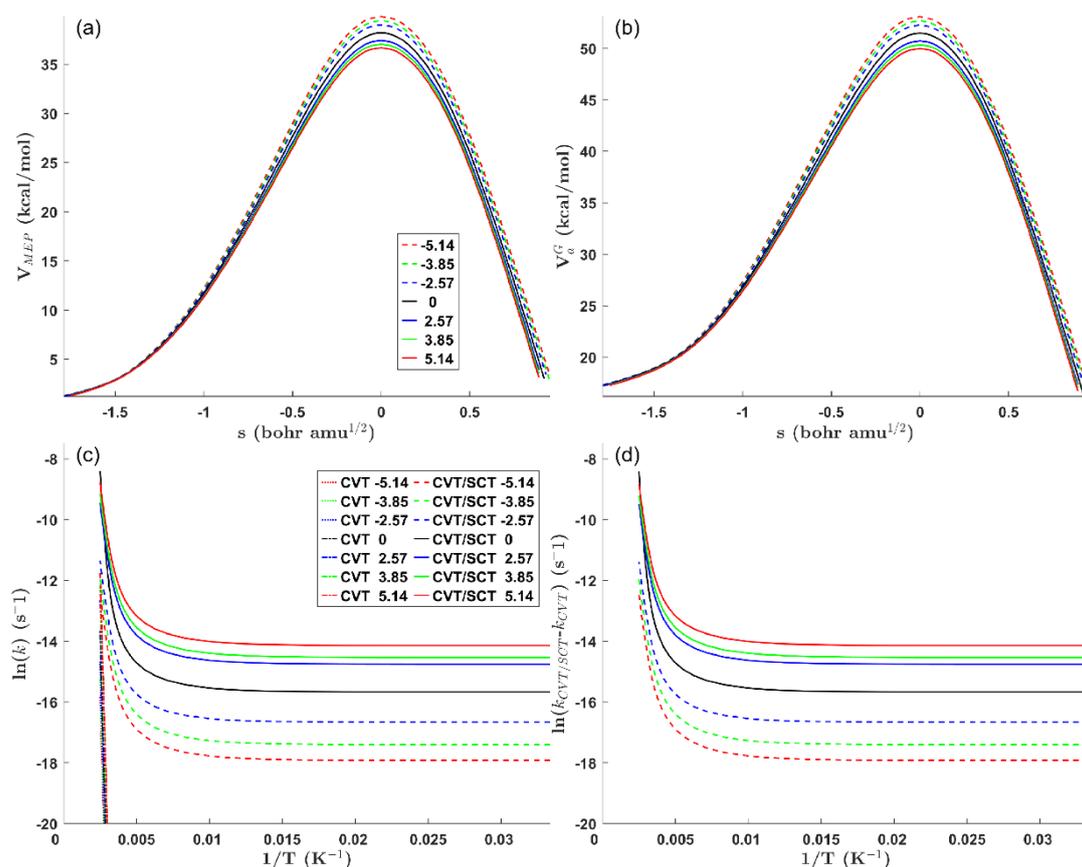
**Table S85.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) for the D-migration of HO-C-OD using the M06-2X method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	3.21E-22	1.38E-17	1.40E-13
35	3.22E-22	1.38E-17	1.40E-13
40	3.22E-22	1.38E-17	1.40E-13
50	3.22E-22	1.38E-17	1.40E-13
60	3.23E-22	1.38E-17	1.40E-13
70	3.24E-22	1.38E-17	1.40E-13
80	3.26E-22	1.39E-17	1.41E-13
90	3.31E-22	1.41E-17	1.42E-13
100	3.40E-22	1.44E-17	1.45E-13
120	3.82E-22	1.58E-17	1.56E-13
140	4.87E-22	1.92E-17	1.83E-13
160	7.49E-22	2.71E-17	2.41E-13
180	1.51E-21	4.72E-17	3.74E-13
200	4.36E-21	1.09E-16	7.37E-13
220	1.94E-20	3.63E-16	1.98E-12
240	1.33E-19	1.80E-15	7.62E-12
260	1.35E-18	1.28E-14	4.17E-11
273.15	7.48E-18	5.50E-14	1.51E-10
280	1.93E-17	1.23E-13	3.08E-10
290	8.19E-17	4.22E-13	9.15E-10
298.15	2.79E-16	1.19E-12	2.29E-09
300	3.70E-16	1.52E-12	2.83E-09
310	1.75E-15	5.69E-12	8.99E-09
320	8.48E-15	2.17E-11	2.88E-08
340	1.94E-13	3.12E-10	2.85E-07
360	3.85E-12	4.02E-09	2.55E-06
373.15	2.47E-11	1.98E-08	9.94E-06
380	6.26E-11	4.41E-08	1.97E-05
400	8.22E-10	4.06E-07	1.31E-04

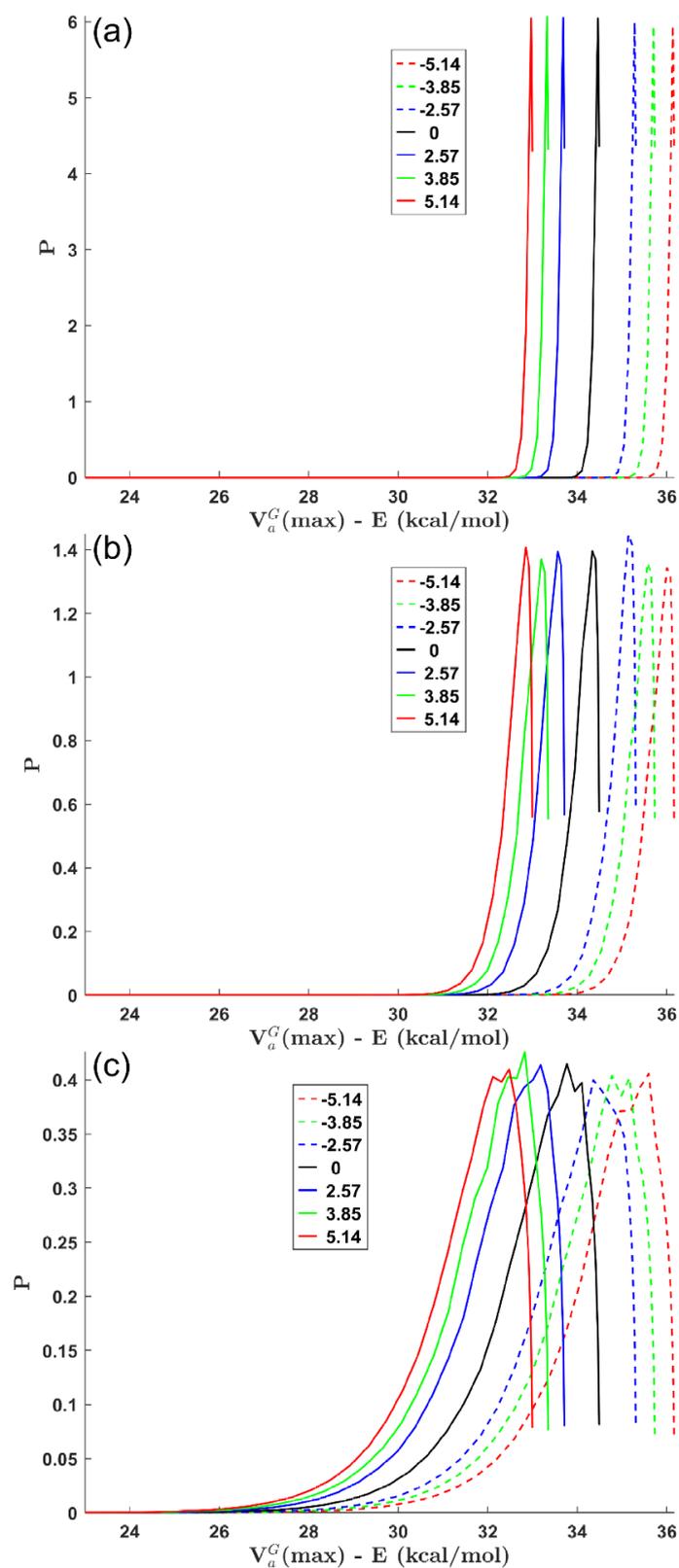
## NC-C-OH

**Table S86.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of NC-C-OH using M06-2X/6-31G(d,p) method under different EEF strengths (V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

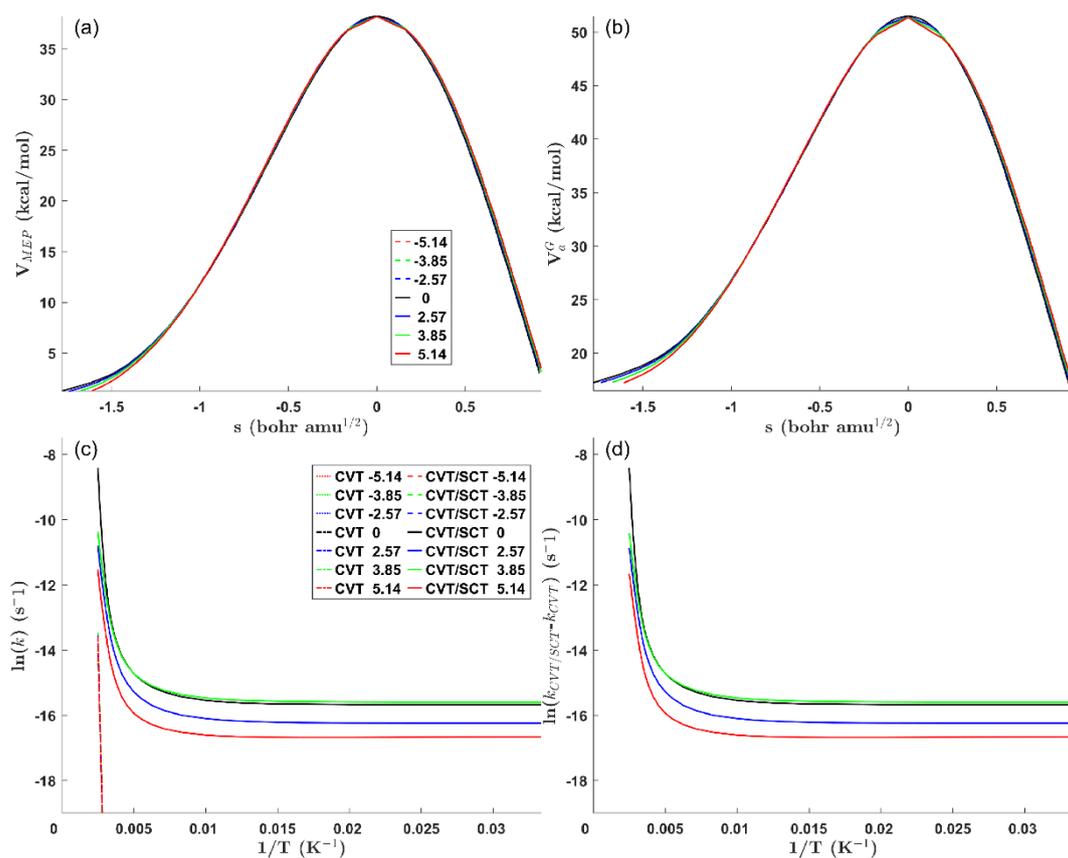
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	39.85	39.43	39.01	38.19	37.41	37.04	36.68
$\Delta V_a^G(\max)$	53.10	52.69	52.28	51.47	50.71	50.34	49.98
$\Omega$	2101	2100	2100	2099	2094	2092	2089
$T_c$	481	481	481	481	479	479	478
<b>Y-EEF Direction</b>							
$\Delta E$	38.18	38.19	38.19	38.19	38.19	38.19	38.18
$\Delta V_a^G(\max)$	51.35	51.40	51.43	51.47	51.43	51.40	51.35
$\Omega$	2094	2096	2097	2099	2097	2096	2094
$T_c$	480	480	480	481	480	480	480
<b>Z-EEF Direction</b>							
$\Delta E$	42.60	41.50	40.40	38.19	35.99	34.89	33.80
$\Delta V_a^G(\max)$	55.81	54.73	53.65	51.47	49.33	48.28	47.26
$\Omega$	2096	2097	2097	2099	2096	2094	2092
$T_c$	480	480	480	481	480	480	479



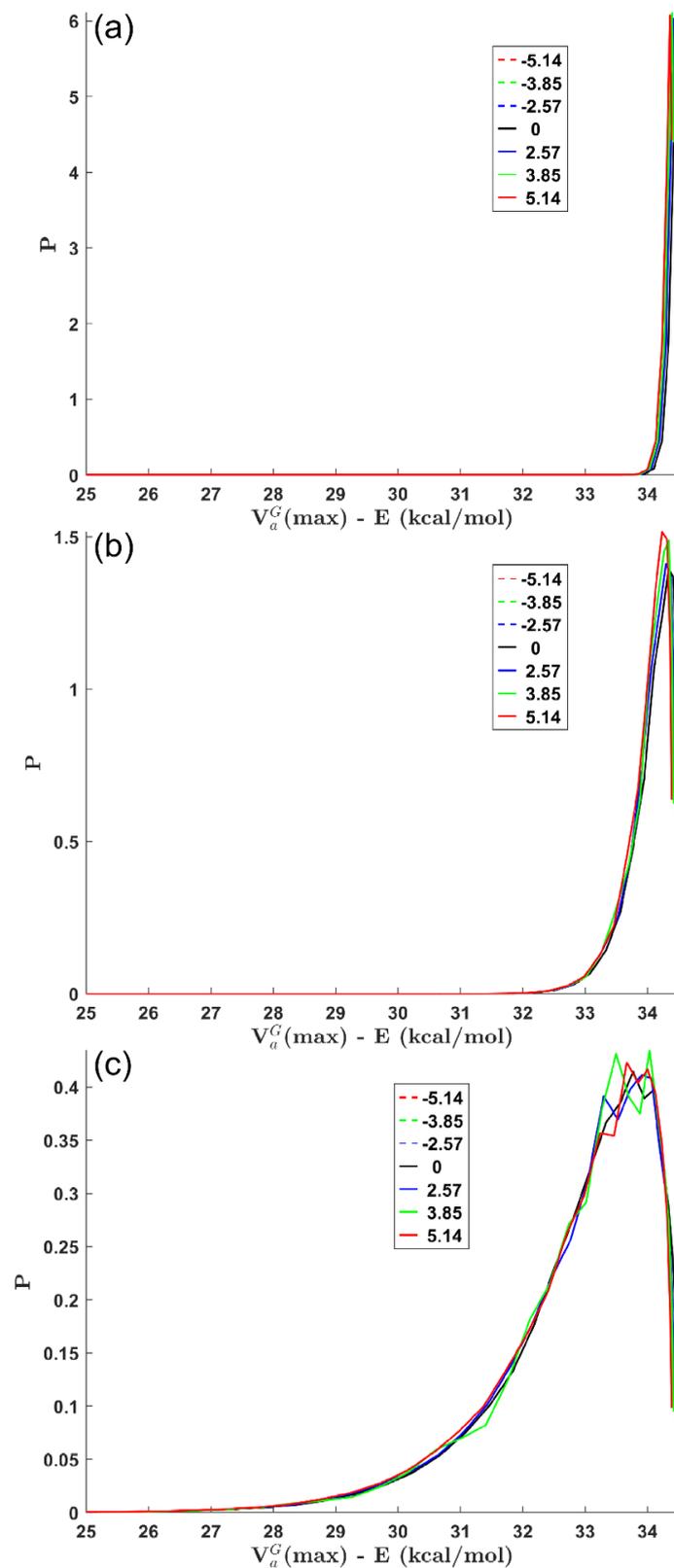
**Figure S52.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



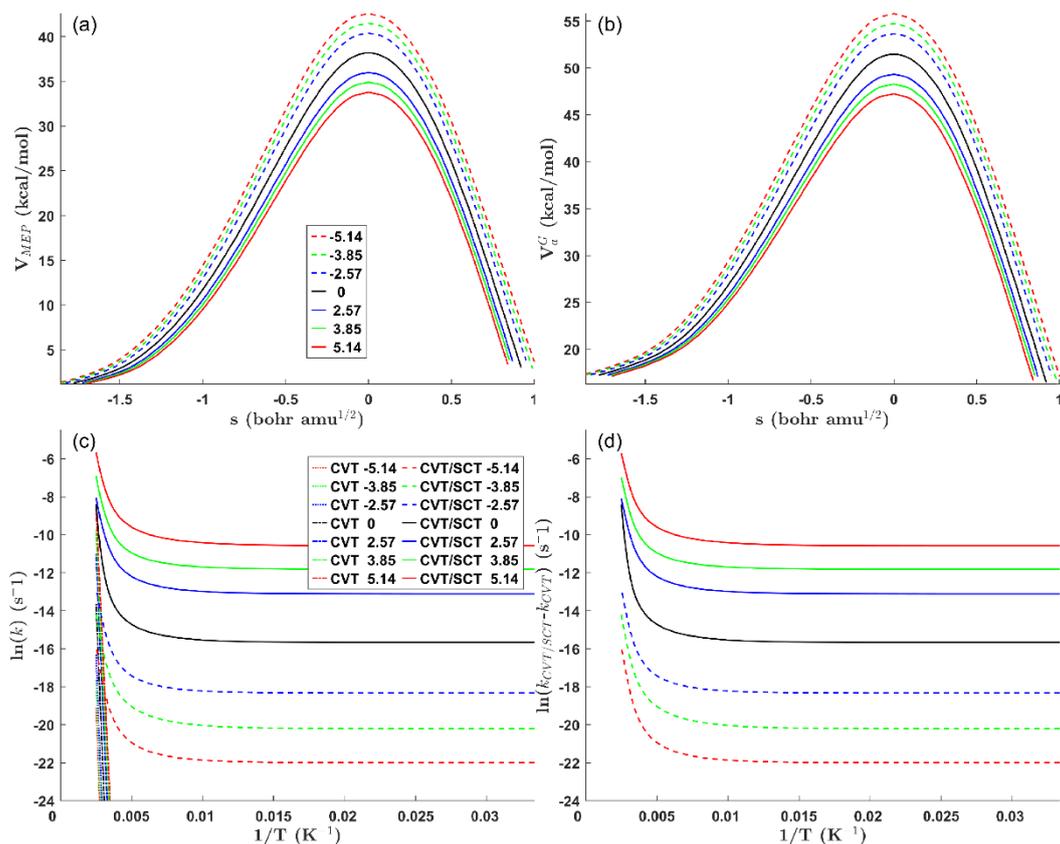
**Figure S53.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of NC-C-OH at (a) 30K, (b) 100K and (c) 200K, using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



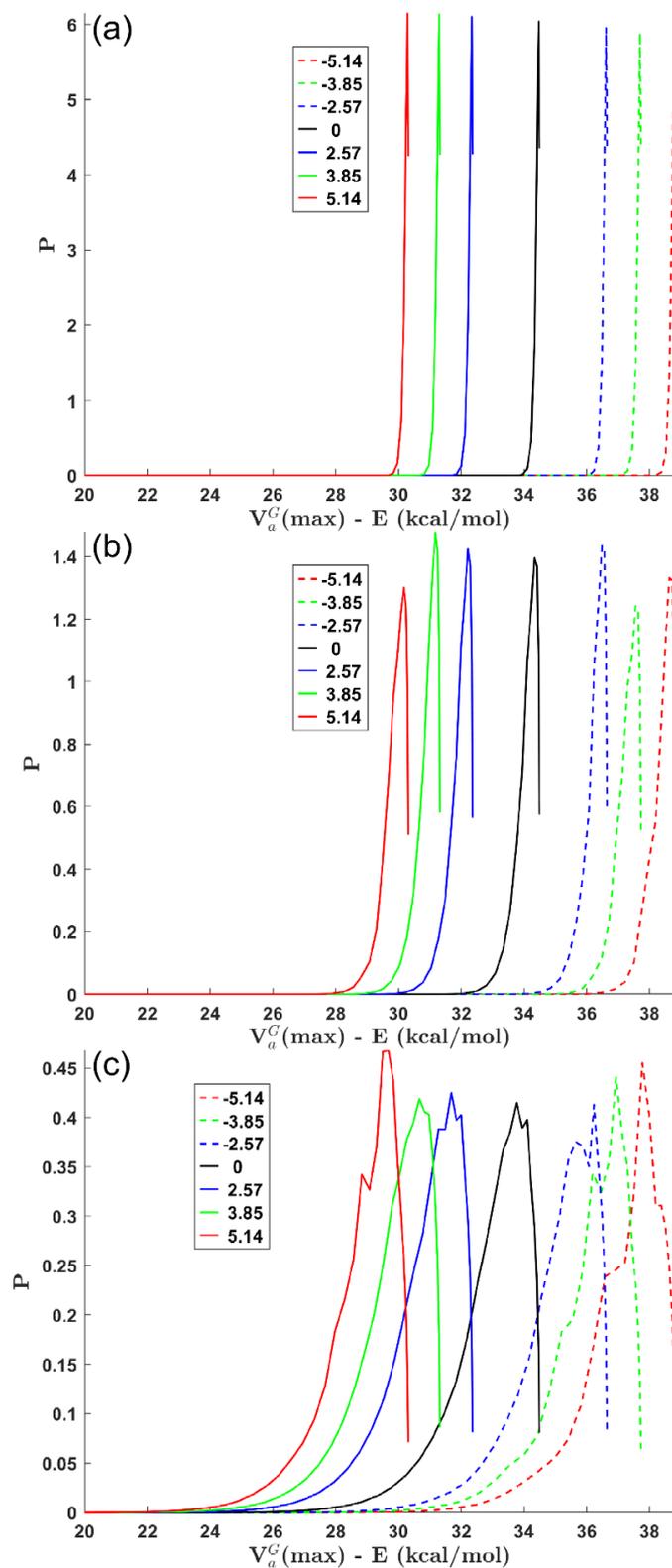
**Figure S54.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



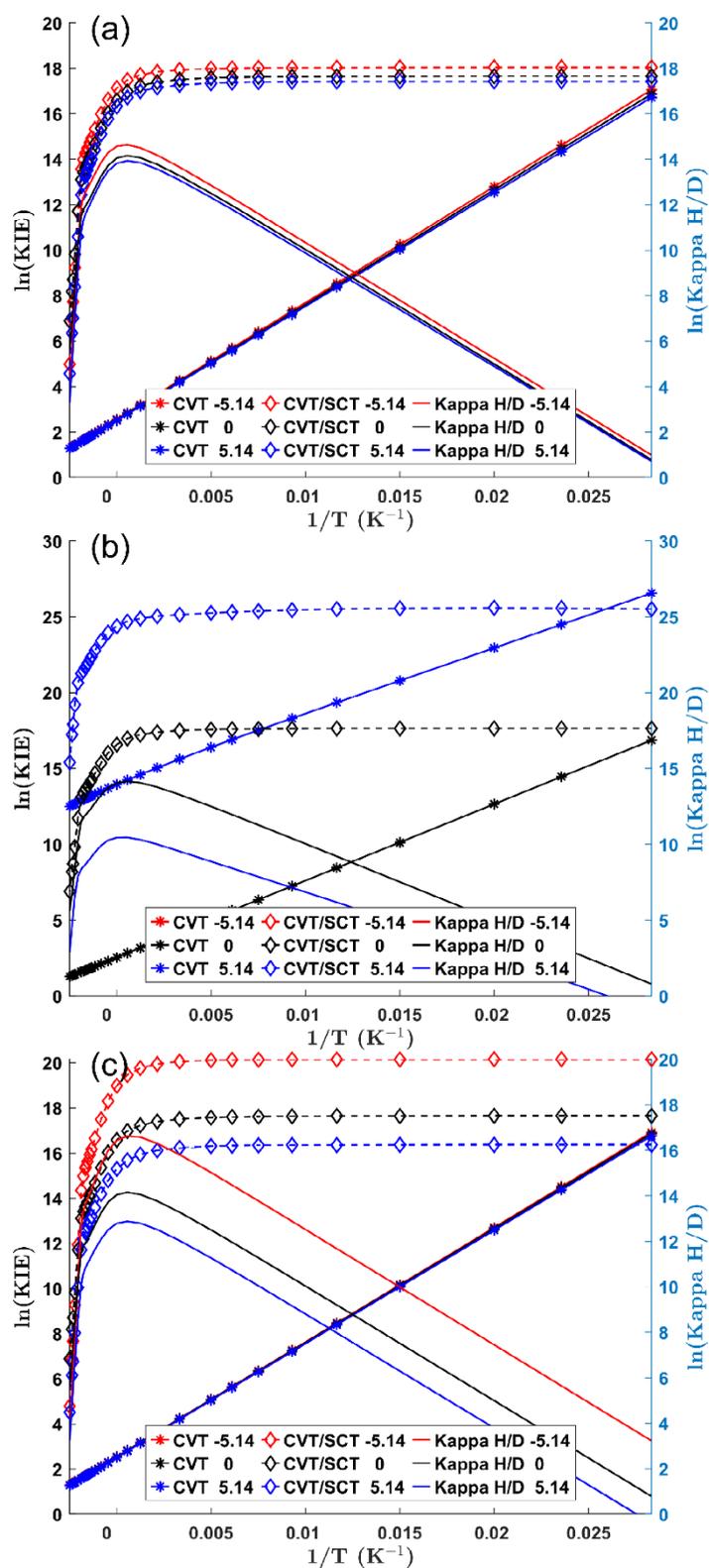
**Figure S55.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of NC-C-OH at (a) 30K, (b) 100K and (c) 200K using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S56.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S57.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of NC-C-OH at (a) 30K, (b) 100K and (c) 200K, using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S58.** Arrhenius plots of  $\ln(\text{H/D KIE})$  and  $\ln(\kappa(\text{H})/\kappa(\text{D}))$  versus  $1/T$  of NC-C-OH using M06-2X/6-31G(d,p) method along direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S87.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.52	0.0	2.52	3.85	5.14
30	1.75E-252	2.54E-249	3.17E-246	2.73E-240	1.25E-234	5.75E-232	2.08E-229
35	8.98E-215	4.60E-212	2.07E-209	2.51E-204	1.80E-199	3.44E-197	5.37E-195
40	1.75E-186	4.10E-184	8.60E-182	2.41E-177	4.27E-173	4.24E-171	3.51E-169
50	7.32E-147	5.76E-145	4.14E-143	1.48E-139	3.74E-136	1.48E-134	5.06E-133
60	1.97E-120	7.47E-119	2.63E-117	2.40E-114	1.64E-111	3.52E-110	6.68E-109
70	1.52E-101	3.44E-100	7.28E-99	2.49E-96	6.74E-94	9.31E-93	1.16E-91
80	2.27E-87	3.48E-86	5.03E-85	8.26E-83	1.11E-80	1.11E-79	1.01E-78
90	2.44E-76	2.76E-75	2.96E-74	2.75E-72	2.16E-70	1.66E-69	1.18E-68
100	1.65E-67	1.46E-66	1.24E-65	7.30E-64	3.71E-62	2.33E-61	1.36E-60
120	2.97E-54	1.83E-53	1.09E-52	3.24E-51	8.60E-50	3.98E-49	1.73E-48
140	8.97E-45	4.27E-44	1.97E-43	3.59E-42	6.01E-41	2.23E-40	7.88E-40
160	1.18E-37	4.62E-37	1.76E-36	2.23E-35	2.64E-34	8.32E-34	2.51E-33
180	4.11E-32	1.39E-31	4.57E-31	4.36E-30	3.94E-29	1.09E-28	2.92E-28
200	1.13E-27	3.39E-27	9.92E-27	7.55E-26	5.50E-25	1.38E-24	3.34E-24
220	4.91E-24	1.33E-23	3.55E-23	2.24E-22	1.37E-21	3.16E-21	7.06E-21
240	5.32E-21	1.33E-20	3.27E-20	1.77E-19	9.36E-19	2.02E-18	4.21E-18
260	1.98E-18	4.64E-18	1.06E-17	5.06E-17	2.36E-16	4.80E-16	9.47E-16
273.15	6.09E-17	1.37E-16	3.02E-16	1.33E-15	5.79E-15	1.14E-14	2.17E-14
280	3.19E-16	7.04E-16	1.53E-15	6.49E-15	2.73E-14	5.26E-14	9.89E-14
290	3.12E-15	6.71E-15	1.42E-14	5.73E-14	2.29E-13	4.33E-13	7.97E-13
298.15	1.79E-14	3.77E-14	7.81E-14	3.04E-13	1.17E-12	2.18E-12	3.94E-12
300	2.63E-14	5.50E-14	1.14E-13	4.38E-13	1.68E-12	3.10E-12	5.60E-12
310	1.93E-13	3.95E-13	7.96E-13	2.94E-12	1.08E-11	1.96E-11	3.47E-11
320	1.25E-12	2.51E-12	4.95E-12	1.76E-11	6.21E-11	1.10E-10	1.92E-10
340	3.79E-11	7.32E-11	1.39E-10	4.58E-10	1.51E-09	2.59E-09	4.37E-09
360	7.91E-10	1.47E-09	2.71E-09	8.34E-09	2.58E-08	4.31E-08	7.05E-08
373.15	4.89E-09	8.92E-09	1.60E-08	4.75E-08	1.42E-07	2.32E-07	3.73E-07
380	1.20E-08	2.17E-08	3.87E-08	1.12E-07	3.28E-07	5.34E-07	8.51E-07
400	1.39E-07	2.45E-07	4.24E-07	1.17E-06	3.25E-06	5.16E-06	8.03E-06

**Table S88.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OH using M06-2X /6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.66E-08	2.76E-08	5.80E-08	1.57E-07	3.90E-07	4.89E-07	7.22E-07
35	1.66E-08	2.76E-08	5.80E-08	1.57E-07	3.90E-07	4.89E-07	7.22E-07
40	1.66E-08	2.76E-08	5.81E-08	1.57E-07	3.90E-07	4.89E-07	7.22E-07
50	1.67E-08	2.77E-08	5.82E-08	1.57E-07	3.91E-07	4.91E-07	7.25E-07
60	1.68E-08	2.80E-08	5.87E-08	1.59E-07	3.94E-07	4.95E-07	7.31E-07
70	1.71E-08	2.85E-08	5.96E-08	1.61E-07	4.01E-07	5.04E-07	7.43E-07
80	1.76E-08	2.92E-08	6.09E-08	1.65E-07	4.11E-07	5.17E-07	7.62E-07
90	1.82E-08	3.02E-08	6.28E-08	1.71E-07	4.25E-07	5.35E-07	7.88E-07
100	1.91E-08	3.16E-08	6.54E-08	1.78E-07	4.43E-07	5.59E-07	8.23E-07
120	2.14E-08	3.54E-08	7.24E-08	1.99E-07	4.94E-07	6.25E-07	9.19E-07
140	2.48E-08	4.10E-08	8.25E-08	2.28E-07	5.67E-07	7.21E-07	1.06E-06
160	2.96E-08	4.87E-08	9.67E-08	2.69E-07	6.69E-07	8.55E-07	1.25E-06
180	3.62E-08	5.96E-08	1.17E-07	3.26E-07	8.11E-07	1.04E-06	1.52E-06
200	4.56E-08	7.51E-08	1.45E-07	4.05E-07	1.01E-06	1.30E-06	1.90E-06
220	5.94E-08	9.79E-08	1.86E-07	5.22E-07	1.31E-06	1.69E-06	2.46E-06
240	8.05E-08	1.33E-07	2.50E-07	7.01E-07	1.75E-06	2.28E-06	3.32E-06
260	1.15E-07	1.91E-07	3.53E-07	9.95E-07	2.48E-06	3.24E-06	4.71E-06
273.15	1.50E-07	2.49E-07	4.58E-07	1.30E-06	3.21E-06	4.20E-06	6.11E-06
280	1.74E-07	2.89E-07	5.29E-07	1.52E-06	3.70E-06	4.86E-06	7.06E-06
290	2.19E-07	3.64E-07	6.62E-07	1.95E-06	4.62E-06	6.08E-06	8.83E-06
298.15	2.66E-07	4.43E-07	8.03E-07	2.44E-06	5.59E-06	7.37E-06	1.07E-05
300	2.79E-07	4.64E-07	8.40E-07	2.57E-06	5.84E-06	7.71E-06	1.12E-05
310	3.59E-07	5.98E-07	1.08E-06	3.49E-06	7.47E-06	9.87E-06	1.43E-05
320	4.66E-07	7.78E-07	1.40E-06	4.90E-06	9.63E-06	1.28E-05	1.85E-05
340	7.98E-07	1.33E-06	2.38E-06	1.07E-05	1.63E-05	2.16E-05	3.13E-05
360	1.37E-06	2.29E-06	4.08E-06	2.64E-05	2.77E-05	3.69E-05	5.34E-05
373.15	1.95E-06	3.26E-06	5.80E-06	5.12E-05	3.92E-05	5.22E-05	7.56E-05
380	2.34E-06	3.91E-06	6.95E-06	7.35E-05	4.68E-05	6.25E-05	9.05E-05
400	3.97E-06	6.66E-06	1.18E-05	2.24E-04	7.93E-05	1.06E-04	1.54E-04

**Table S89.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.57E-239	9.30E-240	5.57E-240	2.73E-240	5.57E-240	9.30E-240	1.57E-239
35	1.13E-203	7.23E-204	4.66E-204	2.51E-204	4.66E-204	7.23E-204	1.13E-203
40	8.95E-177	6.10E-177	4.15E-177	2.41E-177	4.15E-177	6.10E-177	8.95E-177
50	4.23E-139	3.15E-139	2.31E-139	1.48E-139	2.31E-139	3.15E-139	4.23E-139
60	5.71E-114	4.53E-114	3.49E-114	2.40E-114	3.49E-114	4.53E-114	5.72E-114
70	5.23E-96	4.34E-96	3.47E-96	2.49E-96	3.47E-96	4.34E-96	5.23E-96
80	1.58E-82	1.36E-82	1.11E-82	8.26E-83	1.11E-82	1.36E-82	1.58E-82
90	4.87E-72	4.32E-72	3.61E-72	2.75E-72	3.61E-72	4.32E-72	4.87E-72
100	1.22E-63	1.10E-63	9.38E-64	7.30E-64	9.38E-64	1.10E-63	1.22E-63
120	4.93E-51	4.66E-51	4.04E-51	3.24E-51	4.04E-51	4.66E-51	4.93E-51
140	5.13E-42	4.99E-42	4.40E-42	3.59E-42	4.40E-42	4.99E-42	5.13E-42
160	3.03E-35	3.02E-35	2.69E-35	2.23E-35	2.69E-35	3.02E-35	3.03E-35
180	5.68E-30	5.79E-30	5.21E-30	4.36E-30	5.21E-30	5.79E-30	5.68E-30
200	9.53E-26	9.87E-26	8.94E-26	7.55E-26	8.94E-26	9.87E-26	9.53E-26
220	2.75E-22	2.90E-22	2.64E-22	2.24E-22	2.64E-22	2.90E-22	2.75E-22
240	2.13E-19	2.27E-19	2.08E-19	1.77E-19	2.08E-19	2.27E-19	2.13E-19
260	5.96E-17	6.43E-17	5.90E-17	5.06E-17	5.90E-17	6.43E-17	5.96E-17
273.15	1.55E-15	1.68E-15	1.55E-15	1.33E-15	1.55E-15	1.68E-15	1.55E-15
280	7.51E-15	8.18E-15	7.54E-15	6.49E-15	7.54E-15	8.18E-15	7.51E-15
290	6.58E-14	7.20E-14	6.64E-14	5.73E-14	6.64E-14	7.20E-14	6.58E-14
298.15	3.47E-13	3.81E-13	3.52E-13	3.04E-13	3.52E-13	3.81E-13	3.47E-13
300	4.99E-13	5.49E-13	5.07E-13	4.38E-13	5.07E-13	5.49E-13	4.99E-13
310	3.33E-12	3.68E-12	3.40E-12	2.94E-12	3.40E-12	3.68E-12	3.33E-12
320	1.97E-11	2.19E-11	2.03E-11	1.76E-11	2.03E-11	2.19E-11	1.97E-11
340	5.08E-10	5.68E-10	5.27E-10	4.58E-10	5.27E-10	5.68E-10	5.08E-10
360	9.16E-09	1.03E-08	9.58E-09	8.34E-09	9.58E-09	1.03E-08	9.16E-09
373.15	5.19E-08	5.86E-08	5.46E-08	4.75E-08	5.46E-08	5.86E-08	5.19E-08
380	1.22E-07	1.38E-07	1.29E-07	1.12E-07	1.29E-07	1.38E-07	1.22E-07
400	1.26E-06	1.44E-06	1.34E-06	1.17E-06	1.34E-06	1.44E-06	1.26E-06

**Table S90.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	5.83E-08	1.69E-07	8.87E-08	1.57E-07	8.87E-08	1.69E-07	5.83E-08
35	5.81E-08	1.69E-07	8.87E-08	1.57E-07	8.87E-08	1.69E-07	5.81E-08
40	5.78E-08	1.69E-07	8.88E-08	1.57E-07	8.88E-08	1.69E-07	5.78E-08
50	5.74E-08	1.70E-07	8.91E-08	1.57E-07	8.91E-08	1.70E-07	5.74E-08
60	5.73E-08	1.72E-07	9.00E-08	1.59E-07	9.00E-08	1.72E-07	5.74E-08
70	5.77E-08	1.75E-07	9.16E-08	1.61E-07	9.16E-08	1.75E-07	5.77E-08
80	5.85E-08	1.79E-07	9.41E-08	1.65E-07	9.41E-08	1.79E-07	5.85E-08
90	5.98E-08	1.85E-07	9.74E-08	1.71E-07	9.74E-08	1.85E-07	5.98E-08
100	6.16E-08	1.92E-07	1.02E-07	1.78E-07	1.02E-07	1.92E-07	6.16E-08
120	6.68E-08	2.12E-07	1.13E-07	1.99E-07	1.13E-07	2.12E-07	6.68E-08
140	7.43E-08	2.40E-07	1.30E-07	2.28E-07	1.30E-07	2.40E-07	7.43E-08
160	8.48E-08	2.79E-07	1.53E-07	2.69E-07	1.53E-07	2.79E-07	8.48E-08
180	9.94E-08	3.32E-07	1.86E-07	3.26E-07	1.86E-07	3.32E-07	9.94E-08
200	1.20E-07	4.06E-07	2.31E-07	4.05E-07	2.31E-07	4.06E-07	1.20E-07
220	1.51E-07	5.15E-07	2.98E-07	5.22E-07	2.98E-07	5.15E-07	1.51E-07
240	1.98E-07	6.81E-07	4.01E-07	7.01E-07	4.01E-07	6.81E-07	1.98E-07
260	2.76E-07	9.52E-07	5.70E-07	9.95E-07	5.70E-07	9.52E-07	2.76E-07
273.15	3.56E-07	1.23E-06	7.43E-07	1.30E-06	7.43E-07	1.23E-06	3.56E-07
280	4.11E-07	1.41E-06	8.62E-07	1.52E-06	8.62E-07	1.41E-06	4.11E-07
290	5.15E-07	1.77E-06	1.08E-06	1.95E-06	1.08E-06	1.77E-06	5.15E-07
298.15	6.25E-07	2.14E-06	1.32E-06	2.44E-06	1.32E-06	2.14E-06	6.25E-07
300	6.54E-07	2.23E-06	1.38E-06	2.57E-06	1.38E-06	2.23E-06	6.54E-07
310	8.40E-07	2.86E-06	1.78E-06	3.49E-06	1.78E-06	2.86E-06	8.40E-07
320	1.09E-06	3.70E-06	2.32E-06	4.90E-06	2.32E-06	3.70E-06	1.09E-06
340	1.87E-06	6.31E-06	3.98E-06	1.07E-05	3.98E-06	6.31E-06	1.87E-06
360	3.22E-06	1.08E-05	6.88E-06	2.64E-05	6.88E-06	1.08E-05	3.22E-06
373.15	4.61E-06	1.54E-05	9.83E-06	5.12E-05	9.83E-06	1.54E-05	4.61E-06
380	5.56E-06	1.85E-05	1.18E-05	7.35E-05	1.18E-05	1.85E-05	5.56E-06
400	9.92E-06	3.16E-05	2.05E-05	2.24E-04	2.05E-05	3.16E-05	9.92E-06

**Table S91.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	9.46E-272	7.55E-264	5.54E-256	2.73E-240	9.35E-225	3.49E-217	7.51E-210
35	2.73E-231	1.62E-224	8.94E-218	2.51E-204	5.23E-191	1.62E-184	3.12E-178
40	6.14E-201	5.19E-195	4.12E-189	2.41E-177	1.09E-165	5.21E-160	1.65E-154
50	1.98E-158	1.10E-153	5.75E-149	1.48E-139	3.15E-130	1.10E-125	2.77E-121
60	4.49E-130	4.02E-126	3.45E-122	2.40E-114	1.43E-106	8.74E-103	4.06E-99
70	8.27E-110	2.02E-106	4.75E-103	2.49E-96	1.16E-89	2.03E-86	2.83E-83
80	1.33E-94	1.23E-91	1.09E-88	8.26E-83	5.64E-77	3.90E-74	2.19E-71
90	9.11E-83	3.93E-80	1.65E-77	2.75E-72	4.23E-67	1.41E-64	3.93E-62
100	2.71E-73	6.38E-71	1.46E-68	7.30E-64	3.40E-59	6.35E-57	1.00E-54
120	4.53E-59	4.29E-57	3.97E-55	3.24E-51	2.51E-47	1.95E-45	1.32E-43
140	6.74E-49	3.32E-47	1.61E-45	3.59E-42	7.74E-39	3.22E-37	1.19E-35
160	2.93E-41	8.89E-40	2.64E-38	2.23E-35	1.84E-32	4.76E-31	1.11E-29
180	2.61E-35	5.41E-34	1.10E-32	4.36E-30	1.69E-27	3.04E-26	4.98E-25
200	1.52E-30	2.33E-29	3.50E-28	7.55E-26	1.61E-23	2.15E-22	2.65E-21
220	1.22E-26	1.46E-25	1.71E-24	2.24E-22	2.92E-20	3.07E-19	2.98E-18
240	2.22E-23	2.14E-22	2.04E-21	1.77E-19	1.53E-17	1.32E-16	1.05E-15
260	1.28E-20	1.04E-19	8.29E-19	5.06E-17	3.09E-15	2.24E-14	1.51E-13
273.15	5.05E-19	3.70E-18	2.67E-17	1.33E-15	6.65E-14	4.36E-13	2.68E-12
280	2.99E-18	2.09E-17	1.44E-16	6.49E-15	2.94E-13	1.84E-12	1.08E-11
290	3.46E-17	2.26E-16	1.45E-15	5.73E-14	2.27E-12	1.33E-11	7.30E-11
298.15	2.26E-16	1.40E-15	8.53E-15	3.04E-13	1.09E-11	6.04E-11	3.16E-10
300	3.40E-16	2.08E-15	1.26E-14	4.38E-13	1.53E-11	8.43E-11	4.36E-10
310	2.89E-15	1.67E-14	9.51E-14	2.94E-12	9.14E-11	4.75E-10	2.32E-09
320	2.16E-14	1.18E-13	6.34E-13	1.76E-11	4.89E-10	2.41E-09	1.12E-08
340	8.41E-13	4.15E-12	2.02E-11	4.58E-10	1.04E-08	4.65E-08	1.96E-07
360	2.20E-11	9.90E-11	4.41E-10	8.34E-09	1.59E-07	6.50E-07	2.51E-06
373.15	1.55E-10	6.63E-10	2.80E-09	4.75E-08	8.14E-07	3.16E-06	1.16E-05
380	4.08E-10	1.70E-09	6.97E-09	1.12E-07	1.82E-06	6.89E-06	2.47E-05
400	5.67E-09	2.19E-08	8.38E-08	1.17E-06	1.64E-05	5.79E-05	1.93E-04

**Table S92.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OH using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.80E-10	1.69E-09	1.09E-08	1.57E-07	2.01E-06	7.38E-06	2.54E-05
35	2.80E-10	1.69E-09	1.09E-08	1.57E-07	2.01E-06	7.39E-06	2.54E-05
40	2.80E-10	1.69E-09	1.09E-08	1.57E-07	2.01E-06	7.39E-06	2.54E-05
50	2.81E-10	1.70E-09	1.09E-08	1.57E-07	2.02E-06	7.42E-06	2.55E-05
60	2.83E-10	1.72E-09	1.10E-08	1.59E-07	2.04E-06	7.48E-06	2.58E-05
70	2.88E-10	1.75E-09	1.11E-08	1.61E-07	2.07E-06	7.60E-06	2.64E-05
80	2.95E-10	1.80E-09	1.14E-08	1.65E-07	2.12E-06	7.77E-06	2.72E-05
90	3.06E-10	1.88E-09	1.17E-08	1.71E-07	2.19E-06	8.01E-06	2.83E-05
100	3.20E-10	1.98E-09	1.22E-08	1.78E-07	2.29E-06	8.32E-06	2.97E-05
120	3.60E-10	2.28E-09	1.35E-08	1.99E-07	2.54E-06	9.17E-06	3.34E-05
140	4.20E-10	2.71E-09	1.53E-08	2.28E-07	2.90E-06	1.04E-05	3.86E-05
160	5.05E-10	3.31E-09	1.80E-08	2.69E-07	3.40E-06	1.20E-05	4.56E-05
180	6.28E-10	4.16E-09	2.18E-08	3.26E-07	4.09E-06	1.43E-05	5.49E-05
200	8.06E-10	5.37E-09	2.71E-08	4.05E-07	5.04E-06	1.74E-05	6.77E-05
220	1.08E-09	7.15E-09	3.51E-08	5.22E-07	6.43E-06	2.20E-05	8.57E-05
240	1.52E-09	9.93E-09	4.76E-08	7.01E-07	8.51E-06	2.87E-05	1.12E-04
260	2.27E-09	1.46E-08	6.82E-08	9.95E-07	1.18E-05	3.94E-05	1.54E-04
273.15	3.08E-09	1.94E-08	8.94E-08	1.30E-06	1.51E-05	4.99E-05	1.94E-04
280	3.65E-09	2.28E-08	1.04E-07	1.52E-06	1.73E-05	5.69E-05	2.20E-04
290	4.74E-09	2.92E-08	1.32E-07	1.95E-06	2.13E-05	6.98E-05	2.69E-04
298.15	5.94E-09	3.61E-08	1.61E-07	2.44E-06	2.55E-05	8.32E-05	3.19E-04
300	6.26E-09	3.79E-08	1.69E-07	2.57E-06	2.66E-05	8.66E-05	3.32E-04
310	8.37E-09	4.99E-08	2.20E-07	3.49E-06	3.36E-05	1.09E-04	4.13E-04
320	1.13E-08	6.65E-08	2.89E-07	4.90E-06	4.27E-05	1.37E-04	5.18E-04
340	2.09E-08	1.20E-07	5.08E-07	1.07E-05	7.03E-05	2.23E-04	8.30E-04
360	3.88E-08	2.17E-07	8.98E-07	2.64E-05	1.17E-04	3.66E-04	1.34E-03
373.15	5.78E-08	3.19E-07	1.30E-06	5.12E-05	1.62E-04	5.05E-04	1.83E-03
380	7.10E-08	3.89E-07	1.57E-06	7.35E-05	1.93E-04	5.98E-04	2.16E-03
400	1.30E-07	6.92E-07	2.74E-06	2.24E-04	3.21E-04	9.88E-04	3.51E-03

**Table S93.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	6.90E-260	1.30E-247	1.15E-236
35	4.02E-221	1.32E-210	3.22E-201
40	4.85E-192	7.70E-183	1.26E-174
50	2.61E-151	5.92E-144	2.21E-137
60	3.84E-124	5.15E-118	1.55E-112
70	1.00E-104	1.78E-99	8.88E-95
80	3.73E-90	1.46E-85	1.89E-81
90	8.15E-79	9.80E-75	4.45E-71
100	9.73E-70	4.56E-66	8.94E-63
120	4.12E-56	4.71E-53	2.63E-50
140	2.29E-46	9.57E-44	2.18E-41
160	4.76E-39	9.36E-37	1.09E-34
180	2.38E-33	2.60E-31	1.79E-29
200	8.73E-29	5.99E-27	2.71E-25
220	4.79E-25	2.24E-23	7.21E-22
240	6.31E-22	2.15E-20	5.20E-19
260	2.78E-19	7.21E-18	1.37E-16
273.15	9.37E-18	2.08E-16	3.45E-15
280	5.14E-17	1.06E-15	1.64E-14
290	5.36E-16	9.97E-15	1.41E-13
298.15	3.22E-15	5.54E-14	7.28E-13
300	4.78E-15	8.07E-14	1.04E-12
310	3.70E-14	5.72E-13	6.82E-12
320	2.53E-13	3.59E-12	3.97E-11
340	8.41E-12	1.02E-10	9.86E-10
360	1.90E-10	2.02E-09	1.72E-08
373.15	1.23E-09	1.21E-08	9.55E-08
380	3.11E-09	2.92E-08	2.23E-07
400	3.85E-08	3.23E-07	2.23E-06

**Table S94.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	2.43E-16	3.40E-15	1.95E-14
35	2.43E-16	3.40E-15	1.95E-14
40	2.43E-16	3.40E-15	1.95E-14
50	2.45E-16	3.42E-15	1.97E-14
60	2.48E-16	3.46E-15	2.00E-14
70	2.54E-16	3.55E-15	2.05E-14
80	2.64E-16	3.69E-15	2.14E-14
90	2.77E-16	3.89E-15	2.26E-14
100	2.96E-16	4.16E-15	2.43E-14
120	3.50E-16	4.97E-15	2.92E-14
140	4.42E-16	6.36E-15	3.76E-14
160	6.03E-16	8.85E-15	5.26E-14
180	9.22E-16	1.38E-14	8.29E-14
200	1.66E-15	2.55E-14	1.54E-13
220	3.60E-15	5.71E-14	3.47E-13
240	9.20E-15	1.50E-13	9.17E-13
260	2.53E-14	4.22E-13	2.59E-12
273.15	4.92E-14	8.30E-13	5.12E-12
280	6.91E-14	1.17E-12	7.25E-12
290	1.12E-13	1.92E-12	1.19E-11
298.15	1.66E-13	2.86E-12	1.80E-11
300	1.82E-13	3.13E-12	1.97E-11
310	3.05E-13	5.24E-12	3.47E-11
320	6.00E-13	9.93E-12	7.36E-11
340	6.68E-12	8.70E-11	7.87E-10
360	1.33E-10	1.43E-09	1.22E-08
373.15	8.57E-10	8.46E-09	6.75E-08
380	2.16E-09	2.05E-08	1.57E-07
400	2.70E-08	2.28E-07	1.59E-06

**Table S95.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	4.53E-251	1.30E-247	4.53E-251
35	2.59E-214	1.32E-210	2.59E-214
40	9.64E-187	7.70E-183	9.64E-187
50	3.94E-148	5.92E-144	3.94E-148
60	2.25E-122	5.15E-118	2.25E-122
70	5.82E-104	1.78E-99	5.82E-104
80	3.86E-90	1.46E-85	3.86E-90
90	2.22E-79	9.80E-75	2.22E-79
100	9.21E-71	4.56E-66	9.21E-71
120	8.11E-58	4.71E-53	8.11E-58
140	1.50E-48	9.57E-44	1.50E-48
160	1.38E-41	9.36E-37	1.38E-41
180	3.70E-36	2.60E-31	3.70E-36
200	8.32E-32	5.99E-27	8.32E-32
220	3.08E-28	2.24E-23	3.08E-28
240	2.94E-25	2.15E-20	2.94E-25
260	9.86E-23	7.21E-18	9.86E-23
273.15	2.86E-21	2.08E-16	2.86E-21
280	1.46E-20	1.06E-15	1.46E-20
290	1.37E-19	9.97E-15	1.37E-19
298.15	7.65E-19	5.54E-14	7.65E-19
300	1.11E-18	8.07E-14	1.11E-18
310	7.93E-18	5.72E-13	7.93E-18
320	4.99E-17	3.59E-12	4.99E-17
340	1.44E-15	1.02E-10	1.44E-15
360	2.87E-14	2.02E-09	2.87E-14
373.15	1.73E-13	1.21E-08	1.73E-13
380	4.19E-13	2.92E-08	4.19E-13
400	4.70E-12	3.23E-07	4.70E-12

**Table S96.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	4.82E-19	3.40E-15	4.82E-19
35	4.54E-19	3.40E-15	4.54E-19
40	4.44E-19	3.40E-15	4.44E-19
50	4.50E-19	3.42E-15	4.50E-19
60	4.74E-19	3.46E-15	4.74E-19
70	5.10E-19	3.55E-15	5.10E-19
80	5.53E-19	3.69E-15	5.53E-19
90	6.03E-19	3.89E-15	6.03E-19
100	6.60E-19	4.16E-15	6.60E-19
120	7.97E-19	4.97E-15	7.97E-19
140	9.89E-19	6.36E-15	9.89E-19
160	1.30E-18	8.85E-15	1.30E-18
180	1.87E-18	1.38E-14	1.87E-18
200	3.06E-18	2.55E-14	3.06E-18
220	5.89E-18	5.71E-14	5.89E-18
240	1.35E-17	1.50E-13	1.35E-17
260	3.53E-17	4.22E-13	3.53E-17
273.15	6.80E-17	8.30E-13	6.80E-17
280	9.56E-17	1.17E-12	9.56E-17
290	1.56E-16	1.92E-12	1.56E-16
298.15	2.31E-16	2.86E-12	2.31E-16
300	2.52E-16	3.13E-12	2.52E-16
310	4.03E-16	5.24E-12	4.03E-16
320	6.43E-16	9.93E-12	6.43E-16
340	2.00E-15	8.70E-11	2.00E-15
360	1.47E-14	1.43E-09	1.47E-14
373.15	7.64E-14	8.46E-09	7.64E-14
380	1.81E-13	2.05E-08	1.81E-13
400	2.04E-12	2.28E-07	2.04E-12

**Table S97.** The non-tunneling rate constants ( $k_{CVT}$  in  $s^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	4.22E-279	1.30E-247	3.95E-217
35	1.36E-237	1.32E-210	1.79E-184
40	1.87E-206	7.70E-183	5.67E-160
50	7.63E-163	5.92E-144	1.17E-125
60	9.37E-134	5.15E-118	9.16E-103
70	5.77E-113	1.78E-99	2.11E-86
80	2.30E-97	1.46E-85	4.01E-74
90	3.18E-85	9.80E-75	1.44E-64
100	1.67E-75	4.56E-66	6.45E-57
120	6.50E-61	4.71E-53	1.97E-45
140	1.77E-50	9.57E-44	3.23E-37
160	1.22E-42	9.36E-37	4.76E-31
180	1.54E-36	2.60E-31	3.03E-26
200	1.19E-31	5.99E-27	2.14E-22
220	1.21E-27	2.24E-23	3.03E-19
240	2.65E-24	2.15E-20	1.29E-16
260	1.80E-21	7.21E-18	2.19E-14
273.15	7.80E-20	2.08E-16	4.26E-13
280	4.84E-19	1.06E-15	1.79E-12
290	5.95E-18	9.97E-15	1.29E-11
298.15	4.07E-17	5.54E-14	5.86E-11
300	6.20E-17	8.07E-14	8.17E-11
310	5.56E-16	5.72E-13	4.59E-10
320	4.35E-15	3.59E-12	2.32E-09
340	1.86E-13	1.02E-10	4.46E-08
360	5.25E-12	2.02E-09	6.18E-07
373.15	3.89E-11	1.21E-08	2.99E-06
380	1.05E-10	2.92E-08	6.52E-06
400	1.55E-09	3.23E-07	5.44E-05

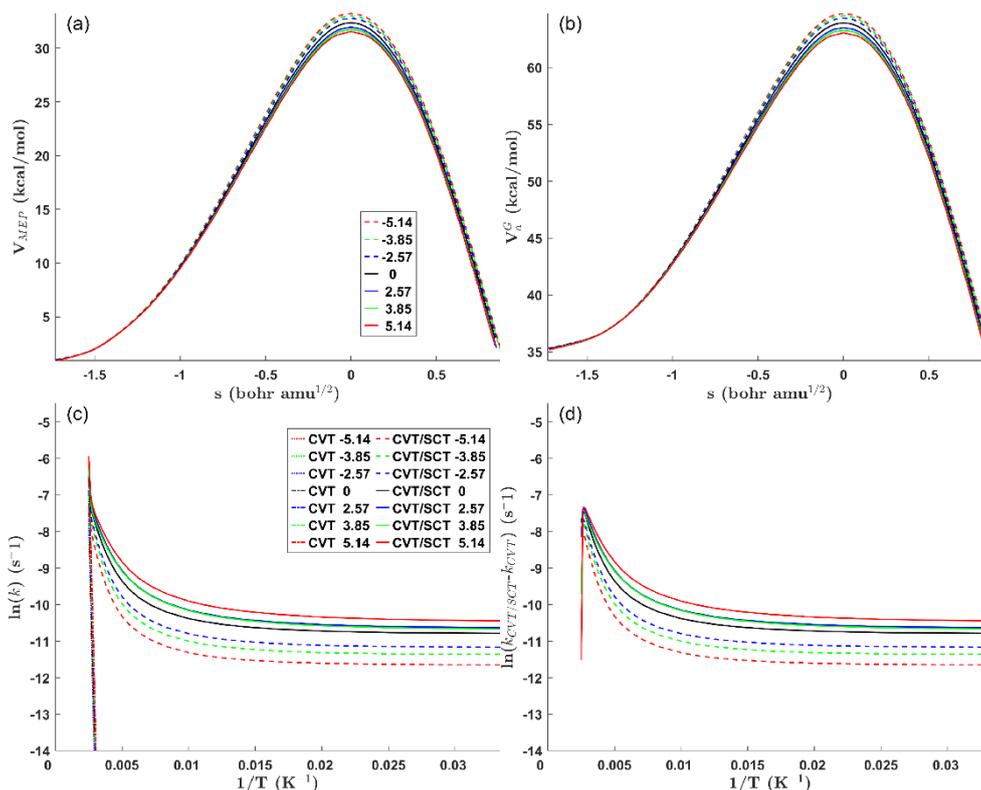
**Table S98.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of NC-C-OD using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	4.96E-19	3.40E-15	1.97E-12
35	4.96E-19	3.40E-15	1.97E-12
40	4.96E-19	3.40E-15	1.97E-12
50	4.98E-19	3.42E-15	1.99E-12
60	5.03E-19	3.46E-15	2.02E-12
70	5.13E-19	3.55E-15	2.07E-12
80	5.29E-19	3.69E-15	2.16E-12
90	5.54E-19	3.89E-15	2.28E-12
100	5.89E-19	4.16E-15	2.45E-12
120	7.03E-19	4.97E-15	2.97E-12
140	9.13E-19	6.36E-15	3.85E-12
160	1.32E-18	8.85E-15	5.44E-12
180	2.22E-18	1.38E-14	8.53E-12
200	4.58E-18	2.55E-14	1.53E-11
220	1.21E-17	5.71E-14	3.22E-11
240	3.87E-17	1.50E-13	7.69E-11
260	1.33E-16	4.22E-13	1.95E-10
273.15	2.94E-16	8.30E-13	3.61E-10
280	4.39E-16	1.17E-12	4.94E-10
290	7.78E-16	1.92E-12	7.80E-10
298.15	1.24E-15	2.86E-12	1.14E-09
300	1.37E-15	3.13E-12	1.24E-09
310	2.61E-15	5.24E-12	2.11E-09
320	6.60E-15	9.93E-12	4.25E-09
340	1.36E-13	8.70E-11	3.61E-08
360	3.63E-12	1.43E-09	4.38E-07
373.15	2.70E-11	8.46E-09	2.10E-06
380	7.28E-11	2.05E-08	4.57E-06
400	1.09E-09	2.28E-07	3.84E-05

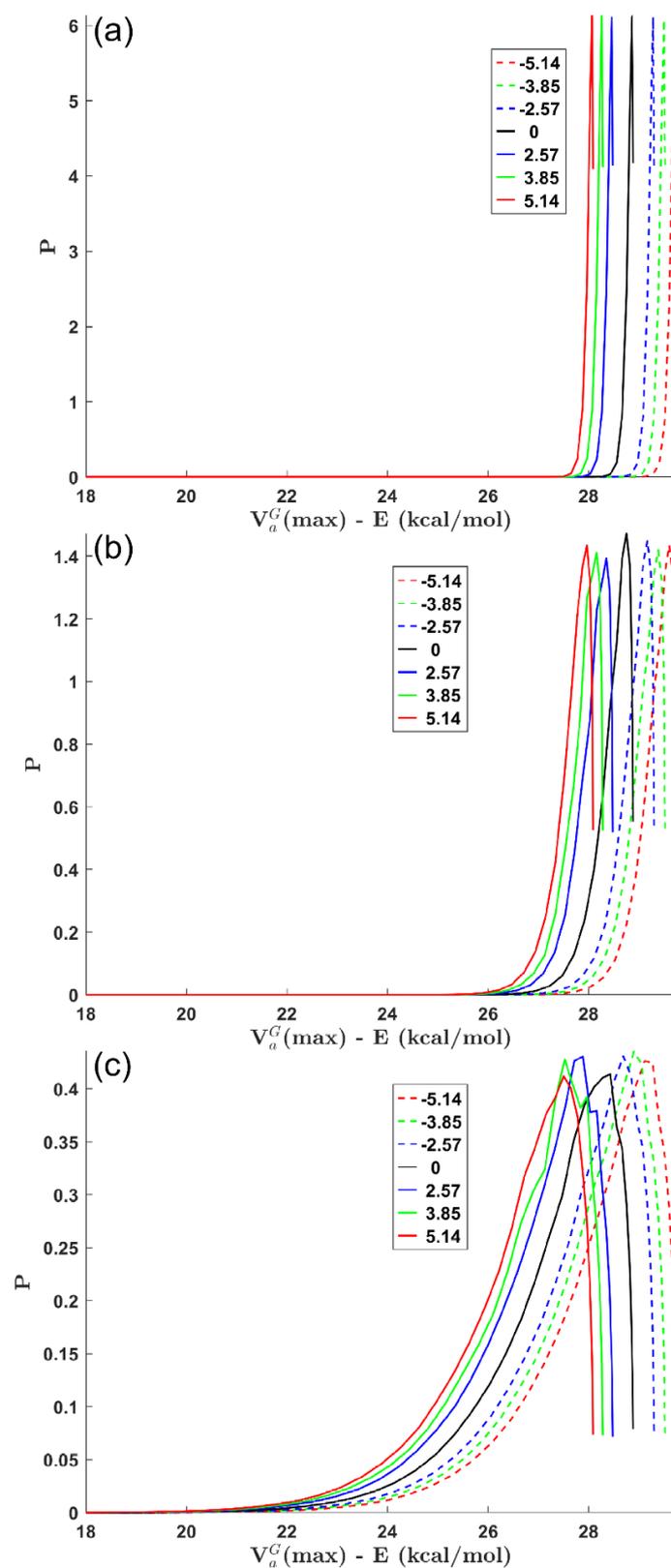
## H<sub>3</sub>C-C-OH

**Table S99.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of H<sub>3</sub>C-C-OH using M06-2X/6-31G(d,p) method under different EEF strengths (V/nm). The  $\Omega$  (in cm<sup>-1</sup>) is the magnitude of the imaginary frequency for the transition state, and T<sub>c</sub> is the crossover temperature (in K).

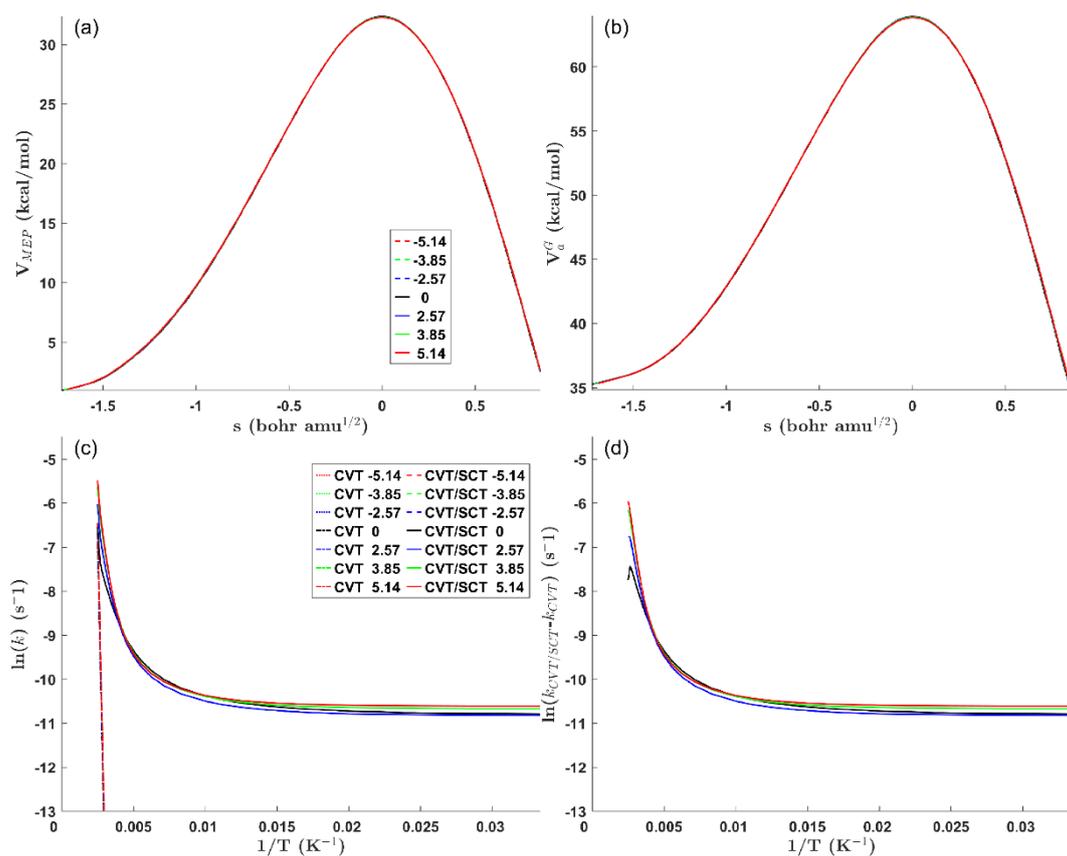
EEF (V/nm)	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
<b>X-EEF Direction</b>							
$\Delta E$	33.24	33.01	32.79	32.36	31.95	31.75	31.55
$\Delta V_a^G(\max)$	64.76	64.55	64.34	63.92	63.49	63.27	63.05
$\Omega$	2043	2041	2038	2031	2024	2020	2016
T <sub>c</sub>	468	467	467	465	464	463	462
<b>Y-EEF Direction</b>							
$\Delta E$	32.30	32.34	32.36	32.36	32.36	32.34	32.30
$\Delta V_a^G(\max)$	63.85	63.90	63.93	63.92	63.93	63.90	63.85
$\Omega$	2026	2028	2030	2031	2030	2028	2026
T <sub>c</sub>	464	464	465	465	465	464	464
<b>Z-EEF Direction</b>							
$\Delta E$	37.70	36.34	35.00	32.36	29.79	28.52	27.27
$\Delta V_a^G(\max)$	69.23	67.88	66.55	63.92	61.34	60.06	58.80
$\Omega$	2038	2039	2038	2031	2018	2010	2001
T <sub>c</sub>	467	467	467	465	462	460	458



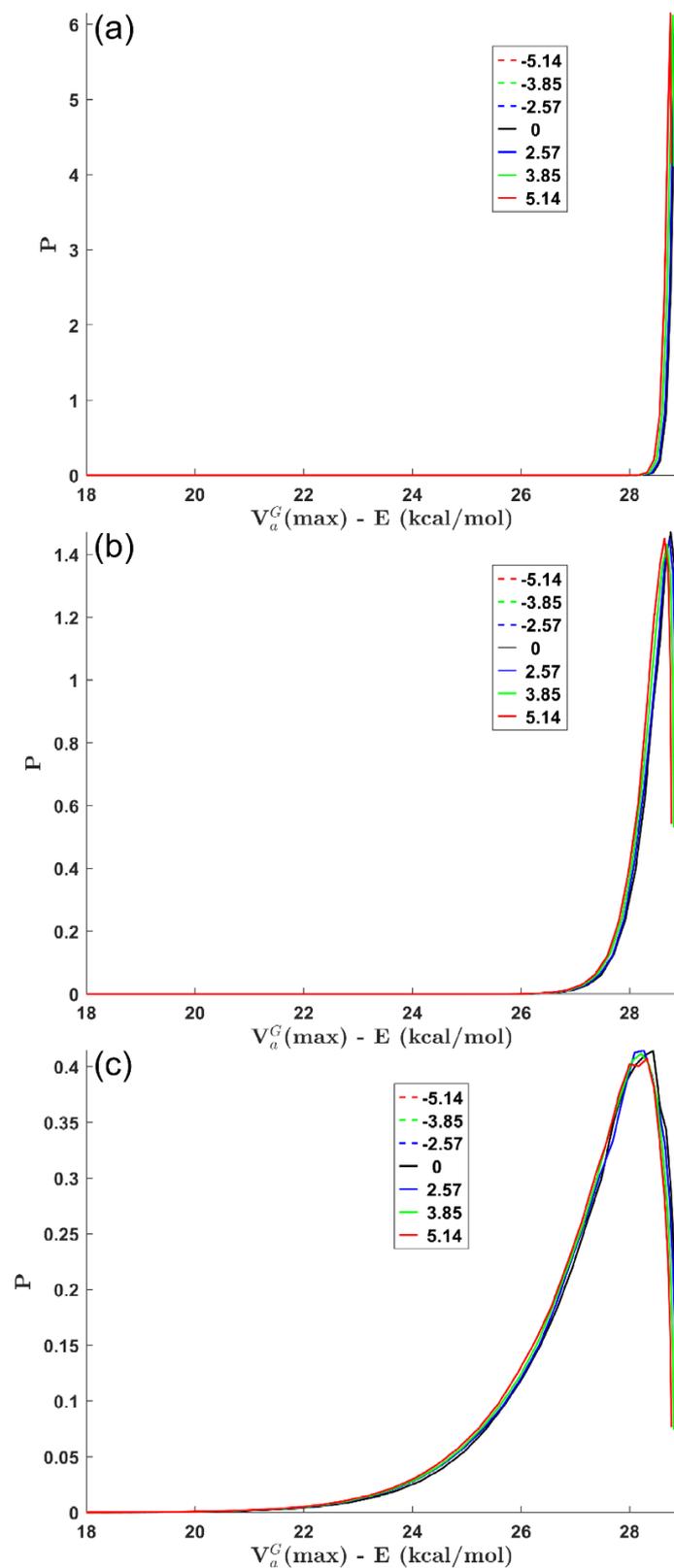
**Figure S59.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of H<sub>3</sub>C-C-OH using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



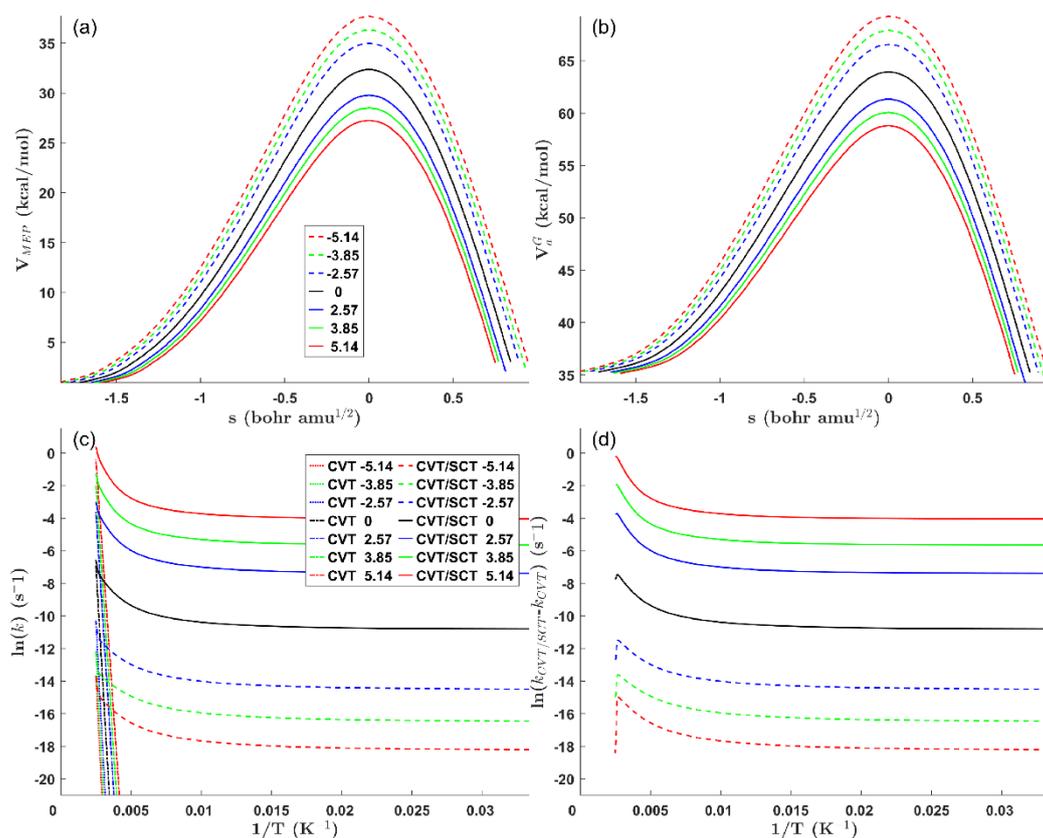
**Figure S60.** Tunneling contributions/probability (P) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of  $\text{H}_3\text{C-C-OH}$  at (a) 30K, (b) 100K and (c) 200K, using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



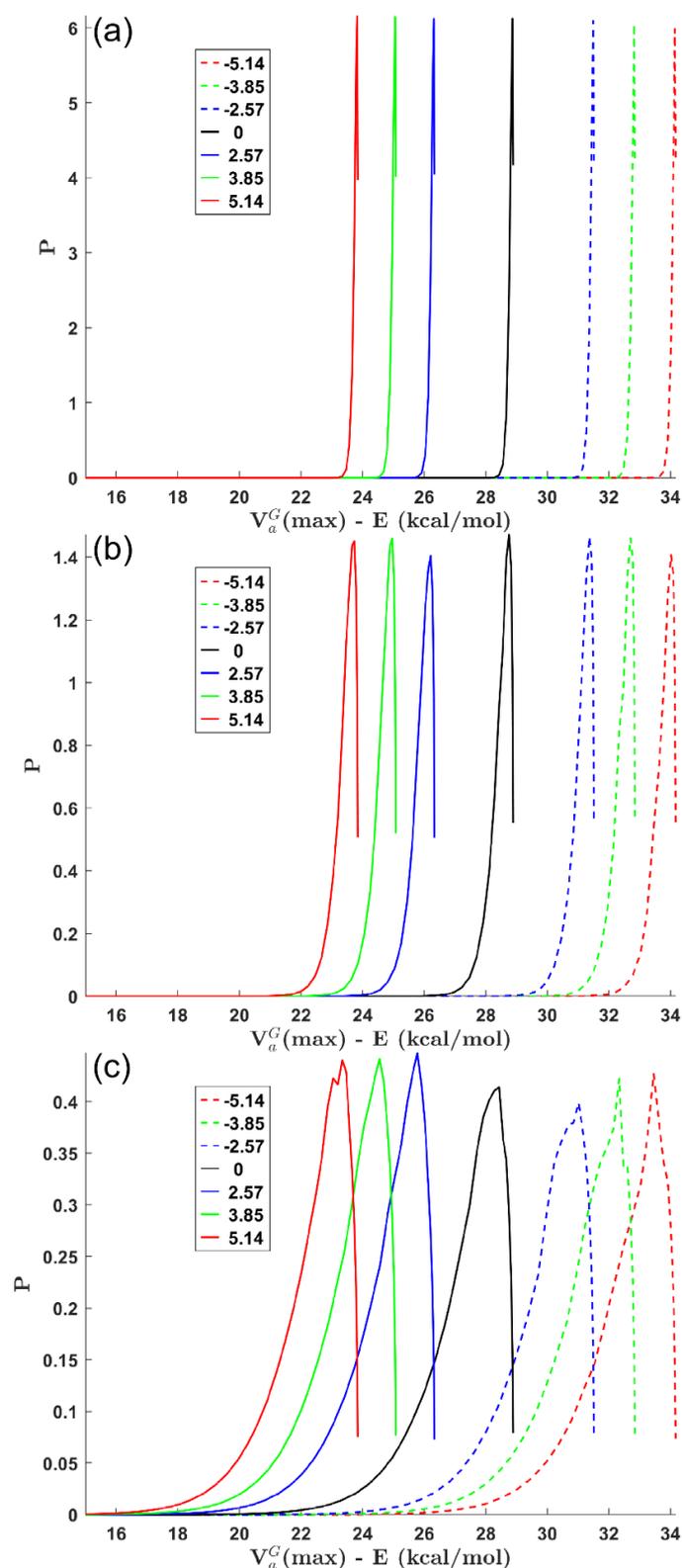
**Figure S61.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of H<sub>3</sub>C-C-OH using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



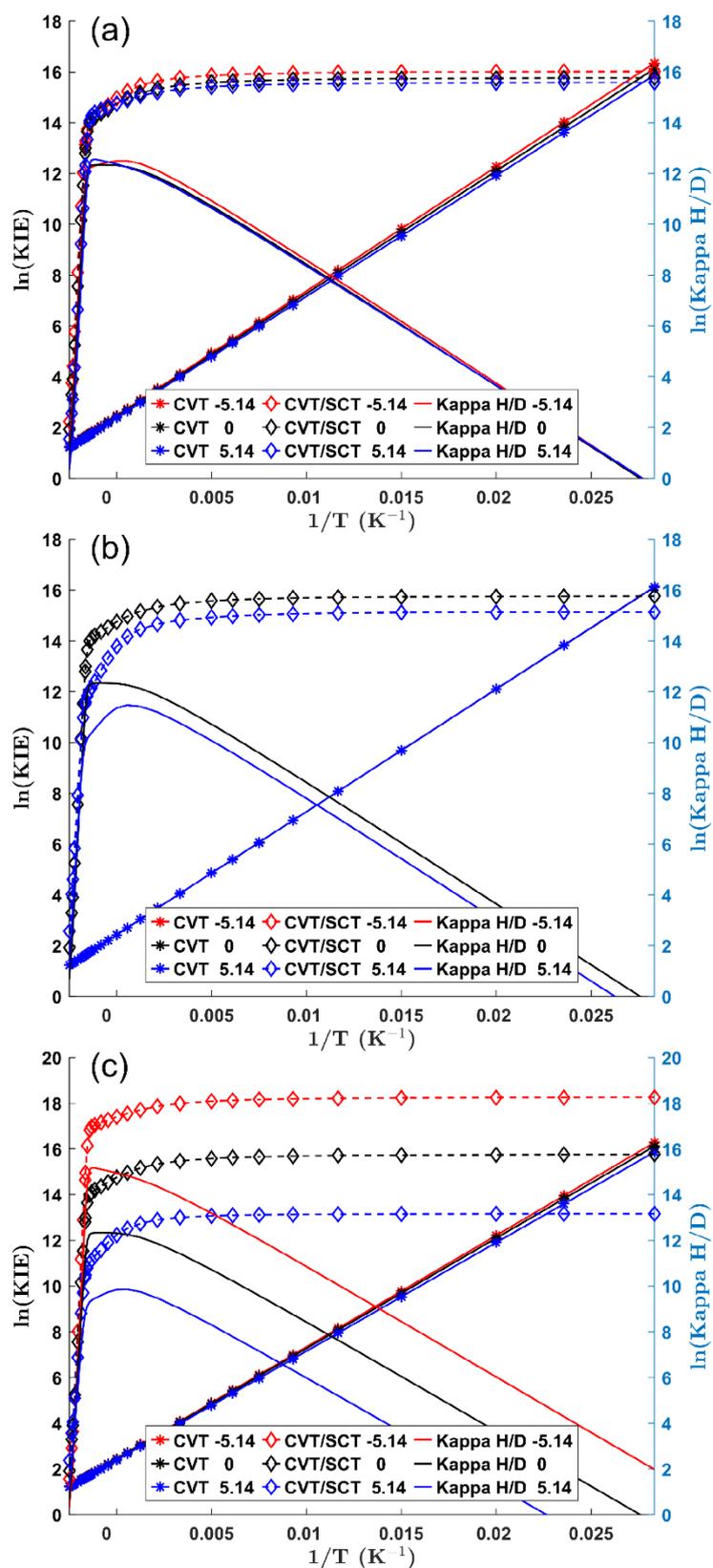
**Figure S62.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of  $\text{H}_3\text{C-C-OH}$  at (a) 30K, (b) 100K and (c) 200K using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths (dash lines: negative direction of Y-EEF; solid lines: positive direction of Y-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S63.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of H<sub>3</sub>C-C-OH using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S64.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of  $\text{H}_3\text{C}-\text{C}-\text{OH}$  at (a) 30K, (b) 100K and (c) 200K, using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 5.14 V/nm; green: 3.85 V/nm, blue: 2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S65.** Arrhenius plots of  $\ln(\text{H/D KIE})$  and  $\ln(\kappa(\text{H})/\kappa(\text{D}))$  versus  $1/T$  of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different EEF strengths (red: -5.14 V/nm; blue: 5.14 V/nm and black: no field (0.0 V/nm)).

**Table S100.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.12E-205	4.55E-204	1.70E-202	1.92E-199	1.65E-196	4.44E-195	1.15E-193
35	1.18E-174	2.81E-173	6.28E-172	2.59E-169	8.41E-167	1.41E-165	2.30E-164
40	2.21E-151	3.54E-150	5.36E-149	1.04E-146	1.63E-144	1.92E-143	2.20E-142
50	8.71E-119	7.99E-118	7.00E-117	4.70E-115	2.66E-113	1.91E-112	1.34E-111
60	4.81E-97	3.04E-96	1.85E-95	6.13E-94	1.76E-92	9.05E-92	4.59E-91
70	1.66E-81	8.07E-81	3.79E-80	7.56E-79	1.34E-77	5.42E-77	2.18E-76
80	7.61E-70	3.03E-69	1.17E-68	1.60E-67	1.96E-66	6.66E-66	2.25E-65
90	9.03E-61	3.08E-60	1.02E-59	1.04E-58	9.60E-58	2.85E-57	8.39E-57
100	1.66E-53	4.99E-53	1.46E-52	1.18E-51	8.69E-51	2.31E-50	6.10E-50
120	1.33E-42	3.33E-42	8.16E-42	4.61E-41	2.42E-40	5.45E-40	1.23E-39
140	8.41E-35	1.84E-34	3.95E-34	1.74E-33	7.16E-33	1.43E-32	2.88E-32
160	6.06E-29	1.20E-28	2.34E-28	8.50E-28	2.93E-27	5.36E-27	9.88E-27
180	2.21E-24	4.06E-24	7.34E-24	2.30E-23	6.88E-23	1.18E-22	2.03E-22
200	1.00E-20	1.73E-20	2.94E-20	8.19E-20	2.19E-19	3.55E-19	5.79E-19
220	9.91E-18	1.62E-17	2.63E-17	6.67E-17	1.62E-16	2.52E-16	3.94E-16
240	3.13E-15	4.92E-15	7.65E-15	1.79E-14	4.04E-14	6.04E-14	9.10E-14
260	4.12E-13	6.25E-13	9.37E-13	2.05E-12	4.34E-12	6.28E-12	9.18E-12
273.15	6.92E-12	1.03E-11	1.51E-11	3.18E-11	6.48E-11	9.22E-11	1.32E-10
280	2.71E-11	3.99E-11	5.81E-11	1.20E-10	2.40E-10	3.39E-10	4.82E-10
290	1.78E-10	2.58E-10	3.71E-10	7.46E-10	1.46E-09	2.03E-09	2.85E-09
298.15	7.50E-10	1.08E-09	1.53E-09	3.02E-09	5.79E-09	7.99E-09	1.11E-08
300	1.03E-09	1.47E-09	2.09E-09	4.11E-09	7.83E-09	1.08E-08	1.50E-08
310	5.32E-09	7.53E-09	1.06E-08	2.03E-08	3.79E-08	5.16E-08	7.11E-08
320	2.49E-08	3.48E-08	4.83E-08	9.08E-08	1.66E-07	2.24E-07	3.06E-07
340	4.15E-07	5.69E-07	7.74E-07	1.40E-06	2.47E-06	3.27E-06	4.38E-06
360	5.08E-06	6.84E-06	9.15E-06	1.60E-05	2.72E-05	3.55E-05	4.69E-05
373.15	2.28E-05	3.04E-05	4.02E-05	6.88E-05	1.15E-04	1.49E-04	1.94E-04
380	4.79E-05	6.35E-05	8.36E-05	1.42E-04	2.34E-04	3.01E-04	3.92E-04
400	3.62E-04	4.73E-04	6.14E-04	1.01E-03	1.63E-03	2.07E-03	2.66E-03

**Table S101.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); positive direction of X-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	8.76E-06	1.17E-05	1.42E-05	2.07E-05	2.42E-05	2.34E-05	2.92E-05
35	8.80E-06	1.17E-05	1.43E-05	2.09E-05	2.46E-05	2.37E-05	2.97E-05
40	8.88E-06	1.18E-05	1.44E-05	2.11E-05	2.50E-05	2.42E-05	3.04E-05
50	9.12E-06	1.22E-05	1.49E-05	2.20E-05	2.63E-05	2.55E-05	3.23E-05
60	9.48E-06	1.27E-05	1.56E-05	2.32E-05	2.80E-05	2.73E-05	3.48E-05
70	9.98E-06	1.35E-05	1.65E-05	2.47E-05	3.01E-05	2.95E-05	3.78E-05
80	1.06E-05	1.44E-05	1.76E-05	2.65E-05	3.27E-05	3.21E-05	4.13E-05
90	1.13E-05	1.54E-05	1.90E-05	2.86E-05	3.57E-05	3.51E-05	4.53E-05
100	1.22E-05	1.67E-05	2.05E-05	3.10E-05	3.91E-05	3.86E-05	5.00E-05
120	1.44E-05	1.98E-05	2.43E-05	3.70E-05	4.76E-05	4.70E-05	6.11E-05
140	1.73E-05	2.39E-05	2.94E-05	4.49E-05	5.86E-05	5.79E-05	7.55E-05
160	2.11E-05	2.94E-05	3.60E-05	5.52E-05	7.29E-05	7.21E-05	9.39E-05
180	2.62E-05	3.67E-05	4.48E-05	6.87E-05	9.15E-05	9.03E-05	1.17E-04
200	3.31E-05	4.66E-05	5.68E-05	8.67E-05	1.16E-04	1.13E-04	1.47E-04
220	4.27E-05	6.01E-05	7.29E-05	1.10E-04	1.46E-04	1.43E-04	1.83E-04
240	5.60E-05	7.85E-05	9.44E-05	1.41E-04	1.85E-04	1.78E-04	2.27E-04
260	7.40E-05	1.03E-04	1.23E-04	1.80E-04	2.31E-04	2.21E-04	2.79E-04
273.15	8.91E-05	1.23E-04	1.46E-04	2.10E-04	2.67E-04	2.53E-04	3.17E-04
280	9.82E-05	1.36E-04	1.60E-04	2.28E-04	2.87E-04	2.71E-04	3.38E-04
290	1.13E-04	1.55E-04	1.82E-04	2.56E-04	3.19E-04	2.99E-04	3.71E-04
298.15	1.27E-04	1.73E-04	2.01E-04	2.81E-04	3.46E-04	3.23E-04	3.99E-04
300	1.30E-04	1.77E-04	2.06E-04	2.87E-04	3.53E-04	3.29E-04	4.06E-04
310	1.49E-04	2.02E-04	2.33E-04	3.21E-04	3.89E-04	3.60E-04	4.42E-04
320	1.70E-04	2.30E-04	2.64E-04	3.57E-04	4.28E-04	3.94E-04	4.81E-04
340	2.21E-04	2.94E-04	3.34E-04	4.40E-04	5.14E-04	4.68E-04	5.66E-04
360	2.86E-04	3.76E-04	4.21E-04	5.43E-04	6.25E-04	5.68E-04	6.83E-04
373.15	3.46E-04	4.50E-04	5.04E-04	6.46E-04	7.50E-04	7.00E-04	8.44E-04
380	3.89E-04	5.05E-04	5.67E-04	7.33E-04	8.67E-04	8.33E-04	1.01E-03
400	6.90E-04	8.89E-04	1.04E-03	1.44E-03	1.92E-03	2.13E-03	2.65E-03

**Table S102.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.36E-198	6.22E-199	2.84E-199	1.92E-199	2.84E-199	6.22E-199	1.36E-198
35	1.40E-168	7.14E-169	3.65E-169	2.59E-169	3.65E-169	7.14E-169	1.40E-168
40	4.59E-146	2.55E-146	1.41E-146	1.04E-146	1.41E-146	2.55E-146	4.59E-146
50	1.59E-114	9.92E-115	6.15E-115	4.70E-115	6.15E-115	9.92E-115	1.59E-114
60	1.74E-93	1.18E-93	7.86E-94	6.13E-94	7.86E-94	1.18E-93	1.74E-93
70	1.91E-78	1.37E-78	9.57E-79	7.56E-79	9.57E-79	1.37E-78	1.91E-78
80	3.71E-67	2.76E-67	2.01E-67	1.60E-67	2.01E-67	2.76E-67	3.71E-67
90	2.26E-58	1.74E-58	1.30E-58	1.04E-58	1.30E-58	1.74E-58	2.26E-58
100	2.45E-51	1.93E-51	1.47E-51	1.18E-51	1.47E-51	1.93E-51	2.45E-51
120	8.92E-41	7.30E-41	5.73E-41	4.61E-41	5.73E-41	7.30E-41	8.92E-41
140	3.20E-33	2.69E-33	2.16E-33	1.74E-33	2.16E-33	2.69E-33	3.20E-33
160	1.52E-27	1.30E-27	1.06E-27	8.50E-28	1.06E-27	1.30E-27	1.52E-27
180	4.00E-23	3.49E-23	2.86E-23	2.30E-23	2.86E-23	3.49E-23	4.00E-23
200	1.39E-19	1.23E-19	1.02E-19	8.19E-20	1.02E-19	1.23E-19	1.39E-19
220	1.12E-16	9.95E-17	8.30E-17	6.67E-17	8.30E-17	9.95E-17	1.12E-16
240	2.96E-14	2.66E-14	2.23E-14	1.79E-14	2.23E-14	2.66E-14	2.96E-14
260	3.35E-12	3.03E-12	2.56E-12	2.05E-12	2.56E-12	3.03E-12	3.35E-12
273.15	5.16E-11	4.70E-11	3.97E-11	3.18E-11	3.97E-11	4.70E-11	5.16E-11
280	1.94E-10	1.77E-10	1.50E-10	1.20E-10	1.50E-10	1.77E-10	1.94E-10
290	1.20E-09	1.10E-09	9.30E-10	7.46E-10	9.30E-10	1.10E-09	1.20E-09
298.15	4.85E-09	4.44E-09	3.77E-09	3.02E-09	3.77E-09	4.44E-09	4.85E-09
300	6.59E-09	6.04E-09	5.12E-09	4.11E-09	5.12E-09	6.04E-09	6.59E-09
310	3.24E-08	2.98E-08	2.53E-08	2.03E-08	2.53E-08	2.98E-08	3.24E-08
320	1.45E-07	1.33E-07	1.13E-07	9.08E-08	1.13E-07	1.33E-07	1.45E-07
340	2.21E-06	2.05E-06	1.75E-06	1.40E-06	1.75E-06	2.05E-06	2.21E-06
360	2.51E-05	2.33E-05	2.00E-05	1.60E-05	2.00E-05	2.33E-05	2.51E-05
373.15	1.08E-04	1.00E-04	8.60E-05	6.88E-05	8.60E-05	1.00E-04	1.08E-04
380	2.22E-04	2.06E-04	1.77E-04	1.42E-04	1.77E-04	2.06E-04	2.22E-04
400	1.58E-03	1.47E-03	1.26E-03	1.01E-03	1.26E-03	1.47E-03	1.58E-03

**Table S103.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); positive direction of Y-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	2.47E-05	2.33E-05	2.00E-05	2.07E-05	2.00E-05	2.33E-05	2.47E-05
35	2.47E-05	2.33E-05	2.01E-05	2.09E-05	2.01E-05	2.33E-05	2.47E-05
40	2.48E-05	2.35E-05	2.03E-05	2.11E-05	2.03E-05	2.35E-05	2.48E-05
50	2.52E-05	2.39E-05	2.07E-05	2.20E-05	2.07E-05	2.39E-05	2.52E-05
60	2.58E-05	2.46E-05	2.15E-05	2.32E-05	2.15E-05	2.46E-05	2.58E-05
70	2.67E-05	2.56E-05	2.26E-05	2.47E-05	2.26E-05	2.56E-05	2.67E-05
80	2.79E-05	2.70E-05	2.40E-05	2.65E-05	2.40E-05	2.70E-05	2.79E-05
90	2.95E-05	2.87E-05	2.56E-05	2.86E-05	2.56E-05	2.87E-05	2.95E-05
100	3.14E-05	3.07E-05	2.76E-05	3.10E-05	2.76E-05	3.07E-05	3.14E-05
120	3.62E-05	3.58E-05	3.25E-05	3.70E-05	3.25E-05	3.58E-05	3.62E-05
140	4.27E-05	4.27E-05	3.90E-05	4.49E-05	3.90E-05	4.27E-05	4.27E-05
160	5.14E-05	5.19E-05	4.77E-05	5.52E-05	4.77E-05	5.19E-05	5.14E-05
180	6.34E-05	6.45E-05	5.96E-05	6.87E-05	5.96E-05	6.45E-05	6.34E-05
200	8.05E-05	8.23E-05	7.62E-05	8.67E-05	7.62E-05	8.23E-05	8.05E-05
220	1.06E-04	1.08E-04	1.00E-04	1.10E-04	1.00E-04	1.08E-04	1.06E-04
240	1.44E-04	1.48E-04	1.35E-04	1.41E-04	1.35E-04	1.48E-04	1.44E-04
260	2.05E-04	2.08E-04	1.84E-04	1.80E-04	1.84E-04	2.08E-04	2.05E-04
273.15	2.63E-04	2.63E-04	2.28E-04	2.10E-04	2.28E-04	2.63E-04	2.63E-04
280	3.00E-04	2.99E-04	2.56E-04	2.28E-04	2.56E-04	2.99E-04	3.00E-04
290	3.66E-04	3.61E-04	3.02E-04	2.56E-04	3.02E-04	3.61E-04	3.66E-04
298.15	4.32E-04	4.22E-04	3.45E-04	2.81E-04	3.45E-04	4.22E-04	4.32E-04
300	4.49E-04	4.37E-04	3.55E-04	2.87E-04	3.55E-04	4.37E-04	4.49E-04
310	5.51E-04	5.29E-04	4.18E-04	3.21E-04	4.18E-04	5.29E-04	5.51E-04
320	6.76E-04	6.40E-04	4.91E-04	3.57E-04	4.91E-04	6.40E-04	6.76E-04
340	1.01E-03	9.32E-04	6.73E-04	4.40E-04	6.73E-04	9.32E-04	1.01E-03
360	1.52E-03	1.35E-03	9.19E-04	5.43E-04	9.19E-04	1.35E-03	1.52E-03
373.15	1.99E-03	1.74E-03	1.15E-03	6.46E-04	1.15E-03	1.74E-03	1.99E-03
380	2.33E-03	2.02E-03	1.32E-03	7.33E-04	1.32E-03	2.02E-03	2.33E-03
400	4.17E-03	3.60E-03	2.42E-03	1.44E-03	2.42E-03	3.60E-03	4.17E-03

**Table S104.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	6.26E-238	2.75E-228	1.49E-218	1.92E-199	8.01E-181	1.09E-171	1.15E-162
35	2.63E-202	4.77E-194	1.06E-185	2.59E-169	2.37E-153	1.60E-145	8.70E-138
40	1.39E-175	2.30E-168	4.70E-161	1.04E-146	9.66E-133	6.88E-126	4.03E-119
50	3.68E-138	2.14E-132	1.53E-126	4.70E-115	7.13E-104	2.17E-98	5.66E-93
60	3.36E-113	2.08E-108	1.60E-103	6.13E-94	1.29E-84	4.81E-80	1.57E-75
70	2.31E-95	2.89E-91	4.52E-87	7.56E-79	7.51E-71	6.25E-67	4.64E-63
80	5.60E-82	2.11E-78	9.98E-75	1.60E-67	1.61E-60	4.34E-57	1.06E-53
90	1.46E-71	2.15E-68	4.03E-65	1.04E-58	1.76E-52	1.99E-49	2.05E-46
100	3.16E-63	2.21E-60	1.97E-57	1.18E-51	4.81E-46	2.69E-43	1.39E-40
120	1.04E-50	2.35E-48	6.87E-46	4.61E-41	2.22E-36	4.36E-34	7.99E-32
140	9.24E-42	9.39E-40	1.24E-37	1.74E-33	1.82E-29	1.69E-27	1.48E-25
160	4.86E-35	2.70E-33	1.96E-31	8.50E-28	2.84E-24	1.50E-22	7.54E-21
180	8.33E-30	2.90E-28	1.32E-26	2.30E-23	3.16E-20	1.08E-18	3.52E-17
200	1.30E-25	3.10E-24	9.74E-23	8.19E-20	5.51E-17	1.33E-15	3.06E-14
220	3.54E-22	6.22E-21	1.44E-19	6.67E-17	2.50E-14	4.54E-13	7.88E-12
240	2.61E-19	3.54E-18	6.36E-17	1.79E-14	4.14E-12	5.91E-11	8.11E-10
260	7.01E-17	7.66E-16	1.11E-14	2.05E-12	3.14E-10	3.66E-09	4.12E-08
273.15	1.78E-15	1.72E-14	2.20E-13	3.18E-11	3.85E-09	3.99E-08	4.00E-07
280	8.53E-15	7.74E-14	9.33E-13	1.20E-10	1.29E-08	1.27E-07	1.20E-06
290	7.35E-14	6.14E-13	6.81E-12	7.46E-10	6.86E-08	6.22E-07	5.46E-06
298.15	3.83E-13	3.00E-12	3.12E-11	3.02E-09	2.46E-07	2.10E-06	1.74E-05
300	5.50E-13	4.25E-12	4.36E-11	4.11E-09	3.26E-07	2.75E-06	2.25E-05
310	3.62E-12	2.60E-11	2.48E-10	2.03E-08	1.40E-06	1.11E-05	8.45E-05
320	2.12E-11	1.42E-10	1.27E-09	9.08E-08	5.51E-06	4.08E-05	2.93E-04
340	5.33E-10	3.15E-09	2.49E-08	1.40E-06	6.71E-05	4.42E-04	2.83E-03
360	9.41E-09	4.98E-08	3.53E-07	1.60E-05	6.21E-04	3.69E-03	2.13E-02
373.15	5.26E-08	2.61E-07	1.73E-06	6.88E-05	2.36E-03	1.32E-02	7.17E-02
380	1.23E-07	5.90E-07	3.79E-06	1.42E-04	4.56E-03	2.47E-02	1.31E-01
400	1.25E-06	5.48E-06	3.22E-05	1.01E-03	2.75E-02	1.37E-01	6.67E-01

**Table S105.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OH}$  using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); positive direction of Z-EEF (2.57 ~ 5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-5.14	-3.85	-2.57	0.0	2.57	3.85	5.14
30	1.25E-08	7.19E-08	5.17E-07	2.07E-05	6.27E-04	3.57E-03	1.77E-02
35	1.27E-08	7.32E-08	5.24E-07	2.09E-05	6.31E-04	3.58E-03	1.78E-02
40	1.30E-08	7.49E-08	5.35E-07	2.11E-05	6.38E-04	3.61E-03	1.79E-02
50	1.38E-08	7.91E-08	5.62E-07	2.20E-05	6.59E-04	3.71E-03	1.83E-02
60	1.48E-08	8.46E-08	5.98E-07	2.32E-05	6.90E-04	3.86E-03	1.90E-02
70	1.61E-08	9.14E-08	6.43E-07	2.47E-05	7.31E-04	4.05E-03	1.99E-02
80	1.76E-08	9.92E-08	6.95E-07	2.65E-05	7.82E-04	4.30E-03	2.11E-02
90	1.93E-08	1.08E-07	7.56E-07	2.86E-05	8.42E-04	4.60E-03	2.25E-02
100	2.13E-08	1.19E-07	8.26E-07	3.10E-05	9.12E-04	4.94E-03	2.42E-02
120	2.61E-08	1.44E-07	9.96E-07	3.70E-05	1.08E-03	5.80E-03	2.82E-02
140	3.24E-08	1.76E-07	1.22E-06	4.49E-05	1.31E-03	6.91E-03	3.35E-02
160	4.05E-08	2.17E-07	1.50E-06	5.52E-05	1.60E-03	8.38E-03	4.05E-02
180	5.11E-08	2.69E-07	1.86E-06	6.87E-05	2.00E-03	1.04E-02	4.99E-02
200	6.45E-08	3.31E-07	2.32E-06	8.67E-05	2.53E-03	1.30E-02	6.27E-02
220	8.13E-08	4.05E-07	2.88E-06	1.10E-04	3.26E-03	1.68E-02	8.06E-02
240	1.02E-07	4.90E-07	3.55E-06	1.41E-04	4.26E-03	2.20E-02	1.06E-01
260	1.26E-07	5.87E-07	4.35E-06	1.80E-04	5.61E-03	2.91E-02	1.42E-01
273.15	1.44E-07	6.57E-07	4.94E-06	2.10E-04	6.73E-03	3.52E-02	1.73E-01
280	1.54E-07	6.96E-07	5.27E-06	2.28E-04	7.39E-03	3.89E-02	1.92E-01
290	1.70E-07	7.53E-07	5.77E-06	2.56E-04	8.48E-03	4.50E-02	2.23E-01
298.15	1.83E-07	8.02E-07	6.20E-06	2.81E-04	9.47E-03	5.07E-02	2.53E-01
300	1.86E-07	8.14E-07	6.30E-06	2.87E-04	9.71E-03	5.20E-02	2.60E-01
310	2.04E-07	8.76E-07	6.86E-06	3.21E-04	1.11E-02	6.00E-02	3.03E-01
320	2.23E-07	9.41E-07	7.46E-06	3.57E-04	1.27E-02	6.91E-02	3.52E-01
340	2.63E-07	1.08E-06	8.73E-06	4.40E-04	1.64E-02	9.12E-02	4.74E-01
360	3.12E-07	1.25E-06	1.03E-05	5.43E-04	2.12E-02	1.20E-01	6.40E-01
373.15	3.71E-07	1.49E-06	1.22E-05	6.46E-04	2.57E-02	1.48E-01	7.96E-01
380	4.34E-07	1.76E-06	1.41E-05	7.33E-04	2.91E-02	1.68E-01	9.06E-01
400	1.24E-06	5.21E-06	3.48E-05	1.44E-03	5.08E-02	2.84E-01	1.51E+00

**Table S106.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	8.96E-213	1.92E-206	1.47E-200
35	9.67E-181	2.57E-175	2.81E-170
40	1.04E-156	5.77E-152	1.47E-147
50	4.73E-123	2.92E-119	9.64E-116
60	1.33E-100	1.90E-97	1.61E-94
70	1.48E-84	7.40E-82	2.37E-79
80	1.62E-72	3.70E-70	5.73E-68
90	3.80E-63	4.71E-61	4.14E-59
100	1.20E-55	9.14E-54	5.12E-52
120	2.19E-44	8.01E-43	2.28E-41
140	2.48E-36	5.38E-35	9.45E-34
160	2.77E-30	4.07E-29	4.98E-28
180	1.43E-25	1.54E-24	1.43E-23
200	8.49E-22	7.21E-21	5.32E-20
220	1.05E-18	7.31E-18	4.50E-17
240	4.01E-16	2.36E-15	1.25E-14
260	6.16E-14	3.16E-13	1.46E-12
273.15	1.13E-12	5.36E-12	2.31E-11
280	4.65E-12	2.11E-11	8.76E-11
290	3.23E-11	1.39E-10	5.49E-10
298.15	1.43E-10	5.89E-10	2.24E-09
300	1.98E-10	8.09E-10	3.05E-09
310	1.08E-09	4.21E-09	1.52E-08
320	5.29E-09	1.97E-08	6.84E-08
340	9.63E-08	3.32E-07	1.07E-06
360	1.27E-06	4.09E-06	1.23E-05
373.15	6.00E-06	1.84E-05	5.34E-05
380	1.29E-05	3.88E-05	1.10E-04
400	1.04E-04	2.94E-04	7.92E-04

**Table S107.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); positive direction of X-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	X-EEF		
	-5.14	0.0	5.14
30	9.69E-13	2.96E-12	4.99E-12
35	9.77E-13	3.00E-12	5.10E-12
40	9.90E-13	3.06E-12	5.26E-12
50	1.03E-12	3.23E-12	5.67E-12
60	1.09E-12	3.47E-12	6.22E-12
70	1.18E-12	3.79E-12	6.91E-12
80	1.29E-12	4.20E-12	7.76E-12
90	1.42E-12	4.70E-12	8.79E-12
100	1.59E-12	5.32E-12	1.01E-11
120	2.05E-12	7.04E-12	1.35E-11
140	2.78E-12	9.79E-12	1.89E-11
160	4.04E-12	1.43E-11	2.72E-11
180	6.32E-12	2.18E-11	3.96E-11
200	1.05E-11	3.40E-11	5.75E-11
220	1.79E-11	5.31E-11	8.19E-11
240	3.04E-11	8.15E-11	1.14E-10
260	5.05E-11	1.22E-10	1.55E-10
273.15	7.00E-11	1.59E-10	2.01E-10
280	8.41E-11	1.90E-10	2.62E-10
290	1.23E-10	3.02E-10	6.03E-10
298.15	2.17E-10	6.36E-10	1.78E-09
300	2.59E-10	7.92E-10	2.34E-09
310	8.86E-10	3.14E-09	1.07E-08
320	3.81E-09	1.38E-08	4.75E-08
340	6.70E-08	2.30E-07	7.45E-07
360	8.93E-07	2.86E-06	8.68E-06
373.15	4.23E-06	1.30E-05	3.79E-05
380	9.12E-06	2.74E-05	7.84E-05
400	7.40E-05	2.10E-04	5.69E-04

**Table S108.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	1.35E-205	1.92E-206	1.35E-205
35	1.38E-174	2.57E-175	1.38E-174
40	2.54E-151	5.77E-152	2.54E-151
50	9.84E-119	2.92E-119	9.84E-119
60	5.40E-97	1.90E-97	5.40E-97
70	1.87E-81	7.40E-82	1.87E-81
80	8.60E-70	3.70E-70	8.60E-70
90	1.03E-60	4.71E-61	1.03E-60
100	1.90E-53	9.14E-54	1.90E-53
120	1.55E-42	8.01E-43	1.55E-42
140	9.92E-35	5.38E-35	9.93E-35
160	7.25E-29	4.07E-29	7.25E-29
180	2.68E-24	1.54E-24	2.68E-24
200	1.23E-20	7.21E-21	1.23E-20
220	1.22E-17	7.31E-18	1.22E-17
240	3.90E-15	2.36E-15	3.90E-15
260	5.16E-13	3.16E-13	5.16E-13
273.15	8.69E-12	5.36E-12	8.69E-12
280	3.41E-11	2.11E-11	3.41E-11
290	2.24E-10	1.39E-10	2.24E-10
298.15	9.45E-10	5.89E-10	9.45E-10
300	1.30E-09	8.09E-10	1.30E-09
310	6.72E-09	4.21E-09	6.72E-09
320	3.14E-08	1.97E-08	3.14E-08
340	5.25E-07	3.32E-07	5.25E-07
360	6.43E-06	4.09E-06	6.43E-06
373.15	2.89E-05	1.84E-05	2.89E-05
380	6.06E-05	3.88E-05	6.06E-05
400	4.58E-04	2.94E-04	4.58E-04

**Table S109.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 V/nm); positive direction of Y-EEF (5.14 V/nm); no field (0.0 V/nm).

T(K)	Y-EEF		
	-5.14	0.0	5.14
30	6.65E-12	2.96E-12	6.65E-12
35	6.67E-12	3.00E-12	6.67E-12
40	6.71E-12	3.06E-12	6.71E-12
50	6.88E-12	3.23E-12	6.88E-12
60	7.20E-12	3.47E-12	7.21E-12
70	7.69E-12	3.79E-12	7.69E-12
80	8.35E-12	4.20E-12	8.35E-12
90	9.20E-12	4.70E-12	9.20E-12
100	1.03E-11	5.32E-12	1.03E-11
120	1.33E-11	7.04E-12	1.33E-11
140	1.82E-11	9.79E-12	1.82E-11
160	2.69E-11	1.43E-11	2.69E-11
180	4.42E-11	2.18E-11	4.42E-11
200	8.27E-11	3.40E-11	8.27E-11
220	1.73E-10	5.31E-11	1.73E-10
240	3.83E-10	8.15E-11	3.83E-10
260	8.44E-10	1.22E-10	8.44E-10
273.15	1.39E-09	1.59E-10	1.39E-09
280	1.80E-09	1.90E-10	1.80E-09
290	2.68E-09	3.02E-10	2.68E-09
298.15	3.97E-09	6.36E-10	3.97E-09
300	4.42E-09	7.92E-10	4.42E-09
310	9.38E-09	3.14E-09	9.38E-09
320	2.77E-08	1.38E-08	2.77E-08
340	3.67E-07	2.30E-07	3.67E-07
360	4.42E-06	2.86E-06	4.42E-06
373.15	1.99E-05	1.30E-05	1.99E-05
380	4.19E-05	2.74E-05	4.19E-05
400	3.20E-04	2.10E-04	3.20E-04

**Table S110.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	5.34E-245	1.92E-206	1.48E-169
35	2.28E-208	2.57E-175	1.08E-143
40	6.87E-181	5.77E-152	2.72E-124
50	2.08E-142	2.92E-119	4.10E-97
60	9.65E-117	1.90E-97	5.56E-79
70	2.12E-98	7.40E-82	5.08E-66
80	1.23E-84	3.70E-70	2.72E-56
90	6.29E-74	4.71E-61	1.01E-48
100	2.35E-65	9.14E-54	1.17E-42
120	1.74E-52	8.01E-43	1.48E-33
140	2.78E-43	5.38E-35	4.84E-27
160	2.27E-36	4.07E-29	3.79E-22
180	5.47E-31	1.54E-24	2.46E-18
200	1.12E-26	7.21E-21	2.80E-15
220	3.83E-23	7.31E-18	8.95E-13
240	3.39E-20	2.36E-15	1.10E-10
260	1.07E-17	3.16E-13	6.53E-09
273.15	2.97E-16	5.36E-12	6.92E-08
280	1.48E-15	2.11E-11	2.17E-07
290	1.36E-14	1.39E-10	1.04E-06
298.15	7.40E-14	5.89E-10	3.48E-06
300	1.07E-13	8.09E-10	4.54E-06
310	7.44E-13	4.21E-09	1.79E-05
320	4.57E-12	1.97E-08	6.52E-05
340	1.25E-10	3.32E-07	6.86E-04
360	2.39E-09	4.09E-06	5.58E-03
373.15	1.40E-08	1.84E-05	1.96E-02
380	3.35E-08	3.88E-05	3.64E-02
400	3.61E-07	2.94E-04	1.98E-01

**Table S111.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{C-C-OD}$  using M06-2X/6-31G(d,p) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.47E-16	2.96E-12	3.40E-08
35	1.51E-16	3.00E-12	3.42E-08
40	1.55E-16	3.06E-12	3.45E-08
50	1.67E-16	3.23E-12	3.55E-08
60	1.83E-16	3.47E-12	3.71E-08
70	2.03E-16	3.79E-12	3.93E-08
80	2.28E-16	4.20E-12	4.22E-08
90	2.59E-16	4.70E-12	4.60E-08
100	2.96E-16	5.32E-12	5.06E-08
120	4.01E-16	7.04E-12	6.35E-08
140	5.66E-16	9.79E-12	8.40E-08
160	8.23E-16	1.43E-11	1.19E-07
180	1.22E-15	2.18E-11	1.83E-07
200	1.79E-15	3.40E-11	3.05E-07
220	2.58E-15	5.31E-11	5.41E-07
240	3.63E-15	8.15E-11	9.77E-07
260	4.97E-15	1.22E-10	1.75E-06
273.15	6.20E-15	1.59E-10	2.55E-06
280	7.59E-15	1.90E-10	3.15E-06
290	1.66E-14	3.02E-10	4.59E-06
298.15	5.83E-14	6.36E-10	7.11E-06
300	8.11E-14	7.92E-10	8.04E-06
310	5.15E-13	3.14E-09	1.85E-05
320	3.13E-12	1.38E-08	5.25E-05
340	8.68E-11	2.30E-07	4.87E-04
360	1.67E-09	2.86E-06	3.92E-03
373.15	9.85E-09	1.30E-05	1.38E-02
380	2.37E-08	2.74E-05	2.58E-02
400	2.58E-07	2.10E-04	1.41E-01

**Table S112.** Computed half-life (hr) for the hydroxycarbenes (R-C-OH: R = H, CH<sub>3</sub>, OH, CN) using M06-2X/6-31G(d,p) method along various X-, Y- and Z-EEF directions with various strengths (0.0 ~ 5.14 V/nm) at low temperature of 30 K.

	Various EEF strengths (V/nm)						
	-5.14	-3.85	-2.52	0	2.52	3.85	5.14
<b>R = H</b>							
<b>X-EEF</b>	2.19	1.93	1.70	1.34	1.08	0.91	1.01
<b>Y-EEF</b>	1.65	1.55	1.49	1.34	1.49	1.55	1.65
<b>Z-EEF</b>	1188.27	196.03	35.65	1.34	0.06	0.01	0.00
<b>R = CH<sub>3</sub></b>							
<b>X-EEF</b>	21.97	16.45	13.56	9.30	7.95	8.23	6.59
<b>Y-EEF</b>	7.79	8.26	9.63	9.30	9.63	8.26	7.79
<b>Z-EEF</b>	15400.00	2677.33	372.34	9.30	0.31	0.05	0.01
<b>R = OH</b>							
<b>X-EEF</b>	31402.9	40526.3	39609.1	47648.5	94362.7	143656.7	317133.4
<b>Y-EEF</b>	70000.0	79218.1	64597.3	47648.5	64597.3	77935.2	70000.0
<b>Z-EEF</b>	99740932.6	13006756.8	1850961.5	47648.5	1336.8	247.7	53.0
<b>R = CN</b>							
<b>X-EEF</b>	11596.4	6974.6	3319.0	1226.1	493.6	393.7	266.6
<b>Y-EEF</b>	3301.9	1139.1	2170.2	1226.1	2170.2	1139.1	3301.9
<b>Z-EEF</b>	687500.0	113905.3	17660.6	1226.1	95.8	26.1	7.6

### 2.3 S<sub>N</sub>2 Reaction

**Table S113.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) comparison of S<sub>N</sub>2 reaction using different DFT functionals and basis sets in gas phase. The values in parentheses are relative to the high-level results calculated by DLPNO-CCSD(T1)/aug-cc-pVTZ//M06-2X/6-31+G(d) method.

Methods	$\Delta E$ ( $\Delta\Delta E$ )
<b>DLPNO-CCSD(T1)</b>	<b>8.8 (0.0)</b>
CCSD(T)/aug-cc-pVTZ	9.1 (0.3)
M06-2X/6-31+G(d)	8.6 (0.2)
B3LYP-D3/6-31+G(d)	5.2 (3.6)
PBE0-D3/6-31+G(d)	6.6 (2.2)
$\omega$ B97X-D/6-31+G(d)	9.4 (0.4)
M06-2X/6-31+G(d)	8.6 (0.2)
M06-2X/6-31G(d,p)	4.6 (2.2)
M06-2X/6-31+G(d,p)	8.4 (0.4)

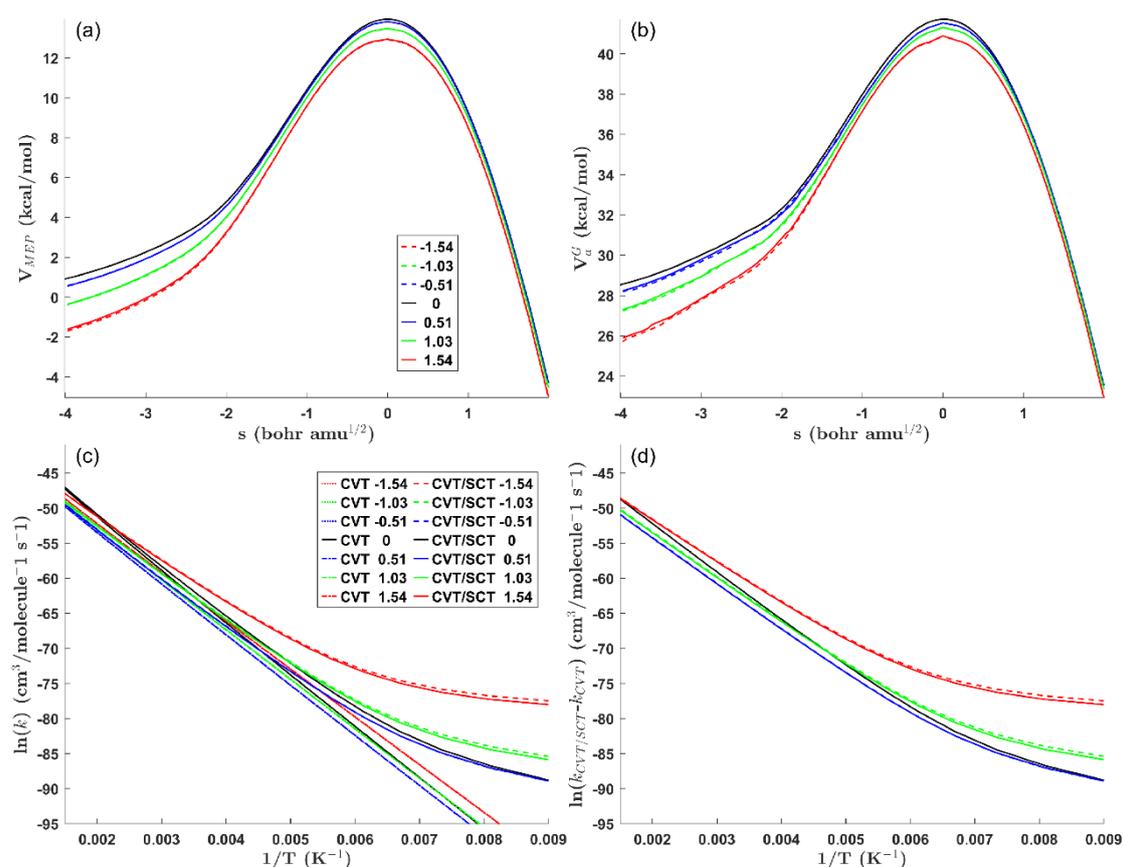
**Table S114.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) comparison of S<sub>N</sub>2 reaction in gas phase, PCM and SMD water solvation model in using M06-2X/6-31+G(d)

	Gas-phase	PCM-H <sub>2</sub> O	SMD-H <sub>2</sub> O
$\Delta E$	-1.8	13.9 (11.8) <sup>a</sup>	14.7

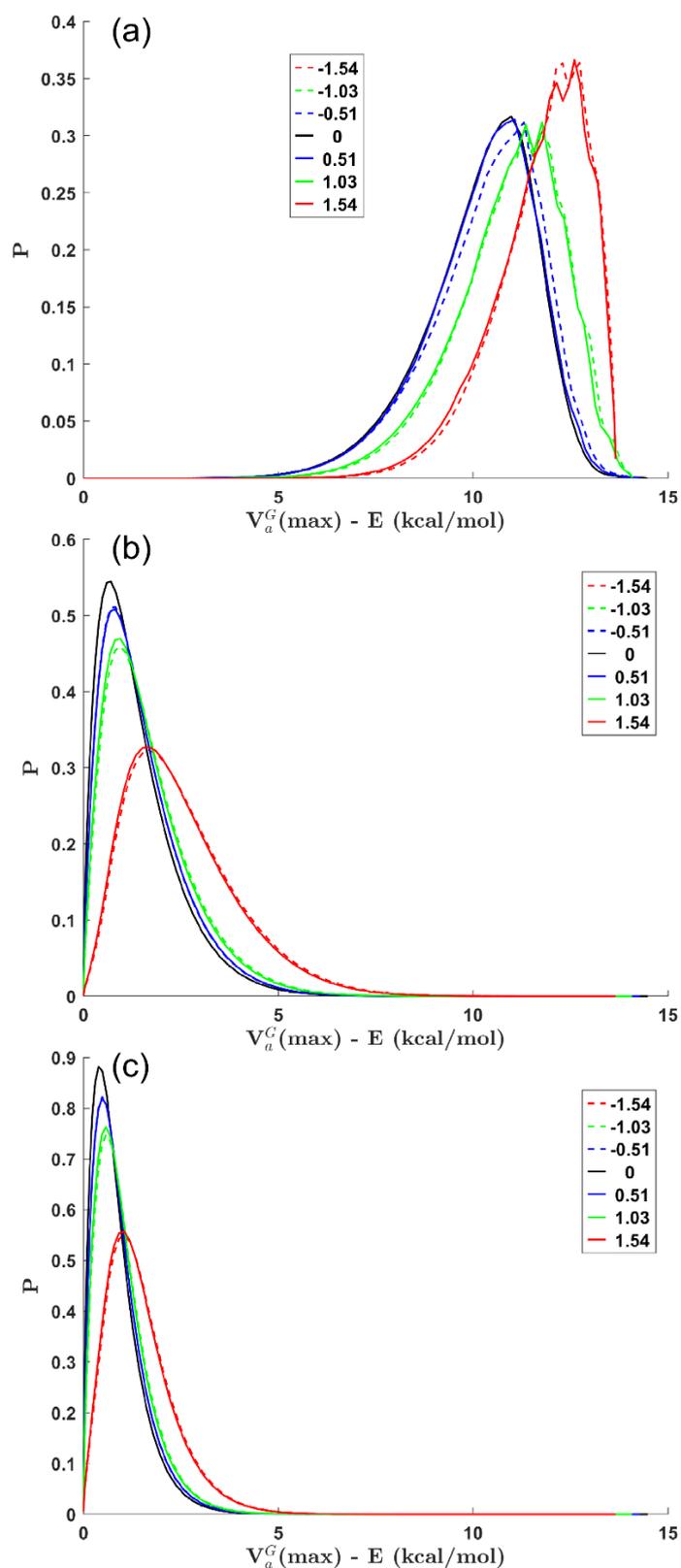
<sup>a</sup>: data in parentheses calculated using B3LYP/6-31++G(d,p) method

**Table S115.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of S<sub>N</sub>2 reaction using M06-2X/6-31+G(d) method under different EEF strengths (V/nm). The  $\Omega$  (in cm<sup>-1</sup>) is the magnitude of the imaginary frequency for the transition state, and T<sub>c</sub> is the crossover temperature (in K).

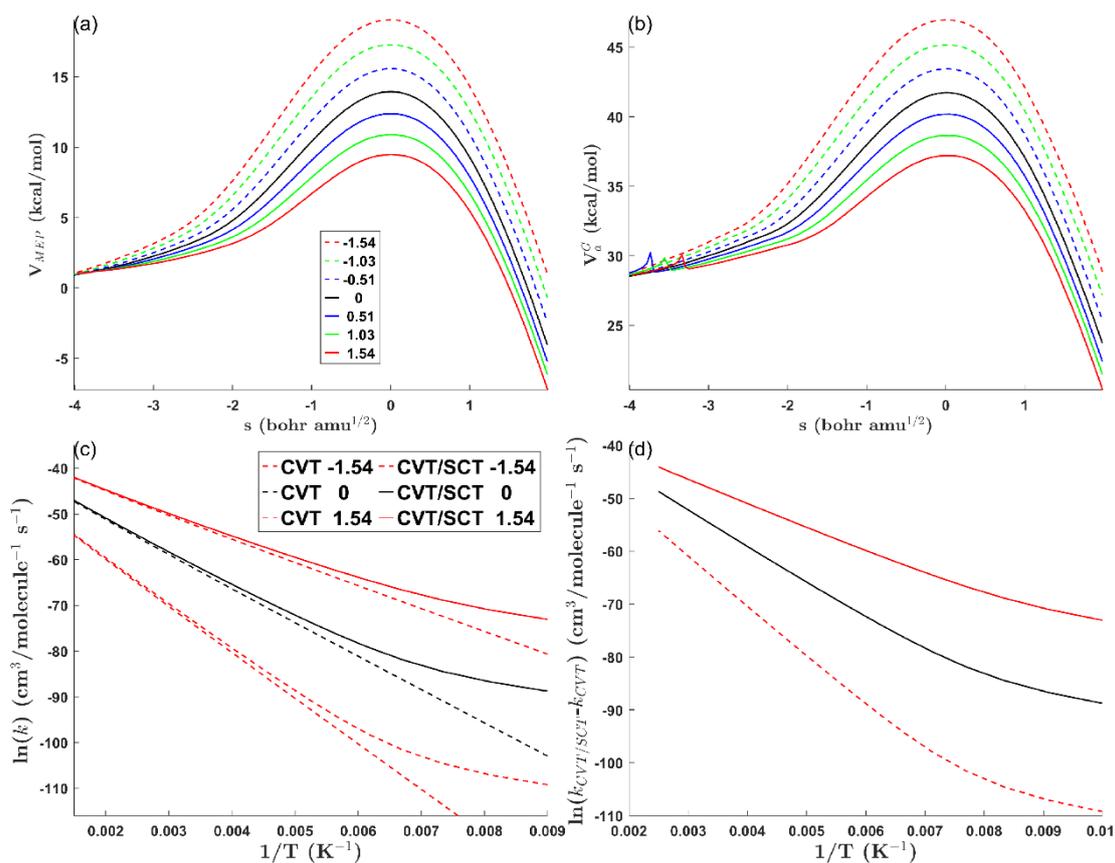
EEF (V/nm)	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
<b>Z-EEF Direction</b>							
$\Delta E$	19.06	17.29	15.59	13.95	12.39	10.89	9.48
$\Delta V_a^G(\max)$	46.96	45.17	43.43	41.73	40.17	38.64	37.19
$\Omega$	638	620	611	608	611	620	636
T <sub>c</sub>	146	142	140	139	140	142	146
<b>X-EEF Direction</b>							
$\Delta E$	12.93	13.48	13.83	13.95	13.83	13.49	12.95
$\Delta V_a^G(\max)$	40.88	41.31	41.53	41.73	41.53	41.32	40.89
$\Omega$	631	625	617	608	598	586	574
T <sub>c</sub>	145	143	141	139	137	134	131



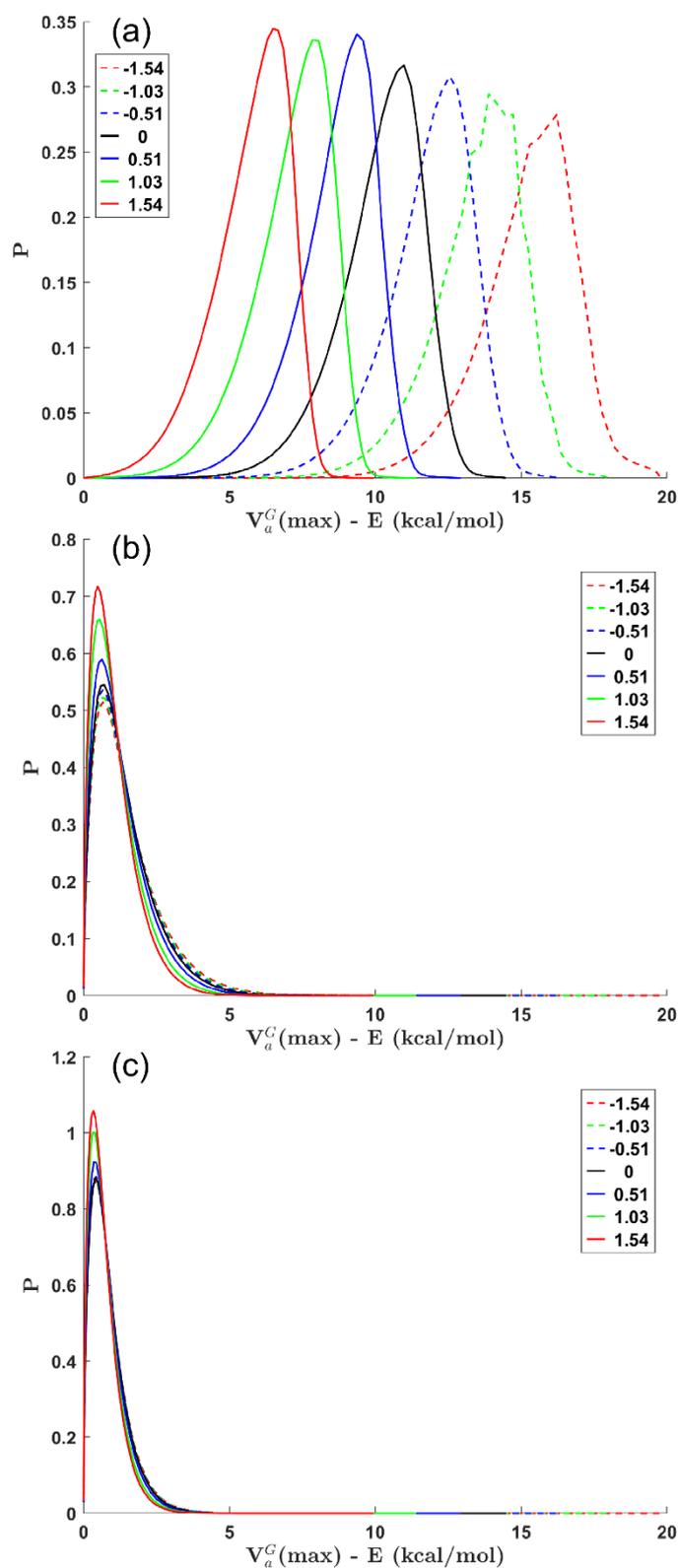
**Figure S66.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $cm^3/molecule^{-1}s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of  $S_N2$  reaction using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 1.54 V/nm; green: 1.03 V/nm, blue: 0.51 V/nm and black: no field (0.0 V/nm)).



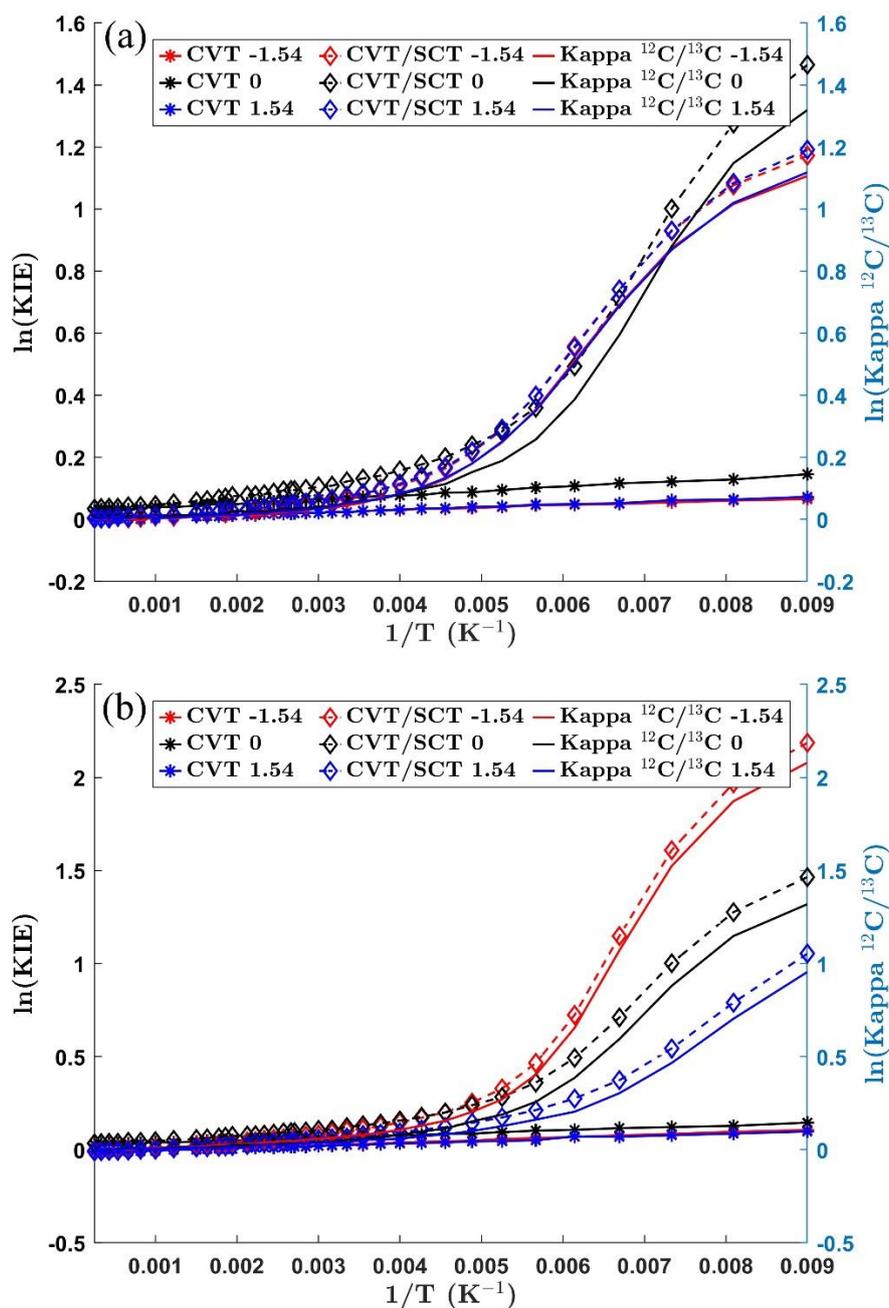
**Figure S67.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the  $\text{S}_{\text{N}}2$  reaction at (a) 100K, (b) 200K and (c) 300K using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths (dash lines: negative direction of X-EEF; solid lines: positive direction of X-EEF; red: 1.54 V/nm; green: 1.03 V/nm, blue: 0.51 V/nm and black: no field (0.0 V/nm)).



**Figure S68.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $cm^3/molecule^{-1}s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of  $S_N2$  reaction using M06-2X/6-31+G(d) method along the Z-EEF direction with various strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 1.54 V/nm; green: 1.03 V/nm, blue: 0.51 V/nm and black: no field (0.0 V/nm)).



**Figure S69.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the  $\text{S}_{\text{N}}2$  reaction at (a) 100K, (b) 200K and (c) 300K using M06-2X/6-31+G(d) method along the Z-EEF direction with various EEF strengths (dash lines: negative direction of Z-EEF; solid lines: positive direction of Z-EEF; red: 1.54 V/nm; green: 1.03 V/nm, blue: 0.51 V/nm and black: no field (0.0 V/nm)).



**Figure S70.** Arrhenius plots of  $\ln \text{KIE}$  ( $^{12}\text{C}/^{13}\text{C}$ ) and  $\ln(\kappa(^{12}\text{C})/\kappa(^{13}\text{C}))$  versus  $1/T$  of  $\text{S}_{\text{N}}2$  reaction along direction (a) X-EEF (b) Z-EEF with different EEF strength (red: -1.54 V/nm; blue 1.54 V/nm and black: no field (0.0 V/nm)).

**Table S116.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-1.54 ~ -0.51 V/nm); positive direction of X-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	3.17E-44	3.09E-45	8.52E-46	1.92E-45	8.27E-46	2.89E-45	3.00E-44
110	1.53E-41	1.82E-42	5.53E-43	1.41E-42	5.34E-43	1.70E-42	1.45E-41
120	2.64E-39	3.70E-40	1.22E-40	3.49E-40	1.18E-40	3.46E-40	2.51E-39
130	2.07E-37	3.34E-38	1.18E-38	3.74E-38	1.14E-38	3.12E-38	1.97E-37
140	8.74E-36	1.59E-36	5.99E-37	2.07E-36	5.73E-37	1.48E-36	8.33E-36
150	2.25E-34	4.55E-35	1.80E-35	6.77E-35	1.72E-35	4.23E-35	2.15E-34
160	3.86E-33	8.57E-34	3.57E-34	1.44E-33	3.39E-34	7.97E-34	3.69E-33
170	4.77E-32	1.15E-32	4.98E-33	2.16E-32	4.73E-33	1.07E-32	4.57E-32
180	4.47E-31	1.16E-31	5.21E-32	2.42E-31	4.94E-32	1.07E-31	4.28E-31
190	3.32E-30	9.17E-31	4.27E-31	2.11E-30	4.04E-31	8.51E-31	3.19E-30
200	2.02E-29	5.93E-30	2.85E-30	1.49E-29	2.69E-30	5.50E-30	1.94E-29
210	1.04E-28	3.22E-29	1.59E-29	8.83E-29	1.50E-29	2.98E-29	1.00E-28
220	4.63E-28	1.50E-28	7.61E-29	4.46E-28	7.19E-29	1.39E-28	4.45E-28
230	1.81E-27	6.15E-28	3.19E-28	1.97E-27	3.01E-28	5.70E-28	1.74E-27
240	6.34E-27	2.25E-27	1.19E-27	7.70E-27	1.12E-27	2.08E-27	6.11E-27
250	2.01E-26	7.41E-27	4.01E-27	2.72E-26	3.77E-27	6.85E-27	1.94E-26
260	5.86E-26	2.23E-26	1.23E-26	8.73E-26	1.16E-26	2.07E-26	5.65E-26
270	1.58E-25	6.22E-26	3.49E-26	2.58E-25	3.28E-26	5.75E-26	1.52E-25
273.15	2.12E-25	8.46E-26	4.78E-26	3.58E-25	4.49E-26	7.82E-26	2.05E-25
280	3.97E-25	1.61E-25	9.21E-26	7.09E-25	8.65E-26	1.49E-25	3.83E-25
290	9.38E-25	3.92E-25	2.28E-25	1.82E-24	2.14E-25	3.63E-25	9.07E-25
300	2.10E-24	9.01E-25	5.31E-25	4.42E-24	4.98E-25	8.33E-25	2.03E-24
310	4.46E-24	1.97E-24	1.17E-24	1.01E-23	1.10E-24	1.82E-24	4.31E-24
320	9.06E-24	4.09E-24	2.47E-24	2.21E-23	2.32E-24	3.78E-24	8.77E-24
340	3.31E-23	1.56E-23	9.68E-24	9.26E-23	9.07E-24	1.44E-23	3.21E-23
350	6.00E-23	2.89E-23	1.81E-23	1.79E-22	1.70E-23	2.67E-23	5.82E-23
360	1.05E-22	5.17E-23	3.27E-23	3.34E-22	3.06E-23	4.77E-23	1.02E-22
380	2.98E-22	1.51E-22	9.79E-23	1.06E-21	9.16E-23	1.40E-22	2.89E-22
400	7.64E-22	4.01E-22	2.64E-22	3.02E-21	2.46E-22	3.70E-22	7.42E-22

**Table S117.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-1.54 ~ -0.51 V/nm); positive direction of X-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	2.26E-34	8.15E-38	2.42E-39	2.77E-39	2.45E-39	5.11E-38	1.31E-34
110	4.55E-34	3.32E-37	1.54E-38	2.15E-38	1.61E-38	2.16E-37	2.75E-34
120	1.18E-33	1.82E-36	1.31E-37	2.13E-37	1.36E-37	1.25E-36	7.61E-34
130	4.03E-33	1.38E-35	1.52E-36	2.85E-36	1.53E-36	1.01E-35	2.81E-33
140	1.80E-32	1.33E-34	2.09E-35	4.57E-35	2.05E-35	1.03E-34	1.35E-32
150	9.69E-32	1.40E-33	2.81E-34	7.11E-34	2.72E-34	1.13E-33	7.68E-32
160	5.65E-31	1.37E-32	3.28E-33	9.45E-33	3.15E-33	1.14E-32	4.66E-31
170	3.24E-30	1.17E-31	3.17E-32	1.03E-31	3.03E-32	9.89E-32	2.74E-30
180	1.72E-29	8.47E-31	2.53E-31	9.05E-31	2.41E-31	7.24E-31	1.48E-29
190	8.26E-29	5.20E-30	1.69E-30	6.60E-30	1.60E-30	4.49E-30	7.20E-29
200	3.56E-28	2.74E-29	9.53E-30	4.05E-29	9.02E-30	2.39E-29	3.13E-28
210	1.38E-27	1.26E-28	4.65E-29	2.13E-28	4.39E-29	1.10E-28	1.22E-27
220	4.82E-27	5.14E-28	1.99E-28	9.81E-28	1.88E-28	4.51E-28	4.31E-27
230	1.54E-26	1.87E-27	7.60E-28	4.00E-27	7.17E-28	1.65E-27	1.39E-26
240	4.54E-26	6.19E-27	2.62E-27	1.46E-26	2.47E-27	5.48E-27	4.10E-26
250	1.24E-25	1.87E-26	8.23E-27	4.87E-26	7.74E-27	1.66E-26	1.12E-25
260	3.15E-25	5.24E-26	2.38E-26	1.49E-25	2.24E-26	4.67E-26	2.88E-25
270	7.55E-25	1.37E-25	6.41E-26	4.22E-25	6.02E-26	1.22E-25	6.91E-25
273.15	9.82E-25	1.82E-25	8.63E-26	5.78E-25	8.10E-26	1.63E-25	9.00E-25
280	1.71E-24	3.34E-25	1.61E-25	1.12E-24	1.51E-25	2.99E-25	1.57E-24
290	3.67E-24	7.72E-25	3.83E-25	2.78E-24	3.59E-25	6.92E-25	3.39E-24
300	7.54E-24	1.69E-24	8.60E-25	6.52E-24	8.07E-25	1.52E-24	6.98E-24
310	1.48E-23	3.54E-24	1.84E-24	1.46E-23	1.73E-24	3.18E-24	1.38E-23
320	2.81E-23	7.10E-24	3.77E-24	3.11E-23	3.53E-24	6.39E-24	2.61E-23
340	9.09E-23	2.54E-23	1.40E-23	1.25E-22	1.31E-23	2.29E-23	8.49E-23
350	1.56E-22	4.57E-23	2.57E-23	2.37E-22	2.40E-23	4.13E-23	1.46E-22
360	2.61E-22	7.96E-23	4.55E-23	4.35E-22	4.25E-23	7.21E-23	2.45E-22
380	6.76E-22	2.23E-22	1.31E-22	1.34E-21	1.23E-22	2.02E-22	6.36E-22
400	1.61E-21	5.68E-22	3.43E-22	3.73E-21	3.21E-22	5.15E-22	1.52E-21

**Table S118.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-1.54 ~ -0.51 V/nm); positive direction of Z-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	3.38E-57	2.99E-53	1.89E-49	1.92E-45	2.61E-42	5.96E-39	9.31E-36
110	2.71E-53	1.05E-49	3.01E-46	1.41E-42	9.37E-40	1.06E-36	8.55E-34
120	4.90E-50	9.58E-47	1.42E-43	3.49E-40	1.27E-37	8.03E-35	3.74E-32
130	2.82E-47	3.09E-44	2.61E-41	3.74E-38	8.20E-36	3.16E-33	9.22E-31
140	6.60E-45	4.40E-42	2.30E-39	2.07E-36	2.94E-34	7.41E-32	1.46E-29
150	7.53E-43	3.26E-40	1.13E-37	6.77E-35	6.60E-33	1.15E-30	1.60E-28
160	4.79E-41	1.42E-38	3.42E-36	1.44E-33	1.01E-31	1.28E-29	1.32E-27
170	1.88E-39	4.01E-37	6.99E-35	2.16E-32	1.13E-30	1.08E-28	8.53E-27
180	4.95E-38	7.86E-36	1.03E-33	2.42E-31	9.79E-30	7.26E-28	4.51E-26
190	9.30E-37	1.13E-34	1.15E-32	2.11E-30	6.78E-29	4.01E-27	2.02E-25
200	1.31E-35	1.26E-33	1.02E-31	1.49E-29	3.89E-28	1.88E-26	7.82E-25
210	1.44E-34	1.12E-32	7.33E-31	8.83E-29	1.90E-27	7.65E-26	2.68E-24
220	1.28E-33	8.19E-32	4.44E-30	4.46E-28	8.09E-27	2.76E-25	8.23E-24
230	9.49E-33	5.07E-31	2.31E-29	1.97E-27	3.05E-26	8.92E-25	2.31E-23
240	5.97E-32	2.71E-30	1.06E-28	7.70E-27	1.03E-25	2.63E-24	5.97E-23
250	3.25E-31	1.27E-29	4.28E-28	2.72E-26	3.20E-25	7.15E-24	1.44E-22
260	1.56E-30	5.31E-29	1.56E-27	8.73E-26	9.09E-25	1.81E-23	3.24E-22
270	6.71E-30	2.00E-28	5.21E-27	2.58E-25	2.40E-24	4.27E-23	6.92E-22
273.15	1.04E-29	2.98E-28	7.49E-27	3.58E-25	3.21E-24	5.54E-23	8.69E-22
280	2.60E-29	6.90E-28	1.60E-26	7.09E-25	5.93E-24	9.55E-23	1.40E-21
290	9.24E-29	2.19E-27	4.56E-26	1.82E-24	1.38E-23	2.02E-22	2.72E-21
300	3.02E-28	6.45E-27	1.22E-25	4.42E-24	3.06E-23	4.09E-22	5.06E-21
310	9.17E-28	1.78E-26	3.05E-25	1.01E-23	6.44E-23	7.94E-22	9.06E-21
320	2.61E-27	4.62E-26	7.26E-25	2.21E-23	1.30E-22	1.48E-21	1.57E-20
340	1.76E-26	2.65E-25	3.54E-24	9.26E-23	4.69E-22	4.65E-21	4.30E-20
350	4.24E-26	5.90E-25	7.34E-24	1.79E-22	8.47E-22	7.87E-21	6.85E-20
360	9.73E-26	1.26E-24	1.46E-23	3.34E-22	1.48E-21	1.30E-20	1.07E-19
380	4.53E-25	5.14E-24	5.25E-23	1.06E-21	4.19E-21	3.27E-20	2.42E-19
400	1.82E-24	1.83E-23	1.67E-22	3.02E-21	1.08E-20	7.59E-20	5.09E-19

**Table S119.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-1.54 ~ -0.51 V/nm); positive direction of Z-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	3.63E-48	3.34E-45	2.30E-42	2.77E-39	3.81E-37	7.47E-35	1.87E-32
110	3.08E-47	2.73E-44	1.80E-41	2.15E-38	2.90E-36	5.79E-34	1.45E-31
120	3.88E-46	3.10E-43	1.88E-40	2.13E-37	2.74E-35	5.51E-33	1.28E-30
130	7.98E-45	5.43E-42	2.86E-39	2.85E-36	3.30E-34	6.13E-32	1.19E-29
140	2.60E-43	1.39E-40	5.81E-38	4.57E-35	4.35E-33	6.78E-31	1.03E-28
150	1.02E-41	3.98E-39	1.23E-36	7.11E-34	5.30E-32	6.55E-30	7.66E-28
160	3.54E-40	9.95E-38	2.23E-35	9.45E-33	5.44E-31	5.29E-29	4.78E-27
170	9.51E-39	1.96E-36	3.25E-34	1.03E-31	4.60E-30	3.55E-28	2.52E-26
180	1.92E-37	2.97E-35	3.76E-33	9.05E-31	3.22E-29	2.00E-27	1.14E-25
190	2.97E-36	3.55E-34	3.50E-32	6.60E-30	1.90E-28	9.67E-27	4.51E-25
200	3.60E-35	3.41E-33	2.68E-31	4.05E-29	9.60E-28	4.07E-26	1.58E-24
210	3.52E-34	2.69E-32	1.73E-30	2.13E-28	4.23E-27	1.52E-25	5.00E-24
220	2.84E-33	1.79E-31	9.53E-30	9.81E-28	1.65E-26	5.08E-25	1.44E-23
230	1.94E-32	1.02E-30	4.59E-29	4.00E-27	5.80E-26	1.55E-24	3.80E-23
240	1.14E-31	5.11E-30	1.96E-28	1.46E-26	1.85E-25	4.33E-24	9.36E-23
250	5.85E-31	2.26E-29	7.51E-28	4.87E-26	5.43E-25	1.13E-23	2.16E-22
260	2.67E-30	9.00E-29	2.61E-27	1.49E-25	1.47E-24	2.73E-23	4.70E-22
270	1.10E-29	3.25E-28	8.35E-27	4.22E-25	3.74E-24	6.26E-23	9.71E-22
273.15	1.68E-29	4.79E-28	1.18E-26	5.78E-25	4.96E-24	8.03E-23	1.21E-21
280	4.10E-29	1.08E-27	2.47E-26	1.12E-24	8.94E-24	1.36E-22	1.91E-21
290	1.41E-28	3.31E-27	6.81E-26	2.78E-24	2.02E-23	2.80E-22	3.62E-21
300	4.46E-28	9.48E-27	1.76E-25	6.52E-24	4.34E-23	5.53E-22	6.58E-21
310	1.32E-27	2.54E-26	4.31E-25	1.46E-23	8.93E-23	1.05E-21	1.16E-20
320	3.66E-27	6.45E-26	1.00E-24	3.11E-23	1.76E-22	1.92E-21	1.96E-20
340	2.37E-26	3.55E-25	4.69E-24	1.25E-22	6.13E-22	5.84E-21	5.23E-20
350	5.61E-26	7.77E-25	9.55E-24	2.37E-22	1.09E-21	9.75E-21	8.22E-20
360	1.27E-25	1.63E-24	1.87E-23	4.35E-22	1.88E-21	1.59E-20	1.26E-19
380	5.72E-25	6.48E-24	6.54E-23	1.34E-21	5.17E-21	3.92E-20	2.81E-19
400	2.24E-24	2.26E-23	2.03E-22	3.73E-21	1.30E-20	8.91E-20	5.81E-19

**Table S120.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of isotopic ( $^{13}\text{C}$ )  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-1.54 ~ -0.51 V/nm); positive direction of X-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	2.97E-44	2.84E-45	7.67E-46	1.66E-45	7.43E-46	2.66E-45	2.79E-44
110	1.44E-41	1.68E-42	5.02E-43	1.24E-42	4.85E-43	1.57E-42	1.36E-41
120	2.50E-39	3.45E-40	1.12E-40	3.09E-40	1.08E-40	3.22E-40	2.36E-39
130	1.97E-37	3.13E-38	1.09E-38	3.33E-38	1.05E-38	2.92E-38	1.87E-37
140	8.34E-36	1.50E-36	5.57E-37	1.86E-36	5.32E-37	1.40E-36	7.93E-36
150	2.15E-34	4.30E-35	1.69E-35	6.11E-35	1.61E-35	4.00E-35	2.05E-34
160	3.71E-33	8.15E-34	3.35E-34	1.31E-33	3.18E-34	7.57E-34	3.54E-33
170	4.60E-32	1.10E-32	4.69E-33	1.98E-32	4.46E-33	1.02E-32	4.39E-32
180	4.32E-31	1.11E-31	4.93E-32	2.22E-31	4.67E-32	1.03E-31	4.13E-31
190	3.21E-30	8.81E-31	4.06E-31	1.95E-30	3.84E-31	8.16E-31	3.08E-30
200	1.96E-29	5.71E-30	2.71E-30	1.38E-29	2.56E-30	5.29E-30	1.88E-29
210	1.01E-28	3.11E-29	1.52E-29	8.19E-29	1.43E-29	2.88E-29	9.72E-29
220	4.51E-28	1.45E-28	7.30E-29	4.15E-28	6.88E-29	1.35E-28	4.33E-28
230	1.77E-27	5.96E-28	3.07E-28	1.84E-27	2.89E-28	5.52E-28	1.70E-27
240	6.19E-27	2.18E-27	1.15E-27	7.21E-27	1.08E-27	2.02E-27	5.96E-27
250	1.97E-26	7.20E-27	3.87E-27	2.55E-26	3.64E-27	6.66E-27	1.90E-26
260	5.74E-26	2.17E-26	1.19E-26	8.20E-26	1.12E-26	2.01E-26	5.53E-26
270	1.55E-25	6.06E-26	3.38E-26	2.43E-25	3.18E-26	5.60E-26	1.49E-25
273.15	2.08E-25	8.25E-26	4.63E-26	3.37E-25	4.35E-26	7.63E-26	2.01E-25
280	3.90E-25	1.57E-25	8.93E-26	6.69E-25	8.39E-26	1.46E-25	3.76E-25
290	9.22E-25	3.84E-25	2.21E-25	1.72E-24	2.07E-25	3.54E-25	8.91E-25
300	2.06E-24	8.82E-25	5.16E-25	4.18E-24	4.84E-25	8.15E-25	1.99E-24
310	4.39E-24	1.93E-24	1.14E-24	9.60E-24	1.07E-24	1.78E-24	4.25E-24
320	8.93E-24	4.01E-24	2.41E-24	2.10E-23	2.26E-24	3.70E-24	8.64E-24
340	3.27E-23	1.53E-23	9.46E-24	8.82E-23	8.86E-24	1.42E-23	3.17E-23
350	5.93E-23	2.84E-23	1.77E-23	1.70E-22	1.66E-23	2.62E-23	5.74E-23
360	1.04E-22	5.09E-23	3.21E-23	3.18E-22	3.00E-23	4.69E-23	1.01E-22
380	2.95E-22	1.49E-22	9.60E-23	1.01E-21	8.98E-23	1.38E-22	2.86E-22
400	7.57E-22	3.95E-22	2.59E-22	2.89E-21	2.42E-22	3.65E-22	7.35E-22

**Table S121.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of isotopic ( $^{13}\text{C}$ )  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-1.54 ~ -0.51 V/nm); positive direction of X-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	X-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	7.00E-35	1.16E-38	3.22E-40	6.40E-40	3.43E-40	6.19E-39	3.98E-35
110	1.55E-34	5.81E-38	2.63E-39	6.00E-39	2.84E-39	3.28E-38	9.30E-35
120	4.66E-34	4.28E-37	3.19E-38	7.82E-38	3.36E-38	2.63E-37	3.00E-34
130	1.92E-33	4.54E-36	5.36E-37	1.40E-36	5.45E-37	3.08E-36	1.34E-33
140	1.03E-32	5.93E-35	9.82E-36	2.79E-35	9.74E-36	4.34E-35	7.76E-33
150	6.50E-32	7.67E-34	1.59E-34	4.96E-34	1.56E-34	5.92E-34	5.16E-32
160	4.24E-31	8.61E-33	2.09E-33	7.12E-33	2.03E-33	6.87E-33	3.48E-31
170	2.61E-30	8.00E-32	2.19E-32	8.11E-32	2.11E-32	6.53E-32	2.20E-30
180	1.46E-29	6.14E-31	1.85E-31	7.41E-31	1.77E-31	5.10E-31	1.25E-29
190	7.23E-29	3.94E-30	1.28E-30	5.53E-30	1.23E-30	3.31E-30	6.27E-29
200	3.19E-28	2.15E-29	7.49E-30	3.46E-29	7.14E-30	1.83E-29	2.79E-28
210	1.25E-27	1.02E-28	3.75E-29	1.85E-28	3.57E-29	8.70E-29	1.11E-27
220	4.45E-27	4.23E-28	1.64E-28	8.60E-28	1.56E-28	3.64E-28	3.96E-27
230	1.44E-26	1.57E-27	6.38E-28	3.54E-27	6.04E-28	1.36E-27	1.29E-26
240	4.27E-26	5.26E-27	2.23E-27	1.31E-26	2.11E-27	4.58E-27	3.84E-26
250	1.17E-25	1.61E-26	7.10E-27	4.38E-26	6.71E-27	1.41E-26	1.06E-25
260	3.00E-25	4.57E-26	2.08E-26	1.35E-25	1.96E-26	4.01E-26	2.73E-25
270	7.22E-25	1.20E-25	5.65E-26	3.84E-25	5.33E-26	1.06E-25	6.59E-25
273.15	9.40E-25	1.61E-25	7.63E-26	5.26E-25	7.19E-26	1.42E-25	8.59E-25
280	1.64E-24	2.97E-25	1.44E-25	1.02E-24	1.35E-25	2.62E-25	1.50E-24
290	3.54E-24	6.91E-25	3.43E-25	2.55E-24	3.23E-25	6.13E-25	3.25E-24
300	7.29E-24	1.53E-24	7.77E-25	6.01E-24	7.31E-25	1.36E-24	6.72E-24
310	1.44E-23	3.22E-24	1.67E-24	1.35E-23	1.57E-24	2.86E-24	1.33E-23
320	2.73E-23	6.48E-24	3.44E-24	2.88E-23	3.24E-24	5.78E-24	2.53E-23
340	8.87E-23	2.34E-23	1.29E-23	1.16E-22	1.21E-23	2.10E-23	8.27E-23
350	1.53E-22	4.23E-23	2.38E-23	2.21E-22	2.23E-23	3.80E-23	1.42E-22
360	2.55E-22	7.41E-23	4.23E-23	4.07E-22	3.97E-23	6.66E-23	2.39E-22
380	6.64E-22	2.09E-22	1.23E-22	1.26E-21	1.15E-22	1.88E-22	6.23E-22
400	1.58E-21	5.35E-22	3.24E-22	3.52E-21	3.03E-22	4.83E-22	1.49E-21

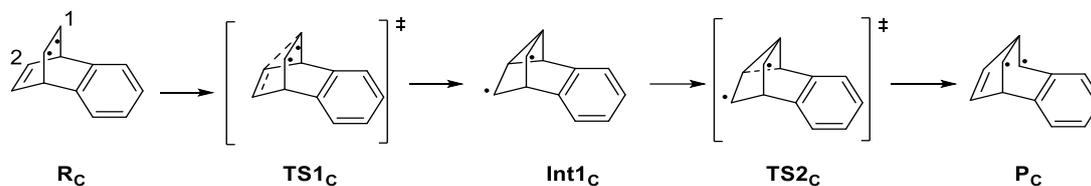
**Table S122.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of isotopic ( $^{13}\text{C}$ )  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-1.54 ~ -0.51 V/nm); positive direction of Z-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	3.04E-57	2.69E-53	1.70E-49	1.66E-45	2.36E-42	5.38E-39	8.44E-36
110	2.46E-53	9.58E-50	2.74E-46	1.24E-42	8.55E-40	9.68E-37	7.84E-34
120	4.50E-50	8.82E-47	1.30E-43	3.09E-40	1.17E-37	7.41E-35	3.46E-32
130	2.61E-47	2.86E-44	2.42E-41	3.33E-38	7.62E-36	2.93E-33	8.60E-31
140	6.16E-45	4.11E-42	2.15E-39	1.86E-36	2.75E-34	6.94E-32	1.36E-29
150	7.07E-43	3.07E-40	1.06E-37	6.11E-35	6.22E-33	1.09E-30	1.52E-28
160	4.52E-41	1.35E-38	3.23E-36	1.31E-33	9.59E-32	1.22E-29	1.26E-27
170	1.79E-39	3.82E-37	6.64E-35	1.98E-32	1.08E-30	1.03E-28	8.16E-27
180	4.73E-38	7.51E-36	9.83E-34	2.22E-31	9.37E-30	6.95E-28	4.34E-26
190	8.91E-37	1.09E-34	1.10E-32	1.95E-30	6.51E-29	3.86E-27	1.95E-25
200	1.26E-35	1.21E-33	9.78E-32	1.38E-29	3.75E-28	1.82E-26	7.56E-25
210	1.39E-34	1.08E-32	7.08E-31	8.19E-29	1.84E-27	7.41E-26	2.60E-24
220	1.24E-33	7.94E-32	4.30E-30	4.15E-28	7.86E-27	2.68E-25	8.02E-24
230	9.22E-33	4.93E-31	2.25E-29	1.84E-27	2.97E-26	8.69E-25	2.25E-23
240	5.81E-32	2.64E-30	1.03E-28	7.21E-27	1.01E-25	2.57E-24	5.84E-23
250	3.18E-31	1.24E-29	4.18E-28	2.55E-26	3.13E-25	7.00E-24	1.41E-22
260	1.53E-30	5.20E-29	1.53E-27	8.20E-26	8.91E-25	1.77E-23	3.19E-22
270	6.58E-30	1.97E-28	5.11E-27	2.43E-25	2.36E-24	4.20E-23	6.81E-22
273.15	1.02E-29	2.93E-28	7.34E-27	3.37E-25	3.16E-24	5.45E-23	8.56E-22
280	2.56E-29	6.78E-28	1.57E-26	6.69E-25	5.84E-24	9.40E-23	1.38E-21
290	9.09E-29	2.16E-27	4.49E-26	1.72E-24	1.36E-23	2.00E-22	2.69E-21
300	2.98E-28	6.37E-27	1.20E-25	4.18E-24	3.02E-23	4.05E-22	4.99E-21
310	9.05E-28	1.76E-26	3.01E-25	9.60E-24	6.37E-23	7.86E-22	8.96E-21
320	2.58E-27	4.57E-26	7.17E-25	2.10E-23	1.28E-22	1.47E-21	1.55E-20
340	1.75E-26	2.62E-25	3.51E-24	8.82E-23	4.66E-22	4.62E-21	4.28E-20
350	4.21E-26	5.86E-25	7.28E-24	1.70E-22	8.42E-22	7.83E-21	6.82E-20
360	9.67E-26	1.25E-24	1.45E-23	3.18E-22	1.48E-21	1.29E-20	1.06E-19
380	4.50E-25	5.12E-24	5.22E-23	1.01E-21	4.19E-21	3.27E-20	2.41E-19
400	1.81E-24	1.83E-23	1.66E-22	2.89E-21	1.08E-20	7.59E-20	5.09E-19

**Table S123.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{cm}^3/\text{molecule}^{-1}\text{s}^{-1}$ ) of isotopic ( $^{13}\text{C}$ )  $\text{S}_{\text{N}}2$  reaction using M06-2X/6-31+G(d) method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-1.54 ~ -0.51 V/nm); positive direction of Z-EEF (0.51 ~ 1.54V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF						
	-1.54	-1.03	-0.51	0.0	0.51	1.03	1.54
100	4.08E-49	4.21E-46	4.47E-43	6.40E-40	1.07E-37	1.93E-35	6.52E-33
110	4.30E-48	4.31E-45	4.27E-42	6.00E-39	9.74E-37	2.08E-34	6.58E-32
120	7.76E-47	6.93E-44	6.01E-41	7.82E-38	1.19E-35	2.77E-33	7.43E-31
130	2.53E-45	1.88E-42	1.30E-39	1.40E-36	1.85E-34	3.93E-32	8.19E-30
140	1.26E-43	6.99E-41	3.47E-38	2.79E-35	2.92E-33	4.98E-31	7.82E-29
150	6.40E-42	2.51E-39	8.65E-37	4.96E-34	3.95E-32	5.22E-30	6.19E-28
160	2.55E-40	7.12E-38	1.73E-35	7.12E-33	4.33E-31	4.42E-29	4.02E-27
170	7.39E-39	1.51E-36	2.66E-34	8.11E-32	3.82E-30	3.06E-28	2.18E-26
180	1.57E-37	2.40E-35	3.19E-33	7.41E-31	2.76E-29	1.77E-27	1.01E-25
190	2.50E-36	2.96E-34	3.04E-32	5.53E-30	1.66E-28	8.70E-27	4.05E-25
200	3.11E-35	2.92E-33	2.38E-31	3.46E-29	8.56E-28	3.71E-26	1.44E-24
210	3.10E-34	2.35E-32	1.55E-30	1.85E-28	3.83E-27	1.40E-25	4.59E-24
220	2.54E-33	1.59E-31	8.68E-30	8.60E-28	1.51E-26	4.73E-25	1.33E-23
230	1.75E-32	9.19E-31	4.22E-29	3.54E-27	5.36E-26	1.45E-24	3.56E-23
240	1.04E-31	4.64E-30	1.82E-28	1.31E-26	1.72E-25	4.09E-24	8.81E-23
250	5.39E-31	2.07E-29	7.02E-28	4.38E-26	5.09E-25	1.07E-23	2.04E-22
260	2.48E-30	8.32E-29	2.46E-27	1.35E-25	1.39E-24	2.61E-23	4.47E-22
270	1.03E-29	3.03E-28	7.90E-27	3.84E-25	3.55E-24	6.00E-23	9.28E-22
273.15	1.57E-29	4.47E-28	1.12E-26	5.26E-25	4.71E-24	7.71E-23	1.16E-21
280	3.86E-29	1.01E-27	2.35E-26	1.02E-24	8.52E-24	1.31E-22	1.84E-21
290	1.33E-28	3.12E-27	6.50E-26	2.55E-24	1.93E-23	2.71E-22	3.48E-21
300	4.23E-28	8.97E-27	1.69E-25	6.01E-24	4.17E-23	5.36E-22	6.35E-21
310	1.26E-27	2.42E-26	4.15E-25	1.35E-23	8.61E-23	1.02E-21	1.12E-20
320	3.50E-27	6.16E-26	9.66E-25	2.88E-23	1.70E-22	1.87E-21	1.91E-20
340	2.29E-26	3.41E-25	4.55E-24	1.16E-22	5.96E-22	5.72E-21	5.12E-20
350	5.42E-26	7.50E-25	9.29E-24	2.21E-22	1.06E-21	9.57E-21	8.06E-20
360	1.23E-25	1.58E-24	1.83E-23	4.07E-22	1.84E-21	1.56E-20	1.24E-19
380	5.57E-25	6.29E-24	6.40E-23	1.26E-21	5.08E-21	3.87E-20	2.77E-19
400	2.19E-24	2.20E-23	2.00E-22	3.52E-21	1.28E-20	8.82E-20	5.74E-19

## 2.4 Triplet Di- $\pi$ -Methane (DPM) Rearrangement



**Figure S71.** Schematic reaction pathway for the triplet Di- $\pi$ -methane (DPM) rearrangement

**Table S124.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) comparison of triplet Di- $\pi$ -methane rearrangement using different DFT functionals and basis sets. The values in parentheses are relative to the high-level results calculated by DLPNO-CCSD(T1)/aug-cc-pVTZ// $\omega$ B97X-D/6-31G(d) method

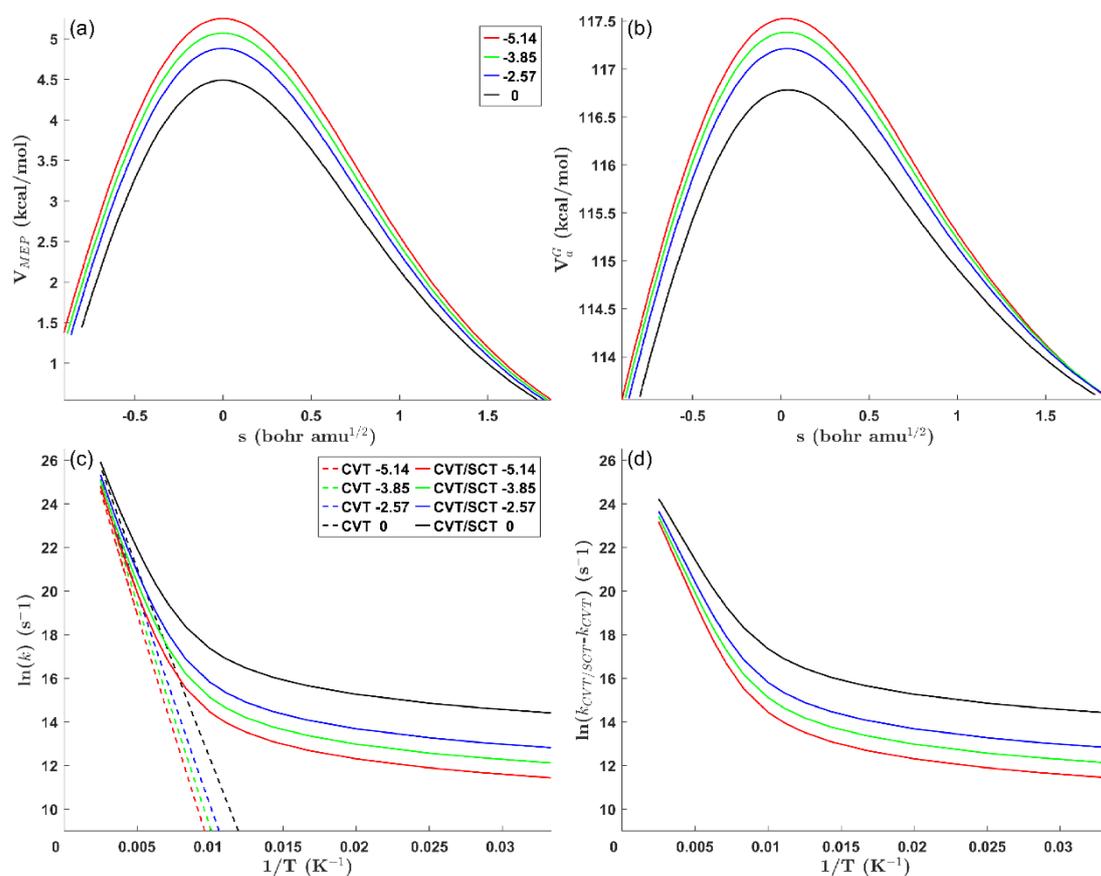
Methods (gas phase)	TS1 $\Delta E$	TS2 $\Delta E$
DLPNO-CCSD(T1)	4.51(0.00)	-5.64(0.00)
$\omega$ B97X-D/6-31G(d)	4.49(0.02)	-4.65(0.99)
M06-2X/6-31G(d)	6.00(1.49)	-3.85(1.79)
B3LYP-D3/6-31G(d)	1.68(2.83)	-4.44(1.20)

**Table S125.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method under different EEF strengths (V/nm). The  $\Omega$  (in  $\text{cm}^{-1}$ ) is the magnitude of the imaginary frequency for the transition state, and  $T_c$  is the crossover temperature (in K).

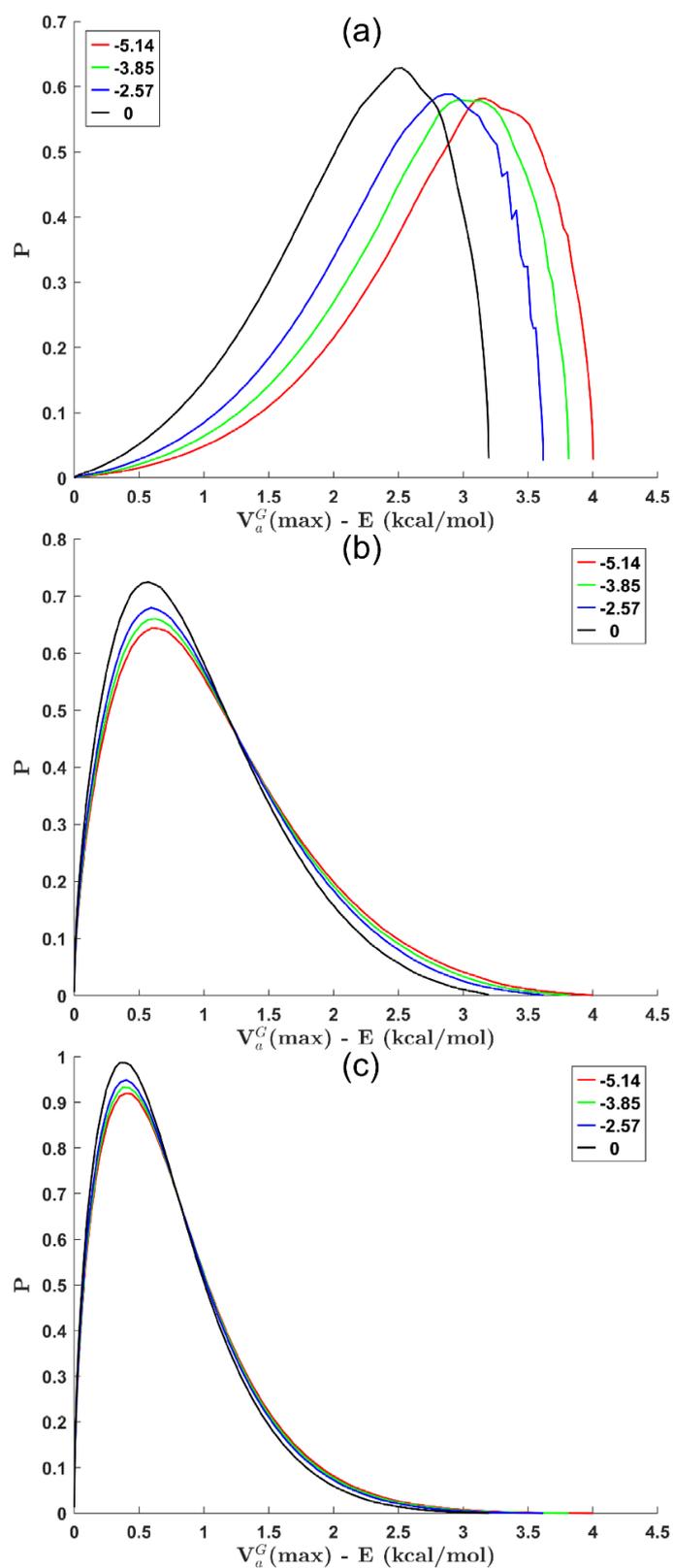
EEF (V/nm)	-5.14	-3.85	-2.57	0.0
<b>X-EEF Direction</b>				
$\Delta E$	5.25	5.07	4.88	4.49
$\Delta V_a^G(\max)$	117.52	117.38	117.21	116.78
$\Omega$	631	626	622	611
$T_c$	144	143	142	140
<b>Y-EEF Direction</b>				
$\Delta E$	3.82	3.99	4.16	4.49
$\Delta V_a^G(\max)$	116.10	116.30	116.48	116.78
$\Omega$	582	590	598	611
$T_c$	133	135	137	140
<b>Z-EEF Direction</b>				
$\Delta E$	3.13	3.53	3.88	4.49
$\Delta V_a^G(\max)$	115.20	115.68	116.10	116.78
$\Omega$	549	570	588	611
$T_c$	126	131	135	140

**Table S126.** Mulliken atomic charge of C-C bond formation reactant for the first step (TS1) of DPM rearrangement of benzobarrelene under X-, Y- and Z-EEF with various strengths

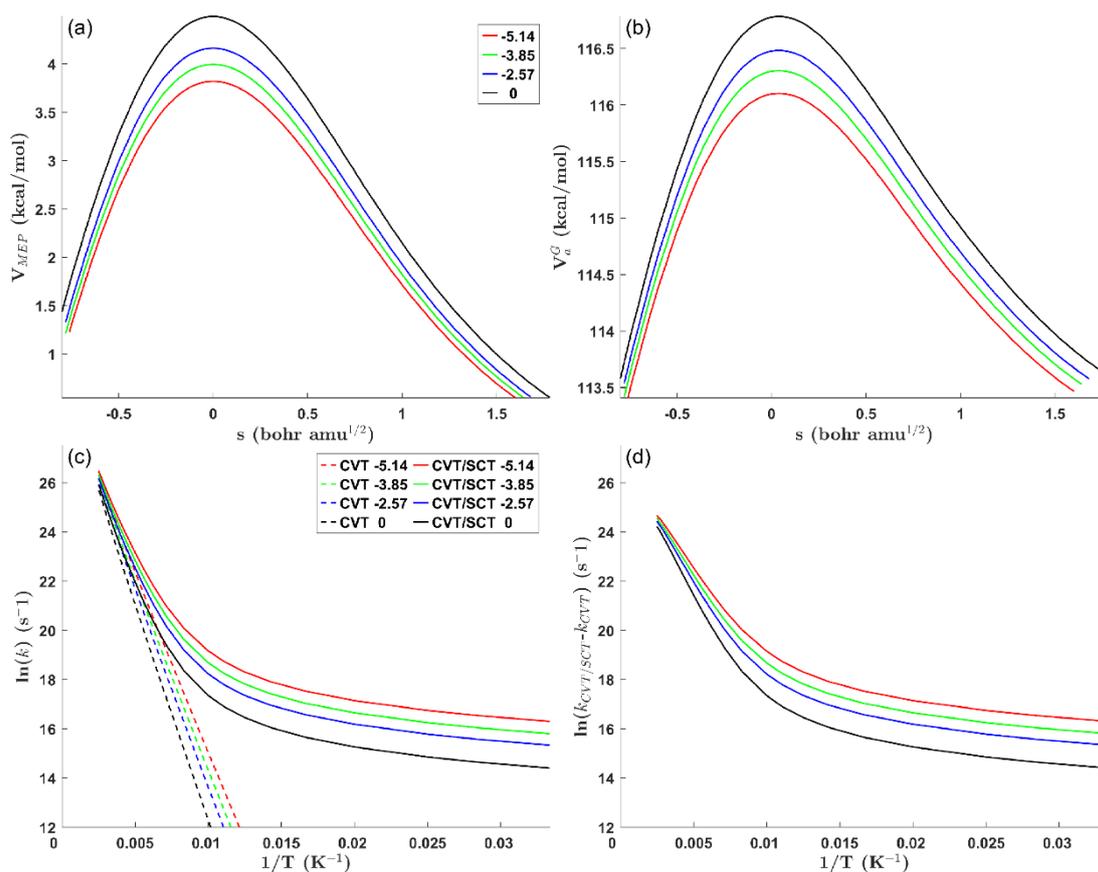
EEF (V/nm)	-5.14	-3.85	-2.57	0.0
	<b>X-EEF Direction</b>			
C1	-0.12	-0.12	-0.13	-0.13
C3	-0.14	-0.14	-0.14	-0.14
	<b>Y-EEF Direction</b>			
C1	-0.13	-0.13	-0.13	-0.13
C3	-0.13	-0.14	-0.14	-0.14
	<b>Z-EEF Direction</b>			
C1	-0.11	-0.11	-0.12	-0.13
C3	-0.15	-0.15	-0.15	-0.14



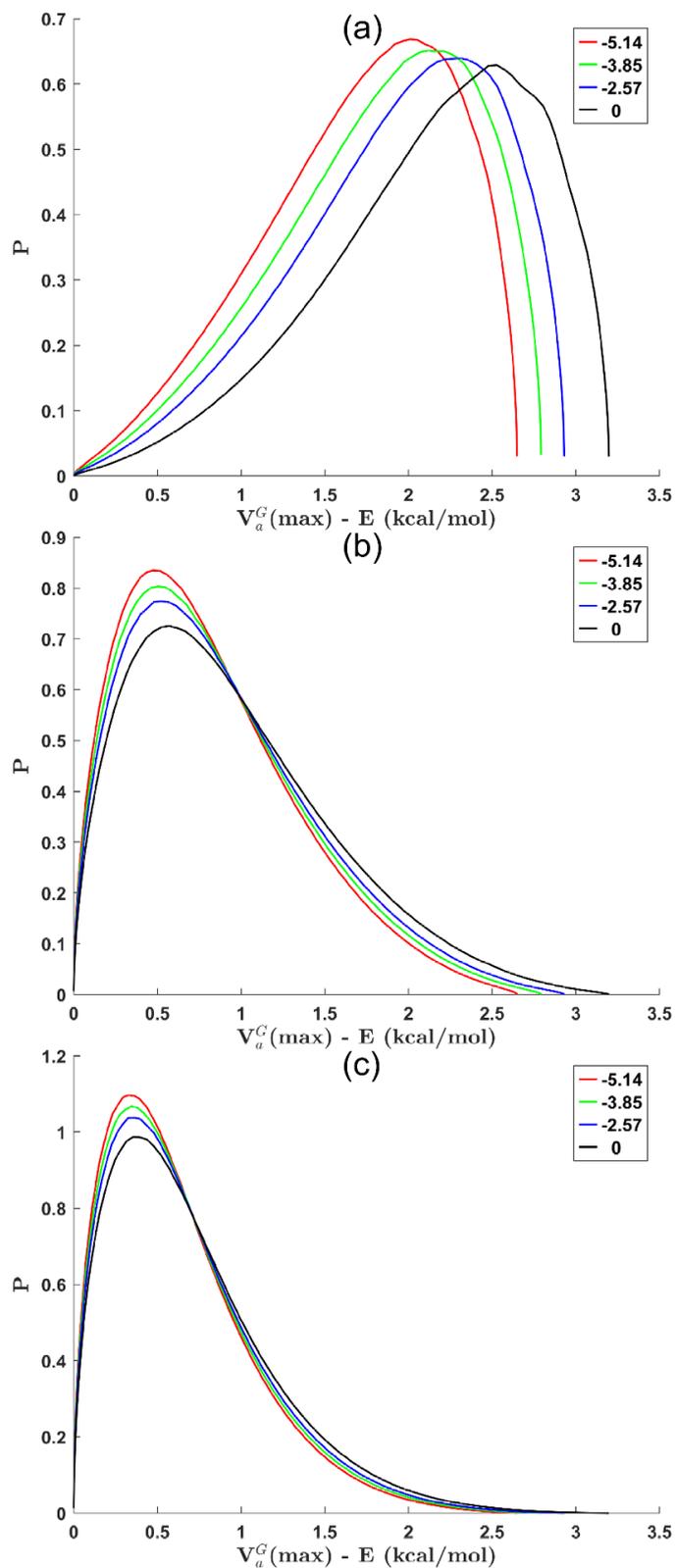
**Figure S72.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method along the X-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm)).



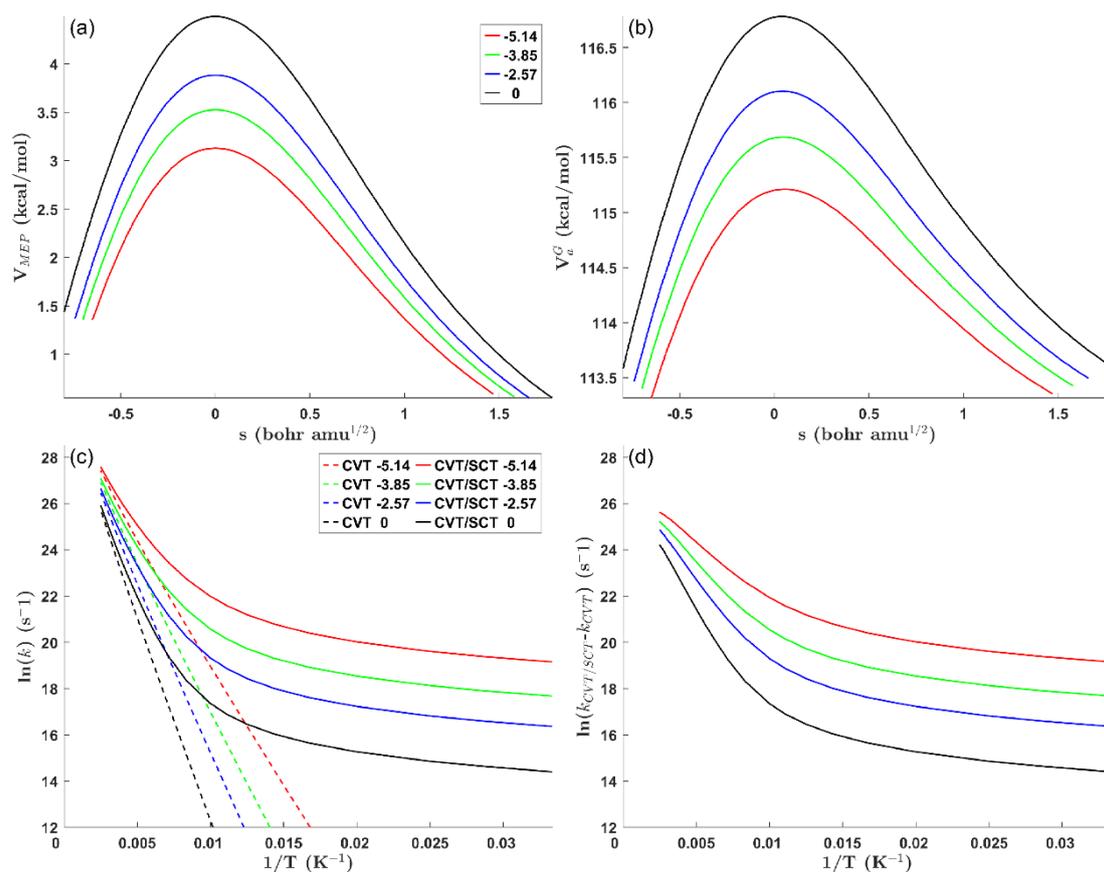
**Figure S73.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the X-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm)).



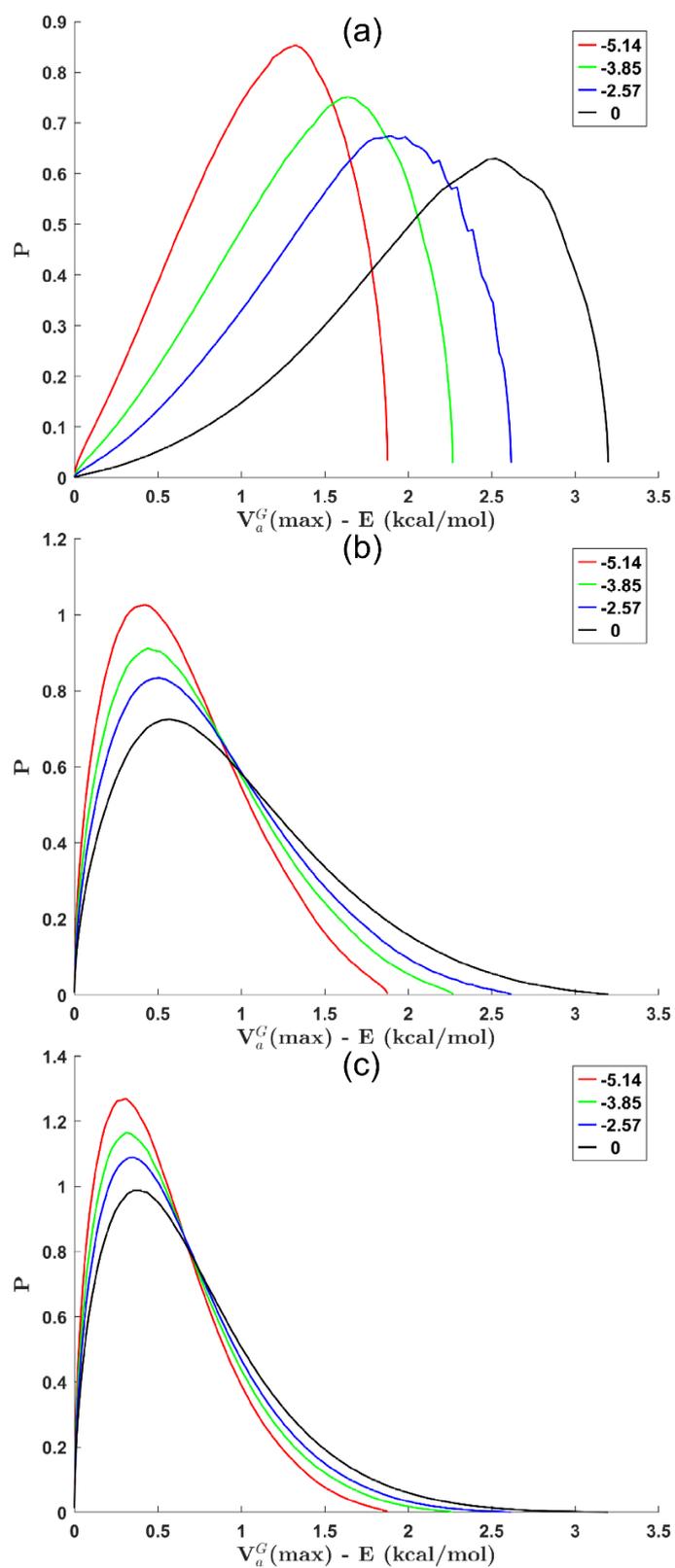
**Figure S74.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method along the Y-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm))



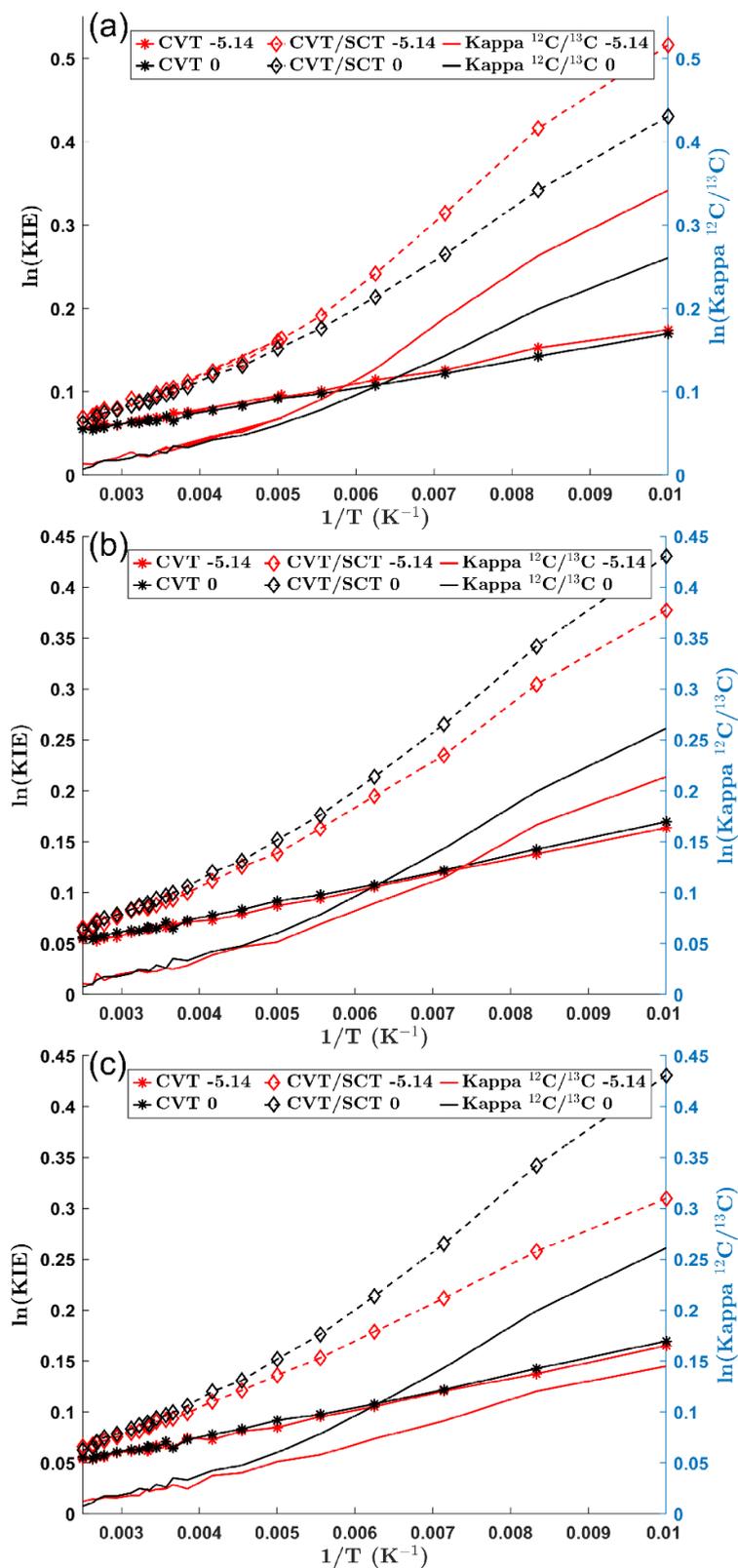
**Figure S75.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the Y-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S76.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method along the Z-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm))



**Figure S77.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the Y-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0.0 V/nm)).



**Figure S78.** Arrhenius plots of  $\ln(\text{KIE})$  ( $^{12}\text{C}/^{13}\text{C}$ ) and  $\ln(\kappa(^{12}\text{C})/\kappa(^{13}\text{C}))$  versus  $1/T$  of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D}/6\text{-}31\text{G(d)}$  method along direction (a) X-EEF (b) Y-EEF (c) Z-EEF with different strengths (red:  $-5.14$  V/nm and black: no field ( $0.0$  V/nm)).

**Table S127.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF			
	-5.14	-3.85	-2.57	0.0
30	4.28E-18	1.02E-16	2.75E-15	3.20E-12
35	7.33E-14	1.11E-12	1.87E-11	7.93E-09
40	1.12E-10	1.20E-09	1.42E-08	2.84E-06
50	3.30E-06	2.21E-05	1.60E-04	1.11E-02
60	3.27E-03	1.59E-02	8.30E-02	2.84E+00
70	4.62E-01	1.80E+00	7.39E+00	1.53E+02
80	1.92E+01	6.32E+01	2.18E+02	3.10E+03
90	3.55E+02	1.02E+03	3.08E+03	3.27E+04
100	3.69E+03	9.58E+03	2.59E+04	2.18E+05
120	1.27E+05	2.81E+05	6.45E+05	3.84E+06
140	1.61E+06	3.20E+06	6.55E+06	3.05E+07
160	1.11E+07	2.02E+07	3.79E+07	1.47E+08
180	5.01E+07	8.57E+07	1.50E+08	5.05E+08
200	1.69E+08	2.75E+08	4.57E+08	1.37E+09
220	4.61E+08	7.19E+08	1.14E+09	3.13E+09
240	1.07E+09	1.61E+09	2.47E+09	6.28E+09
260	2.20E+09	3.21E+09	4.78E+09	1.14E+10
273.15	3.34E+09	4.79E+09	7.00E+09	1.60E+10
280	4.08E+09	5.82E+09	8.43E+09	1.90E+10
290	5.40E+09	7.60E+09	1.09E+10	2.39E+10
298.15	1.53E+08	9.34E+09	1.33E+10	2.86E+10
300	7.02E+09	9.77E+09	1.38E+10	2.97E+10
310	8.97E+09	1.24E+10	1.73E+10	3.64E+10
320	1.13E+10	1.54E+10	2.14E+10	4.42E+10
340	1.72E+10	2.32E+10	3.16E+10	6.28E+10
360	2.52E+10	3.33E+10	4.48E+10	8.60E+10
373.15	3.16E+10	4.14E+10	5.52E+10	1.04E+11
380	3.54E+10	4.62E+10	6.12E+10	1.14E+11
400	4.81E+10	6.21E+10	8.12E+10	1.48E+11

**Table S128.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF			
	-5.14	-3.85	-2.57	0.0
30	9.27E+04	1.83E+05	3.67E+05	1.80E+06
35	1.17E+05	2.31E+05	4.65E+05	2.28E+06
40	1.46E+05	2.87E+05	5.80E+05	2.83E+06
50	2.20E+05	4.32E+05	8.75E+05	4.25E+06
60	3.27E+05	6.41E+05	1.30E+06	6.28E+06
70	4.87E+05	9.53E+05	1.93E+06	9.29E+06
80	7.38E+05	1.44E+06	2.92E+06	1.40E+07
90	1.15E+06	2.25E+06	4.54E+06	2.15E+07
100	1.86E+06	3.64E+06	7.33E+06	3.43E+07
120	5.61E+06	1.08E+07	2.13E+07	9.36E+07
140	1.89E+07	3.49E+07	6.63E+07	2.62E+08
160	6.15E+07	1.08E+08	1.95E+08	6.86E+08
180	1.78E+08	2.99E+08	5.11E+08	1.61E+09
200	4.52E+08	7.25E+08	1.18E+09	3.41E+09
220	1.01E+09	1.56E+09	2.46E+09	6.52E+09
240	2.05E+09	3.05E+09	4.64E+09	1.15E+10
260	3.78E+09	5.48E+09	8.10E+09	1.89E+10
273.15	5.43E+09	7.75E+09	1.13E+10	2.53E+10
280	6.48E+09	9.18E+09	1.32E+10	2.93E+10
290	8.28E+09	1.16E+10	1.65E+10	3.58E+10
298.15	4.17E+08	1.39E+10	1.97E+10	4.17E+10
300	1.04E+10	1.45E+10	2.04E+10	4.32E+10
310	1.30E+10	1.78E+10	2.49E+10	5.17E+10
320	1.60E+10	2.17E+10	3.01E+10	6.12E+10
340	2.34E+10	3.13E+10	4.26E+10	8.37E+10
360	3.30E+10	4.35E+10	5.83E+10	1.11E+11
373.15	4.06E+10	5.31E+10	7.05E+10	1.32E+11
380	4.50E+10	5.87E+10	7.75E+10	1.43E+11
400	5.98E+10	7.70E+10	1.00E+11	1.81E+11

**Table S129.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF			
	-5.14	-3.85	-2.57	0.0
30	3.14E-08	2.84E-09	2.81E-10	3.20E-12
35	2.10E-05	2.67E-06	3.68E-07	7.93E-09
40	2.80E-03	4.62E-04	8.15E-05	2.84E-06
50	2.75E+00	6.50E-01	1.62E-01	1.11E-02
60	2.81E+02	8.44E+01	2.66E+01	2.84E+00
70	7.83E+03	2.80E+03	1.04E+03	1.53E+02
80	9.67E+04	3.93E+04	1.66E+04	3.10E+03
90	6.93E+05	3.12E+05	1.45E+05	3.27E+04
100	3.38E+06	1.65E+06	8.28E+05	2.18E+05
120	3.73E+07	2.06E+07	1.16E+07	3.84E+06
140	2.12E+08	1.27E+08	7.82E+07	3.05E+07
160	7.91E+08	5.09E+08	3.33E+08	1.47E+08
180	2.23E+09	1.51E+09	1.04E+09	5.05E+08
200	5.16E+09	3.64E+09	2.61E+09	1.37E+09
220	1.03E+10	7.54E+09	5.57E+09	3.13E+09
240	1.85E+10	1.39E+10	1.06E+10	6.28E+09
260	3.05E+10	2.35E+10	1.83E+10	1.14E+10
273.15	4.07E+10	3.18E+10	2.51E+10	1.60E+10
280	4.69E+10	3.69E+10	2.93E+10	1.90E+10
290	5.70E+10	4.53E+10	3.63E+10	2.39E+10
298.15	6.62E+10	5.29E+10	4.28E+10	2.86E+10
300	6.84E+10	5.48E+10	4.43E+10	2.97E+10
310	8.12E+10	6.56E+10	5.35E+10	3.64E+10
320	9.54E+10	7.77E+10	6.39E+10	4.42E+10
340	1.28E+11	1.06E+11	8.84E+10	6.28E+10
360	1.67E+11	1.40E+11	1.18E+11	8.60E+10
373.15	1.96E+11	1.66E+11	1.41E+11	1.04E+11
380	2.13E+11	1.80E+11	1.54E+11	1.14E+11
400	2.64E+11	2.26E+11	1.95E+11	1.48E+11

**Table S130.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

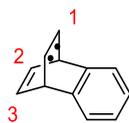
T(K)	Y-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.20E+07	7.29E+06	4.58E+06	1.80E+06
35	1.51E+07	9.18E+06	5.76E+06	2.28E+06
40	1.87E+07	1.14E+07	7.14E+06	2.83E+06
50	2.79E+07	1.70E+07	1.07E+07	4.25E+06
60	4.09E+07	2.49E+07	1.57E+07	6.28E+06
70	5.99E+07	3.66E+07	2.30E+07	9.29E+06
80	8.90E+07	5.45E+07	3.43E+07	1.40E+07
90	1.35E+08	8.30E+07	5.25E+07	2.15E+07
100	2.10E+08	1.30E+08	8.24E+07	3.43E+07
120	5.26E+08	3.33E+08	2.16E+08	9.36E+07
140	1.29E+09	8.49E+08	5.68E+08	2.62E+08
160	2.94E+09	2.00E+09	1.39E+09	6.86E+08
180	6.05E+09	4.27E+09	3.06E+09	1.61E+09
200	1.13E+10	8.23E+09	6.08E+09	3.41E+09
220	1.95E+10	1.46E+10	1.11E+10	6.52E+09
240	3.13E+10	2.40E+10	1.86E+10	1.15E+10
260	4.74E+10	3.71E+10	2.94E+10	1.89E+10
273.15	6.06E+10	4.81E+10	3.85E+10	2.53E+10
280	6.84E+10	5.46E+10	4.40E+10	2.93E+10
290	8.09E+10	6.51E+10	5.29E+10	3.58E+10
298.15	9.22E+10	7.46E+10	6.10E+10	4.17E+10
300	9.48E+10	7.69E+10	6.29E+10	4.32E+10
310	1.10E+11	8.99E+10	7.42E+10	5.17E+10
320	1.27E+11	1.04E+11	8.67E+10	6.12E+10
340	1.65E+11	1.38E+11	1.16E+11	8.37E+10
360	2.09E+11	1.76E+11	1.50E+11	1.11E+11
373.15	2.42E+11	2.05E+11	1.76E+11	1.32E+11
380	2.59E+11	2.21E+11	1.90E+11	1.43E+11
400	3.16E+11	2.72E+11	2.36E+11	1.81E+11

**Table S131.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.37E-02	1.91E-05	5.54E-08	3.20E-12
35	1.43E+00	5.11E-03	3.41E-05	7.93E-09
40	4.74E+01	3.43E-01	4.28E-03	2.84E-06
50	6.65E+03	1.29E+02	3.87E+00	1.11E-02
60	1.86E+05	6.95E+03	3.74E+02	2.84E+00
70	2.06E+06	1.23E+05	1.00E+04	1.53E+02
80	1.28E+07	1.08E+06	1.21E+05	3.10E+03
90	5.36E+07	5.97E+06	8.49E+05	3.27E+04
100	1.71E+08	2.37E+07	4.08E+06	2.18E+05
120	9.97E+08	1.91E+08	4.42E+07	3.84E+06
140	3.61E+09	8.73E+08	2.48E+08	3.05E+07
160	9.62E+09	2.77E+09	9.21E+08	1.47E+08
180	2.09E+10	6.91E+09	2.59E+09	5.05E+08
200	3.94E+10	1.45E+10	5.98E+09	1.37E+09
220	6.68E+10	2.68E+10	1.20E+10	3.13E+09
240	1.04E+11	4.50E+10	2.15E+10	6.28E+09
260	1.53E+11	7.03E+10	3.54E+10	1.14E+10
273.15	1.91E+11	9.11E+10	4.74E+10	1.60E+10
280	2.13E+11	1.03E+11	5.46E+10	1.90E+10
290	2.48E+11	1.23E+11	6.64E+10	2.39E+10
298.15	2.78E+11	1.41E+11	7.72E+10	2.86E+10
300	2.85E+11	1.45E+11	7.98E+10	2.97E+10
310	3.26E+11	1.69E+11	9.48E+10	3.64E+10
320	3.70E+11	1.95E+11	1.12E+11	4.42E+10
340	4.66E+11	2.55E+11	1.50E+11	6.28E+10
360	5.73E+11	3.24E+11	1.96E+11	8.60E+10
373.15	6.50E+11	3.74E+11	2.31E+11	1.04E+11
380	6.91E+11	4.02E+11	2.50E+11	1.14E+11
400	8.20E+11	4.89E+11	3.11E+11	1.48E+11

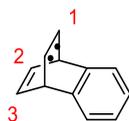
**Table S132.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF			
	-5.14	-3.85	-2.57	0.0
30	2.08E+08	4.73E+07	1.27E+07	1.80E+06
35	2.63E+08	5.98E+07	1.61E+07	2.28E+06
40	3.27E+08	7.44E+07	2.00E+07	2.83E+06
50	4.92E+08	1.12E+08	3.01E+07	4.25E+06
60	7.29E+08	1.66E+08	4.47E+07	6.28E+06
70	1.08E+09	2.46E+08	6.67E+07	9.29E+06
80	1.60E+09	3.69E+08	1.01E+08	1.40E+07
90	2.37E+09	5.60E+08	1.56E+08	2.15E+07
100	3.53E+09	8.59E+08	2.45E+08	3.43E+07
120	7.57E+09	2.02E+09	6.25E+08	9.36E+07
140	1.52E+10	4.52E+09	1.54E+09	2.62E+08
160	2.81E+10	9.30E+09	3.49E+09	6.86E+08
180	4.79E+10	1.75E+10	7.14E+09	1.61E+09
200	7.63E+10	3.02E+10	1.33E+10	3.41E+09
220	1.14E+11	4.86E+10	2.29E+10	6.52E+09
240	1.63E+11	7.38E+10	3.67E+10	1.15E+10
260	2.23E+11	1.07E+11	5.56E+10	1.89E+10
273.15	2.69E+11	1.33E+11	7.12E+10	2.53E+10
280	2.95E+11	1.48E+11	8.03E+10	2.93E+10
290	3.35E+11	1.71E+11	9.51E+10	3.58E+10
298.15	3.69E+11	1.92E+11	1.08E+11	4.17E+10
300	3.78E+11	1.97E+11	1.11E+11	4.32E+10
310	4.23E+11	2.25E+11	1.30E+11	5.17E+10
320	4.72E+11	2.56E+11	1.49E+11	6.12E+10
340	5.78E+11	3.23E+11	1.94E+11	8.37E+10
360	6.94E+11	4.00E+11	2.47E+11	1.11E+11
373.15	7.75E+11	4.55E+11	2.85E+11	1.32E+11
380	8.20E+11	4.85E+11	3.07E+11	1.43E+11
400	9.55E+11	5.79E+11	3.74E+11	1.81E+11



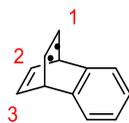
**Table S133.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $^{13}\text{C}$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF	
	-5.14	0.0
30	2.42E-18	1.82E-12
35	4.49E-14	4.90E-09
40	7.27E-11	1.86E-06
50	2.34E-06	7.90E-03
60	2.46E-03	2.14E+00
70	3.61E-01	1.20E+02
80	1.55E+01	2.51E+03
90	2.93E+02	2.71E+04
100	3.10E+03	1.84E+05
120	1.09E+05	3.33E+06
140	1.42E+06	2.70E+07
160	9.90E+06	1.32E+08
180	4.53E+07	4.58E+08
200	1.54E+08	1.25E+09
220	4.24E+08	2.88E+09
240	9.90E+08	5.81E+09
260	2.04E+09	1.06E+10
273.15	3.10E+09	1.50E+10
280	3.81E+09	1.77E+10
290	5.04E+09	2.24E+10
298.15	1.39E+08	2.68E+10
300	6.56E+09	2.78E+10
310	8.40E+09	3.42E+10
320	1.06E+10	4.15E+10
340	1.62E+10	5.91E+10
360	2.37E+10	8.12E+10
373.15	2.98E+10	9.83E+10
380	3.34E+10	1.08E+11
400	4.55E+10	1.40E+11



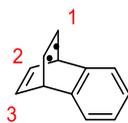
**Table S134.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $^{13}\text{C}$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF	
	-5.14	0.0
30	4.93E+04	1.02E+06
35	6.25E+04	1.29E+06
40	7.81E+04	1.60E+06
50	1.19E+05	2.43E+06
60	1.78E+05	3.65E+06
70	2.68E+05	5.50E+06
80	4.12E+05	8.48E+06
90	6.59E+05	1.35E+07
100	1.11E+06	2.23E+07
120	3.70E+06	6.65E+07
140	1.38E+07	2.01E+08
160	4.83E+07	5.54E+08
180	1.47E+08	1.35E+09
200	3.85E+08	2.93E+09
220	8.82E+08	5.72E+09
240	1.81E+09	1.02E+10
260	3.38E+09	1.70E+10
273.15	4.89E+09	2.29E+10
280	5.85E+09	2.66E+10
290	7.51E+09	3.26E+10
298.15	3.54E+08	3.82E+10
300	9.51E+09	3.95E+10
310	1.19E+10	4.74E+10
320	1.46E+10	5.63E+10
340	2.16E+10	7.74E+10
360	3.05E+10	1.03E+11
373.15	3.77E+10	1.23E+11
380	4.19E+10	1.34E+11
400	5.58E+10	1.70E+11



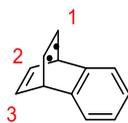
**Table S135.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $^{13}\text{C}$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Y-EEF direction with various strengths at different temperatures (T), negative direction of Y-EEF (-5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF	
	-5.14	0.0
30	1.83E-08	1.82E-12
35	1.32E-05	4.90E-09
40	1.86E-03	1.86E-06
50	1.98E+00	7.90E-03
60	2.14E+02	2.14E+00
70	6.20E+03	1.20E+02
80	7.89E+04	2.51E+03
90	5.78E+05	2.71E+04
100	2.87E+06	1.84E+05
120	3.25E+07	3.33E+06
140	1.88E+08	2.70E+07
160	7.12E+08	1.32E+08
180	2.03E+09	4.58E+08
200	4.73E+09	1.25E+09
220	9.52E+09	2.88E+09
240	1.72E+10	5.81E+09
260	2.84E+10	1.06E+10
273.15	3.80E+10	1.50E+10
280	4.39E+10	1.77E+10
290	5.34E+10	2.24E+10
298.15	6.21E+10	2.68E+10
300	6.42E+10	2.78E+10
310	7.63E+10	3.42E+10
320	8.98E+10	4.15E+10
340	1.21E+11	5.91E+10
360	1.58E+11	8.12E+10
373.15	1.86E+11	9.83E+10
380	2.01E+11	1.08E+11
400	2.50E+11	1.40E+11



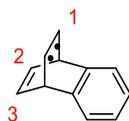
**Table S136.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) of  $^{13}C$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega$ B97X-D/6-31G(d) method along the Y-EEF direction with various strengths at different temperatures (T), negative direction of Y-EEF (-5.14 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF	
	-5.14	0.0
30	7.10E+06	1.02E+06
35	8.97E+06	1.29E+06
40	1.12E+07	1.60E+06
50	1.68E+07	2.43E+06
60	2.50E+07	3.65E+06
70	3.74E+07	5.50E+06
80	5.69E+07	8.48E+06
90	8.91E+07	1.35E+07
100	1.44E+08	2.23E+07
120	3.88E+08	6.65E+07
140	1.02E+09	2.01E+08
160	2.42E+09	5.54E+08
180	5.14E+09	1.35E+09
200	9.84E+09	2.93E+09
220	1.72E+10	5.72E+09
240	2.80E+10	1.02E+10
260	4.29E+10	1.70E+10
273.15	5.52E+10	2.29E+10
280	6.24E+10	2.66E+10
290	7.41E+10	3.26E+10
298.15	8.46E+10	3.82E+10
300	8.71E+10	3.95E+10
310	1.01E+11	4.74E+10
320	1.17E+11	5.63E+10
340	1.53E+11	7.74E+10
360	1.95E+11	1.03E+11
373.15	2.25E+11	1.23E+11
380	2.42E+11	1.34E+11
400	2.96E+11	1.70E+11



**Table S137.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $^{13}\text{C}$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF	
	-5.14	0.0
30	7.96E-03	1.82E-12
35	8.97E-01	4.90E-09
40	3.16E+01	1.86E-06
50	4.81E+03	7.90E-03
60	1.42E+05	2.14E+00
70	1.63E+06	1.20E+02
80	1.04E+07	2.51E+03
90	4.47E+07	2.71E+04
100	1.45E+08	1.84E+05
120	8.69E+08	3.33E+06
140	3.20E+09	2.70E+07
160	8.66E+09	1.32E+08
180	1.90E+10	4.58E+08
200	3.62E+10	1.25E+09
220	6.16E+10	2.88E+09
240	9.67E+10	5.81E+09
260	1.42E+11	1.06E+10
273.15	1.79E+11	1.50E+10
280	1.99E+11	1.77E+10
290	2.32E+11	2.24E+10
298.15	2.61E+11	2.68E+10
300	2.68E+11	2.78E+10
310	3.06E+11	3.42E+10
320	3.48E+11	4.15E+10
340	4.39E+11	5.91E+10
360	5.42E+11	8.12E+10
373.15	6.15E+11	9.83E+10
380	6.55E+11	1.08E+11
400	7.77E+11	1.40E+11

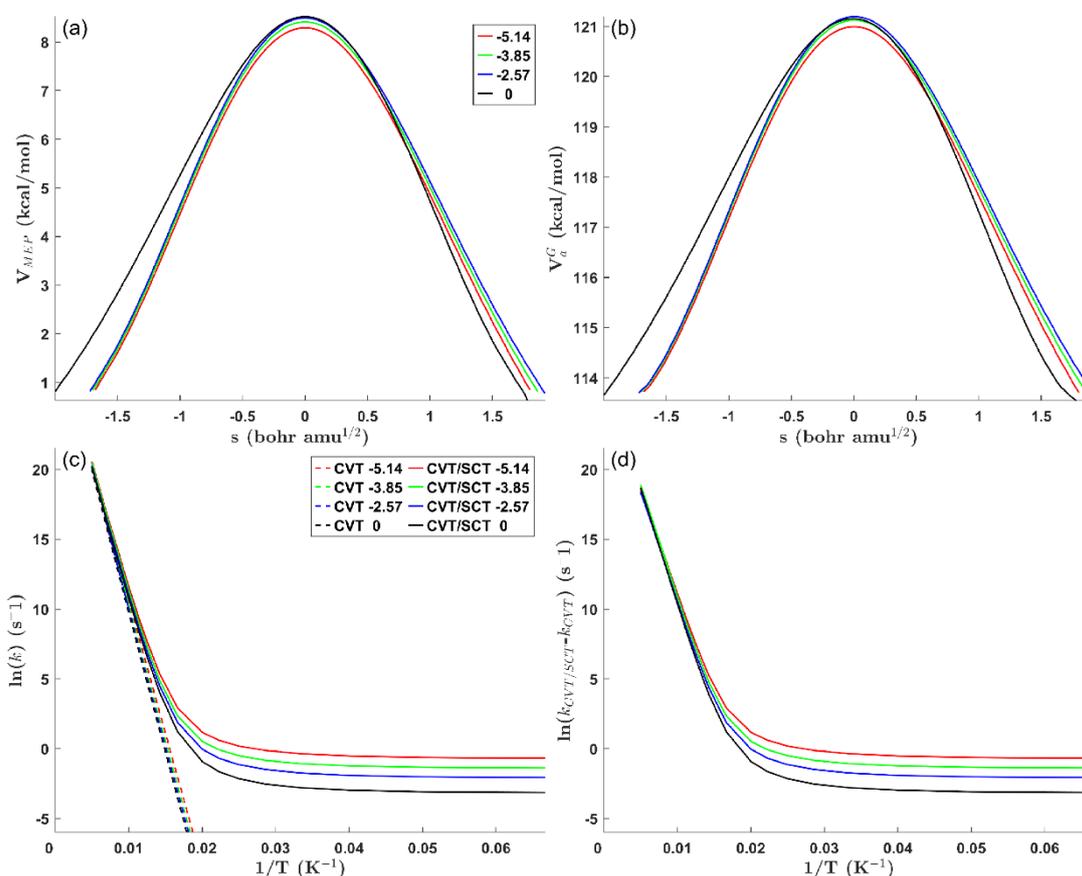


**Table S138.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $^{13}\text{C}$  at C1, C2 and C3 for triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); no field (0.0 V/nm)).

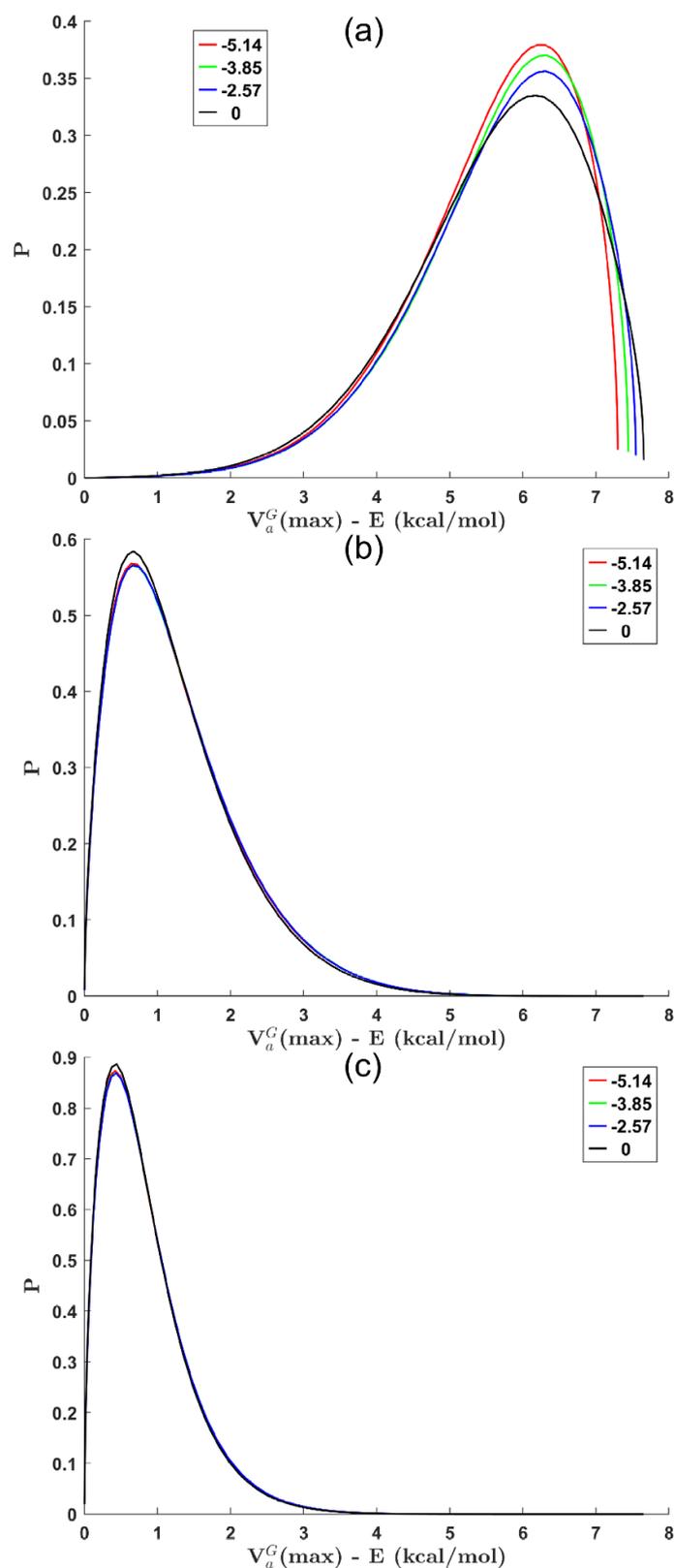
T(K)	Z-EEF	
	-5.14	0.0
30	1.38E+08	1.02E+06
35	1.75E+08	1.29E+06
40	2.18E+08	1.60E+06
50	3.31E+08	2.43E+06
60	4.94E+08	3.65E+06
70	7.39E+08	5.50E+06
80	1.12E+09	8.48E+06
90	1.70E+09	1.35E+07
100	2.59E+09	2.23E+07
120	5.85E+09	6.65E+07
140	1.23E+10	2.01E+08
160	2.35E+10	5.54E+08
180	4.11E+10	1.35E+09
200	6.66E+10	2.93E+09
220	1.01E+11	5.72E+09
240	1.46E+11	1.02E+10
260	2.02E+11	1.70E+10
273.15	2.45E+11	2.29E+10
280	2.69E+11	2.66E+10
290	3.06E+11	3.26E+10
298.15	3.39E+11	3.82E+10
300	3.47E+11	3.95E+10
310	3.90E+11	4.74E+10
320	4.36E+11	5.63E+10
340	5.36E+11	7.74E+10
360	6.46E+11	1.03E+11
373.15	7.23E+11	1.23E+11
380	7.66E+11	1.34E+11
400	8.94E+11	1.70E+11

**Table S139.** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and vibrationally adiabatic ground-state potential energy ( $\Delta V_a^G(\max)$  in kcal/mol) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method under X-, Y- and Z-EEF with different strengths (V/nm).

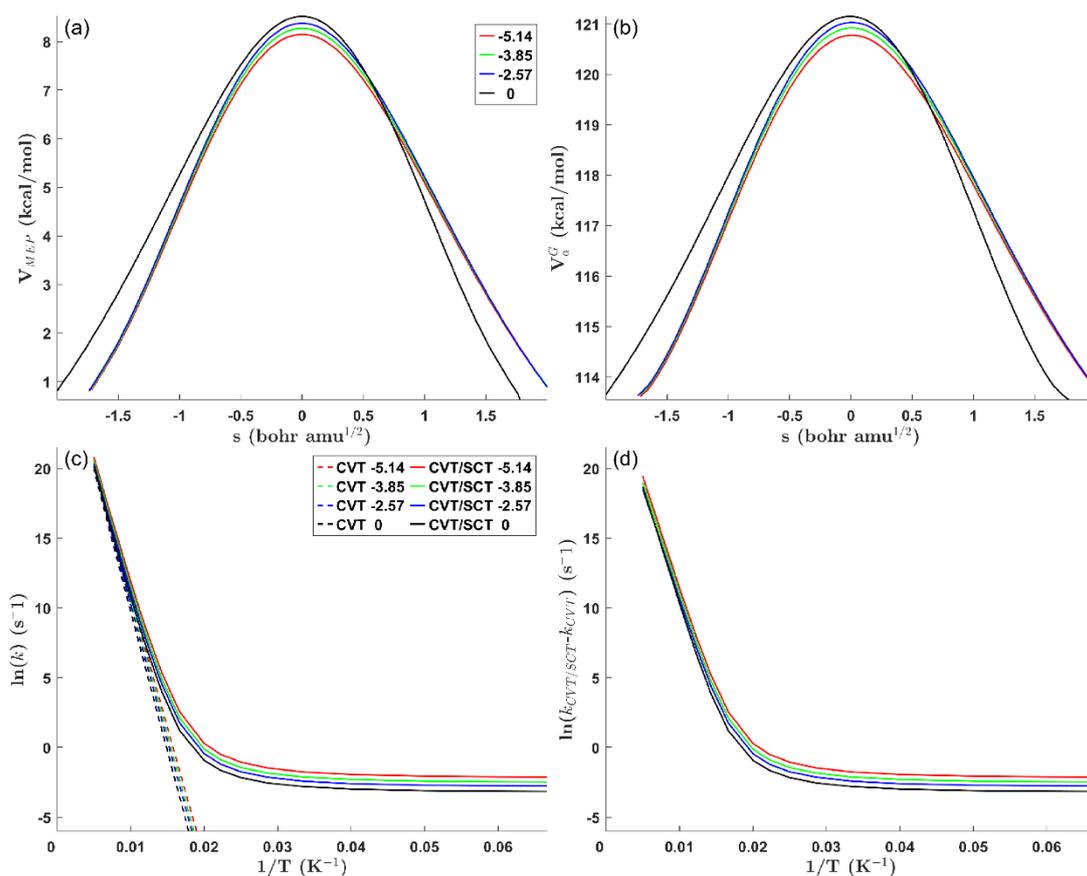
EEF (V/nm)	-5.14	-3.85	-2.57	0.0
<b>X-EEF Direction</b>				
$\Delta E$	8.29	8.42	8.50	8.52
$\Delta V_a^G(\max)$	120.99	121.12	121.19	121.15
<b>Y-EEF Direction</b>				
$\Delta E$	8.15	8.28	8.38	8.52
$\Delta V_a^G(\max)$	120.78	120.92	121.03	121.15
<b>Z-EEF Direction</b>				
$\Delta E$	8.72	8.68	8.63	8.52
$\Delta V_a^G(\max)$	121.20	121.20	121.20	121.15



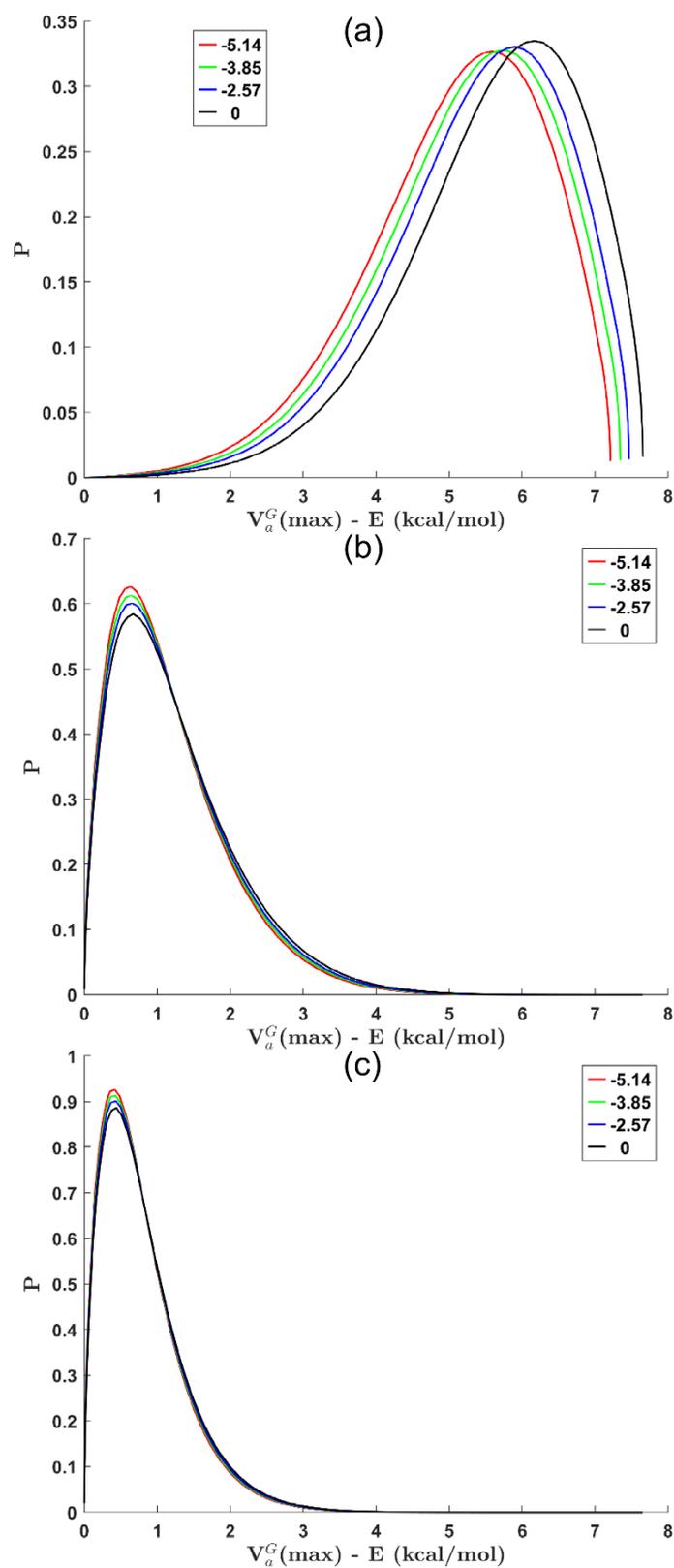
**Figure S79.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method along the X-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm)).



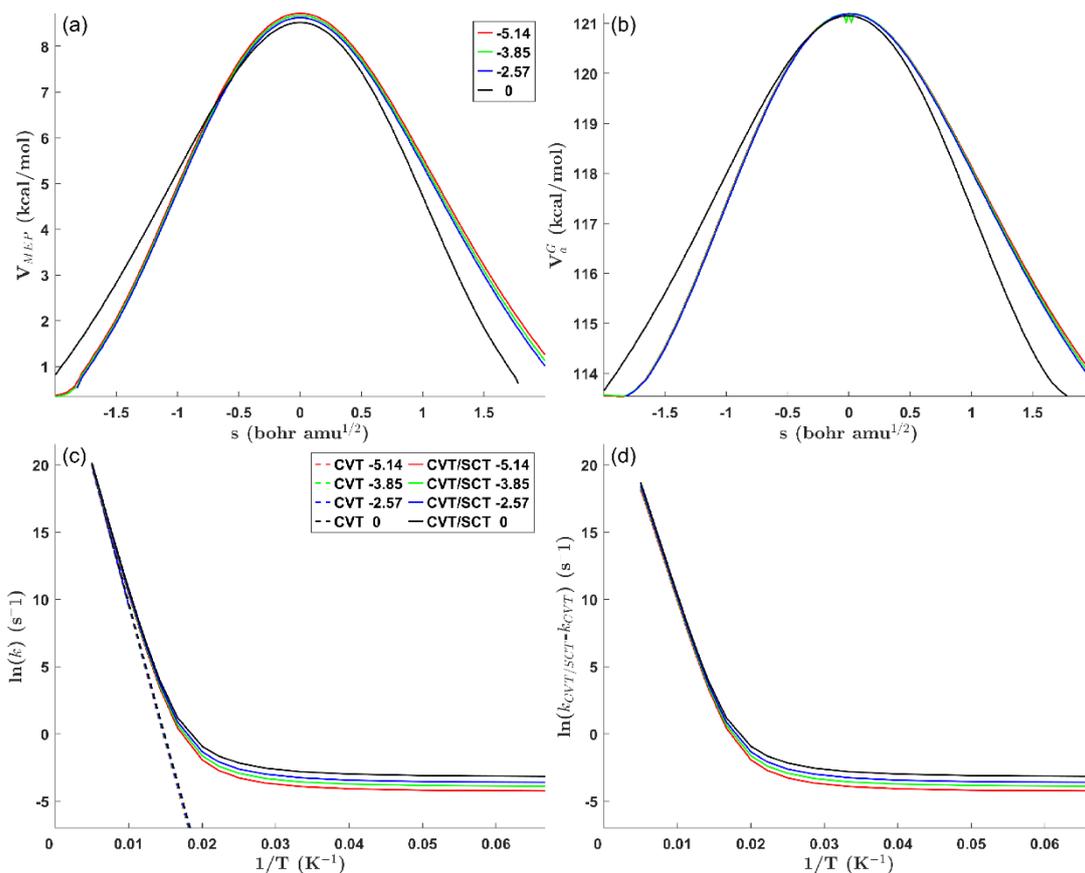
**Figure S80.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the X-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm))



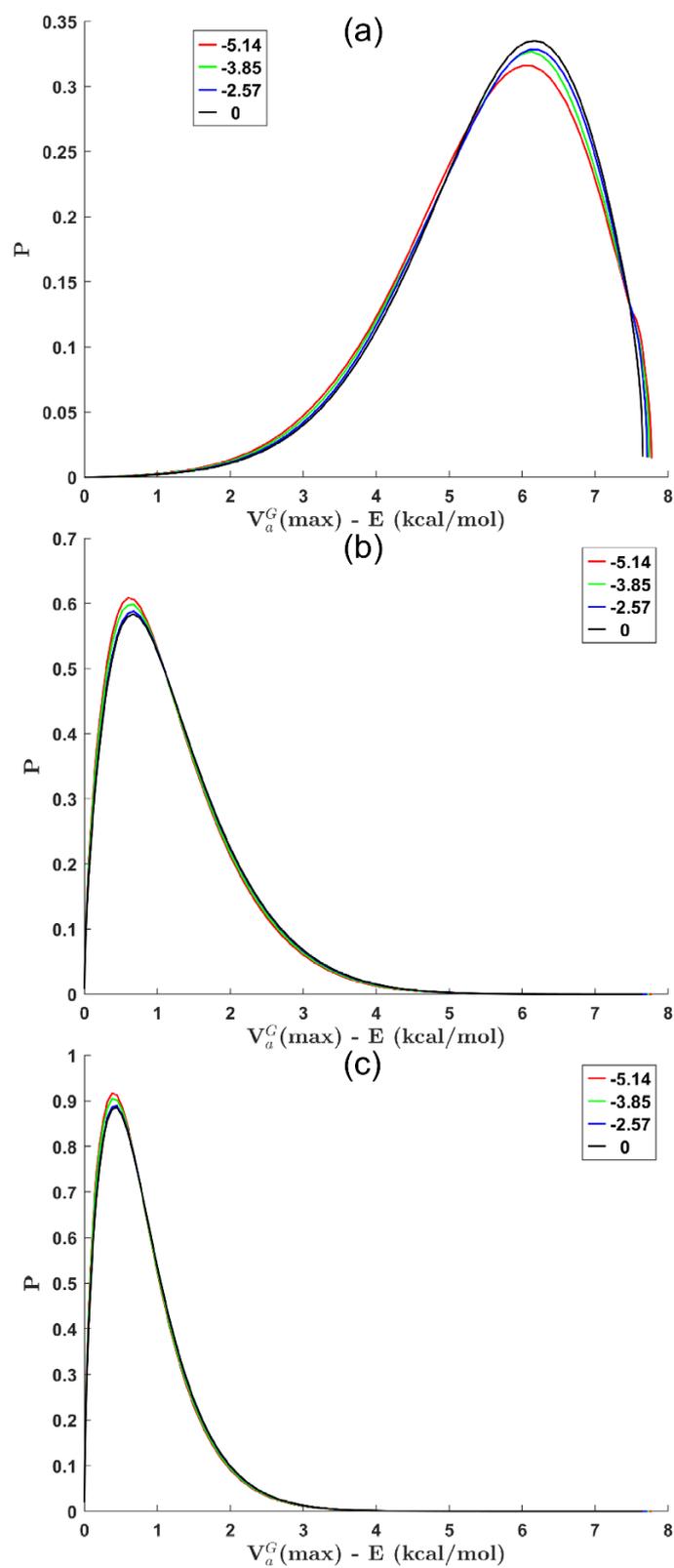
**Figure S81.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method along the Y-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm))



**Figure S82.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the Y-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm))



**Figure S83.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method along the Z-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm))



**Figure S84.** Tunneling contributions/probability ( $P$ ) to the SCT transmission coefficient ( $\kappa_{\text{SCT}}$ ) of the triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega$ B97X-D/6-31G(d) method at (a) 100K, (b) 200K and (c) 300K along the Z-EEF direction with different strengths (red: -5.14 V/nm; green: -3.85 V/nm, blue: -2.57 V/nm and black: no field (0 V/nm))

**Table S140.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF			
	-5.14	-3.85	-2.57	0.0
30	4.37E-42	3.86E-43	6.60E-44	1.08E-44
35	2.01E-34	2.50E-35	5.51E-36	1.17E-36
40	1.14E-28	1.84E-29	4.90E-30	1.26E-30
50	1.34E-20	3.12E-21	1.08E-21	3.65E-22
60	3.32E-15	9.88E-16	4.08E-16	1.65E-16
70	2.43E-11	8.58E-12	4.02E-12	1.85E-12
80	1.95E-08	7.86E-09	4.05E-09	2.05E-09
90	3.60E-06	1.60E-06	8.89E-07	4.86E-07
100	2.36E-04	1.14E-04	6.70E-05	3.89E-05
120	1.28E-01	6.99E-02	4.49E-02	2.84E-02
140	1.18E+01	7.01E+00	4.79E+00	3.23E+00
160	3.56E+02	2.25E+02	1.61E+02	1.14E+02
180	5.10E+03	3.39E+03	2.51E+03	1.84E+03
200	4.33E+04	2.99E+04	2.28E+04	1.71E+04
220	2.51E+05	1.79E+05	1.40E+05	1.07E+05
240	1.09E+06	8.00E+05	6.36E+05	4.96E+05
260	3.80E+06	2.85E+06	2.30E+06	1.82E+06
273.15	7.83E+06	5.95E+06	4.86E+06	3.87E+06
280	1.11E+07	8.51E+06	6.97E+06	5.58E+06
290	1.80E+07	1.39E+07	1.15E+07	9.21E+06
298.15	3.61E+04	2.49E+04	1.90E+04	1.35E+07
300	2.83E+07	2.20E+07	1.82E+07	1.47E+07
310	4.32E+07	3.38E+07	2.82E+07	2.29E+07
320	6.42E+07	5.07E+07	4.24E+07	3.45E+07
340	1.33E+08	1.06E+08	8.95E+07	7.34E+07
360	2.53E+08	2.05E+08	1.74E+08	1.44E+08
373.15	3.73E+08	3.04E+08	2.59E+08	2.15E+08
380	4.52E+08	3.69E+08	3.16E+08	2.62E+08
400	7.63E+08	6.28E+08	5.41E+08	4.52E+08

**Table S141.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega\text{B97X-D/6-31G(d)}$  method along the X-EEF direction with various strengths at different temperatures (T in K), negative direction of X-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	X-EEF			
	-5.14	-3.85	-2.57	0.0
30	5.05E-01	2.49E-01	1.25E-01	4.27E-02
35	5.14E-01	2.54E-01	1.28E-01	4.36E-02
40	5.31E-01	2.62E-01	1.32E-01	4.51E-02
50	5.89E-01	2.90E-01	1.47E-01	5.05E-02
60	6.94E-01	3.42E-01	1.75E-01	6.06E-02
70	8.75E-01	4.34E-01	2.25E-01	7.92E-02
80	1.20E+00	5.99E-01	3.17E-01	1.15E-01
90	1.83E+00	9.29E-01	5.07E-01	1.95E-01
100	3.23E+00	1.68E+00	9.58E-01	3.98E-01
120	1.83E+01	1.03E+01	6.48E+00	3.33E+00
140	1.97E+02	1.22E+02	8.21E+01	5.09E+01
160	2.17E+03	1.48E+03	1.02E+03	7.18E+02
180	1.81E+04	1.32E+04	9.31E+03	7.09E+03
200	1.10E+05	8.49E+04	6.08E+04	4.89E+04
220	5.13E+05	4.11E+05	2.99E+05	2.50E+05
240	1.92E+06	1.58E+06	1.17E+06	1.00E+06
260	5.97E+06	5.04E+06	3.77E+06	3.30E+06
273.15	1.16E+07	9.93E+06	7.49E+06	6.63E+06
280	1.61E+07	1.38E+07	1.05E+07	9.31E+06
290	2.52E+07	2.18E+07	1.66E+07	1.49E+07
298.15	9.45E+04	7.24E+04	5.18E+04	2.13E+07
300	3.83E+07	3.34E+07	2.56E+07	2.30E+07
310	5.70E+07	4.99E+07	3.85E+07	3.48E+07
320	8.27E+07	7.29E+07	5.65E+07	5.12E+07
340	1.64E+08	1.46E+08	1.14E+08	1.04E+08
360	3.03E+08	2.72E+08	2.15E+08	1.97E+08
373.15	4.39E+08	3.95E+08	3.14E+08	2.88E+08
380	5.27E+08	4.76E+08	3.80E+08	3.48E+08
400	8.70E+08	7.89E+08	6.35E+08	5.84E+08

**Table S142.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.84E-41	1.88E-42	2.61E-43	1.08E-44
35	6.86E-34	9.73E-35	1.79E-35	1.17E-36
40	3.34E-28	6.04E-29	1.37E-29	1.26E-30
50	3.17E-20	8.07E-21	2.47E-21	3.65E-22
60	6.81E-15	2.18E-15	8.12E-16	1.65E-16
70	4.49E-11	1.69E-11	7.26E-12	1.85E-12
80	3.34E-08	1.42E-08	6.78E-09	2.05E-09
90	5.81E-06	2.72E-06	1.41E-06	4.86E-07
100	3.63E-04	1.83E-04	1.01E-04	3.89E-05
120	1.84E-01	1.04E-01	6.33E-02	2.84E-02
140	1.60E+01	9.81E+00	6.41E+00	3.23E+00
160	4.64E+02	3.02E+02	2.08E+02	1.14E+02
180	6.43E+03	4.39E+03	3.15E+03	1.84E+03
200	5.32E+04	3.77E+04	2.79E+04	1.71E+04
220	3.02E+05	2.20E+05	1.68E+05	1.07E+05
240	1.29E+06	9.65E+05	7.50E+05	4.96E+05
260	4.42E+06	3.38E+06	2.68E+06	1.82E+06
273.15	9.02E+06	6.99E+06	5.59E+06	3.87E+06
280	1.27E+07	9.93E+06	7.99E+06	5.58E+06
290	2.05E+07	1.61E+07	1.31E+07	9.21E+06
298.15	4.45E+04	3.14E+04	2.32E+04	1.35E+07
300	3.20E+07	2.54E+07	2.07E+07	1.47E+07
310	4.86E+07	3.88E+07	3.18E+07	2.29E+07
320	7.19E+07	5.77E+07	4.76E+07	3.45E+07
340	1.47E+08	1.19E+08	9.95E+07	7.34E+07
360	2.78E+08	2.28E+08	1.92E+08	1.44E+08
373.15	4.08E+08	3.37E+08	2.85E+08	2.15E+08
380	4.93E+08	4.09E+08	3.46E+08	2.62E+08
400	8.25E+08	6.90E+08	5.89E+08	4.52E+08

**Table S143.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Y-EEF direction with various strengths at different temperatures (T in K), negative direction of Y-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Y-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.20E-01	8.49E-02	6.32E-02	4.27E-02
35	1.23E-01	8.67E-02	6.45E-02	4.36E-02
40	1.28E-01	8.98E-02	6.67E-02	4.51E-02
50	1.44E-01	1.01E-01	7.48E-02	5.05E-02
60	1.74E-01	1.21E-01	9.01E-02	6.06E-02
70	2.32E-01	1.60E-01	1.19E-01	7.92E-02
80	3.48E-01	2.38E-01	1.75E-01	1.15E-01
90	6.15E-01	4.16E-01	3.03E-01	1.95E-01
100	1.34E+00	8.95E-01	6.41E-01	3.98E-01
120	1.29E+01	8.36E+00	5.79E+00	3.33E+00
140	2.00E+02	1.29E+02	8.85E+01	5.09E+01
160	2.61E+03	1.71E+03	1.18E+03	7.18E+02
180	2.35E+04	1.57E+04	1.10E+04	7.09E+03
200	1.49E+05	1.01E+05	7.17E+04	4.89E+04
220	7.02E+05	4.87E+05	3.51E+05	2.50E+05
240	2.63E+06	1.86E+06	1.36E+06	1.00E+06
260	8.17E+06	5.87E+06	4.36E+06	3.30E+06
273.15	1.58E+07	1.15E+07	8.61E+06	6.63E+06
280	2.19E+07	1.59E+07	1.20E+07	9.31E+06
290	3.41E+07	2.50E+07	1.90E+07	1.49E+07
298.15	1.27E+05	8.63E+04	6.11E+04	2.13E+07
300	5.16E+07	3.82E+07	2.91E+07	2.30E+07
310	7.63E+07	5.68E+07	4.36E+07	3.48E+07
320	1.10E+08	8.26E+07	6.38E+07	5.12E+07
340	2.16E+08	1.64E+08	1.28E+08	1.04E+08
360	3.95E+08	3.03E+08	2.39E+08	1.97E+08
373.15	5.68E+08	4.39E+08	3.48E+08	2.88E+08
380	6.80E+08	5.26E+08	4.20E+08	3.48E+08
400	1.11E+09	8.68E+08	6.98E+08	5.84E+08

**Table S144.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS2** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.49E-45	2.40E-45	3.92E-45	1.08E-44
35	2.13E-37	3.22E-37	4.90E-37	1.17E-36
40	2.85E-31	4.08E-31	5.89E-31	1.26E-30
50	1.11E-22	1.48E-22	1.99E-22	3.65E-22
60	6.13E-17	7.79E-17	9.95E-17	1.65E-16
70	7.93E-13	9.73E-13	1.20E-12	1.85E-12
80	9.78E-10	1.17E-09	1.40E-09	2.05E-09
90	2.51E-07	2.95E-07	3.47E-07	4.86E-07
100	2.15E-05	2.48E-05	2.87E-05	3.89E-05
120	1.74E-02	1.96E-02	2.21E-02	2.84E-02
140	2.12E+00	2.35E+00	2.60E+00	3.23E+00
160	7.90E+01	8.63E+01	9.44E+01	1.14E+02
180	1.33E+03	1.44E+03	1.56E+03	1.84E+03
200	1.29E+04	1.38E+04	1.48E+04	1.71E+04
220	8.29E+04	8.81E+04	9.39E+04	1.07E+05
240	3.93E+05	4.16E+05	4.40E+05	4.96E+05
260	1.48E+06	1.55E+06	1.64E+06	1.82E+06
273.15	3.17E+06	3.33E+06	3.50E+06	3.87E+06
280	4.60E+06	4.82E+06	5.05E+06	5.58E+06
290	7.67E+06	8.01E+06	8.38E+06	9.21E+06
298.15	1.06E+04	1.14E+04	1.22E+04	1.35E+07
300	1.24E+07	1.29E+07	1.35E+07	1.47E+07
310	1.93E+07	2.01E+07	2.10E+07	2.29E+07
320	2.94E+07	3.06E+07	3.18E+07	3.45E+07
340	6.33E+07	6.56E+07	6.80E+07	7.34E+07
360	1.25E+08	1.30E+08	1.34E+08	1.44E+08
373.15	1.89E+08	1.95E+08	2.01E+08	2.15E+08
380	2.31E+08	2.38E+08	2.46E+08	2.62E+08
400	4.02E+08	4.13E+08	4.25E+08	4.52E+08

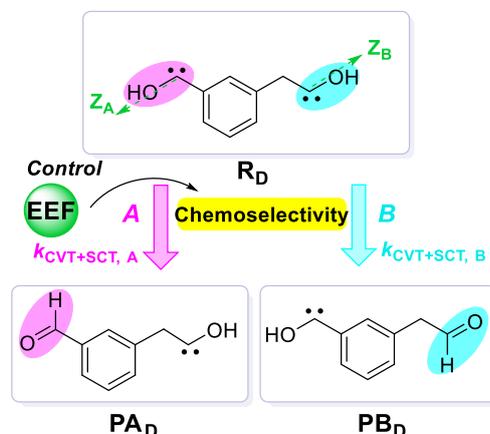
**Table S145.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of triplet Di- $\pi$ -methane rearrangement **TS1** using  $\omega\text{B97X-D/6-31G(d)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 ~ -2.57 V/nm); no field (0.0 V/nm)).

T(K)	Z-EEF			
	-5.14	-3.85	-2.57	0.0
30	1.45E-02	2.06E-02	2.77E-02	4.27E-02
35	1.48E-02	2.10E-02	2.82E-02	4.36E-02
40	1.52E-02	2.17E-02	2.91E-02	4.51E-02
50	1.69E-02	2.40E-02	3.24E-02	5.05E-02
60	2.00E-02	2.84E-02	3.87E-02	6.06E-02
70	2.60E-02	3.67E-02	5.03E-02	7.92E-02
80	3.81E-02	5.35E-02	7.37E-02	1.15E-01
90	6.66E-02	9.22E-02	1.26E-01	1.95E-01
100	1.46E-01	1.98E-01	2.66E-01	3.98E-01
120	1.54E+00	1.93E+00	2.42E+00	3.33E+00
140	2.81E+01	3.33E+01	3.94E+01	5.09E+01
160	4.36E+02	5.01E+02	5.74E+02	7.18E+02
180	4.55E+03	5.15E+03	5.79E+03	7.09E+03
200	3.27E+04	3.66E+04	4.06E+04	4.89E+04
220	1.73E+05	1.91E+05	2.10E+05	2.50E+05
240	7.11E+05	7.83E+05	8.53E+05	1.00E+06
260	2.40E+06	2.63E+06	2.84E+06	3.30E+06
273.15	4.90E+06	5.33E+06	5.74E+06	6.63E+06
280	6.92E+06	7.51E+06	8.08E+06	9.31E+06
290	1.12E+07	1.21E+07	1.30E+07	1.49E+07
298.15	2.76E+04	3.10E+04	3.44E+04	2.13E+07
300	1.75E+07	1.89E+07	2.02E+07	2.30E+07
310	2.66E+07	2.86E+07	3.06E+07	3.48E+07
320	3.96E+07	4.25E+07	4.53E+07	5.12E+07
340	8.19E+07	8.75E+07	9.28E+07	1.04E+08
360	1.57E+08	1.67E+08	1.76E+08	1.97E+08
373.15	2.32E+08	2.46E+08	2.60E+08	2.88E+08
380	2.82E+08	2.99E+08	3.15E+08	3.48E+08
400	4.79E+08	5.05E+08	5.31E+08	5.84E+08

## 2.5 Chemo- or Site-selectivity

### EEF Effect

#### Arene molecule $R_D$



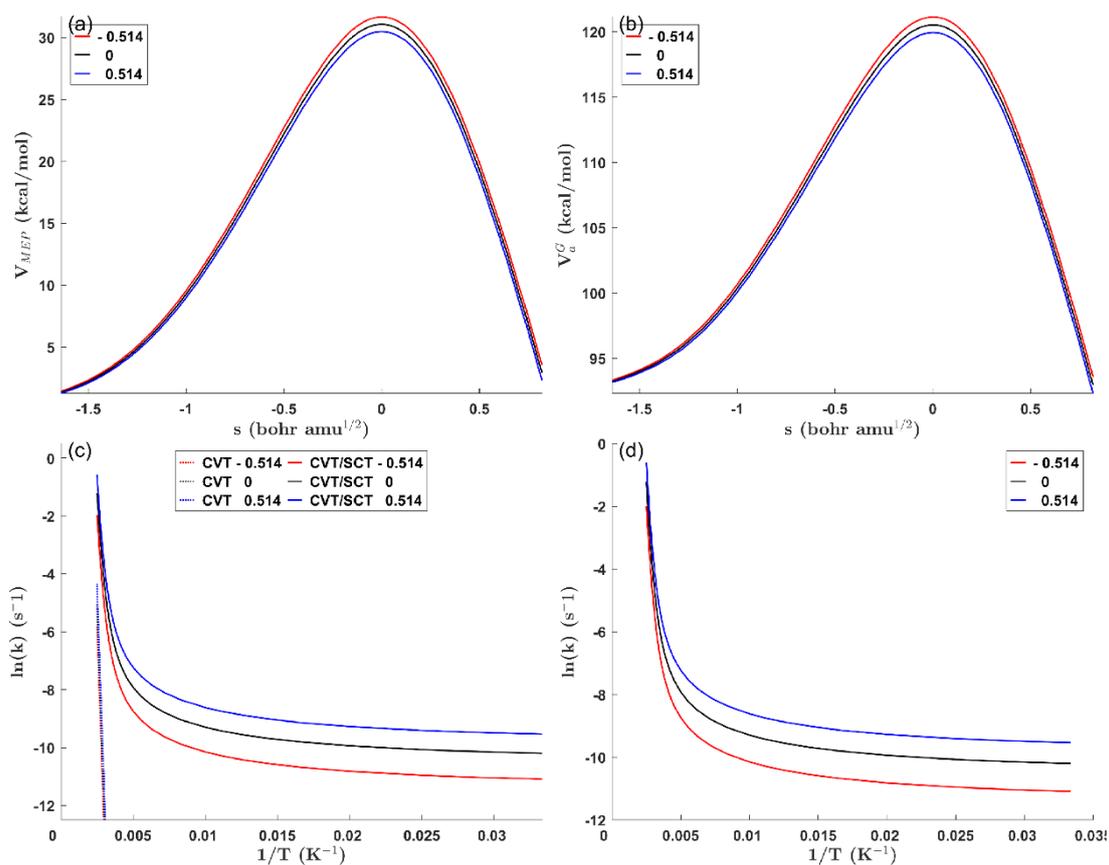
**Figure S85** Schematic chemo-selectivity of the H-migration of one arene molecule bearing two hydroxycarbene groups ( $R_D$ ) under EEF of the  $Z_A$  and  $Z_B$  directions.

**Table S146** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and electronic energies plus zero-point correction energy ( $\Delta V_a^G(\max)$  in kcal/mol) and their difference  $\Delta\Delta E$  and  $\Delta\Delta V_a^G(\max)$  between the chemo-selectivity for the arene molecule bearing two hydroxycarbene groups ( $R_D$ ) at sites A and B under different EEF strengths.

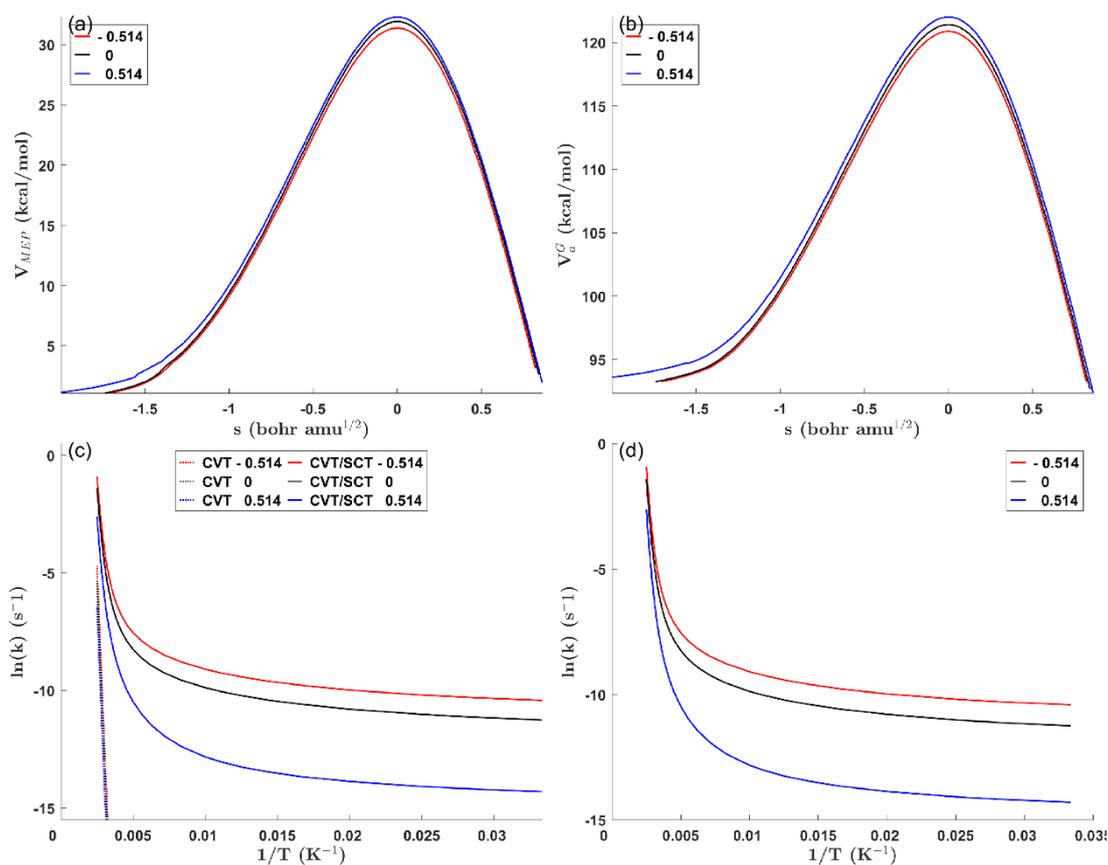
EEF (V/nm)	-0.514	0	0.514
<b><math>Z_A</math>-EEF Direction</b>			
$\Delta E_A$	31.66	31.07	30.48
$\Delta E_B$	31.40	31.93	32.32
$\Delta\Delta E$	-0.26	0.86	1.84
$\Delta V_a^G(\max)_A$	28.12	27.55	26.98
$\Delta V_a^G(\max)_B$	27.87	28.44	29.06
$\Delta\Delta V_a^G(\max)$	-0.25	0.89	2.08
<b><math>Z_B</math>-EEF Direction</b>			
$\Delta E_A$	30.53	31.06	31.59
$\Delta E_B$	32.52	31.93	31.33
$\Delta\Delta E$	1.99	0.87	-0.26
$\Delta V_a^G(\max)_A$	27.00	27.54	28.09
$\Delta V_a^G(\max)_B$	29.09	28.50	27.87
$\Delta\Delta V_a^G(\max)$	2.08	0.96	-0.22

**Table S147** Half-life ( $\tau$  in hr) at 30K, barrier width of PES ( $w$  in bohr) and their difference  $\Delta\Delta\tau$  and  $\Delta\Delta w$  between the chemo-selectivity for the arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at site A and site B under different EEF strengths

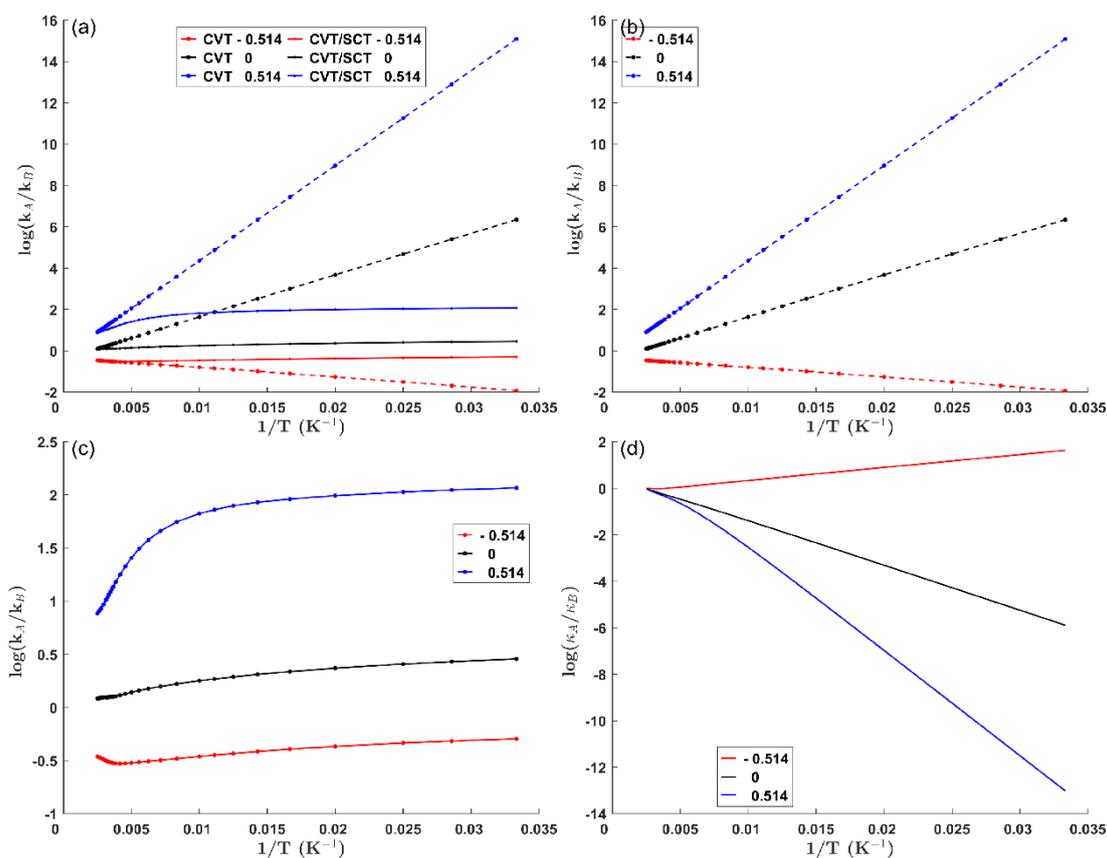
EEF (V/nm)	-0.514	0	0.514
<b>Z<sub>A</sub>-EEF Direction</b>			
$\Delta\tau_A$	12.58	5.17	2.67
$\Delta\tau_B$	6.40	14.81	310.99
$\Delta\Delta\tau$	-6.19	9.63	308.32
$\Delta w_A$	2.49	2.46	2.45
$\Delta w_B$	2.52	2.58	2.85
$\Delta\Delta w$	0.03	0.12	0.40
<b>Z<sub>B</sub>-EEF Direction</b>			
$\Delta\tau_A$	5.22	10.88	15.04
$\Delta\tau_B$	38.81	16.31	5.92
$\Delta\Delta\tau$	33.59	5.44	-9.12
$\Delta w_A$	2.53	2.54	2.57
$\Delta w_B$	2.65	2.59	2.54
$\Delta\Delta w$	0.12	0.06	-0.03



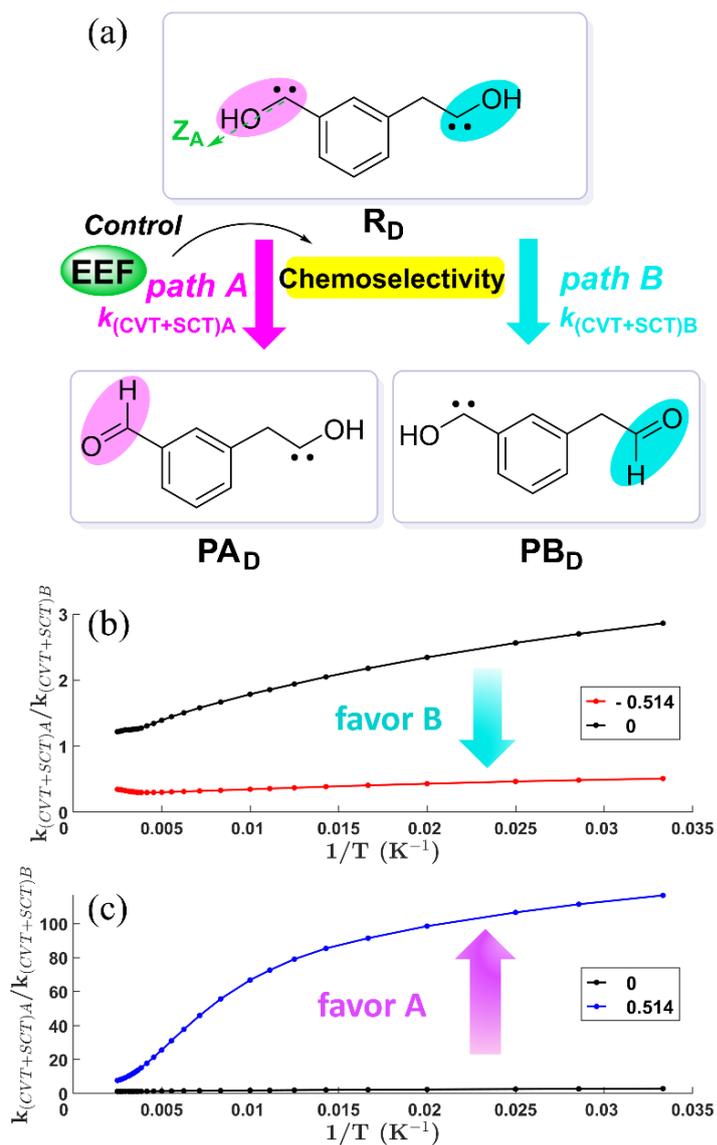
**Figure S86.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**Rd**) at **site A** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>A</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



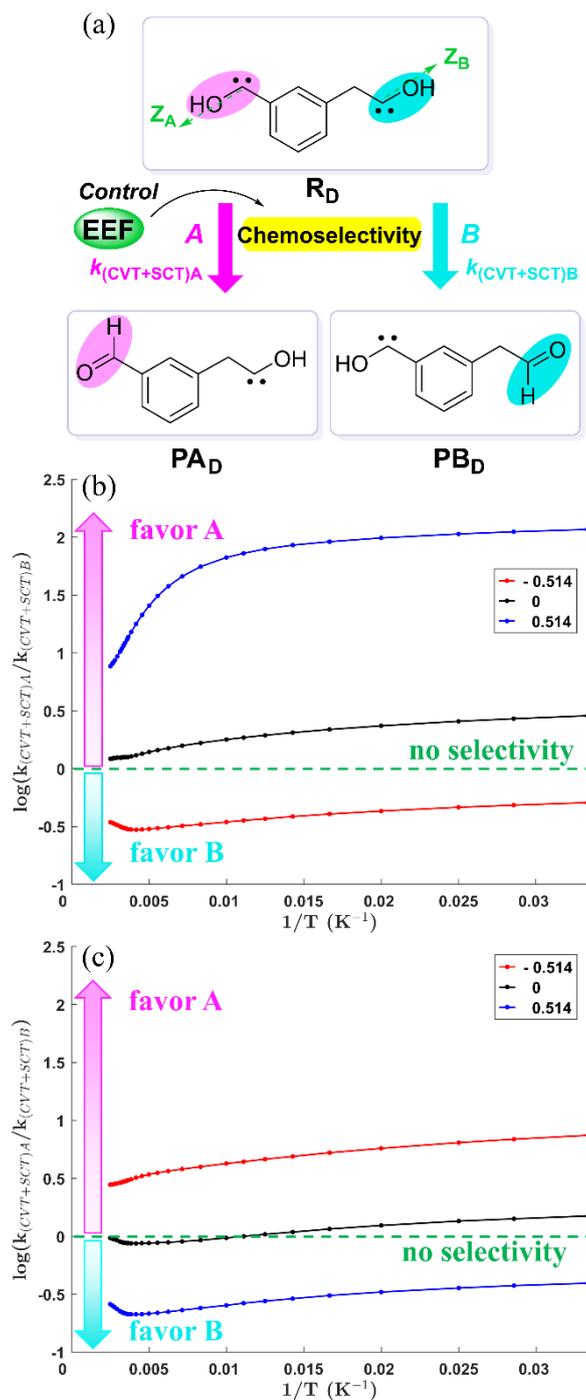
**Figure S87.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**Rd**) at **site B** using  $\omega$ B97X-D/6-31G(d,p) method along **ZA-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S88.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ , dash lines) and overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ ), (c) overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ ) rate constants and (d)  $\ln(\kappa_A/\kappa_B)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at **site A** and **site B** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>A</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S89.** (a) Schematic depicting chemoselectivity during H-migration in  $R_D$  bearing two different hydroxycarbene moieties in a  $Z_A$ -EEF (purple arrow) and  $Z_B$ -EEF (green arrow). Arrhenius plots ( $k_{(CVT+SCT)A}/k_{(CVT+SCT)B}$  vs.  $1/T$ ) for  $R_D$  calculated using the  $\omega$ B97X-D method in the (b)  $Z_A$ -EEF and (c)  $Z_B$ -EEF (red:  $-0.514$  V/nm, black: no-EEF ( $0$  V/nm), blue:  $0.514$  V/nm).



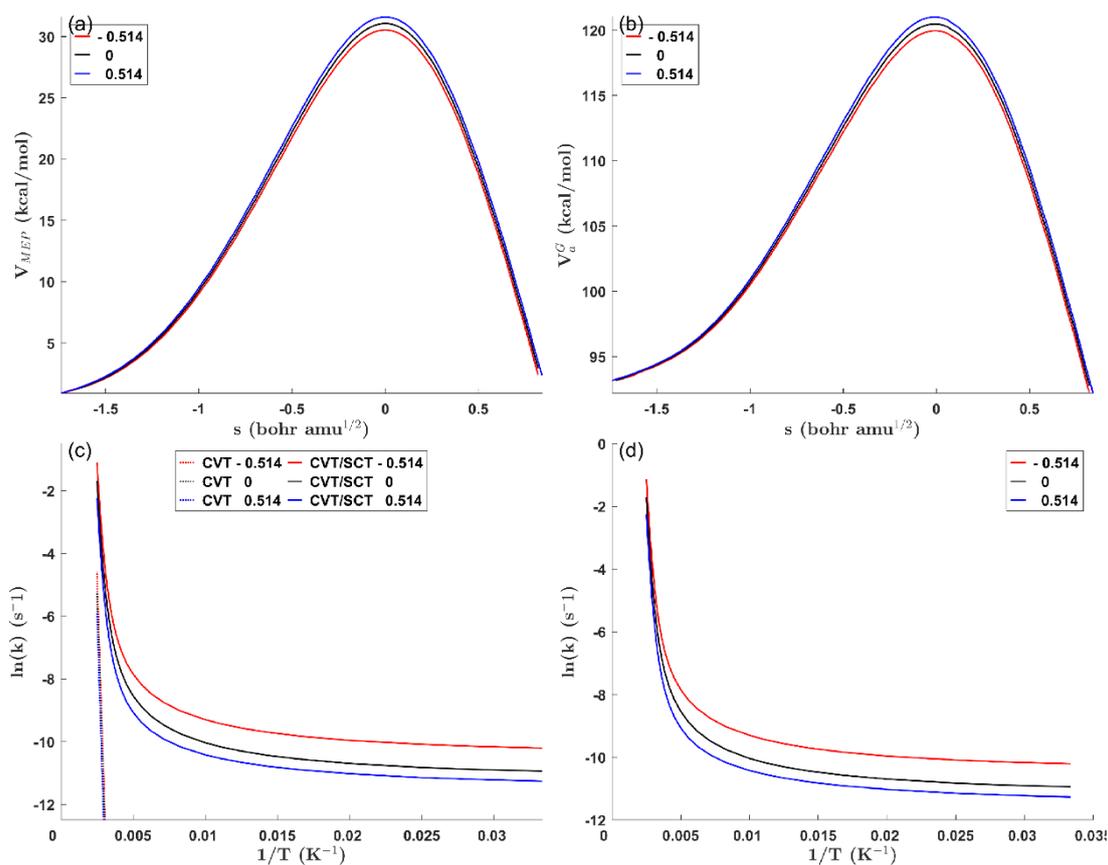
**Figure S90.** (a) Schematic depicting chemoselectivity during H-migration in  $R_D$  bearing two different hydroxycarbene moieties in a  $Z_A$ -EEF and  $Z_B$ -EEF (green arrows). Arrhenius plots ( $\log(k_{(CVT+SCT)A}/k_{(CVT+SCT)B})$  vs.  $1/T$ ) for  $R_D$  calculated using the  $\omega$ B97X-D method in the (b)  $Z_A$ -EEF and (c)  $Z_B$ -EEF (red:  $-0.514$  V/nm, black: no-EEF (0 V/nm), blue:  $0.514$  V/nm). Pink arrow is favourable to selectivity of A path, and light-blue arrow is favourable to selectivity of B path.

**Table S148.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{A-EEF}}$  direction with various strengths at different temperatures (T in K), negative direction of  $Z_{\text{A-EEF}}$  (-0.514 V/nm); positive direction of  $Z_{\text{A-EEF}}$  (0.514 V/nm); no field (0.0 V/nm)).

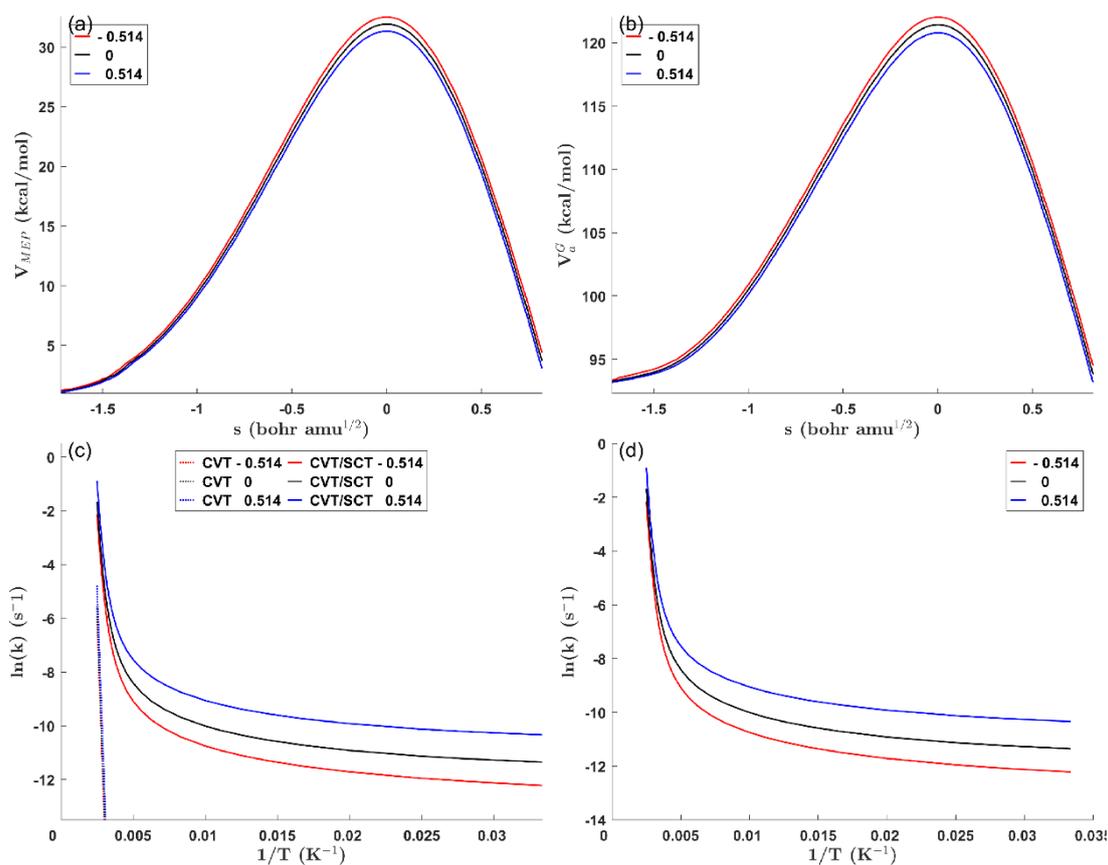
T(K)	$Z_{\text{A-EEF}}$					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	8.33E-194	1.14E-189	1.64E-185	7.07E-192	5.13E-196	1.35E-200
35	1.77E-164	6.21E-161	2.27E-157	8.59E-163	2.48E-166	2.84E-170
40	1.78E-142	2.25E-139	2.95E-136	5.71E-141	4.65E-144	1.60E-147
50	1.16E-111	3.55E-109	1.10E-106	2.13E-110	7.41E-113	1.18E-115
60	4.19E-91	4.94E-89	5.90E-87	5.31E-90	4.89E-92	2.16E-94
70	2.07E-76	1.24E-74	7.45E-73	2.02E-75	3.73E-77	3.41E-79
80	2.20E-65	7.91E-64	2.85E-62	1.78E-64	5.52E-66	8.71E-68
90	8.41E-57	2.04E-55	4.93E-54	5.89E-56	2.74E-57	6.59E-59
100	6.25E-50	1.10E-48	1.94E-47	3.89E-49	2.50E-50	8.44E-52
120	1.30E-39	1.42E-38	1.55E-37	6.80E-39	7.10E-40	3.97E-41
140	3.11E-32	2.43E-31	1.88E-30	1.45E-31	2.13E-32	1.71E-33
160	1.09E-26	6.57E-26	3.94E-25	4.62E-26	8.83E-27	9.25E-28
180	2.27E-22	1.12E-21	5.52E-21	8.96E-22	2.09E-22	2.70E-23
200	6.54E-19	2.76E-18	1.16E-17	2.45E-18	6.71E-19	1.02E-19
220	4.48E-16	1.66E-15	6.11E-15	1.60E-15	5.01E-16	8.73E-17
240	1.04E-13	3.47E-13	1.14E-12	3.59E-13	1.25E-13	2.44E-14
260	1.06E-11	3.21E-11	9.66E-11	3.52E-11	1.35E-11	2.89E-12
273.15	1.53E-10	4.40E-10	1.26E-09	5.00E-10	2.02E-10	4.57E-11
280	5.58E-10	1.56E-09	4.35E-09	1.81E-09	7.49E-10	1.74E-10
290	3.31E-09	8.95E-09	2.40E-08	1.06E-08	4.54E-09	1.09E-09
298.15	1.29E-08	3.41E-08	8.89E-08	4.09E-08	1.81E-08	4.47E-09
300	1.74E-08	4.57E-08	1.18E-07	5.51E-08	2.45E-08	6.09E-09
310	8.27E-08	2.10E-07	5.28E-07	2.58E-07	1.18E-07	3.04E-08
320	3.56E-07	8.78E-07	2.15E-06	1.10E-06	5.19E-07	1.37E-07
340	5.12E-06	1.20E-05	2.77E-05	1.55E-05	7.72E-06	2.15E-06
360	5.49E-05	1.22E-04	2.71E-04	1.64E-04	8.53E-05	2.49E-05
373.15	2.28E-04	4.94E-04	1.06E-03	6.74E-04	3.60E-04	1.08E-04
380	4.60E-04	9.84E-04	2.08E-03	1.35E-03	7.34E-04	2.24E-04
400	3.12E-03	6.43E-03	1.31E-02	9.08E-03	5.11E-03	1.62E-03

**Table S149.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at sites A and B using  $\omega$ B97X-D/6-31G(d,p) method along  $Z_A$ -EEF direction with various strengths at different temperatures (T in K), negative direction of  $Z_A$ -EEF (-0.514 V/nm); positive direction of  $Z_A$ -EEF (0.514 V/nm); no field (0.0 V/nm))

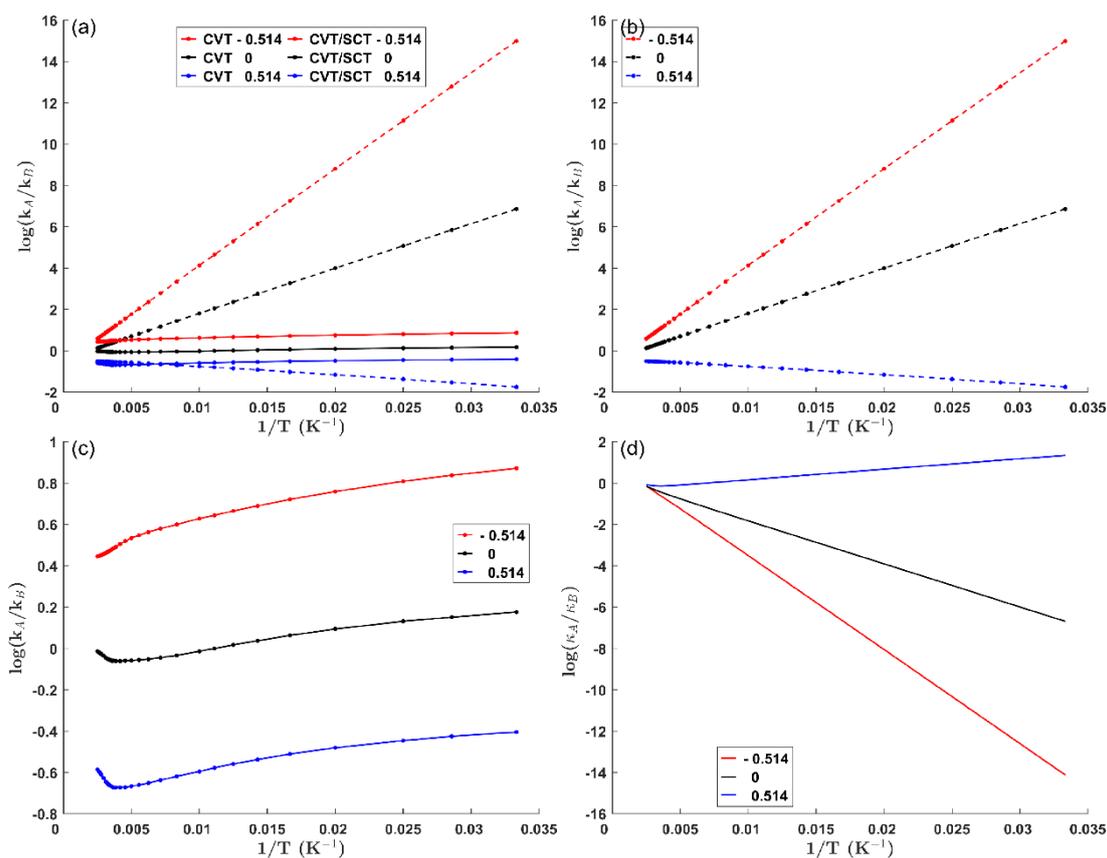
T(K)	$Z_A$ -EEF					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	1.53E-05	3.72E-05	7.22E-05	3.01E-05	1.30E-05	6.19E-07
35	1.63E-05	3.97E-05	7.70E-05	3.37E-05	1.47E-05	6.91E-07
40	1.75E-05	4.23E-05	8.22E-05	3.77E-05	1.65E-05	7.71E-07
50	2.00E-05	4.83E-05	9.39E-05	4.65E-05	2.06E-05	9.53E-07
60	2.30E-05	5.51E-05	1.07E-04	5.67E-05	2.53E-05	1.17E-06
70	2.63E-05	6.27E-05	1.23E-04	6.82E-05	3.06E-05	1.44E-06
80	3.00E-05	7.12E-05	1.40E-04	8.13E-05	3.67E-05	1.77E-06
90	3.43E-05	8.09E-05	1.59E-04	9.61E-05	4.36E-05	2.19E-06
100	3.91E-05	9.18E-05	1.81E-04	1.13E-04	5.14E-05	2.71E-06
120	5.08E-05	1.18E-04	2.35E-04	1.54E-04	7.08E-05	4.22E-06
140	6.63E-05	1.53E-04	3.05E-04	2.07E-04	9.68E-05	6.65E-06
160	8.73E-05	2.00E-04	4.00E-04	2.80E-04	1.33E-04	1.06E-05
180	1.17E-04	2.66E-04	5.32E-04	3.82E-04	1.84E-04	1.71E-05
200	1.60E-04	3.63E-04	7.24E-04	5.31E-04	2.61E-04	2.83E-05
220	2.27E-04	5.12E-04	1.02E-03	7.62E-04	3.81E-04	4.79E-05
240	3.38E-04	7.58E-04	1.50E-03	1.14E-03	5.80E-04	8.42E-05
260	5.36E-04	1.19E-03	2.35E-03	1.80E-03	9.34E-04	1.55E-04
273.15	7.59E-04	1.68E-03	3.28E-03	2.53E-03	1.33E-03	2.39E-04
280	9.24E-04	2.04E-03	3.97E-03	3.06E-03	1.62E-03	3.04E-04
290	1.26E-03	2.76E-03	5.34E-03	4.13E-03	2.20E-03	4.37E-04
298.15	1.65E-03	3.60E-03	6.93E-03	5.35E-03	2.87E-03	5.96E-04
300	1.75E-03	3.83E-03	7.37E-03	5.69E-03	3.06E-03	6.41E-04
310	2.51E-03	5.45E-03	1.04E-02	8.04E-03	4.37E-03	9.61E-04
320	3.68E-03	7.95E-03	1.51E-02	1.16E-02	6.38E-03	1.47E-03
340	8.50E-03	1.82E-02	3.42E-02	2.61E-02	1.46E-02	3.67E-03
360	2.10E-02	4.47E-02	8.37E-02	6.30E-02	3.62E-02	9.72E-03
373.15	3.88E-02	8.30E-02	1.55E-01	1.15E-01	6.76E-02	1.88E-02
380	5.37E-02	1.15E-01	2.15E-01	1.58E-01	9.39E-02	2.66E-02
400	1.39E-01	3.01E-01	5.64E-01	4.03E-01	2.47E-01	7.34E-02



**Figure S91.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at **site A** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>B</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S92.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at **site B** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>B</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S93.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ , dash lines) and overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ ), (c) overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ ) rate constants and (d)  $\ln(\kappa_A/\kappa_B)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at **site A** and **site B** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>B</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).

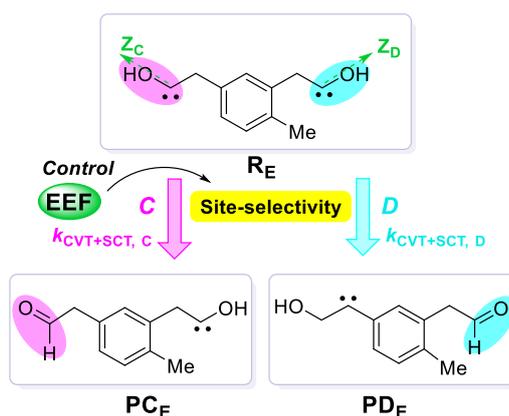
**Table S150.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{B-EEF}}$  direction with various strengths at different temperatures (T), negative direction of  $Z_{\text{B-EEF}}$  (-0.514 V/nm); positive direction of  $Z_{\text{B-EEF}}$  (0.514 V/nm); no field (0.0 V/nm).

T(K)	$Z_{\text{B-EEF}}$					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	1.08E-185	1.37E-189	1.24E-193	1.10E-200	1.87E-196	6.96E-192
35	1.57E-157	7.20E-161	2.48E-164	2.53E-170	1.02E-166	8.44E-163
40	2.10E-136	2.53E-139	2.38E-142	1.53E-147	2.11E-144	5.60E-141
50	8.17E-107	3.81E-109	1.45E-111	1.26E-115	3.81E-113	2.08E-110
60	4.47E-87	5.13E-89	4.98E-91	2.48E-94	2.72E-92	5.18E-90
70	5.73E-73	1.25E-74	2.37E-76	4.13E-79	2.20E-77	1.97E-75
80	2.22E-62	7.84E-64	2.45E-65	1.10E-67	3.40E-66	1.73E-64
90	3.86E-54	1.98E-55	9.13E-57	8.57E-59	1.74E-57	5.71E-56
100	1.53E-47	1.06E-48	6.65E-50	1.13E-51	1.63E-50	3.77E-49
120	1.23E-37	1.33E-38	1.34E-39	5.51E-41	4.80E-40	6.57E-39
140	1.49E-30	2.23E-31	3.13E-32	2.44E-33	1.48E-32	1.39E-31
160	3.12E-25	5.95E-26	1.07E-26	1.35E-27	6.24E-27	4.43E-26
180	4.36E-21	1.00E-21	2.19E-22	4.01E-23	1.50E-22	8.57E-22
200	9.13E-18	2.44E-18	6.22E-19	1.54E-19	4.87E-19	2.33E-18
220	4.81E-15	1.45E-15	4.20E-16	1.33E-16	3.67E-16	1.52E-15
240	8.99E-13	3.01E-13	9.66E-14	3.76E-14	9.24E-14	3.41E-13
260	7.56E-11	2.76E-11	9.68E-12	4.49E-12	1.00E-11	3.34E-11
273.15	9.81E-10	3.76E-10	1.39E-10	7.14E-11	1.50E-10	4.74E-10
280	3.39E-09	1.33E-09	5.06E-10	2.72E-10	5.59E-10	1.71E-09
290	1.87E-08	7.60E-09	2.98E-09	1.72E-09	3.40E-09	1.00E-08
298.15	6.92E-08	2.88E-08	1.16E-08	7.05E-09	1.35E-08	3.87E-08
300	9.22E-08	3.86E-08	1.56E-08	9.61E-09	1.83E-08	5.21E-08
310	4.10E-07	1.77E-07	7.38E-08	4.81E-08	8.88E-08	2.44E-07
320	1.67E-06	7.38E-07	3.17E-07	2.18E-07	3.91E-07	1.04E-06
340	2.15E-05	9.99E-06	4.51E-06	3.44E-06	5.83E-06	1.47E-05
360	2.09E-04	1.02E-04	4.80E-05	4.01E-05	6.46E-05	1.54E-04
373.15	8.18E-04	4.08E-04	1.98E-04	1.75E-04	2.73E-04	6.34E-04
380	1.60E-03	8.11E-04	3.99E-04	3.62E-04	5.58E-04	1.27E-03
400	1.01E-02	5.28E-03	2.69E-03	2.62E-03	3.89E-03	8.52E-03

**Table S151.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**R<sub>D</sub>**) at sites A and B using  $\omega$ B97X-D/6-31G(d,p) method along  $Z_B$ -EEF direction with various strengths at different temperatures (T), negative direction of  $Z_B$ -EEF (-0.514 V/nm); positive direction of  $Z_B$ -EEF (0.514 V/nm); no field (0.0 V/nm))

T(K)	$Z_B$ -EEF					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	3.69E-05	1.77E-05	1.28E-05	4.96E-06	1.18E-05	3.25E-05
35	3.91E-05	1.87E-05	1.36E-05	5.68E-06	1.32E-05	3.62E-05
40	4.16E-05	1.99E-05	1.44E-05	6.46E-06	1.47E-05	4.02E-05
50	4.71E-05	2.26E-05	1.63E-05	8.20E-06	1.82E-05	4.93E-05
60	5.37E-05	2.58E-05	1.84E-05	1.02E-05	2.23E-05	5.96E-05
70	6.12E-05	2.93E-05	2.07E-05	1.25E-05	2.69E-05	7.14E-05
80	6.99E-05	3.35E-05	2.34E-05	1.51E-05	3.22E-05	8.47E-05
90	7.98E-05	3.82E-05	2.64E-05	1.81E-05	3.82E-05	9.97E-05
100	9.14E-05	4.37E-05	2.97E-05	2.15E-05	4.51E-05	1.17E-04
120	1.19E-04	5.74E-05	3.80E-05	2.99E-05	6.20E-05	1.58E-04
140	1.57E-04	7.62E-05	4.89E-05	4.13E-05	8.44E-05	2.12E-04
160	2.09E-04	1.02E-04	6.36E-05	5.71E-05	1.15E-04	2.85E-04
180	2.82E-04	1.40E-04	8.44E-05	7.99E-05	1.59E-04	3.86E-04
200	3.90E-04	1.95E-04	1.15E-04	1.14E-04	2.23E-04	5.34E-04
220	5.56E-04	2.82E-04	1.62E-04	1.68E-04	3.23E-04	7.61E-04
240	8.29E-04	4.24E-04	2.40E-04	2.59E-04	4.88E-04	1.13E-03
260	1.31E-03	6.78E-04	3.78E-04	4.23E-04	7.79E-04	1.78E-03
273.15	1.85E-03	9.61E-04	5.32E-04	6.07E-04	1.10E-03	2.50E-03
280	2.25E-03	1.17E-03	6.47E-04	7.44E-04	1.34E-03	3.02E-03
290	3.04E-03	1.59E-03	8.78E-04	1.02E-03	1.81E-03	4.05E-03
298.15	3.97E-03	2.08E-03	1.15E-03	1.34E-03	2.35E-03	5.25E-03
300	4.22E-03	2.22E-03	1.22E-03	1.43E-03	2.51E-03	5.58E-03
310	6.02E-03	3.18E-03	1.75E-03	2.06E-03	3.56E-03	7.86E-03
320	8.81E-03	4.67E-03	2.58E-03	3.04E-03	5.18E-03	1.14E-02
340	2.02E-02	1.08E-02	6.02E-03	7.06E-03	1.17E-02	2.55E-02
360	4.98E-02	2.70E-02	1.52E-02	1.76E-02	2.87E-02	6.20E-02
373.15	9.21E-02	5.04E-02	2.86E-02	3.27E-02	5.30E-02	1.14E-01
380	1.27E-01	7.00E-02	4.00E-02	4.54E-02	7.32E-02	1.58E-01
400	3.29E-01	1.84E-01	1.07E-01	1.18E-01	1.90E-01	4.12E-01

## Arene molecule $R_E$



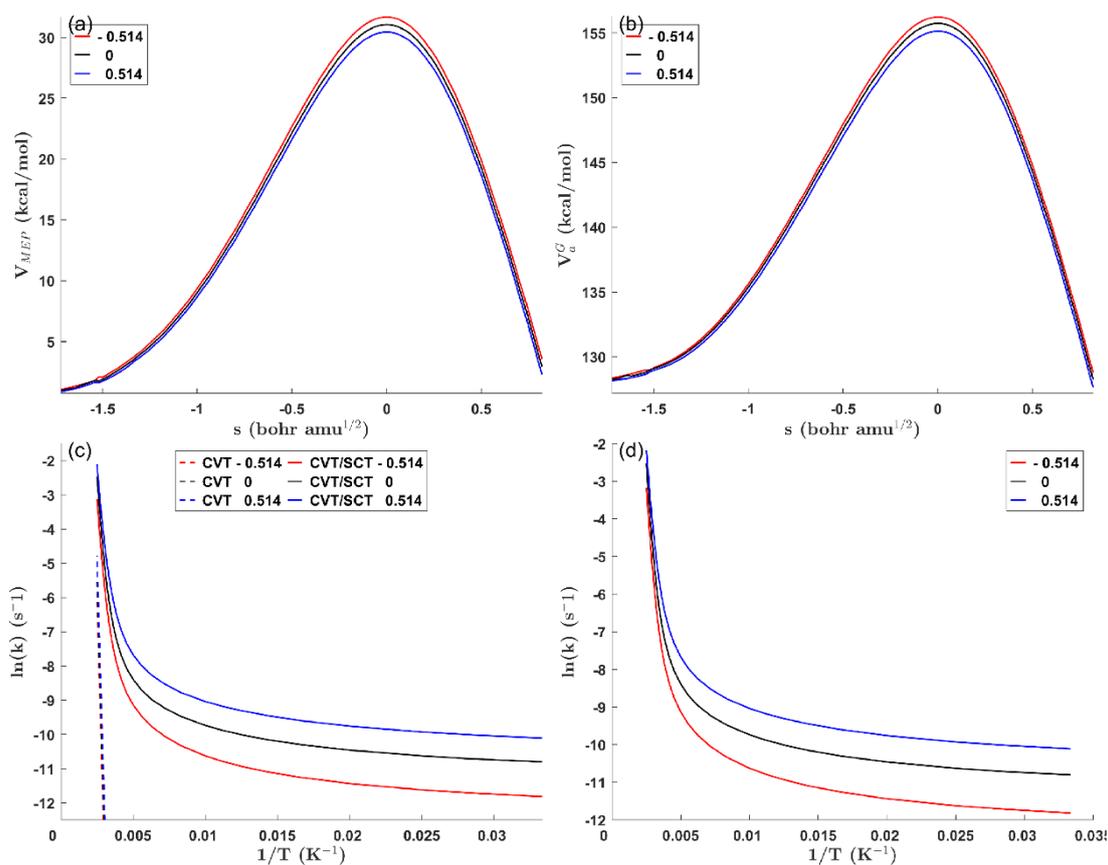
**Figure S94** Schematic site-selectivity of the H-migration of one arene molecule bearing two hydroxycarbene groups ( $R_E$ ) under EEF of the  $Z_C$  and  $Z_D$  directions.

**Table S152** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and electronic energies plus zero-point correction energy ( $\Delta V_a^G(\max)$  in kcal/mol) and their difference  $\Delta\Delta E$  and  $\Delta\Delta V_a^G(\max)$  between the site-selectivity for the arene molecule bearing two hydroxycarbene groups ( $R_E$ ) at sites C and D under different EEF strengths.

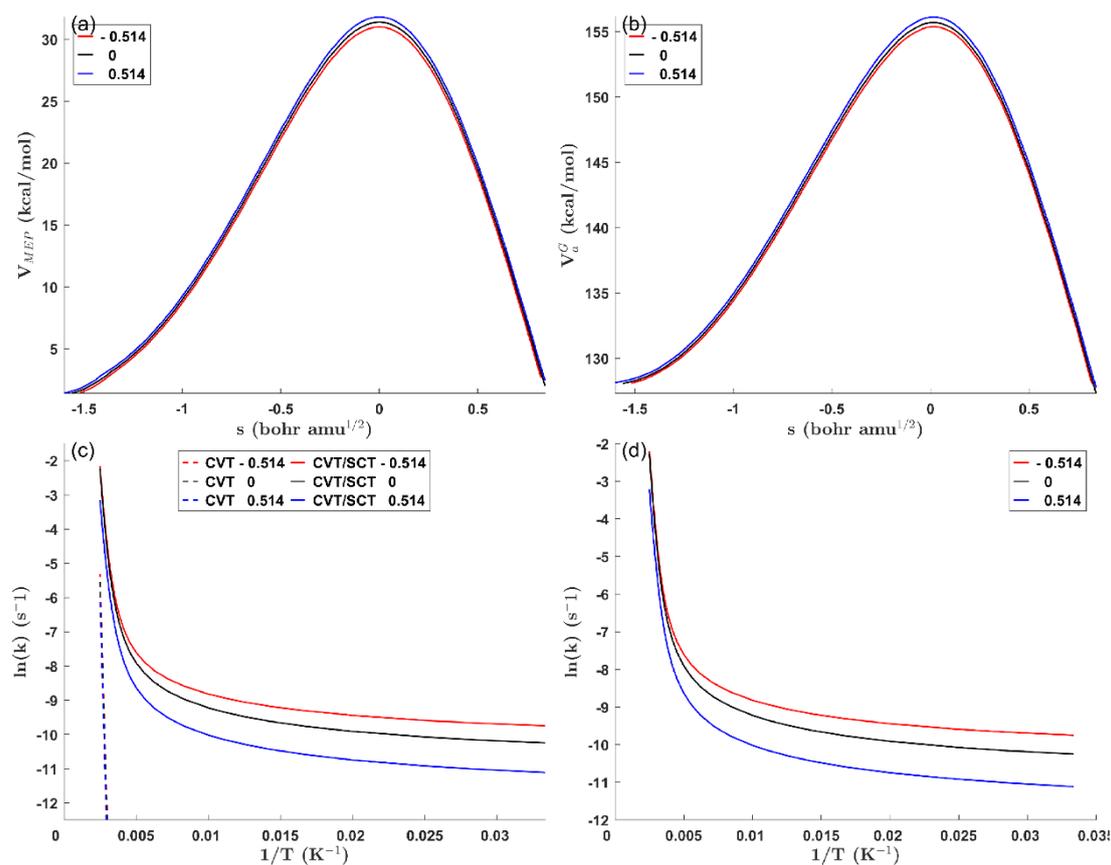
EEF (V/nm)	-0.514	0	0.514
<b><math>Z_C</math>-EEF Direction</b>			
$\Delta E_C$	31.67	31.05	30.43
$\Delta E_D$	30.99	31.39	31.80
$\Delta\Delta E$	0.69	-0.33	-1.37
$\Delta V_a^G(\max)_C$	28.40	27.88	27.23
$\Delta V_a^G(\max)_D$	27.53	27.83	28.20
$\Delta\Delta V_a^G(\max)$	0.87	0.05	-0.97
<b><math>Z_D</math>-EEF Direction</b>			
$\Delta E_C$	30.45	31.05	31.64
$\Delta E_D$	31.91	31.39	30.90
$\Delta\Delta E$	-1.45	-0.34	0.74
$\Delta V_a^G(\max)_C$	27.25	27.85	28.42
$\Delta V_a^G(\max)_D$	28.43	27.84	27.28
$\Delta\Delta V_a^G(\max)$	-1.18	0.01	1.14

**Table S153** Half-life ( $\tau$  in hr) at 30K, barrier width of PES ( $w$  in bohr) and their difference  $\Delta\Delta\tau$  and  $\Delta\Delta w$  between the site-selectivity for the arene molecule bearing two hydroxycarbene groups ( $\mathbf{R_E}$ ) at site C and site D under different EEF strengths

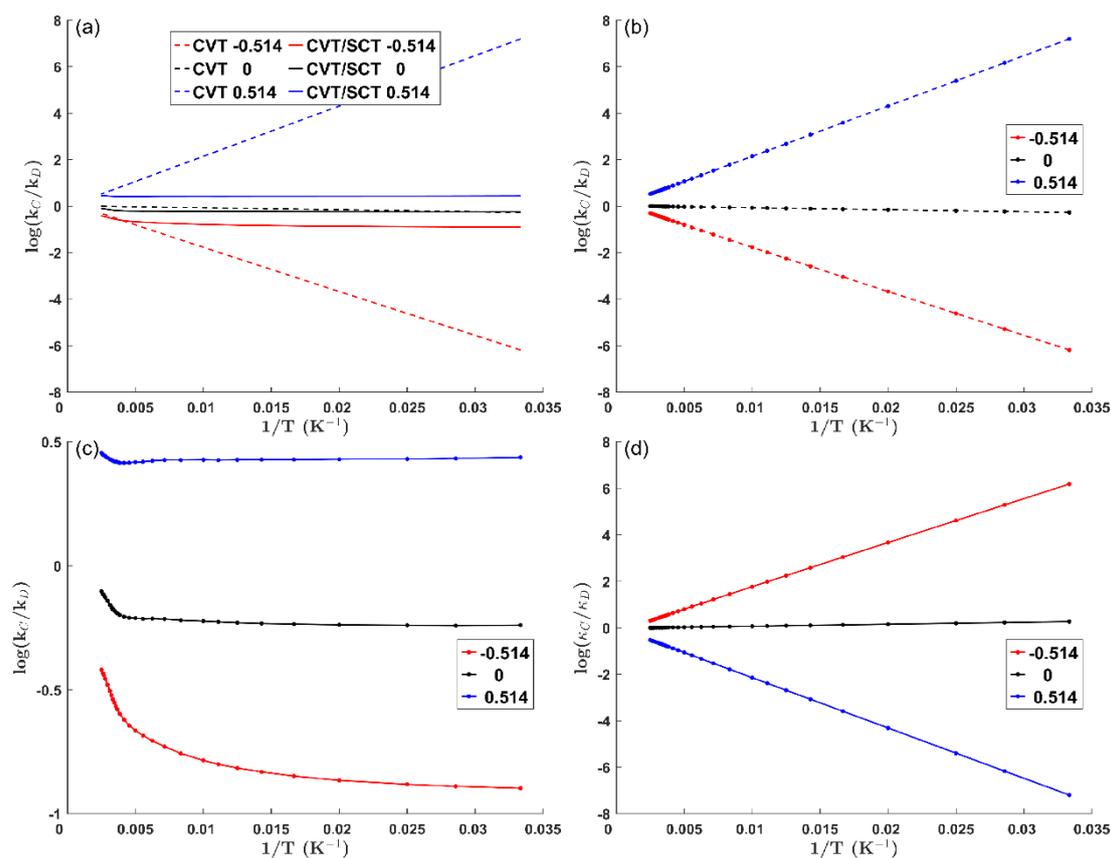
EEF (V/nm)	-0.514	0	0.514
<b>Z<sub>C</sub>-EEF Direction</b>			
$\Delta\tau_C$	26.01	9.44	4.72
$\Delta\tau_D$	3.30	5.44	12.92
$\Delta\Delta\tau$	22.72	4.00	-8.20
$\Delta w_C$	2.66	2.63	2.53
$\Delta w_D$	2.34	2.39	2.44
$\Delta\Delta w$	0.32	0.24	0.10
<b>Z<sub>D</sub>-EEF Direction</b>			
$\Delta\tau_C$	5.48	10.41	20.22
$\Delta\tau_D$	14.37	6.57	4.42
$\Delta\Delta\tau$	-8.88	3.84	15.81
$\Delta w_C$	2.55	2.63	2.66
$\Delta w_D$	2.52	2.50	2.49
$\Delta\Delta w$	0.04	0.13	0.16



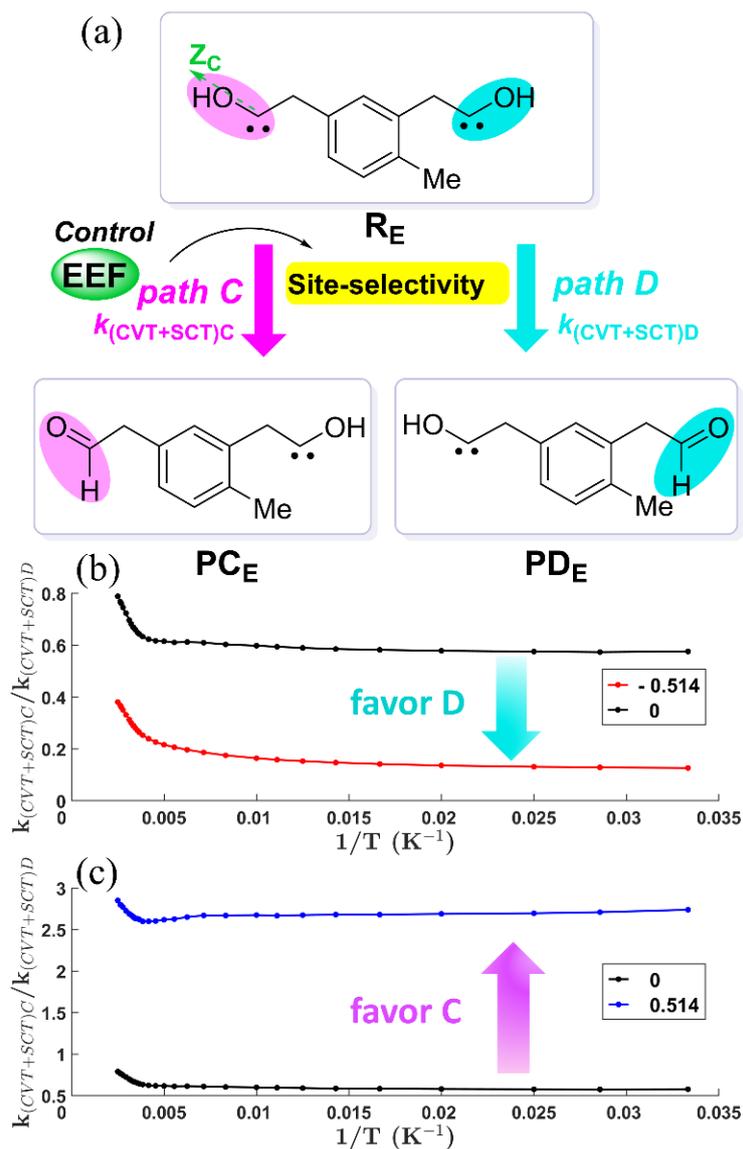
**Figure S95.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at **site C** using  $\omega$ B97X-D/6-31G(d,p) method along **ZC-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



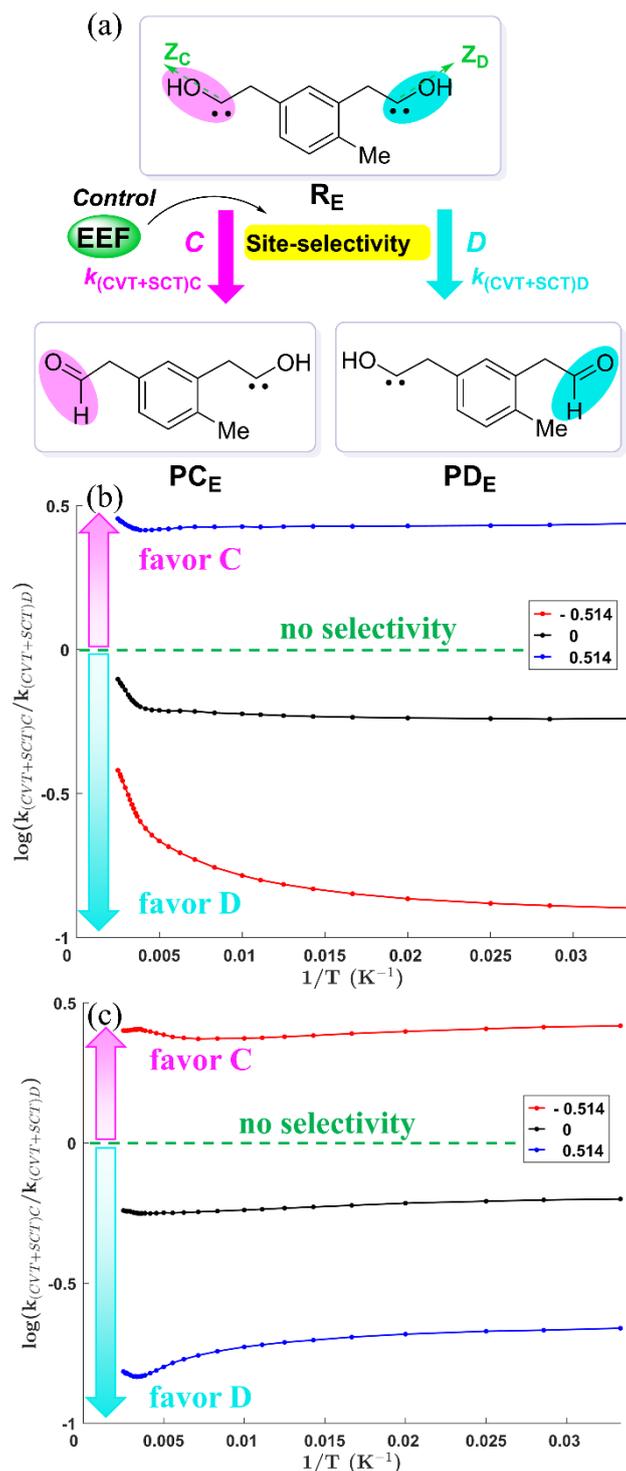
**Figure S96.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at site **D** using  $\omega$ B97X-D/6-31G(d,p) method along **ZC-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S97.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,C}/k_{CVT,D}$ , dash lines) and overall ( $\ln k_{CVT+SCT,C}/k_{CVT+SCT,D}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,C}/k_{CVT,D}$ ), (c) overall ( $\ln k_{CVT+SCT,C}/k_{CVT+SCT,D}$ ) rate constants and (d)  $\ln(k_C/k_D)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups (**RE**) at **site C** and **site D** using  $\omega$ B97X-D/6-31G(d,p) method along **ZC-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S98.** (a) Schematic depicting site-selectivity during the H-migration of  $\mathbf{R_E}$  bearing two different hydroxycarbene moieties in a  $Z_C$ -EEF (purple arrow) and  $Z_D$ -EEF (green arrow). Arrhenius plots ( $k_{(CVT+SCT)C}/k_{(CVT+SCT)D}$  vs.  $1/T$ ) for  $\mathbf{R_E}$  calculated using the  $\omega$ B97X-D method in the (b)  $Z_C$ -EEF and (c)  $Z_D$ -EEF (red:  $-0.514$  V/nm, black: no-EEF ( $0$  V/nm), blue:  $0.514$  V/nm).



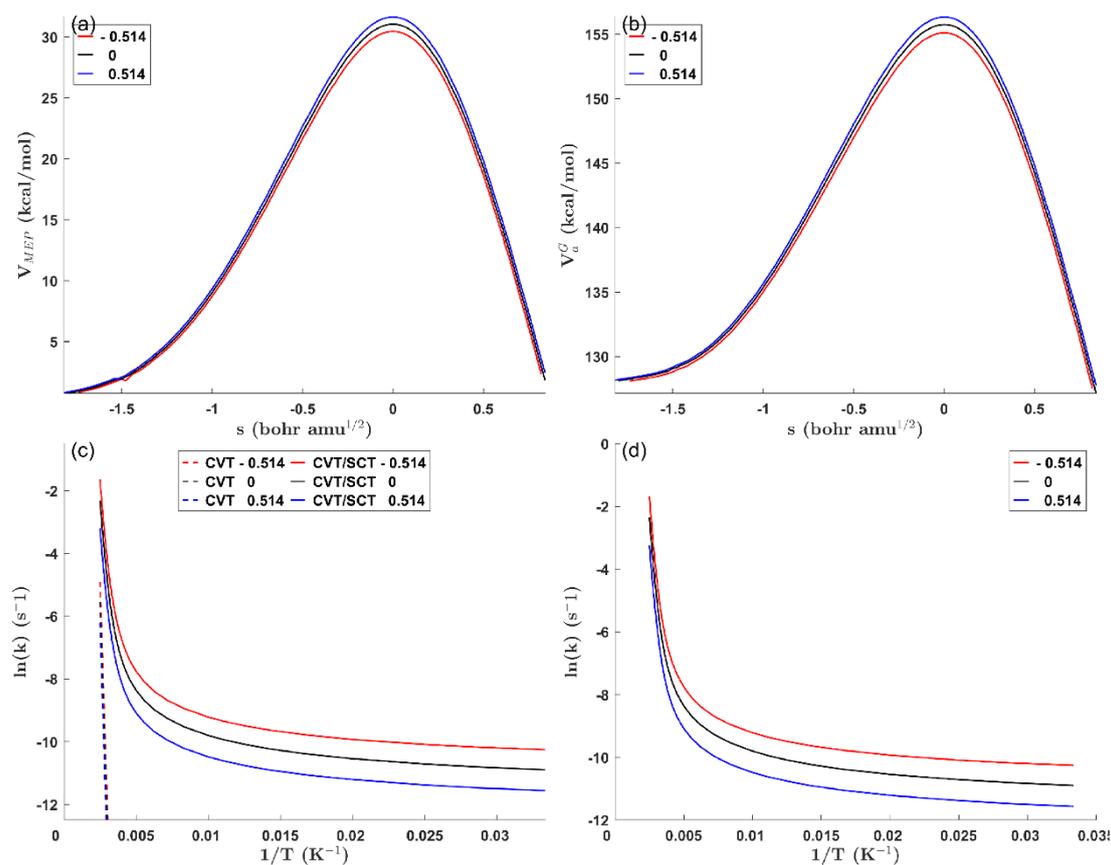
**Figure S99.** (a) Schematic depicting site-selectivity during the H-migration of  $\mathbf{R_E}$  bearing two different hydroxycarbene moieties in a  $Z_C$ -EEF and  $Z_D$ -EEF (green arrows). Arrhenius plots ( $\log(k_{(CVT+SCT)C}/k_{(CVT+SCT)D})$  vs.  $1/T$ ) for  $\mathbf{R_E}$  calculated using the  $\omega$ B97X-D method in the (b)  $Z_C$ -EEF and (c)  $Z_D$ -EEF (red:  $-0.514$  V/nm, black: no-EEF ( $0$  V/nm), blue:  $0.514$  V/nm). Purple arrow is favourable to selectivity of C path, and light-blue arrow is favourable to selectivity of D path.

**Table S154.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at sites C and D using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{C-EEF}}$  direction with various strengths at different temperatures (T in K), negative direction of  $Z_{\text{C-EEF}}$  (-0.514 V/nm); positive direction of  $Z_{\text{C-EEF}}$  (0.514 V/nm); no field (0.0 V/nm)).

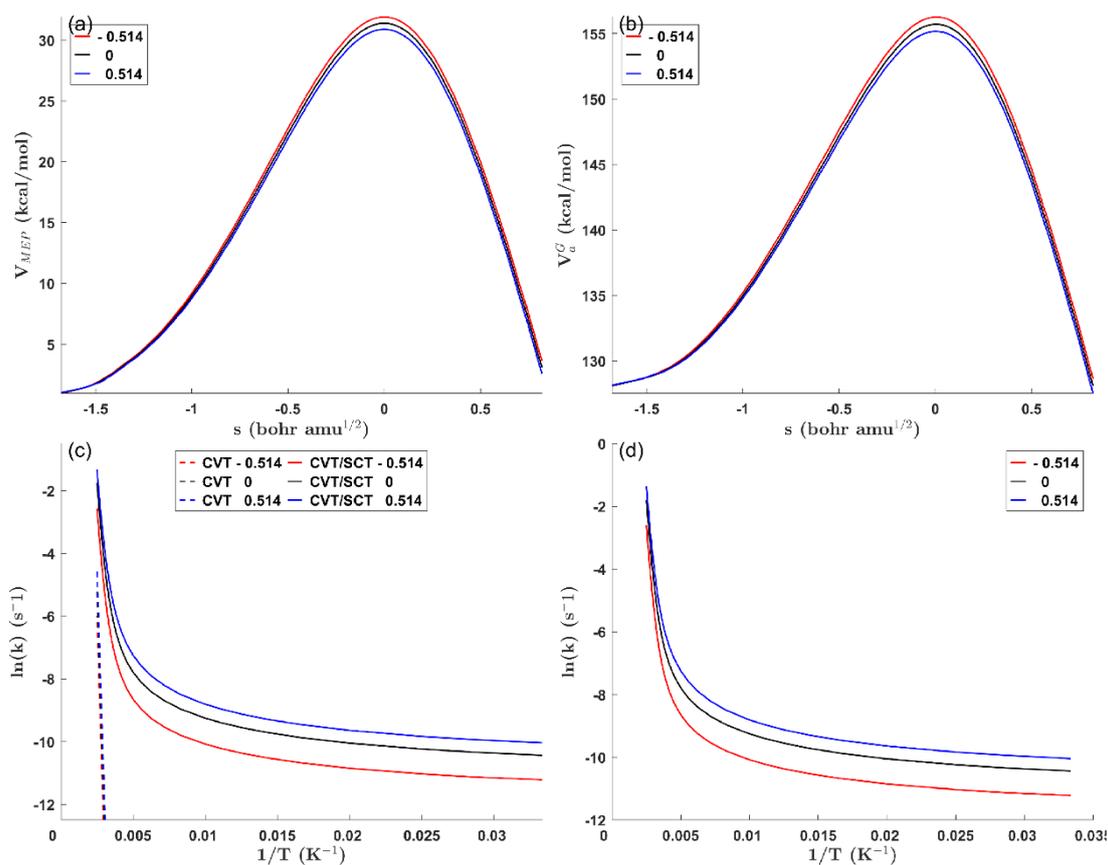
T(K)	$Z_{\text{C-EEF}}$					
	Site C			Site D		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	8.08E-196	4.57E-192	2.50E-187	1.23E-189	8.44E-192	1.60E-194
35	3.37E-166	5.47E-163	6.22E-159	6.53E-161	9.24E-163	4.25E-165
40	5.62E-144	3.58E-141	1.25E-137	2.31E-139	5.65E-141	5.07E-143
50	7.52E-113	1.29E-110	8.64E-108	3.51E-109	1.85E-110	4.24E-112
60	4.37E-92	3.13E-90	6.97E-88	4.78E-89	4.20E-90	1.80E-91
70	3.04E-77	1.17E-75	1.18E-73	1.17E-74	1.49E-75	9.99E-77
80	4.19E-66	1.00E-64	5.63E-63	7.38E-64	1.24E-64	1.16E-65
90	1.96E-57	3.26E-56	1.15E-54	1.88E-55	3.90E-56	4.75E-57
100	1.71E-50	2.12E-49	5.20E-48	1.00E-48	2.48E-49	3.72E-50
120	4.51E-40	3.60E-39	5.09E-38	1.27E-38	4.08E-39	8.37E-40
140	1.29E-32	7.47E-32	7.14E-31	2.13E-31	8.27E-32	2.12E-32
160	5.11E-27	2.34E-26	1.67E-25	5.67E-26	2.54E-26	7.72E-27
180	1.17E-22	4.47E-22	2.53E-21	9.55E-22	4.79E-22	1.66E-22
200	3.67E-19	1.20E-18	5.67E-18	2.32E-18	1.27E-18	4.91E-19
220	2.68E-16	7.77E-16	3.16E-15	1.38E-15	8.15E-16	3.42E-16
240	6.57E-14	1.72E-13	6.17E-13	2.85E-13	1.79E-13	8.07E-14
260	6.96E-12	1.67E-11	5.40E-11	2.61E-11	1.73E-11	8.28E-12
273.15	1.03E-10	2.36E-10	7.17E-10	3.55E-10	2.43E-10	1.20E-10
280	3.81E-10	8.50E-10	2.51E-09	1.26E-09	8.72E-10	4.40E-10
290	2.30E-09	4.95E-09	1.40E-08	7.16E-09	5.07E-09	2.62E-09
298.15	9.09E-09	1.91E-08	5.25E-08	2.71E-08	1.95E-08	1.03E-08
300	1.23E-08	2.57E-08	7.01E-08	3.64E-08	2.62E-08	1.39E-08
310	5.91E-08	1.20E-07	3.16E-07	1.66E-07	1.22E-07	6.59E-08
320	2.58E-07	5.10E-07	1.30E-06	6.93E-07	5.18E-07	2.84E-07
340	3.80E-06	7.14E-06	1.71E-05	9.36E-06	7.22E-06	4.10E-06
360	4.16E-05	7.48E-05	1.70E-04	9.50E-05	7.53E-05	4.41E-05
373.15	1.75E-04	3.06E-04	6.74E-04	3.81E-04	3.07E-04	1.83E-04
380	3.55E-04	6.14E-04	1.33E-03	7.57E-04	6.15E-04	3.70E-04
400	2.44E-03	4.09E-03	8.48E-03	4.91E-03	4.08E-03	2.52E-03

**Table S155.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at sites C and D using  $\omega$ B97X-D/6-31G(d,p) method along  $Z_C$ -EEF direction with various strengths at different temperatures (T in K), negative direction of  $Z_C$ -EEF (-0.514 V/nm); positive direction of  $Z_C$ -EEF (0.514 V/nm); no field (0.0 V/nm))

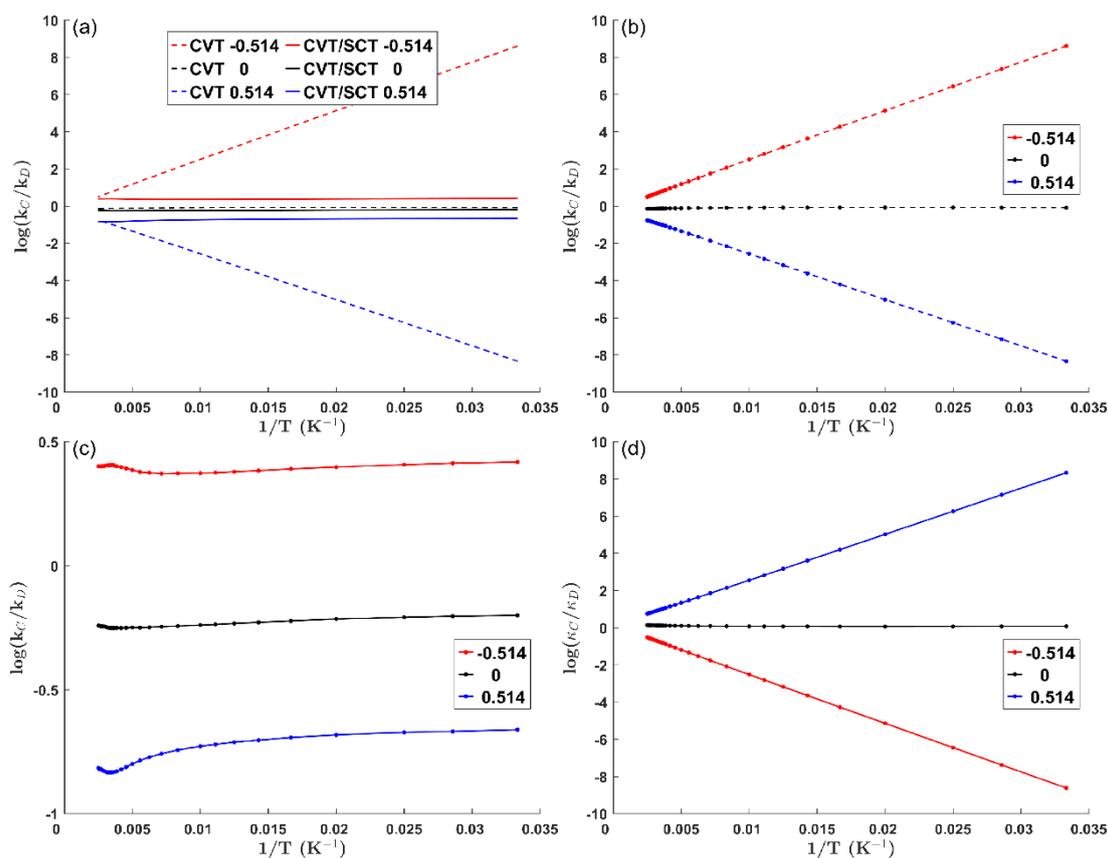
T(K)	$Z_C$ -EEF					
	Site C			Site D		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	7.40E-06	2.04E-05	4.08E-05	5.84E-05	3.54E-05	1.49E-05
35	8.17E-06	2.22E-05	4.47E-05	6.33E-05	3.87E-05	1.65E-05
40	8.99E-06	2.43E-05	4.88E-05	6.84E-05	4.22E-05	1.81E-05
50	1.08E-05	2.87E-05	5.78E-05	7.92E-05	4.96E-05	2.15E-05
60	1.29E-05	3.36E-05	6.78E-05	9.09E-05	5.77E-05	2.53E-05
70	1.52E-05	3.90E-05	7.88E-05	1.03E-04	6.66E-05	2.94E-05
80	1.79E-05	4.50E-05	9.09E-05	1.17E-04	7.63E-05	3.40E-05
90	2.09E-05	5.17E-05	1.04E-04	1.32E-04	8.70E-05	3.90E-05
100	2.43E-05	5.91E-05	1.19E-04	1.48E-04	9.88E-05	4.45E-05
120	3.26E-05	7.66E-05	1.54E-04	1.86E-04	1.27E-04	5.77E-05
140	4.35E-05	9.88E-05	2.00E-04	2.33E-04	1.62E-04	7.49E-05
160	5.81E-05	1.28E-04	2.60E-04	2.95E-04	2.09E-04	9.81E-05
180	7.84E-05	1.68E-04	3.44E-04	3.79E-04	2.75E-04	1.31E-04
200	1.08E-04	2.27E-04	4.66E-04	4.99E-04	3.69E-04	1.78E-04
220	1.54E-04	3.16E-04	6.56E-04	6.79E-04	5.12E-04	2.52E-04
240	2.31E-04	4.63E-04	9.67E-04	9.65E-04	7.43E-04	3.72E-04
260	3.67E-04	7.22E-04	1.51E-03	1.45E-03	1.14E-03	5.81E-04
273.15	5.20E-04	1.01E-03	2.11E-03	1.97E-03	1.57E-03	8.05E-04
280	6.31E-04	1.22E-03	2.54E-03	2.33E-03	1.88E-03	9.66E-04
290	8.53E-04	1.63E-03	3.37E-03	3.04E-03	2.47E-03	1.28E-03
298.15	1.11E-03	2.10E-03	4.29E-03	3.83E-03	3.14E-03	1.62E-03
300	1.17E-03	2.22E-03	4.54E-03	4.04E-03	3.32E-03	1.71E-03
310	1.64E-03	3.09E-03	6.20E-03	5.45E-03	4.53E-03	2.32E-03
320	2.34E-03	4.38E-03	8.55E-03	7.48E-03	6.29E-03	3.18E-03
340	4.84E-03	9.05E-03	1.66E-02	1.46E-02	1.25E-02	6.09E-03
360	1.02E-02	1.91E-02	3.24E-02	2.91E-02	2.56E-02	1.17E-02
373.15	1.66E-02	3.13E-02	5.03E-02	4.59E-02	4.11E-02	1.80E-02
380	2.14E-02	4.03E-02	6.30E-02	5.81E-02	5.25E-02	2.25E-02
400	4.42E-02	8.44E-02	1.22E-01	1.16E-01	1.07E-01	4.28E-02



**Figure S100.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at **site C** using  $\omega$ B97X-D/6-31G(d,p) method along **ZD-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S101.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at site **D** using  $\omega$ B97X-D/6-31G(d,p) method along **ZD-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S102.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,C}/k_{CVT,D}$ , dash lines) and overall ( $\ln k_{CVT+SCT,C}/k_{CVT+SCT,D}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,C}/k_{CVT,D}$ ), (c) overall ( $\ln k_{CVT+SCT,C}/k_{CVT+SCT,D}$ ) rate constants and (d)  $\ln(k_C/k_D)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups (**R<sub>E</sub>**) at **site C** and **site D** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>D</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).

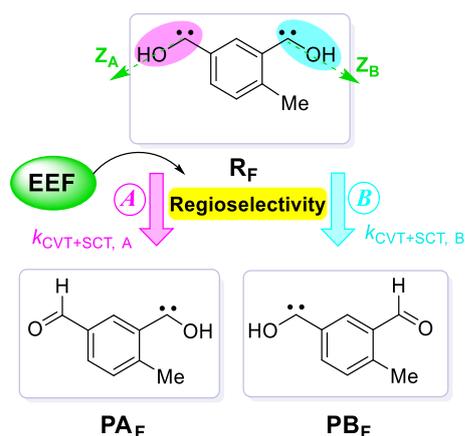
**Table S156.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups (**RE**) at sites C and D using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{D}}\text{-EEF}$  direction with various strengths at different temperatures (T), negative direction of  $Z_{\text{D}}\text{-EEF}$  (-0.514 V/nm); positive direction of  $Z_{\text{D}}\text{-EEF}$  (0.514 V/nm); no field (0.0 V/nm).

T(K)	$Z_{\text{D}}\text{-EEF}$					
	Site C			Site D		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	1.81E-187	8.42E-192	5.32E-196	4.41E-196	1.02E-191	1.15E-187
35	4.74E-159	9.25E-163	2.32E-166	2.01E-166	1.11E-162	3.28E-159
40	9.90E-138	5.68E-141	3.99E-144	3.57E-144	6.73E-141	7.35E-138
50	7.19E-108	1.87E-110	5.58E-113	5.25E-113	2.20E-110	5.92E-108
60	5.99E-88	4.26E-90	3.34E-92	3.25E-92	5.03E-90	5.30E-88
70	1.03E-73	1.51E-75	2.36E-77	2.37E-77	1.80E-75	9.69E-74
80	5.01E-63	1.26E-64	3.30E-66	3.38E-66	1.50E-64	4.91E-63
90	1.04E-54	3.98E-56	1.56E-57	1.62E-57	4.77E-56	1.06E-54
100	4.72E-48	2.53E-49	1.37E-50	1.45E-50	3.06E-49	4.95E-48
120	4.67E-38	4.16E-39	3.65E-40	3.95E-40	5.09E-39	5.16E-38
140	6.60E-31	8.45E-32	1.04E-32	1.15E-32	1.05E-31	7.59E-31
160	1.55E-25	2.60E-26	4.17E-27	4.67E-27	3.26E-26	1.84E-25
180	2.36E-21	4.90E-22	9.60E-23	1.09E-22	6.21E-22	2.88E-21
200	5.30E-18	1.30E-18	3.00E-19	3.45E-19	1.67E-18	6.63E-18
220	2.95E-15	8.35E-16	2.19E-16	2.55E-16	1.08E-15	3.77E-15
240	5.79E-13	1.84E-13	5.39E-14	6.31E-14	2.39E-13	7.53E-13
260	5.07E-11	1.77E-11	5.71E-12	6.74E-12	2.33E-11	6.70E-11
273.15	6.74E-10	2.49E-10	8.47E-11	1.01E-10	3.29E-10	9.00E-10
280	2.36E-09	8.97E-10	3.13E-10	3.72E-10	1.19E-09	3.16E-09
290	1.32E-08	5.22E-09	1.88E-09	2.25E-09	6.93E-09	1.78E-08
298.15	4.94E-08	2.01E-08	7.46E-09	8.93E-09	2.68E-08	6.71E-08
300	6.60E-08	2.70E-08	1.01E-08	1.21E-08	3.60E-08	8.98E-08
310	2.98E-07	1.26E-07	4.85E-08	5.83E-08	1.68E-07	4.08E-07
320	1.22E-06	5.34E-07	2.12E-07	2.55E-07	7.16E-07	1.69E-06
340	1.61E-05	7.45E-06	3.12E-06	3.78E-06	1.01E-05	2.25E-05
360	1.60E-04	7.78E-05	3.42E-05	4.16E-05	1.06E-04	2.26E-04
373.15	6.36E-04	3.18E-04	1.44E-04	1.75E-04	4.34E-04	9.01E-04
380	1.26E-03	6.37E-04	2.92E-04	3.57E-04	8.70E-04	1.78E-03
400	8.01E-03	4.23E-03	2.01E-03	2.48E-03	5.81E-03	1.15E-02

**Table S157.** The overall rate constants ( $k_{CVT+SCT}$  in  $s^{-1}$ ) of one arene molecule bearing two hydroxycarbene groups ( $\mathbf{R_E}$ ) at sites C and D using  $\omega$ B97X-D/6-31G(d,p) method along  $Z_D$ -EEF direction with various strengths at different temperatures (T), negative direction of  $Z_D$ -EEF (-0.514 V/nm); positive direction of  $Z_D$ -EEF (0.514 V/nm); no field (0.0 V/nm))

T(K)	$Z_D$ -EEF					
	Site C			Site D		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	3.51E-05	1.85E-05	9.52E-06	1.34E-05	2.93E-05	4.36E-05
35	3.81E-05	2.03E-05	1.04E-05	1.47E-05	3.24E-05	4.84E-05
40	4.14E-05	2.22E-05	1.14E-05	1.62E-05	3.58E-05	5.35E-05
50	4.85E-05	2.63E-05	1.35E-05	1.94E-05	4.31E-05	6.49E-05
60	5.65E-05	3.08E-05	1.58E-05	2.30E-05	5.14E-05	7.78E-05
70	6.53E-05	3.59E-05	1.83E-05	2.70E-05	6.07E-05	9.24E-05
80	7.52E-05	4.16E-05	2.12E-05	3.14E-05	7.10E-05	1.09E-04
90	8.64E-05	4.80E-05	2.44E-05	3.64E-05	8.27E-05	1.28E-04
100	9.90E-05	5.52E-05	2.79E-05	4.19E-05	9.57E-05	1.49E-04
120	1.30E-04	7.26E-05	3.65E-05	5.51E-05	1.27E-04	2.02E-04
140	1.70E-04	9.54E-05	4.77E-05	7.23E-05	1.68E-04	2.73E-04
160	2.26E-04	1.26E-04	6.26E-05	9.53E-05	2.23E-04	3.70E-04
180	3.06E-04	1.69E-04	8.34E-05	1.28E-04	3.00E-04	5.08E-04
200	4.26E-04	2.33E-04	1.13E-04	1.75E-04	4.13E-04	7.11E-04
220	6.14E-04	3.31E-04	1.59E-04	2.49E-04	5.89E-04	1.03E-03
240	9.27E-04	4.93E-04	2.34E-04	3.71E-04	8.79E-04	1.55E-03
260	1.48E-03	7.81E-04	3.65E-04	5.88E-04	1.39E-03	2.46E-03
273.15	2.10E-03	1.10E-03	5.10E-04	8.29E-04	1.96E-03	3.46E-03
280	2.55E-03	1.33E-03	6.15E-04	1.00E-03	2.37E-03	4.18E-03
290	3.44E-03	1.79E-03	8.22E-04	1.35E-03	3.19E-03	5.60E-03
298.15	4.45E-03	2.31E-03	1.06E-03	1.75E-03	4.11E-03	7.21E-03
300	4.72E-03	2.46E-03	1.12E-03	1.86E-03	4.37E-03	7.64E-03
310	6.61E-03	3.43E-03	1.56E-03	2.60E-03	6.09E-03	1.06E-02
320	9.39E-03	4.88E-03	2.19E-03	3.70E-03	8.63E-03	1.49E-02
340	1.96E-02	1.02E-02	4.50E-03	7.76E-03	1.79E-02	3.03E-02
360	4.21E-02	2.18E-02	9.41E-03	1.67E-02	3.82E-02	6.27E-02
373.15	6.97E-02	3.59E-02	1.53E-02	2.77E-02	6.29E-02	1.01E-01
380	9.04E-02	4.66E-02	1.96E-02	3.59E-02	8.14E-02	1.30E-01
400	1.93E-01	9.88E-02	4.07E-02	7.66E-02	1.72E-01	2.66E-01

## Arene molecule $R_F$



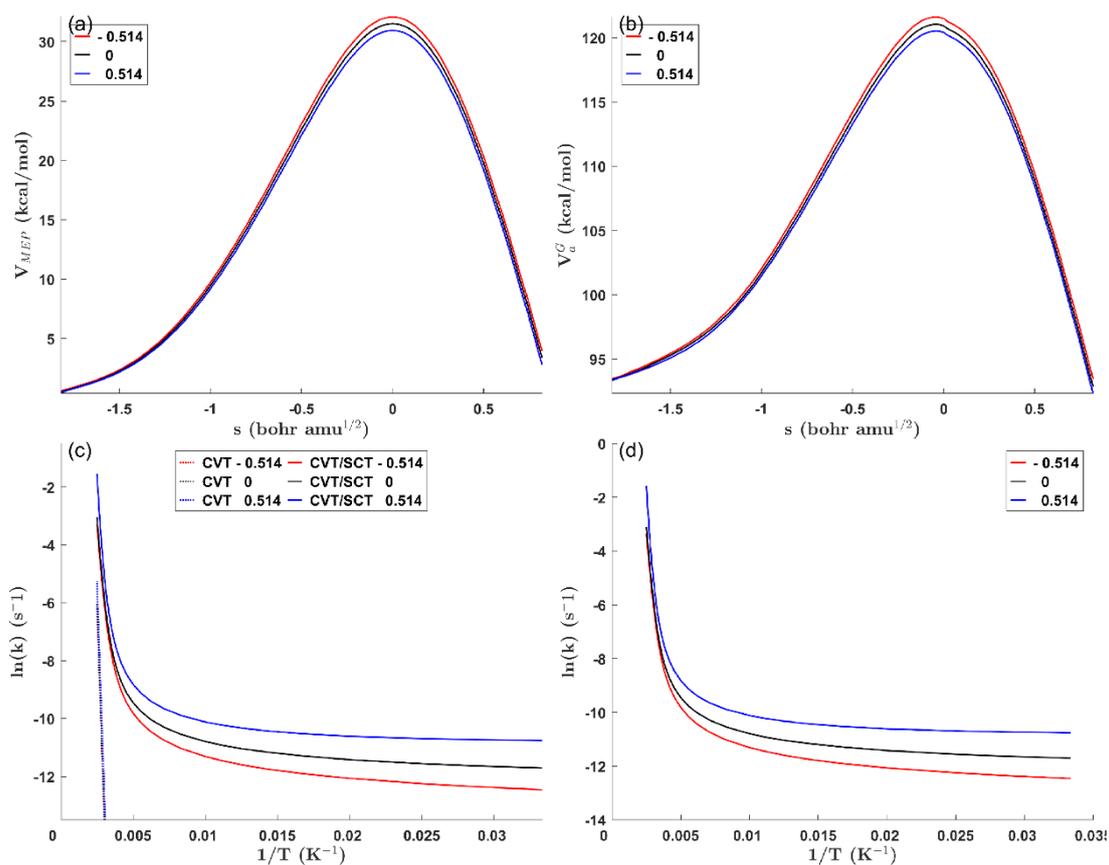
**Figure S103** Schematic site-selectivity of the H-migration of arene molecule bearing two hydroxycarbene groups under EEF of the  $Z_A$  and  $Z_B$  Directions.

**Table S158** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and electronic energies plus zero-point correction energy ( $\Delta V_a^G(\max)$  in kcal/mol) and their difference  $\Delta\Delta E$  and  $\Delta\Delta V_a^G(\max)$  between site-selectivity for arene molecule bearing two hydroxycarbene groups at site A and site B under different EEF strengths.

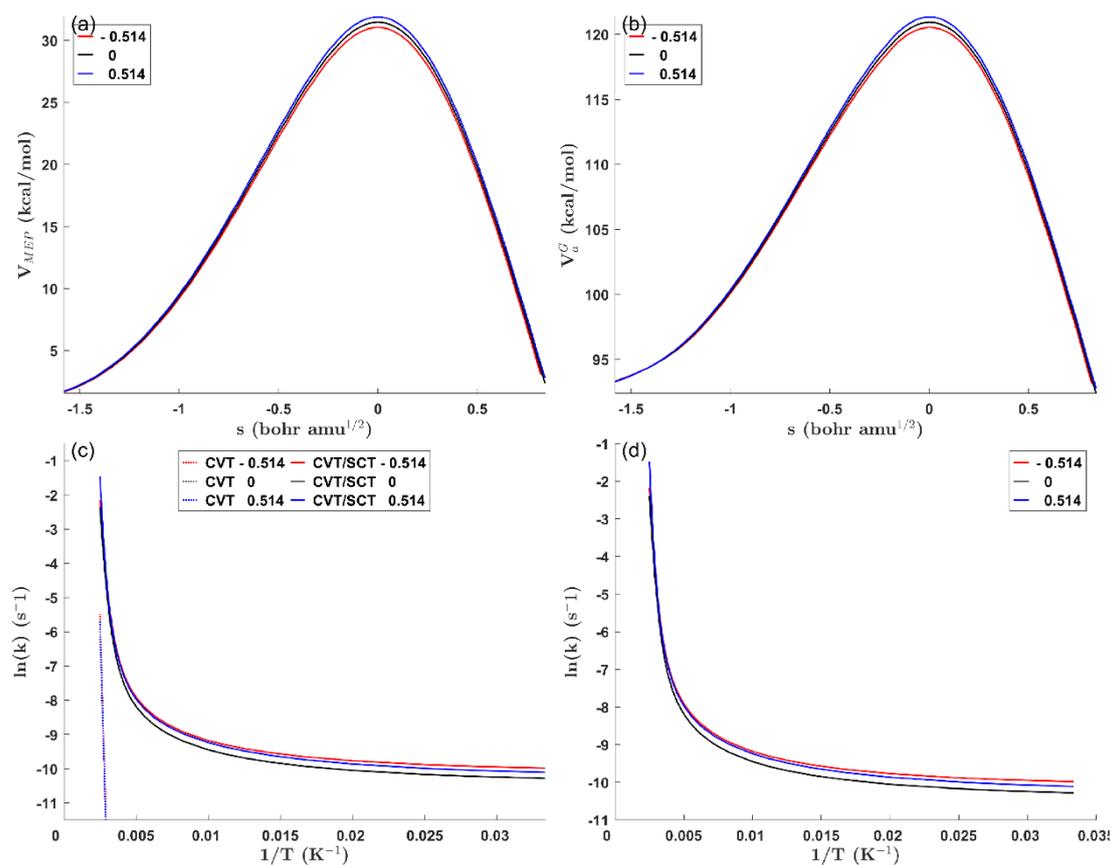
EEF (V/nm)	-0.514	0	0.514
<b><math>Z_A</math>-EEF Direction</b>			
$\Delta E_A$	32.08	31.51	30.94
$\Delta E_B$	31.05	31.48	31.90
$\Delta\Delta E$	-1.02	-0.04	0.95
$\Delta V_a^G(\max)_A$	28.48	27.92	27.35
$\Delta V_a^G(\max)_B$	27.53	27.92	28.27
$\Delta\Delta V_a^G(\max)$	-0.95	0.01	0.92
<b><math>Z_B</math>-EEF Direction</b>			
$\Delta E_A$	31.39	31.51	31.62
$\Delta E_B$	32.05	31.48	30.91
$\Delta\Delta E$	0.66	-0.03	-0.71
$\Delta V_a^G(\max)_A$	27.81	27.94	28.03
$\Delta V_a^G(\max)_B$	28.30	27.79	27.29
$\Delta\Delta V_a^G(\max)$	0.49	-0.15	-0.73

**Table S159** Half-life ( $\tau$  in hr) at 30K, barrier width of PES ( $w$  in bohr) and their difference  $\Delta\Delta\tau$  and  $\Delta\Delta w$  between site-selectivity for arene molecule bearing two hydroxycarbene groups ( $\mathbf{R}_F$ ) at site A and site B under different EEF strengths.

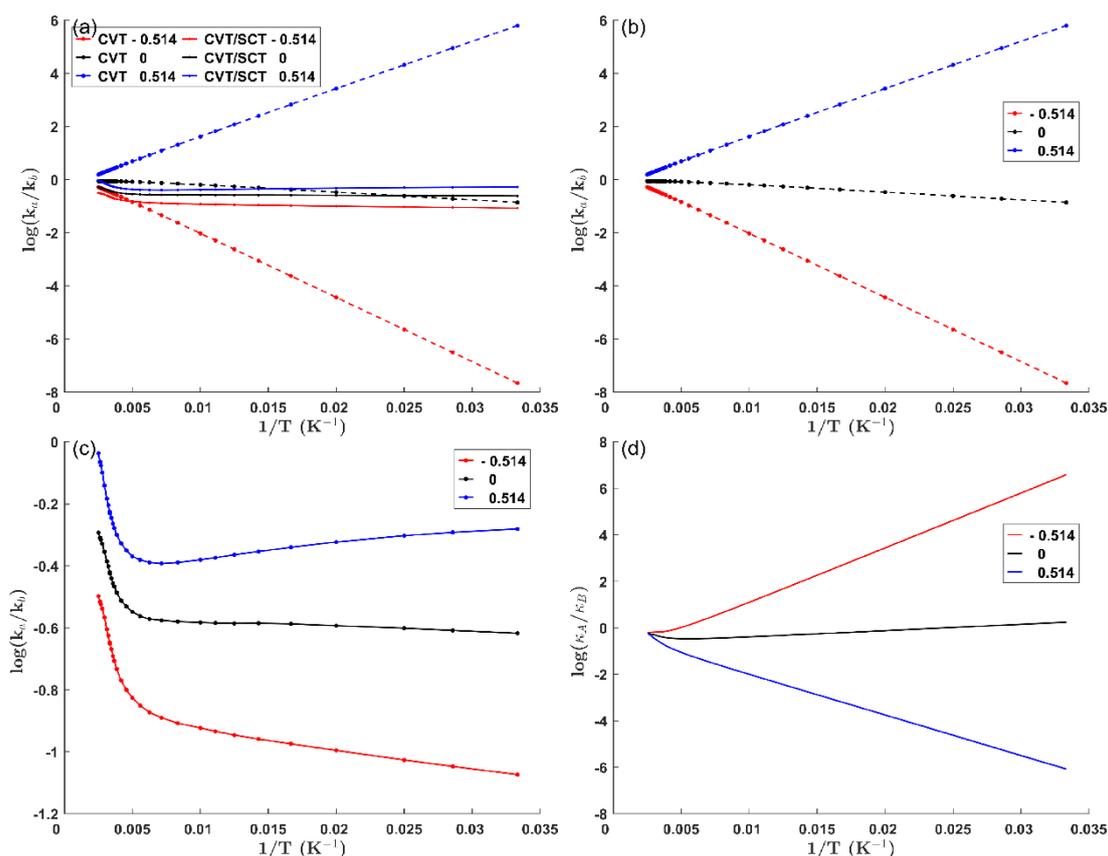
EEF (V/nm)	-0.514	0	0.514
<b>Z<sub>A</sub>-EEF Direction</b>			
$\Delta\tau_A$	49.36	23.25	9.04
$\Delta\tau_B$	4.17	5.61	4.73
$\Delta\Delta\tau$	-45.19	-17.64	-4.31
$\Delta w_A$	2.69	2.66	2.63
$\Delta w_B$	2.42	2.43	2.42
$\Delta\Delta w$	-0.27	-0.23	-0.21
<b>Z<sub>B</sub>-EEF Direction</b>			
$\Delta\tau_A$	7.73	14.26	17.34
$\Delta\tau_B$	6.17	4.53	2.45
$\Delta\Delta\tau$	-1.56	-9.73	-14.90
$\Delta w_A$	2.56	2.58	2.61
$\Delta w_B$	2.49	2.48	2.45
$\Delta\Delta w$	-0.07	-0.10	-0.15



**Figure S104.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants ( $k$ , in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene molecule bearing two hydroxycarbene groups (**R<sub>F</sub>**) at **site A** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>A</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S105.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in  $s^{-1}$ ), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene molecule bearing two hydroxycarbene groups (**R<sub>F</sub>**) at **site B** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>A</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



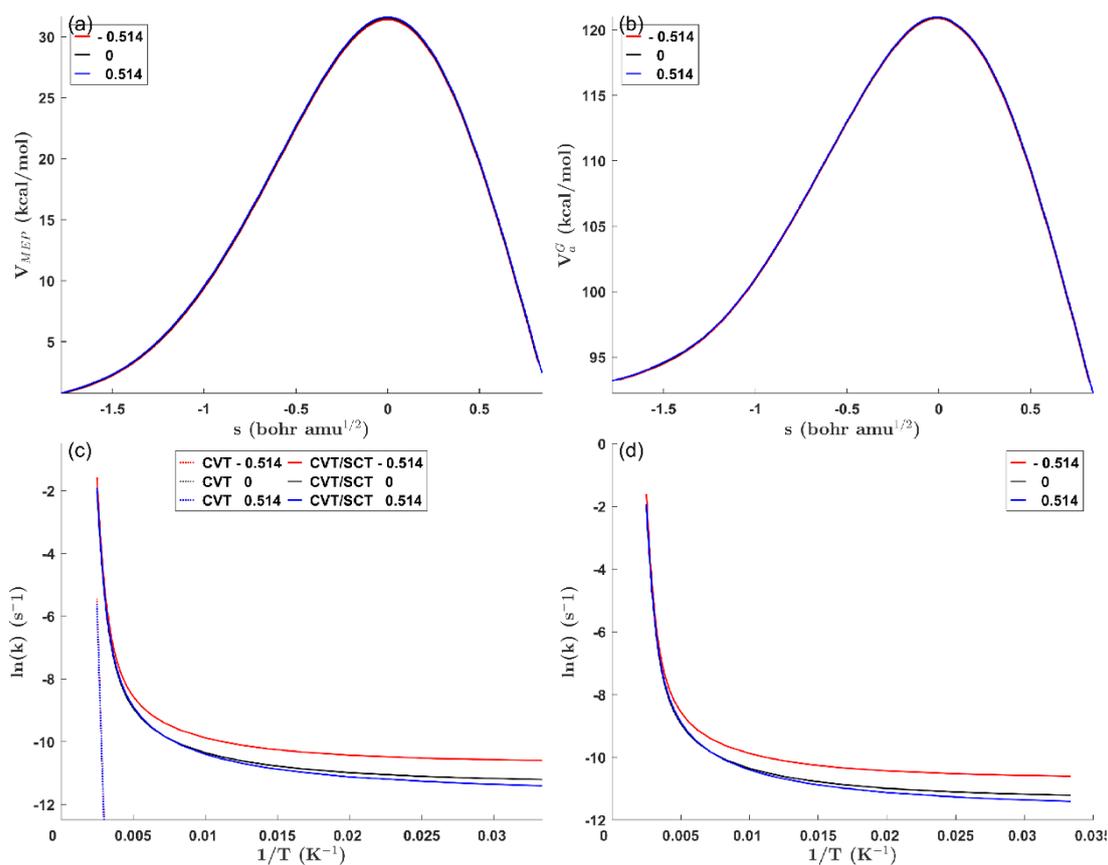
**Figure S106.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ , dash lines) and overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ ), (c) overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ ) rate constants and (d)  $\ln(\kappa_A/\kappa_B)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups ( $\mathbf{R}_F$ ) at **site A** and **site B** ( $\log(X_A/X_B)$ ) using  $\omega$ B97X-D/6-31G(d,p) method along  $\mathbf{Z}_A$ -EEF direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).

**Table S160.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of arene molecule bearing two hydroxycarbene groups (**R<sub>F</sub>**) sites A and B using  $\omega$ B97X-D/6-31G(d,p) method along  $Z_{\text{A}}$ -EEF direction with various strengths at different temperatures (T in K), negative direction of  $Z_{\text{A}}$ -EEF (-0.514 V/nm); positive direction of  $Z_{\text{A}}$ -EEF (0.514 V/nm); no field (0.0 V/nm).

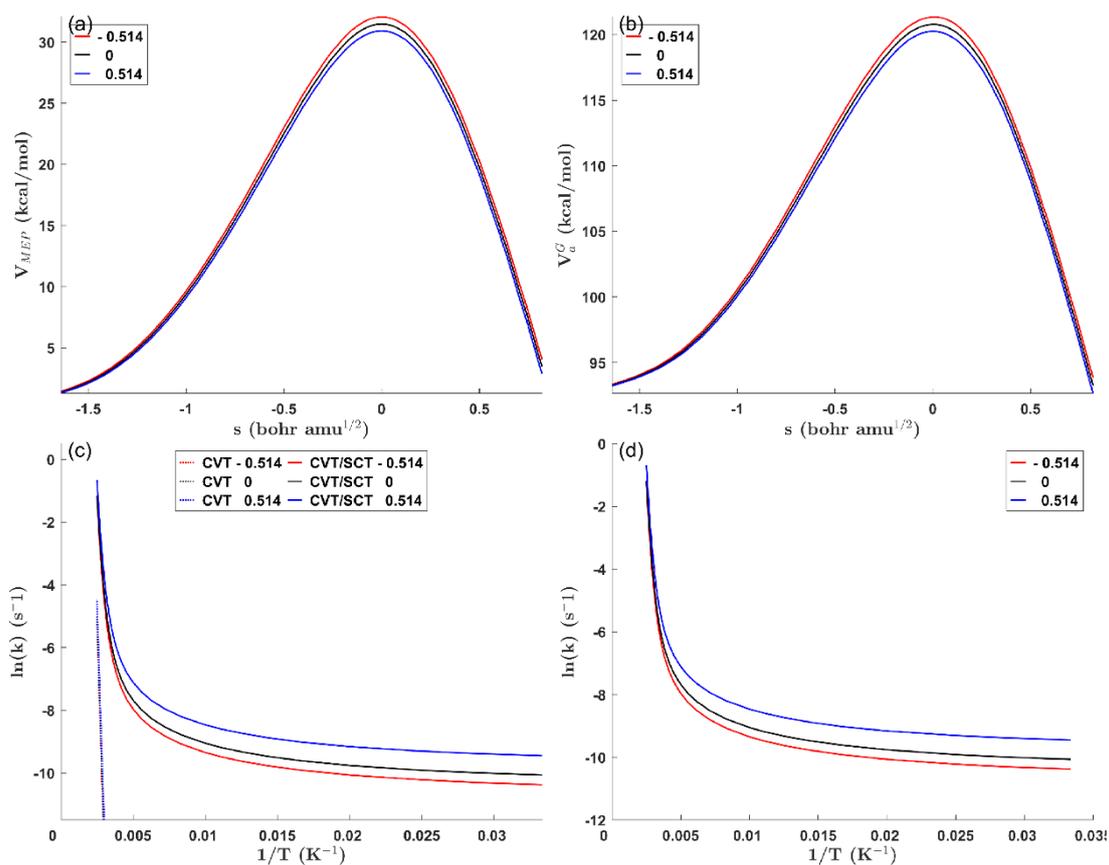
T(K)	$Z_{\text{A}}$ -EEF					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	2.84E-197	2.79E-193	4.06E-189	1.29E-189	2.02E-192	6.54E-195
35	2.03E-167	4.94E-164	1.83E-160	6.48E-161	2.59E-163	2.05E-165
40	5.04E-145	4.32E-142	5.75E-139	2.21E-139	1.78E-141	2.76E-143
50	1.17E-113	2.31E-111	7.34E-109	3.17E-109	6.83E-111	2.75E-112
60	9.79E-93	7.27E-91	8.85E-89	4.15E-89	1.72E-90	1.31E-91
70	8.79E-78	3.24E-76	1.99E-74	9.93E-75	6.58E-76	7.94E-77
80	1.46E-66	3.18E-65	1.17E-63	6.14E-64	5.78E-65	9.86E-66
90	7.91E-58	1.14E-56	2.83E-55	1.54E-55	1.90E-56	4.25E-57
100	7.73E-51	8.05E-50	1.45E-48	8.16E-49	1.26E-49	3.48E-50
120	2.42E-40	1.54E-39	1.72E-38	1.02E-38	2.18E-39	8.36E-40
140	7.74E-33	3.47E-32	2.76E-31	1.71E-31	4.60E-32	2.23E-32
160	3.35E-27	1.15E-26	7.09E-26	4.55E-26	1.46E-26	8.42E-27
180	8.19E-23	2.30E-22	1.16E-21	7.67E-22	2.83E-22	1.86E-22
200	2.69E-19	6.40E-19	2.76E-18	1.87E-18	7.69E-19	5.65E-19
220	2.04E-16	4.25E-16	1.61E-15	1.12E-15	5.02E-16	4.03E-16
240	5.15E-14	9.58E-14	3.26E-13	2.31E-13	1.12E-13	9.69E-14
260	5.60E-12	9.47E-12	2.93E-11	2.13E-11	1.10E-11	1.01E-11
273.15	8.42E-11	1.35E-10	3.96E-10	2.91E-10	1.56E-10	1.49E-10
280	3.13E-10	4.88E-10	1.40E-09	1.03E-09	5.63E-10	5.46E-10
290	1.90E-09	2.86E-09	7.91E-09	5.89E-09	3.29E-09	3.27E-09
298.15	7.58E-09	1.11E-08	2.99E-08	2.24E-08	1.27E-08	1.29E-08
300	1.03E-08	1.49E-08	4.00E-08	3.00E-08	1.72E-08	1.74E-08
310	4.98E-08	7.01E-08	1.82E-07	1.38E-07	8.04E-08	8.33E-08
320	2.19E-07	2.99E-07	7.54E-07	5.74E-07	3.42E-07	3.62E-07
340	3.26E-06	4.22E-06	1.01E-05	7.80E-06	4.82E-06	5.28E-06
360	3.61E-05	4.46E-05	1.02E-04	7.96E-05	5.08E-05	5.75E-05
373.15	1.52E-04	1.83E-04	4.06E-04	3.20E-04	2.08E-04	2.41E-04
380	3.11E-04	3.68E-04	8.05E-04	6.37E-04	4.19E-04	4.88E-04
400	2.16E-03	2.46E-03	5.19E-03	4.16E-03	2.80E-03	3.35E-03

**Table S161.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of arene molecule bearing two hydroxycarbene groups ( $\mathbf{R}_F$ ) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_A\text{-EEF}$  direction with various strengths at different temperatures (T in K), negative direction of  $Z_A\text{-EEF}$  (-0.514 V/nm); positive direction of  $Z_A\text{-EEF}$  (0.514 V/nm); no field (0.0 V/nm))

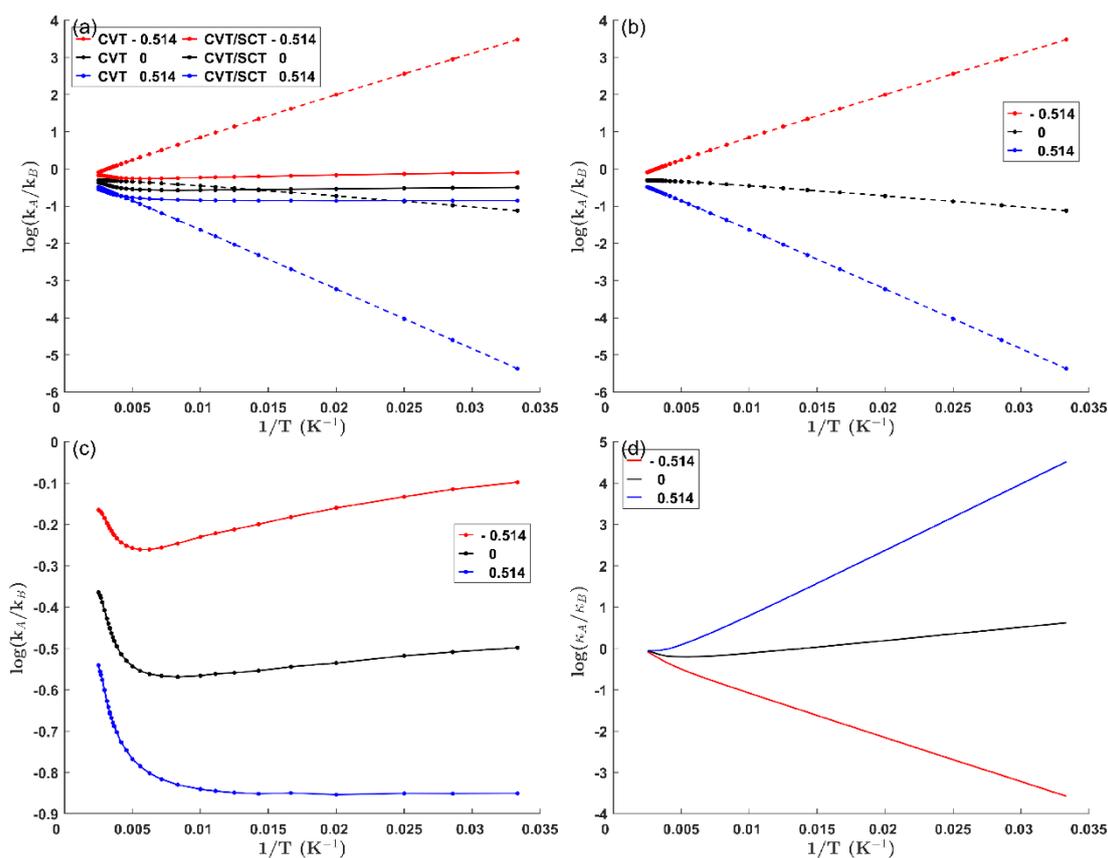
T(K)	$Z_A\text{-EEF}$					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	3.90E-06	8.28E-06	2.13E-05	4.62E-05	3.43E-05	4.07E-05
35	4.35E-06	8.92E-06	2.20E-05	4.85E-05	3.62E-05	4.31E-05
40	4.81E-06	9.59E-06	2.28E-05	5.11E-05	3.83E-05	4.58E-05
50	5.78E-06	1.10E-05	2.47E-05	5.72E-05	4.31E-05	5.20E-05
60	6.82E-06	1.26E-05	2.70E-05	6.43E-05	4.87E-05	5.91E-05
70	7.96E-06	1.43E-05	2.97E-05	7.24E-05	5.50E-05	6.71E-05
80	9.24E-06	1.61E-05	3.29E-05	8.16E-05	6.20E-05	7.61E-05
90	1.07E-05	1.82E-05	3.64E-05	9.19E-05	6.99E-05	8.61E-05
100	1.23E-05	2.06E-05	4.05E-05	1.03E-04	7.88E-05	9.73E-05
120	1.62E-05	2.63E-05	5.06E-05	1.31E-04	1.00E-04	1.24E-04
140	2.15E-05	3.37E-05	6.40E-05	1.67E-04	1.27E-04	1.58E-04
160	2.87E-05	4.37E-05	8.25E-05	2.14E-04	1.63E-04	2.02E-04
180	3.91E-05	5.78E-05	1.09E-04	2.77E-04	2.11E-04	2.62E-04
200	5.46E-05	7.86E-05	1.48E-04	3.66E-04	2.78E-04	3.47E-04
220	7.91E-05	1.11E-04	2.10E-04	4.99E-04	3.77E-04	4.70E-04
240	1.20E-04	1.64E-04	3.13E-04	7.06E-04	5.33E-04	6.65E-04
260	1.96E-04	2.60E-04	4.98E-04	1.06E-03	7.97E-04	9.94E-04
273.15	2.83E-04	3.69E-04	7.11E-04	1.44E-03	1.08E-03	1.35E-03
280	3.48E-04	4.50E-04	8.71E-04	1.71E-03	1.29E-03	1.60E-03
290	4.80E-04	6.13E-04	1.20E-03	2.24E-03	1.69E-03	2.11E-03
298.15	6.34E-04	8.04E-04	1.58E-03	2.84E-03	2.14E-03	2.69E-03
300	6.77E-04	8.57E-04	1.69E-03	3.01E-03	2.26E-03	2.84E-03
310	9.76E-04	1.23E-03	2.46E-03	4.12E-03	3.10E-03	3.94E-03
320	1.43E-03	1.79E-03	3.69E-03	5.76E-03	4.35E-03	5.63E-03
340	3.20E-03	3.98E-03	9.03E-03	1.18E-02	9.01E-03	1.25E-02
360	7.30E-03	9.14E-03	2.44E-02	2.52E-02	1.95E-02	3.07E-02
373.15	1.25E-02	1.58E-02	4.88E-02	4.18E-02	3.27E-02	5.82E-02
380	1.66E-02	2.10E-02	7.07E-02	5.44E-02	4.29E-02	8.22E-02
400	3.72E-02	4.78E-02	2.13E-01	1.17E-01	9.38E-02	2.32E-01



**Figure S107.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene molecule bearing two hydroxycarbene groups (**R<sub>F</sub>**) at **site A** using  $\omega$ B97X-D/6-31G(d,p) method along **Z<sub>B</sub>-EEF** direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).



**Figure S108.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene molecule bearing two hydroxycarbene groups (R<sub>F</sub>) at site B using  $\omega$ B97X-D/6-31G(d,p) method along Z<sub>B</sub>-EEF direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: (0.0 V/nm)).



**Figure S109.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ , dash lines) and overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ ), (c) overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ ) rate constants and (d)  $\ln(\kappa_A/\kappa_B)$  versus  $1/T$  between arene molecule bearing two hydroxycarbene groups ( $\mathbf{R}_F$ ) at **site A** and **site B** using  $\omega$ B97X-D/6-31G(d,p) method along  $\mathbf{Z}_B$ - $\mathbf{EEF}$  direction with different strengths (red: -0.514 V/nm; blue: 0.514 V/nm and black: no field (0.0 V/nm)).

**Table S162.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of arene molecule bearing two hydroxycarbene groups (**R<sub>F</sub>**) sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{B}}\text{-EEF}$  direction with various strengths at different temperatures (T in K), negative direction of  $Z_{\text{B}}\text{-EEF}$  (-0.514 V/nm); positive direction of  $Z_{\text{B}}\text{-EEF}$  (0.514 V/nm); no field (0.0 V/nm).

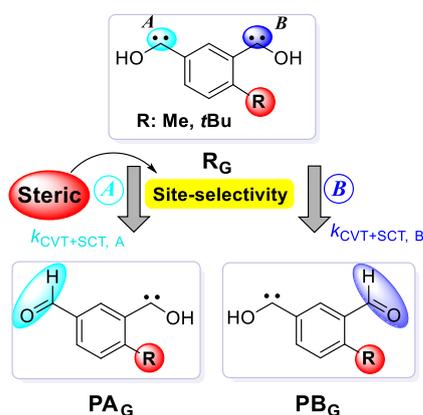
T(K)	$Z_{\text{B}}\text{-EEF}$					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	1.42E-191	1.71E-192	3.98E-193	4.73E-195	2.26E-191	9.25E-188
35	1.45E-162	2.33E-163	6.84E-164	1.62E-165	2.20E-162	2.73E-159
40	8.41E-141	1.67E-141	5.87E-142	2.33E-143	1.24E-140	6.25E-138
50	2.55E-110	6.80E-111	3.09E-111	2.57E-112	3.61E-110	5.20E-108
60	5.49E-90	1.79E-90	9.67E-91	1.32E-91	7.64E-90	4.76E-88
70	1.87E-75	7.03E-76	4.30E-76	8.47E-77	2.58E-75	8.84E-74
80	1.51E-64	6.31E-65	4.24E-65	1.10E-65	2.08E-64	4.54E-63
90	4.70E-56	2.11E-56	1.53E-56	4.92E-57	6.39E-56	9.85E-55
100	2.93E-49	1.41E-49	1.08E-49	4.15E-50	4.00E-49	4.65E-48
120	4.69E-39	2.49E-39	2.09E-39	1.05E-39	6.42E-39	4.91E-38
140	9.32E-32	5.32E-32	4.75E-32	2.90E-32	1.29E-31	7.29E-31
160	2.82E-26	1.70E-26	1.59E-26	1.13E-26	3.94E-26	1.78E-25
180	5.26E-22	3.30E-22	3.21E-22	2.56E-22	7.39E-22	2.80E-21
200	1.38E-18	8.99E-19	9.02E-19	7.93E-19	1.97E-18	6.47E-18
220	8.80E-16	5.87E-16	6.04E-16	5.76E-16	1.26E-15	3.69E-15
240	1.92E-13	1.31E-13	1.38E-13	1.41E-13	2.78E-13	7.38E-13
260	1.84E-11	1.29E-11	1.37E-11	1.49E-11	2.69E-11	6.58E-11
273.15	2.59E-10	1.82E-10	1.96E-10	2.20E-10	3.79E-10	8.84E-10
280	9.28E-10	6.57E-10	7.12E-10	8.13E-10	1.36E-09	3.11E-09
290	5.38E-09	3.84E-09	4.18E-09	4.90E-09	7.93E-09	1.75E-08
298.15	2.07E-08	1.49E-08	1.63E-08	1.94E-08	3.06E-08	6.60E-08
300	2.78E-08	2.00E-08	2.19E-08	2.62E-08	4.11E-08	8.83E-08
310	1.29E-07	9.37E-08	1.03E-07	1.26E-07	1.92E-07	4.01E-07
320	5.47E-07	3.99E-07	4.41E-07	5.50E-07	8.15E-07	1.66E-06
340	7.60E-06	5.61E-06	6.27E-06	8.11E-06	1.14E-05	2.21E-05
360	7.91E-05	5.90E-05	6.65E-05	8.89E-05	1.20E-04	2.22E-04
373.15	3.22E-04	2.42E-04	2.74E-04	3.74E-04	4.90E-04	8.87E-04
380	6.45E-04	4.85E-04	5.51E-04	7.59E-04	9.82E-04	1.76E-03
400	4.28E-03	3.24E-03	3.71E-03	5.25E-03	6.55E-03	1.13E-02

**Table S163.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of arene molecule bearing two hydroxycarbene groups ( $\mathbf{R}_F$ ) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method along  $Z_{\text{B-EEF}}$  direction with various strengths at different temperatures (T in K), negative direction of  $Z_{\text{B-EEF}}$  (-0.514 V/nm); positive direction of  $Z_{\text{B-EEF}}$  (0.514 V/nm); no field (0.0 V/nm))

T(K)	$Z_{\text{B-EEF}}$					
	Site A			Site B		
	-0.514	0.0	0.514	-0.514	0.0	0.514
30	2.49E-05	1.35E-05	1.11E-05	3.12E-05	4.25E-05	7.87E-05
35	2.58E-05	1.42E-05	1.19E-05	3.36E-05	4.58E-05	8.45E-05
40	2.68E-05	1.50E-05	1.28E-05	3.64E-05	4.94E-05	9.08E-05
50	2.94E-05	1.68E-05	1.47E-05	4.25E-05	5.76E-05	1.05E-04
60	3.25E-05	1.91E-05	1.71E-05	4.94E-05	6.69E-05	1.21E-04
70	3.62E-05	2.16E-05	1.97E-05	5.73E-05	7.73E-05	1.40E-04
80	4.05E-05	2.46E-05	2.28E-05	6.60E-05	8.91E-05	1.61E-04
90	4.56E-05	2.80E-05	2.63E-05	7.59E-05	1.02E-04	1.84E-04
100	5.12E-05	3.18E-05	3.03E-05	8.70E-05	1.17E-04	2.10E-04
120	6.47E-05	4.13E-05	4.04E-05	1.14E-04	1.53E-04	2.73E-04
140	8.27E-05	5.40E-05	5.40E-05	1.49E-04	1.99E-04	3.54E-04
160	1.07E-04	7.13E-05	7.28E-05	1.95E-04	2.60E-04	4.61E-04
180	1.41E-04	9.57E-05	9.97E-05	2.57E-04	3.43E-04	6.07E-04
200	1.92E-04	1.32E-04	1.39E-04	3.47E-04	4.61E-04	8.14E-04
220	2.69E-04	1.88E-04	2.01E-04	4.80E-04	6.36E-04	1.12E-03
240	3.95E-04	2.80E-04	3.02E-04	6.92E-04	9.14E-04	1.61E-03
260	6.19E-04	4.45E-04	4.82E-04	1.06E-03	1.39E-03	2.43E-03
273.15	8.68E-04	6.30E-04	6.83E-04	1.46E-03	1.91E-03	3.33E-03
280	1.05E-03	7.67E-04	8.32E-04	1.75E-03	2.28E-03	3.98E-03
290	1.42E-03	1.04E-03	1.13E-03	2.33E-03	3.02E-03	5.26E-03
298.15	1.85E-03	1.37E-03	1.48E-03	3.00E-03	3.88E-03	6.73E-03
300	1.97E-03	1.46E-03	1.58E-03	3.19E-03	4.12E-03	7.14E-03
310	2.81E-03	2.09E-03	2.27E-03	4.48E-03	5.75E-03	9.94E-03
320	4.13E-03	3.09E-03	3.35E-03	6.49E-03	8.27E-03	1.42E-02
340	9.68E-03	7.24E-03	7.90E-03	1.48E-02	1.85E-02	3.15E-02
360	2.51E-02	1.84E-02	2.02E-02	3.75E-02	4.50E-02	7.61E-02
373.15	4.89E-02	3.51E-02	3.85E-02	7.22E-02	8.37E-02	1.41E-01
380	6.99E-02	4.93E-02	5.42E-02	1.03E-01	1.16E-01	1.95E-01
400	2.04E-01	1.34E-01	1.48E-01	2.98E-01	3.10E-01	5.14E-01

## Steric Effect

### Arene molecule $R_G$



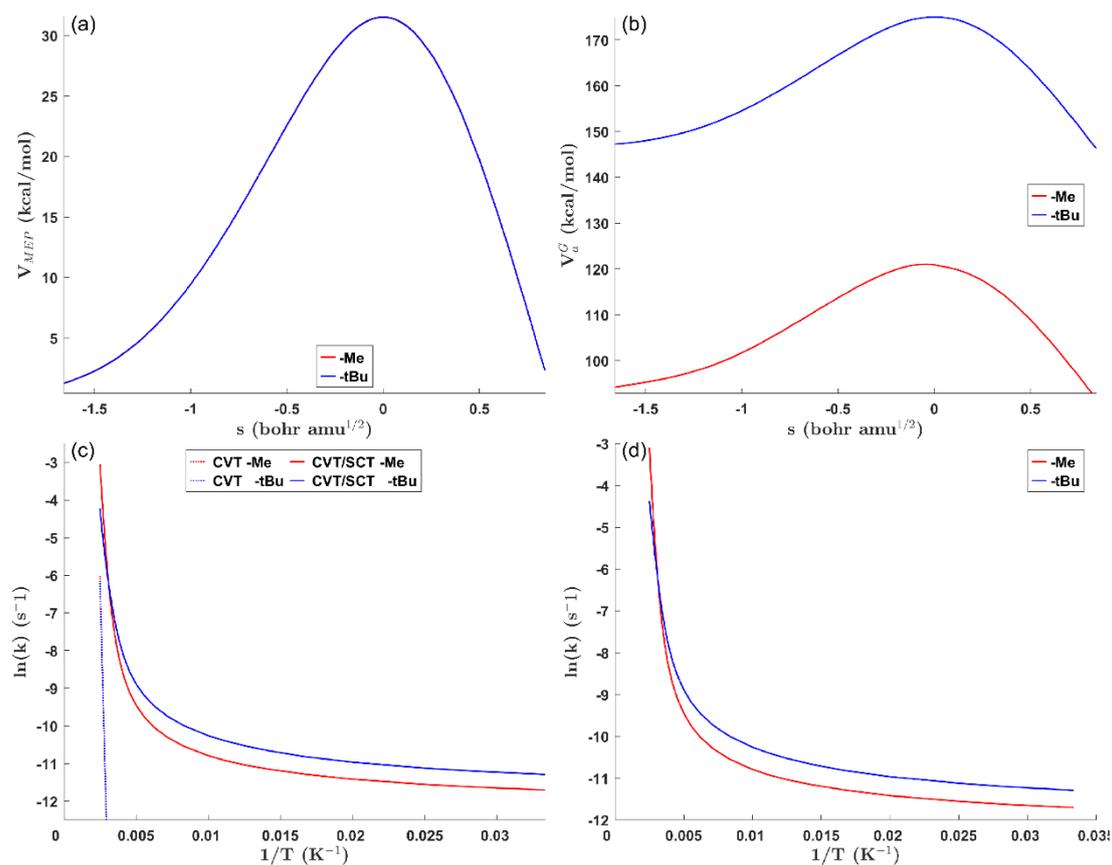
**Figure S110** Schematic site-selectivity of the H-migration of arene derivatives bearing two hydroxycarbene groups ( $R_G$ ) under steric effect.

**Table S164** Computed barrier in terms of electronic energies ( $\Delta E$  in kcal/mol) and electronic energies plus zero-point correction energy ( $\Delta V_a^G(\max)$  in kcal/mol) and their difference  $\Delta\Delta E$  and  $\Delta\Delta V_a^G(\max)$  between site-selectivity for arene derivatives bearing two hydroxycarbene groups ( $R_G$ ) at site A and site B with different groups (R=Me and R=*t*Bu)

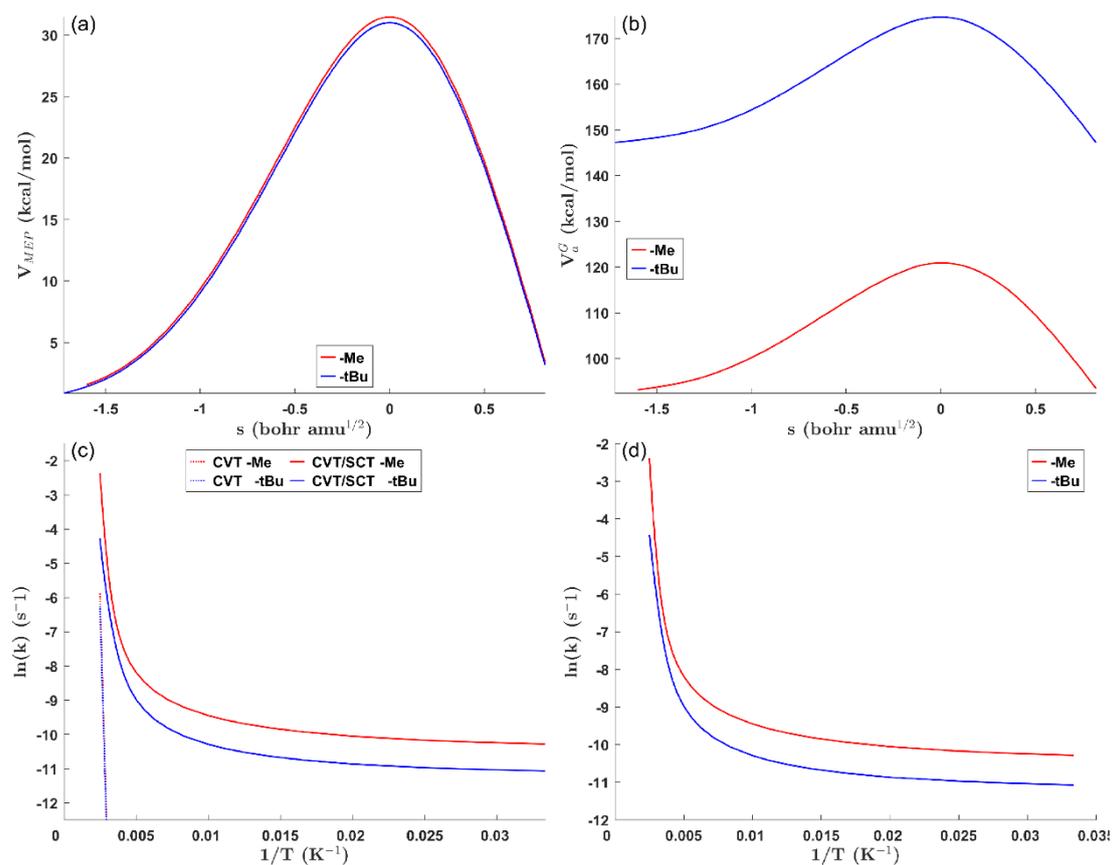
Groups	R=Me	R= <i>t</i> Bu
<b>No-EEF</b>		
$\Delta E_A$	31.51	31.54
$\Delta E_B$	31.48	31.01
$\Delta\Delta E$	-0.04	-0.53
$\Delta V_a^G(\max)_A$	27.92	28.01
$\Delta V_a^G(\max)_B$	27.92	27.67
$\Delta\Delta V_a^G(\max)$	0.01	-0.34

**Table S165** Half-life ( $\tau$  in hr) at 30K, width of PES ( $w$  in bohr) and their difference  $\Delta\Delta\tau$  and  $\Delta\Delta w$  between site-selectivity for arene derivatives bearing two hydroxycarbene groups ( $R_G$ ) at site A and site B with different substituent groups (R=Me and *t*Bu)

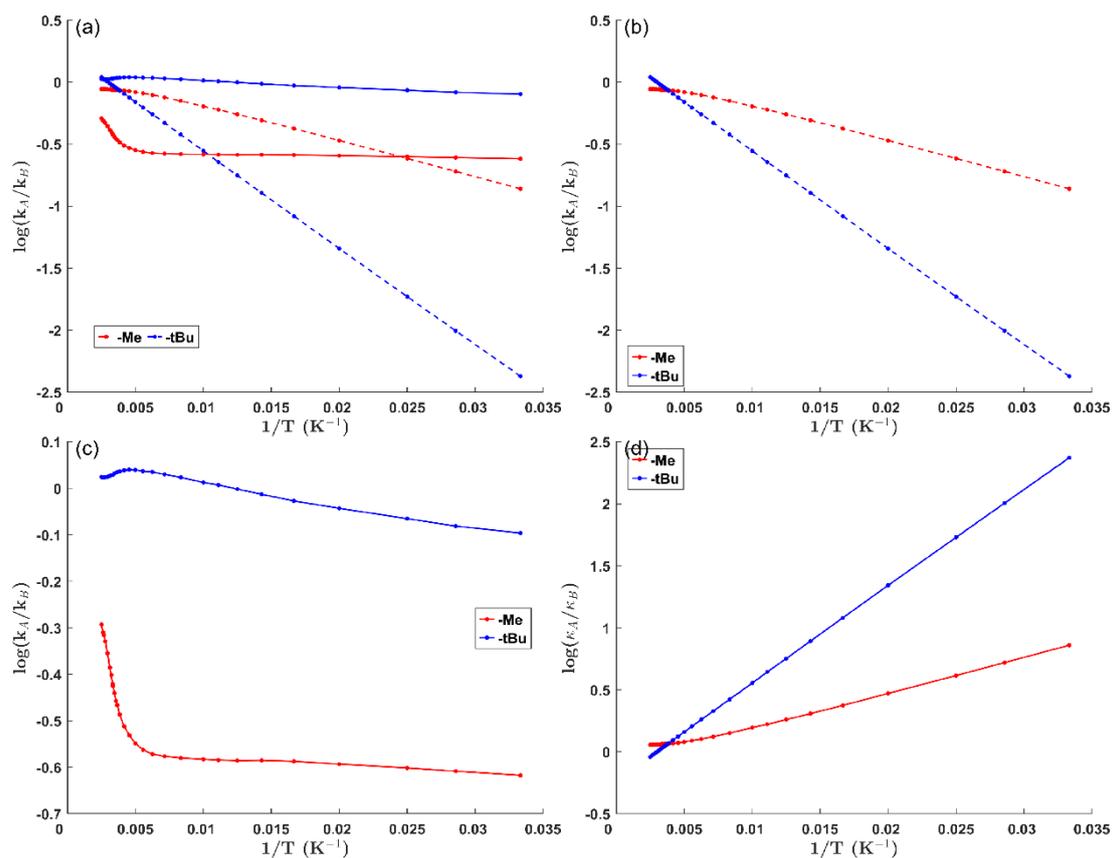
Groups	R=Me	R= <i>t</i> -Bu
<b>No-EEF</b>		
$\Delta\tau_A$	23.25	15.40
$\Delta\tau_B$	5.61	12.34
$\Delta\Delta\tau$	-17.64	-3.06
$\Delta w_A$	2.66	2.49
$\Delta w_B$	2.43	2.54
$\Delta\Delta w$	-0.23	0.05



**Figure S111.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constant ( $k$ , in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene derivatives bearing two hydroxycarbene groups (**R<sub>G</sub>**) at **site A** using  $\omega$ B97X-D/6-31G(d,p) method with different substituent groups (R=Me and  $tBu$ ).



**Figure S112.** (a) Potential energy surface along the minimum energy path ( $V_{MEP}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^G$ ), (c) Arrhenius plots of the non-tunneling ( $k_{CVT}$ ) and overall ( $k_{CVT+SCT}$ ) rate constants (in s<sup>-1</sup>), (d) the tunneling-involving rate constant ( $k_{CVT+SCT} - k_{CVT}$ ) of arene derivatives bearing two hydroxycarbene groups (**R<sub>G</sub>**) at **site B** using  $\omega$ B97X-D/6-31G(d,p) method with different substituent groups (R=Me and *t*Bu).



**Figure S113.** Arrhenius plots of the ratio of (a) the non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ , dash lines) and overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ , solid lines) rate constants (b) non-tunneling ( $\ln k_{CVT,A}/k_{CVT,B}$ ), (c) overall ( $\ln k_{CVT+SCT,A}/k_{CVT+SCT,B}$ ) rate constants and (d)  $\ln(\kappa_A/\kappa_B)$  versus  $1/T$  between arene derivatives bearing two hydroxycarbene groups ( $\mathbf{R}_G$ ) at **site A** and **site B** using  $\omega\text{B97X-D/6-31G(d,p)}$  method with different substituent groups ( $\text{R}=\text{Me}$  and *t*Bu).

**Table S166.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of arene derivatives bearing two hydroxycarbene groups ( $\mathbf{R_G}$ ) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method with different substituent groups ( $\text{R}=\text{Me}$  and  $t\text{Bu}$ ).

No-EEF				
T(K)	Site A		Site B	
	R = Me	R = <i>t</i> Bu	R = Me	R = <i>t</i> Bu
30	2.79E-193	4.00E-193	2.02E-192	9.40E-191
35	4.94E-164	6.31E-164	2.59E-163	6.39E-162
40	4.32E-142	5.07E-142	1.78E-141	2.72E-140
50	2.31E-111	2.42E-111	6.83E-111	5.32E-110
60	7.27E-91	7.09E-91	1.72E-90	8.53E-90
70	3.24E-76	3.01E-76	6.58E-76	2.35E-75
80	3.18E-65	2.87E-65	5.78E-65	1.62E-64
90	1.14E-56	1.00E-56	1.90E-56	4.41E-56
100	8.05E-50	6.96E-50	1.26E-49	2.49E-49
120	1.54E-39	1.30E-39	2.18E-39	3.44E-39
140	3.47E-32	2.89E-32	4.60E-32	6.16E-32
160	1.15E-26	9.52E-27	1.46E-26	1.73E-26
180	2.30E-22	1.89E-22	2.83E-22	3.03E-22
200	6.40E-19	5.27E-19	7.69E-19	7.61E-19
220	4.25E-16	3.50E-16	5.02E-16	4.65E-16
240	9.58E-14	7.93E-14	1.12E-13	9.85E-14
260	9.47E-12	7.87E-12	1.10E-11	9.21E-12
273.15	1.35E-10	1.12E-10	1.56E-10	1.27E-10
280	4.88E-10	4.07E-10	5.63E-10	4.53E-10
290	2.86E-09	2.39E-09	3.29E-09	2.60E-09
298.15	1.11E-08	9.28E-09	1.27E-08	9.93E-09
300	1.49E-08	1.25E-08	1.72E-08	1.33E-08
310	7.01E-08	5.88E-08	8.04E-08	6.14E-08
320	2.99E-07	2.52E-07	3.42E-07	2.58E-07
340	4.22E-06	3.57E-06	4.82E-06	3.53E-06
360	4.46E-05	3.78E-05	5.08E-05	3.63E-05
373.15	1.83E-04	1.56E-04	2.08E-04	1.47E-04
380	3.68E-04	3.13E-04	4.19E-04	2.93E-04
400	2.46E-03	2.11E-03	2.80E-03	1.92E-03

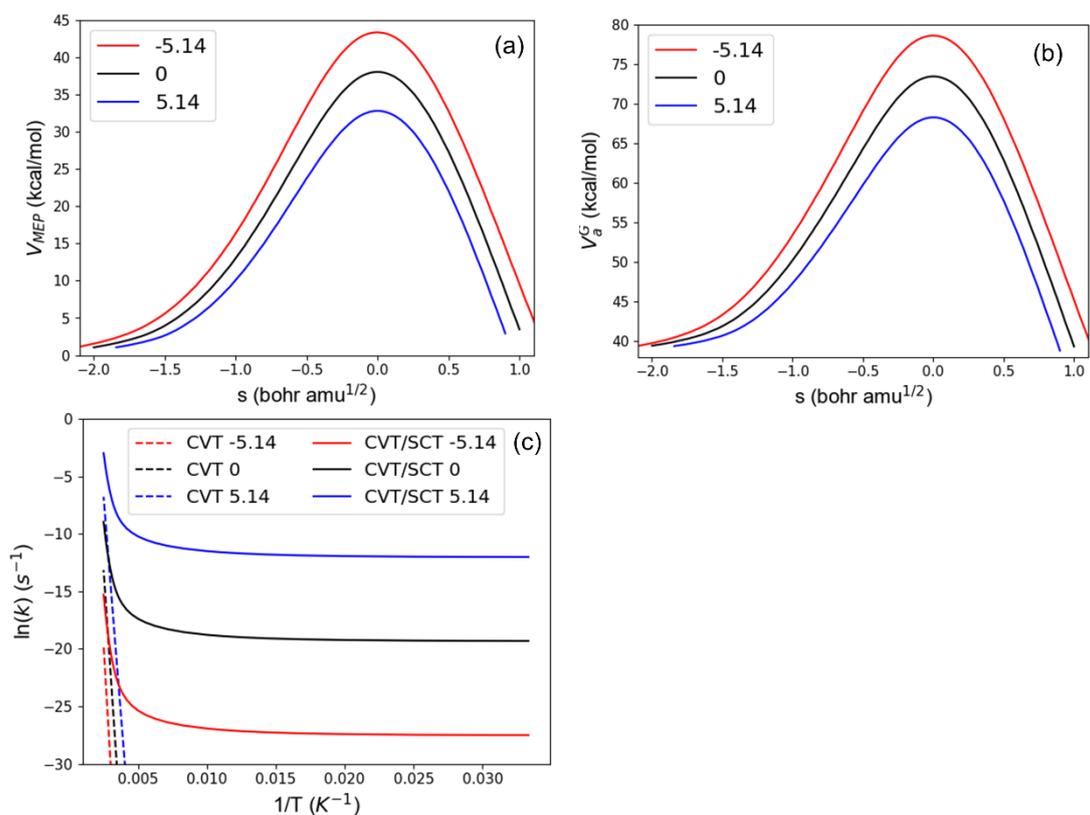
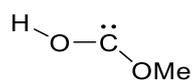
**Table S167.** The overall rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of arene derivatives bearing two hydroxycarbene groups ( $\mathbf{R_G}$ ) at sites A and B using  $\omega\text{B97X-D/6-31G(d,p)}$  method with different substituent group ( $\text{R}=\text{Me}$  and  $t\text{Bu}$ ).

No-EEF				
T(K)	Site A		Site B	
	R = Me	R = <i>t</i> Bu	R = Me	R = <i>t</i> Bu
30	8.28E-06	1.25E-05	3.43E-05	1.56E-05
35	8.92E-06	1.36E-05	3.62E-05	1.64E-05
40	9.59E-06	1.48E-05	3.83E-05	1.72E-05
50	1.10E-05	1.73E-05	4.31E-05	1.91E-05
60	1.26E-05	2.01E-05	4.87E-05	2.14E-05
70	1.43E-05	2.33E-05	5.50E-05	2.40E-05
80	1.61E-05	2.68E-05	6.20E-05	2.69E-05
90	1.82E-05	3.07E-05	6.99E-05	3.02E-05
100	2.06E-05	3.50E-05	7.88E-05	3.40E-05
120	2.63E-05	4.55E-05	1.00E-04	4.31E-05
140	3.37E-05	5.90E-05	1.27E-04	5.51E-05
160	4.37E-05	7.72E-05	1.63E-04	7.12E-05
180	5.78E-05	1.02E-04	2.11E-04	9.37E-05
200	7.86E-05	1.38E-04	2.78E-04	1.26E-04
220	1.11E-04	1.93E-04	3.77E-04	1.76E-04
240	1.64E-04	2.80E-04	5.33E-04	2.56E-04
260	2.60E-04	4.24E-04	7.97E-04	3.90E-04
273.15	3.69E-04	5.72E-04	1.08E-03	5.28E-04
280	4.50E-04	6.73E-04	1.29E-03	6.23E-04
290	6.13E-04	8.59E-04	1.69E-03	7.98E-04
298.15	8.04E-04	1.05E-03	2.14E-03	9.82E-04
300	8.57E-04	1.10E-03	2.26E-03	1.03E-03
310	1.23E-03	1.43E-03	3.10E-03	1.34E-03
320	1.79E-03	1.85E-03	4.35E-03	1.74E-03
340	3.98E-03	3.10E-03	9.01E-03	2.93E-03
360	9.14E-03	5.17E-03	1.95E-02	4.89E-03
373.15	1.58E-02	7.20E-03	3.27E-02	6.82E-03
380	2.10E-02	8.57E-03	4.29E-02	8.12E-03
400	4.78E-02	1.47E-02	9.38E-02	1.39E-02

**Table S168.** Rate constant data, and half-life ( $\tau$ , h) at 30 K for the chemo- or site-selectivities of  $\mathbf{R}_D$  and  $\mathbf{R}_E$  in the  $Z_A$ -,  $Z_B$ -,  $Z_C$ - and  $Z_D$ -EEFs calculated using the  $\omega$ B97X-D method

<b><math>\mathbf{R}_D</math> (Chemoselectivity): <math>Z_A</math>-EEF Direction</b>						
	$k_{(CVT)A}$	$k_{(CVT+SCT)A}$	$k_{(CVT)B}$	$k_{(CVT+SCT)B}$	$\tau_A$	$\tau_B$
<b>-0.514</b>	8.33E-194	1.53E-05	7.07E-192	3.01E-05	12.6	6.4
<b>0</b>	1.14E-189	3.72E-05	5.13E-196	1.30E-05	5.2	14.8
<b>0.514</b>	1.64E-185	7.22E-05	1.35E-200	6.19E-07	2.7	311.0
<b><math>\mathbf{R}_D</math> (Chemoselectivity): <math>Z_B</math>-EEF Direction</b>						
<b>-0.514</b>	1.08E-185	3.69E-05	1.10E-200	4.96E-06	5.2	38.8
<b>0</b>	1.37E-189	1.77E-05	1.87E-196	1.18E-05	10.9	16.3
<b>0.514</b>	1.24E-193	1.28E-05	6.96E-192	3.25E-05	15.0	5.9
<b><math>\mathbf{R}_E</math> (Site-selectivity): <math>Z_C</math>-EEF Direction</b>						
	$k_{(CVT)C}$	$k_{(CVT+SCT)C}$	$k_{(CVT)D}$	$k_{(CVT+SCT)D}$	$\tau_C$	$\tau_D$
<b>-0.514</b>	8.08E-196	7.40E-06	1.23E-189	5.84E-05	26.0	3.3
<b>0</b>	4.57E-192	2.04E-05	8.44E-192	3.54E-05	9.4	5.4
<b>0.514</b>	2.50E-187	4.08E-05	1.60E-194	1.49E-05	4.7	12.9
<b><math>\mathbf{R}_E</math> (Site-selectivity): <math>Z_D</math>-EEF Direction</b>						
<b>-0.514</b>	1.81E-187	3.51E-05	4.41E-196	1.34E-05	5.5	14.4
<b>0</b>	8.42E-192	1.85E-05	1.02E-191	2.93E-05	10.4	6.6
<b>0.514</b>	5.32E-196	9.52E-06	1.15E-187	4.36E-05	20.2	4.4

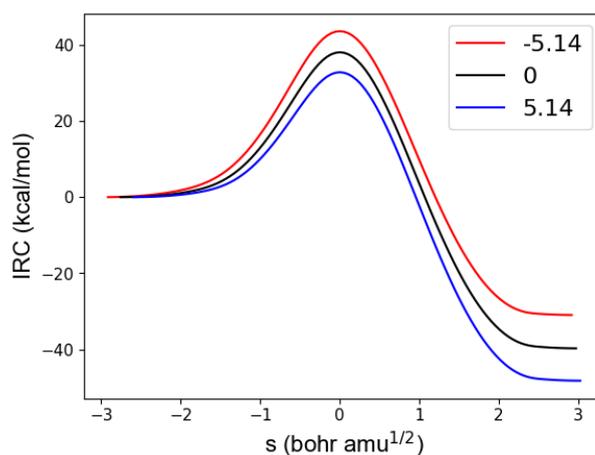
## H<sub>3</sub>CO-C-OH



**Figure S114.** (a) Potential energy surface along the minimum energy path ( $V_{\text{MEP}}$ ), (b) vibrationally adiabatic ground-state potential energy ( $V_a^{\text{G}}$ ), (c) Arrhenius plots of the non-tunneling ( $k_{\text{CVT}}$ ) and overall ( $k_{\text{CVT+SCT}}$ ) rate constant ( $k$ , in  $\text{s}^{-1}$ ).

**Table S169.** Computed rate constants ( $k_{\text{CVT}}$  and  $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ), transmission coefficients ( $\kappa_{\text{SCT}}$ ), and half-life ( $\tau$ ) for the 1,2-H migration in  $\text{H}_3\text{CO-C-OH}$  using the  $\omega\text{B97X-D}$  method in the absence or presence of a Z-EEF (V/nm) at 30, 100, and 200 K.

Z-EEF	$k_{\text{CVT}}$	$k_{\text{CVT+SCT}}$	$\kappa_{\text{SCT}}$	$\tau$
<b>30K</b>				
-5.14	2.33E-277	1.13E-12	4.84E+264	19450.9 (y)
0	4.02E-239	4.06E-09	1.01E+230	1976.0 (d)
5.14	1.10E-201	6.00E-06	5.46E+195	32.1 (h)
<b>100K</b>				
-5.14	6.38E-75	2.00E-12	3.13E+62	10989.8 (y)
0	1.88E-63	6.89E-09	3.67E+54	1164.4 (d)
5.14	3.12E-52	9.99E-06	3.20E+46	19.3 (h)
<b>200K</b>				
-5.14	2.68E-31	9.57E-12	3.58E+19	2296.7(y)
0	1.42E-25	2.79E-08	1.97E+17	287.5 (d)
5.14	5.55E-20	3.60E-05	6.48E+14	5.3 (h)



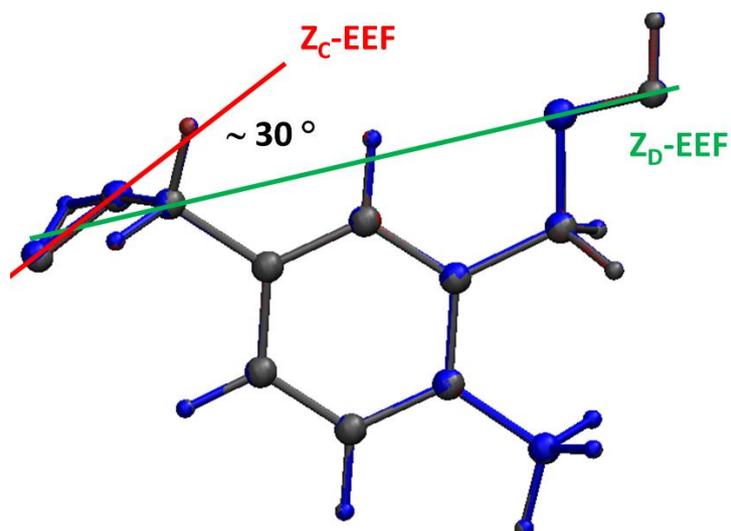
**Figure S115.** Intrinsic Reaction Coordinate (IRC) for  $\text{H}_3\text{CO-CO-H}$  system under various Z-EEFs (-5.14 and 5.14 V/nm) using Gaussian16 program.

**Table S170.** The non-tunneling rate constants ( $k_{\text{CVT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{CO-C-OH}$  using  $\omega\text{B97X-D/6-31G(d,p)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

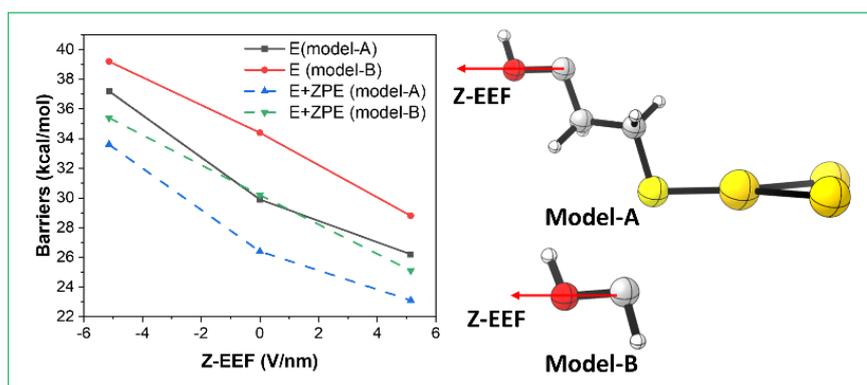
T(K)	Z-EEF		
	-5.14	0.0	5.14
30	2.33E-277	4.02E-239	1.10E-201
35	4.30E-236	2.56E-203	3.14E-171
40	3.90E-205	1.86E-176	2.22E-148
50	8.95E-162	7.85E-139	2.26E-116
60	7.53E-133	9.90E-114	5.12E-95
70	3.55E-112	8.66E-96	9.46E-80
80	1.16E-96	2.53E-82	2.72E-68
90	1.38E-84	7.65E-72	2.26E-59
100	6.38E-75	1.88E-63	3.12E-52
120	2.08E-60	7.46E-51	1.65E-41
140	4.98E-50	7.67E-42	7.78E-34
160	3.11E-42	4.51E-35	4.52E-28
180	3.66E-36	8.46E-30	1.40E-23
200	2.68E-31	1.42E-25	5.55E-20
220	2.59E-27	4.11E-22	4.94E-17
240	5.48E-24	3.19E-19	1.43E-14
260	3.60E-21	8.95E-17	1.75E-12
273.15	1.54E-19	2.33E-15	2.81E-11
280	9.45E-19	1.13E-14	1.08E-10
290	1.15E-17	9.92E-14	6.88E-10
298.15	7.79E-17	5.24E-13	2.84E-09
300	1.19E-16	7.54E-13	3.87E-09
310	1.05E-15	5.04E-12	1.96E-08
320	8.18E-15	2.99E-11	8.93E-08
340	3.44E-13	7.72E-10	1.43E-06
360	9.61E-12	1.39E-08	1.68E-05
373.15	7.07E-11	7.90E-08	7.39E-05
380	1.89E-10	1.86E-07	1.53E-04
400	2.78E-09	1.92E-06	1.12E-03

**Table S171.** The non-tunneling rate constants ( $k_{\text{CVT+SCT}}$  in  $\text{s}^{-1}$ ) of  $\text{H}_3\text{CO-C-OH}$  using  $\omega\text{B97X-D/6-31G(d,p)}$  method along the Z-EEF direction with various strengths at different temperatures (T in K), negative direction of Z-EEF (-5.14 V/nm); positive direction of Z-EEF (5.14 V/nm); no field (0.0 V/nm)).

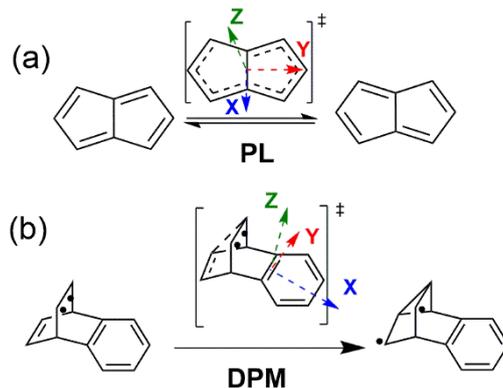
T(K)	Z-EEF		
	-5.14	0.0	5.14
30	1.13E-12	4.06E-09	6.00E-06
35	1.14E-12	4.11E-09	6.07E-06
40	1.16E-12	4.18E-09	6.17E-06
50	1.23E-12	4.40E-09	6.48E-06
60	1.32E-12	4.71E-09	6.91E-06
70	1.44E-12	5.10E-09	7.48E-06
80	1.59E-12	5.59E-09	8.18E-06
90	1.77E-12	6.19E-09	9.01E-06
100	2.00E-12	6.89E-09	9.99E-06
120	2.58E-12	8.71E-09	1.25E-05
140	3.42E-12	1.13E-08	1.58E-05
160	4.66E-12	1.49E-08	2.04E-05
180	6.55E-12	2.01E-08	2.68E-05
200	9.57E-12	2.79E-08	3.60E-05
220	1.48E-11	4.04E-08	4.99E-05
240	2.45E-11	6.20E-08	7.24E-05
260	4.52E-11	1.03E-07	1.12E-04
273.15	7.28E-11	1.52E-07	1.57E-04
280	9.58E-11	1.90E-07	1.91E-04
290	1.48E-10	2.72E-07	2.59E-04
298.15	2.19E-10	3.75E-07	3.40E-04
300	2.41E-10	4.04E-07	3.63E-04
310	4.08E-10	6.23E-07	5.24E-04
320	7.22E-10	9.98E-07	7.84E-04
340	2.55E-09	2.85E-06	1.93E-03
360	1.03E-08	9.27E-06	5.30E-03
373.15	2.76E-08	2.13E-05	1.08E-02
380	4.66E-08	3.32E-05	1.59E-02
400	2.26E-07	1.27E-04	5.01E-02



**Figure S116.** Direction of  $Z_C$ -EEF and  $Z_D$ -EEF for  $R_E$  bearing two different hydroxycarbene moieties. The angle between these two EEF directions is about 30 degrees.



**Figure S117.** Plots of the 1,2-H migration reaction barriers (relative electronic energy ( $\Delta E$ ), and  $\Delta E$  with zero-point correction energy ( $\Delta E+ZPE$ )) as well as model-A and model-B under Z-EEFs (-5.14 and 5.14 V/nm) and no field (0 V/nm).



**Figure S118.** Pentalene (**PL**)  $\pi$  bond-shifting (*Chem. Sci.* **2021**, *12*, 3179-3187) and excited-state Zimmerman di- $\pi$ -methane (**DPM**) rearrangement at 100 K under the EEF of  $\pm 5.14$  V/nm and no field (0 V/nm). The direction of EEF is indicated by the colored arrows.

**Table S172.** Comparison of reaction rates ( $k_{\text{CVT+SCT}}$ ) for pentalene (**PL**)  $\pi$  bond-shifting and excited-state Zimmerman di- $\pi$ -methane (**DPM**) rearrangement at 100 K under the EEF of  $\pm 5.14$  V/nm and no field (0 V/nm).

EEF (V/nm)	<b>PL</b>		EEF (V/nm)	<b>DPM</b>	
	Barriers (kcal/mol)	$k_{\text{CVT+SCT}}$ ( $\text{s}^{-1}$ )		Barriers (kcal/mol)	$k_{\text{CVT+SCT}}$ ( $\text{s}^{-1}$ )
No-field	9.9	$1.76 \times 10^8$	No-field	4.5	$3.34 \times 10^7$
X=5.14	9.4	$1.88 \times 10^8$	X=-5.14	5.3	$1.86 \times 10^6$
Y=5.14	8.1	$2.51 \times 10^8$	Y=-5.14	3.8	$2.10 \times 10^8$
Z=5.14	9.3	$1.30 \times 10^6$	Z=-5.14	3.1	$3.53 \times 10^9$

**Table S173.** Absolute energies of hydroxycarbene connected with  $-(\text{CH}_2)_2\text{-S-Au}_3$  moiety (model-A) computed by  $\omega\text{B97X-D/def2-SVP}$  method under the EEF of  $\pm 5.14$  V/nm and no field (0 V/nm).

	<b>E</b>	<b>E+ZPE</b>	<b>G</b>
<b>0 V/nm</b>			
<b>RC</b>	-997.738827	-997.660856	-997.709010
<b>TS</b>	-997.691243	-997.618753	-997.666811
<b>PC</b>	-997.822124	-997.743999	-997.792554
<b>Z=5.14 V/nm</b>			
<b>RC</b>	-997.765369	-997.688072	-997.736870
<b>TS</b>	-997.723550	-997.651302	-997.699184
<b>PC</b>	-997.864035	-997.786535	-997.835132
<b>Z=-5.14 V/nm</b>			
<b>RC</b>	-997.772857	-997.694690	-997.743131
<b>TS</b>	-997.713628	-997.641102	-997.688099
<b>PC</b>	-997.864035	-997.786535	-997.835132

**Table S174.** Absolute energies of hydroxycarbene (model-B) computed by  $\omega$ B97X-D/def2-SVP method under the EEF of  $\pm 5.14$  V/nm and no field (0 V/nm).

	<b>E</b>	<b>E+ZPE</b>	<b>G</b>
<b>0 V/nm</b>			
<b>RC</b>	-114.290857	-114.263599	-114.285297
<b>TS</b>	-114.236618	-114.215442	-114.237169
<b>PC</b>	-114.375871	-114.348970	-114.370628
<b>Z=5.14 V/nm</b>			
<b>RC</b>	-114.371977	-114.344987	-114.366717
<b>TS</b>	-114.326156	-114.305007	-114.326746
<b>PC</b>	-114.472973	-114.445834	-114.467495
<b>Z=-5.14 V/nm</b>			
<b>RC</b>	-114.384454	-114.357356	-114.379057
<b>TS</b>	-114.321927	-114.300959	-114.322690
<b>PC</b>	-114.454955	-114.428155	-114.449809

## 4. Examples of Polyrate input files

For reproducibility purpose, due to the many Polyrate options, some examples of input files are included (e.g., \*.dat, \*.70 files)

### HO-C-OH

#### *HOCO.H.dat*

```
*General
TITLE
HOCO.H-Z100
END

ATOMS
1 C
2 O
3 H
4 O
5 H
END

NOSUPERMOL
# use AU now
INPUNIT AU

WRITEFU31

MDMOVIE ON

*OPTIMIZATION

OPTMIN OHOOK
OPTTS OHOOK

*SECOND

HESSCAL HHOOK

*REACT1
SPECIES NONLINRP
STATUS 2

*REACT1
# Geometry in a.u.
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.476969
3 1.725052 0.000000 3.068367
4 -2.447965 -0.000002 -0.623219
5 -2.487009 -0.000006 -2.438598
END

# spin multiplicity
ELEC
1 0.00
END

# end of react section

*PROD1
SPECIES NONLINRP
STATUS 2

*PROD1
# Geometry in a.u.
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.239763

3 1.742545 0.000000 -1.162702
4 -2.141100 0.000000 -1.409517
5 -1.679011 0.000006 -3.170007
END

# spin multiplicity
ELEC
1 0.00
END

# end of prod section

*START
SPECIES NONLINTS
STATUS 2

# transform Ang to AU by gview
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.384682
3 1.997874 0.000000 1.129975
4 -2.264751 -0.000000 -1.128991
5 -1.968933 -0.000004 -2.924685
END

# spin multiplicity
ELEC
1 0.00
END

# end of start section

*PATH
SCALEMASS 1.00
RODS ON
INTMU 3
SSTEP 0.002
INH 10 # Hessian
NSTEPS 99999
RPM pagem
SIGN Reactant # reactant

SRANGE
SLP 4.0
SLM -4.0
END

#prsaverp

EXFIRST
END
EXSECOND
END

COORD Curv3

INTDEF
2-1 3-1 4-1 5-4
3-1-2 4-1-2 5-4-1
4-1-2-3 5-4-1-2
END
```

```

PRPATH
COORD 3 1
INTERVAL 1
XMOL
END

PRSAVERP

SPECSTOP
PERCENTDOWN 99.
END

*TUNNEL

QUAD
NQE 40
NQTH 40
END

ZCT
SCT
SCTOPT
LAGRANGE 8
END

QRST
MODE 9
SRW -3.52
END

*RATE
GTLOG
FORWARDK
SIGMAF 1
HOCOH.70

*GRGENERAL
GRRESTART

*GRCOMMON
GRENER
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d,p) int=ultrafine UNITS=AU nosymm
field=Z-100
END

GRFIRST
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d,p) int=ultrafine UNITS=AU Force
nosymm field=Z-100
END

GRSEC
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d,p) UNITS=AU int=ultrafine
Freq=noraman nosymm field=Z-100
END

*GRREACT1
CHARGE 0
MULTIPLICITY 1

*GRSTART
CHARGE 0
MULTIPLICITY 1

*GRPROD1
CHARGE 0
MULTIPLICITY 1

TST
CVT

TEMP
30.
35.
40.
50.
60.
70.
80.
90.
100.
120.
140.
160.
180.
200.
220.
240.
260.
273.15
280.
290.
298.15
300.
310.
320.
340.
360.
373.15
380.
400.
END

field=Z-100
END

GRFIRST
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d,p) UNITS=AU int=ultrafine Force
nosymm field=Z-100
END

GRSEC
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d,p) UNITS=AU int=ultrafine
Freq=noraman nosymm field=Z-100
END

*GRREACT1
CHARGE 0
MULTIPLICITY 1

*GRSTART
CHARGE 0
MULTIPLICITY 1

*GRPROD1
CHARGE 0
MULTIPLICITY 1

```

## SN2 Reaction

### *S<sub>N</sub>2.dat*

```
*General
TITLE
SN2
END

ATOMS
1 C
2 Cl
3 H
4 H
5 H
6 C
7 N
END

RESTART
writeful
END

NOSUPERMOL
writefu31

INPUNIT au

*SECOND
HESSCAL HHOOK

*OPTIMIZATION
OPTTS OHOOK
OPTMIN OHOOK

*REACT1
status 2
GEOM
7 0.0000000 0.0000000 0.0000000
6 0.0000000 0.0000000 2.22260416
END
SPECIES LINRP

*REACT2
status 2
GEOM
1 0.0000000 0.0000000 0.0000000
2 0.0000000 0.0000000 3.39669903
3 1.95287966 0.0000000 -0.64178715
4 -0.97854026 1.69106367 -0.63913965
5 -0.97853837 -1.69106556 -0.63913776
END
SPECIES NONLINRP

*PROD1
status 2
GEOM
7 0.0000000 0.0000000 0.0000000
6 0.0000000 0.0000000 2.18555417
1 -0.02796985 0.0000000 4.94814023
3 -0.99870743 -1.68575165 5.63382762
4 1.90870540 0.00543296 5.65833927
5 -1.00813527 1.68031868 5.63374636
END
SPECIES NONLINRP

*PROD2
status 2
GEOM
2 0.0000000 0.0000000 0.0000000
END
SPECIES ATOMIC

*START
status 2
```

```
GEOM
1 0.0000000 0.0000000 0.0000000
2 0.0000000 0.0000000 4.11719141
3 2.03033390 0.0000000 -0.12136771
4 -1.01305612 1.75649924 -0.17790267
5 -1.01305612 -1.75649924 -0.17790456
6 0.23202067 0.00000378 -4.21929525
7 0.66682792 0.00001512 -6.39008876
END

SPECIES NONLINTS

*PATH
SCALEMASS 1.000000
INTMU 3
SSTEP 0.005
INH 9
NSTEPS 99999
CURV dgrad
RPM pagem

sign reactant

SRANGE
slp 2.
slm -4.
END

SFIRST
NFSTEP 10
FSIZE 0.02
END

COORD curv3
INTDEF
2=1=6
2-1 3-1 4-1 5-1 6-1 7-6
3-1-2 4-1-3 5-1-3 6-1-3 7-6-5
4-1-3-2 5-1-3-4 6-1-3-4 7-6-5-1
END
prsaverp

*TUNNEL
ZCT
SCT

*RATE
forwardk
SIGMAF 1
TST
CVT

TEMP
100.
110.
120.
130.
140.
150.
160.
170.
180.
190.
200.
210.
220.
230.
240.
250.
260.
270.
273.15
```

280.  
290.  
300.  
310.  
320.  
340.

### ***S<sub>N</sub>2.70***

\*GRGENERAL

GRRESTART

\*GRCOMMON

GRENER

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water)  
scf=tight nosymm Field=Z-30  
END

GRFIRST

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water) Force  
scf=tight nosymm Field=Z-30  
END

GRSEC

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water)  
Freq=norman scf=tight nosymm Field=Z-30  
END

\*GRPATH

GRENER

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water)  
scf=tight nosymm Field=Z-30  
END

350.  
360.  
380.  
400.  
END

GRFIRST

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water)  
Force scf=tight nosymm Field=Z-30  
END

GRSEC

%mem=12000mb  
%nprocshared=12  
# m062x/6-31+g(d) Int=ultrafine  
units=au scrf(pcm,solvent=water)  
Freq=norman scf=tight nosymm Field=Z-30  
END

\*GRREACT1

CHARGE -1  
MULTIPLICITY 1

\*GRREACT2

CHARGE 0  
MULTIPLICITY 1

\*GRSTART

CHARGE -1  
MULTIPLICITY 1

\*GRPROD1

CHARGE 0  
MULTIPLICITY 1

\*GRPROD2

CHARGE -1  
MULTIPLICITY 1

## **Triplet DPM Rearrangement**

### ***Triplet DPM Rearrangement-TS1.dat***

\*General

TITLE

Triplet DPM-Field=Z-100  
END

ATOMS

1 C  
2 C  
3 C  
4 C  
5 C  
6 C  
7 C  
8 C  
9 C  
10 C  
11 H  
12 H  
13 H  
14 H

15 H  
16 H  
17 C  
18 C  
19 H  
20 H  
21 H  
22 H  
END

NOSUPERMOL  
# use AU now  
INPUNIT AU

WRITEFU31

MDMOVIE ON

\*OPTIMIZATION

OPTMIN OHOOK

OPTTS OHOOK  
 3 0.00  
 END  
 \*SECOND  
 # end of prod section  
 HESSCAL HHOOK  
 \*REACT1  
 SPECIES NONLINRP  
 STATUS 2  
 # Geometry in a.u.  
 GEOM  
 1 5.222523 -1.220919 0.002464  
 2 2.972478 -2.594223 -0.092958  
 3 0.683733 -1.314711 -0.183670  
 4 0.631817 1.335770 -0.140817  
 5 2.868010 2.695474 -0.035185  
 6 5.171474 1.408338 0.028945  
 7 -1.943762 -2.493735 -0.103549  
 8 -2.018516 2.424627 -0.088075  
 9 -3.385767 1.331581 2.207426  
 10 -2.942749 -1.441198 2.397098  
 11 7.016539 -2.210689 0.123307  
 12 3.006436 -4.647849 -0.039482  
 13 2.824592 4.746771 0.069020  
 14 6.925053 2.464748 0.172734  
 15 -1.877566 -4.556460 -0.151772  
 16 -2.047888 4.487255 -0.152482  
 17 -3.545734 1.199255 -2.209346  
 18 -3.516810 -1.329538 -2.201507  
 19 -4.616408 -2.497569 -3.481308  
 20 -4.707650 2.334298 -3.466736  
 21 -5.249484 2.104621 2.617107  
 22 -2.141469 -2.237047 4.116734  
 END

# spin multiplicity  
 ELEC  
 3 0.00  
 END

# end of react section

\*PROD1  
 SPECIES NONLINRP  
 STATUS 2

\*PROD1  
 # Geometry in a.u.  
 GEOM  
 1 5.334298 -1.164497 0.004263  
 2 3.091665 -2.550181 -0.030247  
 3 0.784890 -1.301542 -0.073837  
 4 0.698919 1.354267 -0.081084  
 5 2.941420 2.722919 -0.053313  
 6 5.256946 1.463850 -0.009534  
 7 -1.815956 -2.564732 -0.023769  
 8 -1.850687 2.523483 -0.035472  
 9 -3.926221 1.133039 1.448290  
 10 -3.196581 -1.435988 2.207817  
 11 7.137319 -2.139517 0.108999  
 12 3.140356 -4.603208 0.044688  
 13 2.884551 4.776217 0.003566  
 14 7.000359 2.542837 0.082515  
 15 -1.667984 -4.625441 -0.010598  
 16 -1.951192 4.574258 -0.013910  
 17 -3.996935 1.126948 -1.432182  
 18 -3.289081 -1.446248 -2.208097  
 19 -2.979347 -2.011771 -4.158962  
 20 -5.354811 2.249780 -2.481875  
 21 -5.213947 2.263447 2.569630  
 22 -2.948376 -2.053387 4.143103  
 END

# spin multiplicity  
 ELEC

3 0.00  
 END  
 # end of prod section  
 \*START  
 SPECIES NONLINTS  
 STATUS 2  
 # transform Ang to AU by gview  
 GEOM  
 1 5.293633 -1.222975 -0.027127  
 2 3.040123 -2.588712 -0.107250  
 3 0.748543 -1.310369 -0.160736  
 4 0.703952 1.337745 -0.119642  
 5 2.947095 2.694163 -0.042532  
 6 5.248202 1.406956 0.002302  
 7 -1.862082 -2.505024 -0.092557  
 8 -1.904771 2.468569 -0.067847  
 9 -3.540537 1.311943 1.956986  
 10 -3.122144 -1.438751 2.260036  
 11 7.086226 -2.216997 0.080979  
 12 3.070553 -4.642792 -0.061752  
 13 2.907339 4.746189 0.053717  
 14 7.004103 2.461294 0.132714  
 15 -1.776525 -4.567105 -0.116371  
 16 -1.937788 4.527961 -0.119480  
 17 -3.669389 1.215159 -1.936993  
 18 -3.499769 -1.362257 -2.149249  
 19 -4.844218 -2.495190 -3.203376  
 20 -5.111870 2.338390 -2.870505  
 21 -5.193618 2.300157 2.653211  
 22 -2.925598 -2.335077 4.093517  
 END

# spin multiplicity  
 ELEC  
 3 0.00  
 END

# end of start section

\*PATH  
 SCALEMASS 1.00  
 RODS ON  
 INTMU 3  
 SSTEP 0.002  
 INH 10 # Hessian  
 NSTEPS 99999  
 RPM pagem  
 SIGN PRODUCT # reactant

SRANGE  
 SLP 2.0  
 SLM -2.0  
 END

SFIRST  
 NFSTEP 10  
 FSIZE 0.005  
 END

EXFIRST  
 END  
 EXSECOND  
 END

COORD CART

PRPATH  
 COORD 9 17  
 INTERVAL 1  
 XMOL  
 END

```

PRSAVERP
40.
SPECSTOP
50.
PERCENTDOWN 99.
60.
END
70.
80.
90.
*TUNNEL
100.
120.
QUAD
140.
NQE 40
160.
NQTH 40
180.
END
200.
220.
ZCT
240.
SCT
260.
SCTOPT
273.15
LAGRANGE 8
280.
END
290.
298.15
*RATE
300.
GTLOG
310.
FORWARDK
320.
SIGMAF 1
340.
TST
360.
CVT
373.15
380.
TEMP
400.
30.
END
35.

```

### ***Triplet DPM Rearrangement-TS1.70***

```

*GRGENERAL
Field=Z-100
END

GRRESTART

*GRCOMMON
GRFIRST
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) UNITS=AU int=ultrafine Force
nosymm Field=Z-100
END

GRENER
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) int=ultrafine UNITS=AU nosymm
Field=Z-100
END

GRSEC
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) UNITS=AU int=ultrafine
Freq=norman nosymm Field=Z-100
END

*GRREACT1
CHARGE 0
MULTIPLICITY 3

*GRSTART
CHARGE 0
MULTIPLICITY 3

*GRPROD1
CHARGE 0
MULTIPLICITY 3

GRFIRST
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) int=ultrafine UNITS=AU Force
nosymm Field=Z-100
END

GRSEC
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) UNITS=AU int=ultrafine
Freq=norman nosymm Field=Z-100
END

*GRPATH
GRENER
%mem=16000mb
%nprocs=16
# wB97XD/6-31g(d) UNITS=AU int=ultrafine nosymm

```

## Site-selectivity

### *HOCPhCOHMe-Z10.dat*

```
*General
18 1.017125 3.955952 0.669540
19 -0.219463 -1.724213 3.043269
END

TITLE
HOCPhCOHMe-Z10
END

ATOMS
1 C
2 O
3 C
4 O
5 C
6 C
7 C
8 C
9 C
10 C
11 H
12 H
13 H
14 H
15 H
16 C
17 H
18 H
19 H
END

NOSUPERMOL
# use AU now
INPUNIT AU

WRITEFU31

MDMOVIE ON

*OPTIMIZATION

OPTMIN OHOOK
OPTTS OHOOK

*SECOND

HESSCAL HHOOK

*REACT1
SPECIES NONLINRP
STATUS 2

*REACT1
# Geometry in a.u.
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.487608
3 1.575157 0.000000 -9.675577
4 2.934844 0.509157 -11.724878
5 4.691623 5.262702 -5.881966
6 4.149154 3.708326 -7.914119
7 2.328846 1.789316 -7.661607
8 1.086332 1.479375 -5.351965
9 1.610448 3.044441 -3.292583
10 3.429236 4.924311 -3.587172
11 6.100133 6.744205 -6.054460
12 5.116333 3.946823 -9.706025
13 -0.287885 -0.033082 -5.176056
14 3.875635 6.149778 -1.999764
15 2.417125 -0.675192 -13.005227
16 0.234963 2.726022 -0.809268
17 -1.753544 3.302551 -1.060507

# spin multiplicity
ELEC
1 0.00
END

# end of react section

*PROD1
SPECIES NONLINRP
STATUS 2

*PROD1
# Geometry in a.u.
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.484840
3 1.495621 0.000000 -9.746888
4 2.277246 0.231412 -11.886802
5 3.478965 5.869596 -6.265166
6 3.169888 4.125285 -8.193538
7 1.836947 1.894625 -7.717560
8 0.821895 1.430523 -5.332273
9 1.110294 3.185875 -3.385026
10 2.457144 5.396140 -3.880520
11 4.519928 7.604866 -6.598057
12 3.942586 4.436368 -10.066815
13 -0.177332 -0.323765 -4.953976
14 2.715515 6.772915 -2.378397
15 0.434044 -1.718385 -9.170378
16 -0.039994 2.733174 -0.809323
17 -2.081706 3.153132 -0.902859
18 0.741400 4.018644 0.621497
19 -0.048139 -1.735735 3.045973
END

# spin multiplicity
ELEC
1 0.00
END

# end of prod section

*START
SPECIES NONLINTS
STATUS 2

# transform Ang to AU by gview
GEOM
1 0.000000 0.000000 0.000000
2 0.000000 0.000000 2.485798
3 1.529819 0.000000 -9.743906
4 2.607475 0.407905 -11.947388
5 4.208289 5.485099 -6.124333
6 3.717055 3.835868 -8.095520
7 2.084631 1.790431 -7.698464
8 0.957952 1.415199 -5.344051
9 1.430939 3.079174 -3.353421
10 3.071277 5.099224 -3.773856
11 5.477133 7.074480 -6.389590
12 4.568496 4.076687 -9.946540
13 -0.270129 -0.202516 -5.060311
14 3.474068 6.399382 -2.235229
15 1.275806 -1.323601 -11.672159
16 0.180433 2.729079 -0.809111
17 -1.821606 3.295483 -0.959879
```

18 1.018540 3.957872 0.639442  
19 -0.186883 -1.727163 3.044365  
END

# spin multiplicity  
ELEC  
1 0.00  
END

# end of start section

\*PATH  
SCALEMASS 1.00  
RODS ON  
INTMU 3  
SSTEP 0.002  
INH 10 # Hessian  
NSTEPS 99999  
RPM pagem  
SIGN product # product

SRANGE  
SLP 4.0  
SLM -4.0  
END

#prsaverp

EXFIRST  
END  
EXSECOND  
END

COORD Curv3

INTDEF  
2-1 3-1 4-3 5-3 6-5 7-6 8-7 9-8 10-9 11-5 12-6  
13-8 14-10 15-4 16-1 17-16 18-16 19-2  
3-1-2 4-3-1 5-3-1 6-5-3 7-6-5 8-7-6 9-8-7 10-9-8 11-5-3  
12-6-5 13-8-7 14-10-9 15-4-3 16-1-2 17-16-1 18-16-1 19-2-1  
4-3-1-2 5-3-1-2 6-5-3-1 7-6-5-3 8-7-6-5 9-8-7-6 10-9-8-7  
11-5-3-1 12-6-5-3 13-8-7-6 14-10-9-8 15-4-3-1  
16-1-2-9 17-16-1-2 18-16-1-2 19-2-1-16  
END

PRPATH  
COORD 15 3  
INTERVAL 1  
XMOL  
END

PRSAVERP

SPECSTOP  
PERCENTDOWN 99.  
END

\*TUNNEL

QUAD

NQE 40  
NQTH 40  
END

ZCT  
SCT  
SCTOPT  
LAGRANGE 8  
END

QRST  
MODE 51  
SRW -1.66  
states 200  
END

\*RATE  
GTLOG  
FORWARDK  
SIGMAF 1  
TST  
CVT  
# PRDELG  
# PRPART rtp

TEMP  
#10.  
#15.  
#20.  
#25.  
30.  
35.  
40.  
50.  
60.  
70.  
80.  
90.  
100.  
120.  
140.  
160.  
180.  
200.  
220.  
240.  
260.  
273.15  
280.  
290.  
298.15  
300.  
310.  
320.  
340.  
360.  
373.15  
380.  
400.  
END

## 5. Cartesian coordinates

### Hydroxycarbenes using $\omega$ B97X-D

#### H-C-OH

R No field  
C 0.01202200 0.00000000 0.00620000  
O -0.00522300 0.00000000 2.48698300  
H 1.72920400 0.00000000 3.06374000  
H -2.06112100 0.00000000 -0.43241300

TS No field  
C 0.01202400 0.00000000 -0.00064300  
O 0.00751200 0.00000000 2.45364400  
H 1.92367800 0.00000000 1.35991700  
H -1.90932700 0.00000000 -0.87102800

P No field  
C -0.00006600 0.00000000 0.01089600  
O 0.00010800 0.00000000 2.28426600  
H 1.77166800 0.00000000 -1.10685300  
H -1.77197000 0.00000000 -1.10658100

R EEF -5.14 V/nm along X direction  
C 0.01784300 0.00000000 0.00519900  
O -0.00447100 0.00000000 2.48346400  
H 1.73150200 0.00000000 3.06954200  
H -2.06999500 0.00000000 -0.43369400

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44653500  
H 1.93346800 0.00000000 1.35439200  
H -1.93848400 0.00000000 -0.86341100

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27297700  
H 1.76266700 0.00000000 -1.11999000  
H -1.78373200 0.00000000 -1.11644300

R EEF -3.85 V/nm along X direction  
C 0.01621800 0.00000000 0.00546100  
O -0.00470500 0.00000000 2.48438600  
H 1.73084400 0.00000000 3.06793000  
H -2.06747600 0.00000000 -0.43326900

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44858300  
H 1.92828900 0.00000000 1.35527800  
H -1.93400500 0.00000000 -0.86441000

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27314900  
H 1.76474200 0.00000000 -1.11925100  
H -1.78044400 0.00000000 -1.11665300

R EEF -2.52 V/nm along X direction  
C 0.01471000 0.00000000 0.00571800  
O -0.00490800 0.00000000 2.48528000  
H 1.73024300 0.00000000 3.06642800

H -2.06516500 0.00000000 -0.43291800

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45055400  
H 1.92334900 0.00000000 1.35600800  
H -1.92994200 0.00000000 -0.86531000

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27327200  
H 1.76694800 0.00000000 -1.11862200  
H -1.77737900 0.00000000 -1.11690600

R EEF 2.52 V/nm along X direction  
C 0.00973800 0.00000000 0.00662700  
O -0.00544400 0.00000000 2.48857200  
H 1.72837100 0.00000000 3.06145200  
H -2.05778200 0.00000000 -0.43213900

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45778600  
H 1.90579100 0.00000000 1.35757600  
H -1.91737900 0.00000000 -0.86796900

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27327200  
H 1.77737700 0.00000000 -1.11690800  
H -1.76694800 0.00000000 -1.11862000

R EEF 3.85 V/nm along X direction  
C 0.00873400 0.00000000 0.00681400  
O -0.00552700 0.00000000 2.48932200  
H 1.72802900 0.00000000 3.06045000  
H -2.05635500 0.00000000 -0.43207500

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45945300  
H 1.90190800 0.00000000 1.35766700  
H -1.91505900 0.00000000 -0.86841800

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27315100  
H 1.78045200 0.00000000 -1.11664500  
H -1.76473700 0.00000000 -1.11925900

R EEF 5.14 V/nm along X direction  
C 0.00782000 0.00000000 0.00698100  
O -0.00559400 0.00000000 2.49004400  
H 1.72773600 0.00000000 3.05954300  
H -2.05508200 0.00000000 -0.43205800

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.46107100  
H 1.89821000 0.00000000 1.35765700  
H -1.91303700 0.00000000 -0.86878900

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27297700  
H 1.78373200 0.00000000 -1.11644300  
H -1.76266700 0.00000000 -1.11999000

R EEF -5.14 V/nm along Y direction  
C 0.01190100 -0.02029600 0.00551000  
O -0.00467700 -0.03137700 2.48672400  
H 1.72864300 0.02786000 3.06414900  
H -2.06098700 0.02381200 -0.43187300

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45505000  
H 1.91453900 0.00000000 1.35723400  
H -1.91177600 0.20776200 -0.86492400

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27349500  
H 1.77213900 0.00000000 -1.11738600  
H -1.77156200 0.03651300 -1.11740900

R EEF -3.85 V/nm along Y direction  
C 0.01195600 -0.01511200 0.00581300  
O -0.00491500 -0.02355900 2.48683700  
H 1.72888800 0.02086600 3.06396900  
H -2.06104800 0.01780700 -0.43210900

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45471700  
H 1.91436500 0.00000000 1.35715600  
H -1.91668800 0.15535300 -0.86576700

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27344000  
H 1.77199900 0.00000000 -1.11748600  
H -1.77167600 0.02729100 -1.11749800

R EEF -2.52 V/nm along Y direction  
C 0.01199200 -0.01001200 0.00602800  
O -0.00508500 -0.01573000 2.48691800  
H 1.72906200 0.01389500 3.06384300  
H -2.06108900 0.01184700 -0.43227900

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45448100  
H 1.91424400 0.00000000 1.35709600  
H -1.92018400 0.10322600 -0.86635900

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27340200  
H 1.77189900 0.00000000 -1.11755600  
H -1.77175500 0.01815300 -1.11756200

R EEF 2.52 V/nm along Y direction  
C 0.01199200 0.01001200 0.00602800

O -0.00508500 0.01573000 2.48691800  
H 1.72906200 -0.01389500 3.06384300  
H -2.06108900 -0.01184700 -0.43227900

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45448100  
H 1.91424400 0.00000000 1.35709600  
H -1.92018400 -0.10322600 -0.86635900

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27340200  
H 1.77189900 0.00000000 -1.11755600  
H -1.77175500 -0.01815300 -1.11756200

R EEF 3.85 V/nm along Y direction  
C 0.01195600 0.01511200 0.00581300  
O -0.00491500 0.02355900 2.48683700  
H 1.72888800 -0.02086600 3.06396900  
H -2.06104800 -0.01780700 -0.43210900

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45471700  
H 1.91436500 0.00000000 1.35715600  
H -1.91668800 -0.15535300 -0.86576700

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27344000  
H 1.77199900 0.00000000 -1.11748600  
H -1.77167600 -0.02729100 -1.11749800

R EEF 5.14 V/nm along Y direction  
C 0.01190100 0.02029600 0.00551000  
O -0.00467700 0.03137700 2.48672400  
H 1.72864300 -0.02786000 3.06414900  
H -2.06098700 -0.02381200 -0.43187300

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45505000  
H 1.91453900 0.00000000 1.35723400  
H -1.91177600 -0.20776200 -0.86492400

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27349500  
H 1.77213900 0.00000000 -1.11738600  
H -1.77156200 -0.03651300 -1.11740900

R EEF -5.14 V/nm along Z direction  
C 0.01361500 0.00000000 -0.00283300  
O 0.00608700 0.00000000 2.45993900  
H 1.72554200 0.00000000 3.08869200  
H -2.07036200 0.00000000 -0.42128800

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43511200  
H 1.92980400 0.00000000 1.30084100  
H -1.92968700 0.00000000 -0.87480200

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.26366600  
H 1.77484100 0.00000000 -1.12416500  
H -1.77484500 0.00000000 -1.12415900

R EEF -3.85 V/nm along Z direction  
C 0.01323000 0.00000000 -0.00045000  
O 0.00317500 0.00000000 2.46657400  
H 1.72644100 0.00000000 3.08238100  
H -2.06796400 0.00000000 -0.42399200

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43968700  
H 1.92592100 0.00000000 1.31471700  
H -1.92800300 0.00000000 -0.87236600

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26602400  
H 1.77410800 0.00000000 -1.12225600  
H -1.77411100 0.00000000 -1.12225000

R EEF -2.52 V/nm along Z direction  
C 0.01283500 0.00000000 0.00184600  
O 0.00032100 0.00000000 2.47328600  
H 1.72735000 0.00000000 3.07612600  
H -2.06562600 0.00000000 -0.42674600

TS EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44440100  
H 1.92201700 0.00000000 1.32870300  
H -1.92632100 0.00000000 -0.87023400

P EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26842600  
H 1.77335900 0.00000000 -1.12052900  
H -1.77336100 0.00000000 -1.12052500

R EEF 2.52 V/nm along Z direction  
C 0.01118700 0.00000000 0.01024600  
O -0.01057300 0.00000000 2.50113900  
H 1.73109600 0.00000000 3.05145500  
H -2.05683000 0.00000000 -0.43833000

TS EEF 2.52 V/nm along Z direction

## HO-C-OH

R No field  
C -0.15063600 0.00117200 0.01235700  
O -0.03882800 -0.00050300 2.51768100  
H 1.72958800 -0.00033600 2.93752200  
O -2.60527800 0.00089400 -0.50126300  
H -2.73498700 0.00209000 -2.31420700

TS No field  
C -0.10365200 0.00069000 0.01750100  
O -0.06690600 -0.00085800 2.43635900  
H 1.89067900 0.00023600 1.18838900  
O -2.37853300 0.00102800 -1.03349700  
H -2.16050000 0.00222000 -2.84149500

P No field  
C -0.05443400 0.00002500 -0.00768900

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46485600  
H 1.90621100 0.00000000 1.38592600  
H -1.91964500 0.00000000 -0.86443500

P EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27851000  
H 1.77021900 0.00000000 -1.11539600  
H -1.77022100 0.00000000 -1.11539400

R EEF 3.85 V/nm along Z direction  
C 0.01076400 0.00000000 0.01215700  
O -0.01318500 0.00000000 2.50842200  
H 1.73205400 0.00000000 3.04532300  
H -2.05475300 0.00000000 -0.44139300

TS EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47041900  
H 1.90220500 0.00000000 1.40059900  
H -1.91800700 0.00000000 -0.86358600

P EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28115700  
H 1.76940000 0.00000000 -1.11454200  
H -1.76940000 0.00000000 -1.11454000

R EEF 5.14 V/nm along Z direction  
C 0.01034200 0.00000000 0.01399500  
O -0.01575800 0.00000000 2.51586100  
H 1.73301900 0.00000000 3.03918500  
H -2.05272300 0.00000000 -0.44453200

TS EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47619000  
H 1.89816800 0.00000000 1.41546800  
H -1.91639500 0.00000000 -0.86294600

P EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28386000  
H 1.76856900 0.00000000 -1.11385200  
H -1.76856900 0.00000000 -1.11385000

O -0.03346100 -0.00010200 2.25031900  
H 1.67494600 0.00007400 -1.18272000  
O -2.20685700 0.00012100 -1.35634200  
H -1.82137400 0.00021500 -3.13534600

R EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49460600  
H 1.75330000 0.00000000 2.99608300  
O -2.45195500 0.00000400 -0.64222000  
H -2.41435700 0.00000600 -2.45925300

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40999500  
H 1.99001500 0.00000000 1.21275100

O -2.27259700 -0.00000200 -1.11113300  
H -1.93600100 -0.00000200 -2.90173200

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25471300  
H 1.73887000 0.00000000 -1.15209100  
O -2.14919600 0.00000000 -1.39504400  
H -1.67239700 -0.00000200 -3.15291700

R EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49785400  
H 1.75178400 0.00000000 2.99860200  
O -2.44574300 -0.00000200 -0.63771900  
H -2.42899800 0.00000000 -2.45504600

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41234200  
H 1.98616700 0.00000000 1.21007000  
O -2.26847200 -0.00000200 -1.10519500  
H -1.95352600 0.00000000 -2.89947400

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25557400  
H 1.73907800 0.00000000 -1.15360100  
O -2.14646000 -0.00000200 -1.38860900  
H -1.68760500 -0.00000400 -3.15093600

R EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50113500  
H 1.75038600 0.00000000 3.00110700  
O -2.43991300 0.00000800 -0.63293900  
H -2.44448600 0.00000200 -2.45035600

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41464400  
H 1.98260300 0.00000000 1.20722400  
O -2.26478700 -0.00000200 -1.09894000  
H -1.97220800 0.00000000 -2.89677000

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25642500  
H 1.73935900 0.00000000 -1.15525800  
O -2.14400300 0.00000400 -1.38204600  
H -1.70359300 0.00000400 -3.14877600

R EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51469200  
H 1.74597000 0.00000000 3.01099100  
O -2.41994800 -0.00000800 -0.61103400  
H -2.51520000 -0.00000400 -2.42641300

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42351600  
H 1.97108000 0.00000000 1.19433600  
O -2.25401900 0.00000000 -1.07066800  
H -2.05899000 0.00000200 -2.88106200

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25976000  
H 1.74138000 0.00000000 -1.16318200  
O -2.13668200 0.00000000 -1.35440900  
H -1.77578400 0.00000000 -3.13812400

R EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51822200  
H 1.74517000 0.00000000 3.01341900  
O -2.41568300 0.00000800 -0.60488100  
H -2.53511400 0.00000600 -2.41904500

TS EEF 3.85 V/nm along X direction  
C -0.10399700 0.00068200 0.02046200  
O -0.06516000 -0.00086000 2.44640100  
H 1.88147400 0.00023400 1.18294400  
O -2.35739800 0.00103200 -1.03498300  
H -2.17383200 0.00222800 -2.84756700

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26058400  
H 1.74216400 0.00000000 -1.16544700  
O -2.13541800 0.00000000 -1.34714300  
H -1.79603400 0.00000000 -3.13489400

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.52182200  
H 1.74449800 0.00000000 3.01582800  
O -2.41167300 0.00000000 -0.59846500  
H -2.55595400 0.00000000 -2.41108400

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42780400  
H 1.96690100 0.00000000 1.18707700  
O -2.25075500 -0.00000800 -1.05452400  
H -2.11010500 -0.00000800 -2.86988500

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26140800  
H 1.74308400 0.00000000 -1.16780800  
O -2.13435200 0.00000000 -1.33973900  
H -1.81720700 0.00000000 -3.13141300

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50851600  
H 1.74812800 0.00000000 3.00640200  
O -2.42646800 0.10824400 -0.62223600  
H -2.47340300 0.28925500 -2.43077500

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41984300  
H 1.97642000 0.00000000 1.20259400  
O -2.25474700 0.14498600 -1.08331000  
H -2.00817700 0.41368200 -2.86839400

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25804400

H 1.74125500 0.00000000 -1.15728000  
O -2.13940900 -0.04535300 -1.37210800  
H -1.76668900 0.35761200 -3.10885200

R EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50820600  
H 1.74804500 0.00000000 3.00625700  
O -2.42771700 0.08090100 -0.62238200  
H -2.47543100 0.21641300 -2.43461600

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41953400  
H 1.97637100 0.00000000 1.20192100  
O -2.25647000 0.10864800 -1.08423500  
H -2.01039900 0.31014600 -2.87782900

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25807100  
H 1.74076900 0.00000000 -1.15803800  
O -2.13961300 -0.03443100 -1.37050000  
H -1.75409700 0.26722600 -3.12438200

R EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50798500  
H 1.74798600 0.00000000 3.00615500  
O -2.42860300 0.05378400 -0.62247600  
H -2.47688800 0.14397800 -2.43732800

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41931500  
H 1.97633500 0.00000000 1.20144500  
O -2.25768700 0.07245800 -1.08490200  
H -2.01195600 0.20657700 -2.88456800

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25808900  
H 1.74044600 0.00000000 -1.15854400  
O -2.13972600 -0.02311900 -1.36943600  
H -1.74496600 0.17754000 -3.13532000

R EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50798500  
H 1.74798600 0.00000000 3.00615500  
O -2.42860300 -0.05378400 -0.62247600  
H -2.47688800 -0.14398000 -2.43732800

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41931500  
H 1.97633500 0.00000000 1.20144500  
O -2.25768700 -0.07246700 -1.08490200  
H -2.01195400 -0.20658700 -2.88456800

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25808800  
H 1.74044800 0.00000000 -1.15854400  
O -2.13972600 0.02310600 -1.36943200  
H -1.74496800 -0.17755900 -3.13531400

R EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50820600  
H 1.74804500 0.00000000 3.00625700  
O -2.42771700 -0.08090100 -0.62238200  
H -2.47543100 -0.21641300 -2.43461600

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41953400  
H 1.97637100 0.00000000 1.20192300  
O -2.25647000 -0.10866100 -1.08423500  
H -2.01039900 -0.31015500 -2.87782900

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25807100  
H 1.74076900 0.00000000 -1.15803800  
O -2.13961300 0.03443100 -1.37050000  
H -1.75409700 -0.26722600 -3.12438200

R EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50851600  
H 1.74812800 0.00000000 3.00640200  
O -2.42646800 -0.10824400 -0.62223600  
H -2.47340300 -0.28925500 -2.43077500

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41984300  
H 1.97642200 0.00000000 1.20259400  
O -2.25474700 -0.14497400 -1.08331000  
H -2.00817700 -0.41367300 -2.86839400

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25804400  
H 1.74125500 0.00000000 -1.15728000  
O -2.13940900 0.04535300 -1.37210800  
H -1.76668900 -0.35761200 -3.10885200

R EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48003400  
H 1.72556400 0.00000000 3.05775000  
O -2.44870600 -0.00002000 -0.62799400  
H -2.47099200 -0.00000900 -2.44065600

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.39480200  
H 1.99160000 0.00000000 1.14977000  
O -2.27121000 0.00002000 -1.11874900  
H -1.96976800 0.00000400 -2.91048200

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.24416800  
H 1.74416100 0.00000000 -1.16332300  
O -2.13861000 -0.00002000 -1.41054500  
H -1.66815500 0.00000400 -3.16604300

R EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000

O 0.0000000 0.0000000 2.48666100  
H 1.73155100 0.0000000 3.04415200  
O -2.44387400 0.0000000 -0.62614200  
H -2.47350300 -0.00000400 -2.43973200

TS EEF -3.85 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.40063900  
H 1.98787600 0.0000000 1.16231100  
O -2.26828100 0.00000200 -1.10947000  
H -1.98213100 0.00000400 -2.90458600

P EEF -3.85 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.24755000  
H 1.74305200 0.0000000 -1.16219700  
O -2.13926500 0.0000000 -1.39923100  
H -1.68695500 0.00000200 -3.16004500

R EEF -2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.49348700  
H 1.73726200 0.0000000 3.03102400  
O -2.43903600 0.0000000 -0.62462300  
H -2.47550800 -0.00000400 -2.43922700

TS EEF -2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.40663300  
H 1.98408700 0.0000000 1.17504500  
O -2.26520800 0.00000200 -1.10085300  
H -1.99344100 0.00000400 -2.89920000

P EEF -2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.25099700  
H 1.74201800 0.0000000 -1.16109700  
O -2.13968700 0.0000000 -1.38846900  
H -1.70484200 0.00000200 -3.15434700

R EEF 2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.52318800  
H 1.75773700 0.0000000 2.98274300  
O -2.41945500 0.00000800 -0.62167900  
H -2.47876800 0.00000800 -2.44132100

TS EEF 2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43240700  
H 1.96825100 0.0000000 1.22778600

## NC-C-OH

R No field  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46760700  
H 1.74214100 0.0000000 3.02113800  
C -2.60047600 0.0000000 -0.88233400  
N -4.49809000 0.0000000 -1.99184000

TS No field  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43620600  
H 1.94615800 0.0000000 1.29458200  
C -2.37516200 0.0000000 -1.37195700

O -2.25157900 -0.00000400 -1.07232400  
H -2.02923200 -0.00000200 -2.88266700

P EEF 2.52 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.26550700  
H 1.73860900 0.0000000 -1.15694900  
O -2.13920300 0.0000000 -1.35052500  
H -1.76778100 0.0000000 -3.13467100

R EEF 3.85 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.53133600  
H 1.76234400 0.0000000 2.97163900  
O -2.41446400 0.00000800 -0.62169600  
H -2.47844300 0.00000400 -2.44286500

TS EEF 3.85 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43936000  
H 1.96411400 0.0000000 1.24139600  
O -2.24785800 -0.00000400 -1.06653400  
H -2.03604800 -0.00000200 -2.87976000

P EEF 3.85 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.26932800  
H 1.73793800 0.0000000 -1.15597000  
O -2.13857200 0.0000000 -1.34223500  
H -1.78147800 0.0000000 -3.13055900

R EEF 5.14 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.53983400  
H 1.76677200 0.0000000 2.96088800  
O -2.40941700 -0.00000600 -0.62200400  
H -2.47768100 -0.00000400 -2.44482100

TS EEF 5.14 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.44654400  
H 1.95990000 0.0000000 1.25517000  
O -2.24401900 -0.00000400 -1.06123800  
H -2.04209200 -0.00000200 -2.87734000

P EEF 5.14 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27323200  
H 1.73734100 0.0000000 -1.15501100  
O -2.13774800 0.0000000 -1.33439900  
H -1.79439200 0.0000000 -3.12678200

N -4.08293800 0.0000000 -2.75048000

P No field  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27066400  
H 1.73388500 0.0000000 -1.15340000  
C -2.36084500 0.0000000 -1.47977300  
N -4.18750400 0.0000000 -2.68372000

R EEF -5.14 V/nm along X direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46067000

H 1.74952800 0.00000000 3.01773300  
C -2.65631500 0.00000000 -0.81544500  
N -4.61148900 0.00000200 -1.82076500

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42611500  
H 1.97108500 0.00000000 1.28092700  
C -2.45271200 0.00000000 -1.29404500  
N -4.27738900 0.00000000 -2.51292500

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26840900  
H 1.71001200 0.00000000 -1.18014200  
C -2.44358100 0.00000200 -1.39158200  
N -4.39321800 -0.00001900 -2.38564000

R EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46232200  
H 1.74748500 0.00000000 3.01862700  
C -2.64129800 0.00000000 -0.83340200  
N -4.58176800 0.00000000 -1.86634300

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42872400  
H 1.96432200 0.00000000 1.28465900  
C -2.43185700 0.00000000 -1.31506500  
N -4.22681400 0.00000000 -2.57727200

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26907800  
H 1.71592100 0.00000000 -1.17317300  
C -2.42250300 0.00000000 -1.41405200  
N -4.34345600 -0.00002100 -2.46176600

R EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46402100  
H 1.74557500 0.00000000 3.01948300  
C -2.62699100 0.00000000 -0.85059300  
N -4.55285100 -0.00000200 -1.91026300

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43126600  
H 1.95792900 0.00000000 1.28817400  
C -2.41201700 0.00000000 -1.33505400  
N -4.17752100 0.00000000 -2.63825700

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26526300  
H 1.71976500 0.00000000 -1.16629200  
C -2.41229700 0.00000000 -1.43348100  
N -4.29561200 0.00000000 -2.53846800

R EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47152700  
H 1.73921200 0.00000000 3.02279200  
C -2.57678400 0.00000000 -0.90999600  
N -4.44866500 0.00000000 -2.06306000

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44104900  
H 1.93563200 0.00000000 1.30010600  
C -2.34240000 0.00000000 -1.40394200  
N -3.99658000 0.00000000 -2.84720200

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27146300  
H 1.74594700 0.00000000 -1.14136700  
C -2.32233100 0.00000000 -1.51984100  
N -4.08465000 0.00000000 -2.81651700

R EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47363000  
H 1.73793100 0.00000000 3.02365600  
C -2.56603000 0.00000000 -0.92208700  
N -4.42648500 0.00000000 -2.09404400

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44345300  
H 1.93079800 0.00000000 1.30252400  
C -2.32754400 0.00000000 -1.41805100  
N -3.95689700 0.00000000 -2.88983500

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27180700  
H 1.75203200 0.00000000 -1.13569000  
C -2.30395900 0.00000000 -1.53857200  
N -4.03449700 0.00000000 -2.87771400

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47584500  
H 1.73677200 0.00000000 3.02455700  
C -2.55603300 0.00000000 -0.93290500  
N -4.40632000 0.00000000 -2.12153000

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44585600  
H 1.92623600 0.00000000 1.30469800  
C -2.31377200 0.00000000 -1.43079700  
N -3.92003600 0.00000000 -2.92836000

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27211900  
H 1.75815100 0.00000000 -1.13025900  
C -2.28629600 0.00000000 -1.55626600  
N -3.98598200 0.00000000 -2.93477400

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46071700  
H 1.74267200 0.00000000 3.02763500  
C -2.61317300 -0.34579400 -0.84455100  
N -4.46015600 -0.93823800 -1.86722000

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000

O 0.0000000 0.0000000 2.42428700  
H 1.95401500 0.0000000 1.28475300  
C -2.36135000 -0.52072600 -1.33550600  
N -3.99134100 -1.22317300 -2.61806400

P EEF -5.14 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.26969400  
H 1.73033000 0.0000000 -1.15809100  
C -2.34922200 -0.33718600 -1.46882600  
N -4.11995200 -0.87231300 -2.63730100

R EEF -3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46119700  
H 1.74272900 0.0000000 3.02766200  
C -2.62033900 -0.25633400 -0.84765600  
N -4.50016300 -0.69993000 -1.88537900

TS EEF -3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43530800  
H 1.94705000 0.0000000 1.29351000  
C -2.35790100 -0.35157600 -1.36364800  
N -4.01104700 -0.86569300 -2.71283000

P EEF -3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27012500  
H 1.73191400 0.0000000 -1.15600600  
C -2.35442400 -0.25039300 -1.47376200  
N -4.14974600 -0.65030400 -2.65848700

R EEF -2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46732200  
H 1.74210300 0.0000000 3.02110600  
C -2.59680400 -0.16652800 -0.88072000  
N -4.47617900 -0.46445700 -1.98143200

TS EEF -2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43580700  
H 1.94655900 0.0000000 1.29408300  
C -2.36769700 -0.23373100 -1.36812800  
N -4.05135300 -0.57861200 -2.73321600

P EEF -2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.26601900  
H 1.73090300 0.0000000 -1.15399200  
C -2.36925300 -0.16536600 -1.47388100  
N -4.17833500 -0.42269400 -2.66906200

R EEF 2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46732200  
H 1.74210300 0.0000000 3.02110600  
C -2.59680400 0.16652800 -0.88072000  
N -4.47617900 0.46445700 -1.98143200

TS EEF 2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43580700  
H 1.94655900 0.0000000 1.29408300  
C -2.36769700 0.23373100 -1.36812800

N -4.05135300 0.57861200 -2.73321600

P EEF 2.52 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27043100  
H 1.73296500 0.0000000 -1.15461400  
C -2.35826200 0.16606200 -1.47675400  
N -4.17180800 0.43223900 -2.67115500

R EEF 3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46695500  
H 1.74205200 0.0000000 3.02107400  
C -2.59188300 0.25395300 -0.87859800  
N -4.44757600 0.70484700 -1.96763500

TS EEF 3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43530800  
H 1.94705000 0.0000000 1.29351000  
C -2.35790100 0.35157600 -1.36364800  
N -4.01104700 0.86569300 -2.71283000

P EEF 3.85 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27012500  
H 1.73191400 0.0000000 -1.15600600  
C -2.35442400 0.25039300 -1.47376200  
N -4.14974600 0.65030400 -2.65848700

R EEF 5.14 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46071500  
H 1.74267000 0.0000000 3.02763500  
C -2.61317300 0.34579400 -0.84454900  
N -4.46015800 0.93823600 -1.86721800

TS EEF 5.14 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.42428700  
H 1.95401500 0.0000000 1.28475300  
C -2.36135000 0.52072600 -1.33550600  
N -3.99134100 1.22317300 -2.61806400

P EEF 5.14 V/nm along Y direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.26969400  
H 1.73033000 0.0000000 -1.15809100  
C -2.34922200 0.33718600 -1.46882600  
N -4.11995200 0.87231300 -2.63730100

R EEF -5.14 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.43701800  
H 1.72376500 0.0000000 3.06927500  
C -2.59145800 0.0000000 -0.97405000  
N -4.35057800 0.0000000 -2.28631600

TS EEF -5.14 V/nm along Z direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.41180400  
H 1.96351500 0.0000000 1.24855200  
C -2.30923100 0.0000000 -1.51007100  
N -3.77331200 0.0000000 -3.14821700

P EEF -5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25889800  
H 1.74736800 0.00000000 -1.14123600  
C -2.30344700 0.00000200 -1.59592900  
N -3.92888200 0.00000400 -3.06104000

R EEF -3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44863800  
H 1.72846700 0.00000000 3.05045200  
C -2.57121300 0.00000200 -0.97322100  
N -4.34782700 0.00000200 -2.27059200

TS EEF -3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41782800  
H 1.95910100 0.00000000 1.25985800  
C -2.32722500 0.00000000 -1.47378500  
N -3.85789600 0.00000000 -3.04877400

P EEF -3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25765100  
H 1.74160600 0.00000000 -1.14354700  
C -2.33062700 -0.00000200 -1.56076100  
N -4.01287800 -0.00000200 -2.95317400

R EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45487600  
H 1.73320500 0.00000000 3.04031400  
C -2.58163000 0.00000000 -0.94177600  
N -4.40115300 0.00000000 -2.17704300

TS EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42390400  
H 1.95473900 0.00000000 1.27129100  
C -2.34432900 0.00000000 -1.43846000  
N -3.93834400 0.00000000 -2.94835400

P EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26476400  
H 1.74067500 0.00000000 -1.14711100  
C -2.33365400 0.00000000 -1.53563900  
N -4.06789600 0.00000000 -2.86951200

R EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48072800  
H 1.75049200 0.00000000 3.00309900  
C -2.61678600 0.00000000 -0.82783500  
N -4.58124600 0.00000000 -1.81253300

TS EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44877800  
H 1.93772800 0.00000000 1.31844200  
C -2.40142500 0.00000000 -1.31154400  
N -4.20504500 0.00000000 -2.56126600

P EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27664500  
H 1.72706300 0.00000000 -1.16011500  
C -2.38514300 0.00000000 -1.42823700  
N -4.28905600 0.00000000 -2.50607300

R EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48745700  
H 1.75448100 0.00000000 2.99442500  
C -2.62403700 0.00000000 -0.80250100  
N -4.61765700 0.00000000 -1.72613100

TS EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45520500  
H 1.93354800 0.00000000 1.33057000  
C -2.41302800 0.00000000 -1.28348500  
N -4.25847700 0.00000000 -2.47039500

P EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27967600  
H 1.72372000 0.00000000 -1.16355200  
C -2.39598500 0.00000000 -1.40447900  
N -4.33253000 0.00000000 -2.42276800

R EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49432800  
H 1.75835700 0.00000000 2.98596300  
C -2.63086300 0.00000000 -0.77810600  
N -4.65130000 0.00000000 -1.64095200

TS EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46174900  
H 1.92938100 0.00000000 1.34282900  
C -2.42369000 0.00000000 -1.25681200  
N -4.30721900 0.00000000 -2.38228400

P EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28274100  
H 1.72044900 0.00000000 -1.16702000  
C -2.40594200 0.00000000 -1.38212000  
N -4.37140100 0.00000000 -2.34375300

## H<sub>3</sub>C-C-OH

R No field

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49604800  
H 1.74095600 0.00000000 3.04098100  
C -2.71574500 -0.00000200 -0.82371500  
H -2.99165900 1.64616600 -2.05157800  
H -2.99165700 -1.64617300 -2.05157800  
H -4.12016800 -0.00000400 0.70189700

TS No field

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46633700  
H 1.91602800 0.00000000 1.37437600  
C -2.52258100 -0.00000800 -1.25841400  
H -4.04456900 -0.00000900 0.14856300  
H -2.66637400 1.65911200 -2.48732500

H -2.66636700 -1.65912900 -2.48732100

P No field

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28045800  
H 1.81044300 0.00000000 -1.06773900  
C -2.34201800 0.00000000 -1.61109400  
H -4.02882200 0.00000600 -0.42702000  
H -2.33877500 1.66284200 -2.84430000  
H -2.33878100 -1.66284100 -2.84430000

R EEF -5.14 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48743200  
H 1.74741000 0.00000000 3.03154100  
C -2.73645300 0.00000200 -0.81574400  
H -3.00613000 -1.65138500 -2.03748500  
H -4.13777400 0.00000000 0.72072100  
H -3.00613200 1.65138700 -2.03748500

TS EEF -5.14 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45592100  
H 1.93445300 0.00000000 1.37050600  
C -2.53464000 -0.00000600 -1.26093000  
H -4.05817100 -0.00001500 0.15111200  
H -2.66573400 1.66224700 -2.48659900  
H -2.66572600 -1.66224700 -2.48661200

P EEF -5.14 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27914500  
H 1.79923900 0.00000000 -1.07114400  
C -2.35747400 0.00000400 -1.60778300  
H -4.03737100 0.00000200 -0.40920700  
H -2.35018200 1.66412000 -2.83921800  
H -2.35018300 -1.66410300 -2.83923000

R EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48958100  
H 1.74564700 0.00000000 3.03390500  
C -2.73089700 -0.00000900 -0.81791700  
H -3.00202000 1.65005500 -2.04116800  
H -3.00201100 -1.65009800 -2.04113900  
H -4.13252100 -0.00000400 0.71597400

TS EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45858600  
H 1.92948300 0.00000000 1.37167500  
C -2.53130600 -0.00000200 -1.26040600  
H -4.05414800 -0.00000200 0.15036000  
H -2.66538600 1.66142900 -2.48691500  
H -2.66538200 -1.66143800 -2.48690900

P EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27953400  
H 1.80175300 0.00000000 -1.07016200  
C -2.35339800 0.00000400 -1.60851700  
H -4.03484100 0.00000000 -0.41359900  
H -2.34706300 1.66374000 -2.84044800  
H -2.34706300 -1.66372900 -2.84045600

R EEF -2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49173200  
H 1.74398400 0.00000000 3.03626400  
C -2.72560000 0.00000000 -0.81998800  
H -2.99821200 1.64877000 -2.04474900  
H -2.99821200 -1.64877300 -2.04474300  
H -4.12787000 0.00000200 0.71121200

TS EEF -2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46120900  
H 1.92476200 0.00000000 1.37270700  
C -2.52818100 0.00001100 -1.25983400  
H -4.05056500 0.00001300 0.14963600  
H -2.66534800 1.66066000 -2.48714900  
H -2.66535800 -1.66062600 -2.48716200

P EEF -2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27988400  
H 1.80445100 0.00000000 -1.06926800  
C -2.34946300 0.00000000 -1.60932200  
H -4.03258500 -0.00000200 -0.41805500  
H -2.34411500 1.66340000 -2.84171500  
H -2.34411400 -1.66339200 -2.84172000

R EEF 2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50043200  
H 1.73832800 0.00000000 3.04571200  
C -2.70686400 -0.00000200 -0.82667600  
H -2.98667000 1.64356700 -2.05770100  
H -2.98666600 -1.64357900 -2.05769300  
H -4.11426800 -0.00000200 0.69331600

TS EEF 2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47133800  
H 1.90819700 0.00000000 1.37555100  
C -2.51786800 0.00000400 -1.25646200  
H -4.03990300 0.00000800 0.14839300  
H -2.66902600 1.65768200 -2.48687700  
H -2.66903100 -1.65767400 -2.48687300

P EEF 2.52 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28087200  
H 1.81732200 0.00000000 -1.06651500  
C -2.33513000 0.00000200 -1.61302400  
H -4.02593700 0.00001100 -0.43583500  
H -2.33427600 1.66244800 -2.84689600  
H -2.33428700 -1.66245300 -2.84688700

R EEF 3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50266000  
H 1.73716700 0.00000000 3.04808800  
C -2.70277800 0.00000000 -0.82780400  
H -2.98482000 1.64227800 -2.06041500  
H -2.98481000 -1.64227100 -2.06042400  
H -4.11189300 -0.00000900 0.68943300

TS EEF 3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47379800  
H 1.90460500 0.00000000 1.37596300

C -2.51585000 0.00000200 -1.25523400  
H -4.03799500 -0.00000400 0.14877400  
H -2.67104200 1.65699200 -2.48635700  
H -2.67103800 -1.65698100 -2.48636800

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28101600  
H 1.82113400 0.00000000 -1.06600600  
C -2.33189100 0.00000200 -1.61402900  
H -4.02479100 0.00001500 -0.44012900  
H -2.33236700 1.66231500 -2.84817600  
H -2.33238000 -1.66231700 -2.84816400

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50492000  
H 1.73610900 0.00000000 3.05047500  
C -2.69893100 -0.00000200 -0.82866000  
H -2.98342300 1.64096700 -2.06287900  
H -2.98342100 -1.64097600 -2.06287100  
H -4.10985400 0.00000000 0.68590300

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47623600  
H 1.90122600 0.00000000 1.37626400  
C -2.51405900 -0.00000600 -1.25380900  
H -4.03633600 -0.00001300 0.14953800  
H -2.67355200 1.65630600 -2.48562200  
H -2.67354200 -1.65631500 -2.48562600

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28111800  
H 1.82521500 0.00000000 -1.06556000  
C -2.32878600 -0.00000200 -1.61505700  
H -4.02382400 -0.00001900 -0.44430900  
H -2.33072100 1.66223200 -2.84941900  
H -2.33070400 -1.66222300 -2.84944000

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49914300  
H 1.74086200 0.00000000 3.04284600  
C -2.69541900 0.31010400 -0.81473100  
H -3.07711800 -0.85175800 -2.48151800  
H -4.12306300 0.02067000 0.66187900  
H -2.82539300 2.27798300 -1.47090300

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46924000  
H 1.91608500 0.00000000 1.37370700  
C -2.48484000 0.44824500 -1.24668700  
H -2.46199100 2.40248000 -1.94194000  
H -2.73165900 -0.76545800 -2.90074400  
H -4.03982200 0.23769400 0.10762900

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28087800  
H 1.81099500 0.00000000 -1.06744800  
C -2.34005400 0.14252700 -1.60658300  
H -2.39849400 2.00217700 -2.51735100  
H -2.27833000 -1.26680700 -3.12151900

H -4.02868400 -0.08969200 -0.44744800

R EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49804700  
H 1.74088300 0.00000000 3.04208400  
C -2.70357900 0.24266000 -0.81667200  
H -3.06170700 -0.99568800 -2.43338600  
H -4.12224100 -0.02612000 0.67221600  
H -2.87417100 2.17692900 -1.55487700

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46809300  
H 1.91599200 0.00000000 1.37389400  
C -2.50083600 0.34306100 -1.25081200  
H -2.52977500 2.25653400 -2.04843200  
H -2.72263200 -0.96283300 -2.83738500  
H -4.04304000 0.15230800 0.12090700

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28069800  
H 1.81075100 0.00000000 -1.06757700  
C -2.34095400 0.10785400 -1.60842800  
H -2.38665500 1.92765700 -2.59613700  
H -2.29095000 -1.36418200 -3.06290100  
H -4.02865400 -0.07335900 -0.43918200

R EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49712300  
H 1.74090900 0.00000000 3.04150800  
C -2.70981900 0.17209400 -0.81917000  
H -3.04293100 -1.16177400 -2.36461100  
H -4.12117500 -0.05480200 0.68332700  
H -2.91810300 2.05654800 -1.66527500

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46718400  
H 1.91597900 0.00000000 1.37410200  
C -2.51264300 0.23422000 -1.25445600  
H -2.58706300 2.08927600 -2.17487500  
H -2.70922600 -1.17730900 -2.75227000  
H -4.04430500 0.08356400 0.13391700

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28056600  
H 1.81058100 0.00000000 -1.06766700  
C -2.34153000 0.07239700 -1.60990000  
H -2.37136000 1.84511200 -2.67966100  
H -2.30615500 -1.46508800 -2.99552100  
H -4.02874700 -0.05053300 -0.43262700

R EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49712300  
H 1.74090900 0.00000000 3.04150800  
C -2.70981900 -0.17209400 -0.81917000  
H -3.04293100 1.16177400 -2.36461100  
H -2.91810300 -2.05654800 -1.66527600  
H -4.12117500 0.05480200 0.68332700

TS EEF 2.52 V/nm along Y direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46718400  
H 1.91597900 0.00000000 1.37410200  
C -2.51264300 -0.23422200 -1.25445700  
H -4.04430500 -0.08356600 0.13391700  
H -2.70922800 1.17730600 -2.75227200  
H -2.58706100 -2.08928000 -2.17487300

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28056600  
H 1.81058300 0.00000000 -1.06766400  
C -2.34153400 -0.07239500 -1.60989600  
H -4.02874300 0.05054600 -0.43261500  
H -2.30616000 1.46508400 -2.99552300  
H -2.37137500 -1.84511600 -2.67965000

R EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49804700  
H 1.74088300 0.00000000 3.04208400  
C -2.70357900 -0.24265800 -0.81667200  
H -3.06170700 0.99568800 -2.43338600  
H -2.87417300 -2.17692800 -1.55487500  
H -4.12224100 0.02612400 0.67221400

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46809300  
H 1.91599200 0.00000000 1.37389400  
C -2.50083600 -0.34306900 -1.25081200  
H -4.04304000 -0.15230600 0.12090500  
H -2.72262800 0.96281600 -2.83739300  
H -2.52977500 -2.25654700 -2.04841900

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28069800  
H 1.81075100 0.00000000 -1.06757700  
C -2.34095400 -0.10785600 -1.60842800  
H -4.02865400 0.07335500 -0.43918000  
H -2.29095200 1.36417900 -3.06290300  
H -2.38665500 -1.92766100 -2.59613500

R EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49914300  
H 1.74086200 0.00000000 3.04284600  
C -2.69541900 -0.31010400 -0.81473100  
H -3.07711600 0.85175700 -2.48151900  
H -2.82539300 -2.27798400 -1.47090300  
H -4.12306300 -0.02067000 0.66187900

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46924000  
H 1.91608500 0.00000000 1.37370700  
C -2.48484000 -0.44824500 -1.24668700  
H -4.03982200 -0.23769600 0.10762900  
H -2.73165900 0.76545800 -2.90074400  
H -2.46198900 -2.40248000 -1.94194000

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28087800  
H 1.81099500 0.00000000 -1.06744800

C -2.34005600 -0.14252500 -1.60658200  
H -4.02868400 0.08969200 -0.44744400  
H -2.27833200 1.26681400 -3.12151300  
H -2.39849600 -2.00217100 -2.51735400

R EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47554400  
H 1.72139800 0.00000000 3.08806900  
C -2.74301800 -0.02198500 -0.79572100  
H -3.03867700 1.53934500 -2.12549900  
H -3.04606800 -1.76359500 -1.88088900  
H -4.11227400 0.08404400 0.75559800

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44472300  
H 1.93281300 0.00000000 1.31734800  
C -2.55056200 -0.00000400 -1.24412400  
H -4.03851300 0.00000000 0.19790400  
H -2.72005000 1.66905800 -2.45758000  
H -2.72004800 -1.66907700 -2.45756700

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26941100  
H 1.80697000 0.00000000 -1.08332900  
C -2.36481000 -0.00000200 -1.59892200  
H -4.02898500 0.00001100 -0.38311000  
H -2.38027000 1.67146500 -2.82277400  
H -2.38028300 -1.67149700 -2.82274200

R EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48032700  
H 1.72654100 0.00000000 3.07585900  
C -2.73639400 -0.00000200 -0.80268400  
H -3.02965500 1.65353200 -2.01768200  
H -3.02965400 -1.65354900 -2.01766700  
H -4.11455000 0.00000400 0.74486000

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44982900  
H 1.92866500 0.00000000 1.33140100  
C -2.54383500 0.00001100 -1.24713100  
H -4.03985600 -0.00000900 0.18667300  
H -2.70731500 1.66679000 -2.46394700  
H -2.70731000 -1.66673500 -2.46399600

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27206400  
H 1.80783400 0.00000000 -1.07927200  
C -2.35933700 -0.00000200 -1.60159800  
H -4.02897000 0.00000900 -0.39340500  
H -2.37039200 1.66944700 -2.82742800  
H -2.37040200 -1.66945300 -2.82742100

R EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48535200  
H 1.73150200 0.00000000 3.06396200  
C -2.72965000 0.00000400 -0.80939800  
H -3.01734200 1.65120000 -2.02836900  
H -3.01734800 -1.65120000 -2.02835700

H -4.11631600 0.00001100 0.73108200

TS EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45512400  
H 1.92448700 0.00000000 1.34558600  
C -2.53693600 0.00000800 -1.25051700  
H -4.04131900 0.00000200 0.17471300  
H -2.69413100 1.66435200 -2.47105400  
H -2.69413300 -1.66432400 -2.47107300

P EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27478700  
H 1.80869700 0.00000000 -1.07533000  
C -2.35371200 -0.00000200 -1.60452900  
H -4.02894700 0.00000000 -0.40417700  
H -2.36017400 1.66732900 -2.83258300  
H -2.36017400 -1.66733800 -2.83257800

R EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50771700  
H 1.74985900 0.00000000 3.01892400  
C -2.70122500 0.00000200 -0.83926200  
H -2.96442200 1.64064600 -2.07732000  
H -2.96442400 -1.64064200 -2.07732000  
H -4.12440100 0.00000400 0.67039000

TS EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47849200  
H 1.90740500 0.00000000 1.40384800  
C -2.50743300 -0.00000800 -1.26777600  
H -4.04821300 -0.00000900 0.11932300  
H -2.63662600 1.65335800 -2.50635000  
H -2.63661900 -1.65337700 -2.50634700

P EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28645600  
H 1.81223900 0.00000000 -1.06048800  
C -2.32968200 0.00000200 -1.61860600  
H -4.02854600 0.00000200 -0.45169000  
H -2.31602500 1.65799200 -2.85791500  
H -2.31603000 -1.65799000 -2.85791300

R EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51396400

H 1.75412600 0.00000000 3.00818800  
C -2.69370400 -0.00000200 -0.84751800  
H -2.95016200 1.63767100 -2.09119100  
H -2.95016800 -1.63768600 -2.09117400  
H -4.12664800 0.00000900 0.65368900

TS EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48496800  
H 1.90301200 0.00000000 1.41890300  
C -2.49954000 -0.00000600 -1.27299800  
H -4.05017200 -0.00000400 0.10348700  
H -2.62094900 1.65026400 -2.51691400  
H -2.62094500 -1.65028300 -2.51690500

P EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28958600  
H 1.81316500 0.00000000 -1.05697000  
C -2.32324900 -0.00000400 -1.62272000  
H -4.02834200 0.00000000 -0.46475600  
H -2.30409900 1.65541800 -2.86544600  
H -2.30410200 -1.65542300 -2.86544800

R EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.52052500  
H 1.75827900 0.00000000 2.99761700  
C -2.68598800 0.00000000 -0.85612000  
H -2.93543600 1.63456800 -2.10574300  
H -2.93543700 -1.63458000 -2.10573000  
H -4.12897400 0.00000400 0.63629700

TS EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49174300  
H 1.89855200 0.00000000 1.43421200  
C -2.49141800 0.00000800 -1.27857600  
H -4.05222100 0.00001100 0.08679500  
H -2.60469600 1.64702900 -2.52817900  
H -2.60470300 -1.64701400 -2.52817900

P EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.29281100  
H 1.81411300 0.00000000 -1.05351000  
C -2.31663500 0.00000000 -1.62707000  
H -4.02807600 -0.00000200 -0.47830700  
H -2.29180400 1.65275300 -2.87346000  
H -2.29180600 -1.65274900 -2.87346400

## Hydroxycarbenes using M06-2X

### H-C-OH

R No field

C 0.01131600 0.00000000 0.00419100  
O -0.00520200 0.00000000 2.48066000  
H 1.72952900 0.00000000 3.06848600  
H -2.06076200 0.00000000 -0.42882600

TS No field

C 0.01068100 0.00000000 0.00315200  
O 0.00396300 0.00000000 2.44842100

H 1.92613200 0.00000000 1.35870000  
H -1.90688700 0.00000000 -0.86838200

P No field

C -0.00006600 0.00000000 0.00860000  
O 0.00010800 0.00000000 2.27909000  
H 1.77215200 0.00000000 -1.10311900  
H -1.77245400 0.00000000 -1.10284500

R EEF -5.14 V/nm along X direction  
C 0.01720600 0.00000000 0.00318800  
O -0.00487400 0.00000000 2.47708800  
H 1.73188600 0.00000000 3.07404100  
H -2.06934000 0.00000000 -0.42980700

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43773300  
H 1.93994100 0.00000000 1.34667600  
H -1.93530700 0.00000000 -0.86168700

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27012700  
H 1.76312300 0.00000000 -1.11510300  
H -1.78424200 0.00000000 -1.10904700

R EEF -3.85 V/nm along X direction  
C 0.01557100 0.00000000 0.00345600  
O -0.00500000 0.00000000 2.47802700  
H 1.73121300 0.00000000 3.07249000  
H -2.06690400 0.00000000 -0.42946300

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43972400  
H 1.93438500 0.00000000 1.34779300  
H -1.93091000 0.00000000 -0.86295900

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27028600  
H 1.76519800 0.00000000 -1.11410200  
H -1.78095600 0.00000000 -1.10961700

R EEF -2.52 V/nm along X direction  
C 0.01404800 0.00000000 0.00371500  
O -0.00509500 0.00000000 2.47893400  
H 1.73059700 0.00000000 3.07105000  
H -2.06467000 0.00000000 -0.42918900

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44164100  
H 1.92907900 0.00000000 1.34876200  
H -1.92691100 0.00000000 -0.86412500

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27039900  
H 1.76741400 0.00000000 -1.11318500  
H -1.77788000 0.00000000 -1.11022400

R EEF 2.52 V/nm along X direction  
C 0.00897100 0.00000000 0.00460000  
O -0.00521800 0.00000000 2.48226400  
H 1.72866900 0.00000000 3.06632800  
H -2.05754200 0.00000000 -0.42868300

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44868000  
H 1.91013400 0.00000000 1.35136300  
H -1.91448400 0.00000000 -0.86776400

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27039900  
H 1.77787800 0.00000000 -1.11022800  
H -1.76741400 0.00000000 -1.11318300

R EEF 3.85 V/nm along X direction  
C 0.00793300 0.00000000 0.00477500  
O -0.00519700 0.00000000 2.48302200  
H 1.72831600 0.00000000 3.06539600  
H -2.05617200 0.00000000 -0.42868100

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45030300  
H 1.90592000 0.00000000 1.35173300  
H -1.91218100 0.00000000 -0.86843900

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27028600  
H 1.78095600 0.00000000 -1.10961900  
H -1.76520000 0.00000000 -1.11410000

R EEF 5.14 V/nm along X direction  
C 0.00698100 0.00000000 0.00492800  
O -0.00515900 0.00000000 2.48374700  
H 1.72801200 0.00000000 3.06456100  
H -2.05495300 0.00000000 -0.42872400

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45187300  
H 1.90190200 0.00000000 1.35200500  
H -1.91016800 0.00000000 -0.86903100

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27012700  
H 1.78424200 0.00000000 -1.10905000  
H -1.76312300 0.00000000 -1.11510100

R EEF -5.14 V/nm along Y direction  
C 0.01117000 -0.02062600 0.00352400  
O -0.00467000 -0.03116300 2.48043500  
H 1.72899000 0.02795100 3.06887100  
H -2.06061300 0.02383700 -0.42832000

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44619700  
H 1.91963000 0.00000000 1.35079900  
H -1.90683300 0.22731000 -0.86392600

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27061800  
H 1.77262100 0.00000000 -1.11133900  
H -1.77202500 0.03717800 -1.11137900

R EEF -3.85 V/nm along Y direction  
C 0.01123600 -0.01537900 0.00381700  
O -0.00490200 -0.02338000 2.48053300  
H 1.72922700 0.02093400 3.06870300  
H -2.06067900 0.01782400 -0.42854300

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44578800  
H 1.91942600 0.00000000 1.35059200  
H -1.91269300 0.16956000 -0.86497300

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27056200  
H 1.77248100 0.00000000 -1.11144700  
H -1.77214800 0.02779000 -1.11146700

R EEF -2.52 V/nm along Y direction  
C 0.01128000 -0.01020500 0.00402500  
O -0.00506800 -0.01559600 2.48060300  
H 1.72939500 0.01394100 3.06858200  
H -2.06072600 0.01185800 -0.42870000

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44550300  
H 1.91928200 0.00000000 1.35043300  
H -1.91680700 0.11241200 -0.86565200

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27052200  
H 1.77238200 0.00000000 -1.11152200  
H -1.77223500 0.01848300 -1.11153200

R EEF 2.52 V/nm along Y direction  
C 0.01128000 0.01020500 0.00402500  
O -0.00506800 0.01559600 2.48060300  
H 1.72939500 -0.01394100 3.06858200  
H -2.06072600 -0.01185800 -0.42870000

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44550300  
H 1.91928200 0.00000000 1.35043300  
H -1.91680700 -0.11241200 -0.86565200

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27052200  
H 1.77238200 0.00000000 -1.11152200  
H -1.77223500 -0.01848300 -1.11153200

R EEF 3.85 V/nm along Y direction  
C 0.01123600 0.01537900 0.00381700  
O -0.00490200 0.02338000 2.48053300  
H 1.72922700 -0.02093400 3.06870300  
H -2.06067900 -0.01782400 -0.42854300

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44578800  
H 1.91942600 0.00000000 1.35059200  
H -1.91269300 -0.16956000 -0.86497300

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27056200  
H 1.77248100 0.00000000 -1.11144700  
H -1.77214800 -0.02779000 -1.11146700

R EEF 5.14 V/nm along Y direction  
C 0.01117000 0.02062600 0.00352400  
O -0.00467000 0.03116300 2.48043500  
H 1.72899000 -0.02795100 3.06887100  
H -2.06061300 -0.02383700 -0.42832000

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44619700  
H 1.91963000 0.00000000 1.35079900  
H -1.90683300 -0.22731000 -0.86392600

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27061800  
H 1.77262100 0.00000000 -1.11133900  
H -1.77202500 -0.03717800 -1.11137900

R EEF -5.14 V/nm along Z direction  
C 0.01280500 0.00000000 -0.00468800  
O 0.00627800 0.00000000 2.45339800  
H 1.72595200 0.00000000 3.09367000  
H -2.07015400 0.00000000 -0.41787200

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42602000  
H 1.93477800 0.00000000 1.29434000  
H -1.92572400 0.00000000 -0.87442600

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26088600  
H 1.77495200 0.00000000 -1.11784500  
H -1.77495600 0.00000000 -1.11784000

R EEF -3.85 V/nm along Z direction  
C 0.01245000 0.00000000 -0.00233900  
O 0.00332000 0.00000000 2.46008800  
H 1.72682500 0.00000000 3.08729200  
H -2.06771600 0.00000000 -0.42053000

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43061200  
H 1.93089500 0.00000000 1.30821400  
H -1.92433300 0.00000000 -0.87189700

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26321600  
H 1.77432100 0.00000000 -1.11600700  
H -1.77432300 0.00000000 -1.11600300

R EEF -2.52 V/nm along Z direction  
C 0.01208300 0.00000000 -0.00007700  
O 0.00042500 0.00000000 2.46685500  
H 1.72771300 0.00000000 3.08097500  
H -2.06534100 0.00000000 -0.42324200

TS EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43534600  
H 1.92699800 0.00000000 1.32215500  
H -1.92291800 0.00000000 -0.86968400

P EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26559400  
H 1.77366900 0.00000000 -1.11435100  
H -1.77367100 0.00000000 -1.11434900

R EEF 2.52 V/nm along Z direction  
C 0.01051300 0.00000000 0.00812200  
O -0.01062000 0.00000000 2.49489700  
H 1.73139800 0.00000000 3.05614800  
H -2.05641000 0.00000000 -0.43465600

TS EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45589700  
H 1.91130400 0.00000000 1.37888300  
H -1.91707700 0.00000000 -0.86366200

P EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27558600  
H 1.77085900 0.00000000 -1.10951700  
H -1.77085900 0.00000000 -1.10951500

R EEF 3.85 V/nm along Z direction  
C 0.01010200 0.00000000 0.00996100  
O -0.01325600 0.00000000 2.50220200  
H 1.73235000 0.00000000 3.05001900  
H -2.05431600 0.00000000 -0.43767200

TS EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46149000  
H 1.90735000 0.00000000 1.39337100  
H -1.91559900 0.00000000 -0.86278300

P EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27821500  
H 1.77010900 0.00000000 -1.10874100  
H -1.77010900 0.00000000 -1.10873900

R EEF 5.14 V/nm along Z direction  
C 0.00968700 0.00000000 0.01171100  
O -0.01584700 0.00000000 2.50965200  
H 1.73331400 0.00000000 3.04390400  
H -2.05227400 0.00000000 -0.44075600

TS EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46728600  
H 1.90338000 0.00000000 1.40800100  
H -1.91411900 0.00000000 -0.86212900

P EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28090000  
H 1.76934200 0.00000000 -1.10813000  
H -1.76934200 0.00000000 -1.10813000

## HO-C-OH

R No field  
C -0.14716200 0.00117000 0.00946600  
O -0.03837500 -0.00049500 2.51252000  
H 1.73000900 -0.00034800 2.94744100  
O -2.59998300 0.00090500 -0.50101600  
H -2.74462600 0.00208400 -2.31632300

TS No field  
C -0.10598900 0.00067700 0.02837200  
O -0.07104200 -0.00086000 2.43739800  
H 1.89365400 0.00024400 1.17992100  
O -2.37428900 0.00103200 -1.03312100  
H -2.16124500 0.00222600 -2.84531300

P No field  
C -0.05227900 0.00002500 -0.00596600  
O -0.03358600 -0.00009800 2.24773200  
H 1.67705700 0.00006800 -1.17858700  
O -2.20555700 0.00012100 -1.35563000  
H -1.82681400 0.00021700 -3.13932600

R EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49179200  
H 1.75395200 0.00000000 3.00523800  
O -2.45168100 0.00009000 -0.63598900  
H -2.43053600 0.00001300 -2.45655600

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40036700  
H 1.99795700 0.00000000 1.19207200  
O -2.26785000 -0.00000400 -1.11787000

H -1.93840400 -0.00000400 -2.91326300

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25042100  
H 1.73715600 0.00000000 -1.15282000  
O -2.15271400 0.00000000 -1.39217700  
H -1.68488600 -0.00000200 -3.15570200

R EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49515000  
H 1.75224500 0.00000000 3.00809200  
O -2.44528400 0.00000200 -0.63161500  
H -2.44494600 0.00000200 -2.45234800

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40266100  
H 1.99372000 0.00000000 1.18939200  
O -2.26347100 -0.00000400 -1.11235700  
H -1.95559300 -0.00000400 -2.91134200

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25127300  
H 1.73746600 0.00000000 -1.15402000  
O -2.14968900 0.00000000 -1.38614500  
H -1.69971700 -0.00000200 -3.15400700

R EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49854000

H 1.75066000 0.00000000 3.01093200  
O -2.43926300 -0.00000800 -0.62697000  
H -2.46018600 -0.00000600 -2.44766100

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40490600  
H 1.98977800 0.00000000 1.18654600  
O -2.25952200 -0.00000400 -1.10654700  
H -1.97391800 -0.00000400 -2.90900200

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25211600  
H 1.73785700 0.00000000 -1.15535400  
O -2.14693000 0.00000000 -1.37998400  
H -1.71531300 -0.00000200 -3.15213200

R EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51256000  
H 1.74552900 0.00000000 3.02218000  
O -2.41857300 0.00000600 -0.60544000  
H -2.53050300 0.00000600 -2.42350900

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41350200  
H 1.97683200 0.00000000 1.17366000  
O -2.24755600 0.00000000 -1.08038700  
H -2.05863400 -0.00000200 -2.89508600

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25541500  
H 1.74031800 0.00000000 -1.16195700  
O -2.13846600 0.00000000 -1.35374900  
H -1.78659700 0.00000200 -3.14252300

R EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51621500  
H 1.74455800 0.00000000 3.02496300  
O -2.41415400 -0.00000800 -0.59929300  
H -2.55062500 -0.00000800 -2.41598000

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41557400  
H 1.97428100 0.00000000 1.17008700  
O -2.24545300 0.00002100 -1.07305300  
H -2.08299700 0.00002100 -2.89028800

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25623600  
H 1.74118700 0.00000000 -1.16390200  
O -2.13695400 0.00000000 -1.34674200  
H -1.80691900 0.00000000 -3.13950900

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51994100  
H 1.74371900 0.00000000 3.02773200  
O -2.40999300 0.00000000 -0.59287700  
H -2.57171600 0.00000000 -2.40784700

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41762200  
H 1.97199400 0.00000000 1.16636600  
O -2.24368800 0.00000600 -1.06535600  
H -2.10885200 0.00000000 -2.88486800

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25705400  
H 1.74219400 0.00000000 -1.16593300  
O -2.13565600 0.00000000 -1.33957100  
H -1.82827500 0.00000000 -3.13622900

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50607500  
H 1.74802000 0.00000000 3.01689800  
O -2.42596100 0.09987000 -0.61639100  
H -2.48973000 0.28660900 -2.42742000

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40997600  
H 1.98280900 0.00000000 1.18225700  
O -2.24900600 0.14369300 -1.09213000  
H -2.00894600 0.42645100 -2.87967500

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25369800  
H 1.74002500 0.00000000 -1.15661100  
O -2.14182400 -0.05162500 -1.37112300  
H -1.78265500 0.38089700 -3.10725700

R EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50579900  
H 1.74794400 0.00000000 3.01676000  
O -2.42699100 0.07461200 -0.61655000  
H -2.49139900 0.21450100 -2.43146400

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40967400  
H 1.98278100 0.00000000 1.18143800  
O -2.25061000 0.10859500 -1.09299200  
H -2.01090400 0.32002700 -2.88998800

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25373000  
H 1.73952000 0.00000000 -1.15741000  
O -2.14200700 -0.03940300 -1.36938900  
H -1.76836900 0.28795100 -3.12472400

R EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50560200  
H 1.74789200 0.00000000 3.01666200  
O -2.42770600 0.04971100 -0.61668600  
H -2.49252000 0.14223400 -2.43440100

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000

O 0.0000000 0.0000000 2.40945500  
H 1.98276000 0.00000000 1.18087700  
O -2.25175300 0.07316500 -1.09368900  
H -2.01217000 0.21387400 -2.89730100

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25375600  
H 1.73915900 0.00000000 -1.15798700  
O -2.14212100 -0.02633000 -1.36813000  
H -1.75745900 0.18878400 -3.13788200

R EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50560400  
H 1.74789200 0.00000000 3.01666200  
O -2.42770600 -0.04971100 -0.61668600  
H -2.49252000 -0.14223200 -2.43440100

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40945300  
H 1.98276000 0.00000000 1.18087700  
O -2.25175300 -0.07316500 -1.09368900  
H -2.01216800 -0.21387400 -2.89730100

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25375600  
H 1.73915900 0.00000000 -1.15798700  
O -2.14212100 0.02633100 -1.36813000  
H -1.75745900 -0.18878400 -3.13788200

R EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50579900  
H 1.74794400 0.00000000 3.01676000  
O -2.42699100 -0.07461400 -0.61655000  
H -2.49139900 -0.21450100 -2.43146400

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40967400  
H 1.98278100 0.00000000 1.18143800  
O -2.25061000 -0.10860100 -1.09299200  
H -2.01090200 -0.32003300 -2.88998800

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25373000  
H 1.73952000 0.00000000 -1.15741000  
O -2.14200700 0.03940300 -1.36938900  
H -1.76836900 -0.28795100 -3.12472400

R EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50607500  
H 1.74802000 0.00000000 3.01689800  
O -2.42596100 -0.09987000 -0.61639100  
H -2.48973000 -0.28660900 -2.42742000

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40997600  
H 1.98280900 0.00000000 1.18225700  
O -2.24900600 -0.14369500 -1.09213000

H -2.00894600 -0.42645300 -2.87967500

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25369800  
H 1.74002500 0.00000000 -1.15661100  
O -2.14182400 0.05162500 -1.37112300  
H -1.78265500 -0.38089900 -3.10725700

R EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47696900  
H 1.72505200 0.00000000 3.06836700  
O -2.44796500 -0.00000200 -0.62321900  
H -2.48700900 -0.00000600 -2.43859800

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.38468200  
H 1.99787400 0.00000000 1.12997500  
O -2.26475100 0.00000000 -1.12899100  
H -1.96893300 -0.00000400 -2.92468500

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.23976300  
H 1.74254500 0.00000000 -1.16270200  
O -2.14110000 0.00000000 -1.40951700  
H -1.67901100 0.00000600 -3.17000700

R EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48375900  
H 1.73116700 0.00000000 3.05464100  
O -2.44305800 -0.00000200 -0.62115100  
H -2.48931500 0.00000400 -2.43751500

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.39057400  
H 1.99418300 0.00000000 1.14227600  
O -2.26201800 0.00000000 -1.11927400  
H -1.98178300 0.00000400 -2.91847700

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.24316100  
H 1.74152900 0.00000000 -1.16158900  
O -2.14172400 -0.00000400 -1.39814500  
H -1.69786700 0.00000000 -3.16400000

R EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49075600  
H 1.73699700 0.00000000 3.04144000  
O -2.43814300 0.00001100 -0.61940500  
H -2.49112100 0.00000900 -2.43684800

TS EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.39662900  
H 1.99043200 0.00000000 1.15478400  
O -2.25911000 0.00000200 -1.11024300  
H -1.99351800 0.00000400 -2.91280200

P EEF -2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.24662600  
H 1.74058400 0.00000000 -1.16049600  
O -2.14210900 0.00000000 -1.38731800  
H -1.71579600 0.00000000 -3.15828900

R EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.52118700  
H 1.75774600 0.00000000 2.99363500  
O -2.41831800 0.00000800 -0.61540100  
H -2.49380600 0.00000600 -2.43822200

TS EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42270900  
H 1.97482300 0.00000000 1.20677000  
O -2.24591200 -0.00000600 -1.08019100  
H -2.03050800 -0.00000400 -2.89525600

P EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26123400  
H 1.73746400 0.00000000 -1.15645600  
O -2.14143300 0.00000000 -1.34902300  
H -1.77906800 0.00000000 -3.13852500

R EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.52951300  
H 1.76238200 0.00000000 2.98281100  
O -2.41328500 -0.00000800 -0.61511600  
H -2.49339600 -0.00000400 -2.43956900

## NC-C-OH

R No field

C -0.19980300 0.00000000 0.12264700  
O 0.06596800 0.00000000 2.57009800  
H 1.85966300 0.00000000 2.94470100  
C -2.90555300 0.00000000 -0.43939400  
N -4.92988200 0.00000000 -1.28116300

TS No field

C -0.15097800 0.00000000 0.08454100  
O 0.06222500 0.00000000 2.50077800  
H 1.90667200 0.00000000 1.19462300  
C -2.66084500 0.00000000 -1.05292600  
N -4.50631100 0.00000000 -2.23117800

P No field

C -0.03926100 0.00000000 -0.00082800  
O -0.02978200 0.00000000 2.26540600  
H 1.68770200 0.00000000 -1.16083700  
C -2.41735000 0.00000000 -1.46739000  
N -4.24427700 0.00000000 -2.66305000

R EEF -5.14 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45490500  
H 1.75118000 0.00000000 3.02290000  
C -2.68646200 0.00000000 -0.78319200  
N -4.66209800 0.00000000 -1.73448400

TS EEF -5.14 V/nm along X direction

TS EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42975600  
H 1.97075500 0.00000000 1.22023800  
O -2.24225900 -0.00000600 -1.07404500  
H -2.03752600 -0.00000400 -2.89212100

P EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26508900  
H 1.73684200 0.00000000 -1.15552600  
O -2.14075100 0.00000000 -1.34061000  
H -1.79292400 0.00000000 -3.13437800

R EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.53818300  
H 1.76683600 0.00000000 2.97235700  
O -2.40820400 -0.00000600 -0.61511400  
H -2.49256700 -0.00000200 -2.44132900

TS EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43704500  
H 1.96660900 0.00000000 1.23389000  
O -2.23847200 -0.00000400 -1.06839900  
H -2.04374000 -0.00000200 -2.88948100

P EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26903300  
H 1.73628900 0.00000000 -1.15462500  
O -2.13987000 0.00000000 -1.33263900  
H -1.80601800 0.00000000 -3.13056700

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.41548100  
H 1.97895200 0.00000000 1.27139100  
C -2.47851300 0.00000000 -1.27366100  
N -4.32663700 0.00000000 -2.44722700

P EEF -5.14 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26399100  
H 1.70784600 0.00000000 -1.18061600  
C -2.45402600 0.00000200 -1.38898500  
N -4.39476800 -0.00001700 -2.39082000

R EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45658100  
H 1.74887600 0.00000000 3.02417500  
C -2.67094800 0.00000200 -0.80139500  
N -4.63266700 0.00000400 -1.78054400

TS EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41814000  
H 1.97166700 0.00000000 1.27558600  
C -2.45749200 0.00000000 -1.29504900  
N -4.27700400 0.00000000 -2.51240500

P EEF -3.85 V/nm along X direction

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.26466800  
H 1.71379100 0.00000000 -1.17335400  
C -2.43302300 0.00000400 -1.41134300  
N -4.34569700 -0.00001700 -2.46512800

R EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45828700  
H 1.74671200 0.00000000 3.02540500  
C -2.65627900 0.00000000 -0.81876400  
N -4.60425700 -0.00000400 -1.82467100

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42070800  
H 1.96478300 0.00000000 1.27952500  
C -2.43751900 0.00000000 -1.31544100  
N -4.22868300 0.00000000 -2.57418800

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26526300  
H 1.71976500 0.00000000 -1.16629200  
C -2.41229700 0.00000000 -1.43348100  
N -4.29561200 0.00000000 -2.53846800

R EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46567800  
H 1.73940100 0.00000000 3.03009600  
C -2.60502800 0.00000000 -0.87920300  
N -4.50195100 0.00000000 -1.97906000

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43039100  
H 1.94075000 0.00000000 1.29294400  
C -2.36669200 0.00000000 -1.38732600  
N -4.04839600 0.00000000 -2.79030300

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26703900  
H 1.74385100 0.00000000 -1.14026700  
C -2.33389400 0.00000000 -1.51632400  
N -4.09419300 0.00000000 -2.80839300

R EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46772100  
H 1.73789500 0.00000000 3.03128300  
C -2.59400500 0.00000000 -0.89166000  
N -4.48008700 0.00000000 -2.01058800

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43274200  
H 1.93552400 0.00000000 1.29568400  
C -2.35156900 0.00000000 -1.40208100  
N -4.00907600 0.00000000 -2.83411600

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26736600  
H 1.74995300 0.00000000 -1.13431400  
C -2.31564300 0.00000000 -1.53515600

N -4.04524200 0.00000000 -2.86836500

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46986400  
H 1.73651300 0.00000000 3.03249800  
C -2.58369500 0.00000000 -0.90292900  
N -4.46006300 0.00000000 -2.03879200

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43508900  
H 1.93058300 0.00000000 1.29816700  
C -2.33756000 0.00000000 -1.41537500  
N -3.97282200 0.00000000 -2.87338100

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26766100  
H 1.75608900 0.00000000 -1.12859600  
C -2.29807400 0.00000000 -1.55299300  
N -3.99788700 0.00000000 -2.92438800

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46071700  
H 1.74267200 0.00000000 3.02763500  
C -2.61317300 -0.34579400 -0.84455100  
N -4.46015600 -0.93823800 -1.86722000

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42428700  
H 1.95401500 0.00000000 1.28475300  
C -2.36135000 -0.52072600 -1.33550600  
N -3.99134100 -1.22317300 -2.61806400

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26533100  
H 1.72827800 0.00000000 -1.15752600  
C -2.36024600 -0.33633000 -1.46583100  
N -4.12934000 -0.85458000 -2.63624100

R EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46119700  
H 1.74272900 0.00000000 3.02766200  
C -2.62033900 -0.25633400 -0.84765600  
N -4.50016300 -0.69993000 -1.88537900

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42487900  
H 1.95315400 0.00000000 1.28558700  
C -2.37891700 -0.38621700 -1.34364700  
N -4.05528800 -0.91369200 -2.64986200

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26573300  
H 1.72981100 0.00000000 -1.15546200  
C -2.36565500 -0.24978000 -1.47054600  
N -4.15841800 -0.63693600 -2.65537800

R EEF -2.52 V/nm along Y direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46155300  
H 1.74276700 0.00000000 3.02770700  
C -2.62530900 -0.16942000 -0.84958900  
N -4.52828600 -0.46507500 -1.89750900

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42529400  
H 1.95256000 0.00000000 1.28619000  
C -2.39127900 -0.25169800 -1.34932900  
N -4.10095900 -0.59965600 -2.67228500

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26601900  
H 1.73090300 0.00000000 -1.15399200  
C -2.36925300 -0.16536600 -1.47388100  
N -4.17833500 -0.42269400 -2.66906200

R EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46155300  
H 1.74276700 0.00000000 3.02770700  
C -2.62530900 0.16942000 -0.84958900  
N -4.52828600 0.46507500 -1.89750900

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42529400  
H 1.95256000 0.00000000 1.28619000  
C -2.39127900 0.25169800 -1.34932900  
N -4.10095900 0.59965600 -2.67228500

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26601900  
H 1.73090300 0.00000000 -1.15399200  
C -2.36925300 0.16536600 -1.47388100  
N -4.17833500 0.42269400 -2.66906200

R EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46119700  
H 1.74272900 0.00000000 3.02766200  
C -2.62033900 0.25633400 -0.84765600  
N -4.50016300 0.69993000 -1.88537900

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42487900  
H 1.95315400 0.00000000 1.28558700  
C -2.37891700 0.38621700 -1.34364700  
N -4.05528800 0.91369200 -2.64986200

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26573300  
H 1.72981100 0.00000000 -1.15546200  
C -2.36565600 0.24978200 -1.47054400  
N -4.15842500 0.63694200 -2.65536500

R EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46071500  
H 1.74267000 0.00000000 3.02763500

C -2.61317300 0.34579400 -0.84454900  
N -4.46015800 0.93823600 -1.86721800

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.42428700  
H 1.95401500 0.00000000 1.28475300  
C -2.36135000 0.52072600 -1.33550600  
N -3.99134100 1.22317300 -2.61806400

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26533100  
H 1.72827800 0.00000000 -1.15752600  
C -2.36024600 0.33632800 -1.46582700  
N -4.12934200 0.85458400 -2.63623500

R EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43701800  
H 1.72376500 0.00000000 3.06927500  
C -2.59145800 0.00000000 -0.97405000  
N -4.35057800 0.00000000 -2.28631600

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40200500  
H 1.96933700 0.00000000 1.24057000  
C -2.33554400 0.00000000 -1.49174500  
N -3.83656700 0.00000000 -3.08858500

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25480300  
H 1.74478300 0.00000000 -1.14074700  
C -2.31556000 0.00000200 -1.59075700  
N -3.94410400 0.00000600 -3.04602400

R EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44311800  
H 1.72880500 0.00000000 3.05831700  
C -2.60196500 -0.00000400 -0.94128600  
N -4.40603200 -0.00000600 -2.18976100

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.40784800  
H 1.96492100 0.00000000 1.25201400  
C -2.35317100 0.00000000 -1.45540000  
N -3.91835400 0.00000000 -2.98840100

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.25765100  
H 1.74160600 0.00000000 -1.14354700  
C -2.33062700 -0.00000200 -1.56076100  
N -4.01287800 -0.00000200 -2.95317400

R EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44928100  
H 1.73364700 0.00000000 3.04776300  
C -2.61168200 0.00000000 -0.90995800  
N -4.45764300 0.00000000 -2.09447900

TS EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.41372900  
H 1.96058400 0.00000000 1.26351500  
C -2.36986300 0.00000000 -1.42016900  
N -3.99563900 0.00000000 -2.88790900

P EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26050800  
H 1.73834700 0.00000000 -1.14652400  
C -2.34521300 0.00000000 -1.53146300  
N -4.07817200 0.00000000 -2.85993900

R EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47477900  
H 1.75132500 0.00000000 3.00905600  
C -2.64438600 0.00000000 -0.79693600  
N -4.62937900 0.00000000 -1.72611600

TS EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43779900  
H 1.94383500 0.00000000 1.31021200  
C -2.42603100 0.00000000 -1.29326900  
N -4.25236900 0.00000000 -2.50027900

P EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27208500  
H 1.72519200 0.00000000 -1.15953500  
C -2.39580100 0.00000000 -1.42584800  
N -4.29197000 0.00000000 -2.50843900

R EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48144000

H 1.75539000 0.00000000 3.00014900  
C -2.65140200 0.00000000 -0.77119800  
N -4.66473200 0.00000000 -1.63664000

TS EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44402000  
H 1.93975600 0.00000000 1.32207700  
C -2.43739600 0.00000000 -1.26531800  
N -4.30340100 0.00000000 -2.40991600

P EEF 3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27504400  
H 1.72192700 0.00000000 -1.16303200  
C -2.40657900 0.00000000 -1.40231700  
N -4.33458600 0.00000000 -2.42730500

R EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48822200  
H 1.75933200 0.00000000 2.99149200  
C -2.65791000 0.00000000 -0.74667800  
N -4.69676500 0.00000000 -1.54958400

TS EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45035200  
H 1.93569800 0.00000000 1.33403900  
C -2.44765700 0.00000000 -1.23902600  
N -4.34917600 0.00000000 -2.32359300

P EEF 5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27803900  
H 1.71871000 0.00000000 -1.16658500  
C -2.41655100 0.00000000 -1.38007300  
N -4.37297400 0.00000000 -2.34997000

## H<sub>3</sub>C-C-OH

R No field  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49118500  
H 1.74063700 0.00000000 3.05061600  
C -2.72304000 0.00000600 -0.80821200  
H -3.00757600 1.64616200 -2.03149600  
H -3.00758200 -1.64613500 -2.03151700  
H -4.10801700 -0.00000200 0.73173800

TS No field  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45673900  
H 1.92151400 0.00000000 1.36686800  
C -2.53138900 0.00000900 -1.24510500  
H -4.03016400 0.00000900 0.18403300  
H -2.68709500 1.65983200 -2.46872400  
H -2.68709900 -1.65980600 -2.46873400

P No field  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27708900  
H 1.80972000 0.00000000 -1.06474400  
C -2.35213400 0.00000200 -1.59789800  
H -4.02232700 -0.00000400 -0.39291000  
H -2.36001800 1.66307500 -2.82782700

H -2.36001200 -1.66306500 -2.82783600

R EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48268700  
H 1.74792000 0.00000000 3.04020000  
C -2.74434100 0.00000800 -0.79886100  
H -3.02386500 -1.65109000 -2.01591200  
H -4.12458800 -0.00000200 0.75241200  
H -3.02386200 1.65113000 -2.01587900

TS EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44659500  
H 1.94141700 0.00000000 1.36180300  
C -2.54445700 -0.00000200 -1.24523900  
H -4.04238500 -0.00001300 0.19053400  
H -2.68936100 1.66277600 -2.46559300  
H -2.68935300 -1.66276300 -2.46561400

P EEF -5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27582300  
H 1.79839400 0.00000000 -1.06947400  
C -2.36857800 0.00000400 -1.59225400

H -4.03024900 -0.00000800 -0.37152800  
H -2.37412400 1.66420900 -2.82050200  
H -2.37411700 -1.66418800 -2.82052300

R EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48481100  
H 1.74594300 0.00000000 3.04280800  
C -2.73860700 0.00000200 -0.80141000  
H -3.01923900 1.64986800 -2.01998000  
H -3.01924300 -1.64986400 -2.01997800  
H -4.11960600 0.00000600 0.74715100

TS EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44919600  
H 1.93606100 0.00000000 1.36326200  
C -2.54084700 0.00000200 -1.24532800  
H -4.03871700 -0.00000900 0.18876100  
H -2.68825000 1.66200900 -2.46651900  
H -2.68824400 -1.66199200 -2.46653800

P EEF -3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27619900  
H 1.80094200 0.00000000 -1.06817200  
C -2.36423700 0.00000400 -1.59359300  
H -4.02787000 0.00000000 -0.37684200  
H -2.37029600 1.66386700 -2.82231700  
H -2.37029600 -1.66384800 -2.82233000

R EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48693200  
H 1.74407100 0.00000000 3.04541200  
C -2.73315400 0.00000200 -0.80383500  
H -3.01497800 1.64863000 -2.02395400  
H -3.01498000 -1.64861900 -2.02396400  
H -4.11521700 -0.00000200 0.74191800

TS EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45174900  
H 1.93096400 0.00000000 1.36458900  
C -2.53746500 0.00000900 -1.24535300  
H -4.03548300 0.00000200 0.18704700  
H -2.68748300 1.66127000 -2.46736500  
H -2.68748500 -1.66123600 -2.46738600

P EEF -2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27653500  
H 1.80366900 0.00000000 -1.06695700  
C -2.36005200 0.00000800 -1.59498400  
H -4.02577200 0.00000400 -0.38219700  
H -2.36665800 1.66356200 -2.82414800  
H -2.36666200 -1.66354500 -2.82415300

R EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49549400  
H 1.73761500 0.00000000 3.05583400  
C -2.71394400 -0.00000400 -0.81178500  
H -3.00180500 1.64367100 -2.03830900  
H -3.00180500 -1.64368100 -2.03830700  
H -4.10261600 -0.00000200 0.72232200

TS EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46159000  
H 1.91300100 0.00000000 1.36868400  
C -2.52622800 0.00000900 -1.24432300  
H -4.02614800 0.00000400 0.18192800  
H -2.68838800 1.65848100 -2.46945500  
H -2.68839200 -1.65844900 -2.46947200

P EEF 2.52 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27748600  
H 1.81663400 0.00000000 -1.06279800  
C -2.34480700 -0.00000600 -1.60092900  
H -4.01978900 -0.00000400 -0.40345500  
H -2.35426000 1.66274200 -2.83148000  
H -2.35426000 -1.66275700 -2.83147600

R EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49768000  
H 1.73626200 0.00000000 3.05845300  
C -2.70976600 0.00000200 -0.81321000  
H -2.99957700 1.64243700 -2.04136400  
H -2.99957500 -1.64244300 -2.04135500  
H -4.10049200 0.00000400 0.71802800

TS EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46397100  
H 1.90908300 0.00000000 1.36942800  
C -2.52399700 0.00000800 -1.24367500  
H -4.02456500 0.00001300 0.18134200  
H -2.68973000 1.65782300 -2.46954000  
H -2.68973700 -1.65781000 -2.46953700

P EEF 3.85 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27762500  
H 1.82045100 0.00000000 -1.06190900  
C -2.34136800 -0.00000800 -1.60246200  
H -4.01882000 -0.00001100 -0.40857400  
H -2.35176700 1.66264400 -2.83326400  
H -2.35175800 -1.66266300 -2.83325800

R EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49989500  
H 1.73501500 0.00000000 3.06108200  
C -2.70582800 0.00000600 -0.81436500  
H -2.99780200 1.64120900 -2.04414600  
H -2.99780800 -1.64119000 -2.04415700  
H -4.09871000 0.00000200 0.71407100

TS EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46632800  
H 1.90538300 0.00000000 1.37007300  
C -2.52199200 0.00000400 -1.24283700  
H -4.02322300 0.00000200 0.18112300  
H -2.69156800 1.65719400 -2.46939100  
H -2.69156800 -1.65718100 -2.46939700

P EEF 5.14 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.27772600  
H 1.82452800 0.00000000 -1.06107000  
C -2.33808000 -0.00000200 -1.60400000  
H -4.01803700 -0.00000400 -0.41356100  
H -2.34953500 1.66259900 -2.83500600  
H -2.34953100 -1.66260200 -2.83500600

R EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49429800  
H 1.74050800 0.00000000 3.05257000  
C -2.70335300 0.30445400 -0.79854000  
H -3.09356800 -0.84746100 -2.46767900  
H -4.11107200 -0.00045900 0.69060800  
H -2.84258400 2.27648200 -1.43702800

TS EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45976500  
H 1.92183100 0.00000000 1.36654100  
C -2.48863000 0.47634000 -1.23298400  
H -2.44772700 2.42461400 -1.93976700  
H -2.76963300 -0.74757200 -2.87167200  
H -4.02206400 0.29131100 0.14665600

P EEF -5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27745900  
H 1.81031100 0.00000000 -1.06438300  
C -2.34966000 0.13837700 -1.59457400  
H -2.40406000 1.98312700 -2.53182600  
H -2.31046300 -1.29665700 -3.08339700  
H -4.02292200 -0.06803000 -0.41124200

R EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49325700  
H 1.74053700 0.00000000 3.05180100  
C -2.71096100 0.24188700 -0.80034700  
H -3.07872000 -0.97809400 -2.42614900  
H -4.11016000 -0.04655500 0.69982400  
H -2.88867600 2.18477000 -1.51101600

TS EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45855200  
H 1.92163500 0.00000000 1.36659900  
C -2.50663800 0.36446000 -1.23747400  
H -2.52374900 2.27218900 -2.04524000  
H -2.75852900 -0.95174600 -2.80859900  
H -4.02695700 0.19568700 0.15865600

P EEF -3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27730000  
H 1.81005000 0.00000000 -1.06454000  
C -2.35079400 0.10460000 -1.59590300  
H -2.39771200 1.91321600 -2.60048200  
H -2.31991200 -1.38475200 -3.03052300  
H -4.02256000 -0.05931900 -0.40405600

R EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49231700  
H 1.74057500 0.00000000 3.05118900  
C -2.71710800 0.17242200 -0.80306400

H -3.05999100 -1.14449800 -2.35814700  
H -4.10893300 -0.07221200 0.71141400  
H -2.93271800 2.06628200 -1.62330900

TS EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45761100  
H 1.92153900 0.00000000 1.36670200  
C -2.51987500 0.24995200 -1.24123500  
H -2.58897300 2.10094500 -2.16667200  
H -2.74196000 -1.16860900 -2.72633900  
H -4.02931000 0.11518800 0.17028700

P EEF -2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27718300  
H 1.80985900 0.00000000 -1.06466300  
C -2.35157200 0.06988800 -1.59695300  
H -2.38719700 1.83517200 -2.67551500  
H -2.33212700 -1.47790200 -2.96857800  
H -4.02238600 -0.04306900 -0.39802900

R EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49231700  
H 1.74057500 0.00000000 3.05118900  
C -2.71710800 -0.17242200 -0.80306400  
H -3.05999100 1.14449800 -2.35814700  
H -2.93271800 -2.06628200 -1.62330900  
H -4.10893300 0.07221200 0.71141400

TS EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45761100  
H 1.92153900 0.00000000 1.36670200  
C -2.51987700 -0.24994700 -1.24123500  
H -4.02931000 -0.11518300 0.17029100  
H -2.74196200 1.16861700 -2.72633500  
H -2.58897700 -2.10093800 -2.16667200

P EEF 2.52 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27718500  
H 1.80986100 0.00000000 -1.06465700  
C -2.35157600 -0.06988800 -1.59695100  
H -4.02238200 0.04306500 -0.39802000  
H -2.33214000 1.47790600 -2.96857200  
H -2.38720700 -1.83516900 -2.67551900

R EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49325700  
H 1.74053700 0.00000000 3.05180100  
C -2.71096100 -0.24188700 -0.80034700  
H -3.07872000 0.97809600 -2.42614900  
H -2.88867600 -2.18476800 -1.51101800  
H -4.11016000 0.04655300 0.69982400

TS EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45855200  
H 1.92163500 0.00000000 1.36659900  
C -2.50663800 -0.36446000 -1.23747400  
H -4.02695700 -0.19568900 0.15865600  
H -2.75853100 0.95174400 -2.80859900  
H -2.52374900 -2.27219100 -2.04524000

P EEF 3.85 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27730000  
H 1.81005000 0.00000000 -1.06454000  
C -2.35079400 -0.10460000 -1.59590100  
H -4.02256000 0.05931700 -0.40405200  
H -2.31991400 1.38475400 -3.03051900  
H -2.39771000 -1.91321400 -2.60048200

R EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49429800  
H 1.74050800 0.00000000 3.05257000  
C -2.70335300 -0.30445400 -0.79854000  
H -3.09356800 0.84746100 -2.46767900  
H -2.84258400 -2.27648200 -1.43702800  
H -4.11107200 0.00045900 0.69060800

TS EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.45976500  
H 1.92183100 0.00000000 1.36654100  
C -2.48863000 -0.47634000 -1.23298400  
H -4.02206400 -0.29131300 0.14665600  
H -2.76963300 0.74757400 -2.87167200  
H -2.44772700 -2.42461400 -1.93976900

P EEF 5.14 V/nm along Y direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27745900  
H 1.81031100 0.00000000 -1.06438300  
C -2.34966000 -0.13838300 -1.59457200  
H -4.02292200 0.06802400 -0.41124200  
H -2.31046300 1.29664700 -3.08340100  
H -2.40405800 -1.98313400 -2.53182000

R EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47055900  
H 1.72061300 0.00000000 3.09826800  
C -2.74930100 -0.03752100 -0.78133400  
H -3.05385500 1.45940600 -2.17752700  
H -3.05887100 -1.82815200 -1.77959400  
H -4.10056600 0.13357500 0.77684800

TS EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.43518000  
H 1.93817400 0.00000000 1.31021900  
C -2.55782100 0.00001100 -1.23219500  
H -4.02409800 0.00000000 0.22955500  
H -2.73772100 1.66909000 -2.44079400  
H -2.73772500 -1.66904600 -2.44082400

P EEF -5.14 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26621100  
H 1.80605200 0.00000000 -1.07989200  
C -2.37446300 0.00000200 -1.58534300  
H -4.02213200 0.00000000 -0.34943900  
H -2.40077700 1.67105700 -2.80618200  
H -2.40077900 -1.67105000 -2.80618800

R EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.47530800  
H 1.72589100 0.00000000 3.08586700  
C -2.74294800 0.00000400 -0.78876400  
H -3.04339800 1.65303900 -1.99979800  
H -3.04339800 -1.65301600 -1.99982200  
H -4.10344000 -0.00000800 0.77120300

TS EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44027400  
H 1.93404500 0.00000000 1.32423000  
C -2.55150700 0.00001100 -1.23483400  
H -4.02544300 0.00000000 0.21929100  
H -2.72578900 1.66695800 -2.44669900  
H -2.72579300 -1.66691700 -2.44672800

P EEF -3.85 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.26882100  
H 1.80697200 0.00000000 -1.07594800  
C -2.36909800 0.00000000 -1.58812300  
H -4.02220800 0.00000600 -0.35966000  
H -2.39106200 1.66918300 -2.81088700  
H -2.39106800 -1.66918600 -2.81088200

R EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48038700  
H 1.73096900 0.00000000 3.07381500  
C -2.73644000 0.00000600 -0.79496500  
H -3.03179500 1.65086200 -2.00976200  
H -3.03180000 -1.65083700 -2.00977700  
H -4.10485700 0.00000200 0.75855100

TS EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.44555600  
H 1.92989300 0.00000000 1.33832900  
C -2.54499900 0.00000900 -1.23787300  
H -4.02690600 0.00000600 0.20828800  
H -2.71338100 1.66470600 -2.45333000  
H -2.71338500 -1.66467400 -2.45334700

P EEF -2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27150300  
H 1.80788800 0.00000000 -1.07211200  
C -2.36359300 -0.00000200 -1.59114200  
H -4.02227200 0.00000200 -0.37031300  
H -2.38103300 1.66722700 -2.81606500  
H -2.38103700 -1.66723600 -2.81605600

R EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50293800  
H 1.74970200 0.00000000 3.02858000  
C -2.70906300 -0.00000200 -0.82262100  
H -2.98188300 1.64095000 -2.05573600  
H -2.98187900 -1.64095800 -2.05573000  
H -4.11158100 -0.00000200 0.70277400

TS EEF 2.52 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46885300  
H 1.91301200 0.00000000 1.39599600  
C -2.51693700 0.00000000 -1.25383600

H -4.03381900 0.00000000 0.15670700  
H -2.65875100 1.65441400 -2.48696400  
H -2.65874900 -1.65441400 -2.48696200

P EEF 2.52 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28300200  
H 1.81157300 0.00000000 -1.05772400  
C -2.34004300 0.00000000 -1.60560100  
H -4.02223600 -0.00000200 -0.41727800  
H -2.33766200 1.65855700 -2.84149500  
H -2.33765800 -1.65855300 -2.84149900

R EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50921900  
H 1.75402600 0.00000000 3.01796600  
C -2.70183100 -0.00000600 -0.83028000  
H -2.96842500 1.63815100 -2.06882200  
H -2.96841700 -1.63816600 -2.06881600  
H -4.11350500 -0.00000600 0.68741600

TS EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47530200  
H 1.90870500 0.00000000 1.41082700  
C -2.50937200 0.00000400 -1.25875700  
H -4.03578400 -0.00000600 0.14183900  
H -2.64375100 1.65150800 -2.49714700  
H -2.64374700 -1.65148100 -2.49717200

P EEF 3.85 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.28609100  
H 1.81252000 0.00000000 -1.05432400  
C -2.33374300 0.00000000 -1.60980200  
H -4.02212100 -0.00000600 -0.43014300  
H -2.32596300 1.65615900 -2.84904300  
H -2.32595500 -1.65615500 -2.84904900

R EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51579900  
H 1.75821900 0.00000000 3.00759900  
C -2.69441800 -0.00000400 -0.83826600  
H -2.95450900 1.63521100 -2.08259800  
H -2.95450500 -1.63523400 -2.08258100  
H -4.11552100 0.00000000 0.67141800

TS EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48204500  
H 1.90435500 0.00000000 1.42585600  
C -2.50156800 0.00001300 -1.26405000  
H -4.03783400 -0.00000400 0.12612800  
H -2.62816400 1.64844800 -2.50806800  
H -2.62816200 -1.64839000 -2.50811000

P EEF 5.14 V/nm along Z direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28927400  
H 1.81348400 0.00000000 -1.05098700  
C -2.32726300 0.00000200 -1.61424100  
H -4.02194700 -0.00000900 -0.44349100  
H -2.31389300 1.65367000 -2.85707200  
H -2.31388000 -1.65365300 -2.85708900

## SN2 Reaction

R1 No field

N 0.00000000 0.00000000 1.02581745  
C 0.00000000 0.00000000 -1.19678671

R2 No field

C 0.00000000 0.00000000 -2.14707366  
H 0.00000000 1.95345792 -2.78708447  
H -1.69174397 -0.97672801 -2.78708447  
H 1.69174397 -0.97672801 -2.78708447  
Cl 0.00000000 0.00000000 1.24962914

TS No field

N -6.47553763 -0.00000769 0.00215658  
C -4.26176795 0.00000554 -0.00185153  
C -0.03094159 0.00000743 -0.00226727  
H -0.19173656 1.76059037 -1.01003404  
H -0.19341464 -0.00756282 2.02608242  
H -0.19173467 -1.75300527 -1.02314686  
Cl 4.08281430 -0.00000202 0.00075441

P1 No field

N 2.71496683 0.00000000 0.00010582  
C 0.52941832 -0.00000189 -0.00028535  
C -2.23331702 0.00000189 0.00006047  
H -2.92687135 1.69258679 0.95333697  
H -2.92763669 -0.02078889 -1.94206097  
H -2.92685812 -1.67179979 0.98934005

P2 No field

Cl 0.00000000 0.00000000 0.00000000

R1 EEF -0.51 V/nm along X direction

N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22260416

R2 EEF -0.51 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.39670091  
H 1.95376027 0.00000000 -0.63890910  
H -0.97516143 1.69249608 -0.64060040  
H -0.97515954 -1.69249608 -0.64060040

TS EEF -0.51 V/nm along X direction

C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 4.11722165  
H 2.02634468 0.00000000 -0.19785629  
H -1.01506868 1.75762741 -0.13964704  
H -1.01507246 -1.75762552 -0.13964893  
C -0.23639160 0.00000378 -4.21885872  
N -0.67495753 -0.00006425 -6.38889445

P1 EEF -0.51 V/nm along X direction

N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18555984  
C 0.03433067 0.00000000 4.94812133  
H 1.01687904 1.68173787 5.62740822  
H -1.89740295 -0.00051967 5.67057525  
H 1.01778044 -1.68121630 5.62739499

P2 EEF -0.51 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 0.00000000

R1 EEF 0.51 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22260416

R2 EEF 0.51 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.39669903  
H 1.95287966 0.00000000 -0.64178715  
H -0.97854026 1.69106367 -0.63913965  
H -0.97853837 -1.69106556 -0.63913776

TS EEF 0.51 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 4.11719141  
H 2.03033390 0.00000000 -0.12136771  
H -1.01305612 1.75649924 -0.17790267  
H -1.01305612 -1.75649924 -0.17790456  
C 0.23202067 0.00000378 -4.21929525  
N 0.66682792 0.00001512 -6.39008876

P1 EEF 0.51 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.1855417  
C -0.02796985 0.00000000 4.94814023  
H -0.99870743 -1.68575165 5.63382762  
H 1.90870540 0.00543296 5.65833927  
H -1.00813527 1.68031868 5.63374636

P2 EEF 0.51 V/nm along X direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF -1.03 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22261361

R2 EEF -1.03 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.39670658  
H 1.95423459 0.00000000 -0.63747291  
H -0.97349469 1.69320851 -0.64133551  
H -0.97349280 -1.69321040 -0.64133173

TS EEF -1.03 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 4.12623187  
H 2.02439259 0.00000000 -0.22673132  
H -1.01535214 1.75873668 -0.11565884  
H -1.01534836 -1.75873857 -0.11565695  
C -0.45084726 -0.00001134 -4.18660297  
N -1.26673873 0.00001512 -6.24507679

P1 EEF -1.03 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18559008  
C 0.06539400 0.00000000 4.94766779  
H 1.05893113 1.68069096 5.61378896  
H -1.85644501 -0.00001512 5.69562547  
H 1.05895759 -1.68067584 5.61378896

P2 EEF -1.03 V/nm along X direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF 1.03 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22261361

R2 EEF 1.03 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.39670469  
H 1.95247526 0.00000000 -0.64322712  
H -0.98025235 1.69034368 -0.63841021  
H -0.98025046 -1.69034746 -0.63840643

TS EEF 1.03 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 4.12603722  
H 2.03142616 0.00000000 -0.08077260  
H -1.01205646 1.75657294 -0.18911064  
H -1.01205646 -1.75657294 -0.18910875  
C 0.43535150 -0.00001134 -4.18912009  
N 1.22970764 -0.00005669 -6.25597484

P1 EEF 1.03 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18557307  
C -0.05897460 0.00000000 4.94767157  
H -1.03373729 -1.68689493 5.62453395  
H 1.87130960 0.00620019 5.67571153  
H -1.04450874 1.68070041 5.62433552

P2 EEF 1.03 V/nm along X direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF -1.54 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22261739

R2 EEF -1.54 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.39671603  
H 1.95473348 0.00000000 -0.63603671  
H -0.97184685 1.69391716 -0.64206872  
H -0.97184118 -1.69392283 -0.64206116

TS EEF -1.54 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 4.13997963  
H 2.02241405 0.00000000 -0.25332167  
H -1.01490617 1.76002547 -0.08859795  
H -1.01490050 -1.76002736 -0.08860173  
C -0.65344677 0.00005480 -4.13996451  
N -1.77752434 0.00011905 -6.04832410

P1 EEF -1.54 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18563732  
C 0.09586584 0.00000000 4.94694403  
H 1.09957160 1.67992751 5.60002230  
H -1.81595761 -0.00008693 5.71980264  
H 1.09972089 -1.67984058 5.60001663

P2 EEF -1.54 V/nm along X direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF 1.54 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22261739

R2 EEF 1.54 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.39671225  
H 1.95209353 0.00000000 -0.64466899  
H -0.98198145 1.68962181 -0.63768456  
H -0.98197579 -1.68962748 -0.63767700

TS EEF 1.54 V/nm along X direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 4.13909713  
H 2.03162269 0.00000000 -0.03806477  
H -1.01106057 1.75693388 -0.19744055  
H -1.01105868 -1.75693388 -0.19744244  
C 0.62331507 0.00000945 -4.14676186  
N 1.71272183 0.00004913 -6.07506751

P1 EEF 1.54 V/nm along X direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18560330  
C -0.08989431 0.00000000 4.94688356  
H -1.06874259 -1.68794184 5.61495114  
H 1.83387033 0.00680302 5.69268884  
H -1.08057606 1.68115205 5.61461666

P2 EEF 1.54 V/nm along X direction  
Cl 0.00000000 0.00000000 0.00000000

R1 EEF -0.51 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22272321

R2 EEF -0.51 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.39291012  
H 1.95292879 0.00000000 -0.64246367  
H -0.97665242 1.69145106 -0.64198368  
H -0.97664676 -1.69145484 -0.64198368

TS EEF -0.51 V/nm along Z direction  
N -0.00113951 0.00000189 0.01509892  
C 0.00031558 -0.00000189 2.22902734  
C 0.00764395 0.00000000 6.41785830  
H -1.00681058 -1.75877258 6.28416012  
H 2.03754131 0.00102234 6.27754419  
H -1.00857747 1.75774835 6.28416201  
Cl 0.01654645 0.00000189 10.55857490

P1 EEF -0.51 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18603416  
C 0.00310482 0.00000000 4.94886210  
H 0.97521056 1.68205912 5.64196290  
H -1.93802830 -0.00000945 5.64625258  
H 0.97522568 -1.68205156 5.64196290

P2 EEF -0.51 V/nm along Z direction  
Cl 0.00000000 0.00000000 0.00000000

R1 EEF 0.51 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22252101

R2 EEF 0.51 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.40059942  
H 1.95370358 0.00000000 -0.63821746

H -0.97704360 1.69212381 -0.63774314  
H -0.97703604 -1.69212759 -0.63774125

TS EEF 0.51 V/nm along Z direction  
N -0.00115462 0.00000378 -0.01626677  
C 0.00019653 -0.00000189 2.19742922  
C 0.00776300 0.00000000 6.47245440  
H -1.00495864 -1.75556572 6.28699282  
H 2.03385635 0.00101667 6.28045059  
H -1.00672743 1.75454527 6.28699282  
Cl 0.01654267 0.00000378 10.55837080

P1 EEF 0.51 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18508930  
C 0.00314828 0.00000000 4.94772449  
H 0.97546568 1.68251266 5.63938342  
H -1.93846860 -0.00006803 5.64372223  
H 0.97558284 -1.68244463 5.63938342

P2 EEF 0.51 V/nm along Z direction  
Cl 0.00000000 0.00000000 0.00000000

R1 EEF -1.03 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22285927

R2 EEF -1.03 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.38931019  
H 1.95257352 0.00000000 -0.64452537  
H -0.97647479 1.69114304 -0.64404538  
H -0.97647290 -1.69114493 -0.64404538

TS EEF -1.03 V/nm along Z direction  
N -0.00120187 0.00000378 0.03003154  
C 0.00037606 0.00000000 2.24409224  
C 0.00761371 0.00000000 6.39120748  
H -1.00747765 -1.76000469 6.28301495  
H 2.03897940 0.00101856 6.27642169  
H -1.00925210 1.75898234 6.28301684  
Cl 0.01648031 0.00000378 10.55863730

P1 EEF -1.03 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18654250  
C 0.00308025 0.00000000 4.94945925  
H 0.97508773 1.68183802 5.64334051  
H -1.93781665 0.00002457 5.64760184  
H 0.97504616 -1.68186259 5.64334051

P2 EEF -1.03 V/nm along Z direction  
Cl 0.00000000 0.00000000 0.00000000

R1 EEF 1.03 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22245298

R2 EEF 1.03 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
Cl 0.00000000 0.00000000 3.40468879  
H 1.95412310 0.00000000 -0.63605183  
H -0.97724958 1.69248852 -0.63557562  
H -0.97724958 -1.69248663 -0.63557562

TS EEF 1.03 V/nm along Z direction

N -0.00121509 0.00000567 -0.03287180  
C 0.00013417 -0.00000189 2.18072592  
C 0.00784237 0.00000000 6.50062833  
H -1.00377378 -1.75356639 6.28873704  
H 2.03157734 0.00101478 6.28229874  
H -1.00554068 1.75254593 6.28873893  
CI 0.01649165 0.00000378 10.55816860

P1 EEF 1.03 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18465466  
C 0.00316907 0.00000000 4.94718402  
H 0.97569433 1.68268651 5.63818155  
H -1.93869726 0.00001890 5.64254304  
H 0.97566221 -1.68270541 5.63817966

P2 EEF 1.03 V/nm along Z direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF -1.54 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22301612

R2 EEF -1.54 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.38582365  
H 1.95223337 0.00000000 -0.64658139  
H -0.97630282 1.69084824 -0.64609951  
H -0.97630282 -1.69084824 -0.64609762

TS EEF -1.54 V/nm along Z direction  
N -0.00127935 0.00000378 0.04455409  
C 0.00042897 0.00000000 2.25875652  
C 0.00759292 0.00000000 6.36492327  
H -1.00799543 -1.76099868 6.28202662  
H 2.04015292 0.00101667 6.27547683  
H -1.00977178 1.75997445 6.28202851  
CI 0.01639149 0.00000378 10.55865810

P1 EEF -1.54 V/nm along Z direction

N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18707729  
C 0.00305758 0.00000000 4.95007342  
H 0.97466065 1.68179645 5.64477859  
H -1.93760689 -0.00029669 5.64901158  
H 0.97517466 -1.68149976 5.64477670

P2 EEF -1.54 V/nm along Z direction  
CI 0.00000000 0.00000000 0.00000000

R1 EEF 1.54 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.22240763

R2 EEF 1.54 V/nm along Z direction  
C 0.00000000 0.00000000 0.00000000  
CI 0.00000000 0.00000000 3.40892934  
H 1.95456152 0.00000000 -0.63384652  
H -0.97746879 1.69287025 -0.63337220  
H -0.97747068 -1.69286836 -0.63337409

TS EEF 1.54 V/nm along Z direction  
N -0.00130202 0.00000567 -0.05023650  
C 0.00007181 -0.00000378 2.16327996  
C 0.00792740 0.00000000 6.52964698  
H -1.00240562 -1.75127982 6.29077605  
H 2.02896951 0.00101478 6.28448515  
H -1.00416685 1.75026125 6.29077605  
CI 0.01642173 0.00000378 10.55769810

P1 EEF 1.54 V/nm along Z direction  
N 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.18424270  
C 0.00318986 0.00000000 4.94666246  
H 0.97576992 1.68295485 5.63703449  
H -1.93892781 -0.00007748 5.64142055  
H 0.97590220 -1.68287737 5.63703449

P2 EEF 1.54 V/nm along Z direction  
CI 0.00000000 0.00000000 0.00000000

## Triplet DPM Rearrangement

### TS1

R No field  
C 5.21727500 -1.22034200 -0.10475700  
C 2.96524200 -2.59405500 -0.13034600  
C 0.67657900 -1.31354000 -0.11769400  
C 0.62435600 1.33535100 -0.03192700  
C 2.86212000 2.69466900 0.00815600  
C 5.16646000 1.40769500 -0.03776100  
C -1.95227100 -2.49144800 -0.05433200  
C -2.02655800 2.42345900 0.03920000  
C -3.40922800 1.29254500 2.31026100  
C -2.94866200 -1.47933300 2.46150200  
H 7.01534800 -2.20943800 -0.13839600  
H 3.00053700 -4.64766800 -0.17472400  
H 2.82252300 4.74741000 0.07756400  
H 6.92487600 2.46572300 -0.01740600  
H -1.88662000 -4.55262200 -0.14502100  
H -2.05478500 4.48658800 0.00019300  
C -3.53876500 1.23581700 -2.11440400  
C -3.51176600 -1.28983700 -2.14457500  
H -4.53690500 -2.43580100 -3.49951000  
H -4.63279800 2.39602600 -3.40404600

H -5.30951600 2.02008400 2.64398900  
H -2.09133400 -2.27619900 4.15742200

TS No field  
C 5.27898368 -1.22999649 -0.05058976  
C 3.02309368 -2.59399949 -0.07203176  
C 0.73294867 -1.31356249 -0.06284576  
C 0.68956767 1.33389951 -0.01539476  
C 2.93505468 2.68817451 0.00592824  
C 5.23561568 1.39946351 -0.01298976  
C -1.88005632 -2.50612549 -0.03564376  
C -1.91269332 2.47456551 -0.00589176  
C -3.63758732 1.30572551 1.94623424  
C -3.19988332 -1.43451649 2.28700124  
H 7.07404468 -2.22521549 -0.06333976  
H 3.05241868 -4.64822749 -0.10081976  
H 2.89931468 4.74216951 0.03885924  
H 6.99589868 2.45442051 0.00312624  
H -1.79571932 -4.56820449 -0.07217976  
H -1.94208232 4.53306751 -0.07066576  
C -3.65802432 1.22027251 -1.87736376

C -3.46343132 -1.35712449 -2.12336676  
H -4.68700932 -2.48125849 -3.31750176  
H -5.04364832 2.35243751 -2.87869276  
H -5.34395032 2.27987251 2.52609824  
H -2.91894632 -2.28160749 4.13698524

P No field

C 5.33128777 -1.16909531 -0.00000228  
C 3.08763370 -2.55332519 -0.00000028  
C 0.78156276 -1.30329208 -0.00000028  
C 0.69700890 1.35234893 -0.00000028  
C 2.94030197 2.71956781 -0.00000228  
C 5.25531290 1.45913169 -0.00000228  
C -1.82018330 -2.56510994 0.00000172  
C -1.85215904 2.52287006 -0.00000028  
C -3.96453511 1.13036817 1.43976172  
C -3.24711624 -1.44106187 2.20740272  
H 7.13620172 -2.14617440 -0.00000228  
H 3.13606959 -4.60764020 -0.00000028  
H 2.88530107 4.77359182 -0.00000228  
H 7.00152696 2.53743261 -0.00000428  
H -1.67300541 -4.62586995 0.00000172  
H -1.95142294 4.57374206 -0.00000028  
C -3.96453711 1.13036717 -1.43975828  
C -3.24711824 -1.44106387 -2.20739928  
H -2.97299427 -2.03590288 -4.14886128  
H -5.28672106 2.25824323 -2.52499328  
H -5.28671706 2.25824323 2.52499372  
H -2.97299227 -2.03589888 4.14886472

R EEF -2.57 V/nm along X direction

C 5.20752600 -1.22704500 -0.01970200  
C 2.95598100 -2.60005800 -0.05137000  
C 0.66982500 -1.31459600 -0.08899700  
C 0.61878000 1.33313600 -0.04250800  
C 2.85586900 2.69341300 0.00450500  
C 5.15806200 1.40257200 0.00624400  
C -1.96260000 -2.49004000 -0.05192800  
C -2.03552900 2.42319500 -0.02718000  
C -3.45025000 1.32482300 2.23858600  
C -2.99359900 -1.44457000 2.43852200  
H 7.00552600 -2.21414200 -0.01790900  
H 2.99426500 -4.65373200 -0.06518000  
H 2.82254900 4.74685400 0.04016200  
H 6.91801600 2.45558300 0.02996500  
H -1.89364800 -4.55235800 -0.11422500  
H -2.05967400 4.48604200 -0.09445000  
C -3.51137100 1.20860100 -2.19104900  
C -3.48483600 -1.31739500 -2.18505900  
H -4.45552100 -2.48196700 -3.56566500  
H -4.55320800 2.35222100 -3.53914300  
H -5.35662000 2.05831100 2.53787700  
H -2.12068900 -2.20004800 4.14645400

TS EEF -2.57 V/nm along X direction

C 5.27602152 -1.23346230 -0.04498296  
C 3.02042852 -2.59713230 -0.06864996  
C 0.73228252 -1.31253430 -0.06240796  
C 0.69054452 1.33284970 -0.01256096  
C 2.93541152 2.68803270 0.01167304  
C 5.23406952 1.39656870 -0.00607996  
C -1.88390248 -2.50368030 -0.04275496  
C -1.91294048 2.47479970 -0.00579196  
C -3.64858848 1.30087170 1.93361004  
C -3.19341748 -1.43479530 2.29254104  
H 7.07105052 -2.22600330 -0.05704396

H 3.05333252 -4.65096730 -0.09809996  
H 2.90575252 4.74187670 0.04508904  
H 6.99578852 2.44667870 0.01151004  
H -1.79573948 -4.56594430 -0.08163996  
H -1.94113848 4.53362170 -0.06771896  
C -3.66267748 1.22331870 -1.87582396  
C -3.46007448 -1.35349330 -2.13361296  
H -4.65278848 -2.47486330 -3.36231196  
H -5.03403748 2.36106870 -2.89295696  
H -5.34368048 2.28245570 2.53604004  
H -2.77257848 -2.22578230 4.14384804

P EEF -2.57 V/nm along X direction

C 5.32514500 -1.16878900 0.00000000  
C 3.08313700 -2.55585900 0.00000000  
C 0.77836100 -1.30369000 0.00000000  
C 0.69383200 1.34864100 0.00000000  
C 2.93365700 2.72003300 0.00000000  
C 5.24867100 1.45947200 0.00000000  
C -1.82665200 -2.56591100 0.00000000  
C -1.86042700 2.51607900 0.00000000  
C -3.97109500 1.12754100 1.44108500  
C -3.25226300 -1.44605300 2.21118500  
H 7.13092200 -2.14149300 0.00000000  
H 3.13799200 -4.60960100 0.00000000  
H 2.88182000 4.77393000 0.00000000  
H 6.99536300 2.53453900 0.00000000  
H -1.67231400 -4.62644100 0.00000000  
H -1.96043100 4.56733900 0.00000000  
C -3.97109500 1.12754100 -1.44108700  
C -3.25226200 -1.44605300 -2.21118600  
H -2.89250700 -1.99658100 -4.15379000  
H -5.28887100 2.25823500 -2.53157300  
H -5.28887100 2.25823500 2.53157300  
H -2.89250900 -1.99658100 4.15378800

R EEF -3.85 V/nm along X direction

C 5.20431900 -1.22878200 -0.02043600  
C 2.95299500 -2.60172100 -0.04833900  
C 0.66723000 -1.31444100 -0.08530600  
C 0.61653900 1.33256500 -0.03917000  
C 2.85350500 2.69341100 0.00461700  
C 5.15510900 1.40146700 0.00409100  
C -1.96614400 -2.48983400 -0.05041600  
C -2.03959900 2.42246200 -0.02390900  
C -3.45216300 1.32344000 2.24220800  
C -2.99552100 -1.44594300 2.44258300  
H 7.00273400 -2.21432000 -0.02127100  
H 2.99320800 -4.65522700 -0.06183200  
H 2.82330100 4.74681300 0.03846000  
H 6.91597000 2.45233600 0.02416400  
H -1.89546000 -4.55216100 -0.11398600  
H -2.06274500 4.48556700 -0.09020200  
C -3.51367300 1.20938900 -2.18991600  
C -3.48656700 -1.31676000 -2.18439400  
H -4.44045600 -2.48091700 -3.57797300  
H -4.54024600 2.35361300 -3.55015800  
H -5.35967200 2.05707200 2.54460800  
H -2.10381200 -2.19395600 4.14452800

TS EEF -3.85 V/nm along X direction

C 5.27871106 -1.22004779 -0.04263965  
C 3.02699406 -2.58997279 -0.06685665  
C 0.73581606 -1.31001779 -0.06210965  
C 0.68725706 1.33450821 -0.01161965  
C 2.92812006 2.69644321 0.01360035

C 5.22984306 1.41029521 -0.00361065  
C -1.87848694 -2.50802079 -0.04566865  
C -1.92031694 2.46939321 -0.00587265  
C -3.65661094 1.28864021 1.92889335  
C -3.18662994 -1.44393279 2.29502635  
H 7.07685306 -2.20611079 -0.05443665  
H 3.06775206 -4.64352379 -0.09628865  
H 2.89567506 4.75018521 0.04687335  
H 6.98950006 2.46314121 0.01424335  
H -1.78256294 -4.57008179 -0.08561565  
H -1.95383294 4.52830521 -0.06673365  
C -3.66882994 1.21411321 -1.87522665  
C -3.45549494 -1.36195679 -2.13756265  
H -4.63036394 -2.48547679 -3.38220665  
H -5.03702594 2.35038921 -2.89987665  
H -5.34920294 2.26895521 2.54245235  
H -2.71003694 -2.21103179 4.14407835

P EEF -3.85 V/nm along X direction

C 5.31651000 -1.17296100 0.00000000  
C 3.07408500 -2.55984900 0.00000000  
C 0.77050000 -1.30524400 0.00000000  
C 0.68769400 1.34584800 0.00000000  
C 2.92705300 2.71759900 0.00000000  
C 5.24150900 1.45550400 0.00000000  
C -1.83717200 -2.56600500 0.00000000  
C -1.86811400 2.51331000 0.00000000  
C -3.97937900 1.12788200 1.44172700  
C -3.26131700 -1.44712400 2.21309900  
H 7.12232000 -2.14478900 0.00000000  
H 3.13091100 -4.61336800 0.00000000  
H 2.87831100 4.77149200 0.00000000  
H 6.98939500 2.52789300 0.00000000  
H -1.68052500 -4.62650100 0.00000000  
H -1.96733800 4.56483600 0.00000000  
C -3.97937900 1.12788200 -1.44172700  
C -3.26131700 -1.44712600 -2.21309900  
H -2.86483000 -1.97830000 -4.15487800  
H -5.29448400 2.26095000 -2.53471700  
H -5.29448400 2.26095000 2.53471500  
H -2.86483200 -1.97830000 4.15487800

R EEF -5.14 V/nm along X direction

C 5.20151900 -1.22985300 -0.02069600  
C 2.95038500 -2.60274500 -0.04489800  
C 0.66466000 -1.31385200 -0.08181200  
C 0.61418800 1.33268500 -0.03627700  
C 2.85111200 2.69408200 0.00439000  
C 5.15238200 1.40117800 0.00201600  
C -1.96948300 -2.48937100 -0.04940100  
C -2.04397400 2.42217300 -0.02095000  
C -3.45357400 1.32227400 2.24594600  
C -2.99708800 -1.44716400 2.44630800  
H 7.00058400 -2.21375600 -0.02384800  
H 2.99268900 -4.65609600 -0.05782600  
H 2.82401700 4.74745100 0.03623200  
H 6.91425200 2.45004800 0.01849500  
H -1.89690000 -4.55169600 -0.11435900  
H -2.06627800 4.48554800 -0.08622400  
C -3.51658000 1.21048900 -2.18883900  
C -3.48855300 -1.31585500 -2.18393500  
H -4.42597700 -2.47950500 -3.59012600  
H -4.52846200 2.35511600 -3.56080900  
H -5.36231400 2.05613100 2.55230700  
H -2.08774900 -2.18847900 4.14226100

TS EEF -5.14 V/nm along X direction

C 5.27486850 -1.23643440 -0.04163268  
C 3.01916050 -2.59984440 -0.06537768  
C 0.73190350 -1.31175340 -0.06191568  
C 0.69142150 1.33237360 -0.01142068  
C 2.93609750 2.68832060 0.01379832  
C 5.23385250 1.39460060 -0.00320568  
C -1.88722250 -2.50184440 -0.04758768  
C -1.91394550 2.47483260 -0.00583068  
C -3.65621850 1.29747360 1.92581432  
C -3.18728050 -1.43475740 2.29860632  
H 7.07073350 -2.22617340 -0.05340068  
H 3.05621450 -4.65336840 -0.09424468  
H 2.91258150 4.74207560 0.04642632  
H 6.99749150 2.44037660 0.01410432  
H -1.79519650 -4.56424340 -0.08838868  
H -1.94115550 4.53399360 -0.06597068  
C -3.66899450 1.22530660 -1.87380868  
C -3.45973550 -1.35126040 -2.13996168  
H -4.62391150 -2.47042240 -3.39945868  
H -5.02824150 2.36758060 -2.90552168  
H -5.34048250 2.28618460 2.55133632  
H -2.66430450 -2.18230340 4.14421732

P EEF -5.14 V/nm along X direction

C 5.31801600 -1.17291600 0.00000000  
C 3.07603300 -2.56127200 0.00000000  
C 0.77247900 -1.30610600 0.00000000  
C 0.68929900 1.34391500 0.00000000  
C 2.92736600 2.71758600 0.00000000  
C 5.24244100 1.45577600 0.00000000  
C -1.83698100 -2.56752300 0.00000000  
C -1.86883600 2.50931900 0.00000000  
C -3.97996100 1.12512400 1.44234200  
C -3.26049700 -1.45064100 2.21503200  
H 7.12476500 -2.14255200 0.00000000  
H 3.13650100 -4.61453900 0.00000000  
H 2.88023900 4.77145600 0.00000000  
H 6.99084000 2.52690500 0.00000000  
H -1.67629900 -4.62784300 0.00000000  
H -1.96902000 4.56103500 0.00000000  
C -3.97996100 1.12512400 -1.44234300  
C -3.26049500 -1.45064100 -2.21503200  
H -2.82964700 -1.96340900 -4.15533000  
H -5.29351200 2.25956700 -2.53774400  
H -5.29351400 2.25956700 2.53774300  
H -2.82964900 -1.96340900 4.15533000

R EEF -2.57 V/nm along X direction

C 5.21415700 -1.22549200 -0.01206000  
C 2.96213200 -2.59945300 -0.05160800  
C 0.67383900 -1.31915600 -0.09669900  
C 0.62134400 1.33071900 -0.05138200  
C 2.85836100 2.69151900 0.00104100  
C 5.16243500 1.40347200 0.01094300  
C -1.95741100 -2.49219400 -0.06004000  
C -2.02886600 2.42353300 -0.03518700  
C -3.44853800 1.32263100 2.22693500  
C -2.99362400 -1.44685600 2.42745400  
H 7.01528400 -2.21126800 -0.00085400  
H 2.99516400 -4.65547400 -0.06264400  
H 2.82082400 4.74390600 0.03651500  
H 6.91755300 2.46541300 0.04074600  
H -1.88806000 -4.55692900 -0.12297600  
H -2.05713800 4.48411800 -0.10033500  
C -3.50879600 1.20725200 -2.19443200

C -3.48370600 -1.31889300 -2.19151200  
H -4.49150700 -2.47952400 -3.54790200  
H -4.57819400 2.35429500 -3.51544000  
H -5.34141300 2.07133700 2.54420900  
H -2.13498900 -2.20415700 4.14317500

TS EEF -2.57 V/nm along X direction

C 5.27723994 -1.23081574 -0.04185867  
C 3.02144994 -2.59574474 -0.06819067  
C 0.73088794 -1.31621574 -0.06415267  
C 0.68721794 1.33137426 -0.01419767  
C 2.93178894 2.68725926 0.01204133  
C 5.23251194 1.39867926 -0.00341467  
C -1.88435006 -2.50428374 -0.04266467  
C -1.91486806 2.47403226 -0.00750167  
C -3.64081406 1.30241626 1.94317433  
C -3.19278206 -1.43587874 2.29134733  
H 7.07569494 -2.22166674 -0.05170467  
H 3.04914294 -4.65191074 -0.09796867  
H 2.89798494 4.73997726 0.04578433  
H 6.98933794 2.45798426 0.01606433  
H -1.79732306 -4.56895174 -0.08234867  
H -1.94642406 4.53107926 -0.06737567  
C -3.65344706 1.22285126 -1.88819767  
C -3.46157506 -1.35224874 -2.13475667  
H -4.68754706 -2.47148174 -3.33214167  
H -5.02622706 2.36225226 -2.89816067  
H -5.33478006 2.28451326 2.54216633  
H -2.80656706 -2.24062674 4.14443733

P EEF -2.57 V/nm along X direction

C 5.33122600 -1.16776800 0.00000000  
C 3.08882500 -2.55485000 0.00000000  
C 0.78187300 -1.30699700 0.00000000  
C 0.69389100 1.34809100 0.00000000  
C 2.93508000 2.71894700 0.00000000  
C 5.25128600 1.46044900 0.00000000  
C -1.82020900 -2.56538500 0.00000000  
C -1.85587200 2.51773200 0.00000000  
C -3.96857800 1.12722800 1.43992100  
C -3.24931700 -1.44265700 2.20898700  
H 7.14034200 -2.13876100 0.00000000  
H 3.13675200 -4.61111500 0.00000000  
H 2.88063400 4.77162800 0.00000000  
H 6.99307200 2.54451500 0.00000000  
H -1.66956200 -4.62863500 0.00000000  
H -1.95896100 4.56716200 0.00000000  
C -3.96857800 1.12722800 -1.43992100  
C -3.24931700 -1.44265700 -2.20898700  
H -2.92320100 -2.00583700 -4.15364000  
H -5.28328700 2.26102600 -2.52704300  
H -5.28328700 2.26102600 2.52704100  
H -2.92320100 -2.00583700 4.15363900

R EEF -3.85 V/nm along X direction

C 5.21388300 -1.22632500 -0.00948300  
C 2.96201300 -2.60103900 -0.04911800  
C 0.67338900 -1.32131800 -0.09662200  
C 0.62048800 1.32869500 -0.05200200  
C 2.85706700 2.69073900 -0.00027800  
C 5.16128800 1.40283500 0.01102300  
C -1.95837100 -2.49307900 -0.06205900  
C -2.02937200 2.42280600 -0.03558700  
C -3.45022600 1.32015900 2.22456200  
C -2.99620200 -1.44940500 2.42624900  
H 7.01674500 -2.20992000 0.00348800

H 2.99435300 -4.65829600 -0.05872100  
H 2.82033600 4.74278700 0.03343900  
H 6.91464300 2.46720100 0.04014500  
H -1.88711900 -4.55931200 -0.12647000  
H -2.05867800 4.48275000 -0.09875900  
C -3.50916400 1.20727300 -2.19500500  
C -3.48434800 -1.31917500 -2.19400700  
H -4.49348900 -2.47791000 -3.55161500  
H -4.57667100 2.35708500 -3.51492400  
H -5.33681700 2.07722000 2.55374700  
H -2.12489200 -2.19969500 4.13994400

TS EEF -3.85 V/nm along X direction

C 5.28004613 -1.21613222 -0.03779152  
C 3.02821913 -2.58816822 -0.06620952  
C 0.73380813 -1.31551322 -0.06465052  
C 0.68243313 1.33213178 -0.01376152  
C 2.92261813 2.69544178 0.01458948  
C 5.22712613 1.41334078 0.00080248  
C -1.87915187 -2.50880422 -0.04568052  
C -1.92292187 2.46826378 -0.00836052  
C -3.64560787 1.29075078 1.94229448  
C -3.18588687 -1.44558522 2.29322648  
H 7.08303513 -2.19972622 -0.04627252  
H 3.06105313 -4.64547422 -0.09632552  
H 2.88391413 4.74768078 0.04852748  
H 6.97919813 2.47995078 0.02168948  
H -1.78494887 -4.57477622 -0.08676152  
H -1.96142087 4.52472878 -0.06588952  
C -3.65457087 1.21367678 -1.89369252  
C -3.45712687 -1.36002622 -2.13980452  
H -4.68179587 -2.48078122 -3.33781152  
H -5.02447687 2.35283778 -2.90757252  
H -5.33576987 2.27260978 2.55107448  
H -2.75458487 -2.23148822 4.14602648

P EEF -3.85 V/nm along X direction

C 5.32488900 -1.17153800 0.00000000  
C 3.08216500 -2.55871700 0.00000000  
C 0.77557400 -1.31031000 0.00000000  
C 0.68768700 1.34471300 0.00000000  
C 2.92873500 2.71605900 0.00000000  
C 5.24474400 1.45682800 0.00000000  
C -1.82757000 -2.56524900 0.00000000  
C -1.86161700 2.51564600 0.00000000  
C -3.97548800 1.12739800 1.44009700  
C -3.25712000 -1.44221300 2.20977100  
H 7.13545600 -2.14082600 0.00000000  
H 3.12848400 -4.61624400 0.00000000  
H 2.87593400 4.76835500 0.00000000  
H 6.98505400 2.54273900 0.00000000  
H -1.67660900 -4.63013100 0.00000000  
H -1.96528400 4.56467300 0.00000000  
C -3.97548800 1.12739800 -1.44009700  
C -3.25711800 -1.44221300 -2.20977300  
H -2.90802900 -1.99119800 -4.15540500  
H -5.28562500 2.26530400 -2.52808200  
H -5.28562500 2.26530400 2.52808000  
H -2.90803100 -1.99119800 4.15540400

R EEF -5.14 V/nm along X direction

C 5.21377900 -1.22639100 -0.00685600  
C 2.96213900 -2.60212900 -0.04659500  
C 0.67308900 -1.32306800 -0.09658400  
C 0.61962300 1.32717200 -0.05270100  
C 2.85565500 2.69073500 -0.00168000

C 5.16014300 1.40302800 0.01110200  
C -1.95915500 -2.49371400 -0.06414700  
C -2.02998100 2.42242400 -0.03605000  
C -3.45195300 1.31793500 2.22214100  
C -2.99880900 -1.45176800 2.42493000  
H 7.01844400 -2.20775700 0.00795400  
H 2.99396400 -4.66080000 -0.05475700  
H 2.81958600 4.74260400 0.03024900  
H 6.91167000 2.47002000 0.03957700  
H -1.88586400 -4.56163800 -0.13003600  
H -2.06045400 4.48188800 -0.09725700  
C -3.50968600 1.20753700 -2.19559600  
C -3.48494200 -1.31930500 -2.19658300  
H -4.49545200 -2.47638700 -3.55525800  
H -4.57553300 2.36022000 -3.51422900  
H -5.33198700 2.08366400 2.56366800  
H -2.11541700 -2.19547000 4.13665600

TS EEF -5.14 V/nm along X direction

C 5.27614931 -1.23107239 -0.03536332  
C 3.02056231 -2.59770039 -0.06478132  
C 0.72941031 -1.31902439 -0.06514532  
C 0.68517331 1.32903561 -0.01388532  
C 2.92862131 2.68731561 0.01548268  
C 5.22977031 1.39872861 0.00283368  
C -1.88793569 -2.50282039 -0.04745632  
C -1.91708069 2.47330261 -0.00901132  
C -3.64217469 1.30009361 1.94281968  
C -3.18675069 -1.43698439 2.29613768  
H 7.07812931 -2.21765739 -0.04289432  
H 3.04697131 -4.65650639 -0.09483532  
H 2.89648831 4.73942561 0.04921468  
H 6.98305131 2.46294361 0.02429668  
H -1.79830569 -4.57080539 -0.08955132  
H -1.95091269 4.52953861 -0.06456532  
C -3.64943469 1.22474261 -1.89822032  
C -3.46119169 -1.34884939 -2.14318932  
H -4.69193269 -2.46468739 -3.34038032  
H -5.01068469 2.37124061 -2.91534532  
H -5.32269369 2.29156961 2.56164268  
H -2.71987769 -2.20843339 4.14792068

P EEF -5.14 V/nm along X direction

C 5.32826600 -1.17105800 0.00000000  
C 3.08629800 -2.56022100 0.00000000  
C 0.77907200 -1.31300300 0.00000000  
C 0.68921200 1.34198400 0.00000000  
C 2.92902400 2.71570800 0.00000000  
C 5.24585900 1.45745800 0.00000000  
C -1.82419100 -2.56654600 0.00000000  
C -1.86058000 2.51221200 0.00000000  
C -3.97457800 1.12445200 1.44033100  
C -3.25514500 -1.44433700 2.21055300  
H 7.14104500 -2.13729200 0.00000000  
H 3.13265500 -4.61914600 0.00000000  
H 2.87625700 4.76774300 0.00000000  
H 6.98385200 2.54666000 0.00000000  
H -1.67130300 -4.63314700 0.00000000  
H -1.96647400 4.56091400 0.00000000  
C -3.97457800 1.12445200 -1.44033100  
C -3.25514500 -1.44433700 -2.21055500  
H -2.88399500 -1.97959900 -4.15685100  
H -5.28097600 2.26561600 -2.52913300  
H -5.28097800 2.26561600 2.52913100  
H -2.88399500 -1.97959900 4.15684900

R EEF -2.57 V/nm along X direction

C 5.21838300 -1.22290700 -0.00775200  
C 2.96690700 -2.59582500 -0.07462900  
C 0.67875400 -1.31506100 -0.13970900  
C 0.62713800 1.33506200 -0.09477200  
C 2.86433300 2.69409100 -0.01562200  
C 5.16806500 1.40603800 0.01948500  
C -1.95038700 -2.49211900 -0.07903800  
C -2.02355700 2.42469300 -0.06041300  
C -3.41611800 1.32935500 2.22056500  
C -2.96515300 -1.44141200 2.41474400  
H 7.01496300 -2.21327500 0.05608000  
H 3.00131300 -4.64991700 -0.015496500  
H 2.82350000 4.74675800 0.05591300  
H 6.92506900 2.46298100 0.10644600  
H -1.88468300 -4.55463100 -0.13334100  
H -2.05110600 4.48719400 -0.12701600  
C -3.52668600 1.20338900 -2.20117100  
C -3.49999900 -1.32366100 -2.19346100  
H -4.55107800 -2.49044300 -3.51209300  
H -4.64261300 2.34234500 -3.49325100  
H -5.30285700 2.08057000 2.56878700  
H -2.14533100 -2.22442600 4.13316500

TS EEF -2.57 V/nm along X direction

C 5.27725964 -1.22763318 -0.02188045  
C 3.02221464 -2.59220318 -0.07314345  
C 0.73137164 -1.31258618 -0.09485645  
C 0.68765464 1.33515182 -0.04946445  
C 2.93222564 2.69019982 0.00008355  
C 5.23311364 1.40198382 0.01256755  
C -1.88063736 -2.50611118 -0.04821745  
C -1.91740136 2.47160182 -0.01954145  
C -3.60233136 1.30723482 1.96463455  
C -3.16992236 -1.43718818 2.29045355  
H 7.07185764 -2.22271618 0.02538155  
H 3.05223664 -4.64667018 -0.06571245  
H 2.89504264 4.74341782 0.06524755  
H 6.99214864 2.45657282 0.08608355  
H -1.79548936 -4.56820318 -0.07889945  
H -1.94850636 4.53054082 -0.07734345  
C -3.67314436 1.21756982 -1.88873445  
C -3.48984536 -1.35945518 -2.12077145  
H -4.77388236 -2.48834318 -3.24788245  
H -5.08586536 2.34615082 -2.85775045  
H -5.28473036 2.28787482 2.59923855  
H -2.91547636 -2.30246818 4.13352855

P EEF -2.57 V/nm along X direction

C 5.33483300 -1.16420800 0.00197500  
C 3.09202200 -2.54975600 -0.01513100  
C 0.78524400 -1.30104900 -0.03674000  
C 0.69920300 1.35460000 -0.04033800  
C 2.94171700 2.72312900 -0.02650700  
C 5.25739400 1.46401700 -0.00481100  
C -1.81573700 -2.56432200 -0.01174800  
C -1.85057600 2.52370400 -0.01766900  
C -3.94438900 1.13159100 1.44387400  
C -3.22012100 -1.43839000 2.20752400  
H 7.13969600 -2.14000000 0.05409300  
H 3.14139700 -4.60373000 0.02220400  
H 2.88537900 4.77694800 0.00190500  
H 7.00245100 2.54323200 0.04104900  
H -1.66747600 -4.62500600 -0.00514000  
H -1.95102800 4.57450700 -0.00693000  
C -3.97959100 1.12850100 -1.43588400

C -3.26614700 -1.44360200 -2.20756400  
H -2.97485500 -2.02445700 -4.15330800  
H -5.31989900 2.25359200 -2.50336700  
H -5.24972200 2.26049300 2.54700200  
H -2.96019500 -2.04526500 4.14550500

R EEF -3.85 V/nm along X direction

C 5.22031200 -1.22234700 -0.00279700  
C 2.96944500 -2.59536000 -0.08376600  
C 0.68104200 -1.31511600 -0.16148700  
C 0.62938700 1.33517100 -0.11753200  
C 2.86616200 2.69443900 -0.02531300  
C 5.16974700 1.40673900 0.02409800  
C -1.94736200 -2.49302200 -0.09102400  
C -2.02111400 2.42450400 -0.07397100  
C -3.40112700 1.33032400 2.21432100  
C -2.95381300 -1.44134000 2.40635400  
H 7.01577700 -2.21253900 0.08935600  
H 3.00361900 -4.64928400 -0.04725500  
H 2.82421400 4.74648200 0.06255400  
H 6.92529500 2.46338200 0.13929900  
H -1.88151800 -4.55564400 -0.14234700  
H -2.04945400 4.48707000 -0.13944100  
C -3.53607000 1.20127900 -2.20521300  
C -3.50850300 -1.32656900 -2.19728700  
H -4.58341700 -2.49403300 -3.49711300  
H -4.67441500 2.33842400 -3.48058200  
H -5.27712800 2.09192800 2.59209100  
H -2.14222300 -2.23041100 4.12501100

TS EEF -3.85 V/nm along X direction

C 5.27963294 -1.21123818 -0.00701723  
C 3.02912594 -2.58263218 -0.07319623  
C 0.73435094 -1.31002218 -0.11091623  
C 0.68284094 1.33777082 -0.06725823  
C 2.92293194 2.69971182 -0.00348423  
C 5.22753394 1.41837682 0.02529077  
C -1.87366506 -2.51145318 -0.05421523  
C -1.92710106 2.46425282 -0.02694523  
C -3.58593706 1.29848182 1.97595077  
C -3.15139606 -1.44753518 2.29164077  
H 7.07620794 -2.20086118 0.07073477  
H 3.06516294 -4.63689718 -0.04708923  
H 2.87882994 4.75227682 0.07745177  
H 6.98226194 2.47773782 0.12758777  
H -1.78239106 -4.57329618 -0.08166923  
H -1.96497506 4.52331782 -0.08148823  
C -3.68379506 1.20554282 -1.89594723  
C -3.49957806 -1.37105818 -2.11919923  
H -4.81049106 -2.50569718 -3.21087523  
H -5.11407006 2.32770282 -2.84781023  
H -5.25735706 2.27801182 2.64011777  
H -2.91807406 -2.32558218 4.13051677

P EEF -3.85 V/nm along X direction

C 5.32983500 -1.16645800 0.00305000  
C 3.08654400 -2.55116900 -0.02269400  
C 0.78026100 -1.30157000 -0.05522000  
C 0.69531200 1.35417600 -0.06063600  
C 2.93836500 2.72186400 -0.03986200  
C 5.25347900 1.46184900 -0.00720200  
C -1.82117100 -2.56376600 -0.01769900  
C -1.85392600 2.52435200 -0.02654300  
C -3.93922800 1.13390800 1.44604500  
C -3.21330300 -1.43587300 2.20766400  
H 7.13354500 -2.14265200 0.08138100

H 3.13481700 -4.60476900 0.03339700  
H 2.88262500 4.77548700 0.00277000  
H 6.99828400 2.54027300 0.06168400  
H -1.67385800 -4.62451900 -0.00779700  
H -1.95357700 4.57518400 -0.01041100  
C -3.99213300 1.12931800 -1.43401000  
C -3.28249100 -1.44361900 -2.20777200  
H -2.98232700 -2.01709100 -4.15597200  
H -5.34075700 2.25384500 -2.49261600  
H -5.23532400 2.26412000 2.55823100  
H -2.95984900 -2.04831100 4.14420300

R EEF -5.14 V/nm along X direction

C 5.22252300 -1.22091900 0.00246400  
C 2.97247800 -2.59422300 -0.09295800  
C 0.68373300 -1.31471100 -0.18367000  
C 0.63181700 1.33577000 -0.14081700  
C 2.86801000 2.69547400 -0.03518500  
C 5.17147400 1.40833800 0.02894500  
C -1.94376200 -2.49373500 -0.10354900  
C -2.01851600 2.42462700 -0.08807500  
C -3.38576700 1.33158100 2.20742600  
C -2.94274900 -1.44119800 2.39709800  
H 7.01653900 -2.21068900 0.12330700  
H 3.00643600 -4.64784900 -0.03948200  
H 2.82459200 4.74677100 0.06902000  
H 6.92505300 2.46474800 0.17273400  
H -1.87756600 -4.55646000 -0.15177200  
H -2.04788800 4.48725500 -0.15248200  
C -3.54573400 1.19925500 -2.20934600  
C -3.51681000 -1.32953800 -2.20150700  
H -4.61640800 -2.49756900 -3.48130800  
H -4.70765000 2.33429800 -3.46673600  
H -5.24948400 2.10462100 2.61710700  
H -2.14146900 -2.23704700 4.11673400

TS EEF -5.14 V/nm along X direction

C 5.27507486 -1.22424129 0.00641197  
C 3.02156486 -2.58997829 -0.07371103  
C 0.72998486 -1.31163529 -0.12719703  
C 0.68539386 1.33647871 -0.08610303  
C 2.92853686 2.69289671 -0.00899303  
C 5.22964386 1.40568971 0.03584097  
C -1.88064014 -2.50629029 -0.05901803  
C -1.92332914 2.46730271 -0.03430803  
C -3.55909514 1.31067671 1.99052497  
C -3.14070214 -1.44001729 2.29357497  
H 7.06766786 -2.21826329 0.11451797  
H 3.05199486 -4.64405829 -0.02821303  
H 2.88878086 4.74492271 0.08725597  
H 6.98554486 2.46002771 0.16625297  
H -1.79508314 -4.56837129 -0.08283203  
H -1.95634614 4.52669471 -0.08594103  
C -3.68794714 1.21389271 -1.90345403  
C -3.51832714 -1.36352329 -2.11571003  
H -4.86277614 -2.49645629 -3.16983703  
H -5.13042814 2.33712371 -2.83696603  
H -5.21217614 2.29889071 2.68674997  
H -2.94415614 -2.33634329 4.12705597

P EEF -5.14 V/nm along X direction

C 5.33429800 -1.16449700 0.00426300  
C 3.09166500 -2.55018100 -0.03024700  
C 0.78489000 -1.30154200 -0.07383700  
C 0.69891900 1.35426700 -0.08108400  
C 2.94142000 2.72291900 -0.05331300

C 5.25694600 1.46385000 -0.00953400  
C -1.81595600 -2.56473200 -0.02376900  
C -1.85068700 2.52348300 -0.03547200  
C -3.92622100 1.13303900 1.44829000  
C -3.19658100 -1.43598800 2.20781700  
H 7.13731900 -2.13951700 0.10899900  
H 3.14035600 -4.60320800 0.04468800  
H 2.88455100 4.77621700 0.00356600  
H 7.00035900 2.54283700 0.08251500

H -1.66798400 -4.62544100 -0.01059800  
H -1.95119200 4.57425800 -0.01391000  
C -3.99693500 1.12694800 -1.43218200  
C -3.28908100 -1.44624800 -2.20809700  
H -2.97934700 -2.01177100 -4.15896200  
H -5.35481100 2.24978000 -2.48187500  
H -5.21394700 2.26344700 2.56963000  
H -2.94837600 -2.05338700 4.14310300

## TS2

R No field

C 5.33128777 -1.16909531 -0.00000228  
C 3.08763370 -2.55332519 -0.00000028  
C 0.78156276 -1.30329208 -0.00000028  
C 0.69700890 1.35234893 -0.00000028  
C 2.94030197 2.71956781 -0.00000228  
C 5.25531290 1.45913169 -0.00000228  
C -1.82018330 -2.56510994 0.00000172  
C -1.85215904 2.52287006 -0.00000028  
C -3.96453511 1.13036817 1.43976172  
C -3.24711624 -1.44106187 2.20740272  
H 7.13620172 -2.14617440 -0.00000228  
H 3.13606959 -4.60764020 -0.00000028  
H 2.88530107 4.77359182 -0.00000228  
H 7.00152696 2.53743261 -0.00000428  
H -1.67300541 -4.62586995 0.00000172  
H -1.95142294 4.57374206 -0.00000028  
C -3.96453711 1.13036717 -1.43975828  
C -3.24711824 -1.44106387 -2.20739928  
H -2.97299427 -2.03590288 -4.14886128  
H -5.28672106 2.25824323 -2.52499328  
H -5.28671706 2.25824323 2.52499372  
H -2.97299227 -2.03589888 4.14886472

TS No field

C -5.32322681 -1.23333932 0.05437220  
C -3.04863781 -2.55872932 -0.08870880  
C -0.76938281 -1.26637732 -0.15573580  
C -0.73690481 1.40605668 -0.10901180  
C -3.02734381 2.70998368 0.08760820  
C -5.30405681 1.39745868 0.15407220  
C 1.83919519 -2.51724832 -0.17569680  
C 1.69936319 2.66727568 -0.20719480  
C 3.99023819 1.29208568 -1.17411480  
C 3.31181619 -1.21666632 -2.24650680  
H -7.10274981 -2.25419632 0.10355420  
H -3.05131781 -4.61356632 -0.12874480  
H -3.01980581 4.76357968 0.15529320  
H -7.07145981 2.43289268 0.28171220  
H 1.69081819 -4.57209032 -0.34167080  
H 1.82671219 4.68359768 0.15120520  
C 4.19015619 0.79800767 1.62579120  
C 3.20378219 -1.56616032 2.16525520  
H 2.90168119 -2.33937432 4.03655220  
H 5.15306419 2.04861568 2.92560620  
H 5.42236719 2.43197668 -2.11173680  
H 2.95304019 -1.53776732 -4.23983380

P No field

C 5.25821400 -1.46145200 -0.10979700  
C 2.90829000 -2.61167100 0.24222900  
C 0.71379500 -1.18835700 0.33189800  
C 0.84319800 1.50791700 0.09759500  
C 3.24454000 2.62198500 -0.28582300

C 5.41139400 1.16097100 -0.38014500  
C -1.91192400 -2.36136300 0.63729100  
C -1.39147600 2.97413300 0.26298000  
C -3.89681300 1.62766700 0.65457300  
C -3.36349300 -0.60484100 2.34191000  
H 6.95914600 -2.60687400 -0.18030100  
H 2.78928600 -4.65432900 0.43617000  
H 3.36697700 4.66335500 -0.48381000  
H 7.23629700 2.05722300 -0.66051600  
H -1.77647900 -4.32236100 1.27851600  
H -1.32089600 5.00634600 -0.02165600  
C -4.49135500 0.25228400 -1.82857300  
C -3.35371500 -1.99482800 -1.83694100  
H -3.25151500 -3.31120600 -3.40378700  
H -5.49389100 1.12774000 -3.38652700  
H -5.37133900 2.91593700 1.31266500  
H -2.96150800 -0.41051100 4.34608300

R EEF -2.52 V/nm along X direction

C 5.32514500 -1.16878900 0.00000000  
C 3.08313700 -2.55585900 0.00000000  
C 0.77836100 -1.30369000 0.00000000  
C 0.69383200 1.34864100 0.00000000  
C 2.93365700 2.72003300 0.00000000  
C 5.24867100 1.45947200 0.00000000  
C -1.82665200 -2.56591100 0.00000000  
C -1.86042700 2.51607900 0.00000000  
C -3.97109500 1.12754100 1.44108500  
C -3.25226300 -1.44605300 2.21118500  
H 7.13092200 -2.14149300 0.00000000  
H 3.13799200 -4.60960100 0.00000000  
H 2.88182000 4.77393000 0.00000000  
H 6.99536300 2.53453900 0.00000000  
H -1.67231400 -4.62644100 0.00000000  
H -1.96043100 4.56733900 0.00000000  
C -3.97109500 1.12754100 -1.44108700  
C -3.25226200 -1.44605300 -2.21118600  
H -2.89250700 -1.99658100 -4.15379000  
H -5.28887100 2.25823500 -2.53157300  
H -5.28887100 2.25823500 2.53157300  
H -2.89250900 -1.99658100 4.15378800

TS EEF -2.52 V/nm along X direction

C 5.22988133 -1.56193967 0.19262125  
C 2.87396833 -2.74436467 0.24984925  
C 0.68096233 -1.30972167 0.20240425  
C 0.82037733 1.35496933 0.12353825  
C 3.19151033 2.51542733 0.01443125  
C 5.38206633 1.06305733 0.06445425  
C -2.00253867 -2.39433067 0.11975725  
C -1.53635267 2.76626633 0.09839925  
C -3.94614667 1.55475633 0.98784625  
C -3.47162867 -0.97801567 2.11693925  
H 6.94343033 -2.68829467 0.23138325

H 2.75241533 -4.79470267 0.31160425  
H 3.31872433 4.56387833 -0.07563875  
H 7.21536033 1.98058433 0.00447825  
H -1.98420267 -4.45213667 0.31691925  
H -1.52023867 4.78236533 -0.28420675  
C -4.05944767 1.03833833 -1.81373975  
C -3.20986467 -1.39588567 -2.28740175  
H -2.81622067 -2.17864267 -4.13879575  
H -4.86476967 2.33947133 -3.17099475  
H -5.33595767 2.79861833 1.85908225  
H -3.14638267 -1.26234367 4.12341925

P EEF -2.52 V/nm along X direction

C 5.25148900 -1.45465100 -0.11729900  
C 2.90475400 -2.61037600 0.23621600  
C 0.71043700 -1.18771000 0.33257300  
C 0.83461500 1.50793000 0.10307900  
C 3.23450000 2.62681100 -0.28280900  
C 5.40211300 1.16919900 -0.38284700  
C -1.91491100 -2.36744600 0.63919600  
C -1.39967000 2.97181500 0.27589300  
C -3.90467300 1.61741900 0.65517000  
C -3.36888000 -0.61438000 2.34585200  
H 6.95503600 -2.59400900 -0.18996500  
H 2.79455600 -4.65340300 0.42855000  
H 3.35798000 4.66837700 -0.47406800  
H 7.22642000 2.06445100 -0.66037300  
H -1.77042300 -4.32827200 1.27934500  
H -1.33226900 5.00577700 0.00492700  
C -4.49342100 0.24362900 -1.82880000  
C -3.34929100 -2.00173300 -1.83714000  
H -3.20255400 -3.29589500 -3.41978800  
H -5.45059600 1.13465100 -3.40823000  
H -5.38252200 2.90523200 1.31463400  
H -2.90936300 -0.39248900 4.33608200

R EEF -3.85 V/nm along X direction

C 5.31651000 -1.17296100 0.00000000  
C 3.07408500 -2.55984900 0.00000000  
C 0.77050000 -1.30524400 0.00000000  
C 0.68769400 1.34584800 0.00000000  
C 2.92705300 2.71759900 0.00000000  
C 5.24150900 1.45550400 0.00000000  
C -1.83717200 -2.56600500 0.00000000  
C -1.86811400 2.51331000 0.00000000  
C -3.97937900 1.12788200 1.44172700  
C -3.26131700 -1.44712400 2.21309900  
H 7.12232000 -2.14478900 0.00000000  
H 3.13091100 -4.61336800 0.00000000  
H 2.87831100 4.77149200 0.00000000  
H 6.98939500 2.52789300 0.00000000  
H -1.68052500 -4.62650100 0.00000000  
H -1.96733800 4.56483600 0.00000000  
C -3.97937900 1.12788200 -1.44172700  
C -3.26131700 -1.44712600 -2.21309900  
H -2.86483000 -1.97830000 -4.15487800  
H -5.29448400 2.26095000 -2.53471700  
H -5.29448400 2.26095000 2.53471500  
H -2.86483200 -1.97830000 4.15487800

TS EEF -3.85 V/nm along X direction

C 5.22918125 -1.56110371 0.19711433  
C 2.87353225 -2.74514371 0.25234133  
C 0.68096725 -1.30989071 0.20183133  
C 0.82131225 1.35337729 0.12140433  
C 3.19143725 2.51590829 0.01371133

C 5.38228325 1.06382929 0.06779533  
C -2.00424175 -2.39413871 0.11695033  
C -1.53649475 2.76371629 0.09406733  
C -3.94524875 1.55506029 0.98862633  
C -3.47032575 -0.97876471 2.11765333  
H 6.94352625 -2.68556471 0.23784733  
H 2.75548325 -4.79552071 0.31464633  
H 3.32020525 4.56408129 -0.07722667  
H 7.21607725 1.97954229 0.00974433  
H -1.98247375 -4.45203071 0.31519233  
H -1.52013575 4.78024129 -0.28724467  
C -4.06040075 1.04021129 -1.81363567  
C -3.21567975 -1.39757371 -2.28941667  
H -2.79257175 -2.16359971 -4.14197967  
H -4.85609475 2.34663029 -3.17220467  
H -5.33166175 2.80123429 1.86483633  
H -3.11321875 -1.24966871 4.12145033

P EEF -3.85 V/nm along X direction

C 5.24699500 -1.45561900 -0.12091800  
C 2.90081400 -2.61218300 0.23531400  
C 0.70741200 -1.18852700 0.33448900  
C 0.83057100 1.50692900 0.10481000  
C 3.23070700 2.62608200 -0.28482300  
C 5.39792500 1.16875800 -0.38692900  
C -1.91851900 -2.36917900 0.64543600  
C -1.40233400 2.97090600 0.28220800  
C -3.90775500 1.61519900 0.66066700  
C -3.37029400 -0.61555200 2.35373600  
H 6.95131700 -2.59323100 -0.19405000  
H 2.79390400 -4.65514400 0.42901700  
H 3.35611500 4.66749100 -0.47477300  
H 7.22272100 2.06207800 -0.66456000  
H -1.77031700 -4.32964600 1.28605600  
H -1.33547600 5.00550300 0.01647100  
C -4.49898200 0.24063800 -1.82184600  
C -3.35216000 -2.00432600 -1.83044600  
H -3.18645700 -3.28844200 -3.41987100  
H -5.43492100 1.13898800 -3.41096600  
H -5.38535500 2.90470500 1.32206000  
H -2.88263500 -0.38050000 4.33636000

R EEF -5.14 V/nm along X direction

C 5.31801600 -1.17291600 0.00000000  
C 3.07603300 -2.56127200 0.00000000  
C 0.77247900 -1.30610600 0.00000000  
C 0.68929900 1.34391500 0.00000000  
C 2.92736600 2.71758600 0.00000000  
C 5.24244100 1.45577600 0.00000000  
C -1.83698100 -2.56752300 0.00000000  
C -1.86883600 2.50931900 0.00000000  
C -3.97996100 1.12512400 1.44234200  
C -3.26049700 -1.45064100 2.21503200  
H 7.12476500 -2.14255200 0.00000000  
H 3.13650100 -4.61453900 0.00000000  
H 2.88023900 4.77145600 0.00000000  
H 6.99084000 2.52690500 0.00000000  
H -1.67629900 -4.62784300 0.00000000  
H -1.96902000 4.56103500 0.00000000  
C -3.97996100 1.12512400 -1.44234300  
C -3.26049500 -1.45064100 -2.21503200  
H -2.82964700 -1.96340900 -4.15533000  
H -5.29351200 2.25956700 -2.53774400  
H -5.29351400 2.25956700 2.53774300  
H -2.82964900 -1.96340900 4.15533000

TS EEF -5.14 V/nm along X direction  
C 5.22933461 -1.55920585 0.19968574  
C 2.87391061 -2.74531185 0.25387374  
C 0.68133661 -1.31010585 0.20073274  
C 0.82200961 1.35205215 0.11830874  
C 3.19114661 2.51701415 0.01069274  
C 5.38277061 1.06575315 0.06851374  
C -2.00561139 -2.39439885 0.11490874  
C -1.53698139 2.76056015 0.09001974  
C -3.94398539 1.55462015 0.99178374  
C -3.46772139 -0.98035185 2.12013974  
H 6.94485361 -2.68150485 0.24212674  
H 2.75995461 -4.79575985 0.31706774  
H 3.32110361 4.56493815 -0.08153026  
H 7.21703461 1.98009015 0.01165574  
H -1.97991839 -4.45238685 0.31404974  
H -1.52106239 4.77756015 -0.28991826  
C -4.06280239 1.04172115 -1.81115526  
C -3.22328939 -1.39988685 -2.28984426  
H -2.77210339 -2.14882185 -4.14348626  
H -4.85041039 2.35327715 -3.17030226  
H -5.32660039 2.80299015 1.87404074  
H -3.07983839 -1.23898785 4.12068174

P EEF -5.14 V/nm along X direction  
C 5.24329700 -1.45653900 -0.12015300  
C 2.89680400 -2.61392700 0.23491800  
C 0.70398600 -1.18949200 0.33267700  
C 0.82636200 1.50601400 0.10240200  
C 3.22765500 2.62531600 -0.28731600  
C 5.39487000 1.16842800 -0.38716300  
C -1.92311300 -2.37081700 0.64446700  
C -1.40545800 2.96978700 0.28088900  
C -3.91183900 1.61315800 0.65614300  
C -3.37492400 -0.61647200 2.35241700  
H 6.94871100 -2.59243900 -0.19047500  
H 2.79302000 -4.65679500 0.43030400  
H 3.35532000 4.66652400 -0.47637400  
H 7.22079400 2.05983600 -0.66197500  
H -1.77211600 -4.33092300 1.28578300  
H -1.33885300 5.00499300 0.02015800  
C -4.50315900 0.23742700 -1.82544600  
C -3.35285900 -2.00688000 -1.83288000  
H -3.16622600 -3.28094000 -3.42856000  
H -5.41567900 1.14296700 -3.42532800  
H -5.38997200 2.90465600 1.31763700  
H -2.86329300 -0.36895000 4.32807400

R EEF -2.52 V/nm along Y direction  
C 5.33122600 -1.16776800 0.00000000  
C 3.08882500 -2.55485000 0.00000000  
C 0.78187300 -1.30699700 0.00000000  
C 0.69389100 1.34809100 0.00000000  
C 2.93508000 2.71894700 0.00000000  
C 5.25128600 1.46044900 0.00000000  
C -1.82020900 -2.56538500 0.00000000  
C -1.85587200 2.51773200 0.00000000  
C -3.96857800 1.12722800 1.43992100  
C -3.24931700 -1.44265700 2.20898700  
H 7.14034200 -2.13876100 0.00000000  
H 3.13675200 -4.61111500 0.00000000  
H 2.88063400 4.77162800 0.00000000  
H 6.99307200 2.54451500 0.00000000  
H -1.66956200 -4.62863500 0.00000000  
H -1.95896100 4.56716200 0.00000000  
C -3.96857800 1.12722800 -1.43992100

C -3.24931700 -1.44265700 -2.20898700  
H -2.92320100 -2.00583700 -4.15364000  
H -5.28328700 2.26102600 -2.52704300  
H -5.28328700 2.26102600 2.52704100  
H -2.92320100 -2.00583700 4.15363900

TS EEF -2.52 V/nm along Y direction  
C 5.23337519 -1.56337099 0.19060737  
C 2.87648319 -2.74428399 0.24944637  
C 0.68115019 -1.31346799 0.20252437  
C 0.81757719 1.35489801 0.12358437  
C 3.19042019 2.51373301 0.01240437  
C 5.38162419 1.06224701 0.06092737  
C -1.99986181 -2.39375499 0.12163637  
C -1.53514481 2.76846101 0.10478937  
C -3.94777381 1.55466101 0.98684737  
C -3.47301581 -0.97548699 2.11572737  
H 6.94986119 -2.68914199 0.23181637  
H 2.74646119 -4.79639899 0.31308037  
H 3.31560919 4.56133201 -0.07802263  
H 7.21105719 1.98912401 0.00046937  
H -1.98636381 -4.45397699 0.31855937  
H -1.52211281 4.78338601 -0.27761563  
C -4.05929081 1.03750301 -1.81355363  
C -3.20620381 -1.39185399 -2.28594763  
H -2.83563381 -2.18181999 -4.13914363  
H -4.87284481 2.33715701 -3.16592163  
H -5.33656081 2.80078701 1.84957037  
H -3.18533181 -1.27030899 4.12571437

P EEF -2.52 V/nm along Y direction  
C 5.26172700 -1.45381800 -0.10775600  
C 2.91357500 -2.60947500 0.24103500  
C 0.71552100 -1.19169800 0.32703600  
C 0.83868200 1.50468400 0.09318400  
C 3.23759000 2.62524100 -0.28871100  
C 5.40804100 1.16900200 -0.37937000  
C -1.90881500 -2.36679400 0.63048100  
C -1.39740400 2.96805200 0.26079000  
C -3.90087600 1.61823900 0.66010800  
C -3.36086400 -0.61591500 2.34251900  
H 6.96899000 -2.59190600 -0.17168500  
H 2.79589100 -4.65388300 0.43865500  
H 3.35787500 4.66562400 -0.48524000  
H 7.22856200 2.07431900 -0.65473000  
H -1.76724800 -4.33093700 1.26927900  
H -1.33422500 5.00122300 -0.00832800  
C -4.49061700 0.25251100 -1.82707900  
C -3.35434600 -1.99622100 -1.84146300  
H -3.23063900 -3.29222900 -3.42501700  
H -5.48029500 1.14195800 -3.38508500  
H -5.37204800 2.90692300 1.32033900  
H -2.93574900 -0.40997200 4.34123700

R EEF -3.85 V/nm along Y direction  
C 5.32488900 -1.17153800 0.00000000  
C 3.08216500 -2.55871700 0.00000000  
C 0.77557400 -1.31031000 0.00000000  
C 0.68768700 1.34471300 0.00000000  
C 2.92873500 2.71605900 0.00000000  
C 5.24474400 1.45682800 0.00000000  
C -1.82757000 -2.56524900 0.00000000  
C -1.86161700 2.51564600 0.00000000  
C -3.97548800 1.12739800 1.44009700  
C -3.25712000 -1.44221300 2.20977100  
H 7.13545600 -2.14082600 0.00000000

H 3.12848400 -4.61624400 0.00000000  
H 2.87593400 4.76835500 0.00000000  
H 6.98505400 2.54273900 0.00000000  
H -1.67660900 -4.63013100 0.00000000  
H -1.96528400 4.56467300 0.00000000  
C -3.97548800 1.12739800 -1.44009700  
C -3.25711800 -1.44221300 -2.20977300  
H -2.90802900 -1.99119800 -4.15540500  
H -5.28562500 2.26530400 -2.52808200  
H -5.28562500 2.26530400 2.52808000  
H -2.90803100 -1.99119800 4.15540400

TS EEF -3.85 V/nm along Y direction

C 5.23379138 -1.56339317 0.19303423  
C 2.87703538 -2.74531517 0.25091323  
C 0.68120538 -1.31530817 0.20212423  
C 0.81720638 1.35317583 0.12201623  
C 3.18945438 2.51353183 0.01180023  
C 5.38105538 1.06243483 0.06262223  
C -2.00003562 -2.39323317 0.12025323  
C -1.53497762 2.76761883 0.10385023  
C -3.94791362 1.55502683 0.98665523  
C -3.47238462 -0.97458417 2.11595623  
H 6.95228638 -2.68708117 0.23657123  
H 2.74606038 -4.79858817 0.31562223  
H 3.31511338 4.56067283 -0.07892777  
H 7.20880538 1.99216183 0.00386523  
H -1.98543962 -4.45499817 0.31868623  
H -1.52302962 4.78259283 -0.27719577  
C -4.05930762 1.03848283 -1.81378377  
C -3.20930662 -1.39194917 -2.28705877  
H -2.81932862 -2.16904917 -4.14247377  
H -4.86682562 2.34264583 -3.16541677  
H -5.33297562 2.80467283 1.84947423  
H -3.16865262 -1.25959717 4.12557323

P EEF -3.85 V/nm along Y direction

C 5.26125500 -1.45455100 -0.10829800  
C 2.91344900 -2.61107500 0.24192500  
C 0.71471500 -1.19426600 0.32740800  
C 0.83657100 1.50211400 0.09172500  
C 3.23479500 2.62399000 -0.29225000  
C 5.40587000 1.16831600 -0.38214400  
C -1.90951600 -2.36832100 0.63346500  
C -1.39897600 2.96595800 0.26123400  
C -3.90216300 1.61637400 0.66744000  
C -3.35899300 -0.61756500 2.34888300  
H 6.97078100 -2.59040500 -0.16983700  
H 2.79514800 -4.65640200 0.44283900  
H 3.35534400 4.66391000 -0.48939600  
H 7.22461900 2.07676400 -0.65713600  
H -1.76561200 -4.33379800 1.27279200  
H -1.33834600 4.99947800 -0.00261900  
C -4.49229800 0.25377900 -1.82018100  
C -3.35916900 -1.99715800 -1.83630600  
H -3.22669500 -3.28443200 -3.42709900  
H -5.47609000 1.14979900 -3.37808900  
H -5.37026200 2.90706900 1.32872900  
H -2.92114200 -0.40464900 4.34435500

R EEF -5.14 V/nm along Y direction

C 5.32826600 -1.17105800 0.00000000  
C 3.08629800 -2.56022100 0.00000000  
C 0.77907200 -1.31300300 0.00000000  
C 0.68921200 1.34198400 0.00000000  
C 2.92902400 2.71570800 0.00000000

C 5.24585900 1.45745800 0.00000000  
C -1.82419100 -2.56654600 0.00000000  
C -1.86058000 2.51221200 0.00000000  
C -3.97457800 1.12445200 1.44033100  
C -3.25514500 -1.44433700 2.21055300  
H 7.14104500 -2.13729200 0.00000000  
H 3.13265500 -4.61914600 0.00000000  
H 2.87625700 4.76774300 0.00000000  
H 6.98385200 2.54666000 0.00000000  
H -1.67130300 -4.63314700 0.00000000  
H -1.96647400 4.56091400 0.00000000  
C -3.97457800 1.12445200 -1.44033100  
C -3.25514500 -1.44433700 -2.21055500  
H -2.88399500 -1.97959900 -4.15685100  
H -5.28097600 2.26561600 -2.52913300  
H -5.28097800 2.26561600 2.52913100  
H -2.88399500 -1.97959900 4.15684900

TS EEF -5.14 V/nm along Y direction

C 5.23463435 -1.56248701 0.19269411  
C 2.87821935 -2.74594301 0.25079911  
C 0.68161335 -1.31706001 0.20132011  
C 0.81668435 1.35166499 0.11990511  
C 3.18805835 2.51406599 0.00963811  
C 5.38038135 1.06362699 0.06166611  
C -1.99974665 -2.39312001 0.12006611  
C -1.53531565 2.76660899 0.10337611  
C -3.94784665 1.55477499 0.98852011  
C -3.47047365 -0.97419401 2.11807611  
H 6.95535735 -2.68389401 0.23762711  
H 2.74671135 -4.80058301 0.31660311  
H 3.31380535 4.56093699 -0.08133389  
H 7.20625335 1.99661399 0.00380811  
H -1.98352265 -4.45661501 0.32023511  
H -1.52501865 4.78178999 -0.27635189  
C -4.06024365 1.03873199 -1.81191589  
C -3.21356465 -1.39296701 -2.28639789  
H -2.80467365 -2.15708701 -4.14396289  
H -4.86276565 2.34723599 -3.16240289  
H -5.32892665 2.80789999 1.85205111  
H -3.15045765 -1.24970501 4.12707111

P EEF -5.14 V/nm along Y direction

C 5.26087300 -1.45533000 -0.10553200  
C 2.91289100 -2.61276500 0.24286200  
C 0.71335100 -1.19682100 0.32472500  
C 0.83429000 1.49967000 0.08712400  
C 3.23242700 2.62289900 -0.29541000  
C 5.40423700 1.16766200 -0.38133700  
C -1.91123200 -2.36982300 0.62989900  
C -1.40094900 2.96411600 0.25497900  
C -3.90446900 1.61467000 0.66437300  
C -3.36066400 -0.61874900 2.34615300  
H 6.97273900 -2.58905600 -0.16220700  
H 2.79370000 -4.65917500 0.44700500  
H 3.35355800 4.66250400 -0.49302200  
H 7.22162500 2.07930000 -0.65328000  
H -1.76584400 -4.33666400 1.27046900  
H -1.34253000 4.99804600 -0.00431600  
C -4.49103200 0.25472200 -1.82436100  
C -3.36156900 -1.99880200 -1.83986600  
H -3.21766600 -3.27765400 -3.43739400  
H -5.46647200 1.15713600 -3.38381100  
H -5.37055500 2.90760600 1.32416600  
H -2.91338800 -0.39856600 4.33898100

R EEF -2.52 V/nm along Z direction  
C 5.33483300 -1.16420800 0.00197500  
C 3.09202200 -2.54975600 -0.01513100  
C 0.78524400 -1.30104900 -0.03674000  
C 0.69920300 1.35460000 -0.04033800  
C 2.94171700 2.72312900 -0.02650700  
C 5.25739400 1.46401700 -0.00481100  
C -1.81573700 -2.56432200 -0.01174800  
C -1.85057600 2.52370400 -0.01766900  
C -3.94438900 1.13159100 1.44387400  
C -3.22012100 -1.43839000 2.20752400  
H 7.13969600 -2.14000000 0.05409300  
H 3.14139700 -4.60373000 0.02220400  
H 2.88537900 4.77694800 0.00190500  
H 7.00245100 2.54323200 0.04104900  
H -1.66747600 -4.62500600 -0.00514000  
H -1.95102800 4.57450700 -0.00693000  
C -3.97959100 1.12850100 -1.43588400  
C -3.26614700 -1.44360200 -2.20756400  
H -2.97485500 -2.02445700 -4.15330800  
H -5.31989900 2.25359200 -2.50336700  
H -5.24972200 2.26049300 2.54700200  
H -2.96019500 -2.04526500 4.14550500

TS EEF -2.52 V/nm along Z direction  
C 5.23333229 -1.56280424 0.20002059  
C 2.87579929 -2.74262124 0.24318959  
C 0.68158629 -1.31063424 0.17799959  
C 0.82102729 1.35745676 0.09864759  
C 3.19493329 2.51429976 -0.00090541  
C 5.38531729 1.06198776 0.06554759  
C -1.99948571 -2.39492324 0.12192959  
C -1.53224571 2.77094976 0.09649759  
C -3.93526171 1.55555076 1.00032359  
C -3.45679071 -0.97589324 2.12381659  
H 6.94502929 -2.69121724 0.28950459  
H 2.74784829 -4.79139924 0.34144759  
H 3.31963429 4.56441776 -0.06235141  
H 7.21861829 1.98446976 0.04830359  
H -1.98737871 -4.45168824 0.32402959  
H -1.51542071 4.79125476 -0.26385141  
C -4.07561371 1.03525976 -1.80077141  
C -3.22448471 -1.39430124 -2.27716841  
H -2.88968671 -2.20342024 -4.12951041  
H -4.91749071 2.32745476 -3.14444441  
H -5.31854971 2.79647576 1.87949759  
H -3.22293671 -1.30625524 4.13242659

P EEF -2.52 V/nm along Z direction  
C 5.26713400 -1.45111000 -0.11306800  
C 2.91683700 -2.60628700 0.21943100  
C 0.71831200 -1.18789000 0.29233900  
C 0.84443400 1.50920400 0.06029700  
C 3.24636200 2.62813600 -0.30627900  
C 5.41702100 1.17175000 -0.38232000  
C -1.90325000 -2.36374200 0.62058300  
C -1.39051200 2.97241800 0.23776200  
C -3.89079600 1.62437300 0.65409700  
C -3.34458200 -0.60950700 2.33564000  
H 6.97385900 -2.58999000 -0.13406500  
H 2.80383100 -4.64588800 0.44493400  
H 3.36882000 4.67266200 -0.47101300  
H 7.24559600 2.07482600 -0.61456600  
H -1.76228700 -4.32248800 1.26512300  
H -1.31518200 5.01224000 0.01601400  
C -4.50415800 0.24828200 -1.82458400

C -3.36444100 -1.99831100 -1.84273500  
H -3.27909800 -3.31941300 -3.40817900  
H -5.52778400 1.12111600 -3.37189400  
H -5.35967500 2.90932300 1.32842900  
H -2.96710900 -0.43477300 4.34425000

R EEF -3.85 V/nm along Z direction  
C 5.32983500 -1.16645800 0.00305000  
C 3.08654400 -2.55116900 -0.02269400  
C 0.78026100 -1.30157000 -0.05522000  
C 0.69531200 1.35417600 -0.06063600  
C 2.93836500 2.72186400 -0.03986200  
C 5.25347900 1.46184900 -0.00720200  
C -1.82117100 -2.56376600 -0.01769900  
C -1.85392600 2.52435200 -0.02654300  
C -3.93922800 1.13390800 1.44604500  
C -3.21330300 -1.43587300 2.20766400  
H 7.13354500 -2.14265200 0.08138100  
H 3.13481700 -4.60476900 0.03339700  
H 2.88262500 4.77548700 0.00277000  
H 6.99828400 2.54027300 0.06168400  
H -1.67385800 -4.62451900 -0.00779700  
H -1.95357700 4.57518400 -0.01041100  
C -3.99213300 1.12931800 -1.43401000  
C -3.28249100 -1.44361900 -2.20777200  
H -2.98232700 -2.01709100 -4.15597200  
H -5.34075700 2.25384500 -2.49261600  
H -5.23532400 2.26412000 2.55823100  
H -2.95984900 -2.04831100 4.14420300

TS EEF -3.85 V/nm along Z direction  
C 5.23356464 -1.56249103 0.20762960  
C 2.87595064 -2.74266703 0.24220460  
C 0.68180064 -1.31107603 0.16564760  
C 0.82229064 1.35687997 0.08482160  
C 3.19614664 2.51413297 -0.00872940  
C 5.38643264 1.06201597 0.06899160  
C -1.99944836 -2.39499203 0.12029060  
C -1.53050136 2.77121897 0.09229160  
C -3.92913336 1.55613597 1.00680660  
C -3.44809736 -0.97550803 2.12787560  
H 6.94443864 -2.68972103 0.32382860  
H 2.74792364 -4.79041103 0.35928560  
H 3.32089064 4.56468197 -0.05657540  
H 7.21956564 1.98500597 0.07444360  
H -1.98709436 -4.45130703 0.32609860  
H -1.51281336 4.79386597 -0.25590740  
C -4.08391336 1.03525797 -1.79474740  
C -3.23623836 -1.39499903 -2.27434940  
H -2.89945336 -2.20011703 -4.12932140  
H -4.93352636 2.32836397 -3.13347140  
H -5.30599936 2.79751097 1.89463960  
H -3.22307836 -1.31279803 4.13578960

P EEF -3.85 V/nm along Z direction  
C 5.26925800 -1.45046000 -0.11590800  
C 2.91835800 -2.60612400 0.21066300  
C 0.71889200 -1.18854700 0.27604600  
C 0.84506700 1.50866200 0.04253200  
C 3.24762200 2.62794900 -0.31958500  
C 5.41904900 1.17223700 -0.38763000  
C -1.90113500 -2.36371600 0.61861000  
C -1.38880900 2.97229300 0.22721300  
C -3.88711300 1.62545800 0.65884800  
C -3.33492000 -0.60837700 2.33865600  
H 6.97763500 -2.58713400 -0.11278100

H 2.80702300 -4.64369200 0.45412800  
H 3.37123300 4.67365000 -0.46980700  
H 7.24943100 2.07713300 -0.59883900  
H -1.75845100 -4.32098300 1.26617600  
H -1.30956000 5.01499100 0.03517300  
C -4.51226700 0.24786200 -1.81646800  
C -3.37317800 -1.99934200 -1.83874600  
H -3.29786600 -3.32359700 -3.40303500  
H -5.54631100 1.11919500 -3.35871400  
H -5.35178600 2.91015700 1.34153600  
H -2.96889100 -0.44268400 4.34937600

R EEF -5.14 V/nm along Z direction

C 5.33429800 -1.16449700 0.00426300  
C 3.09166500 -2.55018100 -0.03024700  
C 0.78489000 -1.30154200 -0.07383700  
C 0.69891900 1.35426700 -0.08108400  
C 2.94142000 2.72291900 -0.05331300  
C 5.25694600 1.46385000 -0.00953400  
C -1.81595600 -2.56473200 -0.02376900  
C -1.85068700 2.52348300 -0.03547200  
C -3.92622100 1.13303900 1.44829000  
C -3.19658100 -1.43598800 2.20781700  
H 7.13731900 -2.13951700 0.10899900  
H 3.14035600 -4.60320800 0.04468800  
H 2.88455100 4.77621700 0.00356600  
H 7.00035900 2.54283700 0.08251500  
H -1.66798400 -4.62544100 -0.01059800  
H -1.95119200 4.57425800 -0.01391000  
C -3.99693500 1.12694800 -1.43218200  
C -3.28908100 -1.44624800 -2.20809700  
H -2.97934700 -2.01177100 -4.15896200  
H -5.35481100 2.24978000 -2.48187500  
H -5.21394700 2.26344700 2.56963000  
H -2.94837600 -2.05338700 4.14310300

TS EEF -5.14 V/nm along Z direction

C 5.23413042 -1.56123194 0.21284536  
C 2.87668542 -2.74221294 0.24013836  
C 0.68230242 -1.31144894 0.15308336  
C 0.82331742 1.35643706 0.07056036  
C 3.19688842 2.51452206 -0.01856864

C 5.38735142 1.06300806 0.06937936  
C -1.99892558 -2.39546494 0.11955936  
C -1.52915258 2.77124306 0.08916636  
C -3.92277158 1.55595806 1.01530336  
C -3.43813758 -0.97584294 2.13366736  
H 6.94415442 -2.68678294 0.35510036  
H 2.74890742 -4.78875694 0.37642436  
H 3.32121142 4.56545006 -0.05315964  
H 7.21990342 1.98683506 0.09631536  
H -1.98592258 -4.45133394 0.32902636  
H -1.51111658 4.79614006 -0.24706664  
C -4.09326858 1.03461106 -1.78669364  
C -3.24882658 -1.39617094 -2.27004964  
H -2.91027058 -2.19670294 -4.12814064  
H -4.95146458 2.32851006 -3.12009964  
H -5.29296158 2.79743306 1.91265136  
H -3.22038958 -1.31973994 4.14089836

P EEF -5.14 V/nm along Z direction

C 5.27140100 -1.44983800 -0.11514500  
C 2.91950100 -2.60595400 0.20274900  
C 0.71898600 -1.18920700 0.25712600  
C 0.84550300 1.50806400 0.02165400  
C 3.24911700 2.62763700 -0.33329500  
C 5.42141100 1.17261100 -0.39011700  
C -1.90000900 -2.36367400 0.61011300  
C -1.38757000 2.97225300 0.21033200  
C -3.88449000 1.62659400 0.65358700  
C -3.32897300 -0.60707500 2.33274100  
H 6.98117300 -2.58411500 -0.08514500  
H 2.80947600 -4.64125400 0.46468200  
H 3.37398800 4.67439100 -0.46940100  
H 7.25360900 2.07926800 -0.57816400  
H -1.75665600 -4.31940500 1.26117200  
H -1.30395900 5.01736700 0.04776100  
C -4.51727700 0.24739200 -1.81940800  
C -3.37878600 -2.00044800 -1.84382900  
H -3.31056100 -3.32763900 -3.40710000  
H -5.55873200 1.11728000 -3.35865700  
H -5.34605100 2.91102600 1.34229200  
H -2.97777300 -0.45034500 4.34624700

## Chemo- or Site-selectivity

### Arene molecule R<sub>D</sub>

R of site A No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50799600  
C 7.19316800 0.00000000 -0.32768400  
C 4.79466800 -0.00595800 0.71633500  
C 2.66306700 0.00169300 -0.86869600  
C 2.99716500 0.01192000 -3.48763600  
C 5.40786700 0.00410100 -4.56109800  
C 7.49048200 0.00884000 -2.95137200  
H 8.85099900 0.00221100 0.88063000  
H 4.53423000 -0.01226600 2.74987400  
H 1.33191000 0.05209400 -4.68441600  
H 9.38239200 0.01980800 -3.75279500  
H -1.74064400 -0.00184100 3.03943100  
C 5.76008400 -0.02827400 -7.39660100  
H 5.16026000 -1.88705500 -8.12888100  
H 7.75488700 0.19375000 -7.92984200  
C 4.02065700 1.77099900 -8.76200000  
O 5.23591400 2.52630600 -10.80010500

H 4.11619700 3.62632900 -11.73000500

TS of site A No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48296100  
C 7.00733200 0.00000000 -1.14268000  
C 4.71429200 -0.00421600 0.11890400  
C 2.46643900 -0.00608500 -1.27748900  
C 2.52837000 -0.00849600 -3.91296700  
C 4.83181400 -0.01847200 -5.19687000  
C 7.05518900 -0.00311400 -3.78134000  
H 8.77008300 0.01126500 -0.09436900  
H 4.60575600 0.00020800 2.16766800  
H 0.76599500 0.02763000 -4.96101300  
H 8.86380500 0.00789100 -4.75574900  
H -1.90693100 0.00603000 1.37624300  
C 4.92939600 -0.07140300 -8.05242900  
H 4.40320300 -1.98079700 -8.70783500  
H 6.84786900 0.27836200 -8.76594000

C 2.95274700 1.57633100 -9.27798800  
O 3.90571400 2.33836100 -11.44652700  
H 2.63264100 3.33946700 -12.28685900

P of site A No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28838200  
C 6.82885100 0.00000000 -1.97607400  
C 4.69453500 -0.00609200 -0.45847400  
C 2.30622500 -0.01109100 -1.58669000  
C 2.06975000 -0.01725500 -4.20907200  
C 4.21017000 -0.02400500 -5.74976600  
C 6.58180700 -0.00446900 -4.60151300  
H 8.69712600 0.01481700 -1.13074500  
H 4.82267600 0.00099800 1.58762400  
H 0.21067200 0.01995900 -5.08156400  
H 8.26702400 0.00881000 -5.77584600  
H -1.80353600 0.00880200 -1.07667200  
C 3.97744600 -0.08640800 -8.59798300  
H 3.51545900 -2.03292100 -9.19111000  
H 5.77192500 0.38843100 -9.52853800  
C 1.76502900 1.40923000 -9.58959300  
O 2.39109600 2.18504000 -11.86812200  
H 0.96323200 3.08769800 -12.55774300

R of site A EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50502800  
C 7.19650500 0.00000000 -0.30557500  
C 4.79352500 -0.01874600 0.72885300  
C 2.66778600 0.01292000 -0.86310600  
C 3.01137200 0.05988400 -3.47996600  
C 5.42608600 0.06920600 -4.54334700  
C 7.50369900 0.04896800 -2.92721200  
H 8.84886000 -0.01785200 0.90974500  
H 4.52596000 -0.05425600 2.76099900  
H 1.34902900 0.11534700 -4.68049800  
H 9.39858500 0.07125000 -3.72137100  
H -1.73858500 -0.01073000 3.04439900  
C 5.79030500 0.08934300 -7.37878300  
H 5.12419500 -1.72731200 -8.15709500  
H 7.79479800 0.25553800 -7.89616300  
C 4.12257000 1.98898700 -8.69512800  
O 5.41285600 2.84069000 -10.65042100  
H 4.33781100 4.01603600 -11.53949100

TS of site A EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47980700  
C 7.01285600 0.00000000 -1.11921900  
C 4.71398200 -0.00964500 0.13231900  
C 2.47210500 -0.00127900 -1.27285600  
C 2.54475200 0.01225100 -3.90742800  
C 4.85374300 0.00963600 -5.18080700  
C 7.07191200 0.01408800 -3.75725500  
H 8.77037000 0.00263000 -0.06239700  
H 4.59726500 -0.01731700 2.18056900  
H 0.78539900 0.05508400 -4.96056100  
H 8.88464700 0.03000700 -4.72400700  
H -1.90925300 0.00307500 1.36993700  
C 4.96363200 -0.01791100 -8.03724300  
H 4.37759600 -1.90180600 -8.71508200  
H 6.89604800 0.28072500 -8.73667400  
C 3.04604900 1.70811800 -9.24620300  
O 4.06042200 2.53162000 -11.36684900  
H 2.82278500 3.59107300 -12.18772700

P of site A EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28694200  
C 6.83674300 0.00000000 -1.95162100  
C 4.69553700 -0.01019100 -0.44355700  
C 2.31206900 -0.00853200 -1.58160100  
C 2.08653800 -0.00353600 -4.20446500  
C 4.23396900 -0.00452000 -5.73516000  
C 6.60105200 0.00770400 -4.57794700  
H 8.70075000 0.00908600 -1.09714300  
H 4.81489200 -0.01135700 1.60304600  
H 0.22997800 0.03844800 -5.08222600  
H 8.29137900 0.02501400 -5.74500600  
H -1.80207800 0.00815600 -1.07944400  
C 4.01333000 -0.04814100 -8.58554900  
H 3.49746900 -1.97767300 -9.18988700  
H 5.82499100 0.38321600 -9.50432500  
C 1.84785200 1.51506000 -9.57319400  
O 2.52879800 2.34848800 -11.81817800  
H 1.12847300 3.30112400 -12.49624600

R of site A EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51103100  
C 7.18978000 0.00000000 -0.34909300  
C 4.79562600 0.00232800 0.70398800  
C 2.65837300 -0.00601100 -0.87408700  
C 2.98337200 -0.02020500 -3.49464400  
C 5.39024600 -0.03947500 -4.57758000  
C 7.47767200 -0.01776300 -2.97426000  
H 8.85285600 0.01583200 0.85225400  
H 4.54204200 0.01552600 2.73854900  
H 1.31555800 0.01025200 -4.68788100  
H 9.36666000 -0.01391600 -3.78252600  
H -1.74264800 0.00432000 3.03452200  
C 5.73121800 -0.10719500 -7.41290200  
H 5.18809400 -1.99624300 -8.11129000  
H 7.71578100 0.16441400 -7.96071800  
C 3.93215500 1.61198400 -8.80660700  
O 5.09046300 2.30374100 -10.89653700  
H 3.93559200 3.34432300 -11.85216700

TS of site A EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48618700  
C 7.00174400 0.00000000 -1.16596300  
C 4.71454000 0.00043500 0.10552000  
C 2.46076500 -0.01050300 -1.28210000  
C 2.51209500 -0.02702900 -3.91839400  
C 4.81004500 -0.04350300 -5.21268100  
C 7.03854100 -0.01822800 -3.80511800  
H 8.76964200 0.01905600 -0.12615100  
H 4.61413900 0.01562600 2.15471900  
H 0.74667100 0.00299100 -4.96127200  
H 8.84303700 -0.01130800 -4.78706200  
H -1.90459900 0.00879700 1.38257000  
C 4.89582300 -0.11846100 -8.06735600  
H 4.42396800 -2.04851300 -8.70303700  
H 6.80008000 0.27745700 -8.79423300  
C 2.86792300 1.45975900 -9.30384000  
O 3.76917900 2.16989400 -11.50875800  
H 2.46686800 3.12004300 -12.36404800

P of site A EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 2.28985800  
C 6.82110000 0.00000000 -1.99951100  
C 4.69345000 -0.00229200 -0.47282700  
C 2.30048500 -0.01340800 -1.59159600  
C 2.05357200 -0.02988600 -4.21347700  
C 4.18726600 -0.04205800 -5.76374100  
C 6.56321600 -0.01568300 -4.62404300  
H 8.69344100 0.02009200 -1.16301700  
H 4.83001200 0.01241700 1.57274600  
H 0.19207800 0.00285900 -5.08091400  
H 8.24349900 -0.00608900 -5.80530900  
H -1.80496100 0.00935400 -1.07393900  
C 3.94308900 -0.12129800 -8.60984100  
H 3.52790300 -2.08115600 -9.19297100  
H 5.72131100 0.39074300 -9.55137100  
C 1.69143800 1.31640100 -9.60287200  
O 2.27142500 2.04043800 -11.90767200  
H 0.82168500 2.90053800 -12.60677100

R of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50799600  
C 7.19316800 0.00000000 -0.32768400  
C 4.79466800 -0.00595800 0.71633500  
C 2.66306700 0.00169300 -0.86869600  
C 2.99716500 0.01192000 -3.48763600  
C 5.40786700 0.00410300 -4.56109800  
C 7.49048200 0.00884000 -2.95137200  
H 8.85099900 0.00220900 0.88063000  
H 4.53423000 -0.01226600 2.74987400  
H 1.33191000 0.05209400 -4.68441600  
H 9.38239200 0.01981000 -3.75279500  
H -1.74064400 -0.00184100 3.03943100  
C 5.76008400 -0.02827200 -7.39660100  
H 5.16025800 -1.88705100 -8.12888100  
H 7.75488700 0.19375000 -7.92984200  
C 4.02065700 1.77100500 -8.76199800  
O 5.23591500 2.52631200 -10.80010100  
H 4.11620100 3.62633700 -11.73000300

TS of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50523200  
C 7.19757900 0.00000000 -0.33240300  
C 4.79885900 -0.00645000 0.71317500  
C 2.66538000 0.00161900 -0.86786300  
C 2.99901000 0.01081100 -3.48608300  
C 5.40830600 0.00658400 -4.55979200  
C 7.49522900 0.01364600 -2.95533400  
H 8.85545300 -0.00065800 0.87529300  
H 4.54047900 -0.01510500 2.74687500  
H 1.32477800 0.03385400 -4.67301300  
H 9.38525700 0.02729900 -3.75926200  
H -1.73990700 -0.00124900 3.04047200  
C 5.74383800 0.01594200 -7.39636800  
H 4.88775400 -1.69527400 -8.20976300  
H 7.74177400 0.04522700 -7.95944800  
C 4.41265800 2.18371500 -8.65736800  
O 5.64656200 3.32544700 -10.45535600  
H 3.59916800 3.98128600 -9.94706500

P of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50308100  
C 7.20159000 0.00000000 -0.33217200  
C 4.80032200 -0.00674800 0.71256900

C 2.66826000 0.00865700 -0.86692000  
C 3.00364000 0.03425700 -3.48586000  
C 5.41027300 0.03096700 -4.56281700  
C 7.49863300 0.01871000 -2.95290800  
H 8.85802300 -0.01738500 0.87720000  
H 4.54184500 -0.02828500 2.74616100  
H 1.32425800 0.05162700 -4.66792600  
H 9.39059700 0.00895700 -3.75484200  
H -1.73961300 -0.00574100 3.04049700  
C 5.73350900 0.15727800 -7.39528400  
H 4.19409400 -0.78334100 -8.39930700  
H 7.51051700 -0.75976100 -7.94877900  
C 5.87569400 2.87396800 -8.31037600  
O 4.75443800 3.67643000 -10.12248500  
H 7.12924000 4.11382400 -7.16568200

R of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50502800  
C 7.19650500 0.00000000 -0.30557500  
C 4.79352500 -0.01874600 0.72885300  
C 2.66778600 0.01292000 -0.86310600  
C 3.01137200 0.05988200 -3.47996600  
C 5.42608600 0.06920600 -4.54334700  
C 7.50369900 0.04896700 -2.92721200  
H 8.84886000 -0.01785200 0.90974500  
H 4.52596000 -0.05425400 2.76099900  
H 1.34902900 0.11534700 -4.68049800  
H 9.39858500 0.07125000 -3.72137100  
H -1.73858500 -0.01073000 3.04439900  
C 5.79030500 0.08934100 -7.37878300  
H 5.12419700 -1.72731600 -8.15709500  
H 7.79479800 0.25553800 -7.89616300  
C 4.12256800 1.98898300 -8.69513000  
O 5.41285200 2.84068500 -10.65042300  
H 4.33780800 4.01603100 -11.53949200

TS of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50239100  
C 7.20056400 0.00000000 -0.31835100  
C 4.79879500 0.01628200 0.72126900  
C 2.66923000 -0.01756700 -0.86400200  
C 3.00875900 -0.07292100 -3.48054600  
C 5.42041500 -0.10709800 -4.54728400  
C 7.50436100 -0.05617600 -2.93958900  
H 8.85470800 0.03356300 0.89369700  
H 4.53609900 0.05850800 2.75388200  
H 1.33668900 -0.07884100 -4.67090200  
H 9.39654000 -0.06297700 -3.73884900  
H -1.73787600 0.01395000 3.04527400  
C 5.76323200 -0.18374800 -7.38238100  
H 4.92730200 -1.93024100 -8.14187300  
H 7.76212500 -0.15578700 -7.94289400  
C 4.41375000 1.91898000 -8.72585500  
O 5.61922400 2.97024200 -10.60051600  
H 3.58595500 3.65617400 -10.08952400

P of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50038300  
C 7.20453300 0.00000000 -0.30667100  
C 4.79795600 0.03463900 0.72659600  
C 2.67306000 -0.02660700 -0.86049700  
C 3.01960600 -0.11890900 -3.47645500  
C 5.43063500 -0.17696900 -4.54064900

C 7.51260700 -0.10857400 -2.92322200  
H 8.85473700 0.04479200 0.91020600  
H 4.53102500 0.10576600 2.75783300  
H 1.34450900 -0.15555500 -4.66444900  
H 9.40835500 -0.15508800 -3.71534900  
H -1.73745800 0.02206100 3.04562600  
C 5.77165500 -0.20077200 -7.37297400  
H 4.22531800 -1.16944600 -8.33980300  
H 7.53326400 -1.18127400 -7.86635100  
C 5.98082300 2.45111000 -8.44968900  
O 5.01542800 3.11869200 -10.40240400  
H 7.13570500 3.77479700 -7.29579900

R of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51103100  
C 7.18978000 0.00000000 -0.34909300  
C 4.79562600 0.00232800 0.70398800  
C 2.65837300 -0.00601100 -0.87408700  
C 2.98337200 -0.02020500 -3.49464400  
C 5.39024600 -0.03947500 -4.57758000  
C 7.47767200 -0.01776300 -2.97426000  
H 8.85285600 0.01583200 0.85225400  
H 4.54204200 0.01552600 2.73854900  
H 1.31555800 0.01025200 -4.68788100  
H 9.36666000 -0.01391600 -3.78252600  
H -1.74264800 0.00431800 3.03452200  
C 5.73121800 -0.10719500 -7.41290200  
H 5.18809400 -1.99624300 -8.11129000  
H 7.71578100 0.16441400 -7.96071800  
C 3.93215500 1.61198400 -8.80660700  
O 5.09046300 2.30374100 -10.89653700  
H 3.93559200 3.34432300 -11.85216700

TS of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50732400  
C 7.19743900 0.00000000 -0.35041600  
C 4.79774100 -0.01663500 0.70095500  
C 2.66158600 0.01134400 -0.87158900  
C 2.99000500 0.05123000 -3.49395400  
C 5.39239600 0.05330500 -4.57048200  
C 7.48962800 0.04269300 -2.96934700  
H 8.85739000 -0.01751400 0.85437800  
H 4.54420400 -0.05080300 2.73521900  
H 1.30783300 0.07336900 -4.67050200  
H 9.37220200 0.07421300 -3.78934600  
H -1.74158900 -0.00848300 3.03609900  
C 5.76552600 0.13462000 -7.41178500  
H 3.97395800 -0.21562400 -8.37807200  
H 7.17215000 -1.26991700 -8.01025900  
C 6.74343200 2.71703400 -8.10664900  
O 9.18219200 2.88171100 -8.43255500  
H 7.93981000 4.70042300 -8.56566500

P of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50578500  
C 7.19798700 0.00000000 -0.36340400  
C 4.80279000 -0.04694600 0.69305900  
C 2.66259100 0.04396600 -0.87370200  
C 2.98484400 0.18569200 -3.49063200  
C 5.38627200 0.23589300 -4.57917900  
C 7.48229400 0.14371800 -2.98243300  
H 8.86141300 -0.07945000 0.83415000  
H 4.55418500 -0.16017700 2.72503300

H 1.30060300 0.25659300 -4.66342300  
H 9.36985000 0.16893400 -3.79389900  
H -1.74133200 -0.03381100 3.03533000  
C 5.68913600 0.50943300 -7.40458900  
H 4.14871800 -0.39269700 -8.44105700  
H 7.47448400 -0.35028500 -8.01639300  
C 5.77460800 3.28060900 -8.14822800  
O 4.47994300 4.21547200 -9.76991800  
H 7.15025200 4.43119600 -7.05099400

R of site A No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49031400  
C 1.52887000 0.00000000 -9.68347800  
O 2.85242000 0.53977000 -11.74423700  
C 4.59786000 5.31279300 -5.91412700  
C 4.06380900 3.74768900 -7.94099500  
C 2.27311300 1.80391600 -7.67407700  
C 1.05000600 1.47976800 -5.35684300  
C 1.56419100 3.05605300 -3.30391900  
C 3.35450300 4.96098100 -3.61137200  
H 5.98349500 6.81419400 -6.09929200  
H 5.01448700 3.99800800 -9.74004200  
H -0.30245100 -0.05121700 -5.17232600  
H 3.79193700 6.19650500 -2.02899400  
H 2.34544400 -0.64727500 -13.02726300  
C 0.20344000 2.72486500 -0.81340800  
H -1.79296200 3.27809000 -1.05756900  
H 0.97678100 3.96634800 0.66090400  
H -0.20040600 -1.72852200 3.03850100

TS of site A No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48840200  
C 1.69135500 0.00000000 -9.72511800  
O 2.82692600 0.40075400 -11.89653200  
C 4.32372700 5.46841600 -6.04164800  
C 3.86450800 3.82289900 -8.02417100  
C 2.21330900 1.78668600 -7.66328500  
C 1.03561200 1.41579100 -5.33415300  
C 1.47788200 3.07464400 -3.33245000  
C 3.13708500 5.08651200 -3.71550200  
H 5.60480700 7.05205600 -6.28098300  
H 4.75457000 4.06136100 -9.85721800  
H -0.20885800 -0.19447600 -5.08069300  
H 3.51396600 6.38377000 -2.16770200  
H 1.46707100 -1.31866300 -11.65925400  
C 0.17473500 2.72641900 -0.81348800  
H -1.82876600 3.27328300 -1.01160900  
H 0.97211500 3.96875700 0.64688800  
H -0.18270600 -1.72965200 3.03971300

P of site A No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48722800  
C 1.77557200 0.00000000 -9.69898200  
O 2.63930400 0.23444700 -11.80513300  
C 3.57353200 5.90125600 -6.16743700  
C 3.34681600 4.14920100 -8.10055600  
C 2.02586500 1.90418300 -7.66234200  
C 0.94075500 1.43245300 -5.31018700  
C 1.14936000 3.19366300 -3.35823600  
C 2.48418600 5.41934000 -3.81476900  
H 4.60203300 7.64888900 -6.47290200  
H 4.17415900 4.46606300 -9.94932900  
H -0.05089600 -0.33240900 -4.96272100

H 2.67867800 6.80180200 -2.30805900  
H 0.70560500 -1.72515200 -9.15951900  
C -0.07068000 2.72867300 -0.81578800  
H -2.11716100 3.10430200 -0.97478300  
H 0.64231800 4.03519200 0.63201700  
H -0.02751100 -1.73823500 3.04115100

R of site A EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48760800  
C 1.57515700 0.00000000 -9.67557700  
O 2.93484400 0.50915700 -11.72487800  
C 4.69162300 5.26270200 -5.88196600  
C 4.14915400 3.70832600 -7.91411900  
C 2.32884600 1.78931600 -7.66160700  
C 1.08633200 1.47937500 -5.35196500  
C 1.61044800 3.04444100 -3.29258300  
C 3.42923600 4.92431100 -3.58717200  
H 6.10013300 6.74420500 -6.05446000  
H 5.11633300 3.94682300 -9.70602500  
H -0.28788500 -0.03308200 -5.17605600  
H 3.87563500 6.14977800 -1.99976400  
H 2.41712500 -0.67519200 -13.00522700  
C 0.23496300 2.72602200 -0.80926800  
H -1.75354400 3.30255100 -1.06050700  
H 1.01712500 3.95595200 0.66954000  
H -0.21946300 -1.72421300 3.04326900

TS of site A EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48579800  
C 1.52981900 0.00000000 -9.74390600  
O 2.60747500 0.40790500 -11.94738800  
C 4.20828900 5.48509900 -6.12433300  
C 3.71705500 3.83586800 -8.09552000  
C 2.08463100 1.79043100 -7.69846400  
C 0.95795200 1.41519900 -5.34405100  
C 1.43093900 3.07917400 -3.35342100  
C 3.07127700 5.09922400 -3.77385600  
H 5.47713300 7.07448000 -6.38959000  
H 4.56849600 4.07668700 -9.94654000  
H -0.27012900 -0.20251600 -5.06031100  
H 3.47406800 6.39938200 -2.23522900  
H 1.27580600 -1.32360100 -11.67215900  
C 0.18043300 2.72907900 -0.80911100  
H -1.82160600 3.29548300 -0.95987900  
H 1.01854000 3.95787200 0.63944200  
H -0.18688300 -1.72716300 3.04436500

P of site A EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48484000  
C 1.49562100 0.00000000 -9.74688800  
O 2.27724600 0.23141200 -11.88680200  
C 3.47896500 5.86959600 -6.26516600  
C 3.16988800 4.12528500 -8.19353800  
C 1.83694700 1.89462500 -7.71756000  
C 0.82189500 1.43052300 -5.33227300  
C 1.11029400 3.18587500 -3.38502600  
C 2.45714400 5.39614000 -3.88052000  
H 4.51992800 7.60486600 -6.59805700  
H 3.94258600 4.43636800 -10.06681500  
H -0.17733200 -0.32376500 -4.95397600  
H 2.71551500 6.77291500 -2.37839700  
H 0.43404400 -1.71838500 -9.17037800  
C -0.03999400 2.73317400 -0.80932300

H -2.08170600 3.15313200 -0.90285900  
H 0.74140000 4.01864400 0.62149700  
H -0.04813900 -1.73573500 3.04597300

R of site A EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49309000  
C 1.46605200 0.00000000 -9.69435400  
O 2.74725800 0.57081300 -11.76923400  
C 4.49985900 5.35748200 -5.95289100  
C 3.96874400 3.78309500 -7.97406300  
C 2.20626200 1.81698900 -7.69027600  
C 1.00678200 1.47957100 -5.36335500  
C 1.51630700 3.06581000 -3.31732900  
C 3.27947400 4.99335000 -3.64015400  
H 5.86375400 6.87680100 -6.15261100  
H 4.89962500 4.04438600 -9.78183900  
H -0.32495700 -0.06824000 -5.16830700  
H 3.71212500 6.23780300 -2.06316400  
H 2.24757300 -0.61798400 -13.05440100  
C 0.17424000 2.72319100 -0.81751900  
H -1.82953500 3.25552100 -1.05109800  
H 0.94235200 3.97497200 0.65135700  
H -0.18292200 -1.73242000 3.03379200

TS of site A EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49101900  
C 1.88001200 0.00000000 -9.69888700  
O 3.08117900 0.39206000 -11.83224700  
C 4.45538600 5.44994400 -5.94306100  
C 4.03399400 3.80859000 -7.93793800  
C 2.36287100 1.78238300 -7.61932800  
C 1.12718400 1.41629700 -5.32050500  
C 1.53299000 3.06954400 -3.30661400  
C 3.21230900 5.07232200 -3.64618500  
H 5.74936000 7.02737600 -6.15193000  
H 4.96810300 4.04448600 -9.74926300  
H -0.13458400 -0.18570300 -5.10211100  
H 3.55867100 6.36635800 -2.08838400  
H 1.69090900 -1.31285600 -11.63966100  
C 0.17004100 2.72366100 -0.81807600  
H -1.83286300 3.25053600 -1.06991200  
H 0.92221900 3.97981000 0.65485700  
H -0.17846600 -1.73211000 3.03512600

P of site A EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48938800  
C 2.28988200 0.00000000 -9.58465900  
O 3.29400900 0.23658800 -11.62574700  
C 3.78033600 5.94347800 -5.97844400  
C 3.69379400 4.18133600 -7.91408900  
C 2.38555500 1.91713000 -7.54388200  
C 1.17364500 1.43519100 -5.25706500  
C 1.24578400 3.20400200 -3.30220100  
C 2.56823000 5.44996700 -3.68930400  
H 4.79427100 7.70757200 -6.23342700  
H 4.62057500 4.50565300 -9.71375700  
H 0.18975100 -0.34360700 -4.96355500  
H 2.65463000 6.83942800 -2.17877200  
H 1.20284100 -1.73360300 -9.11087000  
C -0.09986100 2.72314700 -0.82492100  
H -2.14347800 3.04383400 -1.09824100  
H 0.50601000 4.05386700 0.64984700  
H -0.00478700 -1.74051400 3.03624900

R of site B No field along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.49031400  
C 1.52886500 0.0000000 -9.68347300  
O 2.85239300 0.53979300 -11.74423900  
C 4.59775300 5.31286900 -5.91414800  
C 4.06372900 3.74774800 -7.94101000  
C 2.27307300 1.80393900 -7.67408100  
C 1.04997900 1.47977100 -5.35684100  
C 1.56413600 3.05607400 -3.30392500  
C 3.35440900 4.96104000 -3.61138900  
H 5.98335500 6.81429800 -6.09932000  
H 5.01439600 3.99808200 -9.74006100  
H -0.30244300 -0.05124200 -5.17231500  
H 3.79182200 6.19657700 -2.02901500  
H 2.34544000 -0.64726700 -13.02725900  
C 0.20339900 2.72486700 -0.81340800  
H -1.79301100 3.27806400 -1.05756300  
H 0.97672600 3.96636300 0.66090000  
H -0.20038100 -1.72852600 3.03850100

TS of site B No field along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.46155300  
C 2.69153000 0.0000000 -9.58561900  
O 4.12340900 0.86459900 -11.45058500  
C 3.35117400 6.09542600 -5.80080800  
C 3.66175800 4.38938200 -7.76045600  
C 2.51115400 1.99978100 -7.62990300  
C 1.05881800 1.38006400 -5.51492600  
C 0.72436400 3.08947500 -3.53414600  
C 1.89493900 5.44155400 -3.69827500  
H 4.23784700 7.94314900 -5.88396900  
H 4.78900100 4.87198000 -9.40340000  
H 0.20075300 -0.48304600 -5.44478700  
H 1.66824500 6.79000600 -2.16556300  
H 4.22278400 -0.45210200 -12.70365100  
C -0.85569700 2.39697900 -1.25808400  
H -2.81412100 2.02601400 -1.85045500  
H -0.90990500 3.90993400 0.16237300  
H 0.59399600 -1.82527000 1.36780100

P of site B No field along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27700600  
C 9.43701800 0.0000000 -4.80491000  
O 10.62440200 0.92447100 -6.80511200  
C 2.99918200 0.38212000 -8.02723500  
C 5.58904700 0.59431300 -7.70230000  
C 6.69870000 -0.12508700 -5.40195600  
C 5.16300800 -1.04670800 -3.46170800  
C 2.55466100 -1.28000800 -3.76708200  
C 1.49711300 -0.54958200 -6.06963100  
H 2.12913100 0.92939800 -9.80213400  
H 6.77988700 1.30845800 -9.21046300  
H 6.06619300 -1.58539800 -1.69763800  
H -0.53145000 -0.72323800 -6.34836700  
H 12.39641000 0.99538300 -6.39276500  
C 0.91540100 -2.18880300 -1.61551200  
H 1.90357100 -3.52639900 -0.39204800  
H -0.77411000 -3.13507600 -2.36080000  
H -0.70177100 1.65397000 -1.09130800

R of site B EEF -0.514 V/nm along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000

O 0.0000000 0.0000000 2.48760800  
C 1.57534100 0.0000000 -9.67553000  
O 2.93503700 0.50921500 -11.72481200  
C 4.69146600 5.26288600 -5.88189400  
C 4.14911800 3.70846800 -7.91404600  
C 2.32889400 1.78937500 -7.66156100  
C 1.08634000 1.47939700 -5.35194700  
C 1.61033500 3.04450500 -3.29256600  
C 3.42904200 4.92445600 -3.58712700  
H 6.09991400 6.74445200 -6.05436600  
H 5.11633200 3.94699500 -9.70593000  
H -0.28780900 -0.03312500 -5.17605600  
H 3.87534600 6.14995700 -1.99971800  
H 2.41741000 -0.67517300 -13.00515900  
C 0.23481000 2.72603100 -0.80927700  
H -1.75372300 3.30244100 -1.06056800  
H 1.01687100 3.95602200 0.66953600  
H -0.21936100 -1.72422600 3.04326700

TS of site B EEF -0.514 V/nm along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.45864200  
C 3.14775000 0.0000000 -9.54092100  
O 4.92813900 0.60162300 -11.20211400  
C 4.92634800 5.42385400 -5.14896500  
C 4.98603100 3.85243900 -7.23998400  
C 3.28575300 1.81975400 -7.41814600  
C 1.54887700 1.41640100 -5.47120900  
C 1.46648900 2.99373900 -3.35890300  
C 3.17946200 4.98806400 -3.21812000  
H 6.23606100 6.99466200 -4.99336700  
H 6.33602700 4.16766200 -8.75022300  
H 0.26232400 -0.17416100 -5.63940200  
H 3.15348400 6.22457900 -1.57862300  
H 4.81215400 -0.60220700 -12.56182500  
C -0.40455800 2.52091100 -1.25335000  
H -2.33277300 2.46289600 -2.02379000  
H -0.34200500 3.99784600 0.20367100  
H 0.27247000 -1.90261100 1.36185600

P of site B EEF -0.514 V/nm along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.27549800  
C 9.39753400 0.0000000 -5.00566700  
O 10.53520100 0.98654900 -7.00680900  
C 2.87327700 0.50298900 -8.02998100  
C 5.47311200 0.68790200 -7.77728100  
C 6.64303200 -0.09096600 -5.52680300  
C 5.15693800 -1.04178800 -3.56194100  
C 2.53831300 -1.24475400 -3.79326200  
C 1.42107100 -0.45760700 -6.04863400  
H 1.95540200 1.09678600 -9.76569800  
H 6.62601400 1.42729400 -9.30283100  
H 6.10669000 -1.62462500 -1.83700700  
H -0.61658800 -0.60747500 -6.26984000  
H 12.31699200 1.03533600 -6.63529600  
C 0.95135500 -2.17716600 -1.61414600  
H 1.98749900 -3.48099600 -0.39432000  
H -0.72451900 -3.17065700 -2.32850800  
H -0.73103100 1.64071000 -1.09302600

R of site B EEF 0.514 V/nm along  $Z_B$  direction  
C 0.0000000 0.0000000 0.0000000  
O 0.0000000 0.0000000 2.49309000  
C 1.46605200 0.0000000 -9.69435400  
O 2.74725800 0.57081300 -11.76923400

C 4.49986500 5.35747800 -5.95289100  
C 3.96874800 3.78309100 -7.97406300  
C 2.20626400 1.81698800 -7.69027600  
C 1.00678200 1.47957100 -5.36335500  
C 1.51631100 3.06580800 -3.31732900  
C 3.27947900 4.99334600 -3.64015300  
H 5.86376400 6.87679500 -6.15261100  
H 4.89962900 4.04438200 -9.78183900  
H -0.32495700 -0.06823800 -5.16830700  
H 3.71213200 6.23779900 -2.06316200  
H 2.24757100 -0.61798400 -13.05440100  
C 0.17424200 2.72319100 -0.81751900  
H -1.82953200 3.25552300 -1.05109800  
H 0.94235600 3.97497100 0.65135700  
H -0.18292400 -1.73242000 3.03379200

TS of site B EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46465000  
C 2.48458800 0.00000000 -9.63606300  
O 3.77895500 0.92609800 -11.56660200  
C 2.86962000 6.19889200 -5.97696400  
C 3.23181500 4.47686300 -7.91430700  
C 2.23668600 2.02426600 -7.70827700  
C 0.88429800 1.35738100 -5.54273900  
C 0.49613600 3.08230700 -3.58564500  
C 1.51311900 5.49854000 -3.82368800  
H 3.63611200 8.09605100 -6.12004300  
H 4.27937700 4.99605000 -9.59826100

H 0.14561700 -0.55338200 -5.41667700  
H 1.24159400 6.86148500 -2.31091300  
H 3.92422800 -0.39922200 -12.80692500  
C -0.98690200 2.34173300 -1.25951400  
H -2.94165800 1.87416500 -1.79547700  
H -1.07868600 3.86661200 0.14662600  
H 0.68832400 -1.78929000 1.37447200

P of site B EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27853800  
C 9.41512200 0.00000000 -4.71476500  
O 10.62833600 0.84948300 -6.73105200  
C 3.03414000 0.19735000 -8.06550500  
C 5.61471700 0.45228300 -7.69893200  
C 6.68933100 -0.17824300 -5.35609800  
C 5.12812900 -1.05729100 -3.41661500  
C 2.52965300 -1.33560200 -3.76451400  
C 1.50656800 -0.69127900 -6.10782600  
H 2.19251600 0.67534300 -9.87352800  
H 6.82455800 1.13104300 -9.20813800  
H 6.00411200 -1.52921600 -1.61974200  
H -0.51364100 -0.90051300 -6.41976500  
H 12.39356800 0.95523000 -6.29783200  
C 0.86471600 -2.20654700 -1.61592400  
H 1.81820300 -3.56955200 -0.39244100  
H -0.84506500 -3.11138100 -2.36626300  
H -0.66353000 1.67013100 -1.08963700

## Arene molecule (R<sub>E</sub>)

R of site C EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48982700  
C 6.55596900 0.00000000 -6.70455100  
C 4.87934100 -1.23007600 -8.31439600  
C 2.44434300 -1.79520700 -7.50548100  
C 1.72321900 -1.09585600 -5.06559100  
C 3.39104100 0.12729400 -3.43859800  
C 5.85505400 0.69377000 -4.26466200  
H 8.45325900 0.43358300 -7.36177900  
H 5.47810300 -1.74946200 -10.20947100  
H -0.18359100 -1.48075000 -4.41957400  
C 2.58828300 0.87373600 -0.79351300  
H 2.43787100 2.95446300 -0.68623400  
H 4.03062100 0.37175300 0.61697500  
H -1.67026200 -0.48137800 3.04144000  
C 7.71053900 2.03053600 -2.56481100  
H 6.96352600 3.83923100 -1.88839700  
H 8.16137900 0.90206900 -0.88762900  
H 9.48071100 2.41148200 -3.55706100  
C -1.94597800 -1.92619900 -9.35301400  
C 0.61835800 -3.16002400 -9.23019900  
H 0.18213200 -5.02817600 -8.41047900  
H 1.44744800 -3.51582700 -11.10156000  
O -2.81093500 -2.30369600 -11.66411800  
H -4.48384800 -1.58085500 -11.73631700

TS of site C EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48741700  
C 6.47196100 0.00000000 -6.78857900  
C 4.76003300 -1.17776700 -8.39279900  
C 2.33132400 -1.73379400 -7.54272200

C 1.65563100 -1.06792100 -5.08621900  
C 3.36412800 0.10987800 -3.46304400  
C 5.81701800 0.65934500 -4.32193600  
H 8.36437900 0.42160900 -7.46585400  
H 5.30653100 -1.66350000 -10.31121300  
H -0.23159200 -1.46381800 -4.38818400  
C 2.60928200 0.81289600 -0.79327700  
H 2.53551100 2.89335900 -0.62747800  
H 4.04454100 0.22213600 0.58964400  
H -1.67929600 -0.44356200 3.04411600  
C 7.71724000 1.93912800 -2.62889500  
H 7.00585200 3.74651000 -1.91238700  
H 8.17326900 0.77513800 -0.97789200  
H 9.47830500 2.31056100 -3.63986200  
C -0.30087300 -1.09324100 -11.28390100  
C 0.44830400 -2.98814200 -9.30778900  
H -1.22465300 -3.58565300 -8.25211000  
H 1.29875300 -4.62354800 -10.26475300  
O 0.77138500 -1.35931600 -13.49611600  
H -0.54915700 0.36126700 -13.12909300

P of site C EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48693200  
C 6.42115400 0.00000000 -6.84122300  
C 4.64114100 1.02047700 -8.48187100  
C 2.19034700 1.49384400 -7.64742800  
C 1.57662400 0.93719300 -5.14445800  
C 3.34498700 -0.09315400 -3.48705300  
C 5.81471200 -0.57437300 -4.34306300  
H 8.32427300 -0.37080000 -7.51824600  
H 5.16360500 1.43399700 -10.42552100  
H -0.31887600 1.29118200 -4.44403500

C 2.64076100 -0.71908600 -0.78552500  
H 4.04983200 0.00634400 0.55968400  
H 2.68337400 -2.79052000 -0.52738500  
H -1.69259400 0.38945900 3.04419300  
C 7.77957800 -1.69838400 -2.61360200  
H 8.18772000 -0.45136900 -1.01164100  
H 7.15601400 -3.50750700 -1.82349400  
H 9.55179500 -2.02709700 -3.61984900  
C 0.47066700 5.55456700 -9.40340400  
C 0.26204700 2.69305000 -9.37270500  
H -1.67502600 2.19287700 -8.86013800  
H 0.57113800 2.06508600 -11.32771100  
O -1.30910600 6.96873800 -9.56353000  
H 2.43813700 6.28763000 -9.29287400

R of site C No field along Z<sub>c</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49256300  
C 6.60650800 0.00000000 -6.65440500  
C 4.97094900 -1.30058900 -8.25070100  
C 2.54199400 -1.90301200 -7.45001200  
C 1.78528700 -1.16905900 -5.03092500  
C 3.41251400 0.12500000 -3.41766600  
C 5.86985300 0.72937200 -4.23561300  
H 8.49813200 0.46325100 -7.30733400  
H 5.59638500 -1.84399400 -10.12999400  
H -0.11934000 -1.58142200 -4.39564800  
C 2.57282900 0.91083300 -0.79504600  
H 2.36725100 2.98944000 -0.73938600  
H 4.01750600 0.47864500 0.63635800  
H -1.66566400 -0.50395800 3.03706700  
C 7.68050200 2.14602500 -2.55178700  
H 6.88791800 3.95301200 -1.92370400  
H 8.14331700 1.06657700 -0.84545100  
H 9.44940400 2.54426400 -3.53939800  
C -1.83076900 -2.16637000 -9.32420500  
C 0.76137700 -3.34026800 -9.16281300  
H 0.36462800 -5.20460300 -8.31553100  
H 1.61205600 -3.70545200 -11.02212500  
O -2.66038800 -2.58930800 -11.63777000  
H -4.34759400 -1.90442100 -11.74436900

TS of site C No field along Z<sub>c</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49011000  
C 6.52000900 0.00000000 -6.74209400  
C 4.87014700 -1.30630000 -8.31128100  
C 2.46174200 -1.93591400 -7.45442100  
C 1.74315400 -1.21322000 -5.02620300  
C 3.38939700 0.09425800 -3.43828200  
C 5.82171700 0.71779000 -4.30389600  
H 8.39599800 0.47933900 -7.42634500  
H 5.44830400 -1.83373200 -10.20907900  
H -0.13188600 -1.66349100 -4.32859500  
C 2.59141800 0.85706700 -0.79707500  
H 2.44698800 2.93887500 -0.70192400  
H 4.03441600 0.35821700 0.61431800  
H -1.67453000 -0.46894900 3.03947600  
C 7.65429000 2.13923300 -2.64941400  
H 6.86443300 3.94318500 -2.00974700  
H 8.14442000 1.06013700 -0.95084100  
H 9.40642200 2.54322100 -3.66330700  
C -0.17174800 -1.53596800 -11.23248400  
C 0.64514300 -3.32772400 -9.18398800  
H -1.00809700 -3.96141700 -8.11852600  
H 1.57165000 -4.95585200 -10.08043100

O 0.94219900 -1.82204300 -13.41807000  
H -0.47359200 -0.15923400 -13.12704100

P of site C No field along Z<sub>c</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48901800  
C 6.49866700 0.00000000 -6.75732500  
C 4.90480900 1.45642400 -8.25611500  
C 2.53687100 2.16936900 -7.36070500  
C 1.81711800 1.41103300 -4.93861200  
C 3.39933700 -0.04831100 -3.42378100  
C 5.78603900 -0.77327800 -4.34310800  
H 8.33731100 -0.55610500 -7.48351900  
H 5.50778700 2.02399800 -10.13569800  
H -0.02252400 1.94310000 -4.20185100  
C 2.59151900 -0.85611400 -0.79978900  
H 4.03648700 -0.39057800 0.62153300  
H 2.43298000 -2.93798900 -0.74359100  
H -1.67451200 0.46996000 3.03851500  
C 7.54824800 -2.36130300 -2.76622900  
H 8.08867900 -1.39215000 -1.01776200  
H 6.67119300 -4.15402400 -2.21414200  
H 9.27854800 -2.79998900 -3.80284700  
C 1.09191400 6.58245900 -8.13226600  
C 0.80352300 3.83678100 -8.90069700  
H -1.18167100 3.30963200 -8.68676500  
H 1.29617300 3.70523700 -10.91143000  
O -0.64324600 7.97313600 -7.63299800  
H 3.08267000 7.25188500 -8.04471800

R of site C EEF 0.514 V/nm along Z<sub>c</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49533300  
C 6.65235800 0.00000000 -6.60720100  
C 5.03983000 -1.32562300 -8.20598800  
C 2.60683900 -1.93581500 -7.42300400  
C 1.82331100 -1.18449400 -5.01763700  
C 3.42792700 0.13473400 -3.40207200  
C 5.88849300 0.74781600 -4.20256500  
H 8.54594800 0.47063300 -7.24870100  
H 5.68545700 -1.88018400 -10.07481800  
H -0.08550100 -1.60241800 -4.39890100  
C 2.55834800 0.94469500 -0.79599100  
H 2.30745700 3.01950600 -0.77758700  
H 4.00361700 0.56664600 0.65023800  
H -1.66093200 -0.52575600 3.03280900  
C 7.67399000 2.19614800 -2.51829400  
H 6.86251300 4.00379600 -1.91621700  
H 8.13256600 1.13818800 -0.79696600  
H 9.44711500 2.59828600 -3.49662600  
C -1.74410100 -2.22608500 -9.34097100  
C 0.85024500 -3.39418000 -9.14221000  
H 0.45162400 -5.25320300 -8.28504600  
H 1.72205700 -3.76884900 -10.98930400  
O -2.53629700 -2.65266600 -11.66438300  
H -4.22232100 -1.97049800 -11.80551300

TS of site C EEF 0.514 V/nm along Z<sub>c</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49279500  
C 6.54719500 0.00000000 -6.71320600  
C 4.94044100 -1.39067600 -8.25416400  
C 2.54729500 -2.06739700 -7.38979400  
C 1.80080400 -1.30649900 -4.98167500  
C 3.40422200 0.08544200 -3.42195900  
C 5.82046600 0.75699100 -4.29528300

H 8.41000800 0.51711400 -7.40561300  
H 5.53930500 -1.94562900 -10.13743800  
H -0.06499000 -1.79040300 -4.28174700  
C 2.57697100 0.88885800 -0.80130500  
H 2.38230100 2.96880200 -0.75616700  
H 4.02436400 0.45570000 0.62770500  
H -1.67111400 -0.48820900 3.03484300  
C 7.60532300 2.27280500 -2.67236900  
H 6.76307700 4.07132200 -2.08561000  
H 8.11817000 1.25412500 -0.94307800  
H 9.34963000 2.69822200 -3.69088000  
C -0.07585200 -1.83411200 -11.19428800  
C 0.77678200 -3.54876000 -9.09090500  
H -0.86556300 -4.19914900 -8.01879900  
H 1.75111700 -5.17381100 -9.94065100  
O 1.07389600 -2.13774200 -13.35551600  
H -0.40669800 -0.51780800 -13.12514900

P of site C EEF 0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49153300  
C 6.52191800 0.00000000 -6.71772400  
C 5.17667600 1.86589900 -7.99054600  
C 2.95382800 2.82233900 -6.96235500  
C 2.12745100 1.88789800 -4.63738800  
C 3.46023900 0.02026500 -3.34951300  
C 5.70109400 -0.94777600 -4.40241400  
H 8.24749900 -0.74169700 -7.54767700  
H 5.85907600 2.56369600 -9.79712500  
H 0.39151200 2.60705600 -3.81225600  
C 2.55349200 -0.94580600 -0.81278300  
H 4.00213200 -0.69106700 0.65915900  
H 2.25215000 -3.00886700 -0.93487100  
H -1.66032500 0.52537800 3.03335900  
C 7.19211700 -2.97550300 -3.06926400  
H 7.82343700 -2.35220500 -1.19804300  
H 6.06200400 -4.68783800 -2.78494200  
H 8.86522800 -3.50214400 -4.15730500  
C 2.07559900 7.41433800 -6.95297400  
C 1.49145600 4.92280300 -8.23708300  
H -0.54731400 4.60634500 -8.14966600  
H 2.05510100 5.07539800 -10.22546900  
O 0.52209900 8.74958500 -5.95225400  
H 4.11326300 7.92947700 -6.95014300

R of site D EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48982700  
C 6.55599900 0.00000000 -6.70451700  
C 4.87937500 -1.23007000 -8.31437300  
C 2.44436700 -1.79518000 -7.50547500  
C 1.72322900 -1.09582000 -5.06559200  
C 3.39104700 0.12732200 -3.43858900  
C 5.85506900 0.69377900 -4.26463500  
H 8.45329800 0.43356900 -7.36173000  
H 5.47815200 -1.74946400 -10.20944200  
H -0.18358700 -1.48070300 -4.41958900  
C 2.58826800 0.87377600 -0.79351300  
H 2.43781800 2.95450300 -0.68625600  
H 4.03061200 0.37183400 0.61698300  
H -1.67025400 -0.48140600 3.04144000  
C 7.71055100 2.03054000 -2.56477300  
H 6.96354000 3.83923900 -1.88836200  
H 8.16137700 0.90207100 -0.88759000  
H 9.48072800 2.41148000 -3.55701400  
C -1.94593700 -1.92614200 -9.35304800

C 0.61838900 -3.15998800 -9.23020700  
H 0.18213600 -5.02813200 -8.41048100  
H 1.44749100 -3.51580700 -11.10155800  
O -2.81087600 -2.30363900 -11.66416000  
H -4.48378100 -1.58078500 -11.73637600

TS of site D EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46336500  
C 5.63468900 0.00000000 -7.49826400  
C 4.26411800 2.00290500 -8.51164500  
C 2.23284300 3.02119700 -7.19212100  
C 1.61965100 2.00398200 -4.83640600  
C 2.98134800 0.00174200 -3.80778100  
C 5.02803200 -1.03039400 -5.15412600  
H 7.21897800 -0.77461200 -8.55118800  
H 4.78892300 2.77565900 -10.34089700  
H 0.05873100 2.81153000 -3.78125800  
C 2.31695600 -1.05331300 -1.23614600  
H 3.88978000 -0.88990300 0.11619200  
H 1.92024200 -3.09357500 -1.38637700  
H -1.78333100 0.70527600 1.36636500  
C 6.54451300 -3.19335500 -4.08926100  
H 7.41382200 -2.69653600 -2.27696600  
H 5.36312800 -4.86115600 -3.75252300  
H 8.05625700 -3.74652500 -5.38170200  
C 0.06110800 7.18543900 -6.38175900  
C 0.70823800 5.17416100 -8.29363900  
H -1.17014000 4.45631400 -8.85030000  
H 1.58317300 5.93129700 -10.01880500  
O 0.00419700 9.35196700 -7.61123600  
H -0.47233200 10.64462000 -6.41506500

P of site D EEF -0.514 V/nm along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28020700  
C 7.59703700 0.00000000 -3.59978400  
C 7.16508100 -0.82248300 -6.05954200  
C 4.75781300 -0.68762400 -7.10792200  
C 2.81036000 0.31217200 -5.63846100  
C 3.22787300 1.14820200 -3.17730400  
C 5.65813100 0.98223300 -2.11267700  
H 9.48969600 -0.12694800 -2.81373700  
H 8.72126200 -1.57796200 -7.16666600  
H 0.93885200 0.47760000 -6.46637100  
C 1.02552100 2.12179900 -1.62839300  
H -0.49009700 2.74373000 -2.89586500  
H 1.55018800 3.69762300 -0.40247400  
H -0.73144000 -1.64514300 -1.08378700  
C 6.18158400 1.87345400 0.54344400  
H 5.97351500 3.92884000 0.69445000  
H 4.88060700 1.03442300 1.91284600  
H 8.10789600 1.39790700 1.11211900  
C 2.43147900 -0.02996700 -11.22530500  
C 4.26754600 -1.63616300 -9.76010500  
H 3.27402700 -3.46854800 -9.64783400  
H 6.03769200 -1.99933700 -10.78398200  
O 3.09168600 -0.19061100 -13.62333600  
H 1.88306000 0.77750400 -14.58696100

R of site D No field along Z<sub>C</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49256300  
C 6.60649300 0.00000000 -6.65441400  
C 4.97092300 -1.30057200 -8.25071400  
C 2.54196400 -1.90298100 -7.45002700

C 1.78526500 -1.16903200 -5.03093900  
C 3.41250100 0.12500900 -3.41767300  
C 5.86984300 0.72936800 -4.23561900  
H 8.49811700 0.46324600 -7.30734300  
H 5.59635400 -1.84397100 -10.13001100  
H -0.11936600 -1.58138400 -4.39566200  
C 2.57282700 0.91083900 -0.79504800  
H 2.36724600 2.98944600 -0.73938400  
H 4.01750600 0.47865100 0.63635400  
H -1.66566400 -0.50396000 3.03706700  
C 7.68050400 2.14600200 -2.55178900  
H 6.88793500 3.95299700 -1.92370800  
H 8.14330600 1.06654900 -0.84545200  
H 9.44941100 2.54422600 -3.53939600  
C -1.83081300 -2.16631900 -9.32420300  
C 0.76133700 -3.34021900 -9.16283200  
H 0.36458300 -5.20455900 -8.31556000  
H 1.61200900 -3.70539900 -11.02214600  
O -2.66047100 -2.58928700 -11.63774700  
H -4.34768000 -1.90440100 -11.74432800

TS of site D No field along Zc direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46623200  
C 5.61874600 0.00000000 -7.51138500  
C 4.20312300 1.95476700 -8.55580500  
C 2.15041800 2.94966000 -7.25144900  
C 1.56218600 1.95913700 -4.87803700  
C 2.96803700 0.00351500 -3.81967700  
C 5.03564600 -1.00578300 -5.15074500  
H 7.21710900 -0.75766300 -8.55496200  
H 4.70751200 2.70589200 -10.39943000  
H -0.01609900 2.74905200 -3.83532000  
C 2.32444000 -1.03275800 -1.23485700  
H 3.89919300 -0.84098300 0.11173400  
H 1.95028100 -3.07915900 -1.36493600  
H -1.78774600 0.68818900 1.37269000  
C 6.59663600 -3.12181700 -4.05584700  
H 7.45645200 -2.58234000 -2.25088000  
H 5.45026100 -4.80941000 -3.69664400  
H 8.11883200 -3.66149700 -5.34149300  
C -0.12933900 7.07662100 -6.52505900  
C 0.57385300 5.04296100 -8.39215600  
H -1.28479300 4.26719000 -8.93772600  
H 1.42857100 5.78806500 -10.13212600  
O -0.28063200 9.20459700 -7.81194600  
H -0.79837200 10.51216500 -6.65011500

P of site D No field along Zc direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28149000  
C 7.57064500 0.00000000 -3.65559000  
C 7.12109000 -0.80937400 -6.11636400  
C 4.70693400 -0.66685200 -7.14881400  
C 2.77060800 0.32698500 -5.66049500  
C 3.20609000 1.15042200 -3.19813800  
C 5.64279200 0.97706600 -2.15090600  
H 9.46921700 -0.13094300 -2.88421500  
H 8.66917700 -1.55847300 -7.23879900  
H 0.89519400 0.49996300 -6.47768500  
C 1.01561100 2.12268500 -1.63062300  
H -0.50846500 2.74677100 -2.88689600  
H 1.54907100 3.69735600 -0.40673200  
H -0.72594200 -1.64835000 -1.08211400  
C 6.18601700 1.85884700 0.50478200  
H 5.98597100 3.91466200 0.66306500

H 4.89137800 1.01991800 1.88055600  
H 8.11500500 1.37549300 1.05854000  
C 2.30820900 -0.01803200 -11.22890300  
C 4.19867600 -1.59927600 -9.80268800  
H 3.24667400 -3.45362100 -9.69501900  
H 5.96075800 -1.91624000 -10.85498400  
O 2.91717700 -0.17585600 -13.63751600  
H 1.67762400 0.77138100 -14.58319800

R of site D EEF 0.514 V/nm along Zc direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49533300  
C 6.65235800 0.00000000 -6.60720100  
C 5.03982800 -1.32561700 -8.20599000  
C 2.60683500 -1.93581000 -7.42300600  
C 1.82330900 -1.18448800 -5.01763900  
C 3.42792700 0.13473600 -3.40207200  
C 5.88849300 0.74781400 -4.20256500  
H 8.54594800 0.47063100 -7.24870100  
H 5.68545500 -1.88017800 -10.07482000  
H -0.08550400 -1.60241100 -4.39890200  
C 2.55834800 0.94469500 -0.79599100  
H 2.30745700 3.01950600 -0.77758500  
H 4.00361700 0.56664400 0.65023800  
H -1.66093200 -0.52575800 3.03280900  
C 7.67399200 2.19614000 -2.51829200  
H 6.86251900 4.00379100 -1.91621100  
H 8.13256800 1.13817900 -0.79696600  
H 9.44711900 2.59827800 -3.49662400  
C -1.74410300 -2.22607000 -9.34097700  
C 0.85023900 -3.39416900 -9.14221500  
H 0.45161400 -5.25319100 -8.28505200  
H 1.72205100 -3.76883700 -10.98931000  
O -2.53629900 -2.65264600 -11.66438800  
H -4.22232300 -1.97047500 -11.80551900

TS of site D EEF 0.514 V/nm along Zc direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46922100  
C 5.60768900 0.00000000 -7.52466200  
C 4.08931000 1.83131500 -8.64517900  
C 1.97644300 2.75597600 -7.38565700  
C 1.43292900 1.82358300 -4.97813600  
C 2.94145200 -0.00961500 -3.84463400  
C 5.06896000 -0.94990300 -5.13071200  
H 7.24975800 -0.70545800 -8.53616700  
H 4.55841400 2.53818300 -10.51512100  
H -0.19305300 2.56074200 -3.97073600  
C 2.33860900 -0.99908500 -1.23149500  
H 3.91609000 -0.74276500 0.10107600  
H 2.01327300 -3.05700900 -1.31252100  
H -1.79547500 0.66160500 1.37892400  
C 6.73758700 -2.93804700 -3.95703300  
H 7.56481300 -2.28727400 -2.17321400  
H 5.68208200 -4.67020500 -3.53633500  
H 8.28850600 -3.44324500 -5.22200500  
C -0.54869000 6.77140500 -6.84002700  
C 0.28704000 4.70555400 -8.61440500  
H -1.51894000 3.79963400 -9.13616200  
H 1.10490800 5.42737900 -10.38121300  
O -0.84816400 8.81862800 -8.22722300  
H -1.45545400 10.14418200 -7.13145700

P of site D EEF 0.514 V/nm along Zc direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28279400

C 7.54019700 0.00000000 -3.71895200  
C 7.07102000 -0.79152900 -6.18170100  
C 4.64955400 -0.63803600 -7.19641300  
C 2.72599300 0.34813900 -5.68632400  
C 3.18145900 1.15426800 -3.22177100  
C 5.62508200 0.97037700 -2.19388200  
H 9.44496100 -0.13741300 -2.96374900  
H 8.60973400 -1.53310900 -7.32163000  
H 0.84632200 0.53116800 -6.49125000  
C 1.00476400 2.12410600 -1.63272600  
H -0.52894200 2.75135700 -2.87573200  
H 1.54837200 3.69684600 -0.41048100  
H -0.72002400 -1.65166900 -1.08051200  
C 6.19046000 1.83810000 0.46220500  
H 5.99911200 3.89406800 0.63130300  
H 4.90321400 0.99733900 1.84413000  
H 8.12232400 1.34560500 0.99858800  
C 2.18227000 0.01469500 -11.23750300  
C 4.12130200 -1.54854000 -9.85342300  
H 3.20636800 -3.42168700 -9.75490600  
H 5.87367200 -1.82140000 -10.93349900  
O 2.74283700 -0.13506100 -13.65530800  
H 1.47640400 0.79656000 -14.58148000

R of site C EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49122500  
C 1.67746300 0.00000000 -9.55693700  
O 2.46113900 -0.66484200 -11.83004400  
C -6.54347600 2.54983900 -5.84175600  
C -5.80656000 1.50393200 -3.54453200  
C -3.43111100 0.40959100 -3.28935100  
C -1.81275300 0.39422900 -5.37374600  
C -2.53816600 1.42834100 -7.68230100  
C -4.94417400 2.53269300 -7.93145800  
H -8.40315800 3.40578100 -6.01015900  
H -7.09264800 1.54805900 -1.94411700  
H 0.06532400 -0.40556800 -5.18957900  
C -0.76562700 1.40171100 -9.93207200  
H -0.12207400 3.35284600 -10.31475100  
H -1.73776300 0.80682300 -11.67154800  
H 4.06995800 -1.49736700 -11.62204900  
C -5.79003400 3.69241900 -10.39355100  
H -4.48138300 5.16288500 -11.03722800  
H -5.90226500 2.28189800 -11.90699100  
H -7.65693000 4.55316500 -10.20008600  
C -2.62651200 -0.75912800 -0.80940800  
H -2.44354000 -2.82202200 -1.06066600  
H -4.05217500 -0.47564600 0.67379300  
H 1.68899800 0.41393300 3.04230900

TS of site C EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46744500  
C 5.65595600 0.00000000 -9.82016200  
O 6.82990200 0.37005200 -11.98811600  
C 8.15350800 -0.42794800 -0.79140100  
C 5.80597600 0.53220800 -0.11563800  
C 4.03170800 1.10087400 -1.97597800  
C 4.64751900 0.66617000 -4.49923600  
C 7.00146800 -0.29290400 -5.19266100  
C 8.79148000 -0.85433200 -3.31310300  
H 9.52453700 -0.86163200 0.67438300  
H 5.34379000 0.83357700 1.86128300  
H 3.28456800 1.07141300 -5.97700800

C 7.65554200 -0.74230400 -7.94349100  
H 7.85888300 -2.79610600 -8.26997800  
H 9.50975800 0.06147100 -8.43344300  
H 5.55887000 0.77159100 -13.23195800  
C 11.35380800 -1.90369800 -3.98396400  
H 11.19944000 -3.65778400 -5.07375800  
H 12.44717000 -0.57260000 -5.13435800  
H 12.45255600 -2.31362900 -2.28543600  
C 1.45197500 2.11204900 -1.23312000  
H 0.43585600 2.77624300 -2.90478200  
H 1.63278800 3.65690700 0.14236800  
H -0.95657400 -1.66141000 1.37515600

P of site C EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27831100  
C 10.29147500 0.00000000 0.38025300  
O 12.11971600 1.36633100 1.36796600  
C 4.79462100 0.46541300 -7.19388400  
C 2.81360100 -0.53119700 -5.78159700  
C 3.17209200 -1.12726700 -3.24597800  
C 5.53599600 -0.68492200 -2.16030700  
C 7.53003400 0.31247200 -3.55774200  
C 7.16080100 0.90054700 -6.12430800  
H 4.49558800 0.91288400 -9.17607900  
H 0.98860500 -0.85468900 -6.66644100  
H 5.85524700 -1.13616600 -0.18406500  
C 10.07716300 0.79279100 -2.34486800  
H 10.70428400 2.75407900 -2.63912300  
H 11.52033400 -0.38446500 -3.28926000  
H 12.33461600 0.83156700 3.09913100  
C 9.27460400 1.97745600 -7.70083500  
H 9.92726300 3.79701500 -6.95833000  
H 10.91829800 0.71806400 -7.73360900  
H 8.66799200 2.27340000 -9.65203900  
C 1.03979600 -2.12108200 -1.62077500  
H 1.66810900 -3.64209100 -0.37335000  
H -0.49505900 -2.83172400 -2.81854500  
H -0.74053500 1.63918900 -1.08787400

R of site C No field along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49414500  
C 1.48812200 0.00000000 -9.65000600  
O 2.21211400 -0.59480500 -11.95969000  
C -6.54887100 2.76421300 -5.69312700  
C -5.79551100 1.65134200 -3.43283400  
C -3.45000600 0.48099800 -3.25225200  
C -1.87787300 0.45742400 -5.37129400  
C -2.62042800 1.55744100 -7.64355600  
C -4.99635100 2.73955000 -7.81783400  
H -8.38518500 3.67771700 -5.80553200  
H -7.04580700 1.70099000 -1.80421700  
H -0.02305800 -0.40643700 -5.24926600  
C -0.89780700 1.52004300 -9.93096800  
H -0.18184100 3.45225700 -10.27708300  
H -1.92989900 1.01491900 -11.66354200  
H 3.78584900 -1.50507100 -11.81956700  
C -5.86016000 3.97047700 -10.23852500  
H -4.51880000 5.40820400 -10.88766500  
H -6.05321800 2.59148800 -11.77223300  
H -7.69292500 4.88746900 -9.98734300  
C -2.62552400 -0.75626900 -0.81160400  
H -2.42983700 -2.80920400 -1.12534600  
H -4.04435900 -0.52163100 0.68702200  
H 1.69076700 0.41519600 3.03806500

TS of site C No field along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.46970500  
C 5.19173700 0.00000000 -10.11798700  
O 6.30021100 0.32053000 -12.32449400  
C 7.99841100 -1.27608900 -1.26262300  
C 5.80207800 -0.11052300 -0.42069700  
C 4.02256300 0.75326800 -2.15821900  
C 4.47839200 0.40659000 -4.72842700  
C 6.68067400 -0.75567700 -5.58878200  
C 8.47625800 -1.61821800 -3.83211500  
H 9.37595500 -1.94149600 0.10735500  
H 5.46306600 0.12486000 1.59026900  
H 3.10922100 1.04490200 -6.11527300  
C 7.15868200 -1.10821300 -8.38923800  
H 7.09082000 -3.14613300 -8.84306600  
H 9.07643600 -0.50771500 -8.92263100  
H 5.04416500 0.95797200 -13.48280400  
C 10.87523300 -2.89632400 -4.68514100  
H 10.48013400 -4.55098200 -5.86548900  
H 12.06031400 -1.62321100 -5.80968900  
H 11.99220300 -3.52819400 -3.06825900  
C 1.60515900 1.99176300 -1.23656900  
H 0.57696200 2.81544200 -2.82881900  
H 2.01137000 3.46151100 0.17350500  
H -1.09162500 -1.57394600 1.38114700

P of site C No field along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27907500  
C 10.42952000 0.00000000 -1.21013800  
O 12.43151900 1.34986800 -0.60609800  
C 3.74201400 0.34756800 -7.76897500  
C 2.02535100 -0.62661800 -6.03326700  
C 2.80091200 -1.19371800 -3.58505200  
C 5.31330700 -0.74666100 -2.91600000  
C 7.04664200 0.22720600 -4.64071200  
C 6.25498800 0.78662500 -7.11609500  
H 3.11632400 0.77012800 -9.67873100  
H 0.07880500 -0.95790800 -6.59870900  
H 5.96110400 -1.17792700 -1.01734400  
C 9.76552800 0.70296500 -3.88466800  
H 10.35993100 2.64094800 -4.34961800  
H 11.01641600 -0.52895300 -5.01598500  
H 12.93218500 0.86580700 1.07964600  
C 8.07648300 1.83308600 -9.03975200  
H 8.84153700 3.66397800 -8.44742100  
H 9.69226900 0.56983000 -9.32531500  
H 7.15395600 2.09784600 -10.86726400  
C 0.96012700 -2.15633300 -1.62452800  
H 1.80974000 -3.57272100 -0.38491300  
H -0.68497500 -3.00977900 -2.55593300  
H -0.71594600 1.65009400 -1.08787400

R of site C EEF 0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49704500  
C 1.17823900 0.00000000 -9.78404000  
O 1.74904200 -0.55531900 -12.14346100  
C -6.20996900 3.77041900 -5.41369900  
C -5.55685500 2.46544500 -3.22601300  
C -3.40519700 0.95860000 -3.17898200  
C -1.92215100 0.79474200 -5.35493400  
C -2.56694800 2.08507400 -7.55574800  
C -4.74714500 3.60848100 -7.59538300

H -7.89534100 4.94446700 -5.42417200  
H -6.73440800 2.62649200 -1.55075100  
H -0.21476200 -0.33961200 -5.34117300  
C -0.94407500 1.88993500 -9.90661200  
H 0.05213800 3.70223400 -10.20146200  
H -2.09677500 1.63272000 -11.61695200  
H 3.16065700 -1.70929600 -12.11264700  
C -5.49895800 5.05033100 -9.93535800  
H -3.97974400 6.29630400 -10.58793000  
H -5.94948400 3.77775500 -11.50610300  
H -7.16354100 6.21900800 -9.58053700  
C -2.68865800 -0.47969200 -0.81427000  
H -2.68477300 -2.52130600 -1.23821500  
H -4.07060400 -0.18703400 0.70877000  
H 1.72589300 0.24375400 3.03400900

TS of site C EEF 0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47216900  
C 4.93992600 0.00000000 -10.20142000  
O 5.97281400 0.26784400 -12.44802800  
C 7.98708200 -1.23305600 -1.41964000  
C 5.80788100 -0.07387700 -0.52528400  
C 3.98085900 0.77531000 -2.21981300  
C 4.37055800 0.41931500 -4.79957000  
C 6.55424700 -0.73757200 -5.71278200  
C 8.39910300 -1.58401300 -3.99932300  
H 9.40387400 -1.88661300 -0.08407200  
H 5.51952400 0.16874900 1.49298800  
H 2.96481300 1.04544800 -6.15513500  
C 6.95679900 -1.10199600 -8.52311000  
H 6.88646900 -3.14159500 -8.96613800  
H 8.85667700 -0.49626900 -9.11117800  
H 4.68846300 0.89980100 -13.57869500  
C 10.78038500 -2.85445300 -4.91073900  
H 10.36133500 -4.51671400 -6.07160700  
H 11.92634200 -1.58163900 -6.07507900  
H 11.94527900 -3.47191000 -3.32212300  
C 1.58126300 2.00487500 -1.24062800  
H 0.52330700 2.84170500 -2.80655600  
H 2.01085500 3.46248000 0.17540300  
H -1.07723900 -1.58150100 1.38699000

P of site C EEF 0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.27995500  
C 10.27733800 0.00000000 -3.58824200  
O 12.40346200 1.29623500 -3.57940900  
C 2.15833600 0.29575700 -8.26893300  
C 0.93084400 -0.66063200 -6.15207800  
C 2.29266800 -1.21261100 -3.96900500  
C 4.89211000 -0.77208600 -3.95470900  
C 6.14060900 0.18033700 -6.06856900  
C 4.75683600 0.72684400 -8.27078700  
H 1.07563400 0.70516300 -9.96485900  
H -1.09541000 -0.99339700 -6.21267200  
H 5.99818200 -1.19277700 -2.27852500  
C 8.96591500 0.63385400 -6.02913400  
H 9.44364200 2.54719700 -6.68844800  
H 9.88296000 -0.64648100 -7.40123100  
H 13.31327700 0.84943600 -2.06372900  
C 6.04003200 1.74550500 -10.60078200  
H 6.92794500 3.58144400 -10.24143000  
H 7.53280800 0.47435000 -11.26613800  
H 4.69079700 1.99138900 -12.14302400  
C 0.97911300 -2.15503300 -1.61902400

H 2.20332700 -3.33875600 -0.45028000  
H -0.67664700 -3.29385100 -2.14058200  
H -0.77075300 1.62553700 -1.08756000

R of site D EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49122500  
C 1.67757900 0.00000000 -9.55687200  
O 2.46129000 -0.66497200 -11.82992800  
C -6.54354000 2.54952100 -5.84186000  
C -5.80660300 1.50370100 -3.54460200  
C -3.43111500 0.40945500 -3.28937600  
C -1.81273800 0.39410300 -5.37375800  
C -2.53817300 1.42812900 -7.68234400  
C -4.94422100 2.53238100 -7.93154800  
H -8.40325400 3.40538600 -6.01029900  
H -7.09270600 1.54781700 -1.94420000  
H 0.06536800 -0.40561500 -5.18955300  
C -0.76561700 1.40149500 -9.93210400  
H -0.12220900 3.35265700 -10.31488900  
H -1.73770200 0.80643500 -11.67155200  
H 4.07017500 -1.49735200 -11.62187700  
C -5.79010600 3.69200900 -10.39367900  
H -4.48151600 5.16252200 -11.03737300  
H -5.90225000 2.28144600 -11.90708800  
H -7.65704300 4.55267100 -10.20025800  
C -2.62649700 -0.75918500 -0.80940000  
H -2.44349100 -2.82208400 -1.06060500  
H -4.05216800 -0.47569100 0.67379200  
H 1.68898900 0.41396700 3.04230900

TS of site D EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48869700  
C 2.02673400 0.00000000 -9.40150300  
O 4.09667800 0.35453500 -10.69709600  
C -5.45877300 4.44091900 -5.89317200  
C -5.09950900 3.21292300 -3.59588800  
C -3.10343600 1.53146500 -3.28717400  
C -1.46925900 1.12539300 -5.31871200  
C -1.81553800 2.34644900 -7.62317900  
C -3.84455100 4.03520000 -7.93110200  
H -7.02768400 5.74960700 -6.10283500  
H -6.38522300 3.57333400 -2.03590300  
H 0.11299100 -0.15550200 -5.07831600  
C -0.01854200 1.90970900 -9.80278100  
H 0.87777400 3.66974800 -10.45781800  
H -1.06699100 1.17440900 -11.44803000  
H 3.91165700 -1.41699300 -9.39823200  
C -4.26857400 5.38928800 -10.40127600  
H -2.64795000 6.57337900 -10.91218600  
H -4.55896800 4.05871900 -11.96262500  
H -5.93108700 6.60899500 -10.30025500  
C -2.72859000 0.15495900 -0.81115400  
H -3.23966500 -1.85122400 -1.07027900  
H -3.98266000 0.88841900 0.67247300  
H 1.72966300 -0.16868100 3.04429900

P of site D EEF -0.514 V/nm along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48653500  
C 0.77174900 0.00000000 -11.41692500  
O 1.10599500 -0.36686000 -13.64510900  
C 3.65525000 -5.86788500 -6.12227700  
C 3.74313100 -4.67310700 -3.78212200  
C 2.33704200 -2.49498900 -3.33987100

C 0.83049700 -1.56620800 -5.29440400  
C 0.72348800 -2.75677900 -7.64019400  
C 2.16798700 -4.94165700 -8.08845100  
H 4.76881300 -7.56615800 -6.42706100  
H 4.91791400 -5.45030500 -2.28786800  
H -0.31936400 0.09664600 -4.93762800  
C -0.87499600 -1.61669000 -9.72530000  
H -2.32197500 -0.39153800 -8.89046800  
H -1.81107100 -3.04535000 -10.88540700  
H 1.73386000 1.58321700 -10.42596000  
C 2.08734100 -6.28893000 -10.59957800  
H 0.22745300 -7.13971100 -10.92987400  
H 2.45355500 -5.00807700 -12.18041200  
H 3.48662700 -7.80553000 -10.66312200  
C 2.47054200 -1.16059500 -0.81591200  
H 3.71524100 0.50467400 -0.99829900  
H 3.33043400 -2.36237400 0.64284700  
H -1.53961300 0.80385000 3.04555000

R of site D No field along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49414500  
C 1.48800300 0.00000000 -9.65002600  
O 2.21181600 -0.59486100 -11.95975400  
C -6.54822700 2.76610700 -5.69293300  
C -5.79512500 1.65294200 -3.43270000  
C -3.44991600 0.48199800 -3.25219400  
C -1.87780600 0.45812500 -5.37125000  
C -2.62010600 1.55843500 -7.64345400  
C -4.99573100 2.74115300 -7.81765600  
H -8.38431200 3.68007700 -5.80527900  
H -7.04539500 1.70282900 -1.80406700  
H -0.02321000 -0.40621000 -5.24928100  
C -0.89751300 1.52071400 -9.93088100  
H -0.18102300 3.45275400 -10.27687900  
H -1.92974900 1.01597800 -11.66347900  
H 3.78530200 -1.50556800 -11.81969700  
C -5.85925500 3.97241000 -10.23828100  
H -4.51753800 5.40982900 -10.88736700  
H -6.05267600 2.59354200 -11.77205200  
H -7.69178400 4.88985300 -9.98703600  
C -2.62572100 -0.75558500 -0.81160400  
H -2.43055200 -2.80855400 -1.12544000  
H -4.04448400 -0.52065200 0.68704200  
H 1.69087500 0.41476100 3.03806500

TS of site D No field along Z<sub>D</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49130300  
C 2.01833200 0.00000000 -9.40890500  
O 4.12524700 0.26240600 -10.66345300  
C -5.17212200 4.84028400 -5.81794200  
C -4.89028800 3.55124500 -3.54321300  
C -3.00352200 1.74305600 -3.26811800  
C -1.39840900 1.27160300 -5.30833200  
C -1.66688800 2.55351200 -7.58996100  
C -3.58654100 4.37144500 -7.86488500  
H -6.65681000 6.24703600 -6.00359800  
H -6.15168600 3.96252900 -1.97571700  
H 0.09926500 -0.11184700 -5.09571100  
C 0.10163900 2.04557300 -9.77728600  
H 1.11075100 3.75741400 -10.39453000  
H -0.98960500 1.41336800 -11.43698600  
H 3.80312100 -1.53885600 -9.43132100  
C -3.92548800 5.79187100 -10.31039000  
H -2.23001800 6.87161000 -10.80829300

H -4.30889700 4.50953700 -11.89139700  
H -5.50185500 7.11864700 -10.18412600  
C -2.71282800 0.30236400 -0.81636200  
H -3.31922800 -1.67120800 -1.11748200  
H -3.93749000 1.07026400 0.67484000  
H 1.72022600 -0.26079000 3.03963100

P of site D No field along  $Z_D$  direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48951700  
C 0.93581000 0.00000000 -11.41934700  
O 1.34073700 -0.41114200 -13.62666900  
C 3.51226700 -5.97033900 -6.09004200  
C 3.61912000 -4.77086700 -3.75281400  
C 2.29242000 -2.53936800 -3.33534100  
C 0.84402200 -1.56150000 -5.30963600  
C 0.71932800 -2.75489300 -7.65296300  
C 2.08546100 -4.99503400 -8.07710100  
H 4.56497700 -7.70983100 -6.37756000  
H 4.74838900 -5.58531500 -2.24312500  
H -0.24471400 0.14659600 -4.97477400  
C -0.80320000 -1.55802100 -9.76266200  
H -2.22273600 -0.28540500 -8.95290600  
H -1.76347000 -2.95352600 -10.94265200  
H 1.89746500 1.57749300 -10.41850300  
C 1.98808500 -6.34350500 -10.58654100  
H 0.10080200 -7.11972200 -10.94291900  
H 2.42761700 -5.08063700 -12.16280400  
H 3.32662600 -7.91447700 -10.62812800  
C 2.45088100 -1.19723600 -0.81687000  
H 3.71611800 0.45161100 -1.00971700  
H 3.29877000 -2.40455100 0.64474500  
H -1.52888400 0.82836200 3.04108100

R of site D EEF 0.514 V/nm along  $Z_D$  direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49704500  
C 1.17823900 0.00000000 -9.78404000  
O 1.74904200 -0.55531900 -12.14346100  
C -6.20996900 3.77041900 -5.41369900  
C -5.55685500 2.46544500 -3.22601300  
C -3.40519700 0.95860000 -3.17898200  
C -1.92215100 0.79474200 -5.35493400  
C -2.56694800 2.08507400 -7.55574800  
C -4.74714500 3.60848100 -7.59538300  
H -7.89534100 4.94446700 -5.42417200  
H -6.73440800 2.62649200 -1.55075100  
H -0.21476200 -0.33961200 -5.34117300  
C -0.94407500 1.88993500 -9.90661200  
H 0.05213800 3.70223400 -10.20146200  
H -2.09677500 1.63272000 -11.61695200  
H 3.16065700 -1.70929600 -12.11264700  
C -5.49895800 5.05033100 -9.93535800  
H -3.97974400 6.29630400 -10.58793000  
H -5.94948400 3.77775500 -11.50610300  
H -7.16354100 6.21900800 -9.58053700  
C -2.68865800 -0.47969200 -0.81427000  
H -2.68477300 -2.52130600 -1.23821500

## Arene molecule ( $R_F$ )

R of site A No field along  $Z_A$  direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50847300  
C 7.20567400 0.00000000 -0.31582200

H -4.07060400 -0.18703400 0.70877000  
H 1.72589300 0.24375400 3.03400900

TS of site D EEF 0.514 V/nm along  $Z_D$  direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49396700  
C 2.03477300 0.00000000 -9.40056200  
O 4.17095200 0.23211900 -10.60805700  
C -5.04062500 4.99342000 -5.79659400  
C -4.79490200 3.68279000 -3.52984200  
C -2.95250200 1.82843900 -3.26405900  
C -1.35470600 1.33259800 -5.30386600  
C -1.58623700 2.63647100 -7.57714100  
C -3.46192100 4.50142800 -7.84363100  
H -6.49207500 6.43500200 -5.97719300  
H -6.05102100 4.11235700 -1.96268700  
H 0.10755800 -0.08959800 -5.10022900  
C 0.17842000 2.10250400 -9.76130900  
H 1.23841600 3.79220200 -10.35340000  
H -0.92135300 1.51896400 -11.43263400  
H 3.77075700 -1.59173400 -9.43050800  
C -3.76260700 5.94439100 -10.28055100  
H -2.03877300 6.98043400 -10.77270400  
H -4.17989800 4.68142000 -11.86806500  
H -5.30299500 7.31194300 -10.14781600  
C -2.70159300 0.36281600 -0.82169900  
H -3.34517800 -1.59619200 -1.14175400  
H -3.91711500 1.14376100 0.67073000  
H 1.71600200 -0.29904200 3.03489900

P of site D EEF 0.514 V/nm along  $Z_D$  direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49256900  
C 1.10477400 0.00000000 -11.42064600  
O 1.59012800 -0.45502000 -13.60170800  
C 3.48288200 -6.00861500 -6.05154600  
C 3.58540100 -4.79959800 -3.71877700  
C 2.29695200 -2.54144500 -3.32898600  
C 0.88991600 -1.54638100 -5.32438500  
C 0.77089300 -2.74780300 -7.66378200  
C 2.09994600 -5.01584700 -8.06080800  
H 4.50689800 -7.76814800 -6.31954000  
H 4.68333100 -5.62646700 -2.19252700  
H -0.16885100 0.18509500 -5.01358000  
C -0.69589200 -1.52808400 -9.79950200  
H -2.11151500 -0.23466400 -9.01719700  
H -1.65180800 -2.91026800 -10.99805000  
H 2.03307200 1.59425900 -10.41454900  
C 2.01269100 -6.37087200 -10.56665200  
H 0.11535500 -7.10861800 -10.94940100  
H 2.50168300 -5.12188500 -12.13909700  
H 3.31891000 -7.96903500 -10.58384400  
C 2.45442800 -1.18593200 -0.81751700  
H 3.70732100 0.47111100 -1.02294900  
H 3.31457100 -2.38046100 0.64786300  
H -1.53408000 0.82294000 3.03674800

C 4.80604800 -0.00223900 0.70921800  
C 2.65732600 -0.00605800 -0.86557800  
C 3.02148600 -0.01335100 -3.46820100  
C 5.44803000 -0.01032400 -4.54847200  
C 7.57780100 -0.00051800 -2.94320600

H 8.84677000 0.00743600 0.91866000  
H 4.54793000 0.00592100 2.74439000  
H 1.36623500 -0.01004200 -4.67923600  
H -1.73976200 0.00389700 3.04319700  
C 5.90065100 0.04942000 -7.30643800  
O 3.70326400 -0.21041400 -8.47341200  
H 4.03301400 -0.13456400 -10.26169900  
C 10.23357600 -0.03497700 -3.95954100  
H 11.06360100 -1.91298000 -3.69195000  
H 10.25084600 0.39416100 -5.97249900  
H 11.42018800 1.31182200 -2.93413200

TS of site A No field along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48276100  
C 7.02215900 0.00000000 -1.12348800  
C 4.72519600 -0.00352600 0.11490900  
C 2.46251100 -0.00491000 -1.27338700  
C 2.56105000 -0.00797700 -3.89466900  
C 4.88212100 -0.00233200 -5.18250800  
C 7.14958300 0.00413100 -3.77406600  
H 8.76871400 0.00529100 -0.04432000  
H 4.61586000 0.00187600 2.16496400  
H 0.80859900 -0.00302700 -4.96031800  
H -1.90820700 0.00290800 1.37150900  
C 5.08347700 0.06987300 -7.97214700  
O 2.79198300 -0.20780000 -8.93370300  
H 2.95387200 -0.12153600 -10.74477900  
C 9.70068400 -0.03228800 -5.02968800  
H 10.53246300 -1.92186400 -4.87195800  
H 9.54015200 0.43117100 -7.02860300  
H 10.98882800 1.28574700 -4.09407200

P of site A No field along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28832300  
C 6.85323600 0.00000000 -1.93139300  
C 4.70567100 -0.00243400 -0.44803900  
C 2.30760400 -0.00408000 -1.57842500  
C 2.12198900 -0.00705100 -4.18973800  
C 4.28866700 -0.00278500 -5.72671900  
C 6.69608800 0.00246600 -4.57942600  
H 8.70476600 0.00477300 -1.04492400  
H 4.82256800 0.00284400 1.60008100  
H 0.27486600 -0.00421200 -5.08919300  
H -1.80114600 0.00265300 -1.08022500  
C 4.17685200 0.05355500 -8.52134900  
O 1.78424800 -0.16884500 -9.21772700  
H 1.74480400 -0.10064300 -11.03633600  
C 9.09690900 -0.02907300 -6.10407300  
H 9.99838100 -1.88703600 -5.95836400  
H 8.70854900 0.34756600 -8.08971100  
H 10.43775900 1.36255000 -5.37004100

R of site A EEF -0.514 V/nm along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50547900  
C 7.20849000 0.00000000 -0.30328600  
C 4.80735600 0.00000000 0.71714600  
C 2.66114200 0.00000200 -0.86223900  
C 3.02987300 0.00000800 -3.46241200  
C 5.45940400 0.00000800 -4.54042200  
C 7.58591000 0.00000400 -2.93008200  
H 8.84704200 -0.00000400 0.93452900  
H 4.54556400 -0.00000600 2.75177500  
H 1.37559500 0.00000800 -4.67458700

H -1.73777000 -0.00000200 3.04797100  
C 5.91597500 0.00000400 -7.29528500  
O 3.70190100 0.00004700 -8.46672300  
H 4.04576900 0.00003800 -10.25306500  
C 10.24872800 0.00001100 -3.93064700  
H 11.26672900 -1.66444900 -3.24184700  
H 10.25684000 -0.00005300 -5.98828700  
H 11.26667300 1.66455500 -3.24196300

TS of site A EEF -0.514 V/nm along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47959200  
C 7.02684200 0.00000000 -1.10675400  
C 4.72624800 0.00128100 0.12483500  
C 2.46739200 0.00457900 -1.27021600  
C 2.57311100 0.01025600 -3.88961200  
C 4.89864300 0.00820500 -5.17250200  
C 7.16208600 0.00141500 -3.75670900  
H 8.76971600 -0.00574300 -0.02178100  
H 4.61123800 -0.00538800 2.17458100  
H 0.82296100 0.00793500 -4.95889700  
H -1.91046900 -0.00262100 1.36562600  
C 5.10656200 -0.03831600 -7.95880400  
O 2.80561100 0.15822100 -8.92592100  
H 2.98027500 0.09888600 -10.73603000  
C 9.72039800 0.03209500 -4.99894700  
H 10.95169100 -1.39447100 -4.14865300  
H 9.55635300 -0.29737300 -7.02366700  
H 10.62164300 1.87246800 -4.70457500

P of site A EEF -0.514 V/nm along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28686400  
C 6.85993000 0.00000000 -1.91059700  
C 4.70752500 0.00000000 -0.43494500  
C 2.31296000 -0.00000200 -1.57418000  
C 2.13627200 -0.00000800 -4.18448800  
C 4.30893600 -0.00000900 -5.71603800  
C 6.71212500 -0.00000400 -4.55923800  
H 8.70812600 0.00000400 -1.01720200  
H 4.81711000 0.00000600 1.61359600  
H 0.29151300 -0.00000900 -5.08847900  
H -1.79964400 0.00000200 -1.08296500  
C 4.20561600 0.00000900 -8.50848000  
O 1.80105300 -0.00008700 -9.20973900  
H 1.77526400 -0.00006000 -11.02899200  
C 9.12434400 -0.00002300 -6.06746300  
H 10.25801800 -1.66485100 -5.59478600  
H 8.72710800 0.00013600 -8.08628700  
H 10.25821000 1.66460600 -5.59453600

R of site A EEF 0.514 V/nm along Z<sub>A</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51153000  
C 7.20250700 0.00000000 -0.32999500  
C 4.80532000 -0.00619800 0.70057300  
C 2.65329700 -0.00403100 -0.86930600  
C 3.01202600 -0.00236400 -3.47412300  
C 5.43542700 0.00670300 -4.55825700  
C 7.56858900 0.01132500 -2.95854100  
H 8.84708500 0.00309300 0.90008400  
H 4.55146000 -0.00471500 2.73641900  
H 1.35507800 0.00583700 -4.68295700  
H -1.74174400 0.00222000 3.03845600  
C 5.88363600 0.09392900 -7.31966400  
O 3.69488300 -0.22169000 -8.48227900

H 4.01298800 -0.12130200 -10.27232900  
C 10.21933100 -0.02300400 -3.98675300  
H 11.00834300 -1.93120300 -3.83054800  
H 10.23700200 0.50849000 -5.97548600  
H 11.44038200 1.23959700 -2.89725700

TS of site A EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48600900  
C 7.01735100 0.00000000 -1.14159000  
C 4.72412100 0.00789900 0.10409600  
C 2.45741200 0.00330100 -1.27689000  
C 2.54821900 -0.00257900 -3.90022400  
C 4.86449900 -0.01502700 -5.19325700  
C 7.13638200 -0.01691900 -3.79258400  
H 8.76769200 -0.00131900 -0.06845500  
H 4.62093200 0.00874000 2.15449700  
H 0.79324300 -0.01275800 -4.96185000  
H -1.90591800 -0.00215100 1.37746900  
C 5.05875300 -0.12032100 -7.98557600  
O 2.77970100 0.23389000 -8.94355600  
H 2.92806400 0.11738400 -10.75500400  
C 9.67916800 0.01948300 -5.06358700  
H 11.02263100 -1.17446900 -4.04403400  
H 9.52651800 -0.58996100 -7.02402000  
H 10.43695800 1.94657700 -5.05982900

P of site A EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28982000  
C 6.84639500 0.00000000 -1.95181000  
C 4.70389500 -0.00478500 -0.46086300  
C 2.30223200 -0.00452600 -1.58263700  
C 2.10784900 -0.00472100 -4.19479500  
C 4.26863800 0.00335000 -5.73745500  
C 6.68006700 0.00836000 -4.59941000  
H 8.70138500 0.00432200 -1.07248000  
H 4.82799300 -0.00094500 1.58685300  
H 0.25836000 0.00006800 -5.08965800  
H -1.80262700 0.00339600 -1.07750000  
C 4.14855700 0.08344500 -8.53436000  
O 1.76554300 -0.21302300 -9.22585300  
H 1.71386900 -0.12099200 -11.04397600  
C 9.07112900 -0.02593100 -6.13823200  
H 9.89770500 -1.92402200 -6.11085300  
H 8.68682500 0.47186100 -8.09817700  
H 10.47027400 1.26698100 -5.33690400

R of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50847300  
C 7.20567400 0.00000000 -0.31582200  
C 4.80604800 -0.00223900 0.70921800  
C 2.65732600 -0.00605800 -0.86557800  
C 3.02148600 -0.01335100 -3.46820100  
C 5.44803000 -0.01032500 -4.54847200  
C 7.57780100 -0.00052000 -2.94320600  
H 8.84677000 0.00743600 0.91866000  
H 4.54793000 0.00592100 2.74439000  
H 1.36623500 -0.01004200 -4.67923600  
H -1.73976200 0.00389700 3.04319700  
C 5.90065100 0.04941600 -7.30643800  
O 3.70326400 -0.21041500 -8.47341200  
H 4.03301400 -0.13456600 -10.26169900  
C 10.23357600 -0.03497700 -3.95954100  
H 11.06360100 -1.91298000 -3.69194800

H 10.25084600 0.39415900 -5.97249900  
H 11.42018800 1.31182200 -2.93413400

TS of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50598000  
C 7.21712000 0.00000000 -0.29143400  
C 4.80763000 -0.00000200 0.71784100  
C 2.66288000 -0.00000200 -0.86240300  
C 3.03605400 0.00000200 -3.46355200  
C 5.47104500 0.00000400 -4.50139900  
C 7.60201200 0.00000400 -2.91454700  
H 8.85021500 -0.00000200 0.95342600  
H 4.54032000 -0.00000600 2.75165800  
H 1.40942800 0.00000000 -4.71628200  
H -1.73971500 0.00000200 3.04230700  
C 5.76733500 0.00000200 -7.26231700  
O 3.70170300 0.00001700 -8.63419800  
H 5.68364100 0.00000000 -9.60966900  
C 10.25295300 0.00001300 -3.94292800  
H 11.28075900 -1.66514800 -3.27229800  
H 10.25609600 -0.00004000 -6.00191800  
H 11.28071100 1.66524100 -3.27238700

P of site B No field along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50485000  
C 7.21190100 0.00000000 -0.30094300  
C 4.80144600 -0.00001100 0.71816800  
C 2.66667500 0.00000800 -0.86045300  
C 3.04022500 0.00004000 -3.46679300  
C 5.46513400 0.00005500 -4.50804900  
C 7.59723700 0.00003200 -2.91902900  
H 8.84385600 -0.00001700 0.94440400  
H 4.54007100 -0.00003400 2.75238300  
H 1.41399600 0.00005500 -4.71717200  
H -1.73982100 -0.00000600 3.04128100  
C 5.69953500 0.00009400 -7.30362200  
O 3.90977500 0.00012500 -8.73171900  
H 7.64930600 0.00009600 -8.06617100  
C 10.26117900 0.00004700 -3.93955700  
H 10.63129200 -1.66733600 -5.10518400  
H 10.63130300 1.66748400 -5.10510300  
H 11.62813000 0.00000400 -2.39412100

R of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50547900  
C 7.20849000 0.00000000 -0.30328600  
C 4.80735600 0.00000000 0.71714600  
C 2.66114200 0.00000200 -0.86223900  
C 3.02987300 0.00000800 -3.46241200  
C 5.45940400 0.00000900 -4.54042200  
C 7.58591000 0.00000400 -2.93008200  
H 8.84704200 -0.00000400 0.93452900  
H 4.54556400 -0.00000600 2.75177500  
H 1.37559500 0.00000900 -4.67458700  
H -1.73777000 -0.00000200 3.04797100  
C 5.91597500 0.00000400 -7.29528500  
O 3.70190100 0.00005100 -8.46672300  
H 4.04576900 0.00004200 -10.25306500  
C 10.24872800 0.00001300 -3.93064700  
H 11.26673300 -1.66444300 -3.24184200  
H 10.25684000 -0.00005900 -5.98828700  
H 11.26667100 1.66456000 -3.24196800

TS of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50316800  
C 7.22052200 0.00000000 -0.26147600  
C 4.80534900 -0.00000200 0.73511900  
C 2.66832300 -0.00000400 -0.85545500  
C 3.05378900 0.00000200 -3.45397700  
C 5.49482300 0.00000800 -4.48016800  
C 7.61847400 0.00000600 -2.88168000  
H 8.84618000 -0.00000400 0.99278900  
H 4.52818800 -0.00000600 2.76747900  
H 1.43276300 0.00000200 -4.71382500  
H -1.73768700 0.00000200 3.04739400  
C 5.80732000 0.00000800 -7.23529700  
O 3.75058800 0.00002100 -8.62656000  
H 5.73841100 0.00000800 -9.58303900  
C 10.27536000 0.00001500 -3.89485700  
H 11.29912500 -1.66477000 -3.21727100  
H 10.29075900 -0.00003000 -5.95385900  
H 11.29908100 1.66485700 -3.21734900

P of site B EEF -0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50216500  
C 7.21525500 0.00000000 -0.26126600  
C 4.79733200 0.00000900 0.74092800  
C 2.67301500 -0.00001500 -0.85137300  
C 3.06337800 -0.00005100 -3.45471600  
C 5.49597200 -0.00006400 -4.47963200  
C 7.61808200 -0.00003800 -2.87569800  
H 8.83749700 0.00002100 0.99641900  
H 4.52271900 0.00003800 2.77322700  
H 1.44487800 -0.00006600 -4.71509200  
H -1.73777400 0.00001500 3.04657000  
C 5.75465500 -0.00010400 -7.27008500  
O 3.98223500 -0.00012700 -8.72167000  
H 7.71321300 -0.00011300 -8.01146500  
C 10.29006900 -0.00004900 -3.87596600  
H 10.67014400 -1.66802400 -5.03774500  
H 10.67014100 1.66789200 -5.03779600  
H 11.64401700 -0.00002500 -2.31928400

R of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.51153000  
C 7.20250700 0.00000000 -0.32999400  
C 4.80532000 -0.00620000 0.70057500  
C 2.65329700 -0.00402900 -0.86930600  
C 3.01202800 -0.00235600 -3.47412100  
C 5.43542900 0.00671400 -4.55825600  
C 7.56859000 0.01133100 -2.95853900  
H 8.84708500 0.00309200 0.90008600  
H 4.55146000 -0.00472100 2.73641900  
H 1.35508000 0.00584700 -4.68295700  
H -1.74174400 0.00221900 3.03845600  
C 5.88363800 0.09394200 -7.31966200  
O 3.69488300 -0.22165700 -8.48227900  
H 4.01298800 -0.12126900 -10.27232900  
C 10.21933300 -0.02299400 -3.98674900  
H 11.00835300 -1.93118900 -3.83052900  
H 10.23700200 0.50848400 -5.97548600  
H 11.44037600 1.23961900 -2.89726300

TS of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50885800

C 7.21358300 0.00000000 -0.32312300  
C 4.81014900 0.00002800 0.69954700  
C 2.65724100 0.00001100 -0.86974300  
C 3.01741200 -0.00000200 -3.47357900  
C 5.44599400 -0.00000900 -4.52385300  
C 7.58468300 -0.00001500 -2.94921400  
H 8.85442500 -0.00001300 0.91182300  
H 4.55335000 0.00003800 2.73488100  
H 1.38485400 -0.00001900 -4.71871000  
H -1.74173100 -0.00001100 3.03722200  
C 5.72517900 -0.00003800 -7.29056800  
O 3.65036700 0.00000000 -8.64246700  
H 5.62598100 -0.00005900 -9.63747900  
C 10.22932400 -0.00003000 -3.99340900  
H 11.26129300 -1.66552000 -3.32990300  
H 10.21981500 -0.00017400 -6.05231900  
H 11.26120600 1.66561500 -3.33015000

P of site B EEF 0.514 V/nm along Z<sub>A</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50759600  
C 7.20828600 0.00000000 -0.34363000  
C 4.80597200 -0.00002300 0.69365100  
C 2.66001500 0.00001500 -0.87017600  
C 3.01552400 0.00007700 -3.47958800  
C 5.43207100 0.00010800 -4.53851500  
C 7.57485900 0.00006600 -2.96548000  
H 8.85049000 -0.00003400 0.88848300  
H 4.55899100 -0.00007200 2.72985800  
H 1.38099900 0.00010800 -4.71911300  
H -1.74186000 -0.00001100 3.03596200  
C 5.64022800 0.00018700 -7.33917800  
O 3.83236200 0.00022900 -8.74228100  
H 7.58030700 0.00020800 -8.12440800  
C 10.23014000 0.00009400 -4.00736400  
H 10.58971200 -1.66669800 -5.17693100  
H 10.58974200 1.66700400 -5.17675400  
H 11.61070300 0.00000000 -2.47391500

R of site A No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50154100  
C 9.22387000 0.00000000 1.76650000  
O 11.43579400 -0.16087200 0.59436400  
C 5.54572300 -0.63263500 -4.40560300  
C 7.58169800 -0.48522100 -2.78001300  
C 7.20735800 -0.19074000 -0.15902400  
C 4.74094900 -0.05996900 0.73932500  
C 2.64383000 -0.20483300 -0.88410900  
C 3.05410500 -0.49321300 -3.50365600  
H 5.85984800 -0.85508300 -6.42278900  
H 9.49762400 -0.58750900 -3.50614800  
H 4.45461700 0.17326100 2.75676000  
H 12.72748600 -0.03393200 1.87035500  
H -1.73090900 0.16892500 3.03812300  
C 0.90417400 -0.70256100 -5.35328400  
H 0.69699600 -2.66868900 -5.96902900  
H -0.86700900 -0.11416400 -4.48525900  
H 1.28360100 0.43177600 -7.03915500

TS of site A No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50049200  
C 9.32345500 0.00000000 1.58199400  
O 11.60775700 -0.14680000 0.62040700  
C 5.54806600 -0.67778100 -4.40588900

C 7.58403300 -0.51102000 -2.78198000  
C 7.18865300 -0.19159400 -0.17658400  
C 4.73666800 -0.05236800 0.74561300  
C 2.64607100 -0.21709600 -0.88143500  
C 3.05836400 -0.53168200 -3.50008000  
H 5.86065700 -0.91984900 -6.42047200  
H 9.51421400 -0.61366800 -3.47364900  
H 4.43924800 0.20097800 2.75907700  
H 11.33235200 0.12458600 2.79468500  
H -1.72960800 0.17953200 3.03895500  
C 0.90545300 -0.76483900 -5.34292100  
H 0.66932400 -2.74574100 -5.89771500  
H -0.85792500 -0.12783100 -4.49351200  
H 1.30027800 0.31227500 -7.06196200

P of site A No field along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50172800  
C 9.35467000 0.00000000 1.60590100  
O 11.54901300 -0.08629400 0.96252100  
C 5.56388900 -0.54548700 -4.39620200  
C 7.59376200 -0.41027900 -2.76099300  
C 7.18752900 -0.15320800 -0.15389200  
C 4.73527400 -0.04182700 0.75637100  
C 2.64867900 -0.17502700 -0.88214700  
C 3.06872900 -0.42901300 -3.50365800  
H 5.89079100 -0.74050500 -6.41338900  
H 9.52521600 -0.49207500 -3.44750100  
H 4.39628100 0.16177200 2.77234300  
H 8.82926100 0.20600900 3.62891800  
H -1.73306700 0.14490400 3.03938900  
C 0.92721700 -0.62089200 -5.36552400  
H 0.76746500 -2.56634700 -6.05540100  
H -0.85881500 -0.10151000 -4.48467100  
H 1.28451500 0.58470600 -7.00611900

R of site A EEF -0.514 V/nm along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49885400  
C 9.22271800 0.00000000 1.77234300  
O 11.43581100 -0.20036800 0.60984900  
C 5.54588000 -0.74651200 -4.39009100  
C 7.58233400 -0.57275900 -2.76637700  
C 7.20733900 -0.22361900 -0.15341200  
C 4.74074100 -0.06753300 0.74137200  
C 2.64445500 -0.23912200 -0.87990800  
C 3.05514200 -0.58065300 -3.49219800  
H 5.86012400 -1.01118300 -6.40244900  
H 9.49879700 -0.69580500 -3.48824300  
H 4.45462700 0.20789300 2.75349800  
H 12.72366000 -0.05279900 1.88814000  
H -1.72610100 0.19576400 3.04312000  
C 0.90107700 -0.82408700 -5.33352000  
H 0.64211000 -2.81176400 -5.85372000  
H -0.85489400 -0.15509600 -4.49220400  
H 1.30612400 0.22012100 -7.07098600

TS of site A EEF -0.514 V/nm along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49767100  
C 9.33377900 0.00000000 1.54782200  
O 11.61048600 -0.16955600 0.57363800  
C 5.52946700 -0.80791900 -4.40600800  
C 7.57232800 -0.60873400 -2.79346200  
C 7.18789200 -0.22821300 -0.19585300  
C 4.73966200 -0.06264400 0.73349400

C 2.64335400 -0.25785100 -0.88238300  
C 3.04486600 -0.63279200 -3.49422800  
H 5.83376100 -1.09805400 -6.41576100  
H 9.50023900 -0.73175900 -3.48838700  
H 4.45060700 0.23752900 2.74178600  
H 11.35316700 0.14628900 2.74418600  
H -1.72405500 0.21163600 3.04353700  
C 0.88002700 -0.90496200 -5.31828900  
H 0.58528400 -2.90556300 -5.76437200  
H -0.86232400 -0.17979400 -4.49534300  
H 1.29499000 0.06913800 -7.09323200

P of site A EEF -0.514 V/nm along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49882200  
C 9.37272200 0.00000000 1.54457600  
O 11.55767900 -0.11003700 0.87323100  
C 5.53231500 -0.73855400 -4.40385000  
C 7.57346400 -0.55497500 -2.78640600  
C 7.18606600 -0.20794400 -0.18808300  
C 4.73980700 -0.05800900 0.73537600  
C 2.64345600 -0.23667500 -0.88556800  
C 3.04516100 -0.57997600 -3.49953800  
H 5.84567700 -1.00370600 -6.41536400  
H 9.50078000 -0.66561300 -3.48052500  
H 4.41417300 0.21544800 2.74526900  
H 8.87417600 0.27233400 3.56529500  
H -1.72635800 0.19421100 3.04379100  
C 0.88521400 -0.83249100 -5.33308100  
H 0.62282800 -2.82247700 -5.84169600  
H -0.86849200 -0.15744800 -4.49230000  
H 1.28601000 0.20265200 -7.07659100

R of site A EEF 0.514 V/nm along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50426400  
C 9.22474100 0.00000000 1.76319100  
O 11.43584100 -0.10955500 0.58231700  
C 5.54750100 -0.45655400 -4.42275600  
C 7.58239900 -0.35023400 -2.79418600  
C 7.20785100 -0.13892300 -0.16380900  
C 4.74144900 -0.04578600 0.73788700  
C 2.64381100 -0.14988900 -0.88886500  
C 3.05453900 -0.35693700 -3.51675900  
H 5.86191800 -0.61536700 -6.44567100  
H 9.49798300 -0.42248100 -3.52443700  
H 4.45428800 0.12235400 2.76170900  
H 12.73086300 -0.01625200 1.85721600  
H -1.73659900 0.12475600 3.03308900  
C 0.91017200 -0.51051700 -5.37768300  
H 0.79519500 -2.42395800 -6.15979300  
H -0.88293000 -0.07054500 -4.46898500  
H 1.23541300 0.77760200 -6.96157600

TS of site A EEF 0.514 V/nm along Z<sub>B</sub> direction  
C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50333600  
C 9.31199800 0.00000000 1.62219800  
O 11.60489600 -0.10324100 0.67382200  
C 5.57090500 -0.46065300 -4.40721700  
C 7.59857900 -0.34732000 -2.76977100  
C 7.19006100 -0.13030800 -0.15438500  
C 4.73373200 -0.03569700 0.75980800  
C 2.64981800 -0.14876700 -0.88097200  
C 3.07508600 -0.36266100 -3.50810400  
H 5.89305500 -0.62388000 -6.42804800

H 9.53149900 -0.41619500 -3.45769800  
H 4.42625800 0.13772900 2.78020200  
H 11.30906900 0.08570300 2.85405800  
H -1.73632800 0.12439900 3.03432100  
C 0.93748000 -0.52662300 -5.37559100  
H 0.81824400 -2.44786000 -6.13748100  
H -0.85839500 -0.07128000 -4.48027200  
H 1.27421800 0.74341300 -6.97128400

P of site A EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50470300  
C 9.33381500 0.00000000 1.67527900  
O 11.53794500 -0.03732000 1.06144800  
C 5.59948400 -0.22512300 -4.38381500  
C 7.61614000 -0.16942200 -2.72895500  
C 7.18831300 -0.06329300 -0.11344000  
C 4.72924900 -0.01729900 0.78096700  
C 2.65433100 -0.07278700 -0.87752700  
C 3.09531200 -0.17765100 -3.50583600  
H 5.94196300 -0.30488300 -6.40611400  
H 9.55245400 -0.20290800 -3.40571900  
H 4.37297000 0.06706800 2.80257100  
H 8.77929500 0.08688800 3.70041000  
H -1.73981700 0.06103600 3.03524700  
C 0.97483500 -0.25970500 -5.39915800  
H 0.99459300 -2.06915800 -6.40322800  
H -0.84832300 -0.03459100 -4.47266000  
H 1.22202400 1.22623100 -6.81582000

R of site B No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50154100  
C 9.22387000 0.00000000 1.76649600  
O 11.43579200 -0.16088000 0.59435900  
C 5.54572100 -0.63264500 -4.40560300  
C 7.58169800 -0.48522700 -2.78001300  
C 7.20735800 -0.19074300 -0.15902600  
C 4.74094900 -0.05997000 0.73932400  
C 2.64383000 -0.20483900 -0.88410900  
C 3.05410300 -0.49322200 -3.50365600  
H 5.85984700 -0.85509600 -6.42278900  
H 9.49762200 -0.58751600 -3.50615200  
H 4.45461700 0.17326500 2.75675800  
H 12.72748600 -0.03393800 1.87035000  
H -1.73090900 0.16892800 3.03812300  
C 0.90417000 -0.70258000 -5.35328100  
H 0.69696500 -2.66872000 -5.96898400  
H -0.86700500 -0.11414300 -4.48526900  
H 1.28361200 0.43171800 -7.03917600

TS of site B No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47969400  
C 9.23968000 0.00000000 0.78923500  
O 11.32804900 -0.00005300 -0.59593300  
C 5.00614700 -0.00015300 -5.06318900  
C 7.17951100 -0.00012300 -3.61373400  
C 7.04894000 -0.00004300 -0.95287600  
C 4.67527900 -0.00000900 0.17443900  
C 2.46397100 -0.00004300 -1.28037900  
C 2.60766200 -0.00011100 -3.93340200  
H 5.14033100 -0.00021000 -7.11227800  
H 9.02190900 -0.00015300 -4.51568900  
H 4.53054500 0.00004300 2.22427000  
H 12.73661200 -0.00003000 0.55741700

H -1.90909500 0.00003600 1.36834600  
C 0.28481200 -0.00014700 -5.57331500  
H 0.27500800 -1.66542200 -6.80033100  
H -1.43214100 -0.00006400 -4.43684200  
H 0.27506900 1.66500800 -6.80049200

P of site B No field along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28970300  
C 9.26259800 0.00000000 -0.09102200  
O 11.22337500 0.00004200 -1.64965800  
C 4.53570700 0.00003000 -5.54632400  
C 6.83462600 0.00002600 -4.29558000  
C 6.92923700 0.00001100 -1.64225400  
C 4.65750400 0.00000200 -0.31122500  
C 2.33225700 0.00000800 -1.55934000  
C 2.24739900 0.00002100 -4.21710100  
H 4.49334000 0.00004000 -7.59876400  
H 8.58877100 0.00003400 -5.35831300  
H 4.69284800 -0.00000900 1.73977700  
H 12.72584400 0.00003000 -0.62140800  
H -1.81200600 -0.00000600 -1.04854700  
C -0.21054800 0.00002600 -5.66500200  
H -1.35271600 -1.66731900 -5.22766300  
H -1.35271600 1.66736800 -5.22765000  
H 0.14615500 0.00003400 -7.69712800

R of site B EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.49885400  
C 9.22271900 0.00000000 1.77232800  
O 11.43581100 -0.20042400 0.60983600  
C 5.54586700 -0.74657600 -4.39009600  
C 7.58232500 -0.57280800 -2.76638800  
C 7.20733700 -0.22363600 -0.15342700  
C 4.74074100 -0.06753500 0.74136300  
C 2.64445400 -0.23914500 -0.87991000  
C 3.05513100 -0.58070700 -3.49219800  
H 5.86010400 -1.01127200 -6.40245100  
H 9.49878600 -0.69586500 -3.48825800  
H 4.45463400 0.20791700 2.75348700  
H 12.72366100 -0.05284400 1.88812400  
H -1.72609900 0.19578300 3.04312000  
C 0.90105600 -0.82416500 -5.33350500  
H 0.64203100 -2.81186100 -5.85361000  
H -0.85489400 -0.15509000 -4.49221100  
H 1.30612800 0.21995100 -7.07102000

TS of site B EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.47680100  
C 9.23613800 0.00000000 0.82227100  
O 11.33180400 0.00001700 -0.55138100  
C 5.02534100 0.00007400 -5.04841300  
C 7.19384100 0.00005700 -3.59089100  
C 7.05278600 0.00002100 -0.93140900  
C 4.67485500 0.00000600 0.18719600  
C 2.46930600 0.00002300 -1.27593000  
C 2.62302800 0.00005700 -3.92728900  
H 5.16666300 0.00010000 -7.09734900  
H 9.04028700 0.00007000 -4.48484500  
H 4.52235500 -0.00002300 2.23472100  
H 12.73218200 0.00000900 0.61251000  
H -1.91127900 -0.00002100 1.36219500  
C 0.30407400 0.00007900 -5.57378300  
H 0.29593500 -1.66580700 -6.80029400

H -1.41467600 0.00001300 -4.43966000  
H 0.29588200 1.66605700 -6.80017100

P of site B EEF -0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28838200  
C 9.26207500 0.00000000 -0.06556800  
O 11.22997000 -0.00004700 -1.61529700  
C 4.55121100 -0.00003400 -5.53629100  
C 6.84704900 -0.00003000 -4.27946200  
C 6.93381000 -0.00001300 -1.62646000  
C 4.65849400 -0.00000200 -0.30136200  
C 2.33667900 -0.00000900 -1.55584400  
C 2.25948800 -0.00002500 -4.21298200  
H 4.51356400 -0.00004700 -7.58916400  
H 8.60488100 -0.00004000 -5.33635400  
H 4.68842200 0.00001100 1.74980000  
H 12.72571700 -0.00003400 -0.57670300  
H -1.81119900 0.00000600 -1.05043700  
C -0.19550500 -0.00003000 -5.66640300  
H -1.33890900 -1.66706800 -5.23102500  
H -1.33890700 1.66701500 -5.23104200  
H 0.16619800 -0.00004200 -7.69802000

R of site B EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50426400  
C 9.22474100 0.00000000 1.76319300  
O 11.43584100 -0.10953600 0.58231900  
C 5.54750300 -0.45652000 -4.42275600  
C 7.58240100 -0.35020800 -2.79418400  
C 7.20785300 -0.13891400 -0.16380700  
C 4.74144900 -0.04578400 0.73788900  
C 2.64381300 -0.14987800 -0.88886500  
C 3.05454100 -0.35691100 -3.51676100  
H 5.86192000 -0.61532000 -6.44567300  
H 9.49798500 -0.42244800 -3.52443700  
H 4.45428700 0.12234300 2.76171300  
H 12.73086300 -0.01623800 1.85722000  
H -1.73659900 0.12474800 3.03308900  
C 0.91017600 -0.51047800 -5.37768600  
H 0.79522000 -2.42390400 -6.15983700  
H -0.88293000 -0.07054200 -4.46898100

## Arene molecule (R<sub>G</sub>)

**R = Me**

R of site A

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50847300  
C 7.20567400 0.00000000 -0.31582200  
C 4.80604800 -0.00223900 0.70921800  
C 2.65732600 -0.00605800 -0.86557800  
C 3.02148600 -0.01335100 -3.46820100  
C 5.44803000 -0.01032400 -4.54847200  
C 7.57780100 -0.00051800 -2.94320600  
H 8.84677000 0.00743600 0.91866000  
H 4.54793000 0.00592100 2.74439000  
H 1.36623500 -0.01004200 -4.67923600  
H -1.73976200 0.00389700 3.04319700  
C 5.90065100 0.04942000 -7.30643800  
O 3.70326400 -0.21041400 -8.47341200  
H 4.03301400 -0.13456400 -10.26169900  
C 10.23357600 -0.03497700 -3.95954100  
H 11.06360100 -1.91298000 -3.69195000  
H 10.25084600 0.39416100 -5.97249900

H 1.23540100 0.77767900 -6.96155400

TS of site B EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48265500  
C 9.24293600 0.00000000 0.75693400  
O 11.32407500 -0.00005500 -0.63945300  
C 4.98725400 -0.00009300 -5.07766800  
C 7.16533600 -0.00007600 -3.63610300  
C 7.04504500 -0.00002300 -0.97388400  
C 4.67559400 0.00000000 0.16191700  
C 2.45865400 -0.00002100 -1.28474800  
C 2.59251800 -0.00006200 -3.93942900  
H 5.11448500 -0.00012900 -7.12690800  
H 9.00372300 -0.00010000 -4.54590800  
H 4.53844700 0.00003800 2.21035500  
H 12.74067100 -0.00004500 0.50341400  
H -1.90689900 0.00001700 1.37451900  
C 0.26593000 -0.00007400 -5.57293900  
H 0.25464100 -1.66455300 -6.80074200  
H -1.44931300 -0.00008500 -4.43424000  
H 0.25462000 1.66441500 -6.80072800

P of site B EEF 0.514 V/nm along Z<sub>B</sub> direction

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.29105400  
C 9.26299000 0.00000000 -0.11606900  
O 11.21669100 -0.00004700 -1.68343900  
C 4.52036700 -0.00012500 -5.55624300  
C 6.82230100 -0.00010000 -4.31147000  
C 6.92464700 -0.00004000 -1.65781600  
C 4.65646300 -0.00000900 -0.32096100  
C 2.32783700 -0.00003200 -1.56279800  
C 2.23542200 -0.00009100 -4.22120400  
H 4.47337300 -0.00017200 -7.60827300  
H 8.57278900 -0.00012700 -5.37997100  
H 4.69713000 0.00003800 1.72988800  
H 12.72579300 -0.00002100 -0.66553200  
H -1.81280000 0.00002300 -1.04668800  
C -0.22540700 -0.00011900 -5.66369100  
H -1.36636300 -1.66775200 -5.22438400  
H -1.36634400 1.66755200 -5.22447900  
H 0.12638100 -0.00017600 -7.69632500

H 11.42018800 1.31182200 -2.93413200

TS of site A

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.48276100  
C 7.02215900 0.00000000 -1.12348800  
C 4.72519600 -0.00352600 0.11490900  
C 2.46251100 -0.00491000 -1.27338700  
C 2.56105000 -0.00797700 -3.89466900  
C 4.88212100 -0.00233200 -5.18250800  
C 7.14958300 0.00413100 -3.77406600  
H 8.76871400 0.00529100 -0.04432000  
H 4.61586000 0.00187600 2.16496400  
H 0.80859900 -0.00302700 -4.96031800  
H -1.90820700 0.00290800 1.37150900  
C 5.08347700 0.06987300 -7.97214700  
O 2.79198300 -0.20780000 -8.93370300  
H 2.95387200 -0.12153600 -10.74477900  
C 9.70068400 -0.03228800 -5.02968800

H 10.53246300 -1.92186400 -4.87195800  
H 9.54015200 0.43117100 -7.02860300  
H 10.98882800 1.28574700 -4.09407200

P of site A

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28832300  
C 6.85323600 0.00000000 -1.93139300  
C 4.70567100 -0.00243400 -0.44803900  
C 2.30760400 -0.00408000 -1.57842500  
C 2.12198900 -0.00705100 -4.18973800  
C 4.28866700 -0.00278500 -5.72671900  
C 6.69608800 0.00246600 -4.57942600  
H 8.70476600 0.00477300 -1.04492400  
H 4.82256800 0.00284400 1.60008100  
H 0.27486600 -0.00421200 -5.08919300  
H -1.80114600 0.00265300 -1.08022500  
C 4.17685200 0.05355500 -8.52134900  
O 1.78424800 -0.16884500 -9.21772700  
H 1.74480400 -0.10064300 -11.03633600  
C 9.09690900 -0.02907300 -6.10407300  
H 9.99838100 -1.88703600 -5.95836400  
H 8.70854900 0.34756600 -8.08971100  
H 10.43775900 1.36255000 -5.37004100

R of site B

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50847300  
C 7.20567400 0.00000000 -0.31582200  
C 4.80604800 -0.00223900 0.70921800  
C 2.65732600 -0.00605800 -0.86557800  
C 3.02148600 -0.01335100 -3.46820100  
C 5.44803000 -0.01032500 -4.54847200  
C 7.57780100 -0.00052000 -2.94320600  
H 8.84677000 0.00743600 0.91866000  
H 4.54793000 0.00592100 2.74439000  
H 1.36623500 -0.01004200 -4.67923600  
H -1.73976200 0.00389700 3.04319700  
C 5.90065100 0.04941600 -7.30643800  
O 3.70326400 -0.21041500 -8.47341200  
H 4.03301400 -0.13456600 -10.26169900  
C 10.23357600 -0.03497700 -3.95954100  
H 11.06360100 -1.91298000 -3.69194800  
H 10.25084600 0.39415900 -5.97249900

**R = tBu**

R of site A

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50756600  
C 7.20843300 0.00000000 -0.34880600  
C 4.80714800 0.00306900 0.68880900  
C 2.65893300 0.00371100 -0.86382100  
C 3.03688700 0.00847200 -3.46487700  
C 5.45251800 -0.00143400 -4.56040200  
C 7.62189000 -0.01211100 -2.97051300  
H 8.80353600 0.00182200 0.93004200  
H 4.57238100 0.00175600 2.72706900  
H 1.38156000 0.00791600 -4.67407500  
H -1.73970300 -0.00256100 3.04284200  
C 5.75429600 -0.05860000 -7.34579200  
O 3.50491600 0.20566500 -8.40133300  
H 3.74945600 0.13159100 -10.20288900  
C 10.34622300 -0.02707400 -3.99803500  
C 12.32500800 0.03881700 -1.86914800  
H 14.21005300 0.03696700 -2.71717000  
H 12.17199000 1.74513400 -0.70895200

H 11.42018800 1.31182200 -2.93413400

TS of site B

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50598000  
C 7.21712000 0.00000000 -0.29143400  
C 4.80763000 -0.00000200 0.71784100  
C 2.66288000 -0.00000200 -0.86240300  
C 3.03605400 0.00000200 -3.46355200  
C 5.47104500 0.00000400 -4.50139900  
C 7.60201200 0.00000400 -2.91454700  
H 8.85021500 -0.00000200 0.95342600  
H 4.54032000 -0.00000600 2.75165800  
H 1.40942800 0.00000000 -4.71628200  
H -1.73971500 0.00000200 3.04230700  
C 5.76733500 0.00000200 -7.26231700  
O 3.70170300 0.00001700 -8.63419800  
H 5.68364100 0.00000000 -9.60966900  
C 10.25295300 0.00001300 -3.94292800  
H 11.28075900 -1.66514800 -3.27229800  
H 10.25609600 -0.00004000 -6.00191800  
H 11.28071100 1.66524100 -3.27238700

P of site B

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50485000  
C 7.21190100 0.00000000 -0.30094300  
C 4.80144600 -0.00001100 0.71816800  
C 2.66667500 0.00000800 -0.86045300  
C 3.04022500 0.00004000 -3.46679300  
C 5.46513400 0.00005500 -4.50804900  
C 7.59723700 0.00003200 -2.91902900  
H 8.84385600 -0.00001700 0.94440400  
H 4.54007100 -0.00003400 2.75238300  
H 1.41399600 0.00005500 -4.71717200  
H -1.73982100 -0.00000600 3.04128100  
C 5.69953500 0.00009400 -7.30362200  
O 3.90977500 0.00012500 -8.73171900  
H 7.64930600 0.00009600 -8.06617100  
C 10.26117900 0.00004700 -3.93955700  
H 10.63129200 -1.66733600 -5.10518400  
H 10.63130300 1.66748400 -5.10510300  
H 11.62813000 0.00000400 -2.39412100

H 12.20575500 -1.61720700 -0.63493100  
C 10.80445700 -2.45735200 -5.54297900  
H 10.47203100 -4.13686900 -4.38039400  
H 9.55802500 -2.51506600 -7.18286500  
H 12.77000500 -2.50541900 -6.19093400  
C 10.79288800 2.31818100 -5.67152600  
H 10.41841800 4.05787100 -4.61499500  
H 12.76561500 2.35952200 -6.29743500  
H 9.57195400 2.26314300 -7.33199500

TS of site A

C -0.06619500 -0.00050600 0.00191200  
O -0.13179500 0.71770700 2.37711800  
C 6.89199500 0.81157700 -1.24719500  
C 4.58991800 0.79806000 -0.00440500  
C 2.39778000 0.04360000 -1.26987600  
C 2.57969100 -0.67437400 -3.78727500  
C 4.89667200 -0.68336700 -5.07472700  
C 7.13524000 0.06793200 -3.78269500  
H 8.54164900 1.41141600 -0.19985800

H 4.44963800 1.36417700 1.96397800  
H 0.88008500 -1.26095800 -4.77198700  
H -1.98362400 0.07826900 1.35804300  
C 5.03091600 -1.56758700 -7.73260900  
O 2.70772000 -1.72643200 -8.63586500  
H 2.83720200 -2.35396900 -10.33949100  
C 9.75550900 0.10747800 -5.05085800  
C 10.51281100 -2.60034000 -5.82465400  
H 12.40994000 -2.57687700 -6.65232400  
H 10.55022000 -3.84775600 -4.17396800  
H 9.18802000 -3.35512700 -7.21036100  
C 9.70393300 1.84003500 -7.39491900  
H 8.42224600 1.08843000 -8.82524400  
H 9.09946800 3.75248400 -6.88534600  
H 11.60226500 1.96280100 -8.21050400  
C 11.82209400 1.11940600 -3.27404800  
H 12.06508400 -0.06599700 -1.59624500  
H 13.62341000 1.12116200 -4.28751800  
H 11.45193800 3.06274800 -2.66782000

P of site A

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.28812500  
C 6.84930600 0.00000000 -1.96307100  
C 4.70259300 0.00435000 -0.46733300  
C 2.30907100 0.00154600 -1.57626500  
C 2.13744900 0.00010600 -4.18951300  
C 4.29112000 -0.01321700 -5.73858500  
C 6.73402300 -0.01858000 -4.61345300  
H 8.66381800 0.00564800 -1.02257800  
H 4.84332700 0.00667600 1.57939800  
H 0.28955000 -0.00200900 -5.08474300  
H -1.80113300 -0.00194500 -1.08043400  
C 4.02953300 -0.08446900 -8.52980400  
O 1.61672600 0.20297900 -9.11411700  
H 1.49258800 0.11688900 -10.92778800  
C 9.19852700 -0.03238200 -6.16464200  
C 11.56018500 0.05065400 -4.47099900  
H 13.23914100 0.05172400 -5.67628400  
H 11.63297900 1.76174900 -3.31008900  
H 11.69626400 -1.60025300 -3.23177900  
C 9.35045700 -2.47042300 -7.75690000  
H 9.26598300 -4.14373300 -6.54225100  
H 7.80374100 -2.54555800 -9.11609700  
H 11.14719600 -2.51493700 -8.78366600  
C 9.29554400 2.30554400 -7.90362600  
H 11.10438300 2.34907800 -8.90872400  
H 7.77133400 2.24040300 -9.29049800  
H 9.13210500 4.04967900 -6.80183900

R of site B

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50756600  
C 7.20843100 0.00000000 -0.34880400  
C 4.80714800 0.00310300 0.68880900  
C 2.65893300 0.00370800 -0.86382100  
C 3.03688700 0.00841900 -3.46487700  
C 5.45251800 -0.00151200 -4.56040200  
C 7.62189000 -0.01217200 -2.97051100  
H 8.80353500 0.00184200 0.93004400  
H 4.57238100 0.00183300 2.72707100  
H 1.38156000 0.00784800 -4.67407500  
H -1.73970300 -0.00255900 3.04284200  
C 5.75430100 -0.05868400 -7.34579200  
O 3.50490900 0.20544700 -8.40133600  
H 3.74945600 0.13139300 -10.20289100

C 10.34622300 -0.02716300 -3.99803300  
C 12.32501000 0.03869200 -1.86914600  
H 14.21005300 0.03679500 -2.71716800  
H 12.17203100 1.74501900 -0.70895700  
H 12.20571600 -1.61732500 -0.63492200  
C 10.80443400 -2.45743500 -5.54299200  
H 10.47198800 -4.13695600 -4.38041700  
H 9.55800800 -2.51512800 -7.18288200  
H 12.76998400 -2.50551900 -6.19094200  
C 10.79290900 2.31809800 -5.67151300  
H 10.41844800 4.05778600 -4.61497000  
H 12.76563600 2.35943000 -6.29741700  
H 9.57197500 2.26307800 -7.33198200

TS of site B

C -0.04165900 0.07240100 0.01993100  
O -0.14731900 -0.92235300 2.31709100  
C 7.06759900 -1.10919800 -0.51085700  
C 4.65329000 -1.07626700 0.50405600  
C 2.61354700 -0.06945900 -0.85681700  
C 3.10592900 0.89057900 -3.25419700  
C 5.53341500 0.86770600 -4.29856900  
C 7.59672900 -0.14951900 -2.92482100  
H 8.57367200 -1.90754100 0.61881600  
H 4.32455500 -1.83871200 2.38007300  
H 1.56088200 1.68228000 -4.34969000  
H -1.87986400 -0.81979200 2.86685400  
C 5.79246100 1.94528100 -6.85607800  
O 3.74112100 2.82420100 -7.93377600  
H 5.67532600 2.91300800 -8.99574400  
C 10.30382300 -0.22392900 -3.97951900  
C 12.17664800 -1.42455700 -2.11031300  
H 14.06029200 -1.42590100 -2.96121000  
H 12.29989800 -0.36319000 -0.33905700  
H 11.69398900 -3.38839600 -1.67512600  
C 10.36529700 -1.81029800 -6.42438000  
H 9.68020000 -3.73011300 -6.07147700  
H 9.20340500 -0.95316500 -7.89596900  
H 12.31004600 -1.94009000 -7.12006800  
C 11.22397000 2.48800900 -4.52391900  
H 11.15356300 3.64513200 -2.81052800  
H 13.18457200 2.43727300 -5.18449400  
H 10.07049100 3.38666100 -5.97716300

P of site B

C 0.00000000 0.00000000 0.00000000  
O 0.00000000 0.00000000 2.50527900  
C 7.20849200 0.00000000 -0.32706400  
C 4.80416800 -0.00000800 0.70570300  
C 2.66787500 -0.00000900 -0.85614600  
C 3.05820700 -0.00000900 -3.45539600  
C 5.47542100 0.00000000 -4.52528500  
C 7.64068900 0.00000900 -2.94594200  
H 8.79594900 0.00004000 0.96034800  
H 4.56488500 -0.00001100 2.74286500  
H 1.43480500 -0.00001300 -4.70824900  
H -1.74001300 0.00000800 3.04101100  
C 5.49161100 -0.00000200 -7.34911600  
O 3.57791100 0.00000200 -8.60788400  
H 7.33761100 -0.00001100 -8.30942000  
C 10.38343700 0.00003000 -3.93845300  
C 10.90081800 -2.41359700 -5.49417500  
H 9.71600600 -2.58916600 -7.17091600  
H 12.87220200 -2.42907200 -6.12149400  
H 10.58686600 -4.09410500 -4.33108000  
C 10.90078000 2.41365200 -5.49419400

H 12.87216900 2.42915700 -6.12149800  
H 9.71598000 2.58918300 -7.17094500  
H 10.58679000 4.09416500 -4.33111600  
C 12.33269800 0.00005300 -1.77607300

H 12.17363600 1.68068300 -0.58241800  
H 12.17363200 -1.68054900 -0.58237600  
H 14.23212300 0.00003800 -2.59113900

### H<sub>3</sub>CO-C-OH

#### R Nofield

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.331369  
H 0.926260 0.000000 1.589874  
O -1.276733 0.000002 -0.329478  
C -1.531721 -0.000002 -1.730629  
H -2.113902 -0.891285 -1.973655  
H -2.113927 0.891264 -1.973657  
H -0.588287 0.000009 -2.280285

#### TS Nofield

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.283050  
H 1.045438 0.000000 0.635046  
O -1.184950 0.000002 -0.577634  
C -1.186435 0.000004 -2.005857  
H -1.715000 0.891740 -2.347202  
H -0.163140 0.000003 -2.386924  
H -1.715002 -0.891729 -2.347202

#### P Nofield

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.195790  
H 0.917466 0.000000 -0.620666  
O -1.127706 -0.000003 -0.725489  
C -1.015641 0.000009 -2.141834  
H -1.510240 -0.891819 -2.531387  
H -1.510145 0.891896 -2.531373  
H 0.031735 -0.000045 -2.465054

#### R of Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.313962  
H 0.914299 0.000000 1.616261  
O -1.290447 -0.000002 -0.329576  
C -1.542749 -0.000003 -1.717571  
H -2.126089 0.890908 -1.969025  
H -0.596929 0.000000 -2.268503  
H -2.126084 -0.890916 -1.969025

#### TS of Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.267571  
H 1.055029 0.000000 0.605474  
O -1.197092 0.000002 -0.591930  
C -1.176307 0.000002 -2.005861  
H -1.697712 -0.891729 -2.365681  
H -1.697712 0.891735 -2.365681  
H -0.145056 0.000002 -2.372826

#### P of Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.186980  
H 0.914315 0.000000 -0.628690  
O -1.136795 -0.000000 -0.740733  
C -1.005243 -0.000005 -2.142038  
H -1.491368 -0.892327 -2.547840  
H -1.491382 0.892307 -2.547846

H 0.048555 0.000003 -2.453255

#### R of Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.351762  
H 0.936399 0.000000 1.567072  
O -1.262325 0.000001 -0.334288  
C -1.511644 -0.000000 -1.752447  
H -2.090986 -0.892108 -1.991268  
H -2.090986 0.892107 -1.991270  
H -0.566085 -0.000001 -2.294878

#### TS of Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.300658  
H 1.035103 0.000000 0.666664  
O -1.171407 0.000005 -0.570389  
C -1.183504 0.000003 -2.015086  
H -1.715733 -0.892199 -2.343479  
H -1.715730 0.892205 -2.343481  
H -0.163850 0.000001 -2.400569

#### P of Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.205446  
H 0.921290 0.000000 -0.612074  
O -1.117207 -0.000000 -0.715695  
C -1.018346 -0.000001 -2.148134  
H -1.519039 -0.891720 -2.524887  
H -1.519042 0.891716 -2.524888  
H 0.024761 0.000000 -2.478259

#### R of 3Au model-A no-field

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.309164  
H 0.918508 0.000000 1.607390  
C -1.421566 0.063073 -0.459217  
H -1.641372 1.151330 -0.469980  
H -2.126681 -0.383589 0.267153  
C -1.612599 -0.494964 -1.864155  
H -1.400616 -1.573874 -1.872810  
H -0.903729 -0.010930 -2.549956  
S -3.340374 -0.196571 -2.408982  
Au -3.420701 -1.042331 -4.529021  
Au -3.917355 -3.083476 -6.297986  
Au -3.174845 -0.737040 -7.246376

#### TS of 3Au model-A no-field

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.298635  
H 1.019354 0.000000 0.729509  
C -1.319180 0.006683 -0.698780  
H -1.336720 0.912946 -1.330959  
H -1.305040 -0.828340 -1.423347  
S -4.135485 0.134964 -0.660843  
Au -4.239893 -1.670963 -2.062747  
Au -3.694525 -2.834786 -4.488225  
Au -4.993424 -4.241364 -2.675212

C -2.539874 -0.059094 0.212056  
H -2.535814 -0.989836 0.796007  
H -2.507395 0.765125 0.940542

P of 3Au model-A no-field

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.200727  
H 0.968387 0.000000 -0.569693  
C -1.234750 -0.010330 -0.866321  
H -1.305445 -1.015546 -1.320982  
H -2.118797 0.130505 -0.227531  
S -2.630999 0.857911 -3.069325  
Au -2.362238 2.489974 -4.648683  
Au -1.463323 3.351039 -7.096613  
Au -2.796354 5.039784 -5.572989  
C -1.165948 1.033761 -1.979043  
H -0.246258 0.897767 -2.568427  
H -1.140041 2.044962 -1.547057

R of 3Au model-A Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.326174  
H 0.927943 0.000000 1.585637  
C -1.406567 0.067618 -0.468811  
H -1.622502 1.159055 -0.454305  
H -2.121123 -0.384749 0.248526  
C -1.628576 -0.434128 -1.893013  
H -1.387674 -1.506560 -1.956209  
H -0.939010 0.090875 -2.568071  
S -3.373865 -0.146279 -2.372947  
Au -3.377511 -0.307942 -4.694545  
Au -3.644321 -1.675304 -7.075404  
Au -3.161231 0.901220 -7.167961

TS of 3Au model-A Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.312960  
H 1.008749 0.000000 0.762313  
C -1.303492 0.084260 -0.707324  
H -1.356017 1.153111 -1.001712  
H -1.232659 -0.451529 -1.667942  
S -4.117329 0.401566 -0.496377  
Au -4.140984 0.066982 -2.800999  
Au -3.524602 1.012895 -5.326110  
Au -4.789976 -1.275029 -5.119447  
C -2.539011 -0.307950 0.097298  
H -2.609905 -1.406030 0.140578  
H -2.417681 0.046374 1.133532

P of 3Au model-A Z-EEF 5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.209890  
H 0.970847 0.000000 -0.561997  
C -1.240351 -0.036663 -0.847822  
H -1.592547 -1.086047 -0.852719  
H -2.030108 0.535600 -0.332864  
S -2.699172 0.347351 -3.119500  
Au -2.304433 0.509940 -5.408219  
Au -1.982337 -0.702207 -7.869535  
Au -2.131257 1.914763 -7.775513  
C -1.068738 0.428227 -2.291431  
H -0.336480 -0.213370 -2.805109  
H -0.675131 1.457451 -2.317884

R of 3Au model-A Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.301862  
H 0.909336 0.000000 1.634199  
C -1.441636 0.047052 -0.421145  
H -1.633110 1.107956 -0.674798  
H -2.112614 -0.199181 0.423956  
C -1.762299 -0.823328 -1.634962  
H -1.501254 -1.870286 -1.418509  
H -1.144838 -0.509140 -2.491950  
S -3.514425 -0.737007 -2.185300  
Au -4.613983 -1.156542 -0.174834  
Au -5.015525 -0.134196 2.368971  
Au -5.811284 -2.581382 1.850122

TS of 3Au model-A Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.289853  
H 1.027452 0.000000 0.703151  
C -1.350800 -0.082404 -0.667818  
H -1.325708 0.445721 -1.635049  
H -1.455811 -1.157790 -0.915137  
S -4.112973 -0.376884 -0.255078  
Au -5.106542 -0.599679 1.839726  
Au -5.256131 -1.972506 4.232392  
Au -6.444765 0.359865 4.048523  
C -2.498848 0.354489 0.238235  
H -2.251688 0.051770 1.263446  
H -2.576330 1.452080 0.245043

P of 3Au model-A Z-EEF -5.14 V/nm

C 0.000000 0.000000 0.000000  
O 0.000000 0.000000 1.209890  
H 0.970847 0.000000 -0.561997  
C -1.240351 -0.036663 -0.847822  
H -1.592547 -1.086047 -0.852719  
H -2.030108 0.535600 -0.332864  
S -2.699172 0.347351 -3.119500  
Au -2.304433 0.509940 -5.408219  
Au -1.982337 -0.702207 -7.869535  
Au -2.131257 1.914763 -7.775513  
C -1.068738 0.428227 -2.291431  
H -0.336480 -0.213370 -2.805109  
H -0.675131 1.457451 -2.317884