Supporting Information

Effect of External Electric Fields on the C-H Bond Activation Reactivity of Nonheme Iron-oxo Reagents

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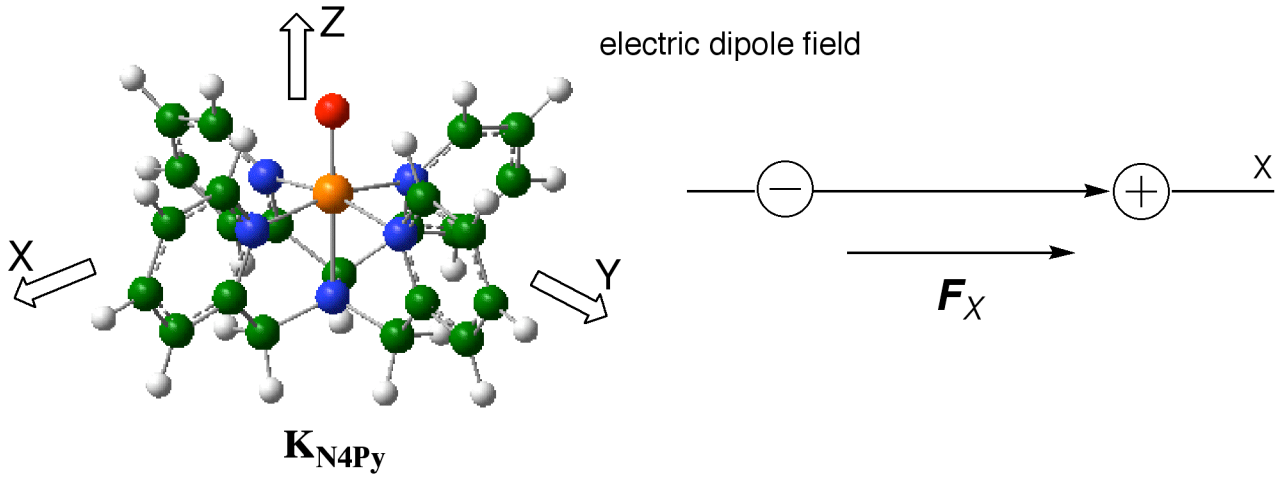
Contents

Abbreviations

EF	electric field
L	N4Py ligand
Bz	Ph-CH_2 (benzyl)
$\mathbf{K_{N4Py}}$	(N4Py)Fe^{IV}=O^{2+}
$\mathbf{K_{N4Py}}$	(TMC(SR))Fe^{IV}=O^{2+}
TE	toluene
CH	cyclohexane

Methods

The stationary-point geometries for the reaction between $\mathbf{K_{N4Py}}$ and **TE** optimized in [Shaik et al. JACS 2006, 128, 8590] were used for the present analyses. Electric dipole field calculations were carried out by single-point calculations on the above geometries, where the Fe-O bond was aligned to the Z-axis. Electric dipole fields were applied in both the + and – directions for each axis. The field strengths applied were 0.0050, 0.0075, 0.0100, and 0.0125 au (see **Part 1**). In the second reaction (**Part 2**), $\mathbf{K_{TMC(SR)}}$ + **CH** we performed geometry optimization in the presence of the EF. This last study was restricted to F_z = -0.0075au. This restriction was applied because the z-oriented field in the negative direction gave the largest effect in the first reaction.



Density functional calculations were performed with the B3LYP functional and the LACVP basis set:

B3LYP: (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.

LACVP: Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310.

Drawings were done with Gaussview and MOLEKEL:

GaussView 3.09; Gaussian Inc.: Pittsburgh, PA, 2002-2003.

MOLEKEL 4.3; (a) Flükiger, P.; Lüthi, H. P.; Portmann, S.; Weber, J. *MOLEKEL 4.3*; Swiss Center for Scientific Computing: Manno, Switzerland, 2000-2002. (b) Portmann, S.; Lüthi, H. P. *CHIMIA* **2000**, *54*, 766-770.

Reference 7 in Full (GAUSSIAN 03)

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004. *Gaussian 03*, Revision C.02.

Part 1 (K_{N4Py})

Table S1. Dependence of energy,[a] spin density and charge of $^3\mathbf{K}_{\mathbf{N4Py}}$ on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.798427	−14.9	14.8	1.07	0.98	−0.05	0.67	−0.33	1.65
−0.0100	−1360.790112	−9.7	13.6	1.06	0.98	−0.04	0.67	−0.32	1.65
−0.0075	−1360.783595	−5.6	12.6	1.06	0.98	−0.04	0.68	−0.32	1.65
−0.0050	−1360.778864	−2.6	11.8	1.06	0.98	−0.04	0.68	−0.32	1.65
0.0000	−1360.774670	0.0	10.9	1.06	0.98	−0.04	0.68	−0.33	1.65
0.0050	−1360.777704	−1.9	11.1	1.06	0.98	−0.04	0.68	−0.33	1.65
0.0075	−1360.781859	−4.5	11.7	1.06	0.98	−0.04	0.67	−0.33	1.65
0.0100	−1360.787804	−8.2	12.5	1.07	0.98	−0.05	0.67	−0.33	1.66
0.0125	−1360.795554	−13.1	13.5	1.07	0.98	−0.05	0.67	−0.33	1.66

(b) Y-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.798374	−14.9	14.8	1.07	0.98	−0.05	0.67	−0.33	1.65
−0.0100	−1360.790073	−9.7	13.6	1.06	0.98	−0.04	0.67	−0.32	1.65
−0.0075	−1360.783568	−5.6	12.6	1.06	0.98	−0.04	0.68	−0.32	1.65
−0.0050	−1360.778848	−2.6	11.8	1.06	0.98	−0.04	0.68	−0.32	1.65
0.0000	−1360.774670	0.0	10.9	1.06	0.98	−0.04	0.68	−0.33	1.65
0.0050	−1360.777711	−1.9	11.1	1.06	0.98	−0.04	0.68	−0.33	1.65
0.0075	−1360.781866	−4.5	11.7	1.06	0.98	−0.04	0.67	−0.33	1.65
0.0100	−1360.787809	−8.2	12.5	1.07	0.98	−0.05	0.67	−0.33	1.66
0.0125	−1360.795554	−13.1	13.6	1.07	0.98	−0.05	0.67	−0.33	1.66

(c) Z-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.741218	21.0	2.8	0.97	1.06	−0.03	0.69	−0.26	1.57
−0.0100	−1360.744738	18.8	4.4	0.99	1.04	−0.03	0.68	−0.27	1.59
−0.0075	−1360.749851	15.6	6.0	1.00	1.03	−0.03	0.68	−0.28	1.60
−0.0050	−1360.756556	11.4	7.6	1.02	1.01	−0.04	0.68	−0.30	1.62
0.0000	−1360.774670	0.0	10.9	1.06	0.98	−0.04	0.68	−0.33	1.65
0.0050	−1360.799271	−15.4	14.1	1.09	0.95	−0.05	0.67	−0.35	1.68
0.0075	−1360.813922	−24.6	15.7	1.11	0.94	−0.05	0.67	−0.37	1.69
0.0100	−1360.830163	−34.8	17.4	1.13	0.92	−0.05	0.67	−0.38	1.71
0.0125	−1360.847994	−46.0	19.0	1.15	0.91	−0.05	0.67	−0.39	1.73

[a] ΔE values are relative to the energy of $^3\mathbf{K}_{\mathbf{N4Py}}$ in the absence of an EF.

Table S2. Dependence of energy,[a] spin density and charge of $^5\mathbf{K}_{\mathbf{N4Py}}$ on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.776495	−1.1	15.9	2.93	0.74	0.33	0.84	−0.32	1.48
−0.0100	−1360.768332	4.0	14.8	2.93	0.74	0.33	0.85	−0.32	1.47
−0.0075	−1360.761976	8.0	13.9	2.93	0.74	0.32	0.85	−0.32	1.47
−0.0050	−1360.757413	10.8	13.1	2.93	0.75	0.32	0.85	−0.32	1.47
0.0000	−1360.753535	13.3	12.3	2.93	0.75	0.32	0.85	−0.32	1.47
0.0050	−1360.756984	11.1	12.6	2.93	0.75	0.32	0.85	−0.32	1.47
0.0075	−1360.761348	8.4	13.1	2.93	0.74	0.32	0.85	−0.32	1.47
0.0100	−1360.767525	4.5	13.9	2.93	0.74	0.33	0.84	−0.32	1.48
0.0125	−1360.775537	−0.5	14.9	2.93	0.74	0.33	0.84	−0.32	1.49

(b) Y-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.776471	−1.1	15.9	2.93	0.74	0.33	0.84	−0.32	1.48
−0.0100	−1360.768328	4.0	14.8	2.93	0.74	0.33	0.85	−0.32	1.47
−0.0075	−1360.761983	8.0	13.8	2.93	0.74	0.32	0.85	−0.32	1.47
−0.0050	−1360.757424	10.8	13.1	2.93	0.75	0.32	0.85	−0.32	1.47
0.0000	−1360.753535	13.3	12.3	2.93	0.75	0.32	0.85	−0.32	1.47
0.0050	−1360.756947	11.1	12.6	2.93	0.75	0.32	0.85	−0.32	1.47
0.0075	−1360.761284	8.4	13.2	2.93	0.74	0.32	0.85	−0.32	1.47
0.0100	−1360.767428	4.5	13.9	2.93	0.74	0.33	0.84	−0.32	1.48
0.0125	−1360.775402	−0.5	14.9	2.93	0.74	0.33	0.84	−0.32	1.48

(c) Z-direction

EF	Energy	ΔE	μ	spin density			charge		
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	Q(Fe)	Q(O)	Q(L)
−0.0125	−1360.713258	38.5	4.1	2.90	0.78	0.32	0.87	−0.25	1.38
−0.0100	−1360.718082	35.5	5.8	2.91	0.77	0.32	0.86	−0.26	1.40
−0.0075	−1360.724532	31.5	7.4	2.92	0.77	0.32	0.86	−0.27	1.41
−0.0050	−1360.732608	26.4	9.0	2.92	0.76	0.32	0.86	−0.29	1.43
0.0000	−1360.753535	13.3	12.3	2.93	0.75	0.32	0.85	−0.32	1.47
0.0050	−1360.781160	−4.1	15.7	2.95	0.73	0.32	0.85	−0.35	1.50
0.0075	−1360.797362	−14.2	17.3	2.96	0.73	0.32	0.84	−0.36	1.52
0.0100	−1360.815190	−25.4	19.0	2.96	0.72	0.32	0.84	−0.38	1.54
0.0125	−1360.834646	−37.6	20.6	2.97	0.71	0.31	0.83	−0.39	1.56

[a] ΔE values are relative to the energy of $^3\mathbf{K}_{\mathbf{N4Py}}$ in the absence of an EF.

Table S3. Dependence of energy,[a] spin density and charge of ^{3}**RC** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.320752	−19.1	15.3	1.06	0.98	−0.05	0.00	0.66	−0.33	1.60	0.07
−0.0100	−1632.310310	−12.5	13.5	1.06	0.98	−0.04	0.00	0.66	−0.33	1.60	0.07
−0.0075	−1632.302070	−7.3	12.0	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.06
−0.0050	−1632.296018	−3.5	10.6	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.06
0.0000	−1632.290373	0.0	9.1	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.06
0.0050	−1632.293564	−2.0	9.5	1.06	0.98	−0.04	0.00	0.67	−0.34	1.61	0.05
0.0075	−1632.298386	−5.0	10.5	1.07	0.98	−0.04	0.00	0.67	−0.34	1.62	0.05
0.0100	−1632.305394	−9.4	11.8	1.07	0.98	−0.05	0.00	0.67	−0.34	1.62	0.05
0.0125	−1632.314598	−15.2	13.4	1.08	0.97	−0.05	0.00	0.67	−0.34	1.62	0.05

(b) Y-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.317080	−16.8	14.9	1.08	0.97	−0.05	0.00	0.67	−0.34	1.63	0.04
−0.0100	−1632.307214	−10.6	13.1	1.07	0.97	−0.04	0.00	0.68	−0.34	1.62	0.04
−0.0075	−1632.299624	−5.8	11.6	1.07	0.97	−0.04	0.00	0.68	−0.34	1.62	0.05
−0.0050	−1632.294303	−2.5	10.3	1.06	0.98	−0.04	0.00	0.68	−0.34	1.61	0.05
0.0000	−1632.290373	0.0	9.1	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.06
0.0050	−1632.295656	−3.3	10.1	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.07
0.0075	−1632.301711	−7.1	11.3	1.06	0.98	−0.04	0.01	0.66	−0.33	1.59	0.07
0.0100	−1632.310284	−12.5	12.9	1.03	0.97	−0.05	0.05	0.65	−0.34	1.57	0.12
0.0125	−1632.322495	−20.2	15.9	1.00	0.95	−0.12	0.17	0.65	−0.35	1.48	0.23

(c) Z-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.274593	9.9	6.9	0.80	0.98	−0.03	0.26	0.64	−0.32	1.35	0.33
−0.0100	−1632.271694	11.7	2.8	0.90	1.01	−0.03	0.12	0.65	−0.30	1.45	0.20
−0.0075	−1632.272713	11.1	2.9	0.99	1.02	−0.03	0.02	0.67	−0.29	1.53	0.10
−0.0050	−1632.276572	8.7	5.1	1.02	1.01	−0.04	0.00	0.67	−0.31	1.56	0.08
0.0000	−1632.290373	0.0	9.1	1.06	0.98	−0.04	0.00	0.67	−0.33	1.60	0.06
0.0050	−1632.312164	−13.7	13.0	1.10	0.95	−0.05	0.00	0.67	−0.36	1.65	0.04
0.0075	−1632.325933	−22.3	15.0	1.12	0.93	−0.05	0.00	0.67	−0.38	1.67	0.04
0.0100	−1632.341636	−32.2	17.0	1.13	0.92	−0.05	0.00	0.67	−0.39	1.69	0.03
0.0125	−1632.359270	−43.2	19.0	1.15	0.90	−0.05	0.00	0.67	−0.41	1.71	0.02

[a] ΔE values are relative to the energy of ^{3}**RC** in the absence of an EF.

Table S4. Dependence of energy,[a] spin density and charge of ^{5}**RC** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.298748	−5.3	15.9	2.92	0.73	0.32	0.03	0.82	−0.33	1.40	0.10
−0.0100	−1632.288437	1.2	14.3	2.92	0.74	0.32	0.01	0.83	−0.33	1.41	0.08
−0.0075	−1632.280380	6.3	12.9	2.93	0.74	0.32	0.01	0.83	−0.32	1.41	0.08
−0.0050	−1632.274540	9.9	11.7	2.93	0.75	0.32	0.01	0.84	−0.32	1.41	0.07
0.0000	−1632.269449	13.1	10.4	2.93	0.75	0.32	0.00	0.84	−0.32	1.42	0.06
0.0050	−1632.273154	10.8	10.9	2.93	0.75	0.32	0.00	0.84	−0.33	1.43	0.06
0.0075	−1632.278306	7.6	11.8	2.93	0.75	0.32	0.00	0.84	−0.33	1.43	0.06
0.0100	−1632.285678	2.9	13.1	2.93	0.74	0.32	0.00	0.84	−0.33	1.44	0.05
0.0125	−1632.295290	−3.1	14.6	2.93	0.74	0.33	0.00	0.84	−0.33	1.45	0.05

(b) Y-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.295461	−3.2	15.8	2.93	0.74	0.33	0.00	0.84	−0.34	1.45	0.05
−0.0100	−1632.285724	2.9	14.1	2.93	0.74	0.32	0.00	0.84	−0.33	1.44	0.05
−0.0075	−1632.278263	7.6	12.7	2.93	0.74	0.32	0.00	0.84	−0.33	1.43	0.05
−0.0050	−1632.273068	10.9	11.5	2.93	0.75	0.32	0.00	0.84	−0.33	1.43	0.06
0.0000	−1632.269449	13.1	10.4	2.93	0.75	0.32	0.00	0.84	−0.32	1.42	0.06
0.0050	−1632.274974	9.7	11.2	2.93	0.75	0.31	0.01	0.83	−0.32	1.41	0.08
0.0075	−1632.281292	5.7	12.2	2.92	0.74	0.31	0.03	0.83	−0.33	1.39	0.11
0.0100	−1632.290161	0.1	13.6	2.91	0.73	0.31	0.06	0.82	−0.34	1.37	0.14
0.0125	−1632.304926	−9.1	17.0	2.81	0.64	0.20	0.35	0.78	−0.39	1.21	0.40

(c) Z-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.261431	18.2	14.6	2.62	0.57	0.13	0.68	0.73	−0.40	0.94	0.73
−0.0100	−1632.253177	23.3	8.9	2.73	0.62	0.18	0.48	0.77	−0.37	1.06	0.53
−0.0075	−1632.250409	25.1	4.0	2.82	0.68	0.24	0.26	0.81	−0.33	1.20	0.32
−0.0050	−1632.253330	23.2	5.8	2.91	0.75	0.30	0.04	0.84	−0.30	1.35	0.12
0.0000	−1632.269449	13.1	10.4	2.93	0.75	0.32	0.00	0.84	−0.32	1.42	0.06
0.0050	−1632.293970	−2.3	14.5	2.95	0.74	0.32	0.00	0.84	−0.35	1.47	0.05
0.0075	−1632.309224	−11.8	16.5	2.96	0.73	0.32	0.00	0.84	−0.37	1.49	0.04
0.0100	−1632.326461	−22.6	18.6	2.96	0.72	0.31	0.00	0.84	−0.39	1.52	0.03
0.0125	−1632.345675	−34.7	20.6	2.97	0.71	0.31	0.00	0.84	−0.40	1.54	0.02

[a] ΔE values are relative to the energy of ^{3}**RC** in the absence of an EF.

Table S5. Dependence of energy,[a] spin density and charge of $^{3}\mathbf{TS_H}$ on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.324176	−34.0	18.8	0.76	0.58	−0.04	0.69	0.01	0.67	−0.57	1.34	0.26	0.31
−0.0100	−1632.307570	−23.6	15.9	0.78	0.60	−0.04	0.66	0.00	0.67	−0.56	1.36	0.22	0.31
−0.0075	−1632.293915	−15.0	13.3	0.79	0.62	−0.04	0.63	−0.01	0.68	−0.55	1.39	0.18	0.30
−0.0050	−1632.283162	−8.2	10.8	0.81	0.65	−0.04	0.60	−0.02	0.69	−0.55	1.41	0.15	0.30
0.0000	−1632.270037	0.0	7.2	0.85	0.69	−0.05	0.54	−0.03	0.70	−0.53	1.46	0.08	0.29
0.0050	−1632.268227	1.1	7.2	0.88	0.72	−0.05	0.49	−0.04	0.71	−0.51	1.50	0.02	0.28
0.0075	−1632.271312	−0.8	8.7	0.90	0.74	−0.05	0.46	−0.05	0.71	−0.50	1.53	−0.01	0.28
0.0100	−1632.277071	−4.4	10.6	0.92	0.75	−0.06	0.44	−0.05	0.71	−0.50	1.55	−0.04	0.27
0.0125	−1632.285495	−9.7	12.9	0.95	0.76	−0.06	0.42	−0.06	0.71	−0.49	1.57	−0.07	0.27

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.302316	−20.3	14.3	0.82	0.65	−0.04	0.58	−0.01	0.69	−0.55	1.42	0.16	0.29
−0.0100	−1632.291580	−13.5	12.4	0.83	0.66	−0.04	0.58	−0.02	0.69	−0.54	1.42	0.14	0.29
−0.0075	−1632.283006	−8.1	10.7	0.83	0.66	−0.04	0.57	−0.02	0.69	−0.54	1.43	0.13	0.29
−0.0050	−1632.276583	−4.1	9.1	0.84	0.67	−0.04	0.56	−0.02	0.70	−0.54	1.44	0.11	0.29
0.0000	−1632.270037	0.0	7.2	0.85	0.69	−0.05	0.54	−0.03	0.70	−0.53	1.46	0.08	0.29
0.0050	−1632.272331	−1.4	7.6	0.86	0.70	−0.05	0.52	−0.04	0.70	−0.52	1.48	0.05	0.29
0.0075	−1632.276645	−4.1	8.7	0.87	0.71	−0.05	0.51	−0.04	0.70	−0.51	1.49	0.04	0.29
0.0100	−1632.283129	−8.2	10.2	0.88	0.72	−0.05	0.50	−0.04	0.70	−0.51	1.50	0.02	0.29
0.0125	−1632.291801	−13.7	11.9	0.89	0.72	−0.06	0.49	−0.05	0.70	−0.51	1.51	0.01	0.29

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.271958	−1.2	9.4	0.69	0.65	−0.03	0.67	0.02	0.67	−0.52	1.26	0.30	0.28
−0.0100	−1632.266545	2.2	7.3	0.72	0.66	−0.03	0.64	0.01	0.68	−0.52	1.30	0.26	0.28
−0.0075	−1632.263668	4.0	5.6	0.75	0.66	−0.04	0.62	0.00	0.68	−0.52	1.34	0.21	0.28
−0.0050	−1632.263320	4.2	5.0	0.78	0.67	−0.04	0.60	−0.01	0.69	−0.52	1.38	0.17	0.28
0.0000	−1632.270037	0.0	7.2	0.85	0.69	−0.05	0.54	−0.03	0.70	−0.53	1.46	0.08	0.29
0.0050	−1632.287013	−10.7	11.5	0.91	0.70	−0.05	0.48	−0.05	0.71	−0.53	1.54	0.00	0.29
0.0075	−1632.299168	−18.3	13.9	0.95	0.71	−0.06	0.45	−0.05	0.71	−0.53	1.58	−0.05	0.29
0.0100	−1632.313806	−27.5	16.3	0.98	0.71	−0.06	0.42	−0.06	0.71	−0.53	1.62	−0.09	0.30
0.0125	−1632.330934	−38.2	18.8	1.02	0.72	−0.06	0.39	−0.06	0.71	−0.54	1.66	−0.14	0.30

[a] ΔE values are relative to the energy of $^{3}\mathbf{TS_H}$ in the absence of an EF.

Table S6. Dependence of energy,[a] spin density and charge of $^{5}\mathbf{TS_H}$ on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.299100	−18.2	13.7	3.55	0.47	0.36	−0.37	−0.01	0.91	−0.49	1.22	0.11	0.25
−0.0100	−1632.288332	−11.5	11.8	3.54	0.47	0.36	−0.36	−0.01	0.91	−0.49	1.23	0.10	0.25
−0.0075	−1632.279765	−6.1	10.1	3.54	0.47	0.36	−0.35	−0.01	0.91	−0.49	1.23	0.09	0.25
−0.0050	−1632.273391	−2.1	8.6	3.53	0.46	0.35	−0.34	−0.01	0.92	−0.48	1.24	0.08	0.25
0.0000	−1632.267252	1.7	7.0	3.51	0.46	0.35	−0.31	−0.01	0.92	−0.48	1.26	0.06	0.24
0.0050	−1632.269862	0.1	8.1	3.49	0.45	0.35	−0.29	0.00	0.91	−0.47	1.28	0.04	0.24
0.0075	−1632.274516	−2.8	9.4	3.48	0.44	0.36	−0.27	0.00	0.91	−0.47	1.29	0.03	0.24
0.0100	−1632.281418	−7.1	11.2	3.46	0.44	0.36	−0.26	0.00	0.91	−0.46	1.31	0.01	0.24
0.0125	−1632.290599	−12.9	13.1	3.45	0.44	0.36	−0.24	0.00	0.90	−0.46	1.32	0.00	0.24

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.286337	−10.2	15.9	3.32	0.43	0.36	−0.11	0.00	0.91	−0.43	1.41	−0.13	0.23
−0.0100	−1632.277071	−4.4	13.6	3.36	0.42	0.36	−0.14	0.00	0.91	−0.43	1.39	−0.10	0.23
−0.0075	−1632.270456	−0.3	11.3	3.40	0.42	0.36	−0.17	0.00	0.92	−0.44	1.36	−0.07	0.23
−0.0050	−1632.266564	2.2	9.2	3.44	0.42	0.36	−0.21	0.00	0.92	−0.45	1.33	−0.03	0.24
0.0000	−1632.267252	1.7	7.0	3.51	0.46	0.35	−0.31	−0.01	0.92	−0.48	1.26	0.06	0.24
0.0050	−1632.279468	−5.9	9.8	3.58	0.51	0.35	−0.43	−0.01	0.91	−0.51	1.18	0.16	0.25
0.0075	−1632.290010	−12.5	12.4	3.61	0.54	0.35	−0.49	−0.01	0.90	−0.52	1.15	0.21	0.26
0.0100	−1632.303523	−21.0	15.3	3.64	0.58	0.35	−0.54	−0.02	0.89	−0.54	1.12	0.27	0.26
0.0125	−1632.320015	−31.4	18.4	3.66	0.61	0.35	−0.60	−0.02	0.88	−0.56	1.09	0.32	0.27

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.287111	−10.7	17.1	3.71	0.79	0.31	−0.76	−0.05	0.88	−0.56	0.89	0.52	0.27
−0.0100	−1632.275447	−3.4	13.5	3.69	0.72	0.32	−0.69	−0.04	0.89	−0.54	0.95	0.44	0.26
−0.0075	−1632.267459	1.6	9.9	3.67	0.64	0.33	−0.60	−0.03	0.90	−0.53	1.02	0.35	0.26
−0.0050	−1632.263345	4.2	6.6	3.63	0.57	0.34	−0.51	−0.02	0.91	−0.51	1.09	0.26	0.25
0.0000	−1632.267252	1.7	7.0	3.51	0.46	0.35	−0.31	−0.01	0.92	−0.48	1.26	0.06	0.24
0.0050	−1632.287244	−10.8	14.1	3.35	0.44	0.34	−0.14	0.00	0.91	−0.45	1.42	−0.12	0.24
0.0075	−1632.302710	−20.5	17.3	3.27	0.48	0.33	−0.08	0.00	0.90	−0.45	1.49	−0.18	0.25
0.0100	−1632.321137	−32.1	20.1	3.21	0.52	0.32	−0.05	0.00	0.89	−0.46	1.54	−0.23	0.26
0.0125	−1632.342119	−45.2	22.6	3.18	0.54	0.30	−0.04	0.00	0.89	−0.47	1.58	−0.27	0.27

[a] ΔE values are relative to the energy of $^{3}\mathbf{TS_H}$ in the absence of an EF.

Table S7. Dependence of energy,[a] spin density and charge of ^{3}**I** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.338464	−31.3	21.3	0.90	0.19	0.17	0.73	0.01	0.67	−0.66	1.28	0.34	0.37
−0.0100	−1632.320981	−20.3	15.8	0.89	0.20	0.01	0.88	0.01	0.67	−0.65	1.42	0.19	0.37
−0.0075	−1632.308954	−12.8	12.8	0.89	0.20	−0.05	0.95	0.01	0.67	−0.65	1.49	0.12	0.38
−0.0050	−1632.299750	−7.0	10.8	0.89	0.20	−0.05	0.96	0.01	0.67	−0.65	1.50	0.11	0.37
0.0000	−1632.288555	0.0	8.0	0.89	0.20	−0.06	0.96	0.01	0.67	−0.64	1.51	0.09	0.37
0.0050	−1632.287047	0.9	7.5	0.90	0.20	−0.06	0.97	0.00	0.68	−0.64	1.53	0.07	0.36
0.0075	−1632.289832	−0.8	8.4	0.90	0.19	−0.06	0.97	0.00	0.68	−0.64	1.54	0.07	0.36
0.0100	−1632.295003	−4.0	9.8	0.91	0.19	−0.07	0.97	0.00	0.67	−0.64	1.55	0.06	0.36
0.0125	−1632.302574	−8.8	11.6	0.91	0.19	−0.07	0.97	0.00	0.67	−0.63	1.56	0.06	0.35

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.320695	−20.2	14.8	0.89	0.20	−0.06	0.95	0.01	0.67	−0.65	1.50	0.11	0.37
−0.0100	−1632.309996	−13.5	13.0	0.89	0.20	−0.06	0.96	0.01	0.67	−0.65	1.50	0.10	0.37
−0.0075	−1632.301449	−8.1	11.3	0.89	0.20	−0.06	0.96	0.01	0.67	−0.65	1.50	0.10	0.37
−0.0050	−1632.295042	−4.1	9.9	0.89	0.20	−0.06	0.96	0.01	0.67	−0.65	1.51	0.10	0.37
0.0000	−1632.288555	0.0	8.0	0.89	0.20	−0.06	0.96	0.01	0.67	−0.64	1.51	0.09	0.37
0.0050	−1632.290713	−1.4	8.2	0.89	0.20	−0.06	0.97	0.00	0.67	−0.64	1.52	0.08	0.37
0.0075	−1632.294964	−4.0	9.1	0.89	0.20	−0.06	0.97	0.00	0.67	−0.64	1.52	0.08	0.37
0.0100	−1632.301365	−8.0	10.5	0.90	0.20	−0.06	0.97	0.00	0.67	−0.64	1.53	0.08	0.36
0.0125	−1632.309931	−13.4	12.1	0.90	0.20	−0.07	0.97	0.00	0.67	−0.64	1.53	0.07	0.36

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.284323	2.7	10.5	0.86	0.22	0.29	0.63	0.01	0.67	−0.61	1.13	0.44	0.37
−0.0100	−1632.278298	6.4	6.1	0.86	0.22	0.12	0.79	0.01	0.67	−0.62	1.29	0.29	0.37
−0.0075	−1632.276745	7.4	3.7	0.86	0.23	−0.01	0.91	0.01	0.67	−0.62	1.42	0.16	0.37
−0.0050	−1632.278527	6.3	4.6	0.87	0.22	−0.05	0.95	0.01	0.67	−0.63	1.46	0.12	0.37
0.0000	−1632.288555	0.0	8.0	0.89	0.20	−0.06	0.96	0.01	0.67	−0.64	1.51	0.09	0.37
0.0050	−1632.306739	−11.4	11.8	0.91	0.18	−0.06	0.97	0.00	0.68	−0.66	1.55	0.07	0.36
0.0075	−1632.318748	−18.9	13.7	0.92	0.17	−0.07	0.97	0.00	0.68	−0.67	1.57	0.06	0.36
0.0100	−1632.332707	−27.7	15.6	0.93	0.17	−0.07	0.97	0.00	0.68	−0.67	1.59	0.05	0.36
0.0125	−1632.348610	−37.7	17.6	0.94	0.16	−0.07	0.97	0.00	0.68	−0.68	1.61	0.04	0.35

[a] ΔE values are relative to the energy of ^{3}**I** in the absence of an EF.

Table S8. Dependence of energy,[a] spin density and charge of ^{5}**I** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.311751	−14.6	12.4	3.98	0.43	0.49	−0.88	−0.02	1.00	−0.76	1.20	0.15	0.42
−0.0100	−1632.302288	−8.6	10.3	3.98	0.43	0.48	−0.87	−0.02	1.00	−0.76	1.19	0.15	0.42
−0.0075	−1632.295015	−4.1	8.4	3.98	0.44	0.47	−0.87	−0.02	1.00	−0.76	1.18	0.16	0.42
−0.0050	−1632.289918	−0.9	6.7	3.98	0.44	0.46	−0.86	−0.02	1.00	−0.76	1.18	0.17	0.41
0.0000	−1632.286173	1.5	4.8	3.98	0.43	0.46	−0.85	−0.02	1.00	−0.76	1.17	0.18	0.41
0.0050	−1632.291132	−1.6	6.3	3.97	0.43	0.45	−0.83	−0.02	1.00	−0.76	1.16	0.19	0.41
0.0075	−1632.296836	−5.2	8.0	3.97	0.43	0.45	−0.83	−0.02	0.99	−0.76	1.16	0.20	0.41
0.0100	−1632.304717	−10.1	9.9	3.96	0.42	0.45	−0.82	−0.02	0.99	−0.77	1.16	0.21	0.41
0.0125	−1632.314826	−16.5	11.9	3.96	0.42	0.44	−0.80	−0.02	0.98	−0.77	1.15	0.23	0.41

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.306347	−11.2	12.1	3.98	0.43	0.48	−0.87	−0.03	1.01	−0.77	1.19	0.16	0.41
−0.0100	−1632.297912	−5.9	10.0	3.98	0.43	0.47	−0.86	−0.03	1.01	−0.77	1.19	0.16	0.41
−0.0075	−1632.291692	−2.0	8.0	3.98	0.43	0.47	−0.86	−0.02	1.01	−0.76	1.18	0.17	0.41
−0.0050	−1632.287673	0.6	6.3	3.98	0.43	0.46	−0.85	−0.02	1.01	−0.76	1.17	0.17	0.41
0.0000	−1632.286173	1.5	4.8	3.98	0.43	0.46	−0.85	−0.02	1.00	−0.76	1.17	0.18	0.41
0.0050	−1632.293520	−3.1	6.9	3.97	0.43	0.45	−0.84	−0.02	0.99	−0.76	1.16	0.19	0.42
0.0075	−1632.300489	−7.5	8.7	3.97	0.43	0.45	−0.83	−0.02	0.99	−0.76	1.16	0.20	0.42
0.0100	−1632.309713	−13.3	10.8	3.96	0.43	0.45	−0.82	−0.02	0.98	−0.76	1.16	0.21	0.42
0.0125	−1632.321276	−20.5	13.1	3.95	0.42	0.43	−0.79	−0.01	0.97	−0.77	1.14	0.23	0.42

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.353468	−40.7	27.0	3.65	0.22	0.09	0.02	0.02	0.84	−0.83	0.61	1.00	0.38
−0.0100	−1632.328695	−25.2	24.3	3.64	0.20	0.10	0.03	0.02	0.84	−0.83	0.64	0.98	0.37
−0.0075	−1632.306659	−11.4	19.9	3.69	0.21	0.14	−0.06	0.02	0.86	−0.83	0.71	0.89	0.37
−0.0050	−1632.291617	−1.9	11.7	3.82	0.28	0.24	−0.35	0.01	0.92	−0.81	0.86	0.64	0.39
0.0000	−1632.286173	1.5	4.8	3.98	0.43	0.46	−0.85	−0.02	1.00	−0.76	1.17	0.18	0.41
0.0050	−1632.302077	−8.5	11.0	4.01	0.41	0.52	−0.93	−0.01	1.01	−0.77	1.26	0.08	0.42
0.0075	−1632.314137	−16.1	13.5	4.01	0.38	0.54	−0.94	0.00	1.01	−0.78	1.29	0.06	0.41
0.0100	−1632.328629	−25.1	16.0	4.02	0.36	0.56	−0.94	0.00	1.01	−0.79	1.32	0.04	0.41
0.0125	−1632.345509	−35.7	18.4	4.02	0.34	0.58	−0.94	0.01	1.01	−0.79	1.35	0.03	0.41

[a] ΔE values are relative to the energy of ^{3}**I** in the absence of an EF.

Table S9. Dependence of energy,[a] spin density and charge of ^{3}**TS**$_{\mathbf{reb}}$ on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.325262	−30.4	16.7	1.68	−0.05	−0.06	0.42	0.00	0.68	−0.69	1.15	0.50	0.36
−0.0100	−1632.310459	−21.2	13.9	1.64	−0.05	−0.06	0.47	0.00	0.68	−0.68	1.19	0.46	0.36
−0.0075	−1632.298252	−13.5	11.2	1.60	−0.06	−0.06	0.51	0.00	0.68	−0.67	1.21	0.42	0.36
−0.0050	−1632.288586	−7.4	8.7	1.57	−0.06	−0.06	0.55	0.00	0.68	−0.67	1.24	0.39	0.36
0.0000	−1632.276753	0.0	4.3	1.51	−0.07	−0.07	0.62	0.00	0.69	−0.66	1.30	0.32	0.35
0.0050	−1632.274805	1.2	4.2	1.44	−0.06	−0.07	0.69	0.00	0.69	−0.64	1.35	0.26	0.35
0.0075	−1632.277531	−0.5	6.2	1.41	−0.06	−0.08	0.72	0.00	0.69	−0.64	1.38	0.23	0.34
0.0100	−1632.282726	−3.7	8.5	1.38	−0.05	−0.09	0.75	0.00	0.69	−0.64	1.41	0.20	0.34
0.0125	−1632.290401	−8.6	10.9	1.35	−0.04	−0.09	0.78	0.00	0.69	−0.63	1.43	0.17	0.34

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.309912	−20.8	13.0	1.53	−0.07	−0.07	0.60	0.00	0.68	−0.67	1.28	0.33	0.37
−0.0100	−1632.298915	−13.9	10.9	1.52	−0.07	−0.07	0.61	0.00	0.69	−0.66	1.28	0.33	0.36
−0.0075	−1632.290114	−8.4	8.9	1.52	−0.07	−0.07	0.61	0.00	0.69	−0.66	1.29	0.33	0.36
−0.0050	−1632.283492	−4.2	7.0	1.51	−0.07	−0.07	0.62	0.00	0.69	−0.66	1.29	0.32	0.36
0.0000	−1632.276753	0.0	4.3	1.51	−0.07	−0.07	0.62	0.00	0.69	−0.66	1.30	0.32	0.35
0.0050	−1632.278665	−1.2	5.1	1.50	−0.07	−0.07	0.63	0.00	0.69	−0.65	1.31	0.31	0.34
0.0075	−1632.282884	−3.8	6.7	1.50	−0.06	−0.07	0.63	0.00	0.68	−0.65	1.31	0.31	0.34
0.0100	−1632.289297	−7.9	8.6	1.50	−0.06	−0.08	0.63	0.00	0.68	−0.65	1.32	0.31	0.34
0.0125	−1632.297926	−13.3	10.6	1.51	−0.06	−0.08	0.63	0.00	0.68	−0.65	1.32	0.31	0.34

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.320707	−27.6	19.5	1.87	0.09	−0.05	0.09	0.00	0.66	−0.72	0.91	0.82	0.33
−0.0100	−1632.304226	−17.2	16.5	1.85	0.06	−0.05	0.14	0.00	0.67	−0.72	0.95	0.76	0.34
−0.0075	−1632.292101	−9.6	13.6	1.82	0.02	−0.03	0.20	0.00	0.68	−0.71	0.99	0.70	0.34
−0.0050	−1632.282278	−3.5	9.4	1.74	−0.03	−0.04	0.32	0.00	0.68	−0.69	1.08	0.59	0.34
0.0000	−1632.276753	0.0	4.3	1.51	−0.07	−0.07	0.62	0.00	0.69	−0.66	1.30	0.32	0.35
0.0050	−1632.289918	−8.3	11.2	1.25	−0.01	−0.08	0.85	0.00	0.70	−0.64	1.49	0.10	0.35
0.0075	−1632.302366	−16.1	14.4	1.16	0.03	−0.09	0.90	0.00	0.70	−0.65	1.55	0.04	0.35
0.0100	−1632.317795	−25.8	17.1	1.12	0.05	−0.09	0.92	0.00	0.70	−0.65	1.60	0.00	0.35
0.0125	−1632.335801	−37.1	19.6	1.09	0.07	−0.09	0.93	0.00	0.70	−0.66	1.63	−0.02	0.35

[a] ΔE values are relative to the energy of ^{3}**TS**$_{\mathbf{reb}}$ in the absence of an EF.

Table S10 Dependence of energy,[a] spin density and charge of ^{5}**TS**$_{\mathbf{reb}}$ [b] on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.358085	−51.0	20.3	3.73	0.10	0.14	0.02	0.01	0.78	−0.77	0.81	0.85	0.34
−0.0100	−1632.340525	−40.0	17.9	3.72	0.09	0.15	0.03	0.01	0.78	−0.77	0.81	0.83	0.34
−0.0075	−1632.325385	−30.5	15.6	3.72	0.09	0.15	0.03	0.01	0.78	−0.77	0.82	0.82	0.35
−0.0050	−1632.312628	−22.5	13.3	3.72	0.08	0.15	0.04	0.01	0.79	−0.77	0.83	0.80	0.35
0.0000	−1632.294217	−11.0	8.9	3.71	0.05	0.16	0.07	0.01	0.79	−0.76	0.85	0.76	0.36
0.0050	−1632.285331	−5.4	5.1	3.71	0.02	0.16	0.11	0.01	0.80	−0.75	0.87	0.72	0.36
0.0075	−1632.284541	−4.9	4.1	3.71	0.00	0.16	0.12	0.01	0.80	−0.74	0.89	0.69	0.37
0.0100	−1632.286259	−6.0	4.7	3.69	−0.03	0.15	0.18	0.01	0.80	−0.73	0.91	0.66	0.37
0.0125	−1632.290513	−8.6	6.4	3.68	−0.07	0.13	0.25	0.01	0.81	−0.72	0.94	0.60	0.38

(b) Y-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.325969	−30.9	14.4	3.73	0.08	0.15	0.04	0.01	0.78	−0.77	0.81	0.81	0.33
−0.0100	−1632.315597	−24.4	12.8	3.72	0.07	0.15	0.04	0.01	0.78	−0.77	0.81	0.80	0.34
−0.0075	−1632.307264	−19.1	11.4	3.72	0.07	0.16	0.05	0.01	0.78	−0.77	0.82	0.79	0.34
−0.0050	−1632.300935	−15.2	10.2	3.72	0.06	0.16	0.05	0.01	0.79	−0.77	0.83	0.78	0.35
0.0000	−1632.294217	−11.0	8.9	3.71	0.05	0.16	0.07	0.01	0.79	−0.76	0.85	0.76	0.36
0.0050	−1632.295394	−11.7	9.2	3.71	0.04	0.16	0.08	0.01	0.79	−0.76	0.85	0.74	0.37
0.0075	−1632.298965	−13.9	10.0	3.71	0.03	0.15	0.09	0.01	0.80	−0.76	0.86	0.73	0.37
0.0100	−1632.304557	−17.4	11.2	3.71	0.03	0.15	0.10	0.01	0.80	−0.75	0.86	0.72	0.38
0.0125	−1632.312214	−22.3	12.6	3.72	0.02	0.14	0.11	0.01	0.80	−0.75	0.87	0.71	0.38

(c) Z-direction

EF	Energy	ΔE	μ	spin density					charge				
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(Bz)	ρ(H)	Q(Fe)	Q(O)	Q(L)	Q(Bz)	Q(H)
−0.0125	−1632.354444	−48.8	20.6	3.71	0.16	0.12	0.01	0.01	0.78	−0.77	0.72	0.90	0.37
−0.0100	−1632.337104	−37.9	18.1	3.71	0.14	0.13	0.01	0.01	0.78	−0.77	0.74	0.88	0.36
−0.0075	−1632.322369	−28.6	15.7	3.71	0.12	0.14	0.02	0.01	0.79	−0.77	0.77	0.86	0.36
−0.0050	−1632.310274	−21.0	13.3	3.72	0.10	0.14	0.03	0.01	0.79	−0.77	0.79	0.83	0.36
0.0000	−1632.294217	−11.0	8.9	3.71	0.05	0.16	0.07	0.01	0.79	−0.76	0.85	0.76	0.36
0.0050	−1632.293635	−10.6	7.7	3.88	0.26	0.31	−0.45	0.00	0.86	−0.72	1.07	0.43	0.36
0.0075	−1632.302755	−16.3	12.1	3.93	0.29	0.37	−0.60	0.00	0.88	−0.71	1.17	0.30	0.36
0.0100	−1632.316938	−25.2	17.1	3.98	0.30	0.46	−0.75	0.00	0.89	−0.71	1.28	0.17	0.36
0.0125	−1632.336197	−37.3	22.0	4.01	0.30	0.55	−0.86	0.00	0.90	−0.71	1.39	0.06	0.36

[a] ΔE values are relative to the energy of ^{3}**TS**$_{\mathbf{reb}}$ in the absence of an EF.

[b] Since ^{5}**TS**$_{\mathbf{reb}}$ is not available the absence of an EF, the optimized geometry with r(C-O) fixed at 2.5 Å was used.

Table S11. Dependence of energy,[a] spin density and charge of ^{3}**P** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.358452	−23.8	13.1	2.00	0.02	−0.03	0.01	0.68	−0.65	1.12	0.84
−0.0100	−1632.346680	−16.4	10.9	1.99	0.02	−0.03	0.01	0.68	−0.65	1.12	0.84
−0.0075	−1632.337049	−10.3	8.8	1.99	0.02	−0.02	0.01	0.68	−0.65	1.12	0.84
−0.0050	−1632.329530	−5.6	6.7	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0000	−1632.320585	0.0	2.6	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0050	−1632.320330	0.2	2.5	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0075	−1632.323263	−1.7	4.4	2.00	0.02	−0.03	0.01	0.69	−0.65	1.12	0.84
0.0100	−1632.328327	−4.9	6.5	2.01	0.02	−0.04	0.01	0.69	−0.65	1.12	0.84
0.0125	−1632.335560	−9.4	8.7	2.02	0.02	−0.06	0.01	0.69	−0.65	1.11	0.84

(b) Y-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.351699	−19.5	12.2	2.00	0.02	−0.03	0.01	0.68	−0.65	1.13	0.84
−0.0100	−1632.341148	−12.9	10.0	1.99	0.02	−0.02	0.01	0.68	−0.65	1.13	0.84
−0.0075	−1632.332796	−7.7	7.9	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
−0.0050	−1632.326623	−3.8	5.8	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0000	−1632.320585	0.0	2.6	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0050	−1632.323528	−1.8	4.4	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0075	−1632.328164	−4.8	6.4	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0100	−1632.334994	−9.0	8.5	2.00	0.02	−0.03	0.01	0.69	−0.65	1.12	0.84
0.0125	−1632.344049	−14.7	10.7	2.01	0.02	−0.04	0.01	0.69	−0.65	1.12	0.84

(c) Z-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.342888	−14.0	10.9	1.98	0.04	−0.02	0.01	0.69	−0.66	1.02	0.94
−0.0100	−1632.333822	−8.3	8.5	1.98	0.03	−0.02	0.01	0.70	−0.66	1.05	0.92
−0.0075	−1632.327130	−4.1	6.2	1.98	0.03	−0.02	0.01	0.70	−0.66	1.06	0.90
−0.0050	−1632.322744	−1.4	4.2	1.99	0.03	−0.02	0.01	0.69	−0.66	1.08	0.88
0.0000	−1632.320585	0.0	2.6	1.99	0.02	−0.02	0.01	0.69	−0.65	1.12	0.84
0.0050	−1632.327717	−4.5	6.3	1.99	0.02	−0.01	0.01	0.68	−0.64	1.15	0.80
0.0075	−1632.334534	−8.8	8.4	1.99	0.01	−0.01	0.01	0.68	−0.63	1.17	0.78
0.0100	−1632.343586	−14.4	10.6	1.98	0.01	−0.01	0.02	0.67	−0.63	1.19	0.76
0.0125	−1632.354901	−21.5	12.9	1.98	0.01	−0.01	0.02	0.66	−0.62	1.21	0.74

[a] ΔE values are relative to the energy of ^{3}**P** in the absence of an EF.

Table S12 Dependence of energy,[a] spin density and charge of ^{5}**P** on the applied electric field

(a) X-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.373256	−33.1	12.8	3.75	0.03	0.20	0.01	0.81	−0.68	0.98	0.90
−0.0100	−1632.361827	−25.9	10.7	3.75	0.03	0.20	0.01	0.81	−0.68	0.97	0.90
−0.0075	−1632.352457	−20.0	8.7	3.75	0.03	0.20	0.01	0.81	−0.68	0.97	0.90
−0.0050	−1632.345123	−15.4	6.7	3.75	0.03	0.20	0.01	0.82	−0.68	0.97	0.90
0.0000	−1632.337018	−10.3	2.3	3.75	0.03	0.21	0.01	0.82	−0.68	0.97	0.89
0.0050	−1632.335904	−9.6	2.8	3.75	0.03	0.20	0.01	0.82	−0.69	0.97	0.90
0.0075	−1632.338618	−11.3	4.4	3.75	0.03	0.20	0.01	0.82	−0.69	0.97	0.90
0.0100	−1632.343355	−14.3	6.3	3.75	0.03	0.20	0.01	0.82	−0.69	0.97	0.90
0.0125	−1632.350134	−18.5	8.3	3.76	0.03	0.20	0.01	0.82	−0.69	0.97	0.90

(b) Y-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.364464	−27.5	11.6	3.75	0.03	0.21	0.01	0.81	−0.68	0.98	0.89
−0.0100	−1632.354623	−21.4	9.5	3.75	0.03	0.21	0.01	0.81	−0.69	0.98	0.89
−0.0075	−1632.346925	−16.5	7.5	3.75	0.03	0.21	0.01	0.82	−0.69	0.98	0.89
−0.0050	−1632.341348	−13.0	5.6	3.75	0.03	0.20	0.01	0.82	−0.69	0.97	0.90
0.0000	−1632.337018	−10.3	2.3	3.75	0.03	0.21	0.01	0.82	−0.68	0.97	0.89
0.0050	−1632.340039	−12.2	4.9	3.75	0.03	0.20	0.01	0.82	−0.69	0.96	0.90
0.0075	−1632.344960	−15.3	6.8	3.75	0.03	0.20	0.01	0.82	−0.69	0.96	0.90
0.0100	−1632.351997	−19.7	8.7	3.75	0.03	0.20	0.01	0.82	−0.69	0.96	0.91
0.0125	−1632.361174	−25.5	10.8	3.76	0.03	0.20	0.01	0.81	−0.69	0.96	0.91

(c) Z-direction

EF	Energy	ΔE	μ	spin density				charge			
(au)	(au)	(kcal/mol)	(debye)	ρ(Fe)	ρ(O)	ρ(L)	ρ(TE)	Q(Fe)	Q(O)	Q(L)	Q(TE)
−0.0125	−1632.355706	−22.0	10.4	3.75	0.05	0.18	0.02	0.83	−0.69	0.87	1.00
−0.0100	−1632.347144	−16.7	7.9	3.76	0.05	0.18	0.01	0.83	−0.69	0.89	0.97
−0.0075	−1632.341046	−12.8	5.6	3.76	0.04	0.19	0.01	0.83	−0.69	0.91	0.95
−0.0050	−1632.337156	−10.4	3.7	3.75	0.04	0.20	0.01	0.83	−0.69	0.93	0.93
0.0000	−1632.337018	−10.3	2.3	3.75	0.03	0.21	0.01	0.82	−0.68	0.97	0.89
0.0050	−1632.344958	−15.3	7.0	3.75	0.02	0.21	0.01	0.81	−0.68	1.01	0.86
0.0075	−1632.352576	−20.1	9.2	3.75	0.02	0.22	0.02	0.80	−0.67	1.02	0.85
0.0100	−1632.362449	−26.3	11.4	3.74	0.02	0.22	0.02	0.79	−0.67	1.04	0.83
0.0125	−1632.374580	−33.9	13.7	3.74	0.02	0.22	0.02	0.79	−0.66	1.07	0.81

[a] ΔE values are relative to the energy of ^{3}**P** in the absence of an EF.

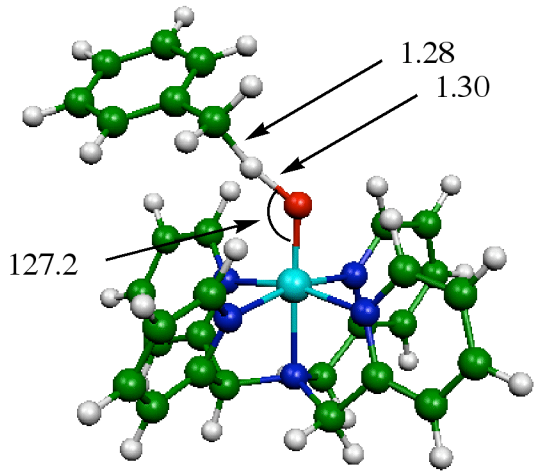
Table S13. Energies of key species along the reaction pathway in the absence of an electric field (B3LYP/LACVP)

	E (au)	ΔE (kcal/mol)
TE	−271.506980	
$^{3}K_{N4Py}$	−1360.774670	
$^{5}K_{N4Py}$	−1360.753535	
^{3}R	−1632.281650	5.5
^{5}R	−1632.260515	18.7
^{3}RC	−1632.290373	0.0
^{5}RC	−1632.269449	13.1
$^{3}TS_{H}$	−1632.270037	12.8
$^{5}TS_{H}$	−1632.267252	14.5
^{3}I	−1632.288555	1.1
^{5}I	−1632.286173	2.6
$^{3}TS_{reb}$	−1632.276753	8.5
$^{5}TS_{reb}$' [a]	−1632.294217	−2.4
^{3}P	−1632.320585	−19.0
^{5}P	−1632.337018	−29.3

[a] Since $^{5}TS_{reb}$ is not available (**see later Figure S13**b in **Part 2**) the absence of an EF, the optimized geometry with r(C-O) fixed at 2.5 Å was used.

Geometries of TS_{H}

$^{3}TS_{H}$



$^{5}TS_{H}$

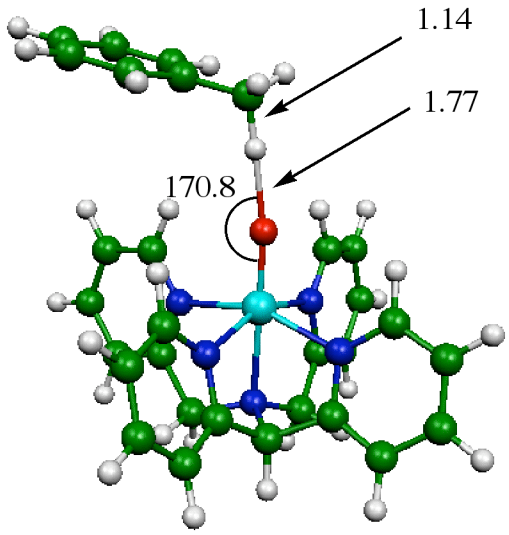


Table S14. Absolute energies and relative energies (with respect to ^{3}**RC**) of key species along the reaction pathway in the presence of an electric field oriented along the X-axis (B3LYP/LACVP)

	X-0.0125		X-0.0100		X-0.0075		X-0.0050	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.798427		−1360.790112		−1360.783595		−1360.778864	
^{5}**K$_{N4Py}$**	−1360.776495		−1360.768332		−1360.761976		−1360.757413	
^{3}**R**	−1632.305407	9.6	−1632.297092	8.3	−1632.290575	7.2	−1632.285844	6.4
^{5}**R**	−1632.283475	23.4	−1632.275312	22.0	−1632.268957	20.8	−1632.264393	19.8
^{3}**RC**	−1632.320752	0.0	−1632.310310	0.0	−1632.30207	0.0	−1632.296018	0.0
^{5}**RC**	−1632.298748	13.8	−1632.288437	13.7	−1632.28038	13.6	−1632.274540	13.5
^{3}**TS$_H$**	−1632.324176	−2.1	−1632.307570	1.7	−1632.293915	5.1	−1632.283162	8.1
^{5}**TS$_H$**	−1632.299100	13.6	−1632.288332	13.8	−1632.279765	14.0	−1632.273391	14.2
^{3}**I**	−1632.338464	−11.1	−1632.320981	−6.7	−1632.308954	−4.3	−1632.299750	−2.3
^{5}**I**	−1632.311751	5.6	−1632.302288	5.0	−1632.295015	4.4	−1632.289918	3.8
^{3}**TS$_{reb}$**	−1632.325262	−2.8	−1632.310459	−0.1	−1632.298252	2.4	−1632.288586	4.7
^{5}**TS$_{reb}$**[a]	−1632.358085	−23.4	−1632.340525	−19.0	−1632.325385	−14.6	−1632.312628	−10.4
^{3}**P**	−1632.358452	−23.7	−1632.346680	−22.8	−1632.337049	−21.9	−1632.329530	−21.0
^{5}**P**	−1632.373256	−32.9	−1632.361827	−32.3	−1632.352457	−31.6	−1632.345123	−30.8

	X+0.0050		X+0.0075		X+0.0100		X+0.0125	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.777704		−1360.781859		−1360.787804		−1360.795554	
^{5}**K$_{N4Py}$**	−1360.756984		−1360.761348		−1360.767525		−1360.775537	
^{3}**R**	−1632.284685	5.6	−1632.288839	6.0	−1632.294784	6.7	−1632.302534	7.6
^{5}**R**	−1632.263964	18.6	−1632.268329	18.9	−1632.274505	19.4	−1632.282517	20.1
^{3}**RC**	−1632.293564	0.0	−1632.298386	0.0	−1632.305394	0.0	−1632.314598	0.0
^{5}**RC**	−1632.273154	12.8	−1632.278306	12.6	−1632.285678	12.4	−1632.295290	12.1
^{3}**TS$_H$**	−1632.268227	15.9	−1632.271312	17.0	−1632.277071	17.8	−1632.285495	18.3
^{5}**TS$_H$**	−1632.269862	14.9	−1632.274516	15.0	−1632.281418	15.0	−1632.290599	15.1
^{3}**I**	−1632.287047	4.1	−1632.289832	5.4	−1632.295003	6.5	−1632.302574	7.5
^{5}**I**	−1632.291132	1.5	−1632.296836	1.0	−1632.304717	0.4	−1632.314826	−0.1
^{3}**TS$_{reb}$**	−1632.274805	11.8	−1632.277531	13.1	−1632.282726	14.2	−1632.290401	15.2
^{5}**TS$_{reb}$**[a]	−1632.285331	5.2	−1632.284541	8.7	−1632.286259	12.0	−1632.290513	15.1
^{3}**P**	−1632.320330	−16.8	−1632.323263	−15.6	−1632.328327	−14.4	−1632.335560	−13.2
^{5}**P**	−1632.335904	−26.6	−1632.338618	−25.2	−1632.343355	−23.8	−1632.350134	−22.3

[a] Since ^{5}**TS$_{reb}$** is not available (**see later Figure S13**b in **Part 2**) in the absence of an EF, the optimized geometry with r(C-O) fixed at 2.5 Å was used.

Table S15. Absolute energies and relative energies (with respect to ^{3}**RC**) of key species along the reaction pathway in the presence of an electric field oriented along the Y-axis (B3LYP/LACVP)

	Y-0.0125		Y-0.0100		Y-0.0075		Y-0.0050	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.798374		−1360.790073		−1360.783568		−1360.778848	
^{5}**K$_{N4Py}$**	−1360.776471		−1360.768328		−1360.761983		−1360.757424	
^{3}**R**	−1632.305354	7.4	−1632.297053	6.4	−1632.290549	5.7	−1632.285829	5.3
^{5}**R**	−1632.283452	21.1	−1632.275308	20.0	−1632.268964	19.2	−1632.264405	18.8
^{3}**RC**	−1632.317080	0.0	−1632.307214	0.0	−1632.299624	0.0	−1632.294303	0.0
^{5}**RC**	−1632.295461	13.6	−1632.285724	13.5	−1632.278263	13.4	−1632.273068	13.3
^{3}**TS$_{H}$**	−1632.302316	9.3	−1632.291580	9.8	−1632.283006	10.4	−1632.276583	11.1
^{5}**TS$_{H}$**	−1632.286337	19.3	−1632.277071	18.9	−1632.270456	18.3	−1632.266564	17.4
^{3}**I**	−1632.320695	−2.3	−1632.309996	−1.7	−1632.301449	−1.1	−1632.295042	−0.5
^{5}**I**	−1632.306347	6.7	−1632.297912	5.8	−1632.291692	5.0	−1632.287673	4.2
^{3}**TS$_{reb}$**	−1632.309912	4.5	−1632.298915	5.2	−1632.290114	6.0	−1632.283492	6.8
^{5}**TS$_{reb}$**[a]	−1632.325969	−5.6	−1632.315597	−5.3	−1632.307264	−4.8	−1632.300935	−4.2
^{3}**P**	−1632.351699	−21.7	−1632.341148	−21.3	−1632.332796	−20.8	−1632.326623	−20.3
^{5}**P**	−1632.364464	−29.7	−1632.354623	−29.7	−1632.346925	−29.7	−1632.341348	−29.5

	Y+0.0050		Y+0.0075		Y+0.0100		Y+0.0125	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.777711		−1360.781866		−1360.787809		−1360.795554	
^{5}**K$_{N4Py}$**	−1360.756947		−1360.761284		−1360.767428		−1360.775402	
^{3}**R**	−1632.284691	6.9	−1632.288846	8.1	−1632.294789	9.7	−1632.302534	12.5
^{5}**R**	−1632.263927	19.9	−1632.268264	21.0	−1632.274408	22.5	−1632.282382	25.2
^{3}**RC**	−1632.295656	0.0	−1632.301711	0.0	−1632.310284	0.0	−1632.322495	0.0
^{5}**RC**	−1632.274974	13.0	−1632.281292	12.8	−1632.290161	12.6	−1632.304926	11.0
^{3}**TS$_{H}$**	−1632.272331	14.6	−1632.276645	15.7	−1632.283129	17.0	−1632.291801	19.3
^{5}**TS$_{H}$**	−1632.279468	10.2	−1632.290010	7.3	−1632.303523	4.2	−1632.320015	1.6
^{3}**I**	−1632.290713	3.1	−1632.294964	4.2	−1632.301365	5.6	−1632.309931	7.9
^{5}**I**	−1632.293520	1.3	−1632.300489	0.8	−1632.309713	0.4	−1632.321276	0.8
^{3}**TS$_{reb}$**	−1632.278665	10.7	−1632.282884	11.8	−1632.289297	13.2	−1632.297926	15.4
^{5}**TS$_{reb}$**[a]	−1632.295394	0.2	−1632.298965	1.7	−1632.304557	3.6	−1632.312214	6.5
^{3}**P**	−1632.323528	−17.5	−1632.328164	−16.6	−1632.334994	−15.5	−1632.344049	−13.5
^{5}**P**	−1632.340039	−27.9	−1632.344960	−27.1	−1632.351997	−26.2	−1632.361174	−24.3

[a] Since ^{5}**TS$_{reb}$** is not available (**see later Figure S13**b in **Part 2**) in the absence of an EF, the optimized geometry with r(C-O) fixed at 2.5 Å was used.

Table S16. Absolute energies and relative energies (with respect to ^{3}**RC**) of key species along the reaction pathway in the presence of an electric field oriented along the Z-axis (B3LYP/LACVP)

	Z-0.0125		Z-0.0100		Z-0.0075		Z-0.0050	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.741218		−1360.744738		−1360.749851		−1360.756556	
^{5}**K$_{N4Py}$**	−1360.713258		−1360.718082		−1360.724532		−1360.732608	
^{3}**R**	−1632.248199	16.6	−1632.251719	12.5	−1632.256832	10.0	−1632.263536	8.2
^{5}**R**	−1632.220238	34.1	−1632.225062	29.3	−1632.231513	25.9	−1632.239589	23.2
^{3}**RC**	−1632.274593	0.0	−1632.271694	0.0	−1632.272713	0.0	−1632.276572	0.0
^{5}**RC**	−1632.261431	8.3	−1632.253177	11.6	−1632.250409	14.0	−1632.253330	14.6
^{3}**TS$_H$**	−1632.271958	1.7	−1632.266545	3.2	−1632.263668	5.7	−1632.263320	8.3
^{5}**TS$_H$**	−1632.287111	−7.9	−1632.275447	−2.4	−1632.267459	3.3	−1632.263345	8.3
^{3}**I**	−1632.284323	−6.1	−1632.278298	−4.1	−1632.276745	−2.5	−1632.278527	−1.2
^{5}**I**	−1632.353468	−49.5	−1632.328695	−35.8	−1632.306659	−21.3	−1632.291617	−9.4
^{3}**TS$_{reb}$**	−1632.320707	−28.9	−1632.304226	−20.4	−1632.292101	−12.2	−1632.282278	−3.6
^{5}**TS$_{reb}$**[a]	−1632.354444	−50.1	−1632.337104	−41.0	−1632.322369	−31.2	−1632.310274	−21.1
^{3}**P**	−1632.342888	−42.9	−1632.333822	−39.0	−1632.32713	−34.1	−1632.322744	−29.0
^{5}**P**	−1632.355706	−50.9	−1632.347144	−47.3	−1632.341046	−42.9	−1632.337156	−38.0

	Z+0.0050		Z+0.0075		Z+0.0100		Z+0.0125	
TE	−271.506980		−271.506980		−271.506980		−271.506980	
^{3}**K$_{N4Py}$**	−1360.799271		−1360.813922		−1360.830163		−1360.847994	
^{5}**K$_{N4Py}$**	−1360.781160		−1360.797362		−1360.815190		−1360.834646	
^{3}**R**	−1632.306251	3.7	−1632.320903	3.2	−1632.337144	2.8	−1632.354975	2.7
^{5}**R**	−1632.288141	15.1	−1632.304342	13.5	−1632.322170	12.2	−1632.341627	11.1
^{3}**RC**	−1632.312164	0.0	−1632.325933	0.0	−1632.341636	0.0	−1632.359270	0.0
^{5}**RC**	−1632.293970	11.4	−1632.309224	10.5	−1632.326461	9.5	−1632.345675	8.5
^{3}**TS$_H$**	−1632.287013	15.8	−1632.299168	16.8	−1632.313806	17.5	−1632.330934	17.8
^{5}**TS$_H$**	−1632.287244	15.6	−1632.302710	14.6	−1632.321137	12.9	−1632.342119	10.8
^{3}**I**	−1632.306739	3.4	−1632.318748	4.5	−1632.332707	5.6	−1632.348610	6.7
^{5}**I**	−1632.302077	6.3	−1632.314137	7.4	−1632.328629	8.2	−1632.345509	8.6
^{3}**TS$_{reb}$**	−1632.289918	14.0	−1632.302366	14.8	−1632.317795	15.0	−1632.335801	14.7
^{5}**TS$_{reb}$**[a]	−1632.293635	11.6	−1632.302755	14.5	−1632.316938	15.5	−1632.336197	14.5
^{3}**P**	−1632.327717	−9.8	−1632.334534	−5.4	−1632.343586	−1.2	−1632.354901	2.7
^{5}**P**	−1632.344958	−20.6	−1632.352576	−16.7	−1632.362449	−13.1	−1632.374580	−9.6

[a] Since ^{5}**TS$_{reb}$** is not available (**see later Figure S13**b in **Part 2**) in the absence of an EF, the optimized geometry with r(C-O) fixed at 2.5 Å was used.

Table S17. Energies and AO-coefficients of d-MOs for $\mathbf{K_{N4Py}}$ (α-spin, in au) under EFs along the Z-axis

(a) $^3\mathbf{K_{N4Py}}$

orbital energy

EF (au)	δ	π*	π*	σ^*_{xy}	σ^*_{z2}	$\Delta\varepsilon(\delta-\sigma^*_{xy})$ (au)
−0.0125	−0.518	−0.502	−0.501	−0.297	−0.284	0.221
−0.0100	−0.515	−0.501	−0.499	−0.295	−0.283	0.220
−0.0075	−0.513	−0.499	−0.497	−0.294	−0.281	0.219
−0.0050	−0.511	−0.497	−0.496	−0.292	−0.279	0.219
0.0000	−0.506	−0.492	−0.493	−0.289	−0.276	0.217
0.0050	−0.501	−0.488	−0.490	−0.286	−0.273	0.215
0.0075	−0.499	−0.486	−0.488	−0.285	−0.272	0.214
0.0100	−0.497	−0.484	−0.486	−0.283	−0.270	0.213
0.0125	−0.494	−0.485	−0.482	−0.282	−0.269	0.212

AO coefficient[a]

EF	δ	π*				π*				σ^*_{xy}	σ^*_{z2}
(au)	dx2−y2	dxz	dyz	2px	2py	dxz	dyz	2px	2py	dxy	dz2
−0.0125	0.633	0.438	0.425	−0.357	−0.346	−0.407	0.419	0.332	−0.341	0.778	0.748
−0.0100	0.628	0.436	0.421	−0.358	−0.345	−0.396	0.408	0.323	−0.333	0.781	0.733
−0.0075	0.622	0.431	0.420	−0.356	−0.348	−0.356	0.368	0.288	−0.297	0.783	0.723
−0.0050	0.615	0.429	0.416	−0.357	−0.347	−0.338	0.346	0.293	−0.300	0.784	0.751
0.0000	0.598	0.423	0.409	−0.357	−0.346	−0.371	0.382	0.318	−0.328	0.785	0.750
0.0050	0.578	0.417	0.402	−0.357	−0.344	−0.347	0.359	0.300	−0.311	0.784	0.744
0.0075	0.567	0.414	0.398	−0.356	−0.342	−0.328	0.340	0.286	−0.296	0.784	0.740
0.0100	0.555	0.408	0.390	−0.355	−0.339	−0.305	0.316	0.267	−0.277	0.784	0.734
0.0125	0.542	0.407	0.388	−0.355	−0.339	−0.277	0.287	0.244	−0.254	0.784	0.725

a. Since the axes are in between the N-ligand atoms, the π* orbitals have mixtures of $2p_{x,y}$ and $3d_{xz,yz}$. These five canonical d-type orbitals were delocalized to the ligand, but the natural orbitals had almost the same amplitudes. See Figure S8.

(b) $^5\mathbf{K}_{\mathbf{N4Py}}$

orbital energy

EF (au)	δ	π*	π*	σ^*_{xy}	σ^*_{z2}	$\Delta\varepsilon(\delta-\sigma^*_{xy})$ (au)
−0.0125	−0.633	−0.524	−0.524	−0.483	−0.352	0.150
−0.0100	−0.630	−0.522	−0.521	−0.480	−0.350	0.150
−0.0075	−0.627	−0.519	−0.519	−0.477	−0.348	0.150
−0.0050	−0.624	−0.520	−0.517	−0.474	−0.345	0.150
0.0000	−0.618	−0.513	−0.512	−0.469	−0.341	0.149
0.0050	−0.611	−0.507	−0.507	−0.463	−0.337	0.148
0.0075	−0.608	−0.504	−0.504	−0.460	−0.335	0.147
0.0100	−0.604	−0.501	−0.501	−0.457	−0.333	0.147
0.0125	−0.600	−0.505	−0.504	−0.455	−0.331	0.146

AO coefficient[a]

EF	δ	π*				π*				σ^*_{xy}	σ^*_{z2}
(au)	dx2−y2	dxz	dyz	2px	2py	dxz	dyz	2px	2py	dxy	dz2
−0.0125	0.635	0.294	−0.343	−0.339	0.395	−0.338	−0.289	0.380	0.324	0.543	0.671
−0.0100	0.625	0.294	−0.337	−0.339	0.389	−0.324	−0.281	0.363	0.315	0.540	0.671
−0.0075	0.613	0.293	−0.331	−0.339	0.383	−0.305	−0.268	0.339	0.298	0.538	0.672
−0.0050	0.596	0.291	−0.325	0.339	0.298	−0.276	−0.245	0.303	0.269	0.536	0.673
0.0000	0.560	0.283	−0.310	−0.329	0.360	−0.249	−0.229	0.298	0.274	0.531	0.674
0.0050	0.508	0.268	−0.289	−0.311	−0.214	−0.260	−0.242	0.303	0.283	0.526	0.674
0.0075	0.477	0.257	−0.273	−0.297	0.315	−0.247	−0.234	0.285	0.270	0.524	0.674
0.0100	0.444	−0.273	0.204	0.312	−0.233	−0.180	−0.257	0.205	0.293	0.521	0.673
0.0125	0.409	0.187	−0.198	−0.215	0.227	−0.231	−0.217	0.293	0.275	0.519	0.673

a. See footnote a) above.

Table S18. Energies and AO-coefficients of d-MOs for $\mathbf{TS_H}$ (α-spin, in au) under EFs along the Z-axis

(a) $^3\mathbf{TS_H}$

energy

EF (au)	δ	π*	π*	σ^*_{xy}	σ^*_{z2}	$\Delta\varepsilon(\delta-\sigma^*_{xy})$ (au)
−0.0125	−0.463	−0.442	−0.411	−0.233	−0.228	0.231
0.0000	−0.476	−0.464	−0.450	−0.253	−0.248	0.223
0.0125	−0.541	−0.486	−0.484	−0.270	−0.268	0.271

AO-coefficient[a]

EF	δ	π*				π*				σ^*_{xy}	σ^*_{z2}
(au)	dx2−y2	dxz	dyz	2px	2py	dxz	dyz	2px	2py	dxy	dz2
−0.0125	0.696	0.407	−0.388	−0.389	0.350	0.266	0.297	−0.259	−0.283	0.632	0.735
0.0000	0.697	−0.388	0.370	0.390	−0.353	0.337	0.365	−0.263	−0.274	0.726	0.730
0.0125	0.555	−0.272	0.361	0.304	−0.319	0.413	0.202	−0.289	−0.063	0.742	0.617

a. See footnote a above in Table S17.

(b) $^5\mathbf{TS_H}$

energy

EF (au)	δ	π*	π*	σ^*_{xy}	σ^*_{z2}	$\Delta\varepsilon(\delta-\sigma^*_{xy})$ (au)
−0.0125	−0.563	−0.418	−0.418	−0.429	−0.359	0.135
0.0000	−0.603	−0.481	−0.478	−0.457	−0.348	0.146
0.0125	−0.616	−0.507	−0.506	−0.463	−0.360	0.153

AO-coefficient

EF	δ	π*				π*				σ^*_{xy}	σ^*_{z2}
(au)	dx2−y2	dxz	dyz	2px	2py	dxz	dyz	2px	2py	dxy	dz2
−0.0125	0.764	−0.391	−0.195	0.524	0.261	0.193	−0.388	−0.258	0.522	0.583	0.494
0.0000	0.511	−0.213	−0.230	0.284	0.311	−0.239	0.196	−0.239	0.196	0.502	0.440
0.0125	0.375	−0.117	−0.298	0.155	0.387	0.160	−0.185	−0.187	0.244	0.452	0.608

Table S19. Effect of EFs along the Z-axis on polarizabilities

$^{3}\mathbf{K_{N4Py}}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	283.3	283.0	255.1	273.8
−0.0100	283.4	283.0	254.8	273.7
−0.0075	283.4	283.1	254.6	273.7
−0.0050	283.5	283.2	254.5	273.7
0.0000	283.8	283.5	254.3	273.8
0.0050	284.2	283.9	254.2	274.1
0.0075	284.5	284.1	254.3	274.3
0.0100	284.8	284.4	254.4	274.5
0.0125	285.1	284.7	254.6	274.8

$^{5}\mathbf{K_{N4Py}}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	282.9	281.9	260.4	275.1
−0.0100	283.3	282.2	260.2	275.2
−0.0075	283.6	282.6	260.1	275.4
−0.0050	284.0	283.0	260.0	275.7
0.0000	284.9	283.9	259.9	276.2
0.0050	285.9	284.9	260.1	277.0
0.0075	286.4	285.4	260.3	277.4
0.0100	287.0	286.0	260.5	277.8
0.0125	287.6	286.5	260.8	278.3

$^{3}\mathbf{RC}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	395.9	601.3	653.5	550.2
−0.0100	393.9	592.6	642.9	543.1
−0.0075	364.5	445.3	435.1	415.0
−0.0050	349.4	371.2	328.3	349.6
0.0000	347.5	362.3	313.1	341.0
0.0050	347.4	361.2	310.0	339.6
0.0075	347.5	361.1	309.3	339.3
0.0100	347.6	361.1	308.9	339.2
0.0125	347.8	361.1	308.7	339.2

$^{5}\mathbf{RC}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	426.3	608.5	849.3	628.0
−0.0100	427.9	619.5	874.9	640.8
−0.0075	429.3	631.6	908.9	656.6
−0.0050	381.5	473.7	591.5	482.2
0.0000	350.9	363.9	328.8	347.9
0.0050	350.6	360.7	318.6	343.3
0.0075	350.9	360.5	317.1	342.8
0.0100	351.3	360.7	316.3	342.8
0.0125	351.7	361.0	316.0	342.9

$^{3}\mathbf{TS_{H}}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	458.8	342.2	407.5	402.8
−0.0100	456.7	342.1	405.8	401.5
−0.0075	453.8	342.1	404.3	400.1
−0.0050	450.3	342.3	402.9	398.5
0.0000	441.8	343.0	399.8	394.8
0.0050	433.1	343.9	397.6	391.5
0.0075	429.3	344.4	397.4	390.4
0.0100	426.2	345.1	398.2	389.8
0.0125	424.0	345.8	400.3	390.0

$^{5}\mathbf{TS_{H}}$

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	340.3	449.3	546.0	445.2
−0.0100	342.1	460.9	588.8	463.9
−0.0075	344.2	467.8	620.1	477.4
−0.0050	346.6	470.7	641.9	486.4
0.0000	352.1	464.0	653.1	489.8
0.0050	356.4	426.0	561.7	448.0
0.0075	357.2	399.8	470.9	409.3
0.0100	358.0	384.4	405.8	382.7
0.0125	358.9	378.4	373.5	370.3

^{3}**I**

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	557.1	399.5	753.6	570.1
−0.0100	516.7	372.4	726.4	538.5
−0.0075	433.0	349.4	532.7	438.4
−0.0050	391.1	342.6	348.3	360.7
0.0000	381.9	340.5	319.9	347.4
0.0050	379.3	340.1	313.6	344.4
0.0075	378.8	340.1	312.1	343.6
0.0100	378.5	340.1	311.0	343.2
0.0125	378.5	340.3	310.5	343.1

^{5}**I**

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	364.5	377.1	401.0	380.9
−0.0100	360.4	372.4	432.3	388.4
−0.0075	358.8	368.1	1521.3	749.4
−0.0050	350.6	357.4	1269.7	659.3
0.0000	344.9	350.6	726.8	474.1
0.0050	347.3	352.0	408.8	369.4
0.0075	348.4	352.8	387.7	362.9
0.0100	349.5	353.6	381.5	361.5
0.0125	350.6	354.5	383.6	362.9

^{3}**TS$_{reb}$**

EF (au)	α_{xx} (au)	α_{yy} (au)	α_{zz} (au)	α_{ave} (au)
−0.0125	392.6	360.7	458.1	403.8
−0.0100	390.4	357.3	509.0	418.9
−0.0075	398.6	351.8	622.1	457.5
−0.0050	401.1	349.1	749.8	500.0
0.0000	395.2	346.1	758.2	499.8
0.0050	382.8	346.5	586.9	438.8
0.0075	375.9	347.0	471.7	398.2
0.0100	372.7	347.5	409.5	376.6
0.0125	371.7	347.9	383.3	367.6

Figure S1. Reaction energy profiles in the presence of EFs in the –X, –Y, and –Z directions for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

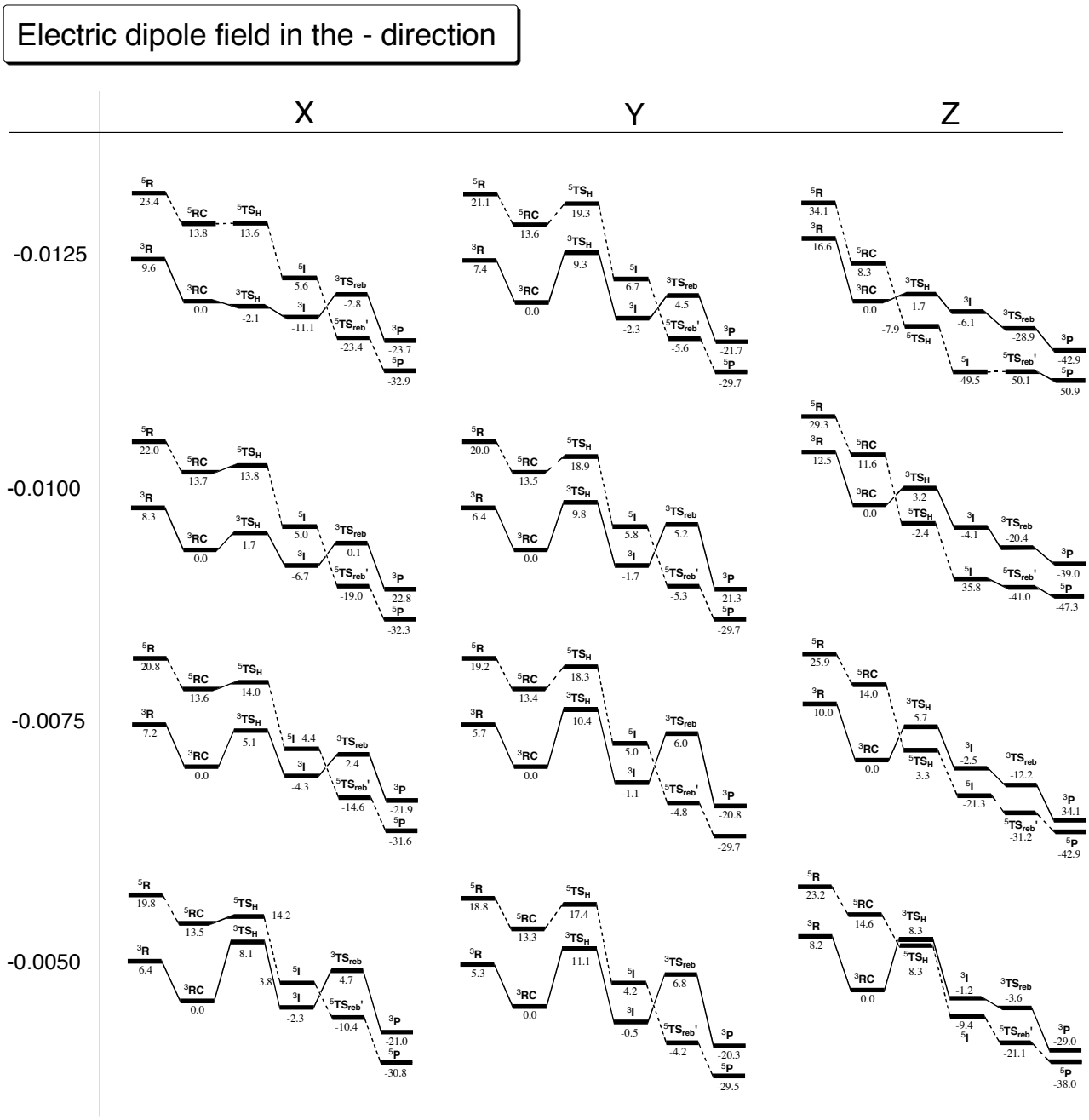


Figure S2. Reaction energy profiles in the presence of EFs in the +X, +Y, and +Z directions for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

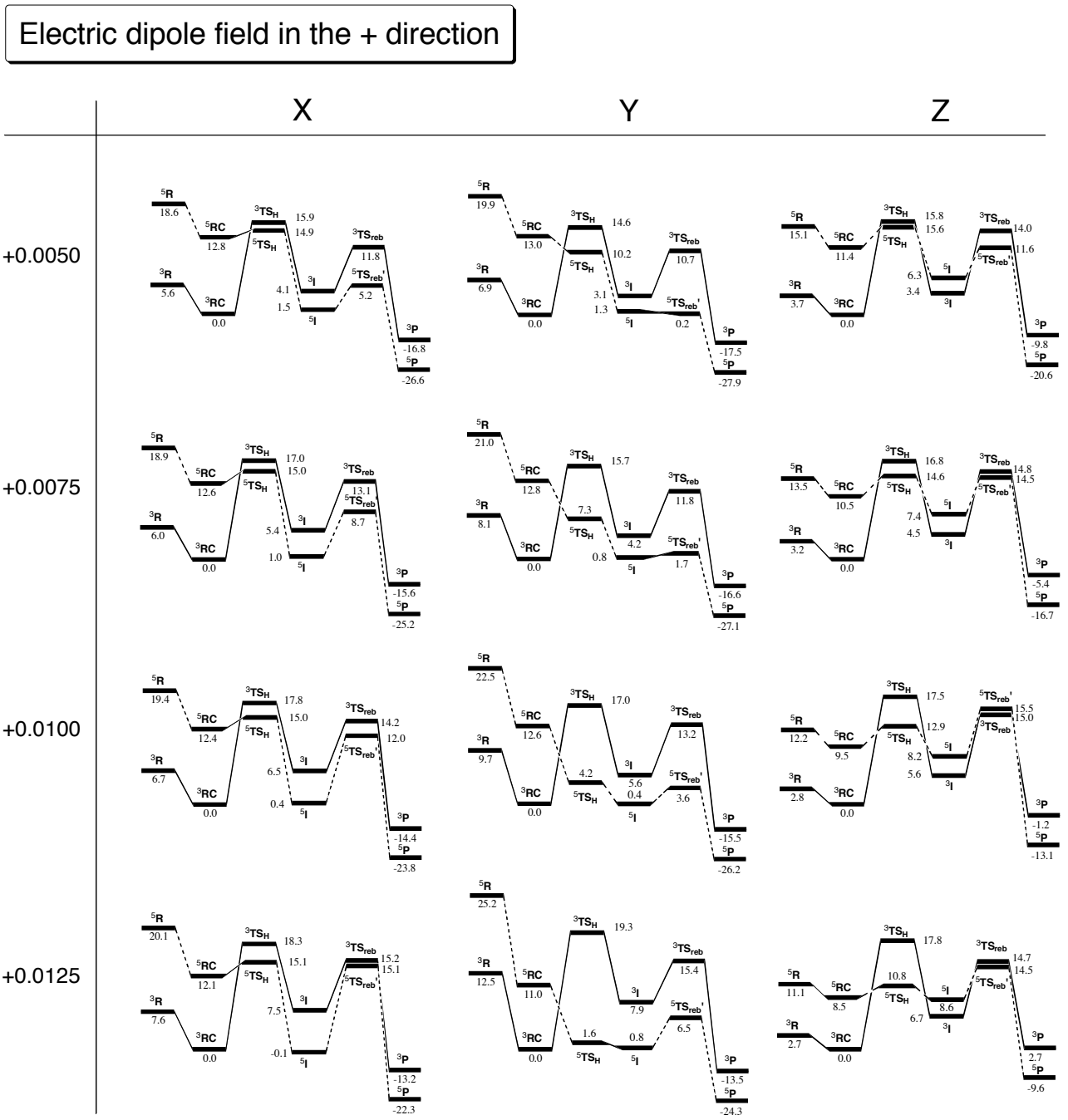
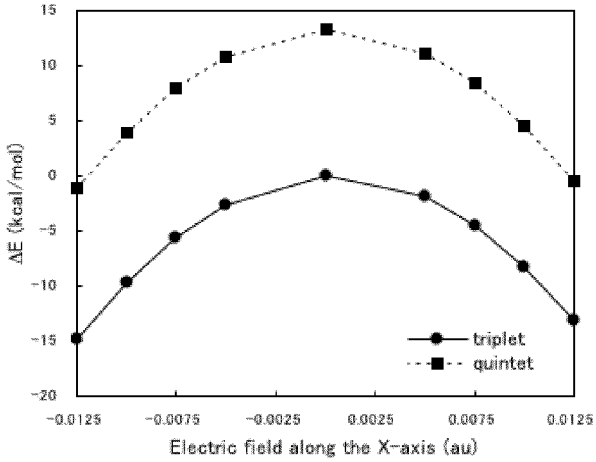
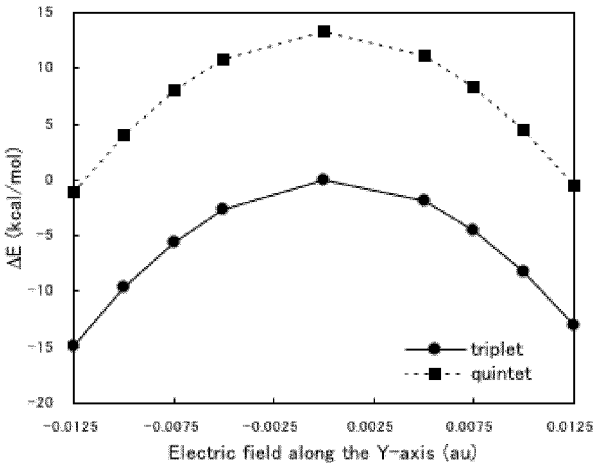


Figure S3. Effect of external EF on the relative energy of $\mathbf{K}_{\mathbf{N4Py}}$ for the reaction of $\mathbf{K}_{\mathbf{N4Py}}$ **with TE.**

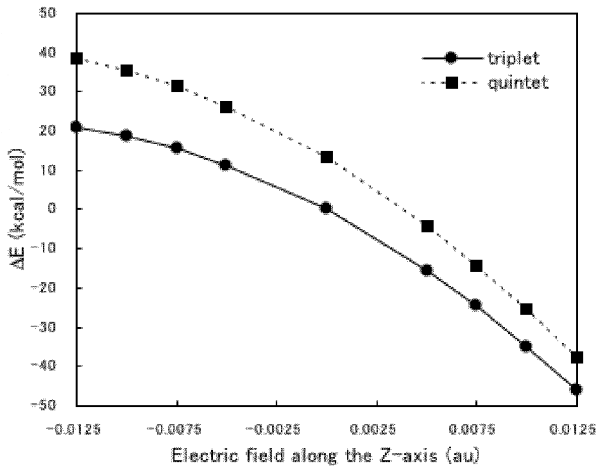
(a) X



(b) Y



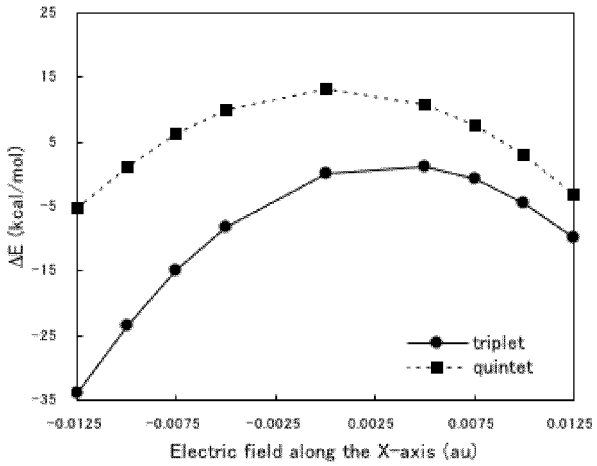
(c) Z



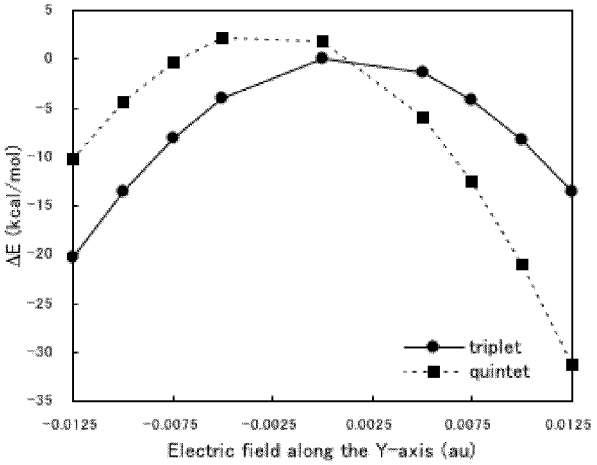
Energies are relative to $^{3}\mathbf{K}_{\mathbf{N4Py}}$ in the absence of an EF.

Figure S4. Effect of external EF on the relative energy of $\mathbf{TS_H}$ for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

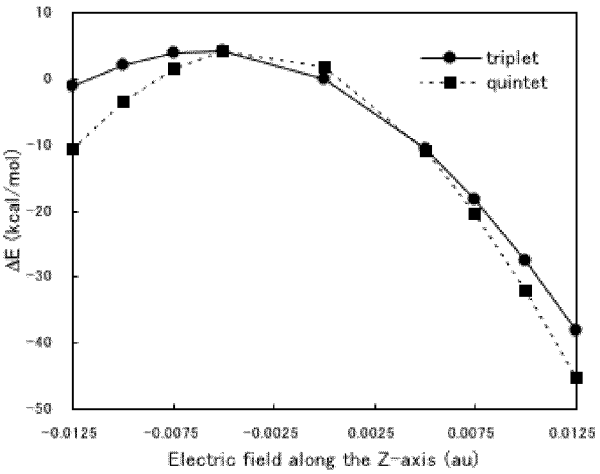
(a) X



(b) Y



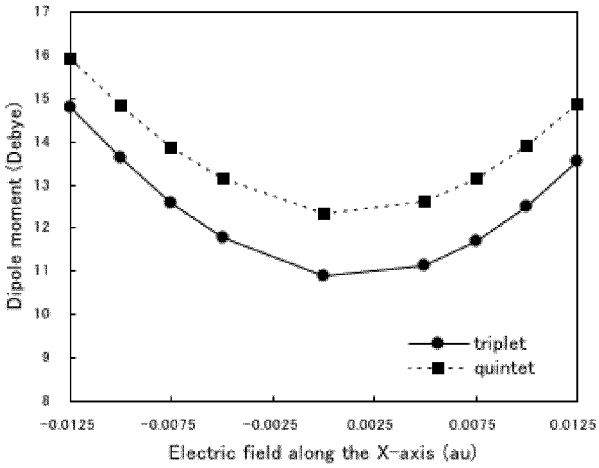
(c) Z



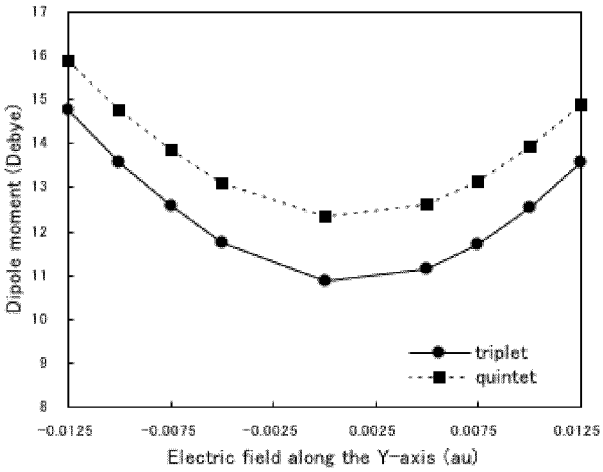
Energies are relative to $^3\mathbf{TS_H}$ in the absence of an EF.

Figure S5. Effect of external EF on the dipole moment of $\mathbf{K_{N4Py}}$ for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

(a) X



(b) Y



(c) Z

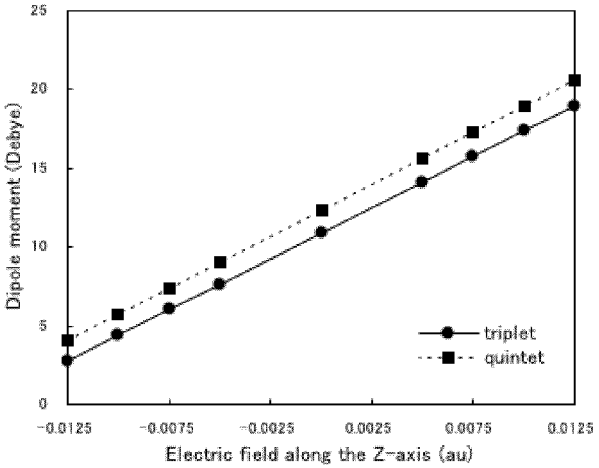
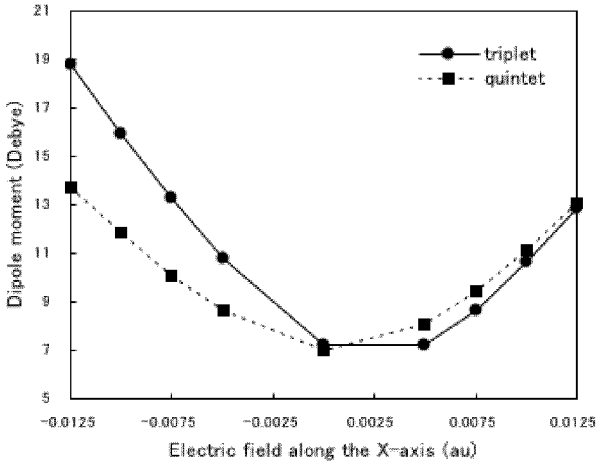
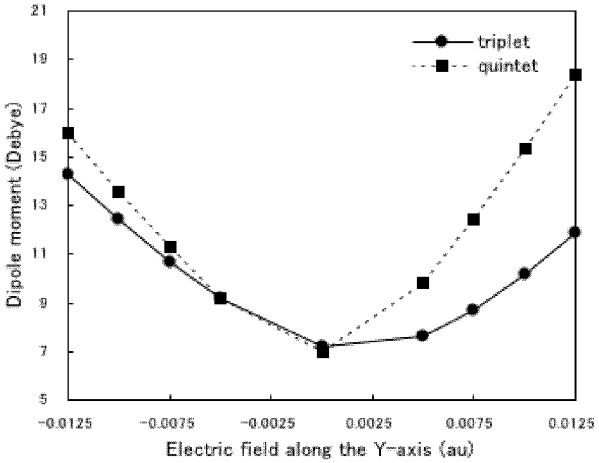


Figure S6. Effect of external EF on the dipole moment of $\mathbf{TS_H}$ for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

(a) X



(b) Y



(c) Z

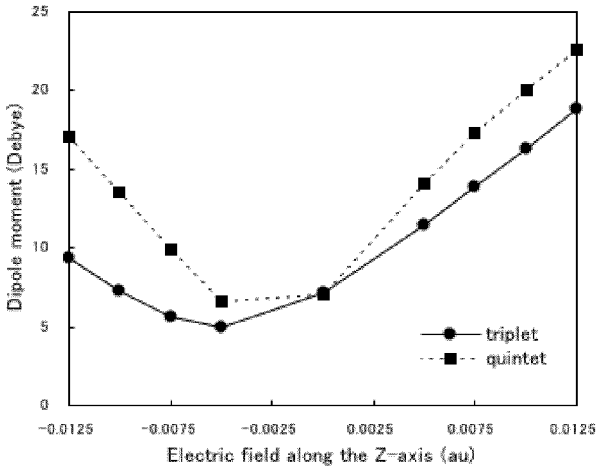
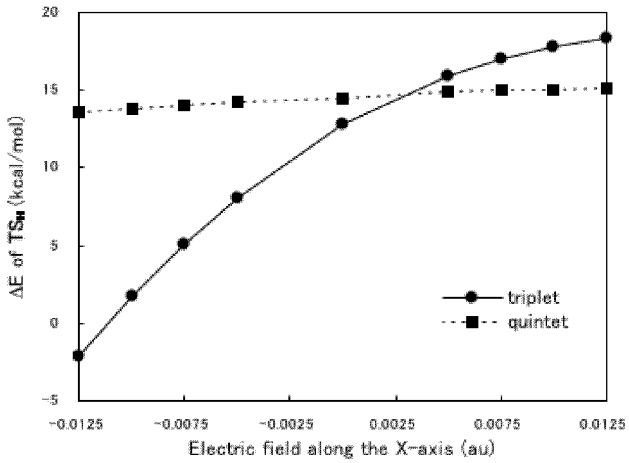
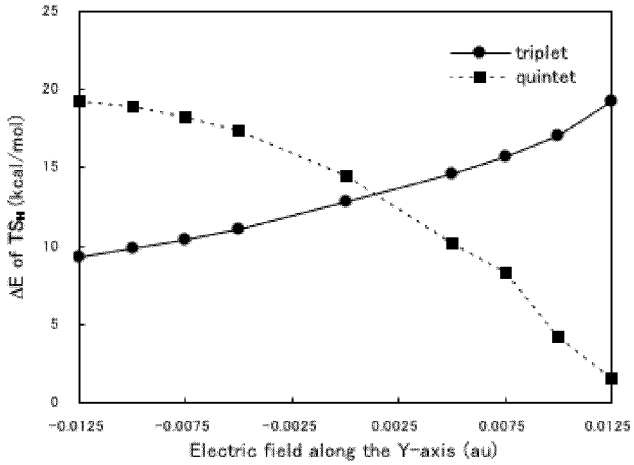


Figure S7. Effect of external EF on the H-abstraction barrier heights in the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

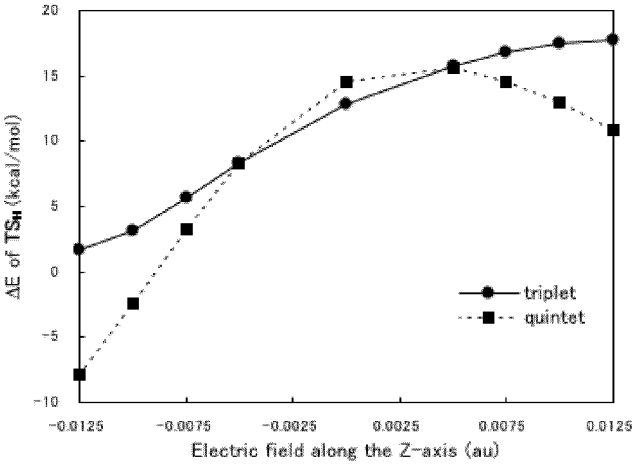
(a) X



(b) Y



(c) Z



See Tables S14-16.

Figure S8. Singly occupied natural orbitals of $^5\mathbf{K}_{\mathbf{N4Py}}$ for the reaction of $\mathbf{K}_{\mathbf{N4Py}}$ **with TE.**

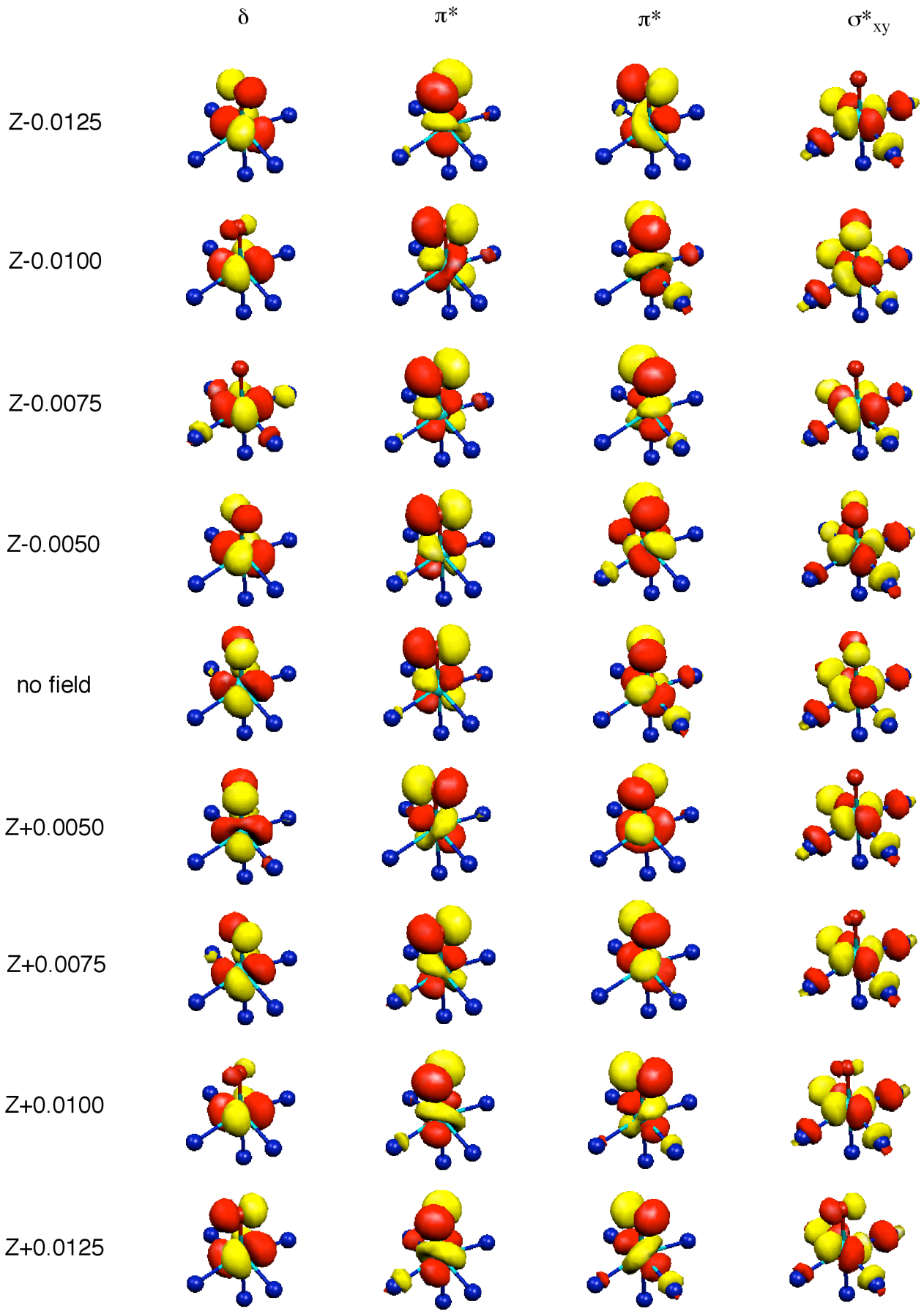


Figure S9. Effect of EFs on dipole moment vectors for $^{3,5}TS_H$ for the reaction of K_{N4Py} **with TE**

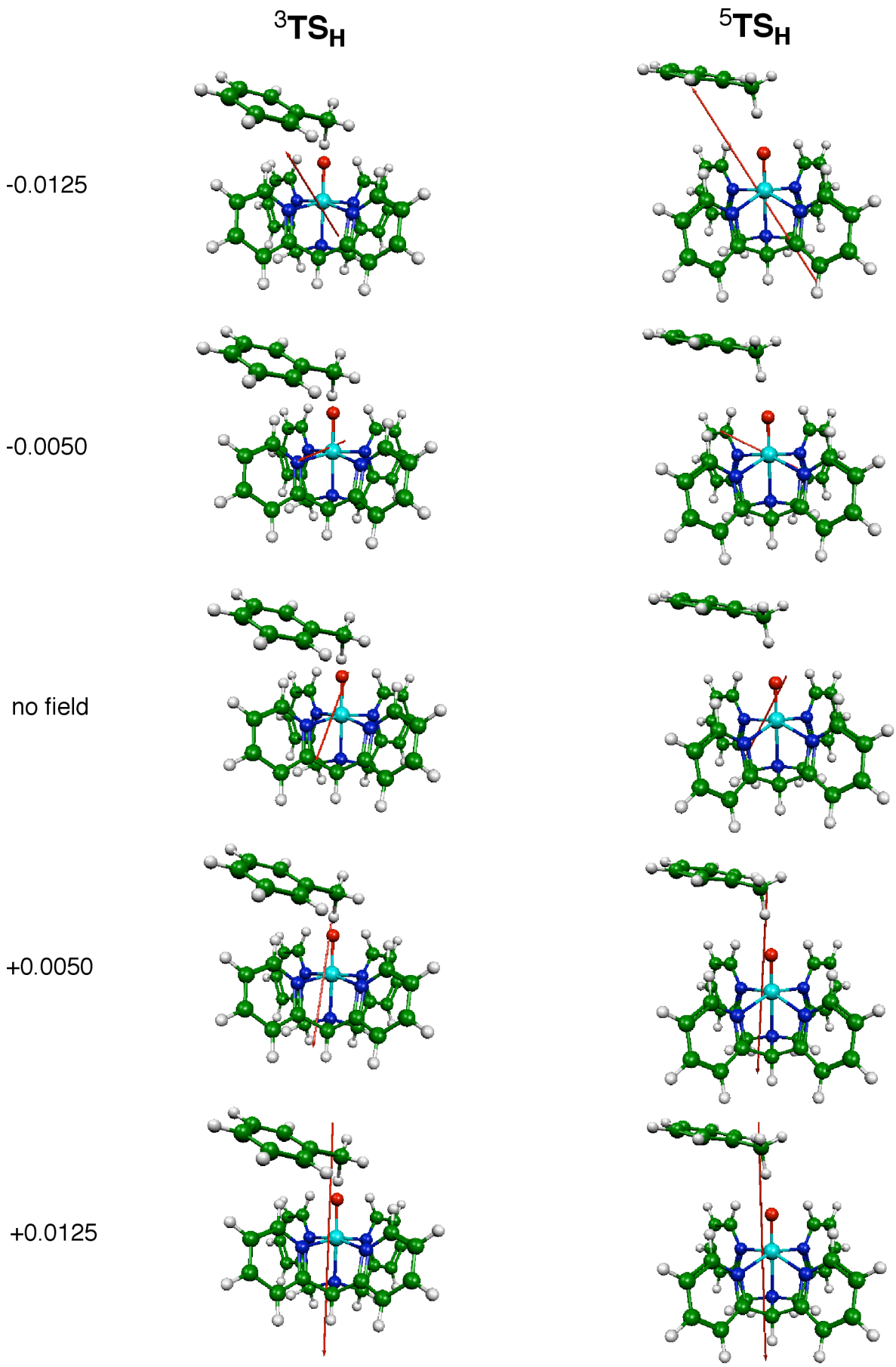


Figure S10. Natural orbitals of $^{3}\mathbf{TS_H}$ for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

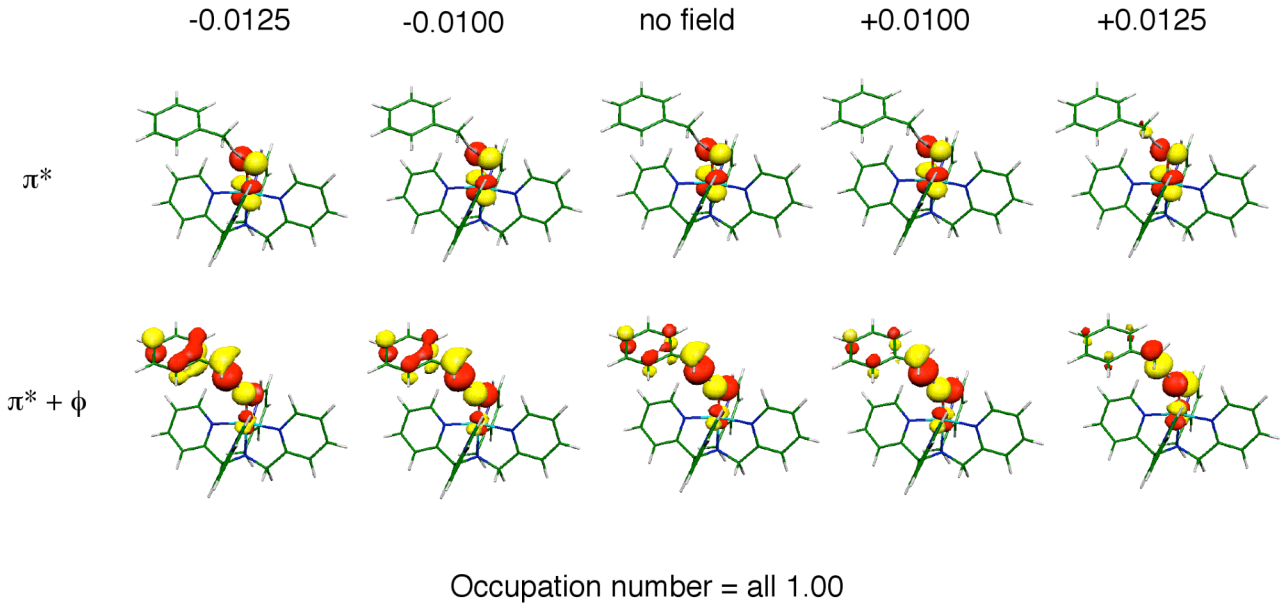


Figure S11. Natural orbitals of ^{5}**TS**$_{\mathbf{H}}$ for the reaction of $\mathbf{K}_{\mathbf{N4Py}}$ **with TE.**

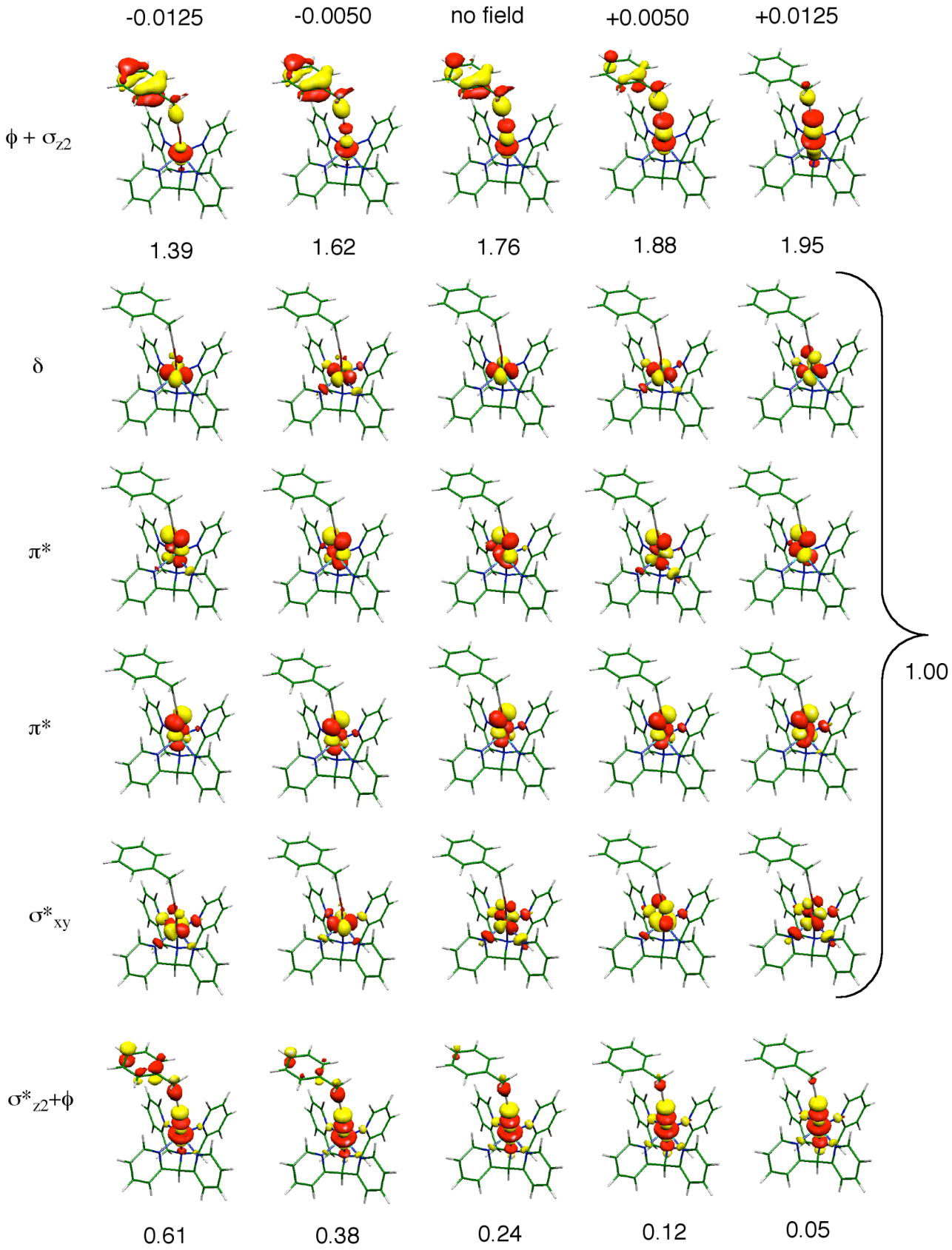


Figure S12. Variation in the ZZ component of polarizability (in au) along the reaction pathway for the reaction of $\mathbf{K_{N4Py}}$ **with TE.**

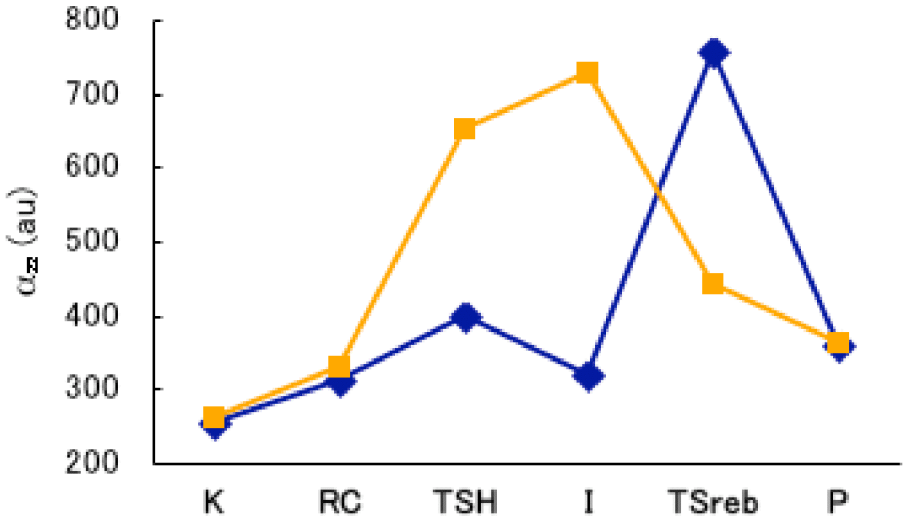
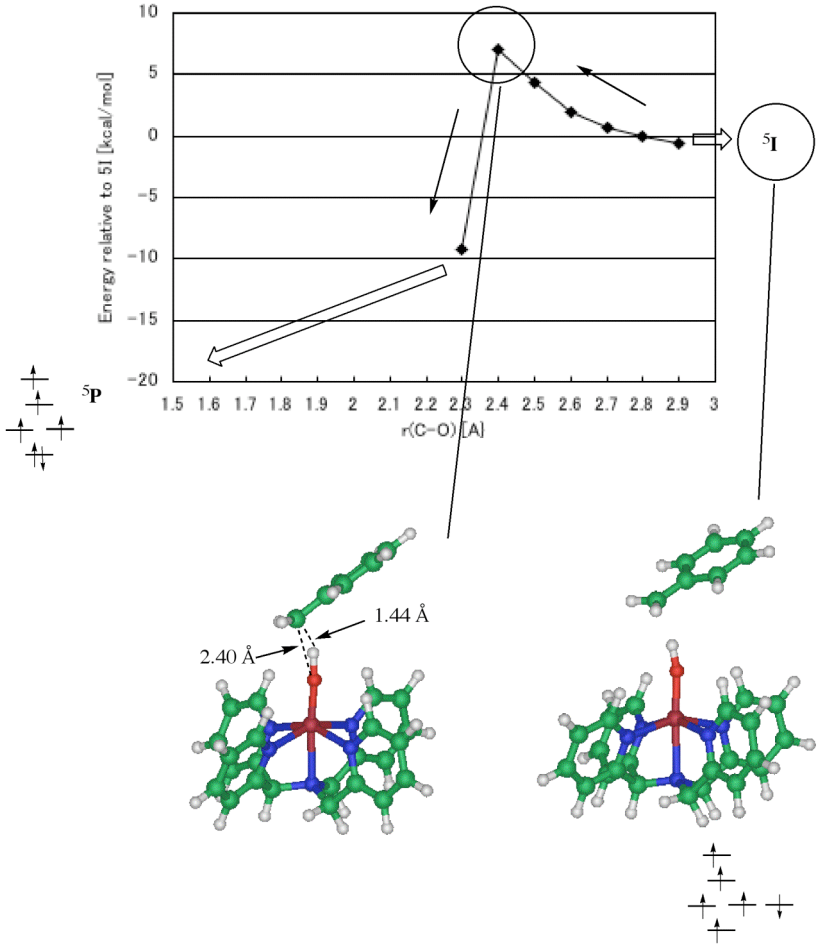


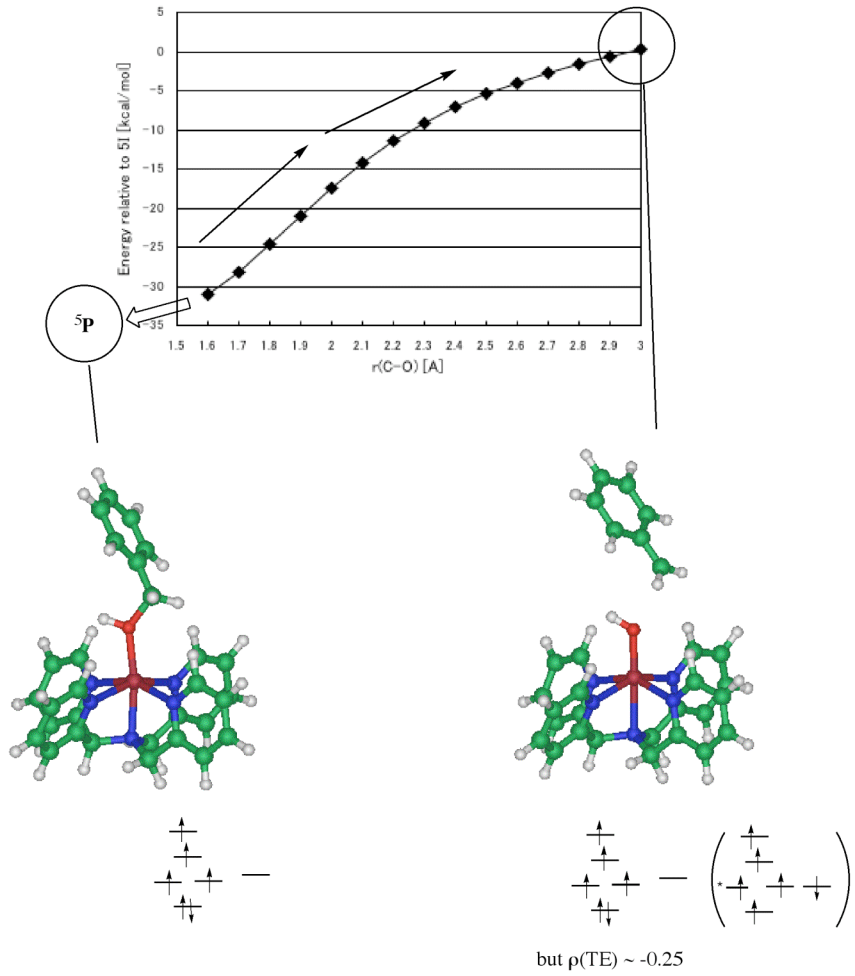
Figure S13. Rebound scans for the reaction between $^5\mathbf{K}_{\mathbf{N4Py}}$ + **TE**

The scan along r(C-O) as a reaction coordinate (in part (a)) leads to a spurious spike (at r=2.4 Å) and a sudden drop in the energy along with drastic geometric and electronic changes. This spike is due to the facts that the rebounding radical bumps into the H of the FeOH moiety rather than into the O atom whereupon the rebound should occur. This is caused by the colinear Fe-O-H-C conformation and the choice of r(C-O) as the variable. Using a backward scan (in paret (b)) from $^5\mathbf{P}$, by increasing r(C-O), the energy of the final species at r=3.0 Å **was very similar to that of $^5\mathbf{I}_\alpha$, to within 0.3 kcal/mol**. In this species the benzyl moiety had a negative spin density value of -0.25, thus indicating that the $\mathbf{I}_{R+}$ and $^5\mathbf{I}_\alpha$ states mix with each other to create a state with an intermediate character, having negative spin density on the benzyl moiety like in the $^5\mathbf{I}_\alpha$ state and a positive charge like in the $\mathbf{I}_{R+}$ state. The similarity in energy and electronic state between $\mathbf{I}_{R+}$ and $^5\mathbf{I}_\alpha$ means that the mixing of the two states ($\mathbf{I}_{R+}$ and $^5\mathbf{I}_\alpha$) is very small, and hence the change from $^5\mathbf{I}_\alpha$ to $\mathbf{I}_{R+}$ is not at all difficult, and subsequently, the system smoothly proceeds toward $^5\mathbf{P}$ without a barrier

(a) Forward scan from $^5\mathbf{I}$ using r(C-O) as a variable



(b) Backward scan from ^{5}**P**



Part 2 ($K_{TMC(SR)}$)

Table S20. Total energies (au) and relative energies (kcal/mol) ($\mathbf{K_{TMC(SR)}}$)

	0	**ΔE**	**Z-0.0075**	**ΔE**
CH	-235.822661		-235.822574	
^{3}**K**	-1406.877654		-1406.889607	
^{5}**K**	-1406.877339		-1406.888129	
^{3}R	-1642.700314	1.1	-1642.712181	4.3
^{5}R	-1642.699999	1.3	-1642.710703	5.2
^{3}RC	-1642.702071	0.0	-1642.718968	0.0
^{5}RC	-1642.701742	0.2	-1642.717754	0.8
$3TS_H$	-1642.659834	26.5	-1642.68541	21.1
^5TS_H	-1642.670409	19.9	-1642.700112	11.8
^{3}I	-1642.675753	16.5	-1642.699677	12.1
$^5I_\alpha$	-1642.681087	13.2	-1642.711006	5.0
$^5I_\beta$	-1642.674443	17.3		
$^3TS_{reb}$	-1642.657182	28.2	-1642.696028	14.4
$^5TS_{reb,\alpha}$	-1642.668341	21.2		
$^5TS_{reb,\beta}$	-1642.671817	19.0		
^{3}P	-1642.726160	-15.1	-1642.771446	-32.9
^{5}P	-1642.751689	-31.1	-1642.797173	-49.1

Table S21. Spin densities ($\mathbf{K}_{TMC(SR)}$)

(a) Without EF

	ρ(Fe)	ρ(O)	ρ(TMCSR)	ρ(CH)
$^3\mathbf{K}_{TMC(SR)}$	1.27	0.81	−0.08	−
$^5\mathbf{K}_{TMC(SR)}$	3.11	0.72	0.16	−
$^3\mathbf{RC}$	1.28	0.81	−0.09	0.00
$^5\mathbf{RC}$	3.12	0.72	0.16	0.00
$^3\mathbf{TS}_H$	1.02	0.51	−0.05	0.52
$^5\mathbf{TS}_H$	3.83	0.06	0.62	−0.51
$^3\mathbf{I}$	1.01	0.10	−0.07	0.97
$^5\mathbf{I}_\alpha$	3.95	0.26	0.73	−0.95
$^5\mathbf{I}_\beta$	3.01	0.10	−0.08	0.97
$^3\mathbf{TS}_{reb}$	1.57	−0.10	−0.08	0.61
$^5\mathbf{TS}_{reb,\alpha}$	3.87	0.23	0.55	−0.65
$^5\mathbf{TS}_{reb,\beta}$	3.34	−0.10	0.05	0.72
$^3\mathbf{P}$	1.92	0.00	0.08	0.00
$^5\mathbf{P}$	3.67	0.00	0.33	0.00

(b) In EF

	ρ(Fe)	ρ(O)	ρ(TMCSR)	ρ(CH)
$^3\mathbf{K}_{TMC(SR)}$	1.25	0.85	−0.10	−
$^5\mathbf{K}_{TMC(SR)}$	3.08	0.72	0.20	−
$^3\mathbf{RC}$	1.25	0.85	−0.10	0.00
$^5\mathbf{RC}$	3.08	0.72	0.20	0.00
$^3\mathbf{TS}_H$	1.03	0.53	−0.08	0.51
$^5\mathbf{TS}_H$	3.82	0.14	0.51	−0.47
$^3\mathbf{I}$	1.00	0.13	−0.08	0.94
$^5\mathbf{I}_\alpha$	3.96	0.33	0.62	−0.92
$^5\mathbf{I}_\beta$	−	−	−	−
$^3\mathbf{TS}_{reb}$	1.63	−0.05	−0.11	0.53
$^5\mathbf{TS}_{reb,\alpha}$	−	−	−	−
$^5\mathbf{TS}_{reb,\beta}$	−	−	−	−
$^3\mathbf{P}$	1.97	0.00	0.03	0.00
$^5\mathbf{P}$	3.70	0.00	0.30	0.00

Table S22. Charges ($\mathbf{K_{TMC(SR)}}$)

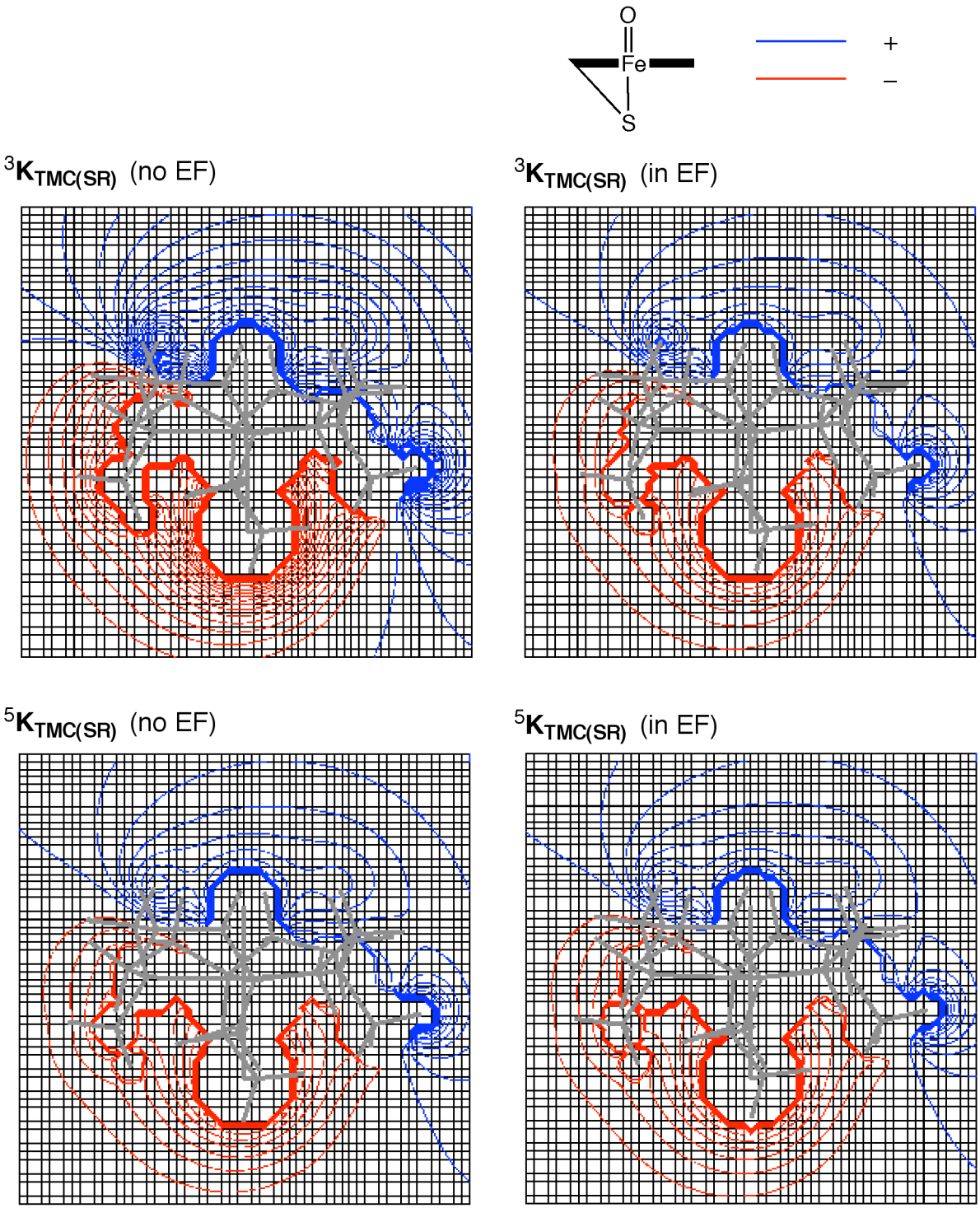
(a) Without EF

	Q(Fe)	Q(O)	Q(TMCSR)	Q(CH)
$^3\mathbf{K_{TMC(SR)}}$	0.29	−0.47	1.18	−
$^5\mathbf{K_{TMC(SR)}}$	0.37	−0.48	1.12	−
$^3\mathbf{RC}$	0.31	−0.49	1.17	0.01
$^5\mathbf{RC}$	0.38	−0.50	1.11	0.01
$^3\mathbf{TS_H}$	0.36	−0.65	1.00	0.29
$^5\mathbf{TS_H}$	0.53	−0.70	0.85	0.32
$^3\mathbf{I}$	0.32	−0.73	1.02	0.39
$^5\mathbf{I_\alpha}$	0.54	−0.81	0.82	0.44
$^5\mathbf{I_\beta}$	0.39	−0.77	0.95	0.43
$^3\mathbf{TS_{reb}}$	0.32	−0.66	0.76	0.58
$^5\mathbf{TS_{reb,\alpha}}$	0.45	−0.70	0.66	0.59
$^5\mathbf{TS_{reb,\beta}}$	0.38	−0.69	0.75	0.56
$^3\mathbf{P}$	0.32	−0.63	0.60	0.71
$^5\mathbf{P}$	0.33	−0.63	0.60	0.70

(b) In EF

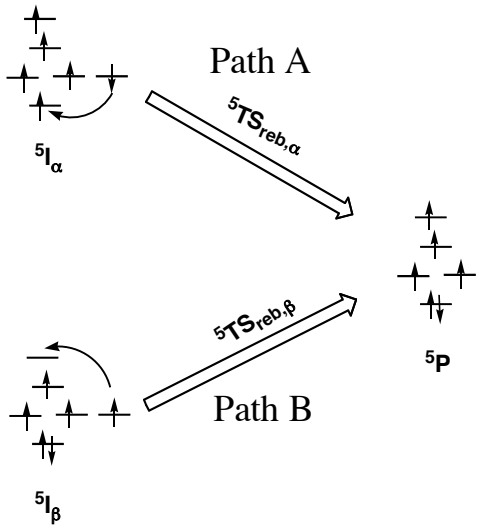
	Q(Fe)	Q(O)	Q(TMCSR)	Q(CH)
$^3\mathbf{K_{TMC(SR)}}$	0.33	−0.43	1.10	−
$^5\mathbf{K_{TMC(SR)}}$	0.40	−0.44	1.03	−
$^3\mathbf{RC}$	0.33	−0.44	1.08	0.02
$^5\mathbf{RC}$	0.39	−0.44	1.02	0.03
$^3\mathbf{TS_H}$	0.41	−0.67	0.82	0.44
$^5\mathbf{TS_H}$	0.57	−0.66	0.69	0.40
$^3\mathbf{I}$	0.36	−0.72	0.90	0.46
$^5\mathbf{I_\alpha}$	0.59	−0.79	0.69	0.51
$^5\mathbf{I_\beta}$	−	−	−	−
$^3\mathbf{TS_{reb}}$	0.37	−0.71	0.39	0.95
$^5\mathbf{TS_{reb,\alpha}}$	−	−	−	−
$^5\mathbf{TS_{reb,\beta}}$	−	−	−	−
$^3\mathbf{P}$	0.36	−0.65	0.54	0.76
$^5\mathbf{P}$	0.38	−0.66	0.53	0.75

Figure S14. Molecular electrostatic potential of $K_{TMC(SR)}$



Summary of Attempts to Find Rebound TSs on the quintet surface for the Reaction of $^5K_{TMC(SR)}$ + CH

The location of the rebound transition states $^5\mathbf{TS}_{\mathbf{reb}}$ connecting quintet interemediates and $^5\mathbf{P}$ posed sometimes difficulties. These two possible paths (A and B) need the following electron reorganizations within the framework of the unrestricted DFT formarism.

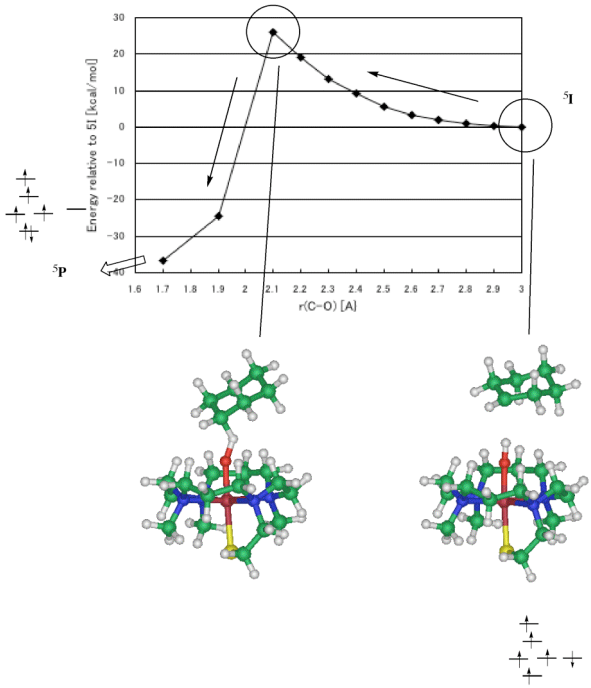


Below we explain several of the trials to locate the corresponding TSs:

Figure S15A. Rebound scans for the reaction to obtain ^{5}**TS**$_{\mathbf{reb,\alpha}}$

As in the corresponding scan of the $\mathbf{K}_{\mathbf{N4Py}}$ reaction, here too the energy increase is due to the high repulsion when the carbon of the cyclohexyl radical bumps into the hydrogen atom of the FeOH moiety, due to the colinear Fe-O-H-C conformation and the use of r(C-O) as the reaction coordinate variable. In this scan, the H atom in fact moves back and form cyclohexane due to this high repulsion. Thus, the point at r=2.1 Å was a poor guess of the rebound transition state. We then changed the search strategy. First, a ^{5}**TS**$_{\mathbf{reb,\alpha}}$**–** like species was generated using a fixed distance of r(C-O)=2.5 Å, while freely optimizing all other parameters. The resultant geometry was found to be a good guess for the TS, and starting from this geometry we were able to locate ^{5}**TS**$_{\mathrm{reb,\alpha}}$ successfully. ^{5}**TS**$_{\mathrm{reb,\beta}}$ was located more easily since the initial geometry of ^{5}**I**$_\beta$ does not cause the articial C---H bumping (see below Figure S15C).

(a) Path a (trial 1)



(b) Path b (trial 2)

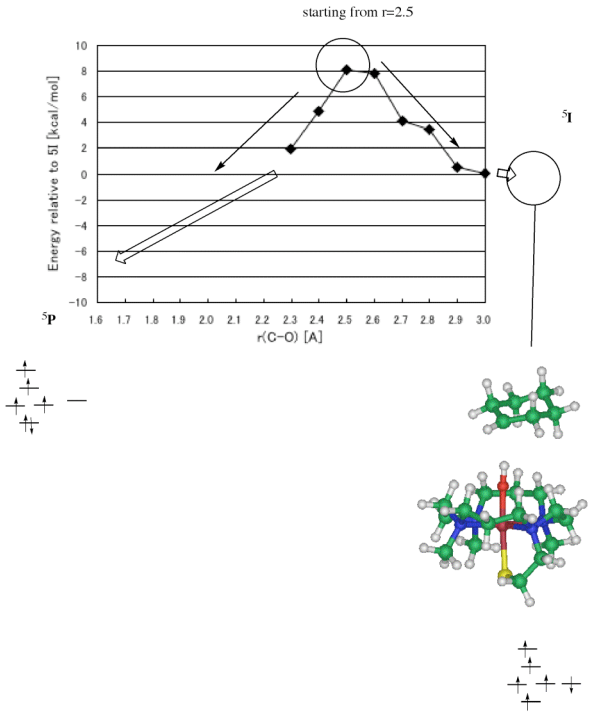
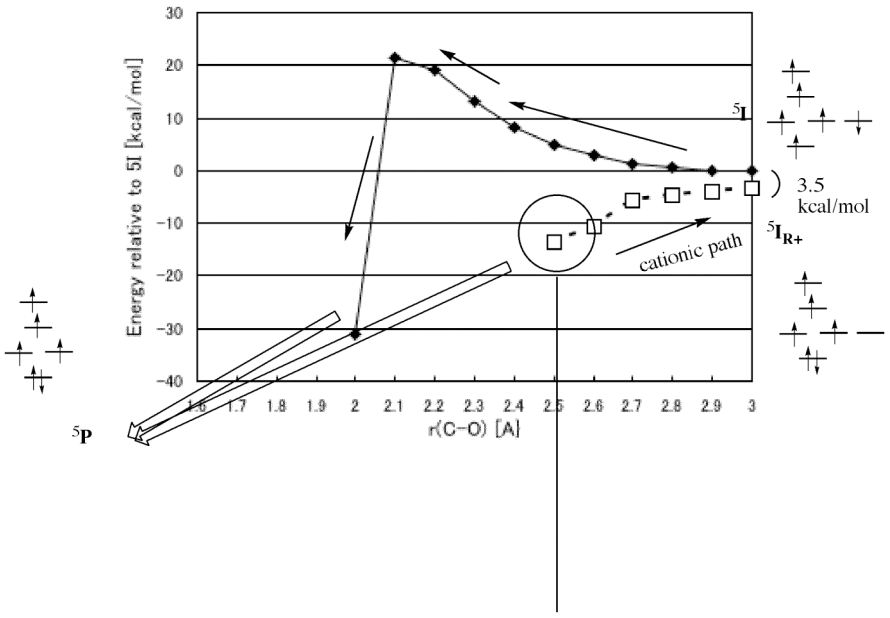


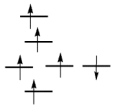
Figure S15B. Energies at the geometries obtained by the energy scan from $^5\mathbf{I}_\alpha$ in the EF presence.

An energy spike was obtained also in the presense of EF, when the same calculation as in Figure 15A(a) was done, due to the collinear Fe-O-H-C conformation at $^5\mathbf{I}_\alpha$, which cased the C---H bumping. So as was done in the $^5\mathbf{TS}_{\mathbf{reb},\alpha}$ optimization without EF, here too, first we attempted to get a good initial structure around r(C-O)=2.5Å, but now the electronic state changed to the cationic one (as in $^5\mathbf{I}_{\mathbf{R+}}$), because the EF strongly stabilizes this state more than the $^5\mathbf{I}_\alpha$ state. At longer r(C-O values) the $^5\mathbf{I}_{\mathbf{R+}}$ state approached the $^5\mathbf{I}_\alpha$ state to within 3.5 kcal/mol. In the energy curve of $^5\mathbf{I}_{\mathbf{R+}}$ no barrier was found and it went smoothly to $^5\mathbf{P}$. Thus, while we could not obtain a $^5\mathbf{TS}_{\mathbf{reb},\alpha}$ in the presense of EF, it seems that the crossover to the $^5\mathbf{I}_{\mathbf{R+}}$ state and then to $^5\mathbf{P}$ should be rather facile.

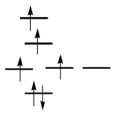
$^5\mathbf{I}_\alpha$ Rebound (in the presence of EF):



starting from $^5\mathbf{TS}_{\mathbf{reb},\alpha}$ optimized without EF



but after single-point calculation with EF, it dropped to

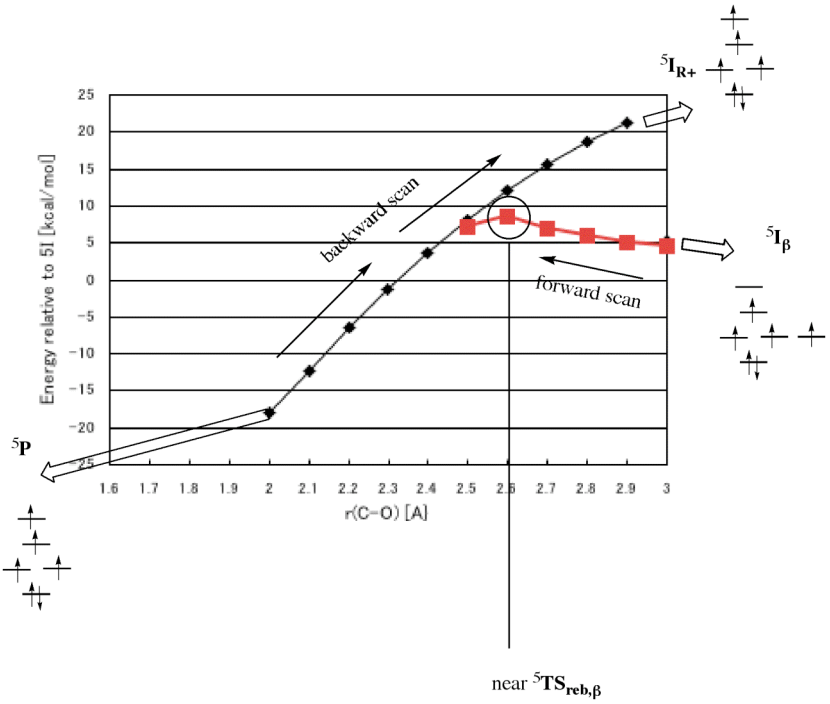


Subsequent backward scan was on the cationic path

Figure S15C. Energies at the geometries obtained by the energy scan from $^5\mathbf{I}_\beta$.

A backward energy scan from $^5\mathbf{P}$ led to spieces $^5\mathbf{I}_{R+}$, which is not an energy minimum. When we ran a forward scan starting from $^5\mathbf{I}_\beta$, an energy maximum (ca 8.5 kcal/mol) was found at r(C-O) = 2.6 Å, and this was used for $^5\mathbf{TS}_{reb,\beta}$ optimization.

$^5\mathbf{I}_\beta$ Rebound (in the absense of EF):



near $^5\mathbf{TS}_{reb,\beta}$

However, when the EF was applied to $^5\mathbf{I}_\beta$, it collapsed to $^5\mathbf{I}_{R+}$ as in Figure S15B; therefore no rebound barrier could be characterized for $^5\mathbf{I}_\beta$ rebound in the EF. Our conclusion from the two trials in Figures 15B and 15C is that the rebound from either $^5\mathbf{I}_\alpha$ or $^5\mathbf{I}_\beta$ is facilitated by the EF.

Cartesian coordinate

```
=== 3KTMC(SR) ===
Fe     0.036376    0.027434   -0.014918
N      0.039693    0.024696    2.145964
N      2.157057   -0.002440    0.161849
N      0.162348   -0.169284   -2.178325
N     -2.054320   -0.016779   -0.275035
C      1.322460   -0.726528    2.410498
H      1.537917   -0.724527    3.488319
H      1.168638   -1.754791    2.084472
C      2.454652   -0.075279    1.649306
H      3.391624   -0.625263    1.804773
H      2.617622    0.944811    2.001138
C      2.657108   -1.280012   -0.494291
H      3.742588   -1.329726   -0.321393
H      2.179029   -2.107646    0.030287
C      2.397642   -1.407992   -1.999882
H      2.839883   -2.367204   -2.302256
H      2.962966   -0.651447   -2.554862
C      0.933937   -1.444442   -2.458025
H      0.408683   -2.255874   -1.954510
H      0.906710   -1.618572   -3.544174
C     -1.278045   -0.315012   -2.627575
H     -1.608067    0.672373   -2.955010
H     -1.320685   -0.974004   -3.505201
C     -2.183993   -0.845060   -1.538984
H     -1.911914   -1.866440   -1.274981
H     -3.228497   -0.835453   -1.881657
C     -2.776764   -0.787415    0.812172
H     -2.480260   -1.832479    0.701955
H     -3.853202   -0.715513    0.604107
C     -2.485041   -0.352017    2.245399
H     -2.653876    0.719645    2.389864
H     -3.219791   -0.854842    2.888188
C     -1.099299   -0.786281    2.718886
H     -0.931093   -1.824080    2.423983
H     -1.033606   -0.724170    3.814573
C      0.089168    1.349310    2.859893
H      0.320193    1.177384    3.919764
H      0.827780    2.005794    2.411165
H     -0.873877    1.847459    2.787651
C      2.923853    1.182979   -0.362464
H      3.985259    1.074522   -0.103274
H      2.528237    2.095179    0.082398
H      2.835944    1.258604   -1.439395
C      0.729708    0.945369   -3.024794
H      1.808332    1.002692   -2.929213
H      0.296130    1.890453   -2.703953
H      0.494565    0.748137   -4.078869
C     -2.697114    1.355121   -0.481392
H     -3.743609    1.294505   -0.152102
H     -2.705702    1.558309   -1.552882
S     -0.118735    2.385759   -0.172363
C     -1.964897    2.492046    0.212976
O     -0.033615   -1.644727    0.114559
H     -2.326573    3.450293   -0.170001
H     -2.120219    2.489072    1.293352

=== 3KTMC(SR) in EF ===
Fe      0.000000    0.000000    0.000000
O       0.000000    0.000000    1.666011
N       2.155457    0.000000    0.218230
N       0.170118   -2.117848   -0.001059
N      -2.172901   -0.121780    0.053362
N      -0.262960    2.094501    0.136635
C       2.355890   -1.317869    0.933934
H       3.429446   -1.538257    1.010549
H       1.955722   -1.208066    1.940983
C       1.648765   -2.419258    0.178182
H       1.761524   -3.377208    0.701048
H       2.079095   -2.538219   -0.818541
C      -0.581303   -2.656914    1.212870
H      -0.419869   -3.744455    1.233571
H      -0.109943   -2.221160    2.093539
C      -2.089834   -2.388262    1.249501
H      -2.451528   -2.846394    2.179835
H      -2.600394   -2.938048    0.450058
C      -2.547547   -0.926323    1.288153
H      -2.115159   -0.421394    2.151289
H      -3.643117   -0.900934    1.379017
C      -2.631444    1.314713    0.206103
H      -2.863423    1.679292   -0.796966
H      -3.563943    1.339912    0.785032
C      -1.592824    2.192946    0.864116
H      -1.417704    1.880637    1.892810
H      -1.931589    3.238169    0.874029
C       0.753208    2.776785    1.038632
H       0.548239    2.435577    2.054743
H       0.548700    3.855176    1.000013
C       2.221754    2.503540    0.728552
H       2.474194    2.731269   -0.313002
H       2.807225    3.206260    1.335794
C       2.654338    1.097348    1.133900
H       2.271990    0.881505    2.133089
H       3.750584    1.028226    1.167479
C       2.980096    0.008884   -1.037366
H       4.020969   -0.237446   -0.787702
H       2.583974   -0.695029   -1.763314
H       2.953115    0.997086   -1.489616
C      -0.261615   -2.843968   -1.242789
H       0.012804   -3.904234   -1.160847
H       0.230260   -2.398321   -2.107101
H      -1.334761   -2.775230   -1.376493
C      -2.931111   -0.659906   -1.132169
H      -2.833334   -1.738144   -1.200008
H      -2.535150   -0.206001   -2.039300
H      -3.997421   -0.426753   -1.011137
C      -0.351003    2.801549   -1.209526
H      -0.026144    3.842226   -1.070754
H      -1.401283    2.825546   -1.504587
S       0.025475    0.280927   -2.383711
C       0.439108    2.126438   -2.320885
H       0.158542    2.566739   -3.282848
H       1.515597    2.259242   -2.196073

=== 5KTMC(SR) ===
Fe     0.020406    0.039369    0.003587
N      0.074393    0.025460    2.255237
N      2.231490   -0.007199    0.179822
N      0.164471   -0.178640   -2.280891
N     -2.122645   -0.008409   -0.314246
C      1.355124   -0.739566    2.453336
H      1.619380   -0.759627    3.521303
H      1.177166   -1.762214    2.120247
C      2.499319   -0.106263    1.668352
H      3.419638   -0.683485    1.832328
H      2.688230    0.906305    2.030554
C      2.686218   -1.281301   -0.508590
H      3.771577   -1.372547   -0.344596
H      2.187130   -2.107274    0.000381
C      2.420051   -1.376330   -2.021155
H      2.886795   -2.318087   -2.341864
H      2.971425   -0.596243   -2.557363
C      0.959937   -1.443392   -2.504419
H      0.439594   -2.248623   -1.984070
H      0.958752   -1.662713   -3.584304
C     -1.283171   -0.352268   -2.677910
H     -1.629032    0.620074   -3.035238
H     -1.350027   -1.043597   -3.530666
C     -2.200627   -0.857326   -1.566962
H     -1.922941   -1.870053   -1.275752
H     -3.235568   -0.871545   -1.939186
C     -2.802346   -0.764627    0.811270
H     -2.516420   -1.812617    0.698488
H     -3.887256   -0.690736    0.648296
C     -2.466286   -0.323343    2.243208
H     -2.605839    0.753772    2.377465
H     -3.218530   -0.794676    2.890268
C     -1.094774   -0.786247    2.757085
H     -0.926857   -1.818763    2.443173
H     -1.082390   -0.756749    3.857142
C      0.132197    1.335089    2.978181
H      0.335712    1.162606    4.044791
H      0.897995    1.977833    2.551013
H     -0.817720    1.857329    2.881673
```

C	2.986080	1.181238	-0.339796
H	4.059253	1.068070	-0.132576
H	2.614829	2.085504	0.142784
H	2.846305	1.285601	-1.410960
C	0.710840	0.939657	-3.120940
H	1.783954	1.038945	-2.985445
H	0.238729	1.874401	-2.821303
H	0.519162	0.738000	-4.184387
C	-2.747301	1.359126	-0.537450
H	-3.803541	1.316268	-0.234952
H	-2.723751	1.563751	-1.608993
S	-0.155189	2.383042	-0.160607
C	-2.018010	2.484717	0.183463
O	-0.047406	-1.639579	0.127674
H	-2.358423	3.452792	-0.194736
H	-2.186960	2.471016	1.261370

=== 5KTMC(SR) in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.670889
N	2.242450	0.000000	0.232555
N	0.230892	-2.209133	0.017407
N	-2.293093	-0.206223	0.092201
N	-0.388542	2.133704	0.150412
C	2.417570	-1.310485	0.955957
H	3.487259	-1.547618	1.049684
H	2.008712	-1.188852	1.958701
C	1.715330	-2.444483	0.217870
H	1.860339	-3.381921	0.771395
H	2.156196	-2.581583	-0.772481
C	-0.532421	-2.724237	1.230097
H	-0.344656	-3.806834	1.296083
H	-0.091763	-2.247925	2.106583
C	-2.052624	-2.498421	1.233415
H	-2.417973	-3.000205	2.139708
H	-2.525234	-3.040684	0.405935
C	-2.578857	-1.055984	1.314187
H	-2.136029	-0.551016	2.173357
H	-3.669910	-1.088625	1.457907
C	-2.746866	1.220651	0.300757
H	-3.057871	1.599431	-0.676143
H	-3.638091	1.231239	0.944109
C	-1.698614	2.142412	0.915850
H	-1.471392	1.832616	1.935119
H	-2.097544	3.166189	0.950970
C	0.660504	2.811388	1.019310
H	0.466504	2.496427	2.046238
H	0.478251	3.893897	0.964935
C	2.133584	2.521517	0.699473
H	2.371029	2.721593	-0.351007
H	2.711143	3.258876	1.273122
C	2.636053	1.141196	1.143837
H	2.234815	0.917628	2.134022
H	3.733281	1.151471	1.219069
C	3.073970	0.026880	-1.008216
H	4.131600	-0.132360	-0.752864
H	2.738966	-0.735170	-1.708708
H	2.969602	0.991100	-1.502717
C	-0.185709	-2.932678	-1.224516
H	0.048720	-4.003164	-1.137206
H	0.340300	-2.508967	-2.081074
H	-1.253404	-2.821815	-1.387125
C	-3.037676	-0.732470	-1.096558
H	-2.869539	-1.799851	-1.213562
H	-2.679963	-0.223796	-1.991832
H	-4.117621	-0.571968	-0.966037
C	-0.538559	2.811165	-1.194636
H	-0.298933	3.878686	-1.079755
H	-1.587588	2.740040	-1.487684
S	0.006397	0.301113	-2.359772
C	0.306996	2.177301	-2.292356
H	0.017568	2.588414	-3.264405
H	1.373127	2.365024	-2.152017

=== 3RC ===

Fe	0.002504	0.017971	-0.014472
O	-0.000693	0.055132	1.664936
N	2.157831	0.012647	0.160768
N	0.180612	-2.104169	-0.011372
N	-2.167478	-0.109889	0.005369
N	-0.261362	2.107098	0.048116
C	2.361757	-1.283121	0.908427
H	3.436432	-1.499015	0.990747
H	1.952620	-1.146775	1.909003
C	1.657083	-2.403925	0.178698
H	1.767312	-3.349869	0.724339
H	2.091557	-2.550917	-0.811524
C	-0.579418	-2.630461	1.196170
H	-0.409064	-3.716745	1.238046
H	-0.128036	-2.169321	2.074921
C	-2.090554	-2.373706	1.202518
H	-2.470619	-2.835606	2.124080
H	-2.580311	-2.922218	0.390481
C	-2.551308	-0.910880	1.233872
H	-2.118178	-0.407832	2.098054
H	-3.648354	-0.886001	1.318628
C	-2.630661	1.326301	0.146137
H	-2.884217	1.675565	-0.856309
H	-3.555467	1.353954	0.737913
C	-1.587692	2.222609	0.775460
H	-1.405702	1.932272	1.809536
H	-1.929465	3.267358	0.757135
C	0.760751	2.813878	0.915999
H	0.568247	2.498195	1.943287
H	0.557895	3.891549	0.847625
C	2.224214	2.529725	0.589659
H	2.452679	2.717197	-0.464157
H	2.824524	3.255326	1.154498
C	2.662841	1.136229	1.035355
H	2.285808	0.949357	2.042868
H	3.760109	1.070980	1.060142
C	2.974339	-0.012471	-1.103661
H	4.018035	-0.245321	-0.852667
H	2.581055	-0.739844	-1.806610
H	2.938772	0.959051	-1.589342
C	-0.241268	-2.846551	-1.251546
H	0.010306	-3.909853	-1.143671
H	0.276966	-2.431968	-2.115349
H	-1.308414	-2.757873	-1.414566
C	-2.917050	-0.651966	-1.187935
H	-2.809756	-1.728294	-1.264181
H	-2.522985	-0.193686	-2.092830
H	-3.985148	-0.426243	-1.071358
C	-0.354710	2.775142	-1.323998
H	-0.034060	3.820522	-1.216827
H	-1.405368	2.786173	-1.616158
S	0.037188	0.218536	-2.374122
C	0.434511	2.064285	-2.411515
H	0.135835	2.445480	-3.392023
H	1.511158	2.215644	-2.312949
H	0.057014	0.239366	4.381796
C	0.009727	0.344708	5.477593
C	-1.213295	1.207835	5.852970
C	-2.534737	0.504079	5.483320
C	-2.621648	-0.900133	6.117709
C	-1.397440	-1.764710	5.750339
C	-0.076145	-1.057010	6.117047
H	0.934966	0.846283	5.792057
H	-1.202428	1.401698	6.935873
H	-1.153660	2.188926	5.361352
H	-3.392162	1.115497	5.794221
H	-2.596637	0.409100	4.385711
H	-2.671769	-0.796471	7.211761
H	-3.549421	-1.400890	5.810347
H	-1.458214	-2.740051	6.250332
H	-1.408985	-1.965404	4.665492
H	0.782234	-1.669436	5.809164
H	-0.013160	-0.959895	7.211148

=== 3RC in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.664691
N	2.156527	0.000000	0.221967
N	0.173596	-2.119888	0.004278
N	-2.170462	-0.123035	0.055387
N	-0.260750	2.093104	0.146972
C	2.356495	-1.316992	0.938751
H	3.430149	-1.535538	1.020096
H	1.951771	-1.206579	1.943926
C	1.651798	-2.420387	0.184241

H	1.764493	-3.376308	0.711034
H	2.083062	-2.543023	-0.811692
C	-0.578036	-2.654749	1.219935
H	-0.410958	-3.741351	1.248600
H	-0.113251	-2.209945	2.099538
C	-2.087288	-2.391104	1.251175
H	-2.449669	-2.847739	2.181922
H	-2.594660	-2.942733	0.450823
C	-2.545688	-0.929683	1.289371
H	-2.115642	-0.426361	2.154920
H	-3.641366	-0.903635	1.379330
C	-2.629762	1.312817	0.215200
H	-2.867618	1.681334	-0.785151
H	-3.558873	1.333880	0.799676
C	-1.590596	2.188454	0.875680
H	-1.417375	1.872456	1.903787
H	-1.929201	3.233795	0.889162
C	0.754832	2.775121	1.049373
H	0.550576	2.433505	2.065521
H	0.549745	3.853509	1.011104
C	2.223087	2.502664	0.737769
H	2.475485	2.732160	-0.303512
H	2.809046	3.203566	1.346663
C	2.652854	1.095484	1.141674
H	2.265064	0.879135	2.138727
H	3.748921	1.024537	1.179761
C	2.983421	0.010888	-1.031396
H	4.026562	-0.222280	-0.777991
H	2.596949	-0.702459	-1.753490
H	2.945479	0.995579	-1.490446
C	-0.259035	-2.846910	-1.236182
H	0.009745	-3.908555	-1.151606
H	0.236991	-2.405373	-2.100398
H	-1.331511	-2.772416	-1.372592
C	-2.927549	-0.657393	-1.132012
H	-2.832774	-1.736107	-1.199792
H	-2.527862	-0.204164	-2.038003
H	-3.993472	-0.421105	-1.013360
C	-0.351369	2.802602	-1.197462
H	-0.030919	3.844370	-1.056029
H	-1.401788	2.822437	-1.492408
S	0.030948	0.286987	-2.384237
C	0.441292	2.133633	-2.310891
H	0.161584	2.578321	-3.271126
H	1.517484	2.267355	-2.183726
H	0.298209	0.613001	4.404280
C	0.238928	0.875154	5.476964
C	-0.939577	1.847055	5.695978
C	-2.294985	1.173418	5.397079
C	-2.471226	-0.125679	6.210499
C	-1.293190	-1.096742	5.992006
C	0.059143	-0.420613	6.296008
H	1.184869	1.362972	5.746517
H	-0.933969	2.187051	6.740418
H	-0.815285	2.749766	5.078804
H	-3.118334	1.867109	5.609485
H	-2.350383	0.933033	4.316574
H	-2.530975	0.127812	7.277662
H	-3.422600	-0.611230	5.956416
H	-1.418512	-1.987880	6.618281
H	-1.296800	-1.443280	4.940806
H	0.887046	-1.114872	6.099486
H	0.107064	-0.179562	7.366506

=== 5RC ===

Fe	0.018898	-0.008275	-0.006954
O	0.053095	-0.036763	1.678471
N	2.269284	0.030983	0.123859
N	0.298259	-2.209537	-0.081179
N	-2.261177	-0.255139	0.079088
N	-0.398092	2.115309	0.145533
C	2.484626	-1.279932	0.830183
H	3.561265	-1.498955	0.896060
H	2.089185	-1.173649	1.840495
C	1.789151	-2.420637	0.094126
H	1.959729	-3.361963	0.634425
H	2.218101	-2.541958	-0.902706
C	-0.441901	-2.773751	1.118651
H	-0.234892	-3.855223	1.151755
H	-0.004122	-2.309464	2.003838
C	-1.967624	-2.576656	1.138706
H	-2.321115	-3.119548	2.026562
H	-2.433529	-3.093981	0.292859
C	-2.516663	-1.145177	1.273826
H	-2.063768	-0.660723	2.140033
H	-3.606028	-1.201700	1.430945
C	-2.735118	1.158131	0.329238
H	-3.074155	1.551796	-0.631534
H	-3.614471	1.139109	0.989479
C	-1.688961	2.089057	0.938025
H	-1.430202	1.761738	1.944672
H	-2.107338	3.104853	0.996296
C	0.660568	2.796644	0.991508
H	0.511680	2.447506	2.015610
H	0.453497	3.876460	0.968917
C	2.125780	2.545909	0.604995
H	2.305590	2.749867	-0.455081
H	2.715123	3.297796	1.147324
C	2.677727	1.173931	1.020488
H	2.323183	0.936486	2.025854
H	3.777573	1.209686	1.045911
C	3.058066	0.074695	-1.147712
H	4.123345	-0.090526	-0.930413
H	2.700321	-0.674285	-1.849838
H	2.942742	1.045441	-1.626153
C	-0.115625	-2.908588	-1.342682
H	0.132672	-3.977365	-1.281859
H	0.402037	-2.461668	-2.191734
H	-1.184229	-2.807205	-1.504244
C	-3.012306	-0.759694	-1.118882
H	-2.805851	-1.812009	-1.291861
H	-2.697775	-0.200960	-1.999425
H	-4.094046	-0.645515	-0.958961
C	-0.589908	2.807395	-1.193067
H	-0.350917	3.874304	-1.074837
H	-1.647179	2.737607	-1.454022
S	-0.025006	0.305259	-2.343815
C	0.224697	2.185875	-2.319450
H	-0.122647	2.564875	-3.284867
H	1.290285	2.407311	-2.239472
H	0.447237	0.101144	4.346323
C	0.801881	0.258256	5.377896
C	-0.399351	0.618270	6.279556
C	-1.369998	-0.570905	6.435042
C	-0.641504	-1.832007	6.943369
C	0.545537	-2.200051	6.028866
C	1.521773	-1.015676	5.872130
H	1.511027	1.098079	5.347209
H	-0.031123	0.912631	7.273788
H	-0.929102	1.491553	5.874438
H	-2.188873	-0.303243	7.115893
H	-1.832759	-0.791798	5.459183
H	-0.267822	-1.646426	7.960991
H	-1.340897	-2.674675	7.016145
H	1.073533	-3.077822	6.423665
H	0.159141	-2.485290	5.036149
H	2.337555	-1.284359	5.184460
H	1.992392	-0.809152	6.844357

=== 5RC in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.669550
N	2.244401	0.000000	0.242526
N	0.226723	-2.208300	0.032146
N	-2.288311	-0.200382	0.095918
N	-0.374031	2.138073	0.161852
C	2.414297	-1.310567	0.967861
H	3.483569	-1.550064	1.062165
H	2.006041	-1.187753	1.970850
C	1.711135	-2.443608	0.229904
H	1.856673	-3.381775	0.782216
H	2.150055	-2.579372	-0.761680
C	-0.534961	-2.715084	1.249463
H	-0.352198	-3.798504	1.318309
H	-0.089424	-2.239151	2.123805
C	-2.054604	-2.482120	1.257479
H	-2.417065	-2.972833	2.170967
H	-2.533920	-3.031007	0.438161
C	-2.575205	-1.036626	1.326736
H	-2.127330	-0.527486	2.180765

H	-3.666192	-1.063029	1.473165
C	-2.734527	1.230644	0.286262
H	-3.019866	1.604260	-0.700484
H	-3.639508	1.252361	0.910088
C	-1.691049	2.148434	0.914704
H	-1.474843	1.836837	1.935796
H	-2.088020	3.173166	0.947501
C	0.670002	2.803500	1.045314
H	0.477510	2.469659	2.066620
H	0.484515	3.886410	1.008374
C	2.142567	2.520464	0.718791
H	2.376071	2.727044	-0.331589
H	2.721427	3.254366	1.295428
C	2.645095	1.137870	1.155078
H	2.249953	0.913741	2.147530
H	3.742935	1.145145	1.223591
C	3.075503	0.022505	-0.998315
H	4.130668	-0.156114	-0.745197
H	2.727308	-0.727839	-1.705210
H	2.987699	0.993096	-1.483949
C	-0.192813	-2.938115	-1.205037
H	0.048343	-4.007063	-1.115827
H	0.325707	-2.514070	-2.066156
H	-1.262234	-2.834793	-1.361572
C	-3.035705	-0.735555	-1.086962
H	-2.875218	-1.805387	-1.190787
H	-2.674261	-0.239140	-1.987797
H	-4.114672	-0.565949	-0.958907
C	-0.505190	2.826693	-1.179572
H	-0.239491	3.887204	-1.057733
H	-1.555471	2.783987	-1.474569
S	0.003341	0.310234	-2.358929
C	0.327202	2.182465	-2.282183
H	0.039871	2.601384	-3.251606
H	1.396298	2.355596	-2.145034
H	0.581354	1.086411	4.263658
C	1.040675	1.126590	5.269723
C	-0.078906	1.136199	6.331970
C	-0.879227	-0.181804	6.319897
C	0.044592	-1.405241	6.485758
C	1.168309	-1.416075	5.428122
C	1.967152	-0.095966	5.440387
H	1.623968	2.055714	5.328069
H	0.371415	1.274370	7.324390
H	-0.748019	1.992378	6.175584
H	-1.633731	-0.171154	7.114648
H	-1.426579	-0.265656	5.363355
H	0.496544	-1.382593	7.486749
H	-0.537360	-2.334136	6.432779
H	1.839437	-2.267849	5.598035
H	0.717027	-1.553356	4.426241
H	2.741307	-0.106843	4.655971
H	2.501145	-0.010395	6.396490

=== 3TSH ===

Fe	-0.026401	-0.119932	-0.006130
O	-0.090241	-0.323425	1.830485
N	2.103839	0.173141	0.213108
N	0.500261	-2.132888	-0.483015
N	-2.167276	-0.546875	-0.110534
N	-0.639190	1.855483	0.464312
C	2.517804	-1.193415	0.692585
H	3.614476	-1.253126	0.754646
H	2.107793	-1.324558	1.690692
C	1.998503	-2.254645	-0.256676
H	2.232392	-3.256969	0.124717
H	2.486019	-2.162233	-1.228569
C	-0.216909	-3.056992	0.480833
H	0.107203	-4.084752	0.255350
H	0.134230	-2.803702	1.477555
C	-1.749108	-3.013429	0.443850
H	-2.090473	-3.767168	1.166970
H	-2.121292	-3.366675	-0.523651
C	-2.423369	-1.695300	0.842103
H	-2.069088	-1.370336	1.818763
H	-3.511168	-1.857193	0.888096
C	-2.859374	0.708200	0.393934
H	-3.252175	1.230879	-0.480198
H	-3.725048	0.425082	1.007101
C	-1.943621	1.613251	1.193300
H	-1.677137	1.141110	2.136232
H	-2.446436	2.571712	1.389989
C	0.278198	2.553910	1.445492
H	0.149389	2.046615	2.401839
H	-0.077273	3.588412	1.553943
C	1.765370	2.547080	1.095925
H	1.952562	2.949152	0.095966
H	2.256953	3.242961	1.789200
C	2.420598	1.180074	1.293615
H	2.072100	0.755351	2.234588
H	3.514280	1.288142	1.339335
C	2.912910	0.524661	-1.007299
H	3.981225	0.451626	-0.761227
H	2.668575	-0.130696	-1.836893
H	2.690688	1.539984	-1.323980
C	0.247115	-2.593975	-1.895770
H	0.618596	-3.620336	-2.018436
H	0.757924	-1.932209	-2.593563
H	-0.812407	-2.576038	-2.123811
C	-2.811626	-0.859483	-1.438616
H	-2.441722	-1.794125	-1.846340
H	-2.574176	-0.067924	-2.144663
H	-3.897607	-0.947831	-1.299522
C	-0.887952	2.739727	-0.753995
H	-0.793863	3.789907	-0.443175
H	-1.920413	2.587821	-1.070404
S	0.010068	0.572473	-2.257885
C	0.017253	2.431227	-1.933852
H	-0.360625	2.928864	-2.831202
H	1.042884	2.769969	-1.773827
H	0.176156	-1.069394	2.718417
C	0.539026	-1.820534	3.824435
C	1.304256	-0.868449	4.735237
C	0.399671	0.209803	5.367305
C	-0.834285	-0.417652	6.044695
C	-1.634376	-1.286491	5.054185
C	-0.747441	-2.379641	4.420394
H	1.178993	-2.590877	3.375612
H	1.759198	-1.467948	5.544275
H	2.145037	-0.405805	4.201423
H	0.975757	0.796347	6.093121
H	0.067619	0.906235	4.583989
H	-0.507835	-1.038417	6.892174
H	-1.476586	0.367697	6.461495
H	-2.489884	-1.751669	5.558503
H	-2.042617	-0.643721	4.260198
H	-1.311365	-2.952567	3.671831
H	-0.469852	-3.107080	5.204475

=== 3TSH in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.824393
N	2.165529	0.000000	0.132721
N	0.204088	-2.105309	-0.205032
N	-2.190254	-0.120461	0.069022
N	-0.293054	2.081088	0.288455
C	2.401825	-1.352552	0.755123
H	3.479701	-1.569236	0.785371
H	2.034620	-1.310281	1.777189
C	1.680923	-2.421824	-0.038881
H	1.794684	-3.399103	0.447572
H	2.112411	-2.506802	-1.038638
C	-0.567891	-2.785385	0.913609
H	-0.401046	-3.868973	0.813765
H	-0.118790	-2.461503	1.848352
C	-2.078703	-2.528792	0.945544
H	-2.465342	-3.118678	1.787631
H	-2.560604	-2.957482	0.058976
C	-2.546209	-1.087794	1.181745
H	-2.102650	-0.693076	2.092860
H	-3.641287	-1.086237	1.290099
C	-2.657092	1.278999	0.432653
H	-2.999651	1.749092	-0.491805
H	-3.528212	1.210857	1.097347
C	-1.580053	2.113843	1.091825
H	-1.337271	1.711835	2.072707
H	-1.925371	3.152003	1.201918
C	0.764359	2.726984	1.165046
H	0.611376	2.335049	2.170402
H	0.560605	3.806681	1.186196

C	2.218351	2.475812	0.770449
H	2.417945	2.756089	-0.269625
H	2.829701	3.153458	1.381391
C	2.685793	1.055955	1.082670
H	2.344067	0.784907	2.080794
H	3.784378	1.004984	1.069186
C	2.946814	0.092548	-1.145953
H	4.007145	-0.109830	-0.936911
H	2.563680	-0.606748	-1.883043
H	2.851547	1.090494	-1.565975
C	-0.215139	-2.685058	-1.526114
H	-0.012850	-3.765503	-1.537191
H	0.337347	-2.196274	-2.328370
H	-1.274411	-2.524608	-1.693465
C	-2.962999	-0.494729	-1.167798
H	-2.811396	-1.539530	-1.421351
H	-2.617886	0.117242	-1.998852
H	-4.035530	-0.341763	-0.984432
C	-0.476209	2.870368	-0.998603
H	-0.209814	3.918961	-0.801312
H	-1.536956	2.849440	-1.253475
S	-0.003096	0.465574	-2.359728
C	0.302218	2.323532	-2.185757
H	-0.044195	2.812946	-3.101682
H	1.374929	2.511741	-2.095602
H	0.225976	-0.622072	2.867304
C	0.508630	-1.199707	4.054000
C	1.377259	-0.207262	4.815672
C	0.598877	1.023284	5.326194
C	-0.672297	0.609274	6.092477
C	-1.579075	-0.288813	5.228804
C	-0.821028	-1.533383	4.719303
H	1.062770	-2.091943	3.728144
H	1.790233	-0.746096	5.687338
H	2.251197	0.093851	4.221224
H	1.249750	1.625204	5.969779
H	0.317923	1.659837	4.471610
H	-0.389416	0.071298	7.007622
H	-1.222822	1.498394	6.419024
H	-2.456190	-0.606118	5.803551
H	-1.954333	0.292423	4.370277
H	-1.454999	-2.141263	4.058257
H	-0.594719	-2.182755	5.583879

=== 5TSH ===

Fe	0.007774	-0.013864	0.004057
O	0.030347	-0.040685	1.818270
N	2.269813	0.026413	0.163411
N	0.317841	-2.232782	-0.125878
N	-2.264837	-0.262641	0.017154
N	-0.434132	2.155409	0.161232
C	2.480504	-1.290083	0.859205
H	3.556782	-1.507442	0.943896
H	2.061499	-1.195251	1.859702
C	1.804786	-2.433540	0.101948
H	1.964827	-3.375211	0.645676
H	2.266903	-2.552857	-0.880252
C	-0.472282	-2.837008	1.015950
H	-0.272778	-3.920845	1.021623
H	-0.071595	-2.403084	1.931723
C	-1.999247	-2.633786	0.976964
H	-2.393062	-3.218022	1.820562
H	-2.426100	-3.110130	0.087789
C	-2.562747	-1.209432	1.153676
H	-2.147064	-0.760886	2.054334
H	-3.657099	-1.282397	1.264402
C	-2.757114	1.142413	0.303480
H	-3.100644	1.550828	-0.649310
H	-3.638346	1.094641	0.959766
C	-1.733094	2.091494	0.932934
H	-1.483043	1.758695	1.937863
H	-2.183035	3.094457	0.996216
C	0.625741	2.822686	1.008712
H	0.464047	2.488498	2.034821
H	0.447586	3.908130	0.977264
C	2.094242	2.546848	0.632973
H	2.274153	2.737618	-0.429001
H	2.687619	3.302764	1.165753
C	2.657902	1.177186	1.055953
H	2.304331	0.938882	2.059861
H	3.757309	1.232892	1.085596
C	3.064854	0.078308	-1.102728
H	4.130726	-0.081030	-0.881872
H	2.714303	-0.669996	-1.809250
H	2.941836	1.047516	-1.581668
C	-0.039008	-2.883704	-1.429856
H	0.232302	-3.948713	-1.411106
H	0.491707	-2.384691	-2.241235
H	-1.104679	-2.799506	-1.621821
C	-2.961076	-0.721855	-1.231701
H	-2.717193	-1.757229	-1.452288
H	-2.627841	-0.112402	-2.070272
H	-4.050563	-0.644023	-1.105702
C	-0.622072	2.856351	-1.166582
H	-0.414656	3.928864	-1.032649
H	-1.673446	2.763236	-1.444778
S	0.026122	0.398691	-2.389632
C	0.218467	2.281141	-2.303700
H	-0.129630	2.689874	-3.256099
H	1.277702	2.529029	-2.208004
H	0.119768	0.054253	3.026620
C	0.384642	0.155923	4.336848
C	-0.540000	1.220182	4.915763
C	-2.002035	0.744519	5.052464
C	-2.089842	-0.607403	5.788632
C	-1.232016	-1.681441	5.089824
C	0.238178	-1.232237	4.948203
H	1.428945	0.486739	4.269227
H	-0.161859	1.485928	5.919401
H	-0.485263	2.146575	4.327440
H	-2.589334	1.505645	5.580089
H	-2.450462	0.640989	4.052547
H	-1.741729	-0.480199	6.824178
H	-3.134030	-0.937895	5.849257
H	-1.276373	-2.626171	5.644960
H	-1.649465	-1.883561	4.092457
H	0.818112	-1.970496	4.377785
H	0.696742	-1.207247	5.953141

=== 5TSH in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.787331
N	2.262611	0.000000	0.207618
N	0.270654	-2.233111	-0.043698
N	-2.281371	-0.214484	0.042878
N	-0.407684	2.174704	0.157153
C	2.444593	-1.308801	0.928469
H	3.515771	-1.542527	1.026645
H	2.026248	-1.190697	1.926327
C	1.753307	-2.453385	0.190778
H	1.897195	-3.385541	0.754404
H	2.214384	-2.596808	-0.789632
C	-0.527590	-2.784418	1.124096
H	-0.345175	-3.870046	1.166583
H	-0.116279	-2.330501	2.024601
C	-2.049824	-2.557143	1.086576
H	-2.443511	-3.099188	1.957313
H	-2.492614	-3.063702	0.220887
C	-2.592326	-1.121236	1.213398
H	-2.177419	-0.649346	2.102217
H	-3.687097	-1.173800	1.324872
C	-2.749634	1.205311	0.295906
H	-3.074458	1.602082	-0.669221
H	-3.636412	1.186422	0.945459
C	-1.715315	2.143548	0.920584
H	-1.482233	1.823571	1.933448
H	-2.145492	3.155345	0.968396
C	0.654002	2.828205	1.017918
H	0.473016	2.503128	2.042938
H	0.492208	3.915716	0.981241
C	2.122711	2.528684	0.665376
H	2.325809	2.719423	-0.393252
H	2.716345	3.272566	1.214166
C	2.658475	1.153080	1.098528
H	2.292019	0.928494	2.099937
H	3.757713	1.189495	1.142355
C	3.073974	0.026375	-1.045321
H	4.136690	-0.135509	-0.809196
H	2.724044	-0.731793	-1.742777
H	2.958896	0.990067	-1.538956

C	-0.101542	-2.919623	-1.319970
H	0.150835	-3.989116	-1.268025
H	0.433871	-2.454122	-2.149131
H	-1.167747	-2.823179	-1.505402
C	-2.986600	-0.696815	-1.187815
H	-2.779402	-1.750425	-1.358673
H	-2.621946	-0.132659	-2.046136
H	-4.074020	-0.576354	-1.072767
C	-0.569213	2.871884	-1.170159
H	-0.351733	3.943142	-1.035950
H	-1.617433	2.787304	-1.464474
S	0.032233	0.410667	-2.442093
C	0.281929	2.286857	-2.296186
H	-0.023607	2.739151	-3.244852
H	1.344993	2.496863	-2.156994
H	0.104756	0.061567	3.104409
C	0.399804	0.204232	4.338411
C	-0.616311	1.159495	4.956131
C	-1.995785	0.515624	5.202248
C	-1.867267	-0.819959	5.961121
C	-0.935219	-1.800258	5.221886
C	0.455559	-1.181683	4.972063
H	1.395424	0.659135	4.236285
H	-0.200516	1.480226	5.927930
H	-0.705479	2.080143	4.361863
H	-2.628487	1.211177	5.764645
H	-2.500599	0.341448	4.236783
H	-1.471882	-0.630235	6.968226
H	-2.855707	-1.271469	6.101870
H	-0.825048	-2.725533	5.798121
H	-1.392923	-2.081163	4.258132
H	1.093263	-1.858122	4.385094
H	0.968707	-1.067566	5.943492

=== 3I ===

Fe	-0.027293	0.100395	-0.037371
O	-0.010613	0.316508	1.831765
N	2.133643	0.032180	0.054105
N	0.122098	-2.038395	0.020223
N	-2.204818	0.033715	0.071063
N	-0.272023	2.192396	-0.016007
C	2.373748	-1.248260	0.812982
H	3.447375	-1.488843	0.809678
H	2.080003	-1.093219	1.851474
C	1.593175	-2.379090	0.176072
H	1.697900	-3.299615	0.765487
H	1.987292	-2.591540	-0.819250
C	-0.636343	-2.555011	1.228875
H	-0.507705	-3.648504	1.254425
H	-0.153606	-2.149381	2.118228
C	-2.138277	-2.243703	1.261127
H	-2.523251	-2.703560	2.182127
H	-2.652321	-2.770361	0.449634
C	-2.557087	-0.768326	1.310297
H	-2.069814	-0.270238	2.146875
H	-3.649255	-0.718623	1.437877
C	-2.644165	1.474364	0.252457
H	-2.982517	1.830482	-0.722614
H	-3.514366	1.509420	0.921831
C	-1.540834	2.354908	0.795700
H	-1.289182	2.061354	1.812564
H	-1.858794	3.407856	0.784767
C	0.815987	2.909737	0.756305
H	0.669327	2.645614	1.804115
H	0.645080	3.990123	0.642776
C	2.254103	2.565094	0.372972
H	2.434246	2.693904	-0.699700
H	2.900352	3.301886	0.869288
C	2.691528	1.183429	0.862100
H	2.352480	1.038649	1.889803
H	3.788646	1.104173	0.842611
C	2.892694	-0.036206	-1.247051
H	3.954336	-0.220635	-1.031493
H	2.496093	-0.816187	-1.889118
H	2.796730	0.902363	-1.785831
C	-0.349330	-2.773237	-1.209152
H	-0.149951	-3.847504	-1.095577
H	0.176867	-2.392652	-2.083455
H	-1.412407	-2.630651	-1.362458
C	-3.006323	-0.486138	-1.096023
H	-2.873663	-1.555460	-1.221223
H	-2.674398	0.008766	-2.005807
H	-4.072401	-0.293246	-0.915182
C	-0.460273	2.816332	-1.395825
H	-0.152084	3.870098	-1.343946
H	-1.527087	2.803522	-1.621575
S	-0.039199	0.225957	-2.378350
C	0.267863	2.086436	-2.512082
H	-0.115848	2.415783	-3.481782
H	1.343840	2.275108	-2.501956
H	0.438320	-0.287141	2.458633
C	1.667074	-0.403986	4.690414
C	0.441133	0.232146	5.286391
C	-0.678090	-0.802131	5.575460
C	-0.135056	-2.038203	6.320835
C	1.012568	-2.706951	5.537849
C	2.164545	-1.705192	5.260688
H	2.375607	0.233250	4.156674
H	0.714976	0.718649	6.242942
H	0.065655	1.032920	4.636739
H	-1.480916	-0.328105	6.152371
H	-1.124378	-1.124442	4.622027
H	0.232495	-1.731268	7.311296
H	-0.945160	-2.759914	6.496480
H	1.399288	-3.575101	6.086285
H	0.622885	-3.087613	4.580345
H	2.924614	-2.158420	4.610884
H	2.681953	-1.504443	6.219849

=== 3I in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.853951
N	2.160508	0.000000	0.144583
N	0.223427	-2.122749	-0.145041
N	-2.178656	-0.148314	0.109323
N	-0.309552	2.068735	0.280423
C	2.429869	-1.346970	0.769206
H	3.510961	-1.547960	0.769933
H	2.105296	-1.312465	1.807706
C	1.703501	-2.428389	-0.001328
H	1.833425	-3.400444	0.491438
H	2.119398	-2.517786	-1.007267
C	-0.526678	-2.795887	0.994818
H	-0.361681	-3.879784	0.897178
H	-0.062465	-2.485271	1.930546
C	-2.036758	-2.539975	1.047392
H	-2.405307	-3.105874	1.913633
H	-2.531389	-2.995737	0.181467
C	-2.508756	-1.095979	1.251838
H	-2.055243	-0.676005	2.147304
H	-3.602202	-1.098908	1.372839
C	-2.661395	1.249787	0.454925
H	-3.014114	1.703771	-0.473991
H	-3.527919	1.179776	1.125069
C	-1.587159	2.096321	1.099484
H	-1.328415	1.696311	2.077011
H	-1.937289	3.132423	1.210270
C	0.747073	2.734223	1.144125
H	0.595406	2.358202	2.155626
H	0.538426	3.813012	1.146602
C	2.202389	2.482066	0.756556
H	2.405676	2.748685	-0.286528
H	2.810000	3.168938	1.360811
C	2.669829	1.067607	1.090815
H	2.316860	0.807891	2.088542
H	3.768171	1.016687	1.088347
C	2.941810	0.098282	-1.135162
H	4.005916	-0.075897	-0.921581
H	2.577307	-0.620041	-1.863296
H	2.823278	1.088170	-1.567265
C	-0.213978	-2.729347	-1.449138
H	-0.004739	-3.808447	-1.444962
H	0.322518	-2.251922	-2.268960
H	-1.276784	-2.579256	-1.601555
C	-2.965535	-0.557022	-1.107987
H	-2.818164	-1.608986	-1.332680
H	-2.632479	0.032049	-1.960527
H	-4.035532	-0.398820	-0.916242
C	-0.514178	2.837436	-1.014352
H	-0.258632	3.892131	-0.837050

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H     -1.576725    2.799255   -1.259111
S     -0.007066    0.410861   -2.337691
C      0.260919    2.280801   -2.199269
H     -0.102380    2.743667   -3.122236
H      1.331522    2.486741   -2.123323
H      0.344306   -0.679165    2.478786
C      1.050983   -1.439291    4.553186
C      0.159715   -0.504786    5.326480
C     -1.251294   -1.086358    5.579416
C     -1.180346   -2.530809    6.110935
C     -0.402958   -3.444882    5.143959
C      1.024485   -2.908106    4.883806
H      1.995171   -1.029698    4.181556
H      0.631395   -0.311609    6.309457
H      0.096980    0.475458    4.835224
H     -1.791415   -0.447084    6.286008
H     -1.824771   -1.074561    4.636834
H     -0.687604   -2.534763    7.092871
H     -2.189845   -2.925568    6.273392
H     -0.344010   -4.463241    5.543898
H     -0.951319   -3.510282    4.187886
H      1.536206   -3.501675    4.111592
H      1.617812   -3.063037    5.805749

=== 5I ===
Fe    -0.086574   -0.004056   -0.010053
O     -0.299522    0.050496    1.839516
N      2.138053   -0.115582    0.433664
N      0.072926   -2.247853   -0.021751
N     -2.362494   -0.089218   -0.269448
N     -0.382755    2.204624    0.014571
C      2.159304   -1.411591    1.196942
H      3.196494   -1.699671    1.430067
H      1.623704   -1.241461    2.129821
C      1.501037   -2.539541    0.400974
H      1.522353   -3.464206    0.994779
H      2.071561   -2.735336   -0.509357
C     -0.894341   -2.736827    1.036400
H     -0.781787   -3.830667    1.110090
H     -0.573539   -2.289493    1.977342
C     -2.386354   -2.427511    0.803795
H     -2.920084   -2.943984    1.614245
H     -2.738101   -2.913208   -0.112778
C     -2.862602   -0.961419    0.856732
H     -2.529616   -0.501414    1.786400
H     -3.964722   -0.956488    0.834646
C     -2.776558    1.358985   -0.093329
H     -2.972164    1.749645   -1.094345
H     -3.730553    1.403535    0.452141
C     -1.765687    2.259938    0.623929
H     -1.661229    1.950755    1.662135
H     -2.146205    3.293101    0.602221
C      0.614324    2.829215    0.964260
H      0.302529    2.551573    1.972908
H      0.527782    3.922694    0.874744
C      2.092662    2.429696    0.787722
H      2.416601    2.557441   -0.249394
H      2.672847    3.164579    1.362804
C      2.492069    1.043442    1.329223
H      1.991229    0.874713    2.284040
H      3.579265    1.024059    1.503879
C      3.087803   -0.173180   -0.720441
H      4.103608   -0.394634   -0.360846
H      2.775273   -0.926373   -1.439787
H      3.096259    0.780504   -1.244623
C     -0.171073   -2.933086   -1.333413
H      0.006207   -4.013859   -1.240328
H      0.495885   -2.516875   -2.089107
H     -1.193919   -2.774669   -1.663419
C     -2.939801   -0.553982   -1.575103
H     -2.737960   -1.609770   -1.733432
H     -2.475080    0.001237   -2.388335
H     -4.029455   -0.406381   -1.581028
C     -0.357361    2.855446   -1.349226
H     -0.082674    3.914982   -1.233856
H     -1.372470    2.827895   -1.749920
S      0.252680    0.300127   -2.393844
C      0.565156    2.168455   -2.355013
H      0.361787    2.553290   -3.357890
H      1.621462    2.347130   -2.142751
H     -0.435203    0.133781    2.810117
C     -0.502140    0.380446    4.979291
C     -1.501894    1.490639    5.166398
C     -2.962787    1.016822    4.974025
C     -3.245992   -0.275568    5.766570
C     -2.273624   -1.401236    5.360418
C     -0.799711   -0.974793    5.562047
H      0.543382    0.657535    4.832109
H     -1.402451    1.889383    6.195226
H     -1.277162    2.338712    4.504424
H     -3.652556    1.813871    5.276018
H     -3.147165    0.827607    3.904522
H     -3.142228   -0.075111    6.843336
H     -4.282803   -0.596662    5.607308
H     -2.476280   -2.311867    5.936594
H     -2.436824   -1.653409    4.301034
H     -0.116817   -1.734450    5.157832
H     -0.595033   -0.947470    6.650673

=== 5I in EF ===
Fe     0.000000    0.000000    0.000000
O      0.000000    0.000000    1.838409
N      2.265151    0.000000    0.227540
N      0.268700   -2.239036   -0.042460
N     -2.290627   -0.220316    0.017254
N     -0.416552    2.184883    0.142493
C      2.436453   -1.310415    0.949057
H      3.505969   -1.547021    1.058318
H      2.007682   -1.191221    1.942344
C      1.751080   -2.454389    0.203664
H      1.894045   -3.387724    0.765964
H      2.218948   -2.594179   -0.774144
C     -0.536993   -2.781086    1.125204
H     -0.356858   -3.866753    1.175986
H     -0.128195   -2.321682    2.024069
C     -2.059668   -2.553221    1.080901
H     -2.455165   -3.087524    1.955668
H     -2.499233   -3.068033    0.218286
C     -2.607860   -1.117593    1.192533
H     -2.205431   -0.637366    2.082861
H     -3.703306   -1.174431    1.295443
C     -2.757812    1.202944    0.254434
H     -3.062482    1.594697   -0.719280
H     -3.657228    1.191700    0.886975
C     -1.732951    2.144145    0.891255
H     -1.510298    1.823250    1.906154
H     -2.169497    3.153366    0.938940
C      0.637222    2.837004    1.013882
H      0.442378    2.516816    2.037978
H      0.481988    3.925321    0.971151
C      2.109994    2.529915    0.681552
H      2.327197    2.716209   -0.375354
H      2.697931    3.274762    1.235020
C      2.639668    1.154609    1.126839
H      2.250741    0.928131    2.119593
H      3.737625    1.194600    1.193735
C      3.095709    0.030118   -1.011459
H      4.158758   -0.099215   -0.757525
H      2.779164   -0.751315   -1.699684
H      2.961588    0.980670   -1.525226
C     -0.095735   -2.935901   -1.314691
H      0.165952   -4.002924   -1.257785
H      0.436104   -2.470320   -2.146229
H     -1.162971   -2.850252   -1.501133
C     -2.987299   -0.714528   -1.212808
H     -2.782742   -1.771233   -1.368799
H     -2.613036   -0.161958   -2.074643
H     -4.075453   -0.588642   -1.110040
C     -0.561939    2.879324   -1.185305
H     -0.339831    3.950052   -1.054482
H     -1.607425    2.799988   -1.490883
S      0.052463    0.408375   -2.439352
C      0.299131    2.286128   -2.300492
H      0.001240    2.730315   -3.255314
H      1.361018    2.497184   -2.153445
H     -0.027455    0.056274    2.838946
C      0.252799    0.201670    4.821595
C     -0.692316    1.288979    5.259653
C     -2.161320    0.815689    5.360631
C     -2.272881   -0.512689    6.133613
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C     -1.411426   -1.612339    5.483105
C      0.071080   -1.183701    5.381095
H      1.274961    0.503882    4.575337
H     -0.372298    1.632374    6.262509
H     -0.604582    2.177260    4.616383
H     -2.763785    1.591560    5.845448
H     -2.574270    0.680015    4.345556
H     -1.947294   -0.359420    7.171523
H     -3.319639   -0.833337    6.185357
H     -1.484326   -2.542919    6.056141
H     -1.801081   -1.828349    4.473184
H      0.660832   -1.920951    4.817617
H      0.501855   -1.193959    6.401191

=== 3TSreb ===
Fe    -0.037020    0.032945    0.004067
O     -0.119110    0.109160    2.077287
N      2.134068   -0.099914    0.331268
N      0.051249   -2.118037   -0.050897
N     -2.246457    0.023163   -0.088037
N     -0.210647    2.124803    0.120602
C      2.212238   -1.415554    1.055942
H      3.263720   -1.709151    1.200416
H      1.757822   -1.268000    2.033919
C      1.489282   -2.496692    0.271069
H      1.507432   -3.445411    0.824595
H      1.999040   -2.674744   -0.676996
C     -0.862154   -2.718200    0.995485
H     -0.788025   -3.814427    0.916902
H     -0.456091   -2.459488    1.976619
C     -2.348793   -2.337668    0.907333
H     -2.846093   -2.863411    1.734621
H     -2.785413   -2.768586    0.000793
C     -2.742406   -0.856181    1.033503
H     -2.360507   -0.430224    1.960324
H     -3.842515   -0.797817    1.057002
C     -2.636828    1.468579    0.148967
H     -2.887622    1.893530   -0.824528
H     -3.552742    1.511000    0.754984
C     -1.545462    2.283947    0.819946
H     -1.395338    1.937183    1.839969
H     -1.837892    3.344972    0.835791
C      0.823568    2.783452    1.007256
H      0.572200    2.508544    2.031177
H      0.701268    3.872262    0.911891
C      2.284517    2.405648    0.756767
H      2.570789    2.567904   -0.286241
H      2.895174    3.107817    1.341122
C      2.641694    0.994836    1.231235
H      2.199547    0.826997    2.213820
H      3.734524    0.892037    1.316441
C      3.008357   -0.159857   -0.890283
H      4.025939   -0.453589   -0.594134
H      2.606619   -0.854747   -1.620944
H      3.047903    0.815194   -1.369360
C     -0.266577   -2.741016   -1.386533
H     -0.111928   -3.827943   -1.335714
H      0.380655   -2.309343   -2.148195
H     -1.295052   -2.543859   -1.668847
C     -2.922169   -0.383810   -1.372513
H     -2.795094   -1.444754   -1.562966
H     -2.467333    0.161896   -2.196377
H     -3.998508   -0.172370   -1.302298
C     -0.253818    2.813067   -1.241634
H      0.041675    3.863806   -1.104787
H     -1.290248    2.810095   -1.582004
S      0.173278    0.293552   -2.374035
C      0.589282    2.135507   -2.310955
H      0.352440    2.567923   -3.287306
H      1.660705    2.269014   -2.143979
H     -0.337944   -0.753952    2.475581
C      0.027445    0.776307    4.283196
C     -1.391067    0.852441    4.775578
C     -2.006782   -0.523133    5.130178
C     -1.043000   -1.374737    5.983804
C      0.308483   -1.570323    5.264836
C      0.967956   -0.213250    4.917901
H      0.468206    1.700032    3.915066
H     -1.388579    1.475908    5.691549
H     -2.024921    1.396306    4.060956
H     -2.958581   -0.373477    5.653852
H     -2.244375   -1.070291    4.205290
H     -0.871093   -0.876000    6.948848
H     -1.497052   -2.349681    6.209865
H      0.994763   -2.164227    5.882058
H      0.143358   -2.151667    4.342680
H      1.864182   -0.354946    4.298932
H      1.340196    0.239305    5.859270

=== 3TSreb in EF ===
Fe     0.000000    0.000000    0.000000
O      0.000000    0.000000    2.002089
N      2.235587    0.000000    0.228042
N      0.225356   -2.120176   -0.131115
N     -2.260048   -0.162344    0.051907
N     -0.314060    2.052196    0.266268
C      2.415825   -1.343891    0.871676
H      3.485726   -1.594731    0.949329
H      2.011738   -1.273090    1.879929
C      1.701769   -2.421074    0.072105
H      1.815854   -3.395584    0.566152
H      2.153369   -2.509125   -0.918447
C     -0.572717   -2.806797    0.960719
H     -0.417444   -3.892134    0.852722
H     -0.129202   -2.529022    1.917872
C     -2.087421   -2.545142    0.978160
H     -2.481339   -3.130844    1.820248
H     -2.550373   -2.988532    0.089067
C     -2.586489   -1.105261    1.183398
H     -2.143602   -0.677393    2.081666
H     -3.680956   -1.133888    1.310227
C     -2.699989    1.247082    0.375426
H     -3.012754    1.705092   -0.566127
H     -3.588191    1.220580    1.023726
C     -1.619998    2.081638    1.041262
H     -1.390775    1.676211    2.024201
H     -1.968807    3.119907    1.146574
C      0.719677    2.707687    1.162510
H      0.546889    2.308278    2.161109
H      0.505544    3.786287    1.180990
C      2.192016    2.478393    0.812136
H      2.410173    2.735310   -0.229865
H      2.769148    3.190217    1.418206
C      2.694104    1.077839    1.172592
H      2.313050    0.816147    2.159804
H      3.794775    1.066447    1.207611
C      3.041470    0.073108   -1.029479
H      4.097609   -0.148104   -0.809348
H      2.654652   -0.617199   -1.774742
H      2.969615    1.072332   -1.453935
C     -0.162464   -2.703699   -1.459281
H      0.031473   -3.786719   -1.466942
H      0.413125   -2.216414   -2.245805
H     -1.215794   -2.530709   -1.654154
C     -3.000494   -0.565708   -1.187584
H     -2.859104   -1.622613   -1.399083
H     -2.609372    0.008534   -2.027068
H     -4.078661   -0.388604   -1.055655
C     -0.468926    2.827729   -1.030989
H     -0.229993    3.884108   -0.833989
H     -1.520299    2.781159   -1.320496
S      0.048170    0.430899   -2.403552
C      0.354448    2.286601   -2.192465
H      0.048116    2.794506   -3.113238
H      1.423602    2.466986   -2.055591
H      0.024783   -0.832488    2.510254
C      0.128114    0.525198    4.864680
C     -1.250649    0.337803    5.379905
C     -1.625845   -1.135948    5.676953
C     -0.490877   -1.874025    6.411211
C      0.824212   -1.808004    5.613034
C      1.240624   -0.343346    5.325479
H      0.369990    1.450132    4.350268
H     -1.298122    0.900397    6.337840
H     -1.986450    0.831219    4.732901
H     -2.546414   -1.161012    6.268311
H     -1.843686   -1.648713    4.726296
H     -0.342329   -1.430868    7.405335
H     -0.773028   -2.918297    6.583726
H      1.630309   -2.312873    6.154540
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H      0.700479   -2.342473    4.656210
H      2.101938   -0.279833    4.648434
H      1.602661    0.098897    6.279117

=== 5TS2,alpha ===
Fe    -0.025847   -0.026196   -0.026530
O     -0.082604   -0.096262    2.007421
N      2.238206    0.104564    0.265002
N      0.379522   -2.215176   -0.171032
N     -2.285771   -0.297201   -0.049528
N     -0.539080    2.181994    0.236562
C      2.456072   -1.222223    0.937352
H      3.532346   -1.410332    1.078219
H      1.973637   -1.164429    1.912429
C      1.858814   -2.370206    0.119823
H      2.031205   -3.319267    0.647592
H      2.369750   -2.446370   -0.842234
C     -0.441103   -2.856967    0.923958
H     -0.209509   -3.934701    0.933172
H     -0.098758   -2.416293    1.859204
C     -1.971074   -2.696589    0.822051
H     -2.384501   -3.329872    1.619830
H     -2.344209   -3.142795   -0.105723
C     -2.581383   -1.296171    1.040866
H     -2.190660   -0.871724    1.964923
H     -3.675018   -1.405191    1.125895
C     -2.828602    1.078491    0.281049
H     -3.170668    1.511750   -0.661016
H     -3.718376    0.977620    0.919691
C     -1.853721    2.045836    0.964915
H     -1.631250    1.689941    1.968775
H     -2.350289    3.025924    1.049401
C      0.482217    2.872952    1.105440
H      0.288215    2.586156    2.143866
H      0.305185    3.958351    1.051260
C      1.968632    2.611068    0.784074
H      2.175094    2.818992   -0.269054
H      2.532531    3.369470    1.344969
C      2.557508    1.245686    1.192696
H      2.196402    0.970720    2.185768
H      3.652894    1.341768    1.260462
C      3.078728    0.214248   -0.968400
H      4.142455    0.099761   -0.709632
H      2.789783   -0.536337   -1.699883
H      2.924299    1.182532   -1.440231
C      0.096024   -2.839861   -1.504294
H      0.387838   -3.900036   -1.503905
H      0.650266   -2.306617   -2.277459
H     -0.961980   -2.769275   -1.742240
C     -2.923056   -0.724850   -1.340602
H     -2.635225   -1.741807   -1.594550
H     -2.573348   -0.071038   -2.137984
H     -4.018629   -0.686831   -1.254369
C     -0.724548    2.914604   -1.073955
H     -0.590389    3.993825   -0.898486
H     -1.757332    2.766002   -1.393507
S      0.082416    0.555198   -2.384274
C      0.184444    2.435153   -2.202755
H     -0.148879    2.879027   -3.144643
H      1.226474    2.727497   -2.054023
H      0.136293    0.653301    2.584861
C      0.106481   -1.127918    4.309384
C      0.875862   -0.071331    5.044607
C      0.024815    1.163927    5.424864
C     -1.323061    0.750606    6.046376
C     -2.113897   -0.171147    5.098066
C     -1.298818   -1.430598    4.724610
H      0.673342   -1.911575    3.816718
H      1.253714   -0.525722    5.982583
H      1.777486    0.220281    4.489742
H      0.591094    1.798364    6.115923
H     -0.166719    1.775140    4.528683
H     -1.140849    0.229595    6.997742
H     -1.914365    1.641928    6.287212
H     -3.062147   -0.471565    5.557882
H     -2.365168    0.380930    4.180995
H     -1.813822   -2.022500    3.959336
H     -1.250757   -2.086101    5.617847

=== 5TS2,beta ===
Fe     0.050132    0.049089    0.021379
O      0.067316   -0.043031    2.028277
N      2.324720    0.161219    0.186581
N      0.419050   -2.148137    0.002924
N     -2.247879   -0.217613    0.120107
N     -0.424558    2.182367    0.156240
C      2.560220   -1.121427    0.935568
H      3.640483   -1.314105    1.030886
H      2.125613   -0.995035    1.926020
C      1.906339   -2.310432    0.229500
H      2.091837   -3.221909    0.815764
H      2.368028   -2.464165   -0.748260
C     -0.352204   -2.716967    1.170982
H     -0.123071   -3.794026    1.230706
H      0.032632   -2.221785    2.061536
C     -1.884129   -2.557817    1.123701
H     -2.264753   -3.141262    1.974346
H     -2.296639   -3.056465    0.240046
C     -2.484090   -1.146240    1.284505
H     -2.045645   -0.668927    2.159604
H     -3.572544   -1.246973    1.431577
C     -2.750532    1.177366    0.401694
H     -3.153472    1.565798   -0.536088
H     -3.593504    1.137215    1.107625
C     -1.706353    2.151148    0.959858
H     -1.438593    1.856798    1.973293
H     -2.151621    3.157402    0.997576
C      0.629547    2.948858    0.924220
H      0.490012    2.725117    1.987117
H      0.420566    4.022905    0.805454
C      2.101598    2.689927    0.552954
H      2.264257    2.838711   -0.517747
H      2.678400    3.484423    1.046542
C      2.709959    1.353767    1.017451
H      2.409023    1.149598    2.047965
H      3.807900    1.443009    1.016518
C      3.107527    0.170230   -1.089292
H      4.178141    0.034645   -0.873390
H      2.758233   -0.611245   -1.759016
H      2.966661    1.116695   -1.607939
C      0.061528   -2.853011   -1.270244
H      0.297323   -3.924839   -1.196840
H      0.618307   -2.411753   -2.097075
H     -0.997622   -2.739545   -1.483543
C     -2.969052   -0.717309   -1.097051
H     -2.682023   -1.741733   -1.319760
H     -2.694248   -0.104090   -1.953618
H     -4.056662   -0.689430   -0.933472
C     -0.662872    2.803800   -1.211814
H     -0.504037    3.890391   -1.134088
H     -1.712137    2.645738   -1.465241
S      0.020438    0.314409   -2.343542
C      0.184775    2.204085   -2.326954
H     -0.178784    2.568002   -3.292434
H      1.238123    2.479515   -2.247997
H      0.366359    0.777289    2.467672
C     -0.193959   -0.572444    4.572083
C      1.205656   -0.658696    5.094160
C      1.851119    0.719933    5.367970
C      0.890482    1.655203    6.127301
C     -0.428420    1.840639    5.352473
C     -1.122495    0.485359    5.082045
H     -0.628673   -1.460551    4.127307
H      1.176722   -1.219025    6.050825
H      1.831678   -1.263106    4.426172
H      2.782374    0.584280    5.929318
H      2.127697    1.189608    4.411303
H      0.675427    1.233172    7.119890
H      1.367365    2.627638    6.298408
H     -1.110209    2.499849    5.901533
H     -0.214764    2.340533    4.394246
H     -1.981070    0.606101    4.409214
H     -1.553564    0.125722    6.038414

=== 3P ===
Fe   -0.002164   -0.002884   -0.204521
O    -0.189933   -0.225978    3.662992
N     2.122863   -0.062166    0.418651
N     0.165069   -2.125192   -0.208138
N    -2.219808   -0.116913   -0.070728
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N	-0.259064	2.053105	0.262450
C	2.241587	-1.439447	1.002567
H	3.298810	-1.692837	1.178694
H	1.736043	-1.430802	1.972500
C	1.620744	-2.447691	0.054301
H	1.707203	-3.466321	0.458578
H	2.137032	-2.437958	-0.906538
C	-0.632048	-2.686398	0.954601
H	-0.450671	-3.772273	0.989287
H	-0.204059	-2.253032	1.864151
C	-2.144920	-2.444975	0.952034
H	-2.544392	-2.992154	1.817644
H	-2.613369	-2.915971	0.082347
C	-2.595873	-0.986814	1.097786
H	-2.143573	-0.549227	1.994619
H	-3.690439	-0.960246	1.226264
C	-2.652912	1.305684	0.167049
H	-2.820445	1.757590	-0.811808
H	-3.616666	1.324048	0.698282
C	-1.614470	2.080216	0.945840
H	-1.478569	1.636140	1.936042
H	-1.944195	3.120691	1.086828
C	0.698144	2.665000	1.270204
H	0.407556	2.282769	2.253697
H	0.519951	3.749972	1.279173
C	2.185481	2.383256	1.081630
H	2.524463	2.654296	0.077907
H	2.727566	3.049144	1.766664
C	2.558647	0.945669	1.444116
H	2.074615	0.674295	2.387757
H	3.647430	0.855919	1.584061
C	3.026072	0.049528	-0.780811
H	4.040604	-0.275968	-0.506963
H	2.643091	-0.534802	-1.613047
H	3.065827	1.082143	-1.118688
C	-0.208520	-2.796610	-1.498525
H	0.025269	-3.869717	-1.452279
H	0.348776	-2.328292	-2.310555
H	-1.267211	-2.677406	-1.702789
C	-2.929351	-0.565140	-1.319909
H	-2.801075	-1.629731	-1.487815
H	-2.504222	-0.027576	-2.167746
H	-4.006225	-0.361586	-1.229510
C	-0.297164	2.898912	-1.013809
H	-0.023492	3.930453	-0.745958
H	-1.329504	2.918388	-1.365900
S	0.172971	0.560527	-2.526168
C	0.571236	2.377312	-2.152324
H	0.360163	2.962160	-3.051925
H	1.637619	2.482373	-1.937351
H	-0.629805	-1.059090	3.925300
C	0.138925	0.545207	4.898336
C	-1.120235	0.753670	5.755201
C	-1.598445	-0.556180	6.421724
C	-0.465364	-1.232695	7.221541
C	0.786580	-1.460751	6.349202
C	1.259715	-0.148997	5.686863
H	0.490986	1.500886	4.498030
H	-0.881267	1.488549	6.539094
H	-1.914609	1.194253	5.139694
H	-2.454231	-0.343660	7.072038
H	-1.974121	-1.257353	5.655295
H	-0.195548	-0.595659	8.074490
H	-0.815969	-2.182932	7.642067
H	1.601080	-1.882142	6.950911
H	0.564418	-2.208958	5.573227
H	2.118454	-0.328634	5.026926
H	1.598399	0.547648	6.465939

=== 3P in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	3.988329
N	2.147816	0.000000	0.559604
N	0.144369	-2.109537	0.314676
N	-2.181101	-0.045648	0.313425
N	-0.199257	2.118324	0.291903
C	2.279770	-1.296737	1.313300
H	3.341315	-1.534368	1.479819
H	1.815382	-1.154495	2.293104
C	1.612766	-2.410495	0.533614
H	1.717757	-3.367949	1.062128
H	2.075375	-2.526733	-0.448688
C	-0.577639	-2.482194	1.602725
H	-0.405253	-3.554679	1.778414
H	-0.086699	-1.929531	2.407641
C	-2.080506	-2.203573	1.665413
H	-2.423191	-2.599752	2.630803
H	-2.625514	-2.785573	0.914538
C	-2.478163	-0.726471	1.630568
H	-1.936116	-0.190292	2.417231
H	-3.555622	-0.634081	1.836837
C	-2.595017	1.401610	0.377661
H	-2.783910	1.726543	-0.647575
H	-3.539508	1.497798	0.932605
C	-1.525171	2.248638	1.022104
H	-1.358425	1.926757	2.053137
H	-1.835696	3.303167	1.051954
C	0.807118	2.807576	1.200330
H	0.563048	2.509598	2.223565
H	0.627878	3.889702	1.128745
C	2.281907	2.502527	0.967912
H	2.579392	2.679597	-0.070838
H	2.854424	3.221092	1.569319
C	2.662297	1.104884	1.445846
H	2.248608	0.939824	2.445045
H	3.755810	1.007042	1.521381
C	2.996587	-0.054380	-0.680542
H	4.007229	-0.401035	-0.419975
H	2.546963	-0.701592	-1.429869
H	3.068239	0.939104	-1.118791
C	-0.314814	-2.960203	-0.829774
H	-0.075934	-4.016412	-0.638779
H	0.185807	-2.622493	-1.738984
H	-1.386971	-2.867637	-0.972101
C	-2.986865	-0.656694	-0.797157
H	-2.873022	-1.735865	-0.814844
H	-2.633931	-0.247603	-1.744746
H	-4.053001	-0.430285	-0.649842
C	-0.274546	2.833074	-1.052953
H	0.035421	3.878370	-0.901180
H	-1.320775	2.846302	-1.364504
S	0.047470	0.365445	-2.418671
C	0.534139	2.186563	-2.173453
H	0.329833	2.726589	-3.104026
H	1.608628	2.248494	-1.983784
H	-0.397443	-0.767621	4.450512
C	0.460277	0.949742	5.066640
C	-0.738872	1.409107	5.908789
C	-1.294004	0.280138	6.806808
C	-0.185977	-0.338836	7.682022
C	0.995201	-0.834437	6.824118
C	1.551722	0.291076	5.922749
H	0.870873	1.785219	4.489004
H	-0.406253	2.239112	6.546642
H	-1.521298	1.808588	5.249829
H	-2.101010	0.673938	7.433583
H	-1.755349	-0.506460	6.183080
H	0.174246	0.414382	8.396042
H	-0.589561	-1.161503	8.281641
H	1.796743	-1.218224	7.464020
H	0.670324	-1.688458	6.203967
H	2.355011	-0.084140	5.274609
H	1.994468	1.069363	6.559175

=== 5P ===

Fe	-0.005655	0.027906	-0.157548
O	0.169982	-0.101027	4.136224
N	2.105684	0.201979	0.732162
N	0.366271	-2.153052	0.334432
N	-2.252115	-0.264360	0.095132
N	-0.524763	2.202294	0.387704
C	2.330646	-1.089447	1.463378
H	3.402160	-1.221232	1.683931
H	1.799576	-1.016416	2.415587
C	1.830950	-2.275661	0.653733
H	2.020839	-3.211193	1.202400
H	2.369179	-2.345587	-0.294244
C	-0.438475	-2.561796	1.546001
H	-0.195036	-3.612691	1.776316
H	-0.098784	-1.949442	2.387204

C	-1.964049	-2.430039	1.436883
H	-2.369970	-2.881439	2.352522
H	-2.358714	-3.043912	0.621226
C	-2.528119	-1.002618	1.374895
H	-2.099152	-0.420645	2.198474
H	-3.619230	-1.042699	1.532355
C	-2.793216	1.136951	0.156919
H	-2.878654	1.482016	-0.875635
H	-3.808909	1.129929	0.583968
C	-1.915871	2.091494	0.953199
H	-1.821505	1.746774	1.987424
H	-2.399790	3.080680	0.987456
C	0.346793	2.874479	1.415857
H	0.081657	2.450503	2.390842
H	0.090290	3.945313	1.445916
C	1.856293	2.706820	1.224923
H	2.158132	2.939938	0.199432
H	2.345922	3.462098	1.854406
C	2.379076	1.340405	1.680206
H	1.907476	1.083270	2.634197
H	3.466996	1.394858	1.847961
C	3.031907	0.296920	-0.446029
H	4.073395	0.154740	-0.120242
H	2.774577	-0.442820	-1.202269
H	2.938893	1.275384	-0.913377
C	0.073137	-3.028077	-0.846077
H	0.364683	-4.068886	-0.641543
H	0.628243	-2.660570	-1.711756
H	-0.985852	-3.006962	-1.088938
C	-2.916535	-0.932148	-1.073543
H	-2.628799	-1.977794	-1.141574
H	-2.597575	-0.427775	-1.986728
H	-4.011116	-0.880545	-0.974713
C	-0.545503	2.992274	-0.914195
H	-0.297221	4.040160	-0.684934
H	-1.570302	2.983329	-1.292166
S	0.057987	0.639339	-2.447062
C	0.368175	2.473654	-2.024596
H	0.165851	3.043202	-2.935812
H	1.425079	2.603331	-1.782966
H	-0.546775	0.507814	4.406967
C	0.737329	-0.742021	5.357345
C	1.242777	0.323926	6.342432
C	0.088175	1.094208	7.020331
C	-0.920135	0.132411	7.681941
C	-1.451743	-0.904902	6.672291
C	-0.297047	-1.679072	6.000807
H	1.576322	-1.318581	4.957932
H	1.837571	-0.182823	7.114960
H	1.919380	1.011399	5.820669
H	0.496920	1.791708	7.760321
H	-0.435780	1.719680	6.277936
H	-0.425044	-0.393417	8.511299
H	-1.751455	0.697234	8.120177
H	-2.129996	-1.609239	7.167473
H	-2.054646	-0.393582	5.903737
H	-0.680145	-2.373427	5.243068
H	0.218737	-2.285647	6.758308

=== 5P in EF ===

Fe	0.000000	0.000000	0.000000
O	0.000000	0.000000	4.248564
N	2.092713	0.000000	0.908131
N	0.176376	-2.212515	0.560010
N	-2.243218	-0.077968	0.310320
N	-0.326775	2.255407	0.534926
C	2.228818	-1.300827	1.654082
H	3.289133	-1.504934	1.866761
H	1.720342	-1.180702	2.613027
C	1.631026	-2.452460	0.866011
H	1.746714	-3.389856	1.430671
H	2.150792	-2.581484	-0.087178
C	-0.632899	-2.491534	1.812106
H	-0.472711	-3.546321	2.087339
H	-0.228906	-1.872855	2.619718
C	-2.139464	-2.227552	1.721013
H	-2.565077	-2.603065	2.661057
H	-2.611143	-2.830746	0.937754
C	-2.558200	-0.756143	1.623074
H	-2.049017	-0.196990	2.413422
H	-3.642201	-0.675489	1.803055
C	-2.672303	1.364513	0.354641
H	-2.744423	1.701771	-0.682297
H	-3.677895	1.438605	0.797076
C	-1.711419	2.249399	1.130908
H	-1.619723	1.898156	2.161359
H	-2.117186	3.272125	1.177164
C	0.605157	2.864565	1.558136
H	0.287140	2.503926	2.541053
H	0.463347	3.955985	1.550764
C	2.087322	2.525734	1.397474
H	2.441008	2.717591	0.379037
H	2.643318	3.221060	2.040119
C	2.431989	1.113135	1.873427
H	1.880383	0.909428	2.795674
H	3.507003	1.044491	2.101066
C	3.049752	0.028606	-0.246332
H	4.078868	-0.117524	0.114003
H	2.799777	-0.744918	-0.971722
H	2.982889	0.986320	-0.758966
C	-0.216488	-3.125645	-0.556435
H	-0.033306	-4.176365	-0.284978
H	0.367399	-2.873630	-1.445090
H	-1.271724	-3.011341	-0.794217
C	-2.986775	-0.719126	-0.821349
H	-2.781062	-1.785804	-0.865054
H	-2.656757	-0.260235	-1.755263
H	-4.071390	-0.582859	-0.694344
C	-0.312085	3.039988	-0.760454
H	0.001651	4.072406	-0.539233
H	-1.337827	3.091753	-1.134976
S	0.119927	0.654117	-2.302870
C	0.561966	2.462494	-1.874170
H	0.408752	3.056911	-2.780472
H	1.624378	2.509346	-1.622175
H	-0.881689	0.262741	4.585111
C	0.865059	-0.250570	5.461834
C	0.925306	1.011990	6.333776
C	-0.411796	1.293003	7.056373
C	-0.887263	0.065195	7.858717
C	-0.985846	-1.186238	6.963540
C	0.349257	-1.469519	6.239510
H	1.842799	-0.460212	5.015867
H	1.711578	0.865214	7.086231
H	1.230344	1.870327	5.720805
H	-0.295397	2.159030	7.716454
H	-1.187431	1.577526	6.322266
H	-0.179507	-0.128330	8.676250
H	-1.853465	0.270825	8.331773
H	-1.270961	-2.059672	7.559672
H	-1.792775	-1.048148	6.222241
H	0.256633	-2.328201	5.561264
H	1.109400	-1.737001	6.986034