

Supporting Information.

What Factors Influence the Rate Constant of Substrate Epoxidation by Compound I of Cytochrome P450 and Analogous Iron(IV)-Oxo Oxidants.

*Devesh Kumar,^{*a} Baharan Karamzadeh,^b G. N. Sastry,^a and Sam P. de Visser^{*b}*

AUTHOR ADDRESS: (a) Molecular Modeling Group, Indian Institute of Chemical Technology, Hyderabad 500-007, India and (b) The Manchester Interdisciplinary Biocenter and the School of Chemical Engineering and Analytical Science, The University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom.

AUTHOR EMAIL ADDRESS: sam.devisser@manchester.ac.uk (SPdV), dkclcre@yahoo.com (DK)

Full Gaussian-03 reference:

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, N.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; 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.; Pople, J. A. Gaussian 03, revision C.02; Gaussian, Inc., Wallingford, CT, 2004.

Table S1. Ionization energies (IE) of substrates taken from the chemistry webbook as well as calculated with UB3LYP. All data represent results after a full geometry optimization in *Jaguar* followed by frequency.

Substrates	IE (chemistry web-book)	IE (B1)	IE (B2)
	kcal/mol	kcal/mol	kcal/mol
Ethene	242.36	235.45	238.90
Propene	224.38	215.89	219.69
1-Butene	220.23	211.11	214.76
<i>trans</i> -2-Butene	209.85	199.78	203.69
1,3-cyclohexadiene	190.25	176.22	181.36
1,4-cyclohexadiene	203.39	189.02	194.46
Styrene	195.09	182.76	187.72

Table S2: RE of substrate for the calculation of epoxidation with Cpd I(SH). RE represents the energy of the substrate in the geometry of the transition state with respect to a fully relaxed structure.

Substrates	RE (B2) from $^2\text{TS}_E$	RE (B2) from $^4\text{TS}_E$
	kcal/mol	kcal/mol
Ethene	2.43	2.80
Propene	1.85	2.93
1-Butene	0.98	1.29
<i>trans</i> -2-Butene	0.36	2.96
1,3-cyclohexadiene	2.06	2.91
1,4-cyclohexadiene	2.55	5.15
Styrene	1.67	3.25

Table S3. Energetic and geometric data of the reaction of 1,4-cyclohexadiene with Cpd I(SH).

	B1			B2	
	ΔE	$\Delta E + \text{ZPE}$	ΔG	ΔE	$\Delta E + \text{ZPE}$
$^2\text{CpdI} + \text{Sub.}$	0.11	0.02	0.34	-0.04	-0.13
$^4\text{CpdI} + \text{Sub.}$	0.00	0.00	0.00	0.00	0.00
^2TSE	11.48	11.10	23.88	13.49	13.09
^4TSE	11.41	11.34	24.17	12.00	11.91
^4I	0.67	1.32	14.57	-4.61	-3.99

B1

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.03	0.61	-0.33	-0.41	0.10	0.45	-0.39	-0.31	-0.05	0.30
^4TSE	1.21	0.87	0.11	0.36	0.45	0.45	-0.40	-0.35	0.01	0.29
^4I	1.81	0.39	-0.12	0.00	0.92	0.48	-0.51	-0.35	0.03	0.35

B2

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.04	0.59	-0.34	-0.42	0.13	0.18	-0.06	0.01	-0.17	0.04
^4TSE	1.34	0.82	0.03	0.33	0.48	0.18	-0.15	-0.02	-0.12	0.11
^4I	1.86	0.35	-0.15	0.01	0.93	0.12	-0.16	0.08	-0.12	0.08

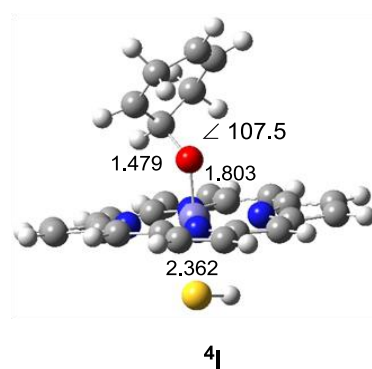
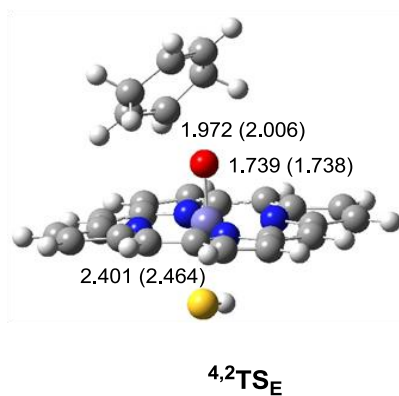


Table S4. Energetic and geometric data for the reaction of 1,3-cyclohexadiene with Cpd I(SH).

	B1			B2	
	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$
$^2\text{CpdI} + \text{Sub.}$	0.11	0.02	0.34	-0.04	-0.13
$^4\text{CpdI} + \text{Sub.}$	0.00	0.00	0.00	0.00	0.00
^2TSE	7.93	7.47	21.31	9.84	9.39
^4TSE	6.35	6.54	18.47	7.69	7.87
^4I	-15.05	-13.94	-2.99	-20.43	-19.32

B1

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.14	0.73	-0.39	-0.47	-0.01	0.48	-0.38	-0.27	-0.07	0.24
^4TSE	1.11	0.92	0.18	0.42	0.37	0.46	-0.38	-0.32	-0.02	0.27
^4I	1.83	0.36	-0.13	-0.06	1.00	0.48	-0.53	-0.34	0.04	0.34

B2

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.16	0.72	-0.10	-0.48	0.00	0.11	-0.06	-0.03	-0.15	0.01
^4TSE	1.21	0.87	0.11	0.41	0.39	0.11	-0.09	-0.01	-0.12	0.11
^4I	1.89	0.31	-0.16	-0.05	1.01	0.19	-0.22	0.06	-0.10	0.07

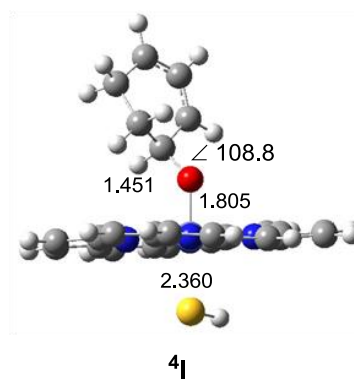
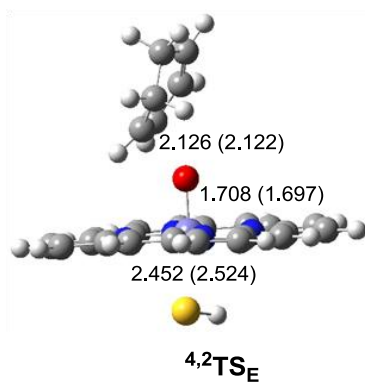


Table S5. Energetic and geometric data for the reaction of 1-Butene with Cpd I(SH).

	B1			B2	
	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$
² CpdI + Sub.	0.11	0.02	0.34	-0.04	-0.13
⁴ CpdI + Sub.	0.00	0.00	0.00	0.00	0.00
² TSE	11.17	11.05	23.53	13.66	13.49
⁴ TSE	9.87	10.38	20.39	10.57	11.03
² I	-3.37	-2.29	9.29	-9.28	-8.24
⁴ I	-3.97	-2.69	8.92	-10.12	-8.89
⁴ TSreb	-2.77	-2.26	10.24	-9.29	-8.83
² P	-31.04	-27.98	-14.97	-42.28	-39.26
⁴ P	-28.72	-27.13	-14.90	-41.03	-39.49

B1

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
² TSE	1.03	0.65	-0.41	-0.49	0.22	0.46	-0.38	-0.28	-0.05	0.25
⁴ TSE	1.18	0.89	0.15	0.40	0.37	0.44	-0.37	-0.33	0.00	0.25
² I	1.84	0.31	-0.14	-0.13	-0.88	0.49	-0.51	-0.34	0.02	0.34
⁴ I	1.86	0.32	-0.12	0.05	0.90	0.48	-0.51	-0.35	0.01	0.36
⁴ TSreb	2.25	-0.04	-0.11	0.21	0.70	0.53	-0.51	-0.39	-0.08	0.44
² P	1.16	0.00	-0.10	-0.06	0.00	0.39	-0.47	-0.55	0.02	0.61
⁴ P	2.57	0.00	-0.02	0.44	0.01	0.59	-0.46	-0.51	-0.18	0.56

B2

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
² TSE	1.09	0.60	-0.42	-0.48	0.22	0.13	-0.13	0.05	-0.15	0.10
⁴ TSE	1.26	0.83	0.12	0.40	0.39	0.11	-0.08	0.03	-0.13	0.07
² I	1.91	0.28	-0.16	-0.12	-0.91	0.16	-0.19	0.08	-0.12	0.06
⁴ I	1.92	0.27	-0.16	0.04	0.93	0.17	-0.19	0.07	-0.13	0.08
⁴ TSreb	2.30	-0.05	-0.16	0.20	0.72	0.21	-0.17	0.00	-0.19	0.14
² P	1.16	-0.01	-0.11	-0.04	0.00	0.19	-0.10	-0.29	-0.11	0.30
⁴ P	2.64	-0.02	-0.08	0.44	0.02	0.26	0.06	-0.28	-0.16	0.12

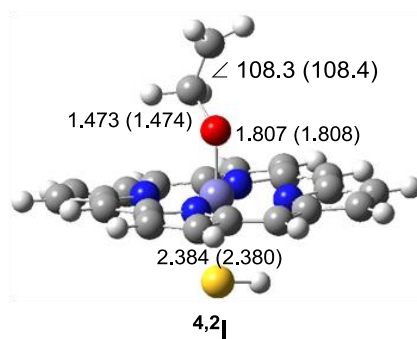
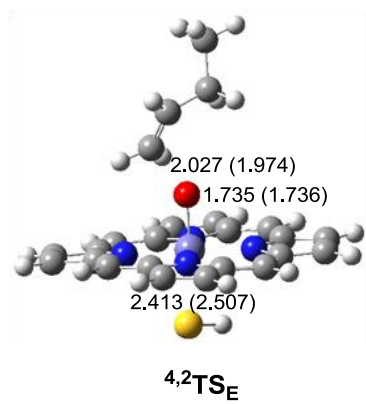


Table S6. Energetic and geometric data for the reaction of *trans*-2-butene with Cpd I(SH).

	B1			B2	
	ΔE	$\Delta E + \text{ZPE}$	ΔG	ΔE	$\Delta E + \text{ZPE}$
$^2\text{CpdI} + \text{Sub.}$	0.11	0.02	0.34	-0.04	-0.13
$^4\text{CpdI} + \text{Sub.}$	0.00	0.00	0.00	0.00	0.00
^2TSE	9.62	9.75	20.68	9.87	10.00
^4TSE	9.23	9.78	21.78	10.28	10.82
^4I	-2.78	-1.78	9.10	-7.83	-6.83

B1

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.65	0.24	-0.27	-0.30	-0.32	0.46	-0.40	-0.32	-0.04	0.30
^4TSE	1.23	0.87	0.10	0.36	0.43	0.45	-0.39	-0.35	0.00	0.29
^4I	1.89	0.33	-0.13	0.02	0.89	0.50	-0.52	-0.36	0.02	0.36

B2

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.74	0.16	-0.28	-0.27	-0.35	0.04	-0.09	0.04	-0.19	0.20
^4TSE	1.33	0.81	0.05	0.35	0.46	0.09	-0.11	-0.01	-0.13	0.16
^4I	1.96	0.28	-0.16	0.01	0.91	0.20	-0.19	0.03	-0.13	0.09

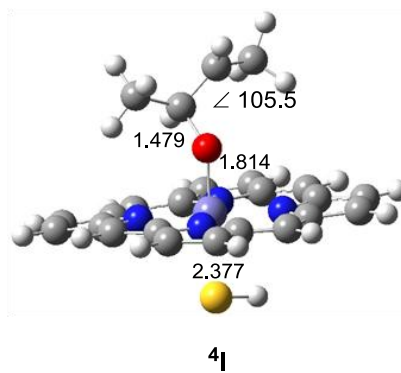
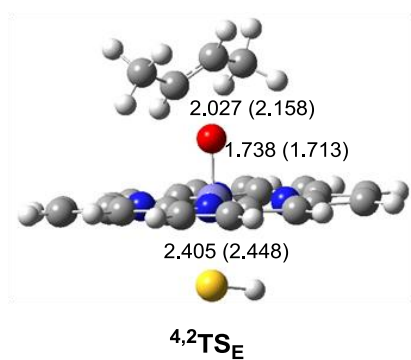


Table S7. Energetic and geometric data for the reaction of Ethene with Cpd I(SH).

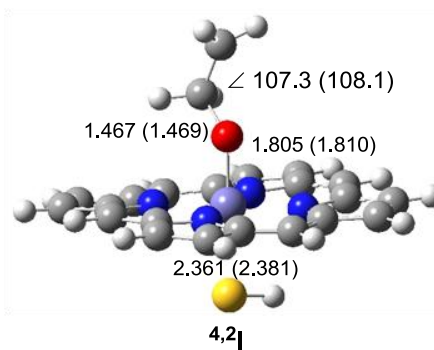
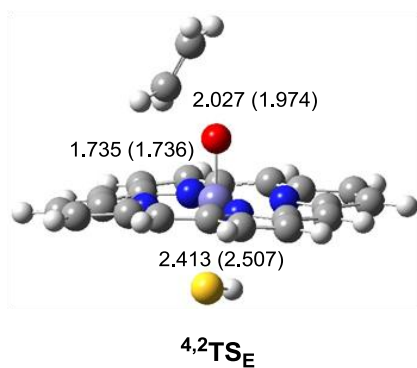
	B1			B2	
	ΔE	$\Delta E+ZPE$	ΔG	ΔE	$\Delta E+ZPE$
$^2\text{CpdI} + \text{Sub.}$	0.11	0.02	0.34	-0.04	-0.13
$^4\text{CpdI} + \text{Sub.}$	0.00	0.00	0.00	0.00	0.00
^2TSE	14.18	14.21	25.12	14.23	14.26
^4TSE	12.90	13.26	24.09	13.74	14.10
^2I	-0.20	0.62	11.90	-6.38	-5.55
^4I	-0.52	0.51	10.02	-7.01	-5.98

B1

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.75	0.19	-0.28	-0.34	-0.32	0.48	-0.40	-0.28	-0.04	0.23
^4TSE	1.11	0.91	0.23	0.45	0.30	0.46	-0.35	-0.28	-0.01	0.18
^2I	1.86	0.31	-0.14	-0.15	-0.88	0.49	-0.50	-0.33	0.02	0.32
^4I	1.81	0.35	-0.12	0.04	0.92	0.48	-0.50	-0.34	0.02	0.33

B2

	Spin Densities					Group Charges				
	Fe	O	Por	SH	Sub.	Fe	O	Por	SH	Sub.
^2TSE	1.80	0.18	-0.31	-0.33	-0.34	0.15	-0.10	0.11	-0.18	0.01
^4TSE	1.20	0.85	0.18	0.45	0.32	0.17	-0.04	0.04	-0.12	-0.05
^2I	1.93	0.29	-0.17	-0.14	-0.91	0.11	-0.13	0.11	-0.12	0.03
^4I	1.88	0.29	-0.15	0.04	0.95	0.10	-0.13	0.10	-0.12	0.05



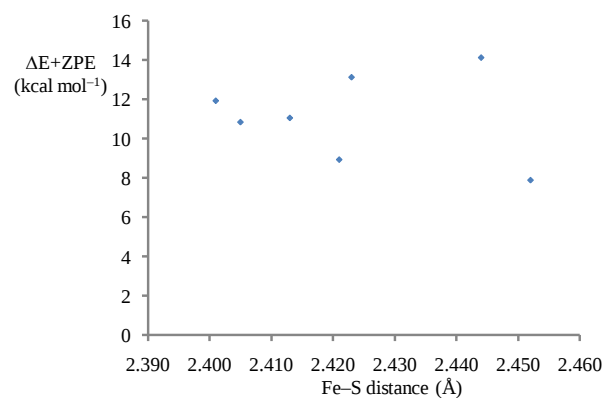


Figure S1: Correlation of Fe–S distance with the barrier height for epoxidation reactions by Cpd I(SH).

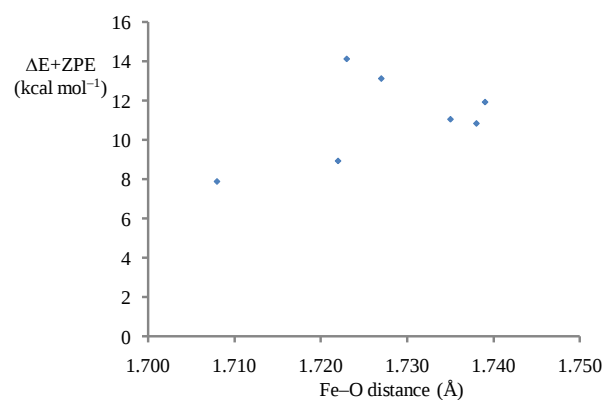


Figure S2: Correlation of Fe–O distance with the barrier height for epoxidation reactions by Cpd I(SH).

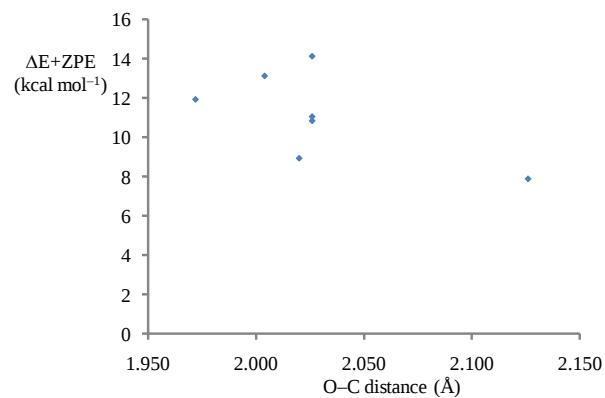


Figure S3: Correlation of O–C distance with the barrier height for epoxidation reactions by Cpd I(SH).

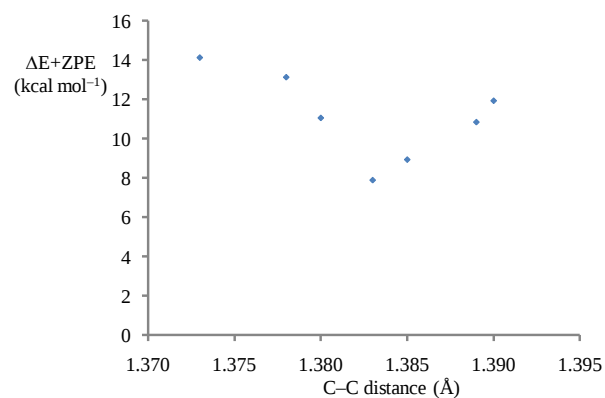


Figure S4: Correlation of C–C distance with the barrier height for epoxidation reactions by Cpdl(SH).

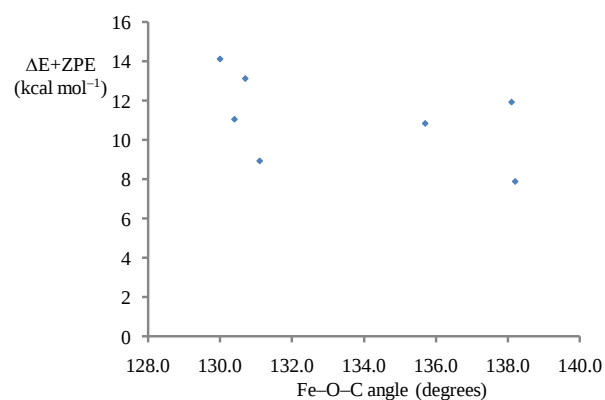


Figure S5: Correlation of Fe–O–C angle with the barrier height for epoxidation reactions by Cpdl(SH).

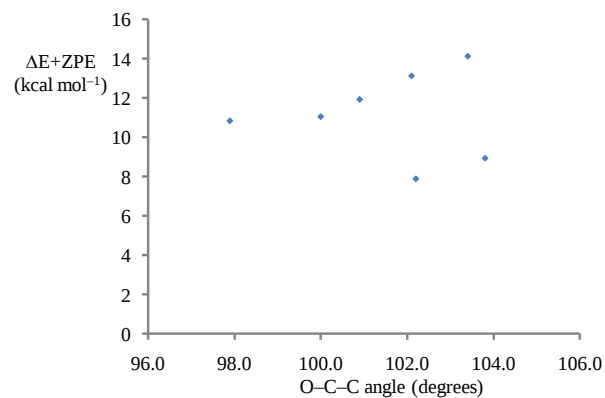


Figure S6: Correlation of O–C–C angle with the barrier height for epoxidation reactions by Cpdl(SH).

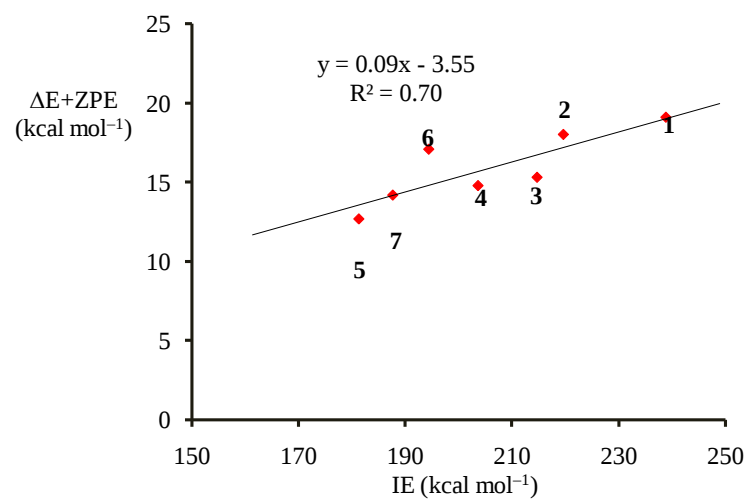


Figure S7: Correlation of solvent corrected ($\epsilon = 5.7$) barrier heights with ionization energy.

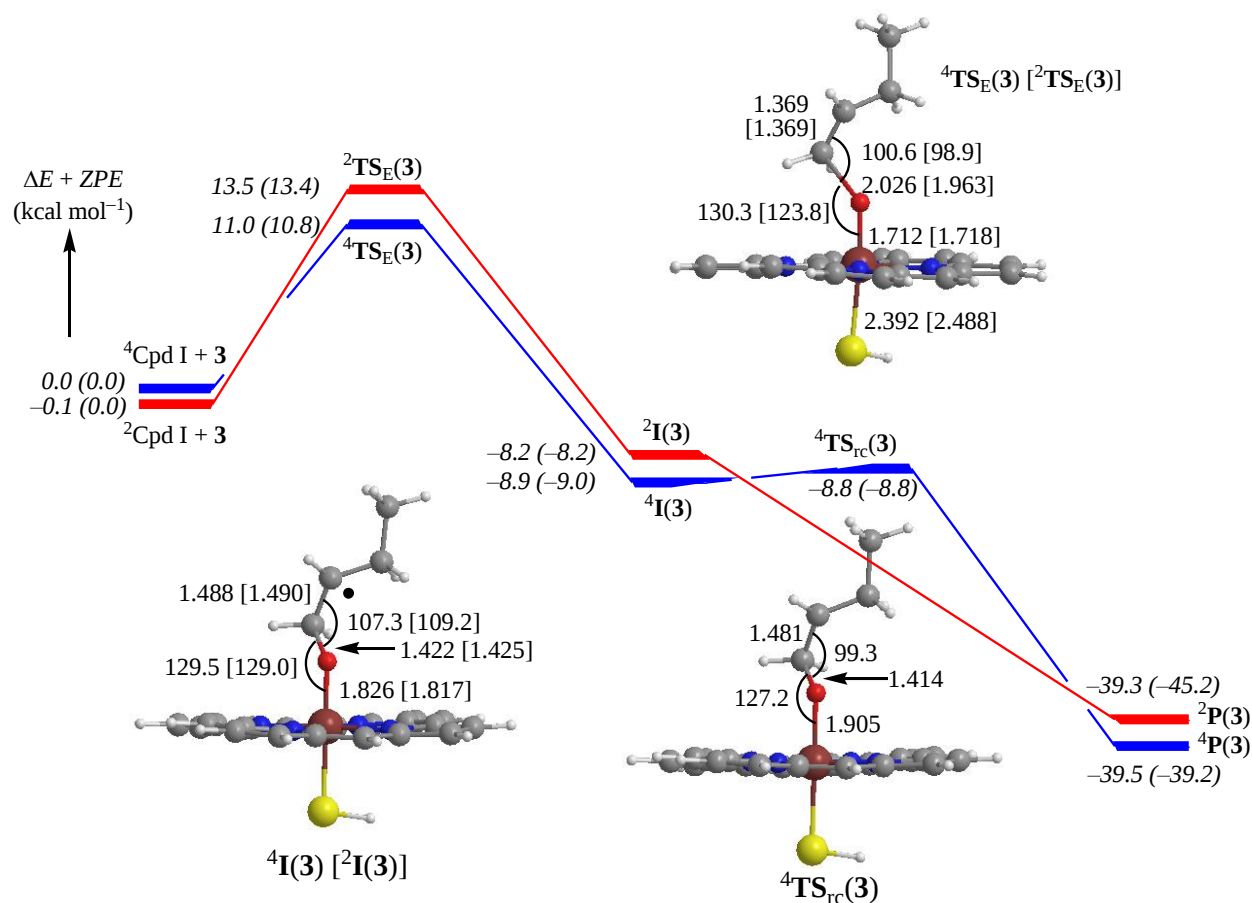


Figure S8. Reaction profile of 1-butene (**3**) epoxidation by ^{4,2}Cpd I(SH) with energies in kcal mol⁻¹. Also shown are optimized geometries of the critical points along the reaction mechanism obtained at UB3LYP/B2 with distances in angstroms, angles in degrees and the value of the imaginary frequency in the transition state in wave numbers. Energies reported outside parenthesis are obtained with basis set B2 on UB3LYP/B1 optimized geometries and contain ZPE corrections with basis set B1. Inside parenthesis are energies (including ZPE) reported at UB3LYP/B2 after a UB3LYP/B2 geometry optimization and frequency.

Table S8. Absolute energies of optimized UB3LYP/B1 structures.

		E (au), B1	ZPE (au)	G (au)	E (au), B2
Cpd I(SH)	⁴ CpdI	-1585.520561	0.289312	-1585.280461	-1586.102247
	² CpdI	-1585.520364	0.289219	-1585.279922	-1586.102317
Ethene	⁴ TS _E	-1664.072005	0.341609	-1663.783955	-1664.688552
	⁴ I _E	-1664.093391	0.342673	-1663.806377	-1664.721619
	² TS _E	-1664.069973	0.341090	-1663.782314	-1664.687771
	² I _E	-1664.092890	0.342350	-1663.803376	-1664.720607
	Substrate	-78.572033	0.051674	-78.541886	-78.608198
1-Butene	⁴ TS _E	-1742.687800	0.399314	-1742.348458	-1743.339741
	⁴ I _E	-1742.709863	0.400545	-1742.366730	-1743.372719
	² TS _E	-1742.685727	0.398307	-1742.343443	-1743.334819
	² I _E	-1742.708908	0.400226	-1742.366136	-1743.371375
	⁴ TS _{reb}	-1742.707947	0.399313	-1742.364619	-1743.371394
	⁴ P	-1742.749302	0.401031	-1742.404691	-1743.421969
	² P	-1742.753003	0.403381	-1742.404800	-1743.423959
	Substrate	-157.182997	0.109218	-157.100483	-157.254341
<i>trans</i> -2-Butene	⁴ TS _E	-1742.694830	0.398993	-1742.352927	-1743.345483
	⁴ I _E	-1742.713970	0.399712	-1742.373138	-1743.374337
	² TS _E	-1742.694216	0.398342	-1742.354683	-1743.346139
	Substrate	-157.189008	0.108770	-157.189008	-157.259617
1,3 cyclohexadiene	⁴ TS _E	-1818.875904	0.413361	-1818.521050	-1819.561231
	⁴ I _E	-1818.910007	0.414834	-1818.555258	-1819.606035
	² TS _E	-1818.873395	0.412342	-1818.516526	-1819.557796
	Substrate	-233.365489	0.123707	-233.270030	-233.471237
1,4 cyclohexadiene	⁴ TS _E	-1818.866962	0.412742	-1818.511604	-1819.554045
	⁴ I _E	-1818.884065	0.413877	-1818.526891	-1819.580518
	² TS _E	-1818.866853	0.412260	-1818.512054	-1819.551677
	Substrate	-233.364604	0.123533	-233.269654	-233.470923

Cartesian Coordinates of all structures described in this work:

²Cpd I

Fe	-0.0037160584308864	0.0064336580819741	0.0107059258134274
N	-0.0024246943150945	-0.0092799284181174	2.0231002994638496
N	2.0148992970174926	-0.0008212749459542	0.0186927430676205
N	-2.0024813613820234	-0.2633319388621611	0.0056514317756367
N	0.0189239131364347	-0.2759830555558580	-1.9921025827884689
C	-1.1092089411735124	-0.0535665492507352	2.8517968289915037
C	2.8528601316871818	-0.0103114341197614	-1.0831443398612381
C	1.0902370027132102	0.1322560496574783	2.8559575972714026
C	2.8417847727594916	0.1382315581142697	1.1241983829771152
C	-2.8388699405280713	-0.2718465207742172	1.1100734705006763
C	1.1315093562877032	-0.2484631732951400	-2.8253494277072009
C	-2.8306314570689413	-0.3553688942932470	-1.0989587035106416
C	-1.0842526132545649	-0.3709477101861339	-2.8357216700409889
C	-0.6993620660789174	0.0593216171705655	4.2365141236357573
C	4.2323081453916158	0.1175421770704543	-0.6596051377849874
C	0.6618416858580412	0.1769046076902504	4.2389181804151912
C	4.2255000822533981	0.2085530735690926	0.7025816361859845
C	-4.2189785619955087	-0.3804953435231058	0.6866360987353302
C	0.7160293777614449	-0.3564640236827452	-4.2077183615840497
C	-4.2140504451161265	-0.4290805361130580	-0.6788311898552941
C	-0.6473746763078621	-0.4317966373339886	-4.2142830272971477
H	-1.3749741304216405	0.0499222724774628	5.0791161178270157
H	5.0790414640238932	0.1328840959596891	-1.3298460892342208
H	1.3261844210247762	0.2815905446406458	5.0840045318960998
H	5.0655235349280785	0.3131247317981534	1.3733738848790407
H	-5.0653337110526735	-0.4125712149122920	1.3568372465545142
H	1.3925475986614828	-0.3684339812720386	-5.0495711472623910
H	-5.0553168370280064	-0.5100016654304377	-1.3514204186286367
H	-1.3102002465916687	-0.5180480782492773	-5.0626595281080862
C	-2.4245438441429852	-0.1817409408684922	2.4302085724631231
C	2.4432292999164007	-0.1181262656742708	-2.4043281080942780
C	-2.4042085604245544	-0.3986871258948436	-2.4211640705654109
C	2.4137647312727788	0.2035276289717433	2.4393681818320543
H	-3.1932263338600957	-0.2024180075198177	3.1957504162136079
H	3.2134289285013788	-0.1029398450078262	-3.1681795811861662
H	-3.1675161294900116	-0.4697534748157446	-3.1888766865292522
H	3.1726848999365989	0.3148203199155226	3.2067026548933928
O	-0.1097788961362226	1.6467866265519220	-0.1131918512012945
S	0.2998997703565072	-2.5678090968996381	-0.1288983105081848
H	-0.8645007488767714	-2.8730481592895396	-0.8091483105277611

⁴Cpd I

Fe	0.0071280916812239	0.0732833942946873	0.0145753128492106
N	-0.0016059910196432	0.0392090824030704	2.0298617784866577

N	2.0178568929209630	-0.0912519800907542	0.0302364188398275
N	-2.0056328905274716	-0.0305420836358360	0.0028496887637697
N	0.0160395303983140	-0.1784544389110838	-1.9903094733058140
C	-1.1110621698100080	0.0855721226818938	2.8547248908292175
C	2.8578818102760488	-0.1440709297205048	-1.0683786744746593
C	1.0956991530085736	0.0781525202588978	2.8677136694260668
C	2.8480973475146474	-0.0436878791976254	1.1413513235106822
C	-2.8439577711395518	0.0215437741564461	1.1049938643612354
C	1.1316687544531565	-0.2148750159024876	-2.8197929969379847
C	-2.8337192739553800	-0.0446497663291797	-1.1052461849223372
C	-1.0878647335503639	-0.1718543700399263	-2.8381980885211147
C	-0.6984431660551670	0.1538831717204301	4.2417575365392892
C	4.2410562992487373	-0.1374180209912457	-0.6375549679739235
C	0.6671665559046314	0.1517147435501913	4.2497234436460296
C	4.2348475372112109	-0.0775392908863021	0.7259330496302094
C	-4.2265751483097409	0.0302201371642151	0.6758103323097561
C	0.7142856830115791	-0.2575271119492803	-4.2047641940373985
C	-4.2203669616763566	-0.0076168810683224	-0.6901411396150404
C	-0.6509018811554838	-0.2323495102808825	-4.2163437298519479
H	-1.3755010761071036	0.1984136525615731	5.0821835895373297
H	5.0899766318559685	-0.1762020923532265	-1.3041071853081618
H	1.3344876388656550	0.1934092906623716	5.0980608390961333
H	5.0773231550318307	-0.0565677514669530	1.4016312723490651
H	-5.0752888816485209	0.0630249392255136	1.3430765691103144
H	1.3912942078626107	-0.2991191328739001	-5.0452620435488811
H	-5.0627592624183100	-0.0125175921392359	-1.3661307360100341
H	-1.3146633038858533	-0.2486646584043838	-5.0682405525296268
C	-2.4305072198017976	0.0686452299248206	2.4276299136855841
C	2.4472889085669789	-0.1898681399540247	-2.3928481386877025
C	-2.4071826645939010	-0.1039494437044393	-2.4271533446878300
C	2.4220303676721615	0.0365394834748646	2.4563112251864121
H	-3.2017160582676363	0.1066565851996164	3.1898749947904554
H	3.2200837865897145	-0.2148892326910867	-3.1536018721866372
H	-3.1709856557810201	-0.1012130722330919	-3.1975983096050240
H	3.1845694041187458	0.0718481253209162	3.2273080292386029
O	0.0239609717348811	1.7244186361128204	-0.0491591366858093
S	0.1202980969237150	-2.4910832148668369	-0.1763000187553427
H	-1.0811659912838600	-2.6943234653515820	-0.8290780287450273

1-butene ²TS_E

Fe	-0.0083140002	0.0261717673	0.0052310950
N	-0.0131418194	-0.0617378192	2.0291137628
N	2.0176252314	-0.0048315973	0.0370127119
N	-2.0032846700	-0.1492768302	-0.0176614621
N	0.0144700299	-0.0540012434	-2.0017323142
C	-1.1283897321	-0.0370861169	2.8488050438
C	2.8567538180	0.1223918512	-1.0600776357
C	1.0842431377	-0.0883352651	2.8738648935
C	2.8416687001	-0.0223938127	1.1513331131
C	-2.8469646769	-0.1280550276	1.0812344924
C	1.1269972418	0.0563245584	-2.8204031611

C	-2.8215781145	-0.3254809813	-1.1242938581
C	-1.0676158945	-0.2363549161	-2.8506524226
C	-0.7195717199	-0.0497034516	4.2403196604
C	4.2368624439	0.1670424464	-0.6215128067
C	0.6435219095	-0.0890867171	4.2552326600
C	4.2273409405	0.0711881025	0.7402593238
C	-4.2215043280	-0.2737985242	0.6511933328
C	0.7292035056	-0.0337131047	-4.2098975503
C	-4.2045446565	-0.4074251001	-0.7082773450
C	-0.6239263255	-0.2241990163	-4.2280331653
H	-1.3994833520	-0.0406443884	5.0794959259
H	5.0878675097	0.2566979828	-1.2807841708
H	1.3046391880	-0.1138737520	5.1089932329
H	5.0687262123	0.0707808290	1.4175465192
H	-5.0735570969	-0.2883029772	1.3151867635
H	1.4086531040	0.0250540682	-5.0479578012
H	-5.0398362152	-0.5475461368	-1.3785125100
H	-1.2719867966	-0.3468246902	-5.0836662691
C	-2.4424573377	-0.0470149080	2.4082153515
C	2.4416186016	0.1677421798	-2.3827561247
C	-2.3855018442	-0.3798768149	-2.4403559631
C	2.4090185786	-0.0769373623	2.4679752585
H	-3.2211285640	-0.0375543902	3.1639228629
H	3.2118618894	0.2525453382	-3.1426995886
H	-3.1365058179	-0.5221878199	-3.2103123176
H	3.1688298093	-0.0885483598	3.2424313044
O	0.0698546934	1.7540777043	0.1558023696
S	0.2035815550	-2.4649622971	0.1871377769
H	1.3461628963	-2.6328152099	-0.5724223681
C	-1.1102761513	3.0012701640	-0.8181143218
H	-1.7687202279	3.1353997989	0.0316904260
H	-1.4329565473	2.2853658790	-1.5653621989
C	-0.1753748619	3.9591883323	-1.1362479700
H	0.0389726835	4.7424581525	-0.4086584328
C	0.6933266261	3.9346586752	-2.3563789069
H	1.6923787174	3.5672179206	-2.0638187487
H	0.3050100254	3.2075141815	-3.0804466808
C	0.8495005255	5.3218223123	-3.0152067909
H	1.2622609729	6.0496616072	-2.3056670970
H	1.5268801807	5.2713800111	-3.8749521480
H	-0.1165103524	5.7039993894	-3.3643212290

1-butene ⁴TS_E

Fe	0.0022486967	-0.0040386047	0.0026425347
N	0.0019398058	-0.0056659347	2.0008827090
N	1.9990173143	-0.0062852573	-0.0157421643
N	-2.0268683686	-0.1501586180	0.0042360190
N	-0.0102811519	-0.1406975517	-2.0288481094
C	-1.1072132039	0.0369733170	2.8343714021
C	2.8253693304	0.0645109154	-1.1312459245
C	1.1091969799	-0.0293596331	2.8310810112

C	2.8387327725	-0.0240224516	1.0866365541
C	-2.8560808353	-0.0941433831	1.1078084775
C	1.0860749837	-0.0535256963	-2.8685453808
C	-2.8537045023	-0.3044633652	-1.0990050823
C	-1.1202012147	-0.2903910182	-2.8495244997
C	-0.6774145651	0.0535164374	4.2180071257
C	4.2102246474	0.0942535756	-0.7103375092
C	0.6861568384	0.0043468889	4.2162986200
C	4.2188549523	0.0317258333	0.6533125933
C	-4.2379481594	-0.2090481806	0.6902241772
C	0.6564920416	-0.1500870061	-4.2472601843
C	-4.2357116421	-0.3448336990	-0.6690775188
C	-0.7015682422	-0.3024082394	-4.2349762225
H	-1.3465454533	0.0856517743	5.0656620814
H	5.0529368583	0.1474962487	-1.3840640540
H	1.3584093625	-0.0068341557	5.0618675044
H	5.0696574226	0.0281176022	1.3191093851
H	-5.0841690697	-0.1977875038	1.3614497135
H	1.3190644457	-0.1145190332	-5.0996701174
H	-5.0799292834	-0.4631778019	-1.3324664863
H	-1.3706967291	-0.4123555882	-5.0757320122
C	-2.4299670305	0.0134037623	2.4255983496
C	2.4061406140	0.0612405672	-2.4512869945
C	-2.4362784754	-0.3746868668	-2.4197324809
C	2.4292549958	-0.0528584150	2.4103345317
H	-3.1922565341	0.0431485730	3.1969444318
H	3.1709888039	0.1158231446	-3.2187820677
H	-3.2021680693	-0.4904705298	-3.1794334615
H	3.1997125488	-0.0674994090	3.1736857798
O	-0.0579459456	1.7287738491	-0.0457065462
S	-0.0902445111	-2.4145266823	-0.0496809719
H	0.9240414440	-2.6222050579	-0.9658583137
C	-1.1834046273	2.9729986980	-1.1822727693
H	-2.1213137919	2.6480436980	-0.7507948660
H	-0.8910618170	2.4901847488	-2.1084706623
C	-0.6275981748	4.1863165457	-0.8299471131
H	-1.0331525009	4.7196582316	0.0296483146
C	0.6109739120	4.7557534331	-1.4512721326
H	1.4590158041	4.5589002439	-0.7736644047
H	0.8403777234	4.2238598945	-2.3832438625
C	0.5220685961	6.2743354616	-1.7077883491
H	0.3071647370	6.8175716437	-0.7775662771
H	1.4662664596	6.6578104492	-2.1108629862
H	-0.2765081139	6.5084003992	-2.4227300546

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Fe	-0.0175369473	-0.0206792525	-0.0088392441
N	-0.0006266835	0.0295327963	2.0020616298
N	1.9950140645	0.0150696963	-0.0373371976
N	-2.0295077541	-0.1309913197	0.0178235067
N	-0.0351897487	-0.1573801593	-2.0231740993

C	-1.0992669188	0.1032474304	2.8421673504
C	2.8093621857	0.0957574425	-1.1567850036
C	1.1182490072	0.0338801649	2.8173154451
C	2.8358936729	0.0301194772	1.0624360775
C	-2.8517034774	-0.0503304611	1.1306325131
C	1.0581604996	-0.0644686274	-2.8717384733
C	-2.8641638336	-0.3279227876	-1.0742071770
C	-1.1477653506	-0.3389543984	-2.8331527243
C	-0.6555882266	0.1590739093	4.2190943224
C	4.1947381833	0.1602193591	-0.7442971216
C	0.7083831343	0.1074393782	4.2040632056
C	4.2116103603	0.1110508121	0.6207091791
C	-4.2326293788	-0.1841066440	0.7237024620
C	0.6176965418	-0.1861141308	-4.2433443530
C	-4.2397786197	-0.3637156200	-0.6309187334
C	-0.7376478168	-0.3636946046	-4.2190944162
H	-1.3156715623	0.2211558054	5.0719710887
H	5.0320492863	0.2277719383	-1.4233658245
H	1.3895823084	0.1239767644	5.0419928381
H	5.0654793541	0.1350930678	1.2819757431
H	-5.0741898933	-0.1549240964	1.4000646423
H	1.2725714121	-0.1472932101	-5.1017516835
H	-5.0887596568	-0.5057484745	-1.2836587072
H	-1.4109441232	-0.4944513837	-5.0535923746
C	-2.4255938760	0.0844966498	2.4431917432
C	2.3796621437	0.0751813003	-2.4742044904
C	-2.4597457746	-0.4361098853	-2.3950364881
C	2.4353374544	0.0175478504	2.3891557890
H	-3.1848708433	0.1382535151	3.2152682616
H	3.1342122496	0.1365700685	-3.2507429172
H	-3.2292844967	-0.5820888259	-3.1448523066
H	3.2101800828	0.0292298968	3.1476506131
O	-0.0556024133	1.7883287718	-0.0937731031
S	0.0269980105	-2.3852613157	0.1137834695
H	1.0024774442	-2.5912442500	-0.8422902246
C	-0.9161657901	2.6912055033	-0.8685776450
H	-1.9310655539	2.6334234312	-0.4560100156
H	-0.9386647647	2.3471492238	-1.9104188081
C	-0.3342089755	4.0527517908	-0.7485035592
H	-0.5642266096	4.6262510374	0.1488402284
C	0.8063750335	4.5093485324	-1.6019750685
H	1.7575904088	4.1746370772	-1.1474331502
H	0.7598838261	4.0088970202	-2.5804095306
C	0.8586243905	6.0392093353	-1.7900098355
H	0.9279535801	6.5509936830	-0.8223378718
H	1.7286773197	6.3321959576	-2.3880886914
H	-0.0419151082	6.4041158020	-2.2971439232

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Fe	-0.0205647577	-0.0087522716	-0.0085835490
N	-0.0079900707	0.0056419325	2.0067445824

N	1.9942040424	0.0160665386	-0.0297774223
N	-2.0297785853	-0.1266685177	0.0138040513
N	-0.0320804770	-0.1333349723	-2.0187716041
C	-1.1077637759	0.0679276748	2.8454063217
C	2.8122956281	0.1055675619	-1.1449473768
C	1.1091950350	-0.0020143422	2.8241570994
C	2.8313901802	0.0151756667	1.0730578517
C	-2.8550605208	-0.0612648332	1.1269531633
C	1.0646536325	-0.0339745513	-2.8643747492
C	-2.8625976303	-0.3157250818	-1.0810798193
C	-1.1420350102	-0.3091868795	-2.8347025366
C	-0.6673819414	0.1037404731	4.2240858810
C	4.1966187440	0.1603487358	-0.7278263760
C	0.6967021274	0.0524291556	4.2111579552
C	4.2088234528	0.0960794317	0.6366104156
C	-4.2346586995	-0.1930585423	0.7156292305
C	0.6277725337	-0.1436582677	-4.2377289845
C	-4.2387345241	-0.3586640985	-0.6408064278
C	-0.7275690996	-0.3221536784	-4.2191682358
H	-1.3293317316	0.1535147199	5.0762972241
H	5.0362405979	0.2324415738	-1.4034345717
H	1.3761558101	0.0574605279	5.0508118821
H	5.0606340627	0.1096056861	1.3007880597
H	-5.0776604105	-0.1727758867	1.3905265364
H	1.2851066219	-0.0968029916	-5.0938178830
H	-5.0861197830	-0.4955827921	-1.2967031949
H	-1.3982720296	-0.4460268934	-5.0569514932
C	-2.4331791829	0.0561282375	2.4420879461
C	2.3851277256	0.1001503014	-2.4634830312
C	-2.4552376569	-0.4120336865	-2.4017710351
C	2.4271049012	-0.0130697897	2.3982432214
H	-3.1949897651	0.0998629993	3.2124680502
H	3.1410153874	0.1684438455	-3.2380761641
H	-3.2224028804	-0.5526504571	-3.1549254347
H	3.2001901635	-0.0122074780	3.1586237573
O	-0.0418057785	1.7985282874	-0.0521425772
S	0.0425665165	-2.3850598514	0.1114665673
H	0.9847295356	-2.5786407775	-0.8801699801
C	-0.9174323214	2.7184732366	-0.7991829711
H	-1.9102975203	2.6854886247	-0.3341800131
H	-0.9997355621	2.3525020602	-1.8311437230
C	-0.3189711230	4.0775558778	-0.7498773247
H	-0.5014589042	4.6803454678	0.1399674771
C	0.7864837258	4.4970763923	-1.6675768413
H	1.7570288278	4.1734822641	-1.2455155770
H	0.6983607770	3.9630318315	-2.6253141129
C	0.8384854850	6.0185310812	-1.9133413783
H	0.9528280481	6.5651637717	-0.9693948402
H	1.6823803009	6.2853282530	-2.5587252463
H	-0.0812763312	6.3724126994	-2.3926293136

1-butene ⁴TS_{reb}

Fe	0.0078386108	-0.0121142863	0.0079989970
N	0.0050699497	-0.0231830909	2.0208063770
N	2.0222613837	-0.0295393544	0.0058394278
N	-2.0067387340	0.0138458101	0.0040133637
N	0.0081043671	-0.0002455810	-2.0143584394
C	-1.1012975683	0.0494479927	2.8506669588
C	2.8525402231	0.0657449155	-1.1004826297
C	1.1121532080	-0.1047635754	2.8491490241
C	2.8507249941	-0.0991266157	1.1136166120
C	-2.8380320691	0.0662201289	1.1123462732
C	1.1172614901	0.0759187685	-2.8433653040
C	-2.8370342490	-0.0742270246	-1.1061884288
C	-1.1002814719	-0.0742335985	-2.8464241373
C	-0.6751162224	0.0158240218	4.2339488405
C	4.2344907962	0.0519020797	-0.6720357200
C	0.6865653343	-0.0863320700	4.2328846294
C	4.2335406451	-0.0577640029	0.6900004400
C	-4.2184760418	0.0251335418	0.6851588759
C	0.6915787042	0.0525328054	-4.2252182448
C	-4.2177104809	-0.0688481440	-0.6785636407
C	-0.6720643194	-0.0476944708	-4.2271833822
H	-1.3438607516	0.0568506003	5.0813758426
H	5.0822895758	0.1116284409	-1.3386952167
H	1.3555890912	-0.1407472967	5.0793113410
H	5.0803397665	-0.1007902454	1.3594238934
H	-5.0663622688	0.0517516402	1.3537578718
H	1.3601581827	0.0979781379	-5.0726332053
H	-5.0647461077	-0.1298261537	-1.3459715268
H	-1.3386606225	-0.0969289135	-5.0759387060
C	-2.4223018832	0.1044216689	2.4351502762
C	2.4382941468	0.1255615641	-2.4224919998
C	-2.4216143459	-0.1246852518	-2.4276639008
C	2.4330834217	-0.1553425617	2.4345139602
H	-3.1890609886	0.1444326276	3.2009698162
H	3.2058011509	0.1848616043	-3.1864850234
H	-3.1882449715	-0.1873679403	-3.1921724533
H	3.1982072449	-0.2126835811	3.2008743095
O	0.0646481025	1.9180095757	0.0141947193
S	-0.0622054623	-2.4475052773	0.0060561730
H	0.9285191341	-2.6454982300	-0.9364537683
C	-0.7898542062	2.8404797056	-0.7190509554
H	-1.8231134430	2.8013609412	-0.3589375866
H	-0.7655858018	2.6444857911	-1.7962557365
C	-0.0916506082	4.0911742160	-0.3603660480
H	-0.2904500431	4.5077630321	0.6244953565
C	1.0688343314	4.6265192802	-1.1302470851
H	1.9916737085	4.1422630089	-0.7666076739
H	0.9795232648	4.3369842736	-2.1854698896
C	1.2248686539	6.1550833209	-1.0001462524
H	1.3448745783	6.4489334673	0.0481109723

H	2.1062694118	6.5011998695	-1.5492510392
H	0.3483693211	6.6785643381	-1.3981192685

1-butene ⁴P

Fe	-0.0178280386	-0.0492810758	0.0014702268
N	-0.0222357260	0.0051359660	2.0151090852
N	1.9935118079	0.0792999167	0.0110020028
N	-2.0273854422	0.1220496086	0.0026034066
N	-0.0101279054	0.1745336054	-2.0045588601
C	-1.1317040134	0.0130854213	2.8477603763
C	2.8331940543	0.1791722122	-1.0918219939
C	1.0850293715	-0.0758510186	2.8494862803
C	2.8262653617	-0.0041399968	1.1197346517
C	-2.8656591892	0.1081426981	1.1085822766
C	1.1013517698	0.2565338782	-2.8332708818
C	-2.8581244926	0.1329919329	-1.1108677000
C	-1.1165577451	0.1883713328	-2.8429104702
C	-0.7078026236	-0.0602175694	4.2286645885
C	4.2129367516	0.1595708945	-0.6613354114
C	0.6572143727	-0.1186450408	4.2298782630
C	4.2084453534	0.0417443429	0.7004139811
C	-4.2453221962	0.1218791718	0.6772721820
C	0.6798823526	0.3193668199	-4.2142804685
C	-4.2404553266	0.1344002322	-0.6898219618
C	-0.6863034685	0.2731502693	-4.2206673862
H	-1.3791153944	-0.0718042897	5.0747268627
H	5.0631149510	0.2213219385	-1.3250048941
H	1.3249093668	-0.1852642116	5.0767241972
H	5.0541414341	-0.0089099970	1.3705915010
H	-5.0956609216	0.1133283826	1.3437900449
H	1.3519284775	0.3849855149	-5.0576319352
H	-5.0848400054	0.1408700917	-1.3628552865
H	-1.3528585440	0.2961434046	-5.0702866266
C	-2.4532988521	0.0642759784	2.4320146629
C	2.4223816889	0.2644332426	-2.4131218837
C	-2.4398060480	0.1577289534	-2.4319542084
C	2.4077775694	-0.0896692003	2.4379219606
H	-3.2218086024	0.0531319484	3.1973131781
H	3.1920373777	0.3302373991	-3.1743798952
H	-3.2041981354	0.1649507454	-3.2010566450
H	3.1723581784	-0.1565455928	3.2044283955
O	-0.0300698094	2.4627288987	0.0435787813
S	-0.0827771298	-2.5397260459	-0.0814749791
H	0.9147287454	-2.6948379328	-1.0264483518
C	-0.8430553636	3.5962674878	-0.4784222391
H	-1.7606989471	3.7841086635	0.0696765020
H	-0.9364264247	3.6126504985	-1.5594366711
C	0.4803487804	3.8724135458	0.1334578904
H	0.4874939923	4.2320908351	1.1593048317
C	1.7220805082	4.1883489468	-0.6759012952
H	2.3820932440	3.3148232439	-0.6333840615

H	1.4579510795	4.3283097674	-1.7302094662
C	2.4668122881	5.4283318738	-0.1558125673
H	2.7733786891	5.2878740507	0.8842683428
H	3.3692407744	5.6192150355	-0.7451266677
H	1.8416942936	6.3287087992	-0.2030217090

1-butene ²P

Fe	0.0073887673	-0.0477518498	-0.0138759665
N	0.0210269350	0.0290432179	1.9956289781
N	2.0211354081	-0.0759251697	-0.0585955058
N	-2.0021848816	0.1257101343	0.0234648375
N	-0.0001761170	0.0243767661	-2.0286381810
C	-1.0677438744	0.0985640916	2.8501300240
C	2.8491807799	-0.1439913249	-1.1729408637
C	1.1414860002	-0.0317569531	2.8074549913
C	2.8606488943	-0.1299722892	1.0454900511
C	-2.8274815027	0.1646054991	1.1389520016
C	1.0899122437	-0.0560872667	-2.8881727752
C	-2.8472517234	0.1181459329	-1.0777520136
C	-1.1272430783	0.0417892505	-2.8425909438
C	-0.6185816597	0.0847859893	4.2270625791
C	4.2322131423	-0.2276051631	-0.7556513125
C	0.7433932687	0.0048162368	4.2007974367
C	4.2391186163	-0.2177151923	0.6109574630
C	-4.2148467851	0.1951095868	0.7260359336
C	0.6355535012	-0.0643116249	-4.2611626011
C	-4.2274599800	0.1660351162	-0.6398898549
C	-0.7294535649	-0.0038061867	-4.2332545995
H	-1.2725778692	0.1286157246	5.0859280719
H	5.0739735457	-0.2878531783	-1.4303382379
H	1.4296339318	-0.0291105233	5.0343330238
H	5.0888932494	-0.2690306643	1.2762643342
H	-5.0558345163	0.2275170354	1.4039387849
H	1.2857752355	-0.1169538540	-5.1220850725
H	-5.0812063812	0.1708388636	-1.3025205544
H	-1.4166570367	0.0017268205	-5.0669638332
C	-2.3952087126	0.1608662171	2.4561407314
C	2.4178612278	-0.1328033308	-2.4923545489
C	-2.4436969020	0.0865644803	-2.4046638800
C	2.4555333881	-0.1054470756	2.3715955096
H	-3.1503777880	0.1973632616	3.2343762663
H	3.1721772677	-0.1960541487	-3.2695606096
H	-3.2204222492	0.0884175347	-3.1625133707
H	3.2305017752	-0.1498040808	3.1296890254
O	0.0060688421	2.1867671936	0.1520288904
S	-0.1295404203	-2.3400801419	0.0280582025
H	0.8373681474	-2.6055759120	-0.9243553572
C	-0.8884882719	3.1462692615	-0.5592216260
H	-1.6158705071	3.6283798174	0.0872579029
H	-1.2715307106	2.7690358456	-1.5018489908
C	0.5565879570	3.4621533836	-0.4498539409

H	0.8476640226	4.1417439312	0.3476523228
C	1.5234035043	3.3589353416	-1.6141230963
H	2.0221161652	2.3893497831	-1.5639768440
H	0.9734598864	3.3726212020	-2.5625207905
C	2.5754672931	4.4795492446	-1.6002399438
H	3.1265665342	4.4895689318	-0.6505667224
H	3.3023260239	4.3366448067	-2.4073962379
H	2.1185463931	5.4681381343	-1.7312605865

trans-2-butene ²TS_E

Fe	-0.0169942968	0.0164452664	-0.0671447128
N	-0.0129669559	0.0077242904	1.9589967427
N	2.0043192393	-0.0129505765	-0.0686991132
N	-2.0216685419	-0.1699527304	-0.0541098702
N	-0.0099448462	-0.1469503760	-2.0717198899
C	-1.1182192535	0.0254227166	2.7904994830
C	2.8362138280	0.0300359434	-1.1759816000
C	1.0970250005	0.0210944092	2.7840428129
C	2.8318046200	0.0141187677	1.0422041876
C	-2.8520385618	-0.1436191228	1.0552700456
C	1.0958088424	-0.1039823716	-2.9073607145
C	-2.8490078067	-0.3321350141	-1.1553057827
C	-1.1148615656	-0.3023269650	-2.8971803631
C	-0.6889591405	0.0638684616	4.1745363012
C	4.2181432889	0.0802758993	-0.7474133798
C	0.6750185357	0.0554171340	4.1707439415
C	4.2152685112	0.0645295750	0.6180270964
C	-4.2293555725	-0.2879024973	0.6371950477
C	0.6718744875	-0.2250608487	-4.2850819705
C	-4.2272645886	-0.4076464245	-0.7236685377
C	-0.6888670563	-0.3496687188	-4.2787455805
H	-1.3582260357	0.0842031596	5.0220680995
H	5.0659037253	0.1165009294	-1.4161402763
H	1.3490146501	0.0713396438	5.0148254049
H	5.0601921425	0.0888301434	1.2907608043
H	-5.0738539210	-0.3052250002	1.3103475245
H	1.3411795892	-0.2265648765	-5.1329614468
H	-5.0699366014	-0.5397605042	-1.3865881978
H	-1.3548959816	-0.4725550042	-5.1204831710
C	-2.4385711951	-0.0323998041	2.3752281939
C	2.4169517707	-0.0006419938	-2.4973727248
C	-2.4322614379	-0.3912685970	-2.4761582803
C	2.4166588412	0.0185710812	2.3644273387
H	-3.2067561754	-0.0239171161	3.1409119931
H	3.1803538336	0.0256443621	-3.2675210413
H	-3.1946606330	-0.5157597775	-3.2374902516
H	3.1854515189	0.0331196164	3.1293540108
O	0.0104271698	1.7265354419	0.0264349178
S	0.0665809330	-2.4246381485	0.0973835757
H	1.2244506162	-2.6188298739	-0.6311686189
C	-1.2158401495	3.1970504411	-0.9686024439

H	-1.6620218214	2.4462532857	-1.6157798436
C	-0.1059082174	3.8704643706	-1.4185312557
H	0.3071909855	4.6562378393	-0.7857254565
C	-2.0187564018	3.6258484630	0.2255536658
H	-2.9127626400	4.1829870131	-0.0926972572
H	-2.3532334525	2.7581220649	0.7996323952
H	-1.4327879031	4.2705984295	0.8878866738
C	0.6450120815	3.5514237650	-2.6695473973
H	0.8760375771	4.4624573684	-3.2382792669
H	1.6079414208	3.0793012396	-2.4237732177
H	0.0955707358	2.8598195434	-3.3149094969

trans-2-butene ⁴TS_E

Fe	0.0026933322	-0.0044541835	0.0026810609
N	0.0024926859	-0.0054602941	1.9963910794
N	2.0083787946	-0.0060616510	-0.0173105859
N	-2.0159969731	-0.1819575868	-0.0015571675
N	-0.0000301147	-0.1200965368	-2.0408959060
C	-1.1059043529	-0.0036358604	2.8312916694
C	2.8350852942	0.0544374592	-1.1326884503
C	1.1117017283	0.0002386199	2.8263094973
C	2.8452377102	0.0080121737	1.0853915530
C	-2.8476836085	-0.1704280000	1.1022674447
C	1.0996576903	-0.0594727214	-2.8761116098
C	-2.8397058352	-0.3203183515	-1.1102326802
C	-1.1079426607	-0.2553256430	-2.8628023267
C	-0.6757502695	0.0206944731	4.2146886119
C	4.2191131527	0.1029171283	-0.7105476208
C	0.6881994409	0.0177054034	4.2117059893
C	4.2258660409	0.0689163852	0.6542905611
C	-4.2257932156	-0.3043389119	0.6803212936
C	0.6733612503	-0.1511986129	-4.2574503404
C	-4.2201046212	-0.4000450434	-0.6823650819
C	-0.6876681114	-0.2737478442	-4.2489664625
H	-1.3447465751	0.0258016150	5.0627133750
H	5.0622962411	0.1507842638	-1.3841402167
H	1.3614318543	0.0236121779	5.0563025882
H	5.0753647246	0.0875261098	1.3214480334
H	-5.0721900917	-0.3292313308	1.3508846892
H	1.3395491820	-0.1335929989	-5.1076672704
H	-5.0616278022	-0.5169241791	-1.3493460815
H	-1.3567203115	-0.3761985194	-5.0910671828
C	-2.4269234439	-0.0680903188	2.4225341216
C	2.4197076936	0.0397927053	-2.4549085811
C	-2.4236910780	-0.3511972954	-2.4330030307
C	2.4321786954	-0.0022264873	2.4089290610
H	-3.1901455057	-0.0715947670	3.1933458956
H	3.1880952368	0.0789006630	-3.2199359140
H	-3.1901875221	-0.4591691370	-3.1931776238
H	3.2007037236	0.0049912700	3.1742710868
O	-0.0584869031	1.7314398483	-0.0461378975

S	-0.0445936933	-2.4075310637	-0.0924452998
H	1.1024286175	-2.5926532978	-0.8423439025
C	-1.1473616225	3.1171836467	-1.0464385932
H	-1.5997242525	2.3826539984	-1.7074719284
C	-0.0892571442	3.8700244078	-1.5402046613
H	0.2948548725	4.6789728909	-0.9180085426
C	-1.9920590622	3.5868479182	0.1102555366
H	-2.8221903180	4.2062431394	-0.2562309169
H	-2.4177464369	2.7407484160	0.6521818141
H	-1.4032642452	4.1853776925	0.8130988442
C	0.6497793769	3.5733496652	-2.8046561480
H	0.8580663479	4.4918540442	-3.3682263556
H	1.6235753911	3.1100693930	-2.5845160643
H	0.1013736053	2.8810072598	-3.4500257595

trans-2-butene ⁴I

Fe	-0.0398359341	-0.0031522373	0.0270473915
N	-0.0562237390	-0.0658021636	2.0364085915
N	1.9804557954	0.1050421912	0.0388183132
N	-2.0352789995	-0.2382523622	0.0070526384
N	-0.0112805022	-0.0359594357	-1.9970579447
C	-1.1691356350	-0.1118685631	2.8589045237
C	2.8099849339	0.2693815609	-1.0594048744
C	1.0485656060	-0.0428044839	2.8717205135
C	2.7983432953	0.1130674485	1.1545429128
C	-2.8784732198	-0.2844796410	1.1068051112
C	1.0947815565	0.1369816704	-2.8157356070
C	-2.8393937451	-0.4049702227	-1.1128424720
C	-1.0992307050	-0.2130517809	-2.8380808716
C	-0.7509996350	-0.1070440079	4.2449561552
C	4.1837510484	0.3775685199	-0.6168592610
C	0.6134424930	-0.0716244086	4.2524518522
C	4.1773621713	0.2744374833	0.7452469577
C	-4.2421113930	-0.4695348319	0.6639545246
C	0.6845742286	0.0794169182	-4.2015626965
C	-4.2171751368	-0.5493780053	-0.7001920249
C	-0.6643499580	-0.1419844521	-4.2151159324
H	-1.4263145036	-0.1376281972	5.0875374763
H	5.0296144922	0.5096613163	-1.2754606634
H	1.2797223765	-0.0622669290	5.1024419809
H	5.0167658735	0.3105314849	1.4242258313
H	-5.0943605049	-0.5387733164	1.3238257663
H	1.3540371610	0.1858807530	-5.0428593972
H	-5.0457117115	-0.6927339639	-1.3780901784
H	-1.3174118942	-0.2479640225	-5.0689064024
C	-2.4843899830	-0.1999674577	2.4334359600
C	2.4039129758	0.2949431286	-2.3851972632
C	-2.4117833485	-0.3990448379	-2.4307085716
C	2.3721592088	0.0271964966	2.4709035587
H	-3.2578937813	-0.2431802458	3.1918927736
H	3.1696069907	0.4187417295	-3.1432919065

H	-3.1625188023	-0.5324392981	-3.2015526274
H	3.1304815502	0.0426242953	3.2458766069
O	-0.1298433551	1.8089927663	0.0283199932
S	0.1377049065	-2.3738035861	0.0151369100
H	1.1796326774	-2.4702250242	-0.8862155438
C	-0.9312454331	2.8242723161	-0.6887091520
H	-1.3112675804	2.3632937250	-1.6093930560
C	0.0182893497	3.9310639447	-1.0023161657
H	0.2474222751	4.6246041717	-0.1946528827
C	-2.0937940046	3.2639259007	0.2080727606
H	-2.7087739769	4.0103284375	-0.3094336069
H	-2.7228692061	2.4108366693	0.4712292735
H	-1.7086451337	3.7085974250	1.1320465007
C	0.8930135606	3.9224337110	-2.2106752554
H	1.2062449325	4.9359298804	-2.4907960695
H	1.8133689347	3.3394014274	-2.0332473996
H	0.3910201774	3.4603525918	-3.0698828818

1,3-cyclohexadiene ²TS_E

Fe	0.0023233802	-0.0040461783	0.0031911521
N	0.0025034857	-0.0083447924	2.0290349671
N	2.0257913972	-0.0057467008	0.0240255347
N	-1.9957107974	-0.2344091984	-0.0019491972
N	0.0242334615	-0.2109747366	-1.9976765279
C	-1.1100458051	-0.0172676825	2.8543157186
C	2.8645811919	0.0315359099	-1.0807083729
C	1.1003082412	0.0948127012	2.8652784185
C	2.8509332678	0.0959238544	1.1356009444
C	-2.8317637863	-0.2356190756	1.1020714303
C	1.1341667310	-0.1480388743	-2.8261630793
C	-2.8169493816	-0.4193060392	-1.1031415098
C	-1.0682130676	-0.3829003235	-2.8360606426
C	-0.6970505809	0.0790861014	4.2403644509
C	4.2431767733	0.1356964986	-0.6493900976
C	0.6655710043	0.1483774164	4.2468245907
C	4.2344232302	0.1742705488	0.7145978331
C	-4.2056320155	-0.4104612806	0.6814646967
C	0.7266756038	-0.2761644392	-4.2090053097
C	-4.1962637654	-0.5265098055	-0.6793866076
C	-0.6311543301	-0.4262563152	-4.2151567918
H	-1.3732716855	0.0855843177	5.0828441526
H	5.0923047647	0.1741450279	-1.3160011557
H	1.3297798133	0.2235511883	5.0954519781
H	5.0753507144	0.2507915715	1.3880098262
H	-5.0516808590	-0.4485779646	1.3518299930
H	1.4029943337	-0.2635997235	-5.0514108275
H	-5.0329714726	-0.6765149573	-1.3456819383
H	-1.2871780305	-0.5591750721	-5.0632895479
C	-2.4237096129	-0.1207366393	2.4250737008
C	2.4506552967	-0.0252549587	-2.4016494345
C	-2.3872202411	-0.4899300373	-2.4204889533

C	2.4235214636	0.1426258366	2.4520447220
H	-3.1972417666	-0.1320287010	3.1859446243
H	3.2187370379	0.0111098339	-3.1671689567
H	-3.1426909605	-0.6345784107	-3.1856339935
H	3.1844167458	0.2256543761	3.2208981713
O	-0.0093050170	1.6926513854	0.0146026497
S	0.3508581345	-2.4844819309	0.3104036516
H	1.0645565451	-2.7203375097	-0.8504517423
C	-1.2186460744	3.2310165120	-0.8051092675
H	-2.0397282796	2.5764720662	-0.5398216911
C	-0.8135949680	4.3188954930	0.1738447808
H	-1.6254899374	4.5159072955	0.8840784319
H	0.0287580890	3.9246742024	0.7591726630
C	-0.7239974300	3.2464174421	-2.0880020105
H	-1.0132882000	2.4737171649	-2.7915425393
C	-0.3919902719	5.6310363043	-0.5281362373
H	-1.2878520770	6.2091221663	-0.8188309460
H	0.1583878626	6.2655600611	0.1768027657
C	0.2404487984	4.2461305532	-2.5000793883
H	0.7842611565	4.0932260458	-3.4282040603
C	0.4315920023	5.3723254329	-1.7688107931
H	1.1309169671	6.1371253226	-2.0973442469

1,3-cyclohexadiene $^4\text{TS}_E$

Fe	0.0030048818	-0.0048712916	0.0021642989
N	0.0026957690	-0.0058993056	2.0016121836
N	2.0050767653	-0.0074046494	-0.0118396402
N	-2.0185004699	-0.2092756734	-0.0021882508
N	-0.0046769800	-0.1626743382	-2.0340628947
C	-1.1066211536	-0.0081146169	2.8340254132
C	2.8321836557	0.0418888771	-1.1263864107
C	1.1079957307	0.0321413191	2.8340978146
C	2.8432055386	0.0299373457	1.0907336556
C	-2.8499967908	-0.1973099888	1.1029172336
C	1.0957909031	-0.0879879202	-2.8705906171
C	-2.8466431046	-0.3347841701	-1.1092101442
C	-1.1128443266	-0.2811543679	-2.8602310852
C	-0.6815975505	0.0429884197	4.2189708276
C	4.2168490424	0.1007401792	-0.7063155677
C	0.6825985541	0.0638924028	4.2192198140
C	4.2239096746	0.0888451659	0.6589335144
C	-4.2298363996	-0.3214578572	0.6829257797
C	0.6696904421	-0.1667242636	-4.2527353945
C	-4.2276182200	-0.4075293385	-0.6804950533
C	-0.6912326619	-0.2883153174	-4.2464820815
H	-1.3531021872	0.0503927197	5.0653559288
H	5.0598691660	0.1416882940	-1.3808268924
H	1.3535476461	0.0939323624	5.0654310462
H	5.0734149543	0.1206063289	1.3256377959
H	-5.0755667502	-0.3440899103	1.3544968370
H	1.3359520289	-0.1404966913	-5.1027359239

H	-5.0713294397	-0.5136325337	-1.3468522038
H	-1.3597645960	-0.3801162240	-5.0902467100
C	-2.4269922277	-0.0913310475	2.4218477034
C	2.4142141000	0.0154915775	-2.4483319627
C	-2.4292944735	-0.3633511369	-2.4321498651
C	2.4293939934	0.0377382698	2.4143969609
H	-3.1909229952	-0.0937419494	3.1923192242
H	3.1817404343	0.0605516615	-3.2139702149
H	-3.1962048270	-0.4573185661	-3.1936942835
H	3.1983226508	0.0659281016	3.1791322826
O	-0.0881354020	1.6997186637	-0.0669548759
S	-0.0567683439	-2.4529153682	-0.1157994472
H	1.1043151932	-2.6417398121	-0.8422315226
C	-1.2713641855	3.1876976943	-1.0193307310
H	-2.0592154861	2.4518905162	-0.9297723921
C	-1.1267835701	4.2345162091	0.0728575758
H	-2.0418737758	4.2871585599	0.6762388235
H	-0.3262363256	3.8893260960	0.7425371259
C	-0.6140649039	3.3583202143	-2.2245033952
H	-0.7190129431	2.6150007563	-3.0087337808
C	-0.7706899397	5.6345320735	-0.4780366144
H	-1.6801318685	6.1379495006	-0.8497033085
H	-0.3928526453	6.2629847647	0.3357583012
C	0.2680864703	4.4838993362	-2.4322501278
H	0.9377126610	4.4697384691	-3.2887097415
C	0.2312360210	5.5650324534	-1.6069358001
H	0.8744294532	6.4236028401	-1.7864196962

1,3-cyclohexadiene ⁴I

Fe	-0.0020701785	-0.0026694472	-0.0028030718
N	0.0035886134	-0.0003887237	2.0097129493
N	2.0111198662	-0.0051659906	-0.0199559673
N	-2.0127593493	-0.0982335263	0.0103240463
N	-0.0090458283	-0.1196221034	-2.0199462542
C	-1.0981329376	0.0745424845	2.8452538094
C	2.8327076415	0.0865981484	-1.1328535713
C	1.1183333539	-0.0218241375	2.8304949724
C	2.8452394069	-0.0213517938	1.0847192109
C	-2.8411639849	-0.0361328325	1.1210948738
C	1.0899609004	-0.0201337692	-2.8604176588
C	-2.8422504263	-0.2811964176	-1.0886589934
C	-1.1172870107	-0.2777270040	-2.8387965702
C	-0.6609533063	0.1073759190	4.2247966830
C	4.2161664519	0.1247630801	-0.7116676839
C	0.7021933677	0.0393951906	4.2159456232
C	4.2243297009	0.0495732765	0.6522183369
C	-4.2194324765	-0.1598826331	0.7046029296
C	0.6565599067	-0.1144621274	-4.2368044568
C	-4.2193258089	-0.3194922778	-0.6527625019
C	-0.6997345632	-0.2818833403	-4.2231768623
H	-1.3245588735	0.1669835335	5.0750545337

H	5.0581544145	0.1947538951	-1.3845866945
H	1.3792196571	0.0379337005	5.0575759296
H	5.0745054308	0.0508615144	1.3185513069
H	-5.0647601745	-0.1385132441	1.3764980353
H	1.3169166989	-0.0652507657	-5.0904155514
H	-5.0648393054	-0.4498832084	-1.3119378706
H	-1.3695322021	-0.3927124996	-5.0634489554
C	-2.4221525766	0.0742252688	2.4383768840
C	2.4103605153	0.0973122071	-2.4529394997
C	-2.4321507897	-0.3730880434	-2.4093138160
C	2.4371082313	-0.0497341500	2.4087561945
H	-3.1856146406	0.1223435357	3.2065954459
H	3.1700373796	0.1658664171	-3.2237673980
H	-3.1988464002	-0.5030414653	-3.1649689352
H	3.2078901172	-0.0589835468	3.1713105756
O	0.0045746616	1.8018435316	-0.0584192389
S	0.0188021751	-2.3610370727	0.0881704211
H	0.9327264975	-2.5619346157	-0.9267404838
C	-0.8785667848	2.7859431972	-0.6559040853
H	-1.6261588549	2.2551066869	-1.2652477199
C	-1.5921931489	3.5633331790	0.4713417908
H	-2.2837546518	2.8961807300	0.9940111251
H	-0.8239680751	3.8726806446	1.1894832012
C	-0.0606680222	3.7048459783	-1.5246237719
H	0.7437352794	3.2543883781	-2.0990470524
C	-2.3248073464	4.8112429101	-0.0714037429
H	-3.2138886750	4.4984539296	-0.6496100658
H	-2.7133063911	5.4040003330	0.7671351294
C	-0.3499177638	5.0658099399	-1.6130043623
H	0.2740235850	5.6900776061	-2.2482168160
C	-1.4209439500	5.6484094183	-0.9390010420
H	-1.6313617499	6.7083702203	-1.0523590061

1,4-cyclohexadiene $^2\text{TS}_E$

Fe	-0.0437391825	-0.0326812541	0.0539915971
N	-0.0611947708	-0.1248461145	2.0709622936
N	1.9837252099	0.0842402164	0.0946914365
N	-2.0338339678	-0.2596026157	0.0170095740
N	0.0007908405	-0.1285779784	-1.9557085231
C	-1.1778656268	-0.1804034481	2.8856360287
C	2.8228879673	0.2359082225	-0.9993910984
C	1.0327099255	-0.0591957893	2.9198175962
C	2.7962166237	0.1418984483	1.2144291201
C	-2.8835095465	-0.3130200096	1.1123332553
C	1.1148663213	0.0273498753	-2.7673678331
C	-2.8391621585	-0.4364494543	-1.0992780011
C	-1.0753025478	-0.3132544721	-2.8114230509
C	-0.7755334756	-0.1605726512	4.2772784434
C	4.1936309717	0.3848500508	-0.5506435440
C	0.5872120634	-0.0882557197	4.2979031984
C	4.1774332858	0.3225485793	0.8121157579

C	-4.2503437688	-0.4914424365	0.6686265686
C	0.7254017374	-0.0621757840	-4.1577304480
C	-4.2223527963	-0.5731536241	-0.6941470448
C	-0.6240174358	-0.2792439711	-4.1847639961
H	-1.4577708431	-0.2003490104	5.1136855484
H	5.0429485552	0.5127213074	-1.2058586017
H	1.2442196565	-0.0533269502	5.1547333695
H	5.0106070342	0.3911008403	1.4960531324
H	-5.1038631452	-0.5630183058	1.3267450356
H	1.4062874862	0.0251061799	-4.9920789293
H	-5.0485089400	-0.7214016411	-1.3739027577
H	-1.2654963264	-0.4021322527	-5.0452739029
C	-2.4896663650	-0.2571901663	2.4417728936
C	2.4191509748	0.2146114621	-2.3246475056
C	-2.3947687476	-0.4692041387	-2.4121907955
C	2.3568838493	0.0591290793	2.5262767534
H	-3.2687420410	-0.3080852612	3.1953511132
H	3.1880145270	0.3304428569	-3.0817076109
H	-3.1385124602	-0.6129284938	-3.1890443365
H	3.1069117081	0.1104465343	3.3084670927
O	0.0149155985	1.7038490567	0.1029711590
S	0.3671438281	-2.4573201922	0.2137879036
H	1.1892652620	-2.5849977079	-0.8897442339
C	-1.0031713385	3.0761892654	-0.9482719246
H	-1.0479874990	2.4615962192	-1.8412430297
C	-2.0651905970	3.0550577827	-0.0742794127
H	-2.8487097230	2.3155485003	-0.2054972428
C	0.0312975706	4.1767471354	-0.9322212326
H	1.0270479830	3.7131396540	-0.9445957322
H	-0.0407536324	4.7572041719	-1.8687153030
C	-2.1540768751	3.9492728210	1.1235923878
H	-3.1483620186	4.4296272389	1.1516076148
H	-2.1261305690	3.3257479269	2.0358995198
C	-0.0999761642	5.0993713315	0.2543369444
H	0.6526389494	5.8803280365	0.3446784757
C	-1.0673742515	4.9958068639	1.1751004530
H	-1.0997271119	5.6885479868	2.0134493997

1,4-cyclohexadiene $^4\text{TS}_E$

Fe	0.0009242441	-0.0095145488	0.0062121452
N	-0.0026456791	-0.0201862620	2.0060460654
N	1.9943342897	-0.0029670647	-0.0103633882
N	-2.0371255708	-0.1518268271	0.0073189228
N	-0.0150012894	-0.1334677817	-2.0231832009
C	-1.1132122601	0.0219479962	2.8374075158
C	2.8218030153	0.0585406287	-1.1255821194
C	1.1032460321	-0.0268606273	2.8369363069
C	2.8333684620	-0.0162892020	1.0934018641
C	-2.8645382398	-0.1014767754	1.1108188800
C	1.0817305141	-0.0468293654	-2.8625069607
C	-2.8631055207	-0.2932294815	-1.0962558409

C	-1.1273806502	-0.2574299590	-2.8447298351
C	-0.6849571341	0.0492336791	4.2214076691
C	4.2067061500	0.0872979587	-0.7036082435
C	0.6789839846	0.0124310020	4.2214858625
C	4.2139517704	0.0344503335	0.6603666256
C	-4.2480360977	-0.2085011291	0.6934360941
C	0.6500421328	-0.1175976876	-4.2421003633
C	-4.2466844568	-0.3330464619	-0.6671481215
C	-0.7100142108	-0.2524111639	-4.2309696063
H	-1.3550865716	0.0821264784	5.0682043507
H	5.0503166960	0.1342894801	-1.3769967199
H	1.3504672295	0.0138059249	5.0677138768
H	5.0641402455	0.0330267877	1.3269326115
H	-5.0940774373	-0.2018356202	1.3653235904
H	1.3126270019	-0.0757690937	-5.0942198856
H	-5.0915074973	-0.4451901913	-1.3312769991
H	-1.3812139372	-0.3395319267	-5.0730644852
C	-2.4366092141	-0.0013969502	2.4291530383
C	2.4031661197	0.0552727690	-2.4458452369
C	-2.4445564045	-0.3445407541	-2.4175460888
C	2.4241102325	-0.0416102023	2.4168716339
H	-3.1977711932	0.0249385170	3.2017452362
H	3.1678754929	0.1069690386	-3.2135629629
H	-3.2092361892	-0.4473596850	-3.1803058975
H	3.1942827583	-0.0483403046	3.1805120680
O	-0.0815459113	1.7265864140	-0.0454899963
S	-0.1036025994	-2.4077055917	-0.0316800951
H	0.8235117286	-2.6182770066	-1.0345918836
C	-0.9089440784	3.1243954811	-1.1636032773
H	-0.7879240393	2.5488327993	-2.0757139418
C	-2.1750911955	3.2020190566	-0.5942510938
H	-2.9533374899	2.5248265214	-0.9309181225
C	0.1205101680	4.2066319079	-0.9210933595
H	1.1015387525	3.7349726574	-0.7830871694
H	0.2106568097	4.8177572332	-1.8371807003
C	-2.4689535020	4.0586463122	0.5995179380
H	-3.4191886076	4.6002004620	0.4496134867
H	-2.6644065418	3.3993949768	1.4664000780
C	-0.2091540536	5.0934661754	0.2538597825
H	0.5516742938	5.8157039021	0.5430041500
C	-1.3608567124	5.0276953988	0.9344533080
H	-1.5342137413	5.6911420973	1.7791763895

1,4-cyclohexadiene ⁴I

Fe	-0.0502330143	-0.0185626043	-0.0005849170
N	-0.1327008780	-0.0891664873	2.0073189809
N	1.9471373924	0.1170198120	0.0729220845
N	-2.0585873983	-0.2717409420	-0.0841338334
N	0.0324010508	-0.0382991397	-2.0198802641
C	-1.2752592007	-0.1301820771	2.7902701761
C	2.8104246302	0.3082015999	-0.9973636094

C	0.9406704125	-0.0753479263	2.8792687289
C	2.7342092490	0.1103458421	1.2142869197
C	-2.9349248576	-0.2931955163	0.9866978174
C	1.1566756196	0.1570823843	-2.8068282918
C	-2.8260365795	-0.4421396456	-1.2258984818
C	-1.0276176184	-0.2474796905	-2.8925475230
C	-0.9038253521	-0.1332582907	4.1898643857
C	4.1678454598	0.4220703704	-0.5107715054
C	0.4598860707	-0.1086874581	4.2445982402
C	4.1219928600	0.2911163967	0.8478729088
C	-4.2872356196	-0.4694204337	0.5033209344
C	0.7906660869	0.0797632990	-4.2033312204
C	-4.2191958885	-0.5695161448	-0.8578000778
C	-0.5508819626	-0.1775848458	-4.2555485737
H	-1.6078630638	-0.1615455190	5.0084877032
H	5.0317014127	0.5763460242	-1.1405596241
H	1.0966600049	-0.1068729253	5.1169196150
H	4.9403347175	0.3224241028	1.5523366743
H	-5.1611334377	-0.5201045978	1.1360035752
H	1.4826633726	0.1987886898	-5.0243993688
H	-5.0264912455	-0.7138283249	-1.5606731977
H	-1.1742481992	-0.3065851114	-5.1280860255
C	-2.5773705772	-0.2055428974	2.3242936576
C	2.4481165860	0.3444336722	-2.3342243222
C	-2.3504405236	-0.4480025630	-2.5286567504
C	2.2757351638	-0.0002322422	2.5167189131
H	-3.3734726114	-0.2374666417	3.0599713827
H	3.2355771605	0.4908760666	-3.0652900357
H	-3.0720619098	-0.5939902872	-3.3249264391
H	3.0135721081	0.0075426256	3.3112337922
O	-0.2527665335	1.7724804052	0.0349223781
S	0.0826198040	-2.3766355783	-0.0332434516
H	1.1701514390	-2.4705189143	-0.8801941817
C	-1.0593803629	2.7248536010	-0.7580884867
H	-1.6381006529	2.1497607621	-1.4864853804
C	-1.9548766333	3.4512896618	0.1875034384
H	-2.9379535707	3.0399837463	0.4001449752
C	-0.0836344120	3.6726800112	-1.4903388281
H	0.7415144313	3.0732388510	-1.8920163159
H	-0.6050766969	4.1044437372	-2.3608273809
C	-1.4104575804	4.5299674558	1.0705381439
H	-2.1782002772	5.3064061703	1.2325707123
H	-1.2130876212	4.1252135674	2.0830198367
C	0.4424020615	4.7791092031	-0.6069485021
H	1.3469408837	5.2831144715	-0.9426998437
C	-0.1455062436	5.1611291841	0.5347518985
H	0.2859556682	5.9638189302	1.1295656139

Ethene ²TS_E

Fe	-0.0122603629	0.0098939623	-0.0087644594
N	-0.0069527444	0.0042391783	2.0145873144

N	2.0167147153	-0.0012561758	-0.0074112701
N	-2.0040678959	-0.1742045349	0.0022280586
N	0.0010121562	-0.1816100219	-2.0064698245
C	-1.1114874819	0.0573167444	2.8456248795
C	2.8453445223	0.0799091712	-1.1147007462
C	1.1040449317	0.0129403745	2.8405754730
C	2.8442920729	0.0206725628	1.1026073868
C	-2.8401843433	-0.1159381520	1.1086146012
C	1.1063029456	-0.1007085699	-2.8436143004
C	-2.8276242159	-0.4027803710	-1.0917276656
C	-1.0937027379	-0.4025715740	-2.8315703626
C	-0.6828625146	0.1056782473	4.2284619472
C	4.2267450896	0.1499905010	-0.6867486055
C	0.6810593083	0.0702846027	4.2252559014
C	4.2264057141	0.1050807069	0.6778409641
C	-4.2143181498	-0.2882171283	0.6923367852
C	0.6887203727	-0.2611015054	-4.2186287501
C	-4.2055210071	-0.4746929801	-0.6607563348
C	-0.6636774136	-0.4566299466	-4.2103908893
H	-1.3512997689	0.1501050147	5.0756234280
H	5.0723143528	0.2175988219	-1.3553638534
H	1.3547899173	0.0850483879	5.0692424989
H	5.0717876858	0.1332028828	1.3497452740
H	-5.0614258391	-0.2831038095	1.3626829970
H	1.3570463583	-0.2387116496	-5.0671496424
H	-5.0443017524	-0.6471752351	-1.3189988736
H	-1.3217953178	-0.6214711455	-5.0508335812
C	-2.4313141865	0.0215035559	2.4266141614
C	2.4233748053	0.0502797228	-2.4341140612
C	-2.4080816318	-0.5178910428	-2.4073270570
C	2.4251625687	0.0078486612	2.4232529829
H	-3.2021331077	0.0560066220	3.1888493305
H	3.1838588649	0.1068275008	-3.2054827931
H	-3.1656405228	-0.6942672985	-3.1630257324
H	3.1911091402	0.0236149793	3.1909959956
O	0.0461174160	1.7252880869	0.0172206415
S	0.1684999200	-2.4410654465	0.2040783895
H	1.1205962700	-2.6455577453	-0.7765130247
C	-1.1418152659	3.0026386580	-1.0022058502
H	-1.9940122782	2.7666072974	-0.3750063530
H	-1.0566027807	2.4348476957	-1.9218017111
C	-0.4503114804	4.1767304578	-0.8379454217
H	0.3370841775	4.4699392289	-1.5250694295
H	-0.6011184942	4.8067415394	0.0327814331

Ethene ⁴TS_E

Fe	0.0017655098	-0.0022539226	0.0017801406
N	0.0017434720	-0.0032729115	1.9993648200
N	1.9988881740	-0.0033045925	-0.0161777189
N	-2.0234691178	-0.1861428750	0.0010499364
N	-0.0111217241	-0.1710929645	-2.0290060987

C	-1.1072015643	0.0279734570	2.8323900451
C	2.8242001146	0.0668598723	-1.1315317432
C	1.1084556635	-0.0158588828	2.8306885583
C	2.8391449340	-0.0074316078	1.0855179838
C	-2.8542030337	-0.1376519569	1.1052972056
C	1.0859692118	-0.0841483416	-2.8694214517
C	-2.8507714887	-0.3567795280	-1.1005926395
C	-1.1180312080	-0.3394250216	-2.8512180193
C	-0.6789909180	0.0512905041	4.2165302905
C	4.2091034703	0.1101204132	-0.7119624205
C	0.6848764905	0.0167192777	4.2157900787
C	4.2187421061	0.0560409041	0.6519703466
C	-4.2339692031	-0.2768058889	0.6897613510
C	0.6597203163	-0.2016442063	-4.2475610994
C	-4.2309428871	-0.4168464118	-0.6689742327
C	-0.6970593992	-0.3646378035	-4.2356582902
H	-1.3491329259	0.0772170418	5.0635333124
H	5.0508905303	0.1660719589	-1.3864071276
H	1.3565675900	0.0144180092	5.0617696630
H	5.0696855482	0.0634854919	1.3173541250
H	-5.0796776577	-0.2766524361	1.3616260079
H	1.3232812437	-0.1704938719	-5.0995286903
H	-5.0738912378	-0.5502815956	-1.3309348973
H	-1.3638447781	-0.4893022407	-5.0763792123
C	-2.4292022662	-0.0169397627	2.4219933818
C	2.4038015293	0.0480052027	-2.4514961676
C	-2.4332924316	-0.4293484807	-2.4209227520
C	2.4284328140	-0.0309582735	2.4093334586
H	-3.1922010647	0.0042923737	3.1930165865
H	3.1684224578	0.1027800474	-3.2192245181
H	-3.1982646113	-0.5561876270	-3.1794970421
H	3.1986920860	-0.0347814082	3.1730897998
O	-0.0551566856	1.7195699691	-0.0434262865
S	-0.0799861817	-2.4443409917	-0.0639311350
H	0.9519667255	-2.6448415808	-0.9636361214
C	-1.1891566802	2.9560379447	-1.1799675888
H	-2.0892594751	2.6473298188	-0.6623729833
H	-0.9566791901	2.4100485151	-2.0868777349
C	-0.6375992197	4.1928251185	-0.9531621861
H	0.1881573398	4.5607514374	-1.5507841465
H	-0.9364129496	4.7993341341	-0.1051833070

Ethene ⁴I

Fe	0.0035526757	-0.0146917561	0.0027400840
N	0.0060289150	0.0005709461	2.0140104309
N	2.0175126979	-0.0079602150	-0.0106931429
N	-2.0098483829	-0.0998382424	0.0134267089
N	-0.0005526623	-0.1292762511	-2.0115196228
C	-1.0979252969	0.0754634909	2.8477079678
C	2.8421926654	0.0686292070	-1.1225670429
C	1.1192394367	-0.0201640100	2.8373928098

C	2.8499218755	-0.0203717882	1.0952987103
C	-2.8395498496	-0.0260735163	1.1216195707
C	1.1014748285	-0.0474474468	-2.8511365235
C	-2.8395347586	-0.2689401508	-1.0873351169
C	-1.1097246053	-0.2842168271	-2.8327270206
C	-0.6634879697	0.1044611667	4.2281618883
C	4.2256620418	0.1032956720	-0.6990767932
C	0.6999840891	0.0367983749	4.2220624990
C	4.2306253637	0.0403782822	0.6651303759
C	-4.2191482311	-0.1349436599	0.7028941974
C	0.6702206595	-0.1512684023	-4.2266742389
C	-4.2187025479	-0.2929537290	-0.6543020159
C	-0.6883483746	-0.3046195524	-4.2151408936
H	-1.3290569400	0.1613644433	5.0771466640
H	5.0696033124	0.1619982985	-1.3709581597
H	1.3751192318	0.0324127702	5.0652986609
H	5.0793534501	0.0416794068	1.3334229084
H	-5.0652247571	-0.1053573536	1.3736414046
H	1.3329599788	-0.1172197379	-5.0792173085
H	-5.0646899861	-0.4133331271	-1.3152469415
H	-1.3568381155	-0.4166288684	-5.0563702609
C	-2.4215490758	0.0814539868	2.4391206318
C	2.4220935282	0.0664073295	-2.4429038865
C	-2.4267905772	-0.3651324172	-2.4063754676
C	2.4392011789	-0.0455630267	2.4185157037
H	-3.1858754292	0.1329192234	3.2064835723
H	3.1831379368	0.1211798820	-3.2134511691
H	-3.1924674651	-0.4898322293	-3.1640394545
H	3.2083035907	-0.0550743194	3.1828025474
O	-0.0090027987	1.7937746357	-0.0537709142
S	0.0259981455	-2.3735010011	0.1027887011
H	0.8962425485	-2.5845260922	-0.9487359642
C	-0.8841746283	2.7148605909	-0.7865780273
H	-1.8910919681	2.6378457914	-0.3575899759
H	-0.9284321139	2.4005974736	-1.8361115290
C	-0.3168327340	4.0794185668	-0.6344346952
H	0.4506476436	4.4357427381	-1.3139196123
H	-0.4736423282	4.6317796866	0.2859471489