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Energetics of Non-Heme Iron Reactivity: Can Ab Initio Calculations Provide the Right Answer?

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S1 Suporting information

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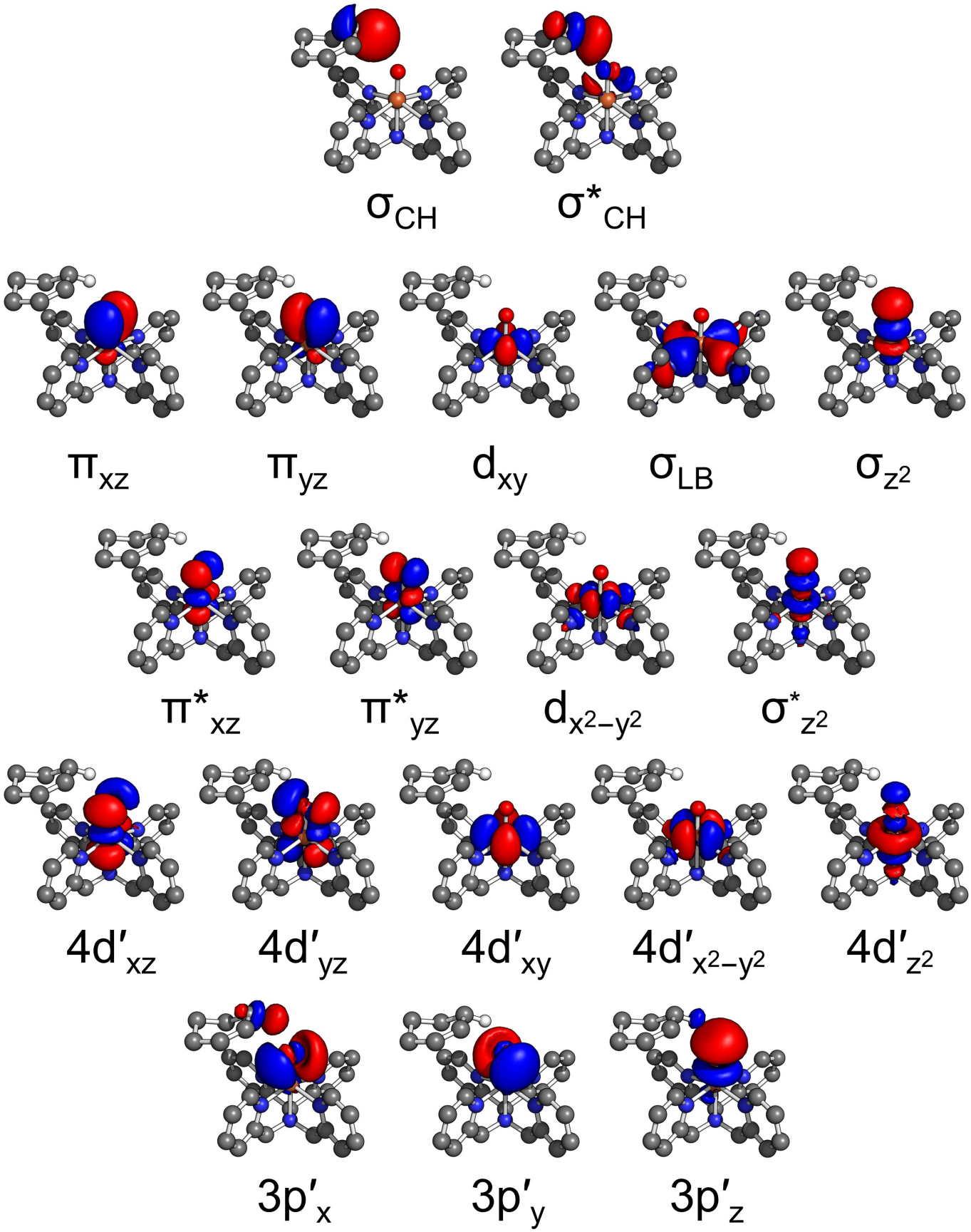

Fig. S1 Full CAS(14,19) active space used in the hydrogen atom transfer reaction for the example of ^{5}RC. Note that the active space for the triplet includes the same orbitals except the double-shell counterparts of the $d_{x^2-y^2}$ and $\sigma^*_{z^2}$ orbitals, yielding a CAS(14,17) active space.

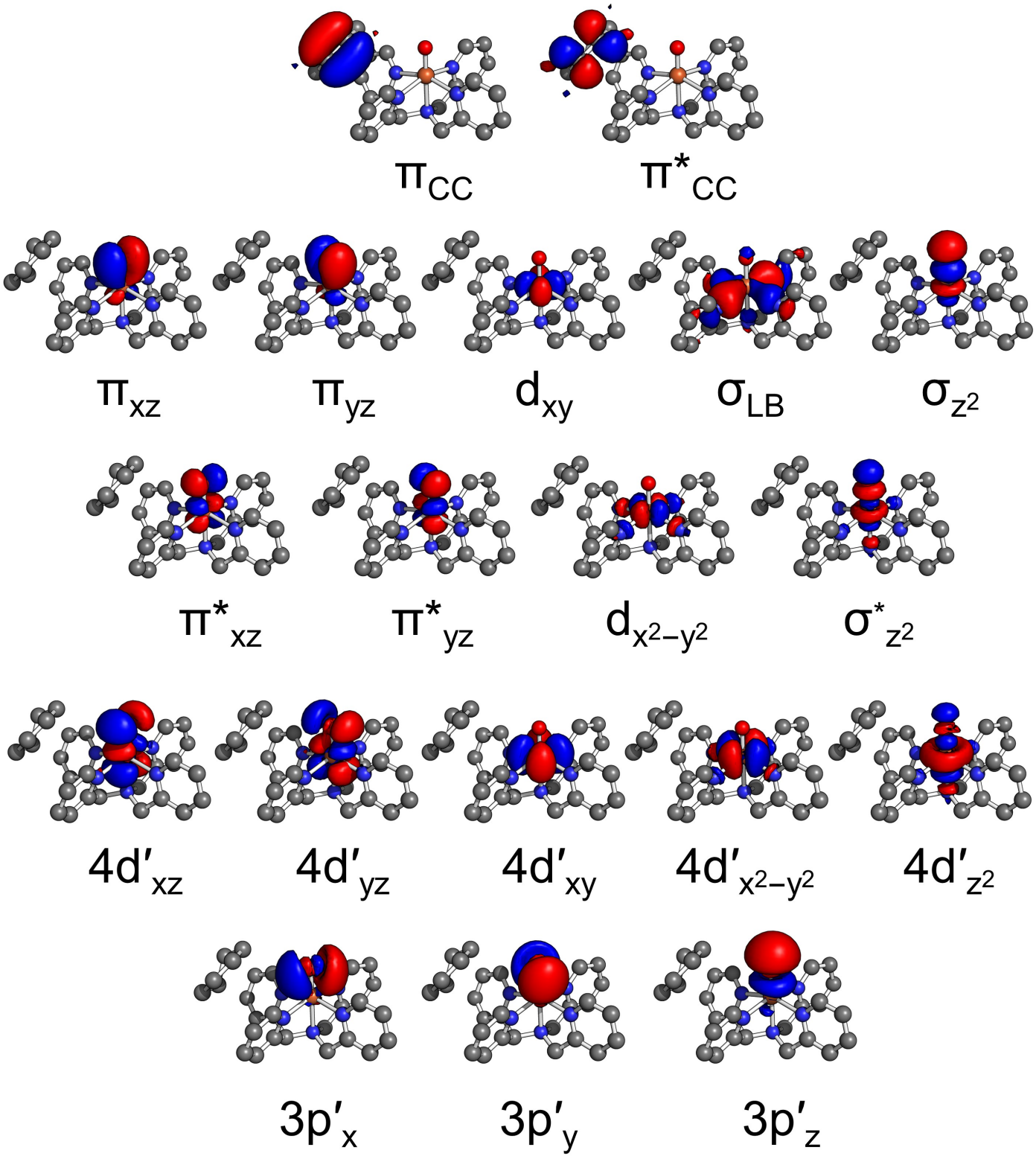

Fig. S2 Full CAS(14,19) active space used in the epoxidation reaction for the example of ^{5}RC. Note that the active space for the triplet includes the same orbitals except the double-shell counterparts of the $d_{x^2-y^2}$ and $\sigma^*_{z^2}$ orbitals, yielding a CAS(14,17) active space.

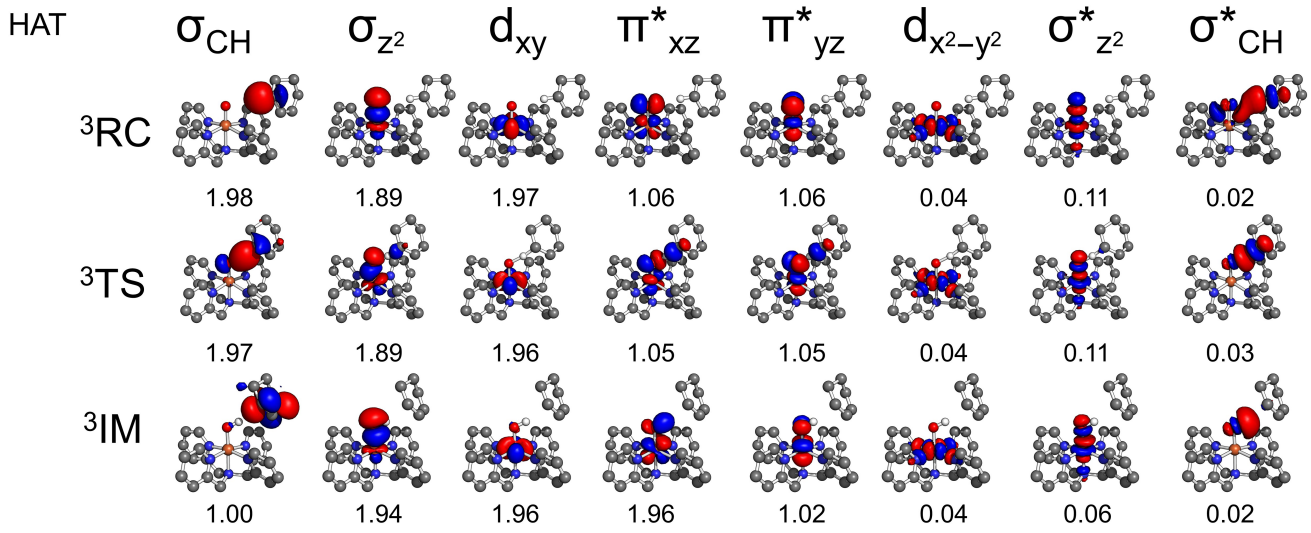

Fig. S3 Selected orbitals of active space for triplet hydrogen atom transfer including NOONs.

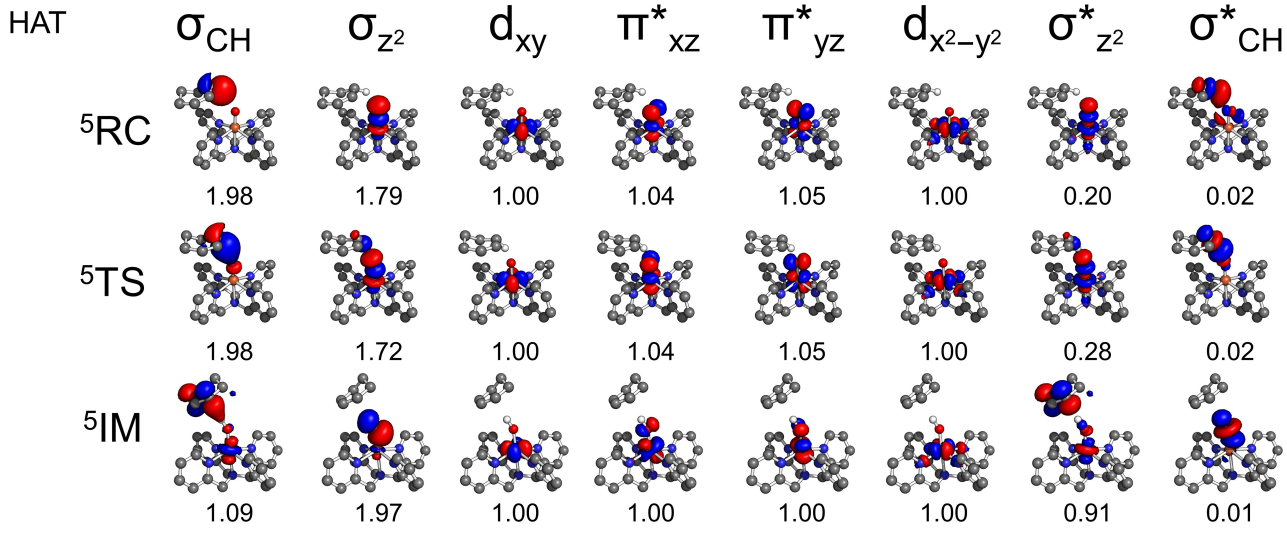

Fig. S4 Selected orbitals of active space for quintet hydrogen atom transfer including NOONs.

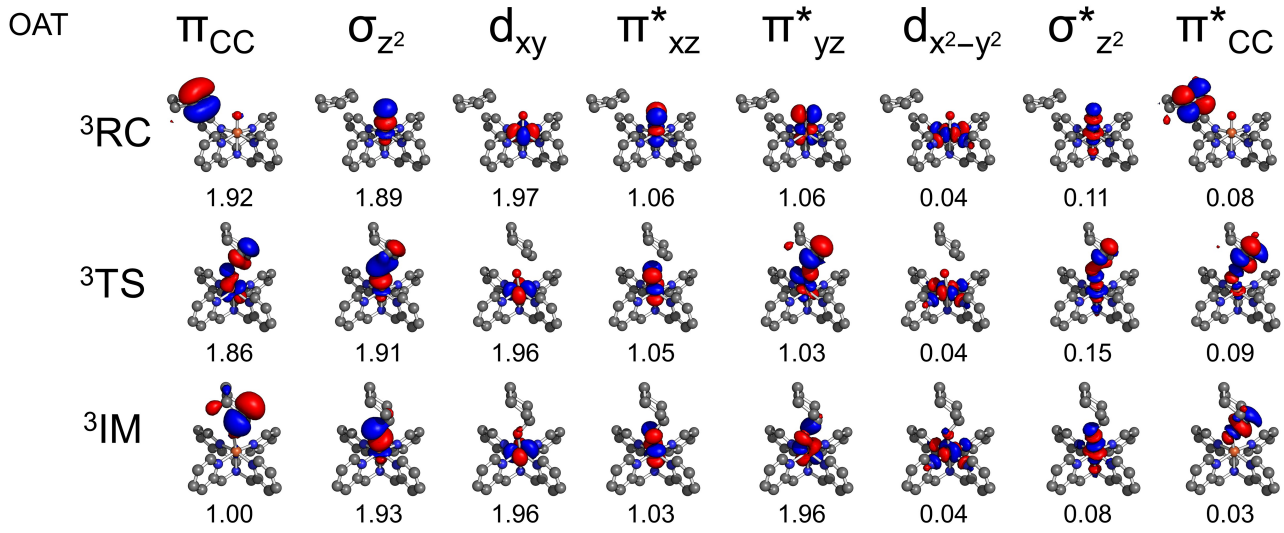

Fig. S5 Selected orbitals of active space for triplet epoxidation including NOONs.

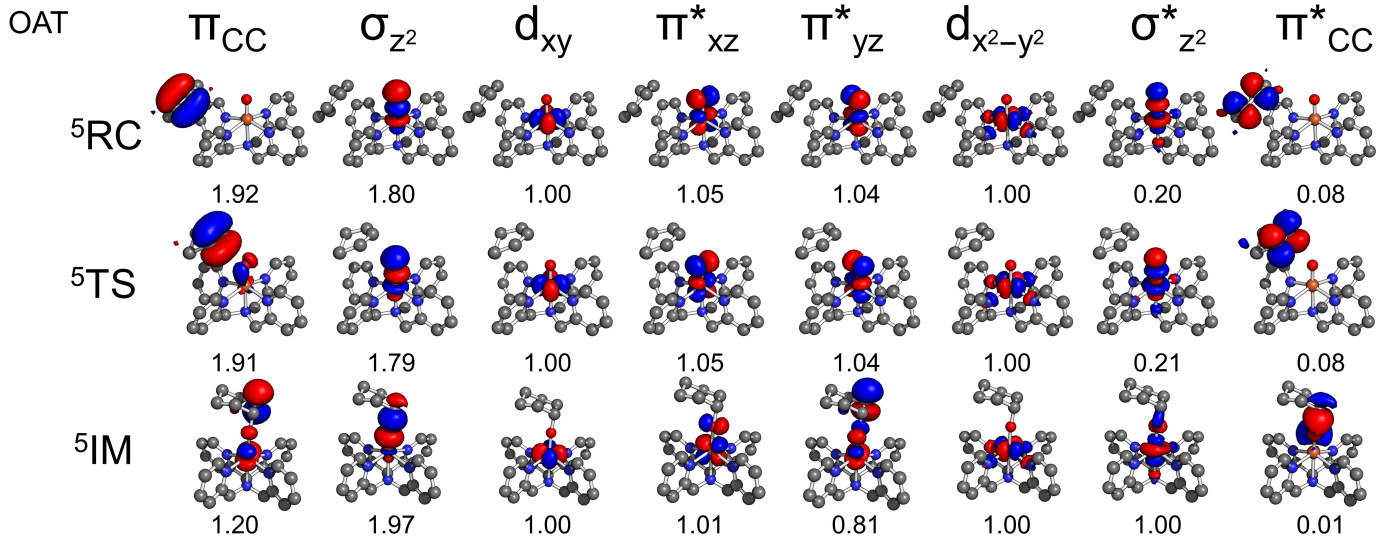

Fig. S6 Selected orbitals of active space for quintet epoxidation including NOONs.

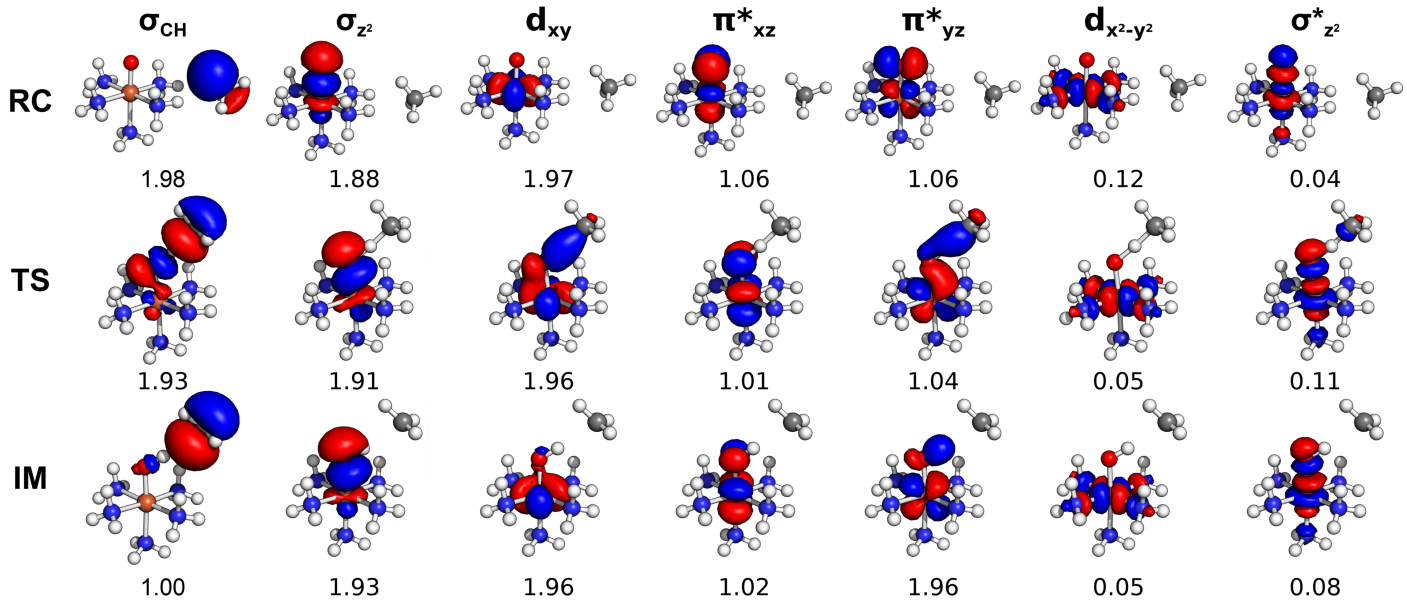

Fig. S7 Selected orbitals of active space for triplet hydrogen atom transfer of the small model system $[FeO(NH_3)_5]^{2+}$ including NOONs.

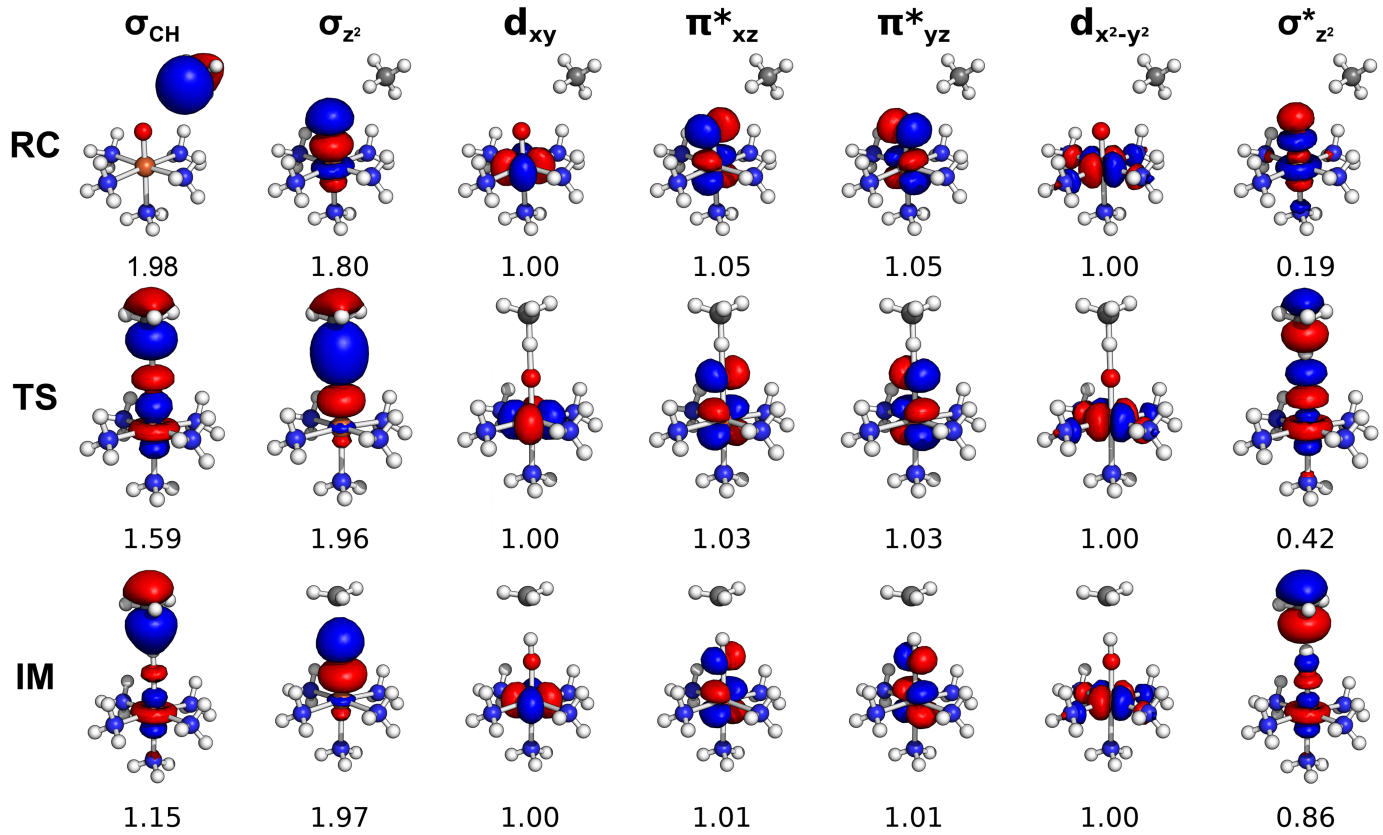

Fig. S8 Selected orbitals of active space for quintet hydrogen atom transfer of the small model system $[FeO(NH_3)_5]^{2+}$ including NOONs.

Table S1 Selected geometries for the reaction with cyclohexene

HAT	Fe-O	Fe-N_{ax}	Fe-N_{eq1}	Fe-N_{eq2}	Fe-N_{eq3}	Fe-N_{eq4}	O-H	H-C	A(Fe-O-H)
^{3}SR	1.62	2.10	1.99	1.99	1.98	1.98			
^{3}RC	1.62	2.10	1.99	1.99	1.98	1.98	2.56	1.10	103.5
^{3}TS	1.72	2.07	1.99	1.99	1.98	1.98	1.35	1.25	118.5
^{3}IM	1.78	2.04	1.99	1.98	1.97	1.97	0.98	2.19	114.1
^{5}SR	1.61	2.12	2.13	2.13	2.09	2.09			
^{5}RC	1.60	2.18	2.18	2.19	2.11	2.12	2.36	1.11	151.2
^{5}TS	1.66	2.24	2.16	2.17	2.12	2.13	1.59	1.16	162.8
^{5}IM	1.78	2.31	2.17	2.16	2.14	2.15	0.98	2.01	153.6
Epoxidation	Fe-O	Fe-N_{ax}	Fe-N_{eq1}	Fe-N_{eq2}	Fe-N_{eq3}	Fe-N_{eq4}	O-C_1	O-C_2	A(Fe-O-C)
^{3}RC	1.62	2.10	1.99	1.99	1.98	1.97	4.05	5.10	127.0
^{3}TS1	1.72	2.09	2.04	1.99	1.99	1.98	1.99	2.62	132.8
^{3}IM1	1.79	2.06	2.06	2.05	1.99	1.98	1.43	2.38	130.0
^{3}TS2	1.90	2.15	2.04	2.02	2.02	1.99	1.42	2.11	131.0
^{3}IM2	2.15	2.22	2.09	2.07	2.00	1.99	1.45	1.46	147.2
^{5}RC	1.60	2.18	2.22	2.15	2.14	2.11	4.38	5.28	107.1
^{5}TS1	1.61	2.19	2.22	2.15	2.13	2.10	2.84	3.34	147.5
^{5}IM1	1.80	2.30	2.21	2.19	2.16	2.15	1.43	2.28	171.1
^{5}TS2	1.83	2.30	2.22	2.19	2.17	2.16	1.42	2.19	174.1
^{5}IM2	2.09	2.25	2.27	2.21	2.20	2.19	1.47	1.48	137.9

Table S2 T_1 diagnostic obtained from DLPNO-CCSD(T0) and LUCCSD(T0) calculations

HAT	DLPNO-CCSD(T0)	LUCCSD(T0)
^{3}SR	0.013	0.061
^{3}RC	0.012	0.056
^{3}TS	0.014	0.056
^{3}IM	0.013	0.059
^{5}SR	0.015	0.041
^{5}RC	0.015	0.039
^{5}TS	0.020	0.041
^{5}IM	0.056	0.036
EPOXIDATION		
^{3}RC	0.012	0.059
^{3}TS1	0.014	0.056
^{3}IM1	0.012	0.044
^{3}TS2	0.014	0.039
^{3}IM2	0.013	0.041
^{5}RC	0.015	0.039
^{5}TS1	0.016	0.039
^{5}IM1	0.035	0.034
^{5}TS2	0.025	0.033
^{5}IM2	0.013	0.033

Table S3 Canonical coupled cluster results obtained with two different versions of ORCA program package and with and without *QROs True keyword*

	CCSD(T) ORCA 4.0	CCSD(T) *QROs True* ORCA 4.0	CCSD(T) ORCA 4.2	CCSD(T) *QROs True* ORCA 4.2
^{3}SR	0.0	0.0	0.0	0.0
^{5}SR	0.6	0.7	1.2	1.2
^{3}RC	-5.0	-5.0	-4.9	-4.9
^{5}RC	-2.9	-2.8	-2.1	-2.2
^{3}TS	24.6	24.6	25.9	25.9
^{5}TS	14.3	14.9	16.0	15.8
^{3}IM	13.6	13.9	15.0	15.2
^{5}IM	2.5	3.6	4.3	5.6

Table S4 Correlation Energy Contributions and Spin-State Spliting of Quintet (HS) and Triplet (LS) States of $[FeO(NH_3)_5]^{2+}$ using NormalnPNO

	HS				LS						
	E_{can}	E_{DLPNO}	Δ mE$_h$	E_{can}/E_{DLPNO}	E_{can}	E_{DLPNO}	Δ mE$_h$	E_{can}/E_{DLPNO}	ΔE_{can}/ kcal/mol	ΔE_{DLPNO}/ /kcal/mol	$\Delta\Delta E$/ kcal/mol
SD	-2.08828	-2.10369	15.4	0.993	-2.13566	-2.14277	7.1	0.997	29.7	24.5	5.2
(T0)	-	-0.09422	-9.5	1.101	-	-0.10444	-12.7	1.121	-	6.4	2.0
(T1)	-0.10369	-0.10228	-1.4	1.014	-0.11713	-0.11468	-2.4	1.021	8.4	7.8	0.7
E_{corr}	-2.19198	-2.20597	14.0	0.994	-2.25279	-2.25745	4.7	0.998	38.2	32.3	5.9

Table S5 Correlation Energy Contributions and Spin-State Spliting of Quintet (HS) and Triplet(LS) States of $[FeO(NH_3)_5]^{2+}$ using TightPNO

	HS				LS						
	E_{can}	E_{DLPNO}	Δ mE$_h$	E_{can}/E_{DLPNO}	E_{can}	E_{DLPNO}	Δ mE$_h$	E_{can}/E_{DLPNO}	ΔE_{can}/ kcal/mol	ΔE_{DLPNO}/ /kcal/mol	$\Delta\Delta E$/ kcal/mol
SD	-2.08828	-2.10095	12.7	0.994	-2.13566	-2.14229	6.6	0.997	29.7	25.9	3.8
(T0)	-	-0.09568	-8.0	1.084	-	-0.10596	-11.2	1.105	-	6.5	2.0
(T1)	-0.10369	-0.10387	0.2	0.998	-0.11713	-0.11658	-0.5	1.005	8.4	8.0	0.5
E_{corr}	-2.19198	-2.20482	12.8	0.994	-2.25279	-2.25887	6.1	0.997	38.2	33.9	4.2

Table S6 Electronic energies and five lowest frequencies for ^{3}SR structure

^{3}SR	
Zero-point correction=	0.410371
Thermal correction to Energy=	0.432965
Thermal correction to Enthalpy=	0.433909
Thermal correction to Gibbs Free Energy=	0.359069
Sum of electronic and zero-point Energies=	-2500.074656
Sum of electronic and thermal Energies=	-2500.052062
Sum of electronic and thermal Enthalpies=	-2500.051118
Sum of electronic and thermal Free Energies=	-2500.125959
Entropy correction=	0.07484
Entropy correction after Truhlar's correction=	0.07437
Frequencies –	38.4576
	39.3141
	61.0906
	81.5916
	92.6693

Table S7 Electronic energies and five lowest frequencies for ^{5}SR structure

^{5}SR	
Zero-point correction=	0.408446
Thermal correction to Energy=	0.432016
Thermal correction to Enthalpy=	0.43296
Thermal correction to Gibbs Free Energy=	0.354233
Sum of electronic and zero-point Energies=	-2500.059202
Sum of electronic and thermal Energies=	-2500.035632
Sum of electronic and thermal Enthalpies=	-2500.034687
Sum of electronic and thermal Free Energies=	-2500.113414
Entropy correction=	0.078727
Entropy correction after Truhlar's correction=	0.077651
Frequencies –	26.3029
	30.3261
	52.8768
	57.892
	77.1284

Table S8 Electronic energies and five lowest frequencies for ^{3}RC HAT structure

^{3}RC HAT	
Zero-point correction=	0.557226
Thermal correction to Energy=	0.587271
Thermal correction to Enthalpy=	0.588216
Thermal correction to Gibbs Free Energy=	0.495559
Sum of electronic and zero-point Energies=	-2734.451397
Sum of electronic and thermal Energies=	-2734.421351
Sum of electronic and thermal Enthalpies=	-2734.420407
Sum of electronic and thermal Free Energies=	-2734.513064
Entropy correction=	0.092656
Entropy correction after Truhlar's correction=	0.091092
Frequencies –	26.6793
	31.6614
	37.5992
	41.8991
	44.5621

Table S9 Electronic energies and five lowest frequencies for ^{5}RC HAT structure

^{5}RC HAT	
Zero-point correction=	0.557267
Thermal correction to Energy=	0.588396
Thermal correction to Enthalpy=	0.58934
Thermal correction to Gibbs Free Energy=	0.491035
Sum of electronic and zero-point Energies=	-2734.436181
Sum of electronic and thermal Energies=	-2734.405052
Sum of electronic and thermal Enthalpies=	-2734.404108
Sum of electronic and thermal Free Energies=	-2734.502413
Entropy correction=	0.098305
Entropy correction after Truhlar's correction=	0.095148
Frequencies –	15.6852
	25.4568
	28.8187
	30.1802
	33.6136

Table S10 Electronic energies and five lowest frequencies for ^{3}RC epoxidation structure

^{3}RC epoxidation	
Zero-point correction=	0.557121
Thermal correction to Energy=	0.587222
Thermal correction to Enthalpy=	0.588166
Thermal correction to Gibbs Free Energy=	0.494682
Sum of electronic and zero-point Energies=	-2734.448638
Sum of electronic and thermal Energies=	-2734.418537
Sum of electronic and thermal Enthalpies=	-2734.417593
Sum of electronic and thermal Free Energies=	-2734.511077
Entropy correction=	0.093484
Entropy correction after Truhlar's correction=	0.091504
Frequencies –	18.3668
	31.3801
	38.187
	39.911
	43.4541

Table S11 Electronic energies and five lowest frequencies for ^{5}RC epoxidation structure

^{5}RC epoxidation	
Zero-point correction=	0.557909
Thermal correction to Energy=	0.588837
Thermal correction to Enthalpy=	0.589781
Thermal correction to Gibbs Free Energy=	0.492868
Sum of electronic and zero-point Energies=	-2734.43882
Sum of electronic and thermal Energies=	-2734.407891
Sum of electronic and thermal Enthalpies=	-2734.406947
Sum of electronic and thermal Free Energies=	-2734.50386
Entropy correction=	0.096913
Entropy correction after Truhlar's correction=	0.09424
Frequencies –	19.6774
	21.835
	30.9605
	31.9001
	44.0127

Table S12 Electronic energies and five lowest frequencies for ^{3}TS HAT structure

^{3}TS HAT	
Zero-point correction=	0.550868
Thermal correction to Energy=	0.580371
Thermal correction to Enthalpy=	0.581315
Thermal correction to Gibbs Free Energy=	0.490451
Sum of electronic and zero-point Energies=	-2734.439075
Sum of electronic and thermal Energies=	-2734.409573
Sum of electronic and thermal Enthalpies=	-2734.408628
Sum of electronic and thermal Free Energies=	-2734.499492
Entropy correction=	0.090863
Entropy correction after Truhlar's correction=	0.087971
Frequencies –	-1206.9845
	27.6147
	38.3043
	39.7609
	41.5099

Table S13 Electronic energies and five lowest frequencies for ^{5}TS HAT structure

^{5}TS HAT	
Zero-point correction=	0.551424
Thermal correction to Energy=	0.582104
Thermal correction to Enthalpy=	0.583048
Thermal correction to Gibbs Free Energy=	0.486844
Sum of electronic and zero-point Energies=	-2734.4384
Sum of electronic and thermal Energies=	-2734.407721
Sum of electronic and thermal Enthalpies=	-2734.406776
Sum of electronic and thermal Free Energies=	-2734.502981
Entropy correction=	0.096204
Entropy correction after Truhlar's correction=	0.091895
Frequencies –	-389.1801
	21.4135
	25.5564
	31.704
	35.1666

Table S14 Electronic energies and five lowest frequencies for ^{3}TS epoxidation structure

^{3}TS epoxidation	
Zero-point correction=	0.555518
Thermal correction to Energy=	0.58504
Thermal correction to Enthalpy=	0.585984
Thermal correction to Gibbs Free Energy=	0.494768
Sum of electronic and zero-point Energies=	-2734.429486
Sum of electronic and thermal Energies=	-2734.399964
Sum of electronic and thermal Enthalpies=	-2734.39902
Sum of electronic and thermal Free Energies=	-2734.490236
Entropy correction=	0.091216
Entropy correction after Truhlar's correction=	0.087933
Frequencies –	-395.949
	23.6629
	35.01
	35.6711
	40.8114

Table S15 Electronic energies and five lowest frequencies for ^{5}TS epoxidation structure

^{5}TS epoxidation	
Zero-point correction=	0.556604
Thermal correction to Energy=	0.58691
Thermal correction to Enthalpy=	0.587854
Thermal correction to Gibbs Free Energy=	0.492829
Sum of electronic and zero-point Energies=	-2734.436352
Sum of electronic and thermal Energies=	-2734.406047
Sum of electronic and thermal Enthalpies=	-2734.405102
Sum of electronic and thermal Free Energies=	-2734.500128
Entropy correction=	0.095025
Entropy correction after Truhlar's correction=	0.090938
Frequencies –	-39.9939
	22.3846
	28.3874
	30.6164
	34.7118

Table S16 Electronic energies and five lowest frequencies for ^{3}IM HAT structure

^{3}IM HAT	
Zero-point correction=	0.554765
Thermal correction to Energy=	0.585138
Thermal correction to Enthalpy=	0.586083
Thermal correction to Gibbs Free Energy=	0.492552
Sum of electronic and zero-point Energies=	-2734.466649
Sum of electronic and thermal Energies=	-2734.436276
Sum of electronic and thermal Enthalpies=	-2734.435332
Sum of electronic and thermal Free Energies=	-2734.528862
Entropy correction=	0.09353
Entropy correction after Truhlar's correction=	0.091771
Frequencies –	22.1707
	31.8216
	37.1968
	39.257
	46.8059

Table S17 Electronic energies and five lowest frequencies for ^{5}IM HAT structure

^{5}IM HAT	
Zero-point correction=	0.550816
Thermal correction to Energy=	0.582879
Thermal correction to Enthalpy=	0.583823
Thermal correction to Gibbs Free Energy=	0.48323
Sum of electronic and zero-point Energies=	-2734.471807
Sum of electronic and thermal Energies=	-2734.439744
Sum of electronic and thermal Enthalpies=	-2734.4388
Sum of electronic and thermal Free Energies=	-2734.539392
Entropy correction=	0.100592
Entropy correction after Truhlar's correction=	0.096627
Frequencies –	10.2993
	15.6641
	28.604
	30.3942
	33.1138

Table S18 Electronic energies and five lowest frequencies for ^{3}IM epoxidation structure

^{3}IM epoxidation	
Zero-point correction=	0.557202
Thermal correction to Energy=	0.586743
Thermal correction to Enthalpy=	0.587687
Thermal correction to Gibbs Free Energy=	0.496686
Sum of electronic and zero-point Energies=	-2734.4524
Sum of electronic and thermal Energies=	-2734.422859
Sum of electronic and thermal Enthalpies=	-2734.421914
Sum of electronic and thermal Free Energies=	-2734.512916
Entropy correction=	0.091001
Entropy correction after Truhlar's correction=	0.08936
Frequencies –	16.0063
	36.3879
	37.9651
	49.4936
	53.4423

Table S19 Electronic energies and five lowest frequencies for ^{5}IM epoxidation structure

^{5}IM epoxidation	
Zero-point correction=	0.554547
Thermal correction to Energy=	0.585428
Thermal correction to Enthalpy=	0.586373
Thermal correction to Gibbs Free Energy=	0.490883
Sum of electronic and zero-point Energies=	-2734.472153
Sum of electronic and thermal Energies=	-2734.441272
Sum of electronic and thermal Enthalpies=	-2734.440328
Sum of electronic and thermal Free Energies=	-2734.535817
Entropy correction=	0.095489
Entropy correction after Truhlar's correction=	0.093629
Frequencies –	27.7868
	28.8745
	30.6613
	36.5774
	48.1228

Table S20 Electronic energies and five lowest frequencies for ^{3}TS2 epoxidation structure

^{3}TS2 epoxidation	
Zero-point correction=	0.555757
Thermal correction to Energy=	0.585229
Thermal correction to Enthalpy=	0.586173
Thermal correction to Gibbs Free Energy=	0.495399
Sum of electronic and zero-point Energies=	-2734.44848
Sum of electronic and thermal Energies=	-2734.419007
Sum of electronic and thermal Enthalpies=	-2734.418063
Sum of electronic and thermal Free Energies=	-2734.508838
Entropy correction=	0.090774
Entropy correction after Truhlar's correction=	0.08787
Frequencies –	-393.6157
	25.9293
	33.0698
	35.8105
	47.3002

Table S21 Electronic energies and five lowest frequencies for ^{5}TS2 epoxidation structure

^{5}TS2 epoxidation	
Zero-point correction=	0.554029
Thermal correction to Energy=	0.584435
Thermal correction to Enthalpy=	0.585379
Thermal correction to Gibbs Free Energy=	0.490728
Sum of electronic and zero-point Energies=	-2734.472559
Sum of electronic and thermal Energies=	-2734.442154
Sum of electronic and thermal Enthalpies=	-2734.441209
Sum of electronic and thermal Free Energies=	-2734.53586
Entropy correction=	0.094651
Entropy correction after Truhlar's correction=	0.090938
Frequencies –	-186.4397
	26.4034
	28.6743
	30.0986
	39.0263

Table S22 Electronic energies and five lowest frequencies for ^{3}IM2 epoxidation structure

^{3}IM epoxidation	
Zero-point correction=	0.558127
Thermal correction to Energy=	0.588144
Thermal correction to Enthalpy=	0.589088
Thermal correction to Gibbs Free Energy=	0.495904
Sum of electronic and zero-point Energies=	-2734.481098
Sum of electronic and thermal Energies=	-2734.451081
Sum of electronic and thermal Enthalpies=	-2734.450137
Sum of electronic and thermal Free Energies=	-2734.543321
Entropy correction=	0.093184
Entropy correction after Truhlar's correction=	0.08962
Frequencies –	16.8734
	32.2921
	35.9417
	44.1411
	48.3055

Table S23 Electronic energies and five lowest frequencies for ^{5}IM2 epoxidation structure

^{5}IM epoxidation	
Zero-point correction=	0.557467
Thermal correction to Energy=	0.58797
Thermal correction to Enthalpy=	0.588914
Thermal correction to Gibbs Free Energy=	0.494393
Sum of electronic and zero-point Energies=	-2734.504129
Sum of electronic and thermal Energies=	-2734.473626
Sum of electronic and thermal Enthalpies=	-2734.472682
Sum of electronic and thermal Free Energies=	-2734.567203
Entropy correction=	0.094521
Entropy correction after Truhlar's correction=	0.091291
Frequencies –	27.8788
	30.8189
	37.994
	49.1487
	52.6328

S2 Cartesian Coordinates of the Molecules Studied in This Work

^{3}SR optimized with B3LYP-D3BJ/def2-SVP

51

Fe	0.057162	-0.000002	-0.666025
N	-0.124150	-0.000002	1.421630
N	-1.386451	-1.357321	-0.493092
N	-1.386451	1.357320	-0.493090
N	1.430051	-1.376429	-0.311329
N	1.430052	1.376424	-0.311330
O	0.185769	-0.000002	-2.277830
C	-1.693611	-2.327395	-1.361686
C	-2.730870	-3.223290	-1.096087
C	-3.446447	-3.097443	0.095765
C	-3.116430	-2.072997	0.994425
C	-2.076797	-1.215985	0.660138
C	-1.625732	-0.000001	1.455284
C	-2.076795	1.215984	0.660140
C	-3.116428	2.072997	0.994429
C	-3.446445	3.097444	0.095769
C	-2.730869	3.223290	-1.096083
C	-1.693611	2.327395	-1.361683
C	2.261083	-1.855117	-1.253004
C	3.268010	-2.762597	-0.938273
C	3.417541	-3.169004	0.389881
C	2.548384	-2.662838	1.359580
C	1.552447	-1.767358	0.974792
C	0.513013	-1.240401	1.937268
C	0.513016	1.240395	1.937269
C	1.552443	1.767360	0.974789
C	2.548372	2.662849	1.359574
C	3.417528	3.169017	0.389874
C	3.268002	2.762602	-0.938278
C	2.261081	1.855114	-1.253007
H	-1.101336	-2.366051	-2.278298
H	-2.970166	-4.003860	-1.820059
H	-4.259549	-3.788741	0.328079
H	-3.659668	-1.947638	1.932660
H	-2.036568	-0.000002	2.476128
H	-3.659664	1.947638	1.932664
H	-4.259546	3.788742	0.328085
H	-2.970165	4.003861	-1.820055
H	-1.101337	2.366050	-2.278296
H	2.095034	-1.489819	-2.268338
H	3.925162	-3.136499	-1.724983
H	4.204172	-3.872953	0.670098
H	2.638534	-2.963801	2.405177
H	2.638518	2.963818	2.405169
H	4.204153	3.872972	0.670088
H	3.925152	3.136504	-1.724990
H	2.095035	1.489812	-2.268340
H	0.950787	-1.069883	2.931860
H	-0.262199	-2.010873	2.067999
H	0.950799	1.069872	2.931856
H	-0.262197	2.010865	2.068011

[5]SR optimized with B3LYP-D3BJ/def2-SVP

51

Fe	0.076358	-0.000015	-0.803732
N	-0.110415	-0.000020	1.312332
N	-1.495855	-1.414093	-0.518927
N	-1.495845	1.414086	-0.518918
N	1.509468	-1.453998	-0.357169
N	1.509455	1.453972	-0.357177
O	0.230217	-0.000019	-2.402972
C	-1.880618	-2.398048	-1.339891
C	-2.930691	-3.253295	-0.999836
C	-3.579244	-3.069520	0.222462
C	-3.169678	-2.033024	1.073158
C	-2.120048	-1.221463	0.661118
C	-1.610960	-0.000008	1.412873
C	-2.120032	1.221462	0.661132
C	-3.169641	2.033041	1.073187
C	-3.579194	3.069551	0.222500
C	-2.930647	3.253321	-0.999801
C	-1.880594	2.398055	-1.339871
C	2.384646	-1.947497	-1.248921
C	3.421958	-2.790024	-0.859563
C	3.553386	-3.108363	0.494806
C	2.639721	-2.585280	1.414894
C	1.615829	-1.761533	0.951504
C	0.521238	-1.238812	1.851845
C	0.521264	1.238754	1.851858
C	1.615813	1.761522	0.951491
C	2.639675	2.585315	1.414865
C	3.553314	3.108424	0.494767
C	3.421892	2.790064	-0.859598
C	2.384609	1.947495	-1.248941
H	-1.336369	-2.491066	-2.282914
H	-3.230623	-4.046762	-1.686288
H	-4.401208	-3.726238	0.516153
H	-3.660614	-1.865384	2.033507
H	-1.957088	-0.000012	2.457681
H	-3.660573	1.865405	2.033538
H	-4.401142	3.726284	0.516203
H	-3.230565	4.046798	-1.686247
H	-1.336350	2.491073	-2.282896
H	2.235175	-1.646958	-2.288678
H	4.115643	-3.181654	-1.605255
H	4.362708	-3.758404	0.834818
H	2.719410	-2.820853	2.477968
H	2.719362	2.820902	2.477936
H	4.362612	3.758501	0.834767
H	4.115557	3.181712	-1.605298
H	2.235140	1.646943	-2.288694
H	0.898614	-1.066861	2.870599
H	-0.252551	-2.017250	1.932998
H	0.898697	1.066759	2.870584
H	-0.252522	2.017186	1.933092

^{3}RC HAT optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	0.711158	0.019188	-0.421954
N	1.310916	-0.096860	1.582655
N	-0.251530	-1.643420	0.086460
N	-0.799172	1.010454	0.403505
N	2.370864	-1.012669	-0.730053
N	1.812323	1.660109	-0.411863
O	0.235898	0.106068	-1.966841
C	-0.640092	-2.633026	-0.725219
C	-1.300215	-3.754254	-0.220697
C	-1.546924	-3.835324	1.150657
C	-1.136580	-2.789362	1.988672
C	-0.493315	-1.701473	1.414170
C	-0.044036	-0.441833	2.136878
C	-0.981326	0.672481	1.698566
C	-1.953166	1.281913	2.478598
C	-2.756580	2.265473	1.886674
C	-2.561166	2.597060	0.546823
C	-1.563642	1.942025	-0.174847
C	2.880861	-1.251534	-1.950383
C	4.098161	-1.905951	-2.112606
C	4.803152	-2.308830	-0.975855
C	4.262415	-2.054800	0.287019
C	3.031764	-1.407296	0.378622
C	2.327756	-1.174788	1.695742
C	1.830436	1.237098	1.983265
C	2.316257	2.022338	0.786567
C	3.182245	3.108250	0.900497
C	3.513949	3.835068	-0.245562
C	2.972971	3.452691	-1.475507
C	2.125299	2.350245	-1.521771
H	-0.426584	-2.503995	-1.787781
H	-1.617585	-4.546353	-0.900499
H	-2.059732	-4.703771	1.569631
H	-1.318585	-2.821847	3.064154
H	-0.042974	-0.572724	3.229388
H	-2.082758	0.999199	3.524539
H	-3.533397	2.762394	2.471459
H	-3.179403	3.348109	0.053729
H	-1.370130	2.144113	-1.229628
H	2.284082	-0.902904	-2.795505
H	4.485131	-2.088727	-3.116269
H	5.765805	-2.816033	-1.070130
H	4.787679	-2.360713	1.193881
H	3.587036	3.384110	1.876167
H	4.189293	4.690729	-0.177846
H	3.205865	3.995551	-2.392866
H	1.675001	1.992825	-2.449827
H	3.051046	-0.948173	2.492867
H	1.824871	-2.108799	1.989214
H	2.627076	1.136247	2.735060
H	1.019544	1.804798	2.464471
H	-2.259592	-0.466519	-1.856435
C	-4.690449	-0.146698	0.355579

C	-5.686293	0.704175	-0.386295
C	-5.596782	0.505163	-1.903684
C	-4.139914	0.501314	-2.374386
C	-3.341942	-0.627272	-1.707487
C	-3.653415	-0.753799	-0.238364
H	-4.849791	-0.286871	1.430813
H	-5.525132	1.769547	-0.127046
H	-6.172122	1.284477	-2.425763
H	-4.081572	0.410272	-3.469638
H	-3.680592	1.474586	-2.121086
H	-3.563781	-1.589818	-2.207319
H	-3.010163	-1.402426	0.363276
H	-6.703187	0.476842	-0.025706
H	-6.063008	-0.459168	-2.168696

^{3}TS HAT optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	-0.461202	-0.037145	-0.214928
N	-1.488644	0.392857	1.528821
N	0.178147	1.830569	0.039565
N	0.946143	-0.575683	1.086882
N	-2.117259	0.600533	-1.088206
N	-1.348462	-1.795700	-0.051567
O	0.342400	-0.423581	-1.679995
C	0.577998	2.702676	-0.893453
C	0.959588	4.000675	-0.552338
C	0.910107	4.390733	0.787456
C	0.473915	3.475218	1.754255
C	0.113269	2.200121	1.337014
C	-0.344639	1.063916	2.237804
C	0.789546	0.052682	2.272762
C	1.617258	-0.209510	3.355885
C	2.633875	-1.161918	3.196738
C	2.781608	-1.806361	1.969003
C	1.913529	-1.483959	0.924815
C	-2.372706	0.470208	-2.399708
C	-3.599569	0.844867	-2.941113
C	-4.583235	1.355280	-2.090848
C	-4.306345	1.483781	-0.727145
C	-3.052358	1.101543	-0.254898
C	-2.625595	1.288178	1.183637
C	-1.931015	-0.895532	2.127412
C	-2.070042	-1.972193	1.074448
C	-2.835463	-3.120903	1.265187
C	-2.835786	-4.105541	0.273444
C	-2.072851	-3.911629	-0.880419
C	-1.341197	-2.734228	-1.011112
H	0.595272	2.338627	-1.921996
H	1.289775	4.691029	-1.330105
H	1.201202	5.401695	1.080796
H	0.410795	3.752945	2.807805
H	-0.607104	1.420744	3.245336
H	1.469363	0.306366	4.306133
H	3.299128	-1.397913	4.030107
H	3.563876	-2.550217	1.812205

H	1.985353	-1.948116	-0.059452
H	-1.559229	0.053349	-2.997294
H	-3.778265	0.730008	-4.011279
H	-5.558933	1.649324	-2.483644
H	-5.054256	1.880702	-0.037976
H	-3.420179	-3.244954	2.178724
H	-3.428441	-5.013919	0.401237
H	-2.047390	-4.657813	-1.675998
H	-0.729199	-2.505533	-1.886379
H	-3.470447	1.129651	1.870091
H	-2.307137	2.332942	1.318787
H	-2.870372	-0.765425	2.684787
H	-1.177375	-1.222418	2.859688
H	1.617078	-0.022580	-1.838343
C	4.546793	0.110282	-0.376450
C	5.193460	-1.096293	-0.993189
C	4.857114	-1.217510	-2.483724
C	3.347966	-1.071571	-2.717380
C	2.805765	0.233212	-2.137630
C	3.486337	0.736681	-0.941342
H	4.994440	0.529035	0.530813
H	4.866769	-2.009611	-0.454455
H	5.211481	-2.179417	-2.883217
H	3.104598	-1.140028	-3.787457
H	2.832789	-1.925406	-2.238317
H	2.604349	1.020870	-2.883886
H	3.126567	1.670770	-0.498104
H	6.283258	-1.049489	-0.837715
H	5.390841	-0.426255	-3.035922

^{3}IM HAT optimized with B3LYP-D3BJ/def2-SVP

67

Fe	-0.472651	-0.032182	-0.182353
N	-1.585566	0.360585	1.487697
N	0.211376	1.801965	0.171255
N	0.849364	-0.642139	1.166861
N	-2.047243	0.666037	-1.147684
N	-1.408194	-1.769734	-0.156029
O	0.450623	-0.407524	-1.660946
C	0.705593	2.688230	-0.700942
C	1.104803	3.960462	-0.289684
C	0.971969	4.309340	1.055695
C	0.439331	3.379172	1.958406
C	0.068608	2.131310	1.473932
C	-0.477026	0.977585	2.300570
C	0.629249	-0.062074	2.368969
C	1.381743	-0.388642	3.487465
C	2.392023	-1.352783	3.347476
C	2.610649	-1.939758	2.102231
C	1.814751	-1.555205	1.020826
C	-2.215961	0.578096	-2.475977
C	-3.397186	0.996663	-3.083605
C	-4.423007	1.505393	-2.283625
C	-4.234596	1.589554	-0.901020
C	-3.022732	1.165002	-0.360977

C	-2.678827	1.298846	1.105013
C	-2.101174	-0.936001	2.013000
C	-2.205225	-1.968910	0.913663
C	-3.010929	-3.101421	1.008330
C	-2.970923	-4.045458	-0.021947
C	-2.130432	-3.827771	-1.116048
C	-1.361479	-2.667144	-1.152188
H	0.784233	2.357712	-1.737925
H	1.513294	4.662547	-1.018213
H	1.274148	5.299733	1.403052
H	0.312534	3.625022	3.014124
H	-0.802156	1.303176	3.300038
H	1.183581	0.086833	4.449549
H	2.998890	-1.638994	4.209158
H	3.393711	-2.685350	1.957456
H	1.938539	-1.977240	0.022814
H	-1.370921	0.160782	-3.028115
H	-3.508665	0.916953	-4.166019
H	-5.364226	1.833163	-2.730222
H	-5.017808	1.984615	-0.251150
H	-3.656536	-3.245705	1.876758
H	-3.593132	-4.941500	0.030312
H	-2.073137	-4.542774	-1.938176
H	-0.687637	-2.417853	-1.974761
H	-3.564650	1.142528	1.737830
H	-2.339855	2.329182	1.291140
H	-3.068007	-0.793716	2.517481
H	-1.401845	-1.309027	2.776412
H	1.377753	-0.098757	-1.641038
C	4.387178	-0.175888	-0.185700
C	4.927831	-1.405435	-0.855815
C	5.096414	-1.202048	-2.368476
C	3.836116	-0.602644	-3.008298
C	3.358654	0.607205	-2.254046
C	3.663560	0.774604	-0.904578
H	4.607105	-0.000868	0.870468
H	4.248478	-2.265744	-0.673411
H	5.359080	-2.152255	-2.855889
H	4.023177	-0.342282	-4.062011
H	3.029611	-1.364539	-3.037225
H	2.830547	1.396066	-2.798327
H	3.340691	1.686550	-0.392440
H	5.885585	-1.697350	-0.395547
H	5.939543	-0.512666	-2.537990

[5]RC HAT optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	0.406014	0.069370	-0.424467
N	1.710231	0.243133	1.317907
N	2.358202	-0.501534	-1.216250
N	0.470704	-1.981427	0.349801
N	0.938223	2.121371	-0.565221
N	-1.010672	0.644465	1.031267
O	-0.542170	-0.035845	-1.715043
C	2.771692	-0.456319	-2.487666

C	4.064740	-0.845812	-2.842703
C	4.932839	-1.284756	-1.841808
C	4.488037	-1.329048	-0.513314
C	3.185276	-0.929241	-0.240479
C	2.526075	-1.003234	1.130559
C	1.572993	-2.190489	1.098614
C	1.820967	-3.415010	1.707056
C	0.893450	-4.449559	1.521395
C	-0.239512	-4.222336	0.739390
C	-0.420315	-2.962302	0.164585
C	0.337557	2.987332	-1.397720
C	0.583819	4.355437	-1.325557
C	1.464714	4.825594	-0.348191
C	2.079446	3.915443	0.516809
C	1.799971	2.557208	0.376036
C	2.503228	1.497678	1.194107
C	0.857681	0.224608	2.538612
C	-0.525666	0.778126	2.285168
C	-1.305539	1.329937	3.298606
C	-2.612583	1.733472	3.004373
C	-3.099392	1.579359	1.705339
C	-2.260808	1.035632	0.736503
H	2.047570	-0.105639	-3.227173
H	4.378635	-0.804293	-3.886937
H	5.951423	-1.592275	-2.088818
H	5.145149	-1.668638	0.289331
H	3.280151	-1.125859	1.923411
H	2.716521	-3.563743	2.313091
H	1.059270	-5.423942	1.986336
H	-0.978812	-5.007040	0.571236
H	-1.290509	-2.726527	-0.451872
H	-0.353999	2.556273	-2.125564
H	0.087056	5.036511	-2.018286
H	1.671492	5.894234	-0.256899
H	2.772808	4.257604	1.287612
H	-0.900175	1.438890	4.306427
H	-3.240872	2.166911	3.785717
H	-4.111197	1.877671	1.427810
H	-2.600197	0.906689	-0.293802
H	2.768303	1.885979	2.188856
H	3.451448	1.259130	0.689057
H	1.349311	0.764840	3.361562
H	0.750340	-0.819204	2.870039
H	-2.648934	-0.397526	-2.705237
C	-3.694372	-0.667990	-2.470829
C	-3.731482	-1.780600	-1.417517
C	-5.141059	-1.958118	-0.845728
C	-5.624887	-0.668065	-0.172691
C	-5.308189	0.557276	-0.990718
C	-4.455058	0.553993	-2.028611
H	-4.119142	-1.032529	-3.424950
H	-3.046410	-1.514144	-0.589500
H	-5.175368	-2.796900	-0.133051
H	-6.711218	-0.714570	0.010574
H	-5.170980	-0.569250	0.834190
H	-5.838589	1.482401	-0.737628

H	-4.320372	1.469651	-2.614965
H	-3.361953	-2.725024	-1.849891
H	-5.828308	-2.217884	-1.668418

[5]TS HAT optimized with B3LYP-D3BJ/def2-SVP

67

Fe	0.289833	0.014933	-0.343513
N	1.825553	0.379302	1.248564
N	2.156175	-0.370086	-1.353084
N	0.656971	-1.958504	0.470377
N	0.615165	2.100115	-0.555073
N	-0.938717	0.507480	1.325014
O	-0.867948	-0.228291	-1.507767
C	2.384014	-0.313538	-2.670408
C	3.648004	-0.576582	-3.201111
C	4.687522	-0.902438	-2.328452
C	4.437569	-0.961535	-0.951026
C	3.150707	-0.688462	-0.501357
C	2.703877	-0.790027	0.951664
C	1.862851	-2.055518	1.063042
C	2.297064	-3.239782	1.647913
C	1.447084	-4.352765	1.606488
C	0.202912	-4.242178	0.983387
C	-0.160047	-3.016763	0.421898
C	-0.173687	2.877538	-1.314714
C	-0.049356	4.263470	-1.317146
C	0.914550	4.848308	-0.491363
C	1.724621	4.030686	0.300655
C	1.553729	2.647625	0.239519
C	2.458153	1.693964	0.990453
C	1.151841	0.313820	2.565070
C	-0.306612	0.712923	2.496166
C	-0.991671	1.204506	3.607301
C	-2.358845	1.471193	3.496335
C	-3.000466	1.247517	2.275554
C	-2.249728	0.769753	1.205440
H	1.530565	-0.055994	-3.302272
H	3.808327	-0.526730	-4.279240
H	5.688382	-1.110266	-2.713327
H	5.230966	-1.213953	-0.245179
H	3.576327	-0.845073	1.622240
H	3.276375	-3.296696	2.126497
H	1.758307	-5.297527	2.057678
H	-0.480104	-5.091280	0.928706
H	-1.118546	-2.870588	-0.081867
H	-0.916356	2.355029	-1.922047
H	-0.699430	4.870426	-1.949144
H	1.033563	5.933645	-0.461026
H	2.484565	4.462349	0.955020
H	-0.463529	1.373636	4.547773
H	-2.914843	1.855595	4.354316
H	-4.064871	1.449073	2.145971
H	-2.695863	0.600020	0.222117
H	2.800816	2.153996	1.930219
H	3.359765	1.537329	0.378745

H	1.681998	0.928881	3.308736
H	1.197713	-0.722488	2.933101
H	-2.248153	-0.518669	-2.236723
C	-3.364247	-0.788832	-2.392919
C	-3.664774	-2.000384	-1.510106
C	-5.149844	-2.081545	-1.139532
C	-5.595767	-0.804063	-0.418735
C	-5.126266	0.434093	-1.125771
C	-4.143575	0.419640	-2.059808
H	-3.387035	-1.004395	-3.477168
H	-3.080030	-1.907028	-0.574901
H	-5.343353	-2.964614	-0.512021
H	-6.692652	-0.770602	-0.315127
H	-5.211611	-0.798244	0.622500
H	-5.651679	1.372761	-0.919608
H	-3.918423	1.338567	-2.611899
H	-3.327354	-2.924417	-2.003307
H	-5.749630	-2.206553	-2.056502

[5]IM HAT optimized with B3LYP-D3BJ/def2-SVP

67

Fe	0.188370	-0.098773	-0.255268
N	1.974349	0.663979	0.998998
N	1.903020	-0.225827	-1.585390
N	1.082823	-1.886663	0.574108
N	0.129112	2.022211	-0.573381
N	-0.696156	0.327988	1.646926
O	-1.205285	-0.702317	-1.178362
C	1.862939	-0.231714	-2.923525
C	3.026876	-0.324770	-3.687819
C	4.255062	-0.412765	-3.030207
C	4.286683	-0.408865	-1.629847
C	3.082298	-0.315031	-0.941153
C	2.953572	-0.372726	0.575416
C	2.376830	-1.741055	0.916894
C	3.108155	-2.786814	1.469281
C	2.467448	-4.017194	1.665007
C	1.126935	-4.157545	1.301573
C	0.462500	-3.059108	0.754396
C	-0.924233	2.613584	-1.161729
C	-1.050300	3.997508	-1.225796
C	-0.052747	4.784751	-0.644123
C	1.034885	4.161805	-0.028192
C	1.100399	2.767945	-0.016478
C	2.297532	2.032059	0.548190
C	1.599029	0.599401	2.425371
C	0.107113	0.728411	2.648538
C	-0.421249	1.173129	3.860866
C	-1.807660	1.184841	4.032190
C	-2.628387	0.760136	2.984017
C	-2.030789	0.343199	1.798844
H	0.873842	-0.164662	-3.383187
H	2.965978	-0.329300	-4.777209
H	5.184225	-0.484121	-3.599936
H	5.231664	-0.476097	-1.087758

H	3.940934	-0.244461	1.048116
H	4.155318	-2.647300	1.743772
H	3.014358	-4.857590	2.098188
H	0.599792	-5.103280	1.436473
H	-0.584529	-3.107942	0.445502
H	-1.679531	1.945687	-1.580960
H	-1.915498	4.447003	-1.715468
H	-0.122325	5.874540	-0.666372
H	1.827872	4.752008	0.435403
H	0.243937	1.502123	4.661691
H	-2.242023	1.526857	4.974201
H	-3.715386	0.757535	3.077690
H	-2.619057	0.022933	0.935861
H	2.752795	2.619113	1.361353
H	3.055710	1.973774	-0.247841
H	2.137244	1.361679	3.010622
H	1.912492	-0.374759	2.831246
H	-2.075591	-0.604641	-1.618661
C	-3.880444	-0.638878	-2.501804
C	-4.074245	-2.107682	-2.248425
C	-5.208304	-2.367789	-1.247224
C	-5.080201	-1.489945	0.005886
C	-4.862925	-0.048571	-0.348559
C	-4.306363	0.313366	-1.571940
H	-3.481206	-0.311663	-3.466689
H	-3.127892	-2.544967	-1.865392
H	-5.236900	-3.431497	-0.969292
H	-5.971719	-1.592364	0.645164
H	-4.234144	-1.847634	0.631164
H	-5.178094	0.730257	0.351981
H	-4.206795	1.375959	-1.816316
H	-4.265797	-2.629507	-3.199542
H	-6.169498	-2.140985	-1.736647

^{3}RC epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	0.620047	0.069745	-0.330904
N	1.745442	0.029628	1.438367
N	2.322997	-0.645818	-1.074174
N	0.238453	-1.801667	0.227404
N	1.309797	1.917102	-0.449779
N	-0.795760	0.749455	0.862765
O	-0.233745	0.092560	-1.704562
C	2.753023	-0.560976	-2.338263
C	3.986183	-1.097778	-2.712356
C	4.773199	-1.725632	-1.745564
C	4.307777	-1.811492	-0.425953
C	3.068958	-1.259369	-0.129350
C	2.357920	-1.322568	1.213995
C	1.202111	-2.295284	1.036531
C	1.123181	-3.576779	1.563910
C	0.011320	-4.363849	1.231170
C	-0.970232	-3.842725	0.387510
C	-0.825070	-2.543345	-0.101887
C	0.867864	2.816069	-1.345469

C	1.314686	4.133870	-1.330887
C	2.231927	4.523358	-0.351971
C	2.681824	3.579724	0.574935
C	2.204840	2.272796	0.495913
C	2.702829	1.165575	1.396277
C	0.799050	0.105855	2.582808
C	-0.496059	0.772211	2.180156
C	-1.377478	1.326130	3.105016
C	-2.592277	1.852442	2.655057
C	-2.888752	1.809029	1.292189
C	-1.958979	1.252934	0.418992
H	2.086450	-0.065548	-3.047248
H	4.316338	-1.023395	-3.749711
H	5.743642	-2.149652	-2.012754
H	4.899199	-2.298438	0.351357
H	3.035665	-1.631907	2.023955
H	1.908477	-3.956228	2.219973
H	-0.081598	-5.376521	1.629631
H	-1.845040	-4.429759	0.103787
H	-1.555979	-2.083496	-0.767410
H	0.144482	2.447666	-2.075494
H	0.941083	4.840581	-2.073494
H	2.593863	5.552883	-0.308280
H	3.400025	3.853439	1.350279
H	-1.117745	1.342088	4.165296
H	-3.296752	2.291632	3.364709
H	-3.824500	2.195299	0.887715
H	-2.144722	1.198017	-0.654162
H	2.904511	1.544604	2.409040
H	3.664956	0.804623	1.001957
H	1.260031	0.625855	3.435523
H	0.574583	-0.915372	2.926295
H	-2.641930	-0.788823	-2.155831
C	-3.744404	-0.773800	-2.070945
C	-4.221214	-1.527784	-0.822957
C	-5.706412	-1.261405	-0.558784
C	-5.964733	0.230909	-0.320261
C	-5.212225	1.105249	-1.289927
C	-4.229393	0.653829	-2.084761
H	-4.106077	-1.286927	-2.981397
H	-3.638404	-1.192390	0.056995
H	-6.064830	-1.853309	0.297273
H	-7.043122	0.448817	-0.394377
H	-5.692111	0.505384	0.718369
H	-5.521067	2.154121	-1.364304
H	-3.768934	1.332869	-2.811065
H	-4.038224	-2.609867	-0.933702
H	-6.286812	-1.594179	-1.435765

^{3}TS1 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	-0.166315	-0.058509	-0.000025
N	-2.197657	0.406264	0.171825
N	-0.274044	1.477550	-1.335952
N	-0.026075	1.335596	1.417192

N	-0.808953	-1.341276	-1.366925
N	-0.613590	-1.412430	1.389066
O	1.500481	-0.461427	0.078043
C	0.461729	1.734461	-2.424713
C	0.227293	2.851170	-3.228095
C	-0.811183	3.719771	-2.893167
C	-1.592457	3.439301	-1.765973
C	-1.291883	2.309636	-1.015191
C	-2.024899	1.893204	0.247747
C	-1.084426	2.172128	1.409013
C	-1.216131	3.194400	2.340239
C	-0.209109	3.345517	3.303118
C	0.882727	2.475627	3.296213
C	0.941640	1.470016	2.329661
C	-0.068564	-2.333648	-1.887210
C	-0.607497	-3.269116	-2.765211
C	-1.962266	-3.180387	-3.093168
C	-2.731293	-2.160530	-2.528655
C	-2.122080	-1.249261	-1.667060
C	-2.870593	-0.085259	-1.057862
C	-2.725075	-0.213269	1.413231
C	-1.879833	-1.386670	1.850260
C	-2.345991	-2.355859	2.737319
C	-1.473192	-3.359406	3.163499
C	-0.159231	-3.362532	2.689578
C	0.234630	-2.371001	1.795792
H	1.255634	1.028497	-2.658832
H	0.854368	3.027934	-4.103238
H	-1.019509	4.600735	-3.504033
H	-2.424382	4.085674	-1.480976
H	-2.978202	2.432881	0.356856
H	-2.082327	3.858000	2.319253
H	-0.280933	4.137633	4.051563
H	1.684636	2.570570	4.029977
H	1.765683	0.757829	2.255775
H	0.972066	-2.365782	-1.566908
H	0.024978	-4.058296	-3.174463
H	-2.418926	-3.903280	-3.772533
H	-3.795989	-2.072104	-2.753303
H	-3.377557	-2.321234	3.093116
H	-1.816116	-4.129153	3.858192
H	0.554842	-4.125651	3.002796
H	1.241626	-2.304477	1.380288
H	-3.915389	-0.360991	-0.850230
H	-2.907263	0.730351	-1.795256
H	-3.776026	-0.512649	1.285218
H	-2.713015	0.538123	2.217576
H	2.814606	1.632408	-0.779799
C	3.590306	0.862559	-0.909081
C	4.469380	0.754262	0.341560
C	5.435700	-0.427095	0.235406
C	4.679071	-1.749269	0.050362
C	3.587997	-1.654688	-0.963552
C	2.958514	-0.456012	-1.279124
H	4.207618	1.187119	-1.768198
H	3.823473	0.620117	1.225762

H	6.079661	-0.485059	1.125372
H	5.364096	-2.572241	-0.211077
H	4.219699	-2.056791	1.014431
H	3.220058	-2.583899	-1.411880
H	2.296164	-0.473122	-2.148495
H	5.022208	1.694192	0.489552
H	6.107080	-0.272897	-0.626256

^{3}IM1 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67

Fe	-0.162409	-0.037338	-0.011505
N	-1.959941	0.818524	0.499959
N	-0.096066	1.609135	-1.227575
N	0.491044	1.127040	1.459128
N	-1.260261	-1.022668	-1.336285
N	-0.669323	-1.401950	1.338805
O	1.414204	-0.848310	-0.251265
C	0.492494	1.814681	-2.413787
C	0.392941	3.031517	-3.089968
C	-0.350225	4.064571	-2.520720
C	-0.986327	3.842699	-1.293492
C	-0.836545	2.603888	-0.683347
C	-1.454221	2.226221	0.650924
C	-0.327696	2.178766	1.667414
C	-0.085448	3.105817	2.672745
C	1.047071	2.924763	3.478691
C	1.883772	1.830114	3.252202
C	1.570431	0.938678	2.224808
C	-0.854103	-2.109861	-2.014167
C	-1.713885	-2.815758	-2.850341
C	-3.039531	-2.392116	-2.966203
C	-3.462136	-1.279868	-2.234880
C	-2.543860	-0.612465	-1.426417
C	-2.903998	0.621137	-0.633886
C	-2.438860	0.203582	1.769146
C	-1.820735	-1.156206	1.995318
C	-2.359586	-2.085780	2.882908
C	-1.677662	-3.285307	3.101531
C	-0.477891	-3.517948	2.425436
C	-0.005022	-2.550727	1.542490
H	1.059147	0.985329	-2.833760
H	0.895353	3.156299	-4.050403
H	-0.445396	5.027789	-3.026527
H	-1.594841	4.617864	-0.824550
H	-2.244397	2.933306	0.945599
H	-0.761603	3.948265	2.828199
H	1.269030	3.634313	4.278755
H	2.772572	1.663058	3.862623
H	2.176038	0.063328	1.984938
H	0.180321	-2.415630	-1.861052
H	-1.347284	-3.689448	-3.391214
H	-3.741198	-2.928597	-3.608468
H	-4.496114	-0.933650	-2.288483
H	-3.297114	-1.871252	3.399600
H	-2.080272	-4.029003	3.792585

H	0.086345	-4.440114	2.572353
H	0.919811	-2.658249	0.972986
H	-3.941437	0.565330	-0.272700
H	-2.852821	1.496871	-1.297546
H	-3.536955	0.144293	1.780435
H	-2.155097	0.857985	2.607468
H	2.824245	1.201057	-1.003872
C	3.332562	0.256004	-1.256170
C	4.413225	-0.073050	-0.220547
C	5.092920	-1.409865	-0.522433
C	4.062918	-2.553540	-0.590307
C	2.920811	-2.210846	-1.484914
C	2.278984	-0.860472	-1.392398
H	3.807291	0.395838	-2.242440
H	3.964458	-0.111337	0.787186
H	5.856841	-1.636122	0.236856
H	4.537712	-3.492688	-0.911651
H	3.686930	-2.741905	0.439470
H	2.474539	-2.972790	-2.131136
H	1.676963	-0.692615	-2.305194
H	5.156904	0.738725	-0.197102
H	5.618505	-1.341308	-1.489743

^{3}TS2 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	-0.150811	-0.054798	-0.057685
N	-1.759998	0.994177	0.908090
N	0.010926	1.743727	-0.998392
N	0.849458	0.766509	1.495037
N	-1.652215	-0.599204	-1.298564
N	-0.721322	-1.547467	1.129472
O	1.227009	-1.125008	-0.817991
C	0.437866	2.050213	-2.232040
C	0.410547	3.353509	-2.728479
C	-0.087164	4.374517	-1.919317
C	-0.560235	4.052714	-0.642608
C	-0.500013	2.728833	-0.221992
C	-0.985118	2.250529	1.137206
C	0.242984	1.881377	1.950452
C	0.736303	2.591837	3.038398
C	1.893361	2.119483	3.670907
C	2.498431	0.950589	3.204852
C	1.938238	0.291786	2.110277
C	-1.540065	-1.570682	-2.218865
C	-2.624490	-1.986423	-2.985378
C	-3.866695	-1.384130	-2.771062
C	-3.978507	-0.387474	-1.799659
C	-2.844649	-0.010811	-1.079941
C	-2.871216	1.106936	-0.059090
C	-2.104867	0.216171	2.117591
C	-1.701450	-1.241668	2.005532
C	-2.270381	-2.218769	2.822239
C	-1.803444	-3.532020	2.739719
C	-0.781144	-3.831098	1.836710
C	-0.269270	-2.808766	1.042370

H	0.812209	1.228587	-2.841145
H	0.774830	3.555434	-3.736912
H	-0.121099	5.405225	-2.278527
H	-0.981241	4.818058	0.011783
H	-1.570465	3.035917	1.641427
H	0.225458	3.489495	3.391089
H	2.308442	2.654754	4.527619
H	3.392425	0.547289	3.682954
H	2.354596	-0.631375	1.705897
H	-0.550482	-2.019104	-2.314491
H	-2.496760	-2.775510	-3.727884
H	-4.741397	-1.692793	-3.347493
H	-4.937291	0.095335	-1.600321
H	-3.068017	-1.951797	3.518377
H	-2.235045	-4.311373	3.371347
H	-0.387673	-4.844156	1.740611
H	0.521307	-2.968704	0.307802
H	-3.843266	1.130991	0.457731
H	-2.784519	2.064084	-0.595163
H	-3.179924	0.296410	2.340624
H	-1.581031	0.649323	2.983416
H	2.793220	1.046399	-1.135211
C	3.246794	0.134948	-1.555012
C	4.322741	-0.422995	-0.616904
C	4.871795	-1.755024	-1.128191
C	3.753173	-2.798884	-1.253855
C	2.561918	-2.282386	-1.964310
C	2.133073	-0.862187	-1.879084
H	3.719916	0.427953	-2.508247
H	3.906642	-0.567370	0.393012
H	5.660567	-2.135845	-0.463027
H	4.099597	-3.720966	-1.751127
H	3.438904	-3.134890	-0.241529
H	1.870515	-2.984954	-2.439190
H	1.591210	-0.553461	-2.793152
H	5.134791	0.312372	-0.512998
H	5.339561	-1.605461	-2.115824

^{3}IM2 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67

Fe	-0.148334	-0.043153	-0.103141
N	-1.505993	1.032503	1.286626
N	0.236201	1.835141	-0.673059
N	1.117912	0.304780	1.523243
N	-1.877040	-0.042736	-1.235921
N	-0.876132	-1.653108	0.814041
O	1.199506	-1.006452	-1.480209
C	0.631281	2.293324	-1.869480
C	0.792207	3.653892	-2.128487
C	0.520128	4.569586	-1.111226
C	0.082675	4.092846	0.129266
C	-0.051034	2.720251	0.310906
C	-0.500943	2.076155	1.616540
C	0.716817	1.389080	2.215615
C	1.384043	1.826967	3.355172

C	2.504766	1.109783	3.789428
C	2.903590	-0.023143	3.077866
C	2.175549	-0.397207	1.948227
C	-2.031554	-0.760488	-2.360200
C	-3.248873	-0.842201	-3.028796
C	-4.347522	-0.162555	-2.495872
C	-4.182250	0.577109	-1.324064
C	-2.924924	0.624260	-0.718777
C	-2.666108	1.482695	0.507491
C	-1.823221	0.048522	2.332134
C	-1.690654	-1.391681	1.862618
C	-2.353615	-2.419601	2.535592
C	-2.167635	-3.741505	2.130563
C	-1.326901	-3.999716	1.045968
C	-0.708762	-2.925860	0.414202
H	0.815557	1.545824	-2.641405
H	1.120987	3.984014	-3.115101
H	0.633437	5.642126	-1.282326
H	-0.160840	4.779907	0.941624
H	-0.881554	2.845577	2.308639
H	1.031473	2.706205	3.897339
H	3.051519	1.427813	4.679735
H	3.764555	-0.614984	3.392346
H	2.440999	-1.281608	1.367058
H	-1.144217	-1.284824	-2.721817
H	-3.334334	-1.433345	-3.941806
H	-5.322625	-0.211398	-2.985167
H	-5.021332	1.117911	-0.881540
H	-3.011623	-2.181480	3.373792
H	-2.677315	-4.556422	2.648821
H	-1.156398	-5.015583	0.686587
H	-0.061019	-3.079256	-0.448407
H	-3.572792	1.524665	1.132619
H	-2.487950	2.513098	0.162677
H	-2.837501	0.210406	2.731310
H	-1.140362	0.190444	3.183708
H	3.178838	0.927797	-2.446270
C	3.352581	-0.159601	-2.489708
C	4.142353	-0.645874	-1.271032
C	4.247527	-2.173263	-1.260186
C	2.877675	-2.868926	-1.195004
C	1.816726	-2.201777	-2.045461
C	2.039815	-0.878572	-2.659478
H	3.930352	-0.341032	-3.412956
H	3.656087	-0.284056	-0.350434
H	4.872503	-2.515067	-0.421704
H	2.969940	-3.918393	-1.513885
H	2.499983	-2.907047	-0.157873
H	1.079451	-2.859633	-2.521801
H	1.464018	-0.636171	-3.562062
H	5.146406	-0.197518	-1.287682
H	4.767355	-2.495450	-2.178073

[5]RC epoxidation optimized with B3LYP-D3BJ/def2-SVP

67

Fe	-0.632467	-0.036742	-0.576060
N	-1.195764	0.103411	1.526584
N	0.585570	1.653362	0.176509
N	0.892334	-1.204240	0.384434
N	-2.293337	1.253749	-0.739862
N	-2.031464	-1.651588	-0.444429
O	-0.235997	-0.146544	-2.127011
C	1.108425	2.673058	-0.510730
C	1.867443	3.659954	0.121795
C	2.078897	3.566089	1.497232
C	1.522075	2.494542	2.208769
C	0.776576	1.555112	1.507343
C	0.171666	0.300715	2.121214
C	1.035859	-0.874350	1.689245
C	1.945604	-1.528042	2.506205
C	2.722274	-2.557275	1.950734
C	2.567341	-2.882067	0.605443
C	1.638654	-2.171260	-0.158345
C	-2.863238	1.588549	-1.909763
C	-4.054091	2.307000	-1.959365
C	-4.668224	2.667483	-0.757200
C	-4.069033	2.309284	0.453848
C	-2.866845	1.604321	0.430577
C	-2.101998	1.273813	1.692220
C	-1.839053	-1.176269	1.934847
C	-2.533806	-1.872476	0.787053
C	-3.583652	-2.768237	0.982818
C	-4.101243	-3.454355	-0.119865
C	-3.559663	-3.223961	-1.387042
C	-2.523484	-2.302448	-1.511016
H	0.919037	2.689301	-1.586497
H	2.288291	4.480490	-0.461302
H	2.670492	4.321618	2.018851
H	1.667468	2.397837	3.286124
H	0.134111	0.379483	3.218532
H	2.048916	-1.249237	3.556297
H	3.441246	-3.096010	2.571535
H	3.163447	-3.664121	0.135892
H	1.491914	-2.372055	-1.220735
H	-2.341060	1.261602	-2.812059
H	-4.492069	2.570718	-2.923267
H	-5.608984	3.222548	-0.760461
H	-4.528213	2.580812	1.406406
H	-3.987063	-2.933459	1.983778
H	-4.922418	-4.162613	0.011083
H	-3.936614	-3.743363	-2.269443
H	-2.067319	-2.065418	-2.475188
H	-2.793374	1.109818	2.532157
H	-1.493298	2.151470	1.957015
H	-2.535832	-1.008522	2.769650
H	-1.055975	-1.851464	2.311634
H	2.320642	0.120505	-2.298509
C	3.409560	0.154729	-2.505848

C	4.090733	1.206101	-1.624415
C	4.236646	0.699365	-0.186780
C	5.117646	-0.555391	-0.145452
C	4.792239	-1.519856	-1.254323
C	4.008878	-1.212053	-2.300198
H	3.488981	0.432802	-3.569956
H	3.536264	2.156346	-1.657334
H	3.234645	0.456069	0.213100
H	6.184302	-0.272940	-0.217138
H	5.025800	-1.062811	0.832035
H	5.251943	-2.512905	-1.202585
H	3.819744	-1.967381	-3.070745
H	5.093318	1.423189	-2.029738
H	4.655288	1.480030	0.467856

[5]TS1 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	0.348756	0.013189	-0.351684
N	1.344560	0.049047	1.598304
N	-0.859971	-1.383778	0.887109
N	-0.789308	1.486761	0.720181
N	1.760626	-1.515549	-0.653965
N	1.906847	1.411001	-0.739854
O	-0.358561	0.030088	-1.798859
C	-1.639197	-2.395524	0.491516
C	-2.346917	-3.172795	1.410371
C	-2.226681	-2.881384	2.769532
C	-1.402701	-1.823078	3.175475
C	-0.734586	-1.095202	2.197367
C	0.131225	0.125395	2.477819
C	-0.673586	1.348468	2.057414
C	-1.306533	2.220151	2.934871
C	-2.079501	3.259124	2.397664
C	-2.192678	3.387036	1.012808
C	-1.525858	2.472533	0.195486
C	2.008661	-2.073432	-1.850975
C	3.060975	-2.965156	-2.034867
C	3.880992	-3.265169	-0.943983
C	3.617518	-2.674584	0.295076
C	2.535464	-1.803488	0.412540
C	2.122520	-1.211283	1.742287
C	2.204107	1.261093	1.670346
C	2.695029	1.708377	0.312196
C	3.855796	2.462652	0.148620
C	4.185861	2.926043	-1.128341
C	3.351162	2.619409	-2.206171
C	2.216817	1.847512	-1.971375
H	-1.701294	-2.576004	-0.583455
H	-2.980116	-3.988985	1.059220
H	-2.766223	-3.472495	3.512821
H	-1.285343	-1.574345	4.231760
H	0.396395	0.179033	3.545187
H	-1.201428	2.096738	4.014233
H	-2.588175	3.961962	3.061233
H	-2.790793	4.182149	0.564988

H	-1.583018	2.509430	-0.894527
H	1.340917	-1.782879	-2.665422
H	3.236184	-3.407654	-3.016665
H	4.722527	-3.952460	-1.056005
H	4.243033	-2.893567	1.162681
H	4.489954	2.690389	1.007630
H	5.089448	3.520868	-1.279321
H	3.576510	2.965901	-3.215923
H	1.530302	1.558705	-2.770755
H	3.003236	-1.050799	2.382081
H	1.495028	-1.952807	2.259485
H	3.049220	1.096917	2.355876
H	1.610049	2.082385	2.099417
H	-2.158236	-1.699115	-2.426400
C	-3.088959	-1.257711	-2.832137
C	-4.228994	-1.323906	-1.805004
C	-4.179149	-0.154254	-0.816938
C	-4.279771	1.180208	-1.562287
C	-3.327551	1.240801	-2.725275
C	-2.781194	0.143603	-3.281812
H	-3.333821	-1.876375	-3.712218
H	-4.211704	-2.289941	-1.274137
H	-3.226210	-0.179917	-0.257334
H	-5.312505	1.328541	-1.931483
H	-4.105558	2.026840	-0.876233
H	-3.103166	2.224514	-3.152581
H	-2.104911	0.255830	-4.134688
H	-5.194715	-1.290699	-2.336241
H	-4.987650	-0.240792	-0.074326

[5]IM1 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	-0.046737	-0.126931	-0.240150
N	-1.368866	1.215722	1.083712
N	0.288683	1.897908	-0.992126
N	1.275438	0.562285	1.390298
N	-1.962108	-0.180544	-1.236052
N	-0.907087	-1.534174	1.136857
O	0.880447	-1.204997	-1.339981
C	0.693844	2.245492	-2.219306
C	0.871193	3.580060	-2.585319
C	0.611831	4.572814	-1.638646
C	0.179602	4.202935	-0.359431
C	0.028246	2.849174	-0.075552
C	-0.384524	2.309609	1.287870
C	0.858479	1.720053	1.938093
C	1.544659	2.329878	2.983866
C	2.699869	1.712095	3.476734
C	3.120332	0.507253	2.911587
C	2.373890	-0.038296	1.866564
C	-2.225217	-1.061892	-2.215030
C	-3.502573	-1.217857	-2.744560
C	-4.539156	-0.439157	-2.223058
C	-4.259899	0.469134	-1.199807
C	-2.950048	0.579657	-0.731445

C	-2.558829	1.610337	0.305240
C	-1.709555	0.458017	2.304364
C	-1.713235	-1.042335	2.094885
C	-2.465331	-1.889026	2.910710
C	-2.360837	-3.270412	2.734790
C	-1.512440	-3.768542	1.742444
C	-0.807384	-2.861820	0.957252
H	0.878772	1.428573	-2.920287
H	1.203654	3.831958	-3.593578
H	0.738117	5.627588	-1.892627
H	-0.040372	4.955818	0.399609
H	-0.782190	3.127793	1.910580
H	1.181732	3.266072	3.411800
H	3.259026	2.165343	4.298234
H	4.011223	-0.008577	3.273032
H	2.657483	-0.982318	1.398110
H	-1.378939	-1.654324	-2.568310
H	-3.680597	-1.939802	-3.542957
H	-5.556801	-0.540715	-2.606538
H	-5.049821	1.089453	-0.771713
H	-3.121209	-1.471417	3.677171
H	-2.939125	-3.950757	3.363835
H	-1.404271	-4.840818	1.572615
H	-0.142764	-3.187684	0.155066
H	-3.412077	1.825813	0.967992
H	-2.340334	2.549101	-0.226488
H	-2.680230	0.783147	2.710776
H	-0.963851	0.681509	3.082486
H	3.613451	-0.190400	-0.707401
C	3.929887	-0.846219	-1.549170
C	4.339317	-2.226598	-1.001965
C	3.131428	-3.085143	-0.611277
C	2.158875	-3.231646	-1.783564
C	1.692253	-1.875396	-2.308602
C	2.810791	-0.915295	-2.522552
H	4.790095	-0.324192	-1.998591
H	5.023343	-2.100409	-0.148661
H	2.598674	-2.633151	0.244357
H	2.654570	-3.759669	-2.615872
H	1.278899	-3.838218	-1.512569
H	1.093246	-2.004842	-3.226632
H	2.687496	-0.120500	-3.264478
H	4.911887	-2.756597	-1.780782
H	3.467291	-4.077209	-0.273957

[5]TS2 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67			
Fe	-0.037412	-0.113671	-0.247716
N	-1.314225	1.240625	1.099829
N	0.293711	1.908382	-1.027764
N	1.335888	0.566524	1.354542
N	-1.983907	-0.163398	-1.199444
N	-0.881291	-1.519866	1.154666
O	0.855575	-1.224293	-1.393878
C	0.657266	2.257824	-2.267176

C	0.827190	3.591774	-2.638701
C	0.604230	4.584428	-1.682615
C	0.212094	4.214050	-0.390986
C	0.064649	2.860153	-0.103534
C	-0.316043	2.326593	1.272136
C	0.937965	1.733025	1.897908
C	1.647426	2.348468	2.925301
C	2.805354	1.726891	3.405903
C	3.204613	0.511115	2.848700
C	2.435490	-0.038646	1.822613
C	-2.285190	-1.049781	-2.161933
C	-3.581456	-1.207410	-2.643361
C	-4.596866	-0.423567	-2.089147
C	-4.278234	0.491005	-1.083158
C	-2.951529	0.601893	-0.664577
C	-2.520749	1.639283	0.350151
C	-1.629315	0.489465	2.330696
C	-1.663939	-1.011316	2.123390
C	-2.421611	-1.841289	2.951442
C	-2.348241	-3.224759	2.776649
C	-1.524979	-3.741083	1.772712
C	-0.813218	-2.849047	0.976432
H	0.811376	1.441643	-2.976702
H	1.125066	3.843586	-3.657745
H	0.726013	5.639068	-1.939309
H	0.018134	4.966782	0.375283
H	-0.691004	3.151634	1.900199
H	1.298851	3.291841	3.349395
H	3.381998	2.184466	4.212777
H	4.095441	-0.009864	3.202875
H	2.701528	-0.992822	1.364273
H	-1.453231	-1.645746	-2.542402
H	-3.790081	-1.934301	-3.429774
H	-5.628164	-0.525897	-2.433960
H	-5.050684	1.115773	-0.630351
H	-3.058188	-1.409284	3.726172
H	-2.931335	-3.892217	3.414980
H	-1.441674	-4.815507	1.602402
H	-0.168170	-3.190591	0.164934
H	-3.353328	1.871040	1.033552
H	-2.307053	2.569741	-0.197839
H	-2.581749	0.830204	2.766718
H	-0.856468	0.701238	3.085218
H	3.581234	-0.244725	-0.762751
C	3.854870	-0.936106	-1.590239
C	4.249293	-2.312345	-1.025508
C	3.034519	-3.153621	-0.618782
C	2.063257	-3.314165	-1.790350
C	1.609800	-1.967611	-2.342662
C	2.710498	-0.986329	-2.529326
H	4.710315	-0.440641	-2.080010
H	4.938503	-2.180442	-0.177515
H	2.504783	-2.682206	0.227846
H	2.554127	-3.864134	-2.611496
H	1.176654	-3.906209	-1.509871
H	1.011080	-2.101806	-3.259886

H	2.552284	-0.159086	-3.227787
H	4.814150	-2.859325	-1.798175
H	3.363611	-4.141645	-0.264074

[5]IM2 epoxidation optimized with B3LYP-D3BJ/def2-SVP

67

Fe	0.046345	0.101253	-0.263164
N	0.357899	-1.692620	1.063764
N	-1.316992	-1.420376	-1.109962
N	-1.569487	0.245046	1.320701
N	1.836368	-0.791621	-1.145847
N	1.470866	0.875986	1.216916
O	-0.243907	1.441214	-1.844925
C	-1.773904	-1.543322	-2.362382
C	-2.587494	-2.605008	-2.759781
C	-2.924785	-3.577249	-1.817145
C	-2.428890	-3.459648	-0.514369
C	-1.625786	-2.365834	-0.202120
C	-1.060453	-2.117411	1.189488
C	-1.852521	-0.976603	1.812526
C	-2.818443	-1.178701	2.795798
C	-3.513885	-0.071461	3.291171
C	-3.206736	1.195598	2.793414
C	-2.222590	1.307385	1.810918
C	2.655044	-0.184018	-2.016792
C	3.903779	-0.698402	-2.357762
C	4.319338	-1.886650	-1.753483
C	3.467338	-2.516499	-0.843650
C	2.224279	-1.944257	-0.569102
C	1.214544	-2.637062	0.321968
C	0.973074	-1.246145	2.328453
C	1.828857	-0.006613	2.168598
C	2.903993	0.237052	3.026173
C	3.617703	1.429779	2.903612
C	3.238096	2.343173	1.917746
C	2.163250	2.019635	1.094697
H	-1.469210	-0.769757	-3.070303
H	-2.941994	-2.667146	-3.789841
H	-3.557235	-4.423865	-2.092747
H	-2.657617	-4.211033	0.243669
H	-1.173231	-3.026209	1.803293
H	-3.018074	-2.182946	3.174075
H	-4.276134	-0.197390	4.063113
H	-3.714444	2.088321	3.161917
H	-1.946610	2.282780	1.407568
H	2.291946	0.749028	-2.454635
H	4.536359	-0.174449	-3.075864
H	5.295536	-2.317740	-1.985659
H	3.761560	-3.447757	-0.355658
H	3.176049	-0.500912	3.783438
H	4.461000	1.640619	3.564706
H	3.767777	3.287340	1.782334
H	1.846040	2.699081	0.301636
H	1.725527	-3.330955	1.008978
H	0.575560	-3.256419	-0.324946

H	1.564553	-2.055567	2.785494
H	0.174703	-1.007530	3.046960
H	-2.718893	1.750261	-0.945910
C	-2.499358	2.556201	-1.666751
C	-2.200996	3.885343	-0.952179
C	-0.747398	4.003853	-0.483141
C	0.215685	3.919280	-1.669978
C	-0.044196	2.716209	-2.534736
C	-1.368731	2.070415	-2.544883
H	-3.402238	2.653136	-2.288500
H	-2.896238	4.013361	-0.108650
H	-0.506970	3.204542	0.239445
H	0.099098	4.804436	-2.319269
H	1.270989	3.924405	-1.350363
H	0.587787	2.601632	-3.422885
H	-1.647420	1.504832	-3.440545
H	-2.410853	4.719016	-1.642386
H	-0.594496	4.955459	0.046364