Electronic Supplementary Information

Structure and Spin State of Nonheme $Fe^{IV}O$ Complexes Depending on Temperature: Predictive Insights from DFT Calculations and Experiments

Na Young Lee,[†] Debasish Mandal,[‡] Seong Hee Bae,[†] Mi Sook Seo,[†]
Yong-Min Lee,[†] Sason Shaik,[‡] Kyung-Bin Cho,[†,*] and Wonwoo Nam[†,*]

[†] *Department of Chemistry and Nano Science, Ewha Womans University, Seoul 03760, Korea.*

[‡] *Institute of Chemistry and The Lise Meitner-Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel.*

*Corresponding authors: workforkyung@ewha.ac.kr, wwnam@ewha.ac.kr

Table of Contents

Energy Abbreviations Used in Energy Tables S1, S2, S4 – S6, and S9 – S23	S3
Methods	S4
DFT Methods	S4
Free-Energy Calculations	S4
Comparison of calculated energy barrier (ΔG) to experimental rate-limiting constant k_2	S5
Materials for Experiments	S6
Instrumentation	S6
Spin State Measurement	S6
Kinetic Measurements and Product Analysis	S7
References	S7
Table S1	S9
Table S2	S10
Table S3	S11
Table S4	S12
Table S5	S13
Table S6	S14
Table S7	S15
Table S8	S16

Additional Data - All the Data for DFT calculations:	
Energies (Tables S9 – S23)	S17
Mulliken Spin Density Distribution (Tables S24 –S38)	S32
Selected Geometries (Tables S39 – S53)	S47
Cartesian Coordinates	S62

Energy Abbreviations Used in Tables S1, S2, S4 – S6, and S9 – S23:

ΔLACVP = Relative electronic energy using LACVP basis set

ΔΔDef2-TZVPP = Correction to ΔLACVP due to use of Def2-TZVPP basis set

$\Delta\Delta E$ = Relative electronic energy using Def2-TZVPP basis set

$\Delta\Delta Z_0$ = Correction to ΔLACVP due to zero-point vibration energy

$\Delta\Delta E_{(\text{Thermal})}$ = Thermal corrections to $\Delta\Delta Z_0$

$-T\Delta\Delta S$ = Correction to ΔLACVP due to entropy

ΔΔDisp = Correction to ΔLACVP due to dispersion

$\Delta\Delta G_{\text{corr}}$ = Correction to ΔLACVP due to change of standard states (RT•ln(V))

ΔΔTun = Correction to ΔLACVP due to tunneling

Methods

DFT Methods. DFT[S1] calculations were performed using the B3LYP functional[S2] as implemented in the Gaussian 09 (G09) package.[S3] The geometries for the reactivity studies were optimized using the LACVP basis set, which uses Los Alamos ECP on transition metals[S4] (slightly tweaked as implemented in the Jaguar program[S5]), and 6-31G on the rest of the atoms.[S6] The stationary points were confirmed by frequency calculations, and the transition states were connected with the ground states on both sides by performing IRC calculations and continuing relaxing the geometry down to the ground state from the end geometry obtained by IRC. The high molecular charge (2+) made it necessary to perform the optimizations in solvent to avoid artificial results (*vide infra*).[S7] Solvent (acetonitrile) effects were included using CPCM model[S8] with UFF cavity, per G09 default. Single-point energy evaluations on the optimized geometry were done with the Def2-TZVPP basis set (ΔE),[S9] as tests indicated that using this large basis set for geometry optimizations was unnecessary (Table S7). Def2-TZVPP was however used in the optimization and frequency calculations of the structures generating the data of Table 1 in the Text, as this system is smaller. MECP was found using a shell program to G09 that iterates to the same energy and geometry for two different electron configurations, at LACVP level.[S10] No frequency calculations have been done on this structure as it is not in a potential energy minimum at either spin state, and its Def2-TZVPP energy was estimated using an average of the $S = 1$ and $S = 2$ Def2-TZVPP energies.

Free-Energy Calculations. Free-energy calculations were done and is presented in Tables S6 – S20. Dispersion effects were added using DFT-D3 program[S11] with Becke-Johnson cutoff as a single-point correction to the optimized geometry. Tests with including dispersion in the optimizations did not improve the results, see Table S8. In previous trials, we have found that using gas-phase optimizations in HAT reactions for highly charged species such as the current system (2+) can cause a hydride transfer (*i.e.*, one proton and two electrons) rather than a net hydrogen atom transfer from the substrate to the metal-oxo species, possibly due to self-interaction errors (SIE). Most of the time, performing optimizations in solvent avoids these artificial results;[S7] hence the solvent effects were included during optimizations. However, in doing that, other problems may arise. Adding thermal contributions then becomes in principle inaccurate since the standard solvent models are parameterized to yield good solvation free energies and not any other property. This means that thermal effects are already included, to a

certain extent, in the obtained electronic energies, hence possibly double counting the thermal contributions[S12] (the same consideration applies to the dispersion correction as well). On the other hand, gas-phase frequency calculations on the structure obtained *via* optimization including solvent effects may not be meaningful either since the structure may not be in a stationary point without the solvent. This leaves us in principle with no easily available options to calculate in a uniform manner the free energies and at the same time avoid SIE, for highly charge systems, unless one is prepared to enlarge the model system to include counter ions.[S13] This is more time consuming and sometimes leading to 'reactions' between the transition metal complex and the counter ions, which may or may not be realistic.

Assuming though that the above described errors are negligible in the cases where no hydride transfers occur, the free energies (ΔG) can still be calculated by adding zero-point vibration energy (ΔZ_0), thermal corrections to Z_0 ($\Delta E_{(\text{Thermal})}$) and entropy ($-T\Delta S$). By consensus, dispersion effects are needed as well (ΔDisp). Also, if the energy of separated reactants in solvent is evaluated, there is a correction factor of RT•ln(V) due to change of standard states (ΔG_{corr}, either subtracted from the complexed states or added to the non-complexed states, depending on the reference state).[S14] The volume V can be estimated from the ideal gas law PV = nRT. In C-H activation reactions, tunneling (ΔTun) may be an issue as well.[S15] We have estimated the magnitude of the tunneling effects using Eckart algorithm[S16] implemented in TheRate Program.[S17] In the current study, ΔG manages to correctly reproduce experimental trends that can be estimated by comparing calculated values to each other, but the overall second-order rate values (k_2) are a bit low compared to experiments.

Comparison of Calculated Energy Barrier (ΔG) to Experimental Rate-Limiting Constant k_2. A commonly cited goal is to reproduce the experimental rate constants within 3 – 5 kcal mol^{-1}. Our experience with current methods on similar systems is that while this seems plausible with ΔE, ΔG frequently shows too low value in comparison. Indeed, in this case, experiments place the rate-limiting barriers for cyclohexene oxidation at 12.2, 11.3 and 14.9 kcal mol^{-1} (converted from the second order rates using Eyring equation; see Table 3 in the Text), for the $Fe^{IV}O$ species bearing Me_3NTB, TQA and TPA ligands, respectively. This is far from the theoretically calculated ΔG barriers of 6.5, 5.1 and 9.4 kcal mol^{-1}, but to gauge temperature effects, ΔG has to be used. The positive side is that ΔG gives excellent match to experimental results (*i*) – (*iv*) by

comparing theoretical values with each other, presumably canceling out calculation errors, and indicates that the error is due to an across-the-board constant amount missing to the barrier of ~6 kcal mol^{-1}, possibly in the form of formation entropies. This should make relative energy comparisons valid, as verified by the agreement to experiments (*i*) – (*iv*) and the current experiments on **3**. Therefore, the paper's main conclusion, that TBP structure preference for **1** and **2** at 233 K should warrant serious considerations, is still valid.

Materials for Experiments. All chemicals were purchased from Aldrich and TCI with the maximum purity available, and used as received unless otherwise indicated. Solvents for air- and moisture-sensitive manipulations were dried and deoxygenated under an argon atmosphere prior to use.[S18] All air- and moisture-sensitive manipulations were carried out using standard Schlenk line techniques or in a drybox under an argon atmosphere. Ligand, tris(2-pyridylmethyl)amine (TPA), and its iron(II) complex, $[Fe^{II}(TPA)(CH_3CN)_2](CF_3SO_3)_2$, were prepared by literature method.[S19] $[Fe^{II}(TPA)(CH_3CN)_2](CF_3SO_3)_2$ was synthesized by reacting $Fe(CF_3SO_3)_2{\cdot}2CH_3CN$ (0.84 mmol, 0.37 g) and TPA ligand (0.70 mmol, 0.20 g) in dry box in anhydrous CH_3CN at ambient temperature. The resulting solution was filtered and added to a large volume of Et_2O. The product was obtained as orange-red solid power in 76% yield (0.38 g).

Instrumentation. UV-vis spectra were recorded on a Hewlett Packard Agilent 8453 UV-visible spectrophotometer equipped with an UNISOKU cryostat system (USP-203; UNISOKU, Japan). ^{1}H NMR spectra were measured with Bruker model digital AVANCE III 400 FT-NMR spectrometer. Product analysis was performed with an Agilent Technologies 6890N gas chromatograph (GC) (HP-5 column, 30 m × 0.32 mm × 0.25 μm film thickness) with a flame ionization detector and Thermo Finnigan (Austin, Texas, USA) FOCUS DSQ (dual stage quadrupole) mass spectrometer interfaced with Finnigan FOCUS gas chromatograph (GC-MS).

Spin State Measurement. The effective magnetic moments (μ_{eff}, B.M.) of the $[(TPA)Fe^{IV}(O)(CH_3CN)]^{2+}$ complex ($\mathbf{3}_{Oh}$) was determined using the modified ^{1}H NMR method of Evans at 233 K.[S20] A WILMAD® coaxial insert (sealed capillary) tube containing the blank acetonitrile-d_3 solvent only was inserted into the normal NMR tube containing an acetonitrile-d_3 solution of $\mathbf{3}_{Oh}$ (2.0 mM). The chemical shift of the solvent peak in the presence of the paramagnetic metal complex $\mathbf{3}_{Oh}$ was compared to that of the solvent peak in the inner coaxial insert tube. The magnetic moment was calculated using the equation $\mu = 0.0618(\Delta\nu T / 2fM)^{1/2}$,

where f is the oscillator frequency (MHz) of the superconducting spectrometer, T is the absolute temperature, M is the molar concentration of the metal ion, and Δv is the difference in frequency (Hz) between the two reference signals.[S20] The magnetic moment of 3.1 B.M. for $\mathbf{3}_{Oh}$ obtained indicates that this intermediate possesses an $S = 1$ spin state in CD_3CN at 233 K.

Kinetic Measurements and Product Analysis. The kinetic experiments were run at least in triplicate, and the data reported represent the average of these reactions. The $Fe^{IV}(O)$ intermediate, $[(TPA)Fe^{IV}(O)(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$), was generated by reacting $[Fe^{II}(TPA)]^{2+}$ (1.0 mM) with 1.2 equiv of peracetic acid (35%) in CH_3CN at 233 K. Subsequently, appropriate amounts of substrates were added to reaction solutions at the given temperatures, and pseudo-first-order fitting of the kinetic data allowed us to determine k_{obs} (s^{-1}) values. All reaction traces were collected at 725nm, using a 1-cm optical path length at given temperature. The pseudo-first-order rate constants increased proportionally with the concentrations of substrates, from which second-order rate constants were determined. The ratio of $k_{2(H)}/k_{2(D)}$ for the oxidation of cyclohexene-h_{10} and cyclohexene-d_{10} by $\mathbf{3}_{Oh}$ was determined to be 86(5).

Products formed in the oxidations of cyclohexene by $\mathbf{3}_{Oh}$ were identified by comparison of the mass peaks and retention time of the products with respect to authentic samples by GC and GC-MS, and the product yields were determined by comparing the responsive peak areas of products against standard curves prepared with known authentic compounds using decane as an internal standard. The product yields were listed in Table 2 in the Text.

References

S1 W. Kohn and L. J. Sham, *Phys. Rev.*, 1965, **140**, A1133.

S2 (*a*) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098; (*b*) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 1372; (*c*) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (*d*) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

S3 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G.

Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision D.01*, Gaussian Inc.; Wallingford, CT, 2009.

S4 (*a*) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270; (*b*) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

S5 A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. A. Friesner, *Int. J. Quantum Chem.*, 2013, **113**, 2110.

S6 (*a*) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (*b*) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654.

S7 (*a*) A. J. Johansson, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Chem. Phys.*, 2008, **129**, 154301; (*b*) A. J. Johansson, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Phys. Chem. C*, 2007, **111**, 12397.

S8 M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669.

S9 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.

S10 J. N. Harvey, M. Aschi, H. Schwarz and W. Koch, *Theor. Chem. Acc.*, 1998, **99**, 95.

S11 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456.

S12 J. Ho, A. Klamt and M. L. Coote, *J. Phys. Chem. A*, 2010, **114**, 13442.

S13 D. Janardanan, D. Usharani, H. Chen and S. Shaik, *J. Phys. Chem. Lett.*, 2011, **2**, 2610.

S14 (*a*) P. Winget, C. J. Cramer and D. G. Truhlar, *Theor. Chem. Acc.*, 2004, **112**, 217; (*b*) A. Lewis, J. A. Bumpus, D. G. Truhlar and C. J. Cramer, *J. Chem. Educ.*, 2004, **81**, 596.

S15 D. Mandal, R. Ramanan, D. Usharani, D. Janardanan, B. Wang and S. Shaik, *J. Am. Chem. Soc.*, 2015, **137**, 722.

S16 C. Eckart, *Phys. Rev.*, 1930, **35**, 1303.

S17 W. T. Duncan, R. L. Bell and T. N. Truong, *J. Comput. Chem.*, 1998, **19**, 1039.

S18 W. L. F. Armarego and C. L. L. Chai, *Purification of Laboratory Chemicals, 6th edition*, Pergamon Press, Oxford, 2009.

S19 M. H. Lim, J.-U. Rohde, A. Stubna, M. R. Bukowski, M. Costas, R. Y. N. Ho, E. Münck, W. Nam and L. Que Jr., *Proc. Natl. Acad. Sci. USA*, 2003, **100**, 3665.

S20 (*a*) D. F. Evans, *J. Chem. Soc.*, 1959, 2003; (*b*) D. F. Evans and D. A. Jakubovic, *J. Chem. Soc. Dalt. Trans.*, 1988, 2927.

Table S1. $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) in kcal mol^{-1}

	T (K)	Def2-TZVPP ($\Delta\boldsymbol{E}^a$)	$\Delta\Delta Z_0$	$\Delta\Delta E_{thermal}$	$-T\Delta\Delta S$	$\Delta\Delta$Disp	$\Delta\Delta G_{corr}{}^b$	$\Delta\boldsymbol{G}^c$
$\mathbf{3}_{TBP}$ (Triplet) + CH_3CN	233.15	**16.36**	-1.49	+0.15	-8.45	+3.47	+1.37	**11.41**
	4.00	**16.36**	-1.49	+0.03	-0.09	+3.47	+0.02	**18.31**
$\mathbf{3}_{TBP}$ (Quintet) + CH_3CN	233.15	**7.50**	-2.06	+0.32	-9.13	+5.62	+1.37	**3.62**
	4.00	**7.50**	-2.06	+0.03	-0.09	+5.62	+0.02	**11.02**
$\mathbf{3}_{Oh}$ (Triplet)	233.15	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
	4.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
$\mathbf{3}_{Oh}$ (Quintet)	233.15	**6.54**	-1.29	+0.53	-1.23	+2.38	+0.00	**6.94**
	4.00	**6.54**	-1.29	+0.00	+0.00	+2.38	+0.00	**7.63**

[a] Electronic energy. [b] Free energy correction for change of standard state upon complexation. [c] Sum of the six previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S2. Cyclohexene HAT by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{1}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 1**										
$Fe^{IV}O$ + substrate	-10.14	+9.54	**-0.60**	+1.98	-0.29	+9.84	-6.35	-1.37		**3.21**
H[1]*AT*[e]										
Reactant Complex	-11.16	+10.90	**-0.25**	+2.31	+0.43	+15.84	-10.78	-2.73		**4.81**
Transition State	1.20	+14.43	**15.63**	-1.43	-0.12	+19.18	-15.16	-2.73	-2.58	**12.78**
Intermediate	-15.46	+8.56	**-6.91**	+0.16	+0.57	+16.49	-13.03	-2.73		**-5.45**
MECP[f]	-3.81	+9.34	**5.53**							
H[2]*AT*[e]										
Reactant Complex	-11.76	+11.22	**-0.54**	+2.45	+0.30	+16.41	-10.55	-2.73		**5.34**
Transition State	3.46	+14.42	**17.88**	-1.44	-0.14	+18.98	-15.25	-2.73	-3.55	**13.74**
Intermediate	-15.40	+8.44	**-6.96**	+0.44	+0.47	+16.75	-11.69	-2.73		**-3.72**
Dissociation										
$Fe^{III}OH$ + substrate•	-13.07	+6.22	**-6.85**	-0.32	-0.01	+9.10	-6.26	-1.37		**-5.70**
Rebound										
Transition State	-4.67	+9.43	**4.76**	-0.56	+0.58	+16.69	-12.57	-2.73		**6.16**
Product	-36.27	+8.66	**-27.61**	+2.34	+0.35	+17.47	-17.01	-2.73		**-27.20**
Desaturation										
Transition State	-1.82	+9.24	**7.42**	-1.81	+0.67	+15.99	-13.65	-2.73		**5.89**
Product	-31.99	+6.15	**-25.84**	-0.21	+1.15	+14.84	-14.61	-2.73		**-27.39**
***S* = 2**										
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
$Fe^{IV}O$ + substrate	-3.22	+5.53	**2.31**	+0.79	+0.22	+7.94	-6.70	-1.37		**3.19**
H[1]*AT*[e]										
Reactant Complex	-4.27	+7.10	**2.83**	+1.05	+0.91	+14.32	-11.75	-2.73		**4.62**
Transition State	0.03	+9.04	**9.07**	-1.36	+0.60	+15.90	-13.96	-2.73	-0.13	**7.39**
Intermediate	-18.96	+5.99	**-12.98**	-1.93	+1.22	+14.36	-13.88	-2.73		**-15.94**
MECP[f]	-3.79	+6.77	**2.98**							
H[2]*AT*[e]										
Reactant Complex	-4.66	+7.14	**2.48**	+1.21	+0.76	+14.89	-10.53	-2.73		**6.07**
Transition State	1.91	+9.11	**11.02**	-1.85	+0.68	+15.47	-13.01	-2.73	-0.20	**9.38**
Intermediate	-18.26	+5.05	**-13.21**	-2.04	+1.26	+13.85	-12.13	-2.73		**-14.99**
Dissociation										
$Fe^{III}OH$ + substrate•	-14.80	+2.29	**-12.51**	-2.88	+0.87	+6.24	-6.61	-1.37		**-16.26**
Rebound										
Transition State	-16.04	+6.18	**-9.86**	-2.56	+1.24	+14.39	-12.73	-2.73		**-12.25**
Product	-53.20	+9.42	**-43.78**	+1.54	+0.71	+16.20	-14.26	-2.73		**-42.31**
Desaturation										
Transition State	-14.83	+4.52	**-10.31**	-2.86	+1.38	+13.41	-10.48	-2.73		**-11.59**
Product	-47.26	+11.72	**-35.54**	-1.39	+1.75	+12.25	-11.09	-2.73		**-36.77**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] Depending on which hydrogens abstracted (at the cyclohexene 2 or 5 position), different energy barriers are obtained (see main Text). [f] The average Def2-TZVPP energy was calculated to be 4.26 kcal mol^{-1}.

Table S3. Selected Geometries of Cyclohexene HAT Reaction by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{1}_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	D(O-H)[c]	A(Fe-O-H)[a]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.65	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.66	2.93	1.10	3.96	5.98	171.04
Transition State	1.76	1.31	1.28	2.59	4.36	123.26
Intermediate	1.81	0.98	2.52	3.44	4.96	115.01
MECP	1.65	2.85	1.10	3.87	5.90	172.23
H^2AT						
Reactant Complex	1.66	2.74	1.10	3.82	4.07	137.10
Transition State	1.76	1.28	1.30	2.56	3.20	125.08
Intermediate	1.81	0.98	2.54	3.37	3.65	114.30
Dissociation						
$Fe^{III}OH$ + substrate•	1.81	0.98	∞	∞	∞	113.08
Rebound						
Transition State	1.95	0.98	2.43	2.47	2.85	107.78
Product	2.33	0.98	2.03	1.50	2.63	100.89
Desaturation						
Transition State	1.97	0.98	3.77	3.74	1.76	106.55
Product	2.19	0.98	3.46	3.31	0.98	112.32
***S* = 2**						
$Fe^{IV}O$ + substrate	1.65	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.65	2.82	1.10	3.79	5.46	166.46
Transition State	1.70	1.61	1.16	2.76	4.47	170.50
Intermediate	1.80	0.98	2.17	3.14	4.80	155.78
MECP	1.65	2.85	1.10	3.87	5.90	172.23
H^2AT						
Reactant Complex	1.65	2.76	1.10	3.86	4.44	135.24
Transition State	1.71	1.54	1.17	2.71	3.28	159.65
Intermediate	1.80	0.98	2.22	3.19	3.44	149.51
Dissociation						
$Fe^{III}OH$ + substrate•	1.82	0.97	∞	∞	∞	143.03
Rebound						
Transition State	1.89	0.97	2.38	2.78	2.81	134.04
Product	2.15	0.98	2.06	1.51	2.63	116.93
Desaturation						
Transition State	1.89	0.98	2.93	3.55	2.13	123.72
Product	2.12	0.97	3.35	3.27	0.98	115.40

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to. [c] H-atom participating in the desaturation reaction.

Table S4. Cyclohexene HAT by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 1**										
$Fe^{IV}O$ + substrate	-7.25	+8.66	**1.42**	+2.30	-0.34	+9.75	-7.52	-1.37		**4.24**
H[1]*AT*[e]										
Reactant Complex	-8.98	+10.65	**1.67**	+2.72	+0.18	+17.13	-13.14	-2.73		**5.82**
Transition State	5.09	+14.17	**19.26**	-0.87	-0.30	+19.71	-18.30	-2.73	-2.84	**13.92**
Intermediate	-14.06	+8.62	**-5.45**	+1.03	+0.27	+17.26	-14.22	-2.73		**-3.84**
H[2]*AT*[e]										
Reactant Complex	-8.80	10.32	**1.52**	2.63	0.22	16.62	-11.83	-2.73		**6.43**
Transition State	5.86	14.23	**20.09**	-1.15	-0.23	19.61	-17.84	-2.73	-3.08	**14.67**
Intermediate	-13.73	8.35	**-5.38**	0.90	0.33	16.77	-13.74	-2.73		**-3.85**
Dissociation										
$Fe^{III}OH$ + substrate•	-11.38	+6.06	**-5.32**	+0.42	-0.19	+9.55	-7.60	-1.37		**-4.52**
Rebound										
Transition State	-6.62	+8.28	**1.67**	-0.16	+0.49	+16.79	-13.08	-2.73		**2.97**
Product	-38.73	+4.29	**-34.44**	+2.86	+0.56	+15.33	-14.04	-2.73		**-32.47**
Desaturation										
Transition State	-5.31	+6.36	**1.05**	-0.93	+0.63	+15.66	-11.17	-2.73		**2.50**
Product	-31.88	+5.76	**-26.13**	+0.48	+0.96	+15.85	-17.15	-2.73		**-28.72**
***S* = 2**										
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
$Fe^{IV}O$ + substrate	-4.03	+5.00	**0.97**	+1.00	+0.19	+7.84	-4.87	-1.37		**3.76**
H[1]*AT*[e]										
Reactant Complex	-5.14	+6.57	**1.44**	+1.05	+0.91	+13.90	-10.19	-2.73		**4.38**
Transition State	-0.38	+8.72	**8.34**	-1.22	+0.54	+16.30	-16.01	-2.73	-0.14	**5.07**
Intermediate	-19.37	+5.48	**-13.89**	-1.49	+1.06	+15.00	-14.37	-2.73		**-16.43**
H[2]*AT*[e]										
Reactant Complex	-5.59	6.64	**1.05**	1.34	0.73	14.93	-9.38	-2.73		**5.93**
Transition State	1.30	8.97	**10.26**	-1.47	0.53	16.44	-15.21	-2.73	-0.21	**7.61**
Intermediate	-19.18	5.23	**-13.94**	-1.61	1.14	14.60	-14.44	-2.73		**-16.98**
Dissociation										
$Fe^{III}OH$ + substrate•	-15.37	+2.41	**-12.96**	-1.99	+0.60	+7.01	-7.71	-1.37		**-16.41**
Rebound										
Transition State	-19.17	+5.21	**-13.97**	-1.84	+0.80	+15.65	-14.38	-2.73		**-16.46**
Product	-52.28	+8.58	**-43.70**	+2.25	+0.61	+16.11	-16.34	-2.73		**-43.80**
Desaturation		Not found								

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] Depending on which hydrogens abstracted (at the cyclohexene 2 or 5 position), different energy barriers are obtained (see main Text).

Table S5. Cyclohexene OAT by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**Δ*G***[d]
***S* = 1**									
OAT									
Reactant Complex	-8.78	+10.36	**1.58**	+2.75	+0.21	+16.38	-12.31	-2.73	**5.88**
Transition State 1	8.40	+15.92	**24.32**	+2.20	-0.35	+20.32	-21.08	-2.73	**22.69**
Intermediate	-1.59	+11.85	**10.26**	+3.24	-0.49	+20.79	-20.65	-2.73	**10.42**
Transition State 2	3.25	+12.51	**15.76**	+2.08	-0.37	+20.36	-20.38	-2.73	**14.72**
Product	-21.22	+7.52	**-13.70**	+3.88	-0.02	+18.69	-22.01	-2.73	**-15.90**
***S* = 2**									
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	-4.76	+6.08	**1.33**	+1.30	+0.88	+13.91	-9.06	-2.73	**5.62**
Transition State	-1.10	+8.23	**7.13**	+0.43	+0.55	+16.34	-17.72	-2.73	**3.99**
Product	-38.56	+7.45	**-31.11**	+2.75	+0.38	+17.37	-18.21	-2.73	**-31.56**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr}$.

Table S6. Energy effects of raising small frequencies (< 100 cm^{-1}) to 100 cm^{-1} at 233.15 K.

Species	No. of Vibrations under 100 cm^{-1}	$\Delta E_{thermal}$ - $T\Delta S$ before change[a] (kcal mol^{-1})	$\Delta E_{thermal}$ - $T\Delta S$ after change[b] (kcal mol^{-1})	Change[c] (kcal mol^{-1})	Relative difference[d] $\Delta\Delta E_{thermal}$ - $T\Delta\Delta S$ (kcal mol^{-1})
$^3\mathbf{1}_{Oh}$	13	-7.13	-2.81	+4.32	**+0.66**
$^5\mathbf{1}_{TBP}$ + $NCCH_3$	9	-5.61	-1.95	+3.66	**+0.00**
$^5\mathbf{2}_{Oh}$	10	-6.68	-2.16	+4.52	**+1.53**
$^5\mathbf{2}_{TBP}$ + $NCCH_3$	7	-4.50	-1.51	+2.99	**+0.00**
$^3\mathbf{3}_{Oh}$	6	-4.07	-1.30	+2.77	**+1.49**
$^5\mathbf{3}_{TBP}$ + $NCCH_3$	5	-2.36	-1.08	+1.28	**+0.00**

[a] This is the energy contribution $\Delta E_{thermal}$ - $T\Delta S$ arising from vibrations less than 100 cm^{-1} (only). [b] All the vibration frequencies less than 100 cm^{-1} has been changed to 100 cm^{-1}, and the energy contribution from these frequencies (only) has been recalculated. See reference 33 in the Text. [c] Change occurred between the two previous columns. [d] Energy difference relative to the quintet TBP structure. These values should be *added* to Table 1 (last column) to obtain the *total* relative energies.

Table S7. Basis set effect (LACVP versus Def2-TZVPP) on geometry optimization[a]

	Fe-O (Å)	O-H (Å)	H-C (Å)	RMSD (Å)	$\Delta\Delta G$ (kcal mol^{-1})
$^3\mathbf{3}_{Oh}$ + C_6H_{10}	1.66/1.63	∞/∞	1.10/1.10	0.04 ($^3\mathbf{3}_{Oh}$), 0.01 (C_6H_{10})	0.00/0.00
Reactant, Triplet	1.66/1.63	2.69/5.14[b]	1.10/1.10	1.22[b]	3.33/4.78
TS, Triplet	1.76/1.73	1.34/1.33	1.26/1.26	0.11	11.11[c]/11.65[c]

[a] The values are presented as optimized with LACVP/Def2-TZVPP. [b] Large RMSD caused by the substrate being at a longer distance from the FeO moiety in Def2-TZVPP optimization than with LACVP. [c] These values do not include the tunnelling effects.

Table S8. Dispersion (D3-BJ) effect on geometry optimization[a]

	Fe-O (Å)	O-H (Å)	H-C (Å)	RMSD (Å)	$\Delta\Delta G$ (kcal mol^{-1})
^{3}**3**$_{Oh}$ + C_6H_{10}	1.66/1.66	∞/∞	1.10/1.10	0.07 (^{3}**3**$_{Oh}$), 0.01 (C_6H_{10})	0.00/0.00
Reactant, Triplet	1.66/1.66	2.69/2.69[b]	1.10/1.10	2.57[b]	3.33/2.75
TS, Triplet[b]	1.76/1.76	1.34/1.34	1.25/1.26	0.51	9.40/9.97
Intermediate, Triplet	1.82/1.81	0.98/0.99	2.44/2.23	1.16[c]	-9.36/-8.30

[a] The values are presented as without/with dispersion in optimization. [b] The hydrogen pointing to the FeO moiety is different without/with dispersion optimization, causing large mismatch in RMSD since the substrate is oriented so differently. However, at the TS, the same H-atom is transferred. [c] Large RMSD caused by a small variation in the orientation of the substrate relative to the FeOH moiety.

All the Data for DFT calculations: Energies

Table S9. $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) in kcal mol^{-1}

	T (K)	Def2-TZVPP (**Δ*E***[a])	ΔΔZ_0	ΔΔ$E_{thermal}$	-TΔΔS	ΔΔDisp	ΔΔG_{corr}[b]	**Δ*G***[c]
1$_{TBP}$ (Triplet) + CH_3CN	233.15	**12.26**	0.32	-0.09	+0.92	-2.49	+0.00	**10.91**
	4.00	**12.26**	0.32	+0.00	+0.01	-2.49	+0.00	**10.09**
1$_{TBP}$ (Quintet) + CH_3CN	233.15	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
	4.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
1$_{Oh}$ (Triplet)	233.15	**-0.58**	+1.88	-0.27	+9.90	-6.05	-1.37	**3.52**
	4.00	**-0.58**	+1.88	-0.03	+0.10	-6.05	-0.02	**-4.71**
1$_{Oh}$ (Quintet)	233.15	**2.15**	+0.73	+0.21	+8.16	-7.23	-1.37	**2.66**
	4.00	**2.15**	+0.73	-0.03	+0.09	-7.23	-0.02	**-4.30**

[a] Electronic energy. [b] Free energy correction for change of standard state upon complexation. [c] Sum of the six previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr}$.

Table S10. $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) in kcal mol^{-1}

	T (K)	Def2-TZVPP (ΔE^a)	$\Delta\Delta Z_0$	$\Delta\Delta E_{thermal}$	$-T\Delta\Delta S$	$\Delta\Delta$Disp	$\Delta\Delta G_{corr}{}^b$	ΔG^c
$\mathbf{2}_{TBP}$ (Triplet) + CH_3CN	233.15	**12.04**	+0.54	-0.13	+0.84	-4.26	+0.00	**9.04**
	4.00	**12.04**	+0.54	+0.00	+0.01	-4.26	+0.00	**8.33**
$\mathbf{2}_{TBP}$ (Quintet) + CH_3CN	233.15	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
	4.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
$\mathbf{2}_{Oh}$ (Triplet)	233.15	**1.56**	+2.11	-0.29	+9.61	-7.30	-1.37	**4.33**
	4.00	**1.56**	+2.11	-0.03	+0.10	-7.30	-0.02	**-3.59**
$\mathbf{2}_{Oh}$ (Quintet)	233.15	**0.88**	+1.00	+0.18	+7.95	-8.46	-1.37	**0.18**
	4.00	**0.88**	+1.00	-0.03	+0.09	-8.46	-0.02	**-6.55**

[a] Electronic energy. [b] Free energy correction for change of standard state upon complexation. [c] Sum of the six previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S11. $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) in kcal mol^{-1}

	T (K)	Def2-TZVPP ($\Delta \boldsymbol{E}^a$)	$\Delta\Delta Z_0$	$\Delta\Delta E_{thermal}$	$-T\Delta\Delta S$	$\Delta\Delta$Disp	$\Delta\Delta G_{corr}{}^b$	$\Delta \boldsymbol{G}^c$
$\mathbf{3}_{TBP}$ (Triplet) + CH_3CN	233.15	**16.36**	-1.49	+0.15	-8.45	+3.47	+1.37	**11.41**
	4.00	**16.36**	-1.49	+0.03	-0.09	+3.47	+0.02	**18.31**
$\mathbf{3}_{TBP}$ (Quintet) + CH_3CN	233.15	**7.50**	-2.06	+0.32	-9.13	+5.62	+1.37	**3.62**
	4.00	**7.50**	-2.06	+0.03	-0.09	+5.62	+0.02	**11.02**
$\mathbf{3}_{Oh}$ (Triplet)	233.15	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
	4.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
$\mathbf{3}_{Oh}$ (Quintet)	233.15	**6.54**	-1.29	+0.53	-1.23	+2.38	+0.00	**6.94**
	4.00	**6.54**	-1.29	+0.00	+0.00	+2.38	+0.00	**7.63**

[a] Electronic energy. [b] Free energy correction for change of standard state upon complexation. [c] Sum of the six previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S12. Cyclohexene HAT by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 1**										
$Fe^{IV}O$ + substrate	-10.14	+9.54	**-0.60**	+1.98	-0.29	+9.84	-6.35	-1.37		**3.21**
H^1*AT*[e]										
Reactant Complex	-11.16	+10.90	**-0.25**	+2.31	+0.43	+15.84	-10.78	-2.73		**4.81**
Transition State	1.20	+14.43	**15.63**	-1.43	-0.12	+19.18	-15.16	-2.73	-2.58	**12.78**
Intermediate	-15.46	+8.56	**-6.91**	+0.16	+0.57	+16.49	-13.03	-2.73		**-5.45**
MECP[f]	-3.81	+9.34	**5.53**							
H^2*AT*[e]										
Reactant Complex	-11.76	+11.22	**-0.54**	+2.45	+0.30	+16.41	-10.55	-2.73		**5.34**
Transition State	3.46	+14.42	**17.88**	-1.44	-0.14	+18.98	-15.25	-2.73	-3.55	**13.74**
Intermediate	-15.40	+8.44	**-6.96**	+0.44	+0.47	+16.75	-11.69	-2.73		**-3.72**
Dissociation										
$Fe^{III}OH$ + substrate•	-13.07	+6.22	**-6.85**	-0.32	-0.01	+9.10	-6.26	-1.37		**-5.70**
Rebound										
Transition State	-4.67	+9.43	**4.76**	-0.56	+0.58	+16.69	-12.57	-2.73		**6.16**
Product	-36.27	+8.66	**-27.61**	+2.34	+0.35	+17.47	-17.01	-2.73		**-27.20**
Desaturation										
Transition State	-1.82	+9.24	**7.42**	-1.81	+0.67	+15.99	-13.65	-2.73		**5.89**
Product	-31.99	+6.15	**-25.84**	-0.21	+1.15	+14.84	-14.61	-2.73		**-27.39**
***S* = 2**										
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
$Fe^{IV}O$ + substrate	-3.22	+5.53	**2.31**	+0.79	+0.22	+7.94	-6.70	-1.37		**3.19**
H^1*AT*[e]										
Reactant Complex	-4.27	+7.10	**2.83**	+1.05	+0.91	+14.32	-11.75	-2.73		**4.62**
Transition State	0.03	+9.04	**9.07**	-1.36	+0.60	+15.90	-13.96	-2.73	-0.13	**7.39**
Intermediate	-18.96	+5.99	**-12.98**	-1.93	+1.22	+14.36	-13.88	-2.73		**-15.94**
MECP[f]	-3.79	+6.77	**2.98**							
H^2*AT*[e]										
Reactant Complex	-4.66	+7.14	**2.48**	+1.21	+0.76	+14.89	-10.53	-2.73		**6.07**
Transition State	1.91	+9.11	**11.02**	-1.85	+0.68	+15.47	-13.01	-2.73	-0.20	**9.38**
Intermediate	-18.26	+5.05	**-13.21**	-2.04	+1.26	+13.85	-12.13	-2.73		**-14.99**
Dissociation										
$Fe^{III}OH$ + substrate•	-14.80	+2.29	**-12.51**	-2.88	+0.87	+6.24	-6.61	-1.37		**-16.26**
Rebound										
Transition State	-16.04	+6.18	**-9.86**	-2.56	+1.24	+14.39	-12.73	-2.73		**-12.25**
Product	-53.20	+9.42	**-43.78**	+1.54	+0.71	+16.20	-14.26	-2.73		**-42.31**
Desaturation										
Transition State	-14.83	+4.52	**-10.31**	-2.86	+1.38	+13.41	-10.48	-2.73		**-11.59**
Product	-47.26	+11.72	**-35.54**	-1.39	+1.75	+12.25	-11.09	-2.73		**-36.77**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] Depending on which hydrogens abstracted (at the cyclohexene 2 or 5 position), different energy barriers are obtained (see main Text). [f] The average Def2-TZVPP energy was calculated to be 4.26 kcal mol^{-1}.

Table S13. Cyclohexene OAT by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**Δ*G***[d]
***S* = 1**									
OAT									
Reactant Complex	-10.89	+10.59	**-0.30**	+2.03	+0.51	+15.09	-9.52	-2.73	**5.08**
Transition State 1	5.29	+16.45	**21.74**	+1.51	-0.13	+19.39	-18.33	-2.73	**21.44**
Intermediate	-5.93	+12.38	**6.44**	+2.27	-0.17	+19.58	-17.65	-2.73	**7.73**
Transition State 2	0.08	+13.08	**13.15**	+1.24	-0.08	+18.96	-17.47	-2.73	**13.08**
Product	-21.30	+7.27	**-14.03**	+2.62	+0.26	+17.83	-18.42	-2.73	**-14.47**
***S* = 2**									
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	-4.02	+6.78	**2.75**	+0.99	+0.94	+14.29	-11.03	-2.73	**5.20**
Transition State	-0.15	+8.42	**8.26**	+0.18	+0.60	+16.22	-14.86	-2.73	**7.67**
Product	-36.21	+6.87	**-29.34**	+1.62	+0.71	+16.05	-14.66	-2.73	**-28.36**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S14. Cyclohexene HAT by $[(Me_3NTB)Fe^{IV}O]^{2+}$ ($\mathbf{1}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	$\Delta \boldsymbol{E}^a$	$\Delta\Delta Z_0$	$\Delta\Delta E_{thermal}{}^b$	$-T\Delta\Delta S^b$	ΔΔDisp	$\Delta\Delta G_{corr}{}^{b,c}$	ΔΔTun^b	$\boldsymbol{\Delta G}^d$
***S* = 2**										
$Fe^{IV}O$ (TBP) + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
HAT										
Reactant Complex	-1.05	+1.43	**0.39**	+0.28	+0.72	+5.62	-4.38	-1.37		**1.26**
Transition State	3.90	+4.19	**8.09**	-2.23	+0.33	+8.54	-6.75	-1.37	-0.15	**6.47**
Intermediate	-14.78	+1.36	**-13.43**	-2.52	+0.93	+6.79	-6.07	-1.37		**-15.66**
Dissociation										
$Fe^{III}OH$ + substrate•	-10.58	-1.58	**-12.16**	-3.46	+0.62	-1.40	+0.61	+0.00		**-15.78**
Rebound										
Transition State	-12.42	+1.02	**-11.40**	-3.27	+0.97	+6.92	-5.49	-1.37		**-13.64**
Product	-49.14	+8.42	**-40.72**	+0.90	+0.41	+9.02	-7.71	-1.37		**-39.47**
Desaturation		Not found								

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$.

Table S15. Cyclohexene OAT by $[(Me_3NTB)Fe^{IV}O]^{2+}$ ($\mathbf{1}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**Δ*G***[d]
***S* = 2**									
$Fe^{IV}O$ (TBP) + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	-1.13	+1.37	**0.23**	+0.53	+0.60	+6.59	-3.80	-1.37	**2.79**
Transition State	4.10	+4.57	**8.67**	-0.58	+0.36	+8.96	-8.04	-1.37	**8.01**
Product	-32.18	+2.62	**-29.56**	+1.12	+0.30	+8.95	-7.55	-1.37	**-28.10**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S16. Cyclohexene HAT by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 1**										
$Fe^{IV}O$ + substrate	-7.25	+8.66	**1.42**	+2.30	-0.34	+9.75	-7.52	-1.37		**4.24**
H[1]*AT*[e]										
Reactant Complex	-8.98	+10.65	**1.67**	+2.72	+0.18	+17.13	-13.14	-2.73		**5.82**
Transition State	5.09	+14.17	**19.26**	-0.87	-0.30	+19.71	-18.30	-2.73	-2.84	**13.92**
Intermediate	-14.06	+8.62	**-5.45**	+1.03	+0.27	+17.26	-14.22	-2.73		**-3.84**
H[2]*AT*[e]										
Reactant Complex	-8.80	10.32	**1.52**	2.63	0.22	16.62	-11.83	-2.73		**6.43**
Transition State	5.86	14.23	**20.09**	-1.15	-0.23	19.61	-17.84	-2.73	-3.08	**14.67**
Intermediate	-13.73	8.35	**-5.38**	0.90	0.33	16.77	-13.74	-2.73		**-3.85**
Dissociation										
$Fe^{III}OH$ + substrate•	-11.38	+6.06	**-5.32**	+0.42	-0.19	+9.55	-7.60	-1.37		**-4.52**
Rebound										
Transition State	-6.62	+8.28	**1.67**	-0.16	+0.49	+16.79	-13.08	-2.73		**2.97**
Product	-38.73	+4.29	**-34.44**	+2.86	+0.56	+15.33	-14.04	-2.73		**-32.47**
Desaturation										
Transition State	-5.31	+6.36	**1.05**	-0.93	+0.63	+15.66	-11.17	-2.73		**2.50**
Product	-31.88	+5.76	**-26.13**	+0.48	+0.96	+15.85	-17.15	-2.73		**-28.72**
***S* = 2**										
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
$Fe^{IV}O$ + substrate	-4.03	+5.00	**0.97**	+1.00	+0.19	+7.84	-4.87	-1.37		**3.76**
H[1]*AT*[e]										
Reactant Complex	-5.14	+6.57	**1.44**	+1.05	+0.91	+13.90	-10.19	-2.73		**4.38**
Transition State	-0.38	+8.72	**8.34**	-1.22	+0.54	+16.30	-16.01	-2.73	-0.14	**5.07**
Intermediate	-19.37	+5.48	**-13.89**	-1.49	+1.06	+15.00	-14.37	-2.73		**-16.43**
H[2]*AT*[e]										
Reactant Complex	-5.59	6.64	**1.05**	1.34	0.73	14.93	-9.38	-2.73		**5.93**
Transition State	1.30	8.97	**10.26**	-1.47	0.53	16.44	-15.21	-2.73	-0.21	**7.61**
Intermediate	-19.18	5.23	**-13.94**	-1.61	1.14	14.60	-14.44	-2.73		**-16.98**
Dissociation										
$Fe^{III}OH$ + substrate•	-15.37	+2.41	**-12.96**	-1.99	+0.60	+7.01	-7.71	-1.37		**-16.41**
Rebound										
Transition State	-19.17	+5.21	**-13.97**	-1.84	+0.80	+15.65	-14.38	-2.73		**-16.46**
Product	-52.28	+8.58	**-43.70**	+2.25	+0.61	+16.11	-16.34	-2.73		**-43.80**
Desaturation		Not found								

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] Depending on which hydrogens abstracted (at the cyclohexene 2 or 5 position), different energy barriers are obtained (see main Text).

Table S17. Cyclohexene OAT by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**Δ*G***[d]
***S* = 1**									
OAT									
Reactant Complex	-8.78	+10.36	**1.58**	+2.75	+0.21	+16.38	-12.31	-2.73	**5.88**
Transition State 1	8.40	+15.92	**24.32**	+2.20	-0.35	+20.32	-21.08	-2.73	**22.69**
Intermediate	-1.59	+11.85	**10.26**	+3.24	-0.49	+20.79	-20.65	-2.73	**10.42**
Transition State 2	3.25	+12.51	**15.76**	+2.08	-0.37	+20.36	-20.38	-2.73	**14.72**
Product	-21.22	+7.52	**-13.70**	+3.88	-0.02	+18.69	-22.01	-2.73	**-15.90**
***S* = 2**									
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	-4.76	+6.08	**1.33**	+1.30	+0.88	+13.91	-9.06	-2.73	**5.62**
Transition State	-1.10	+8.23	**7.13**	+0.43	+0.55	+16.34	-17.72	-2.73	**3.99**
Product	-38.56	+7.45	**-31.11**	+2.75	+0.38	+17.37	-18.21	-2.73	**-31.56**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr}$.

Table S18. Cyclohexene HAT by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 2**										
$Fe^{IV}O$ (TBP) + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
HAT										
Reactant Complex	-1.10	+1.51	**0.41**	+0.19	+0.59	+5.83	-4.56	-1.37		**1.09**
Transition State	5.56	+3.67	**9.22**	-2.27	+0.14	+9.01	-7.27	-1.37	-0.13	**7.33**
Intermediate	-11.94	+0.69	**-11.25**	-2.51	+0.84	+5.95	-6.11	-1.37		**-14.44**
Dissociation										
$Fe^{III}OH$ + substrate•	-7.93	-2.10	**-10.04**	-3.09	+0.36	-1.27	+1.10	+0.00		**-12.94**
Rebound										
Intermediate[e]	-12.11	0.75	**-11.36**	-2.07	0.69	7.12	-6.14	-1.37		**-13.12**
Transition State 1	-12.02	0.47	**-11.55**	-3.28	0.59	7.75	-5.92	-1.37		**-13.78**
Intermediate ($[subs]^+$)	-19.90	3.65	**-16.25**	-2.33	1.12	5.70	-1.67	-1.37		**-14.80**
Transition State 2	-19.15	3.08	**-16.07**	-2.57	0.81	6.73	-3.65	-1.37		**-16.12**
Product	-47.06	4.36	**-42.70**	1.46	0.15	9.58	-8.83	-1.37		**-41.70**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] The substrate radical intermediate repositions itself slightly in preparation for the electron transfer, and this repositioning can be seen as the rate-limiting barrier for the rebound reaction.

Table S19. Cyclohexene OAT by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**Δ*G***[d]
***S* = 2**									
$Fe^{IV}O$ (TBP) + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	-0.64	+1.04	**0.40**	+0.43	+0.53	+6.48	-4.20	-1.37	**2.28**
Transition State	6.05	+4.82	**10.87**	-0.54	+0.19	+8.93	-10.02	-1.37	**8.06**
Product	-29.58	+2.11	**-27.47**	+1.84	+0.02	+9.66	-8.97	-1.37	**-26.29**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

Table S20. Cyclohexene HAT by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 1**										
$Fe^{IV}O$ + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
HAT										
Reactant Complex	-0.74	+0.94	**0.20**	+0.50	+0.66	+5.94	-2.60	-1.37		**3.33**
Transition State	8.96	+5.02	**13.99**	-3.34	+0.17	+8.84	-7.18	-1.37	-1.71	**9.40**
Intermediate	-8.82	-0.29	**-9.11**	-1.35	+0.62	+7.76	-5.92	-1.37		**-9.36**
MECP[e]	10.38	-0.63	**9.75**							
Dissociation										
$Fe^{III}OH$ + substrate•	-6.12	-2.82	**-8.94**	-2.08	+0.19	-0.28	-0.17	+0.00		**-11.27**
Rebound										
Transition State	2.37	+0.23	**2.60**	-2.18	+0.64	+7.73	-5.29	-1.37		**2.13**
Product	-25.57	-0.76	**-26.33**	+0.28	+0.67	+7.64	-9.47	-1.37		**-28.57**
Desaturation										
Transition State	8.68	-0.59	**8.09**	-4.07	+1.02	+5.97	-2.13	-1.37		**7.51**
Product	-20.42	-3.58	**-24.00**	-2.32	+1.45	+5.00	-7.25	-1.37		**-28.49**
***S* = 2**										
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	17.19	-9.59	**7.60**	-2.24	+0.83	-9.48	+5.74	+1.37		**3.83**
$Fe^{IV}O$ + substrate	10.86	-4.13	**6.73**	-1.38	+0.55	-1.47	+2.48	+0.00		**6.91**
HAT										
Reactant Complex	9.39	-2.52	**6.88**	-1.07	+1.25	+4.49	-1.56	-1.37		**8.62**
Transition State	15.16	-0.60	**14.57**	-4.04	+1.00	+5.97	-6.36	-1.37	-0.19	**9.58**
Intermediate	-2.25	-3.88	**-6.13**	-4.21	+1.59	+4.25	-6.09	-1.37		**-11.95**
MECP[e]	10.39	-3.08	**7.30**							
Dissociation										
$Fe^{III}OH$ + substrate•	2.05	-7.08	**-5.03**	-5.15	+1.34	-3.50	-0.32	+0.00		**-12.67**
Rebound										
Transition State	-0.80	-3.97	**-4.76**	-5.11	+1.71	+3.92	-5.14	-1.37		**-10.75**
Product	-37.32	+1.13	**-36.19**	-1.02	+1.27	+5.49	-6.23	-1.37		**-38.05**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$. [e] The average Def2-TZVPP energy was calculated to be 8.53 kcal mol^{-1}.

Table S21. Cyclohexene OAT by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	$\Delta \boldsymbol{E}^a$	$\Delta\Delta Z_0$	$\Delta\Delta E_{thermal}{}^b$	$-T\Delta\Delta S^b$	ΔΔDisp	$\Delta\Delta G_{corr}{}^{b,c}$	$\boldsymbol{\Delta G}^d$
***S* = 1**									
OAT									
Reactant Complex	-1.31	+1.48	**0.17**	+0.48	+0.62	+6.48	-3.93	-1.37	**2.45**
Transition State 1	12.23	+7.06	**19.28**	-0.31	+0.09	+9.48	-9.97	-1.37	**17.21**
Intermediate	3.36	+4.14	**7.50**	+0.49	+0.08	+9.85	-10.64	-1.37	**5.92**
Transition State 2	7.29	+3.56	**10.85**	-0.50	+0.08	+9.93	-9.29	-1.37	**9.70**
Product	-11.88	-2.02	**-13.89**	0.67	+0.48	+8.50	-10.64	-1.37	**-16.25**
***S* = 2**									
$Fe^{IV}O$ (TBP) + CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	9.56	-2.56	**6.99**	-1.24	+1.31	+4.14	-1.57	-1.37	**8.27**
Transition State 1	13.92	-1.46	**12.46**	-2.02	+0.96	+6.37	-7.50	-1.37	**8.90**
Intermediate	0.62	-0.05	**0.57**	-1.42	+0.82	+7.71	-9.49	-1.37	**-3.19**
Transition State 2	0.63	+0.24	**0.88**	-1.86	+0.62	+8.08	-9.40	-1.37	**-3.05**
Product	-23.00	-2.87	**-25.88**	-0.42	+1.03	+6.15	-7.12	-1.37	**-27.60**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr}$.

Table S22. Cyclohexene HAT by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ***E***[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	ΔΔTun[b]	**Δ*G***[d]
***S* = 2**										
$Fe^{IV}O$ (Oh) – CH_3CN + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00		**0.00**
HAT										
Reactant Complex	15.76	-7.96	**7.80**	-1.82	+1.03	-2.98	+1.43	+0.00		**5.45**
Transition State	21.66	-5.58	**16.08**	-4.81	+0.75	-1.66	+0.98	+0.00	-0.20	**11.14**
Intermediate	4.77	-8.67	**-3.90**	-4.71	+1.30	-3.06	+1.57	+0.00		**-8.80**
Dissociation										
$Fe^{III}OH$ + substrate•	9.47	-11.55	**-2.09**	-5.65	+0.56	-11.16	+6.76	+1.37		**-10.21**
Rebound										
Transition State	5.07	-9.42	**-4.36**	-5.43	+1.19	-2.88	+2.05	+0.00		**-9.43**
Product	-33.45	-4.85	**-38.30**	-1.13	+0.78	-1.25	+0.29	+0.00		**-39.62**
Desaturation		Not found								

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp + \Delta\Delta G_{corr} + \Delta\Delta Tun$.

Table S23. Cyclohexene OAT by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) in kcal mol^{-1}

	ΔLACVP	ΔΔDef2-TZVPP	Δ**E**[a]	ΔΔZ_0	ΔΔ$E_{thermal}$[b]	-TΔΔS[b]	ΔΔDisp	ΔΔG_{corr}[b,c]	**ΔG**[d]
***S* = 2**									
$Fe^{IV}O$ (TBP) + substrate	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
OAT									
Reactant Complex	15.70	-7.96	**7.74**	-1.84	+1.04	-3.22	+1.76	+0.00	**5.48**
Transition State	20.58	-6.51	**14.08**	-2.86	+0.78	-1.66	+0.13	+0.00	**10.46**
Product	-17.50	-6.95	**-24.45**	-1.02	+0.66	-0.60	+0.06	-0.15	**-25.35**

[a] Sum of the two previous columns. [b] T = 233.15 K. [c] Free energy correction for change of standard state upon complexation. [d] $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta\text{Disp} + \Delta\Delta G_{corr}$.

All the Data for DFT calculations: Mulliken Spin Density Distribution

Table S24. Mulliken Spin Density Distribution of $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/Def2-TZVPP Level

	Fe	O	4 × ligated N	CH_3CN	Rest
1$_{TBP}$ (Triplet) + CH_3CN	1.36	0.70	-0.08	0.00	0.01
1$_{TBP}$ (Quintet) + CH_3CN	3.04	0.65	0.17	0.00	0.15
1$_{Oh}$ (Triplet)	1.18	0.87	-0.04	-0.01	0.00
1$_{Oh}$ (Quintet)	3.09	0.65	0.14	0.03	0.10

Table S25. Mulliken Spin Density Distribution of $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/Def2-TZVPP Level

	Fe	O	4 × ligated N	CH_3CN	Rest
$\mathbf{2}_{TBP}$ (Triplet) + CH_3CN	1.54	0.53	-0.11	0.00	0.04
$\mathbf{2}_{TBP}$ (Quintet) + CH_3CN	3.06	0.71	0.10	0.00	0.13
$\mathbf{2}_{Oh}$ (Triplet)	1.16	0.88	-0.05	0.00	0.02
$\mathbf{2}_{Oh}$ (Quintet)	3.10	0.69	0.10	0.03	0.08

Table S26. Mulliken Spin Density Distribution of $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/Def2-TZVPP Level

	Fe	O	4 × ligated N	CH_3CN	Rest
$\mathbf{3}_{TBP}$ (Triplet) + CH_3CN	1.36	0.73	-0.11	0.00	0.01
$\mathbf{3}_{TBP}$ (Quintet) + CH_3CN	3.07	0.69	0.11	0.00	0.12
$\mathbf{3}_{Oh}$ (Triplet)	1.21	0.86	-0.06	0.01	-0.01
$\mathbf{3}_{Oh}$ (Quintet)	3.12	0.66	0.11	0.08	0.03

Table S27. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.16	0.89	-0.04	0.00	-0.01	0.00
H[1]*AT*						
Reactant Complex	1.16	0.89	-0.04	0.00	-0.01	0.00
Transition State	0.90	0.67	-0.03	0.47	-0.01	0.00
Intermediate	0.89	0.16	-0.04	0.99	-0.01	0.01
MECP	1.18	0.88	-0.06	0.00	0.00	0.00
H[2]*AT*						
Reactant Complex	1.17	0.88	-0.04	0.00	-0.01	0.00
Transition State	0.91	0.64	-0.03	0.48	-0.01	0.00
Intermediate	0.90	0.15	-0.04	0.99	-0.01	0.01
Dissociation						
$Fe^{III}OH$ + substrate•	0.90	0.15	-0.04	±1.00	-0.01	0.01
Rebound						
Transition State	1.49	-0.10	-0.03	0.65	-0.03	0.01
Product	2.01	0.01	0.00	0.01	-0.03	0.01
Desaturation						
Transition State	1.56	-0.07	-0.03	0.56	-0.03	0.01
Product	1.99	0.02	0.01	0.01	-0.04	0.01
***S* = 2**						
$Fe^{IV}O$ + substrate	3.05	0.69	0.12	0.00	0.03	0.11
H[1]*AT*						
Reactant Complex	3.06	0.68	0.12	0.00	0.03	0.10
Transition State	3.65	0.26	0.20	-0.22	0.03	0.09
Intermediate	4.18	0.37	0.28	-0.95	0.03	0.10
MECP	3.07	0.66	0.14	0.00	0.03	0.10
H[2]*AT*						
Reactant Complex	3.06	0.68	0.12	0.00	0.03	0.10
Transition State	3.73	0.21	0.21	-0.26	0.03	0.09
Intermediate	4.19	0.36	0.29	-0.96	0.03	0.10
Dissociation						
$Fe^{III}OH$ + substrate•	4.20	0.35	0.30	±1.00	0.03	0.10
Rebound						
Transition State	4.13	0.34	0.23	-0.81	0.02	0.08
Product	3.80	0.02	0.10	0.01	0.01	0.07
Desaturation						
Transition State	4.19	0.32	0.27	-0.91	0.03	0.10
Product	3.82	0.02	0.11	0.01	0.01	0.03

Table S28. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{1}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.16	0.89	-0.04	0.00	-0.01	0.00
OAT						
Reactant Complex	1.16	0.89	-0.04	0.00	-0.01	0.00
Transition State 1	0.87	0.68	-0.03	0.49	-0.01	0.00
Intermediate	0.85	0.19	-0.04	1.00	-0.01	0.02
Transition State 2	1.42	-0.07	-0.03	0.69	-0.02	0.01
Product	2.00	0.01	0.00	0.02	-0.04	0.01
***S* = 2**						
$Fe^{IV}O$ + substrate	3.05	0.69	0.12	0.00	0.03	0.11
OAT						
Reactant Complex	3.06	0.68	0.12	0.00	0.03	0.11
Transition State	3.57	0.31	0.18	-0.17	0.03	0.09
Product	3.80	0.01	0.09	0.02	0.01	0.07

Table S29. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(Me_3NTB)Fe^{IV}O]^{2+}$ ($\mathbf{1}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.01	0.67	0.16	0.00	0.15
HAT					
Reactant Complex	3.02	0.66	0.16	0.00	0.16
Transition State	3.63	0.27	0.21	-0.26	0.14
Intermediate	4.12	0.38	0.31	-0.96	0.15
Dissociation					
$Fe^{III}OH$ + substrate•	4.13	0.38	0.32	±1.00	0.17
Rebound					
Transition State	4.12	0.34	0.28	-0.88	0.13
Product	3.81	0.01	0.09	0.02	0.08

Table S30. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(Me_3NTB)Fe^{IV}O]^{2+}$ ($\mathbf{1}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.01	0.67	0.16	0.00	0.15
OAT					
Reactant Complex	3.02	0.66	0.16	0.00	0.16
Transition State	3.70	0.27	0.20	-0.31	0.13
Product	3.80	0.01	0.09	0.02	0.09

Table S31. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.13	0.91	-0.05	0.00	-0.01	0.02
H^1AT						
Reactant Complex	1.14	0.90	-0.05	0.00	-0.01	0.02
Transition State	0.89	0.66	-0.04	0.48	-0.01	0.01
Intermediate	0.92	0.15	-0.05	0.98	-0.01	0.01
H^2AT						
Reactant Complex	1.14	0.90	-0.05	0.00	-0.01	0.02
Transition State	0.89	0.67	-0.05	0.48	-0.01	0.01
Intermediate	0.92	0.15	-0.05	0.99	-0.01	0.01
Dissociation						
$Fe^{III}OH$ + substrate•	0.92	0.14	-0.05	±1.00	-0.02	0.01
Rebound						
Transition State	1.30	0.01	-0.07	0.78	-0.02	0.01
Product	2.02	0.00	-0.01	0.00	-0.02	0.01
Desaturation						
Transition State	1.55	0.03	-0.03	0.49	-0.02	-0.01
Product	1.98	0.01	0.04	0.00	-0.04	0.00
***S* = 2**						
$Fe^{IV}O$ + substrate	3.07	0.72	0.08	0.00	0.03	0.09
H^1AT						
Reactant Complex	3.08	0.72	0.08	0.00	0.03	0.09
Transition State	3.66	0.33	0.15	-0.25	0.03	0.07
Intermediate	4.21	0.35	0.28	-0.94	0.03	0.08
H^2AT						
Reactant Complex	3.08	0.72	0.08	0.00	0.03	0.09
Transition State	3.73	0.28	0.17	-0.29	0.03	0.07
Intermediate	4.21	0.34	0.28	-0.95	0.03	0.08
Dissociation						
$Fe^{III}OH$ + substrate•	4.22	0.34	0.30	±1.00	0.04	0.09
Rebound						
Transition State	4.21	0.34	0.28	-0.94	0.03	0.08
Product	3.81	0.01	0.12	0.01	0.01	0.03

Table S32. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.13	0.91	-0.05	0.00	-0.01	0.02
OAT						
Reactant Complex	1.14	0.90	-0.05	0.00	-0.01	0.02
Transition State 1	0.84	0.68	-0.04	0.52	-0.01	0.01
Intermediate	0.85	0.19	-0.05	1.00	-0.01	0.02
Transition State 2	1.30	0.00	-0.04	0.75	-0.02	0.01
Product	1.99	0.01	0.03	0.01	-0.03	0.00
***S* = 2**						
$Fe^{IV}O$ + substrate	3.07	0.72	0.08	0.00	0.03	0.09
OAT						
Reactant Complex	3.08	0.72	0.08	0.00	0.03	0.09
Transition State	3.59	0.38	0.14	-0.21	0.02	0.07
Product	3.81	0.01	0.10	0.02	0.01	0.05

Table S33. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.03	0.74	0.09	0.00	0.14
HAT					
Reactant Complex	3.03	0.74	0.10	0.00	0.14
Transition State	3.69	0.35	0.17	-0.32	0.11
Intermediate	4.15	0.38	0.31	-0.96	0.12
Dissociation					
$Fe^{III}OH$ + substrate•	4.15	0.37	0.33	±1.00	0.14
Rebound					
Intermediate[a]	4.15	0.38	0.31	-0.96	0.12
Transition State 1	4.15	0.37	0.31	-0.94	0.11
Intermediate ($[subs]^+$)	3.79	0.09	0.07	0.01	0.05
Transition State 2	3.79	0.09	0.07	0.01	0.05
Product	3.81	0.01	0.10	0.01	0.07

[a] The substrate radical intermediate repositions itself slightly in preparation for the electron transfer, and this repositioning can be seen as the rate-limiting barrier for the rebound reaction.

Table S34. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.03	0.74	0.09	0.00	0.14
OAT					
Reactant Complex	3.03	0.73	0.09	0.00	0.14
Transition State	3.85	0.32	0.19	-0.46	0.10
Product	3.81	0.01	0.10	0.02	0.07

Table S35. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ (**3**$_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.19	0.89	-0.06	0.00	-0.01	0.01
HAT						
Reactant Complex	1.19	0.88	-0.06	0.00	-0.01	0.00
Transition State	0.92	0.68	-0.04	0.45	-0.01	0.00
Intermediate	0.93	0.14	-0.05	0.99	-0.01	0.01
MECP	1.22	0.87	-0.09	0.00	0.00	0.00
Dissociation						
$Fe^{III}OH$ + substrate•	0.93	0.13	-0.05	±1.00	-0.01	0.01
Rebound						
Transition State	1.48	-0.08	-0.03	0.66	-0.03	0.00
Product	2.00	0.01	0.03	0.01	-0.04	-0.01
Desaturation						
Transition State	1.71	-0.03	0.00	0.37	-0.03	-0.01
Product	1.99	0.02	0.03	0.01	-0.04	-0.01
***S* = 2**						
$Fe^{IV}O$ + substrate	3.09	0.70	0.09	0.00	0.03	0.09
HAT						
Reactant Complex	3.10	0.70	0.09	0.00	0.03	0.08
Transition State	3.72	0.28	0.18	-0.28	0.03	0.07
Intermediate	4.18	0.37	0.30	-0.96	0.03	0.07
MECP	3.11	0.69	0.09	0.00	0.03	0.08
Dissociation						
$Fe^{III}OH$ + substrate•	4.20	0.36	0.31	±1.00	0.04	0.10
Rebound						
Transition State	4.16	0.33	0.26	-0.84	0.03	0.07
Product	3.81	0.02	0.14	0.02	0.01	0.01

Table S36. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	CH_3CN	Rest
***S* = 1**						
$Fe^{IV}O$ + substrate	1.19	0.89	-0.06	0.00	-0.01	0.01
OAT						
Reactant Complex	1.19	0.88	-0.06	0.00	-0.01	0.01
Transition State 1	0.88	0.69	-0.04	0.48	-0.01	0.00
Intermediate	0.91	0.22	-0.05	0.93	-0.01	0.00
Transition State 2	1.48	-0.07	-0.03	0.65	-0.03	-0.01
Product	1.99	0.01	0.03	0.02	-0.04	-0.01
***S* = 2**						
$Fe^{IV}O$ + substrate	3.09	0.70	0.09	0.00	0.03	0.09
OAT						
Reactant Complex	3.10	0.70	0.09	0.00	0.03	0.08
Transition State 1	3.57	0.36	0.16	-0.18	0.03	0.07
Intermediate	4.10	0.37	0.26	-0.82	0.03	0.06
Transition State 2	4.08	0.37	0.24	-0.78	0.03	0.06
Product	3.80	0.01	0.11	0.02	0.01	0.06

Table S37. Mulliken Spin Density Distribution of Cyclohexene HAT Reaction by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.04	0.72	0.11	0.00	0.13
HAT					
Reactant Complex	3.05	0.71	0.11	0.00	0.13
Transition State	3.67	0.32	0.19	-0.29	0.11
Intermediate	4.14	0.38	0.32	-0.95	0.11
Dissociation					
$Fe^{III}OH$ + substrate•	4.14	0.38	0.34	±1.00	0.14
Rebound					
Transition State	4.15	0.34	0.30	-0.90	0.11
Product	3.79	0.01	0.11	0.01	0.08

Table S38. Mulliken Spin Density Distribution of Cyclohexene OAT Reaction by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) at B3LYP/Def2-TZVPP//B3LYP/LACVP Level

	Fe	O	4 × ligated N	Substrate	Rest
***S* = 2**					
$Fe^{IV}O$ + substrate	3.04	0.72	0.11	0.00	0.13
OAT					
Reactant Complex	3.05	0.71	0.11	0.00	0.13
Transition State	3.56	0.38	0.17	-0.22	0.11
Product	3.78	0.01	0.11	0.02	0.08

All the Data for DFT calculations: Selected Geometries

Table S39. Selected Distances of $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{1}_{Oh}$) at B3LYP/Def2-TZVPP Level in Å

	D(Fe-O)	D(Fe-N_{eq})[a]	D(Fe-N_{ax})	D(Fe-$NCCH_3$)
$\mathbf{1}_{TBP}$ (Triplet) + CH_3CN	1.60	1.94	2.19	∞
$\mathbf{1}_{TBP}$ (Quintet) + CH_3CN	1.62	2.00	2.18	∞
$\mathbf{1}_{Oh}$ (Triplet)	1.62	1.97	2.21	2.01
$\mathbf{1}_{Oh}$ (Quintet)	1.62	2.05	2.21	2.33

[a] The average value of the ligand nitrogens in the equatorial plane, excluding solvent as well as the axial ligand N.

Table S40. Selected Distances of $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/Def2-TZVPP Level in Å.

	D(Fe-O)	D(Fe-N_{eq})[a]	D(Fe-N_{ax})	D(Fe-$NCCH_3$)
$\mathbf{2}_{TBP}$ (Triplet) + CH_3CN	1.59	2.03	2.05	∞
$\mathbf{2}_{TBP}$ (Quintet) + CH_3CN	1.62	2.09	2.05	∞
$\mathbf{2}_{Oh}$ (Triplet)	1.63	2.07	2.08	1.99
$\mathbf{2}_{Oh}$ (Quintet)	1.62	2.17	2.08	2.19

[a] The average value of the ligand nitrogens in the equatorial plane, excluding solvent as well as the axial ligand N.

Table S41. Selected Distances of $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) at B3LYP/Def2-TZVPP Level in Å.

	D(Fe-O)	D(Fe-N_{eq})[a]	D(Fe-N_{ax})	D(Fe-$NCCH_3$)
$\mathbf{3}_{TBP}$ (Triplet) + CH_3CN	1.60	1.97	2.09	∞
$\mathbf{3}_{TBP}$ (Quintet) + CH_3CN	1.62	2.03	2.09	∞
$\mathbf{3}_{Oh}$ (Triplet)	1.63	1.99	2.11	1.99
$\mathbf{3}_{Oh}$ (Quintet)	1.62	2.09	2.12	2.23

[a] The average value of the ligand nitrogens in the equatorial plane, excluding solvent as well as the axial ligand N.

Table S42. Selected Geometries of Cyclohexene HAT Reaction by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	D(O-H)[c]	A(Fe-O-H)[a]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.65	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.66	2.93	1.10	3.96	5.98	171.04
Transition State	1.76	1.31	1.28	2.59	4.36	123.26
Intermediate	1.81	0.98	2.52	3.44	4.96	115.01
MECP	1.65	2.85	1.10	3.87	5.90	172.23
H^2AT						
Reactant Complex	1.66	2.74	1.10	3.82	4.07	137.10
Transition State	1.76	1.28	1.30	2.56	3.20	125.08
Intermediate	1.81	0.98	2.54	3.37	3.65	114.30
Dissociation						
$Fe^{III}OH$ + substrate•	1.81	0.98	∞	∞	∞	113.08
Rebound						
Transition State	1.95	0.98	2.43	2.47	2.85	107.78
Product	2.33	0.98	2.03	1.50	2.63	100.89
Desaturation						
Transition State	1.97	0.98	3.77	3.74	1.76	106.55
Product	2.19	0.98	3.46	3.31	0.98	112.32
***S* = 2**						
$Fe^{IV}O$ + substrate	1.65	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.65	2.82	1.10	3.79	5.46	166.46
Transition State	1.70	1.61	1.16	2.76	4.47	170.50
Intermediate	1.80	0.98	2.17	3.14	4.80	155.78
MECP	1.65	2.85	1.10	3.87	5.90	172.23
H^2AT						
Reactant Complex	1.65	2.76	1.10	3.86	4.44	135.24
Transition State	1.71	1.54	1.17	2.71	3.28	159.65
Intermediate	1.80	0.98	2.22	3.19	3.44	149.51
Dissociation						
$Fe^{III}OH$ + substrate•	1.82	0.97	∞	∞	∞	143.03
Rebound						
Transition State	1.89	0.97	2.38	2.78	2.81	134.04
Product	2.15	0.98	2.06	1.51	2.63	116.93
Desaturation						
Transition State	1.89	0.98	2.93	3.55	2.13	123.72
Product	2.12	0.97	3.35	3.27	0.98	115.40

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to. [c] H-atom participating in the desaturation reaction.

Table S43. Selected Geometries of Cyclohexene OAT Reaction by $[(Me_3NTB)Fe^{IV}O(CH_3CN)]^{2+}$ (**1**$_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.65	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.65	4.34	4.33	1.34	130.78	146.40
Transition State 1	1.77	1.96	2.62	1.40	125.07	148.81
Intermediate						
Transition State 2	1.91	1.50	2.19	1.48	127.48	163.88
Product	2.32	1.53	1.53	1.48	126.14	149.60
***S* = 2**						
$Fe^{IV}O$ + substrate	1.65	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.65	3.98	4.50	1.34	167.15	152.95
Transition State	1.69	2.71	2.70	1.36	147.27	175.15
Product	2.18	1.53	1.52	1.48	128.52	142.64

[a] C-atom participating in the initial *S* = 1 O-C bond formation (and the same C-atom in *S* = 2). [b] C-atom participating in the other O-C bond formation.

Table S44. Selected Geometries of Cyclohexene HAT Reaction by $[(Me_3NTB)Fe^{IV}O]^{2+}$ (**1**$_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	A(Fe-O-H)[a]
***S* = 2**					
$Fe^{IV}O$ + substrate	1.65	∞	1.10	∞	∞
HAT					
Reactant Complex	1.65	2.73	1.10	3.83	167.90
Transition State	1.70	1.59	1.16	2.75	173.61
Intermediate	1.79	0.98	2.20	3.18	175.63
Dissociation					
$Fe^{III}OH$ + substrate•	1.79	0.97	∞	∞	178.11
Rebound					
Transition State	1.84	0.97	2.35	3.01	145.33
Product	2.13	0.98	2.08	1.52	118.30

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to.

Table S45. Selected Geometries of Cyclohexene OAT Reaction by $[(Me_3NTB)Fe^{IV}O]^{2+}$ ($\mathbf{1}_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 2**						
$Fe^{IV}O$ + substrate	1.65	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.65	3.57	4.10	1.34	159.06	142.57
Transition State	1.71	2.42	2.75	1.37	167.57	158.89
Product	2.16	1.54	1.53	1.48	128.87	128.54

[a] C-atom participating in the initial O-C bond formation. [b] C-atom participating in the other O-C bond formation.

Table S46. Selected Geometries of Cyclohexene HAT Reaction by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	D(O-H)[c]	A(Fe-O-H)[a]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.67	2.80	1.10	3.87	5.46	139.08
Transition State	1.77	1.34	1.28	2.57	4.20	126.78
Intermediate	1.82	0.98	2.55	3.37	5.12	114.47
H^2AT						
Reactant Complex	1.66	2.88	1.10	3.95	4.15	144.07
Transition State	1.77	1.32	1.28	2.57	3.12	122.35
Intermediate	1.82	0.98	2.52	3.35	3.32	114.11
Dissociation						
$Fe^{III}OH$ + substrate•	1.82	0.98	∞	∞	∞	112.89
Rebound						
Transition State	1.91	0.98	2.57	2.83	3.09	110.41
Product	3.87	0.98	2.03	1.48	2.64	80.80
Desaturation						
Transition State	1.89	0.98	3.60	4.01	2.21	110.36
Product	2.15	0.98	3.20	3.26	0.98	111.26
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞	∞
H^1AT						
Reactant Complex	1.66	2.73	1.10	3.81	5.55	163.22
Transition State	1.70	1.64	1.16	2.79	4.53	169.25
Intermediate	1.81	0.99	2.19	3.16	4.98	145.28
H^2AT						
Reactant Complex	1.66	2.79	1.10	3.85	3.96	142.78
Transition State	1.71	1.58	1.17	2.74	3.30	158.55
Intermediate	1.82	0.99	2.18	3.12	2.88	137.94
Dissociation						
$Fe^{III}OH$ + substrate•	1.82	0.97	∞	∞	∞	137.92
Rebound						
Transition State	1.82	0.99	2.18	3.12	2.85	136.79
Product	2.17	0.98	2.06	1.52	2.62	109.16

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to. [c] H-atom participating in the desaturation reaction.

Table S47. Selected Geometries of Cyclohexene OAT Reaction by $[(TQA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{2}_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	5.57	4.37	1.34	114.40	116.62
Transition State 1	1.78	1.98	2.63	1.40	126.14	147.72
Intermediate	1.83	1.46	2.43	1.50	127.90	146.63
Transition State 2	1.89	1.50	2.25	1.49	129.45	160.83
Product	2.39	1.53	1.54	1.48	128.76	149.04
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	3.91	4.22	1.34	172.11	168.50
Transition State	1.70	2.64	2.86	1.36	150.93	174.46
Product	2.20	1.54	1.54	1.48	128.97	148.18

[a] C-atom participating in the initial *S* = 1 O-C bond formation (and the same C-atom in *S* = 2). [b] C-atom participating in the other O-C bond formation.

Table S48. Selected Geometries of Cyclohexene HAT Reaction by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	A(Fe-O-H)[a]
***S* = 2**					
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞
HAT					
Reactant Complex	1.66	3.30	1.10	4.40	148.77
Transition State	1.71	1.60	1.17	2.76	174.31
Intermediate	1.78	0.98	2.21	3.18	171.99
Dissociation					
$Fe^{III}OH$ + substrate•	1.78	0.97	∞	∞	172.85
Rebound					
Intermediate[c]	1.78	0.98	2.21	3.18	170.13
Transition State 1	1.80	0.98	2.28	3.24	164.74
Intermediate ($[subs]^+$)	1.94	0.98	4.14	4.72	119.05
Transition State 2	1.94	0.98	3.16	3.52	117.97
Product	2.15	0.98	2.07	1.53	112.40

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to. [c] The substrate radical intermediate repositions itself slightly in preparation for the electron transfer, and this repositioning can be seen as the rate-limiting barrier for the rebound reaction.

Table S49. Selected Geometries of Cyclohexene OAT Reaction by $[(TQA)Fe^{IV}O]^{2+}$ ($\mathbf{2}_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	4.08	4.37	1.34	161.92	146.79
Transition State	1.73	2.28	2.74	1.38	165.66	152.70
Product	2.17	1.55	1.54	1.48	140.80	139.23

[a] C-atom participating in the initial O-C bond formation. [b] C-atom participating in the other O-C bond formation.

Table S50. Selected Geometries of Cyclohexene HAT Reaction by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	D(O-H)[c]	A(Fe-O-H)[a]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞	∞
HAT						
Reactant Complex	1.66	2.69	1.10	3.75	4.43	147.35
Transition State	1.76	1.34	1.26	2.59	3.25	124.41
Intermediate	1.82	0.98	2.44	3.36	3.63	116.07
MECP	1.65	2.41	1.10	3.47	4.29	163.26
Dissociation						
$Fe^{III}OH$ + substrate•	1.82	0.98	∞	∞	∞	114.20
Rebound						
Transition State	1.94	0.98	2.43	2.37	3.65	109.82
Product	2.26	0.98	2.04	1.50	2.81	105.17
Desaturation						
Transition State	1.96	0.98	3.67	3.69	1.74	110.21
Product	2.17	0.97	3.46	3.21	0.98	113.61
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞	∞
HAT						
Reactant Complex	1.66	2.72	1.10	3.72	4.46	156.89
Transition State	1.71	1.55	1.17	2.71	3.37	170.32
Intermediate	1.79	0.98	2.16	3.14	3.68	162.50
MECP	1.65	2.41	1.10	3.47	4.29	163.26
Dissociation						
$Fe^{III}OH$ + substrate•	1.80	0.97	∞	∞	∞	151.68
Rebound						
Transition State	1.87	0.98	2.30	2.89	3.96	135.45
Product	2.15	0.98	2.05	1.50	2.82	108.92

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to. [c] H-atom participating in the desaturation reaction.

Table S51. Selected Geometries of Cyclohexene OAT Reaction by $[(TPA)Fe^{IV}O(CH_3CN)]^{2+}$ ($\mathbf{3}_{Oh}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 1**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	4.12	4.85	1.34	135.98	126.57
Transition State 1	1.77	1.99	2.60	1.40	126.44	146.34
Intermediate	1.82	1.50	2.40	1.49	127.93	149.88
Transition State 2	1.92	1.50	2.14	1.48	129.64	164.14
Product	2.25	1.53	1.53	1.48	130.82	149.29
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	4.62	4.39	1.34	130.90	135.89
Transition State 1	1.69	2.56	2.78	1.36	167.77	162.97
Intermediate	1.81	1.49	2.36	1.49	175.85	138.60
Transition State 2	1.83	1.48	2.32	1.49	174.77	136.21
Product	2.17	1.53	1.53	1.48	137.39	128.82

[a] C-atom participating in the initial O-C bond formation. [b] C-atom participating in the other O-C bond formation.

Table S52. Selected Geometries of Cyclohexene HAT Reaction by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-H)[a]	D(H-C)[a,b]	D(O-C)[b]	A(Fe-O-H)[a]
***S* = 2**					
$Fe^{IV}O$ + substrate	1.66	∞	1.10	∞	∞
HAT					
Reactant Complex	1.66	2.70	1.10	3.67	171.11
Transition State	1.70	1.55	1.17	2.71	168.72
Intermediate	1.78	0.98	2.12	3.10	162.68
Dissociation					
$Fe^{III}OH$ + substrate•	1.78	0.97	∞	∞	179.13
Rebound					
Transition State	1.82	0.98	2.09	3.07	142.56
Product	2.13	0.98	2.07	1.52	115.89

[a] H-atom participating in the first HAT. [b] C-atom where the H-atom in the first HAT reaction is attached to.

Table S53. Selected Geometries of Cyclohexene OAT Reaction by $[(TPA)Fe^{IV}O]^{2+}$ ($\mathbf{3}_{TBP}$) at B3LYP/LACVP Level in Å and °

	D(Fe-O)	D(O-C)[a]	D(O-C)[b]	D(C-C)[a,b]	A(Fe-O-C)[a]	A(Fe-O-C)[b]
***S* = 2**						
$Fe^{IV}O$ + substrate	1.66	∞	∞	1.34	∞	∞
OAT						
Reactant Complex	1.66	4.59	4.12	1.34	127.50	128.94
Transition State	1.69	2.55	2.72	1.36	165.69	161.23
Product	2.11	1.53	1.54	1.49	139.33	140.59

[a] C-atom participating in the initial O-C bond formation. [b] C-atom participating in the other O-C bond formation.

DFT calculated coordinates

Coordinates are given in xyz-file format with (charge/multiplicity) given in parenthesis at the respective comment lines.

1_{TBP} without substrate

```
63
TBP with Def2-TZVPP (2/3)
Fe 0.54151 -0.27288 0.76417
O 0.68363 1.11598 1.53972
C -2.56217 1.91362 -3.09451
C -2.59236 3.20327 -2.58706
C -2.10750 -1.15037 -3.72096
C -1.83033 0.97549 -2.37420
C -1.91592 3.54553 -1.40460
N -1.59794 -0.37818 -2.59320
C 4.62069 -2.30412 -2.01195
C -1.15356 1.31404 -1.19098
C -1.18690 2.61048 -0.68793
C -0.82178 -0.81568 -1.58723
C -0.30906 -2.20043 -1.38034
N -0.53683 0.15736 -0.73795
C 1.92150 -2.64893 -0.39920
N 3.81777 -1.25760 -1.38967
C 2.66463 -1.39068 -0.71254
C 5.22121 0.78604 -1.92166
N 0.50172 -2.28145 -0.11658
C 4.14386 0.09485 -1.37764
N 2.21736 -0.22426 -0.25947
C 5.24016 2.15855 -1.72674
C 3.12376 0.74408 -0.66363
C -0.13893 -3.18282 0.88702
C 4.22309 2.81486 -1.01386
C 3.15151 2.12330 -0.47209
C -1.09867 -2.36887 1.69333
N -0.95366 -1.05093 1.77948
N -2.12282 -2.81159 2.44263
C -2.56714 -4.18821 2.62797
C -1.94078 -0.58803 2.63619
C -2.25324 0.69447 3.08012
C -2.68272 -1.70047 3.06542
C -3.31813 0.81729 3.95820
C -3.75130 -1.58039 3.94750
C -4.05483 -0.30016 4.38451
H -3.08360 1.65352 -4.00408
H -3.15044 3.96419 -3.11450
H -1.96650 4.56399 -1.04556
H -0.66423 2.86541 0.22198
H -1.78932 -2.18357 -3.63228
H -3.19462 -1.11339 -3.72746
H -1.72121 -0.73879 -4.65097
H -1.13911 -2.90380 -1.32820
H 0.30415 -2.50227 -2.22842
H 1.98907 -3.38850 -1.19556
H 2.34885 -3.09503 0.49813
H 4.13879 -3.26610 -1.87894
H 4.72433 -2.10061 -3.07552
H 5.60449 -2.33449 -1.54817
H 6.00597 0.28360 -2.46832
H 6.05820 2.73753 -2.13219
H 4.27997 3.88685 -0.88503
H 2.37085 2.62501 0.07948
H 0.63310 -3.57374 1.54903
H -0.61441 -4.03619 0.40609
H -2.04046 -4.84046 1.94038
H -2.36535 -4.50828 3.64841
H -3.63431 -4.25296 2.42912
H -4.31714 -2.43799 4.28124
H -4.87725 -0.15893 5.07187
H -3.58907 1.79689 4.32693
H -1.68277 1.55109 2.75426

63
TBP with Def2-TZVPP (2/5)
Fe -0.01979 0.17597 0.04593
O -0.03767 1.68811 0.62257
C -3.09365 1.71204 -4.29434
C -2.99909 3.08412 -4.11586
C -2.93857 -1.43363 -4.14696
C -2.42917 0.91849 -3.36643
C -2.26906 3.64032 -3.05292
N -2.31231 -0.46629 -3.25220
C 4.41157 -2.24702 -1.74816
C -1.69854 1.46689 -2.30187
C -1.60654 2.84512 -2.13108
C -1.55625 -0.71044 -2.17334
C -1.20079 -2.03570 -1.58567
N -1.16367 0.41278 -1.57249
C 1.26639 -2.01464 -1.52680
N 3.64149 -1.23233 -1.03659
C 2.31026 -1.13825 -0.91807
C 5.51191 0.24212 -0.15945
N 0.01160 -1.86060 -0.73173
C 4.19177 -0.14604 -0.35715
N 1.94538 -0.07112 -0.20710
C 5.71337 1.39353 0.58692
C 3.11277 0.58207 0.16582
C -0.00455 -2.78728 0.43907
C 4.63817 2.12653 1.11495
C 3.32351 1.73507 0.91644
C -0.74137 -2.12311 1.55439
N -0.85978 -0.79612 1.57878
N -1.28507 -2.69727 2.63627
C -1.32145 -4.11513 2.97794
C -1.52542 -0.47367 2.75426
C -1.91968 0.75222 3.28214
C -1.79634 -1.67206 3.43118
C -2.58069 0.73083 4.50034
C -2.45920 -1.69854 4.65273
C -2.84552 -0.47267 5.17385
H -3.65663 1.28843 -5.11311
H -3.50038 3.74163 -4.81234
H -2.22392 4.71586 -2.95278
H -1.04423 3.26805 -1.31199
H -2.59774 -2.43385 -3.90427
H -4.02036 -1.38826 -4.03907
H -2.66310 -1.20420 -5.17356
H -2.02352 -2.37279 -0.95418
H -1.03568 -2.80244 -2.34179
H 1.07199 -1.67771 -2.54559
H 1.56445 -3.06111 -1.58150
H 3.74665 -3.01491 -2.12712
H 4.93858 -1.78883 -2.58257
H 5.12808 -2.69988 -1.06694
H 6.34149 -0.31922 -0.56377
H 6.72325 1.73508 0.76636
H 4.84302 3.01829 1.69090
H 2.49380 2.29543 1.32092
H 1.02485 -2.96524 0.75177
H -0.43205 -3.75093 0.16431
H -0.95202 -4.70402 2.14593
H -0.69777 -4.29871 3.85044
H -2.34645 -4.40776 3.19257
H -2.66537 -2.62215 5.17359
H -3.36399 -0.44322 6.12202
H -2.90125 1.66284 4.94471
H -1.71338 1.67492 2.76045

63
TBP with LACVP (2/5)
Fe -0.00830 0.11008 0.03773
O -0.02665 1.65053 0.62628
C -3.08932 1.74142 -4.27709
C -2.96537 3.12008 -4.09244
C -2.99607 -1.43139 -4.14659
C -2.42731 0.92636 -3.35574
C -2.20914 3.66152 -3.02761
N -2.33670 -0.47611 -3.24530
C 4.46288 -2.21885 -1.81331
C -1.66951 1.46189 -2.28884
C -1.54815 2.84348 -2.11027
C -1.56563 -0.75094 -2.16572
C -1.22087 -2.07796 -1.57542
N -1.14333 0.38112 -1.56363
C 1.28112 -2.04743 -1.55461
N 3.66995 -1.22456 -1.07623
C 2.32247 -1.16582 -0.94880
C 5.53034 0.28848 -0.18251
N 0.02096 -1.89356 -0.72874
C 4.21050 -0.12614 -0.37695
N 1.94597 -0.10012 -0.20991
C 5.71564 1.44182 0.58278
C 3.11393 0.58013 0.16889
C 0.02550 -2.83261 0.45908
C 4.62312 2.15177 1.13176
C 3.30626 1.73336 0.93601
C -0.72696 -2.16667 1.56311
N -0.85169 -0.82263 1.57237
N -1.29279 -2.72126 2.66241
C -1.34071 -4.14323 3.03095
C -1.54007 -0.47450 2.74500
C -1.94073 0.76668 3.24916
C -1.82164 -1.67218 3.44173
C -2.62246 0.76571 4.46696
C -2.50393 -1.67791 4.66073
C -2.89929 -0.43511 5.16008
H -3.67126 1.33265 -5.09384
H -3.46239 3.79201 -4.78281
H -2.14272 4.73846 -2.92272
H -0.96959 3.25072 -1.29079
H -2.67464 -2.44419 -3.90999
H -4.07972 -1.36339 -4.02960
H -2.72167 -1.20407 -5.17820
H -2.03194 -2.41335 -0.92083
H -1.05879 -2.85522 -2.32789
H 1.06033 -1.71524 -2.57426
H 1.57745 -3.09933 -1.60565
H 3.80985 -3.00063 -2.19745
H 4.97288 -1.73693 -2.65010
H 5.19779 -2.66667 -1.14204
H 6.37073 -0.25128 -0.60126
H 6.72265 1.80192 0.76004
H 4.81520 3.04280 1.71867
H 2.46468 2.27308 1.35147
H 1.06586 -2.99065 0.76126
H -0.38952 -3.80498 0.17833
H -0.97856 -4.75174 2.20418
H -0.71356 -4.32010 3.90738
H -2.37160 -4.42460 3.25243
H -2.71793 -2.59456 5.19642
H -3.43188 -0.39016 6.10319
H -2.94849 1.70744 4.89370
H -1.72285 1.68216 2.71378

64
FeOH TBP with LACVP (2/6)
Fe 0.01465 -0.13199 -0.28407
O -0.01474 1.54622 0.33322
C -3.06219 1.20784 -4.74078
C -2.97013 2.59208 -4.58009
C -2.89785 -1.95535 -4.55501
C -2.39395 0.42317 -3.79737
C -2.23824 3.16736 -3.51624
N -2.27163 -0.97256 -3.66084
C 4.49908 -2.69447 -2.12526
C -1.66151 0.99093 -2.73040
C -1.57256 2.37848 -2.57694
C -1.50865 -1.21287 -2.56214
C -1.15262 -2.54221 -1.97754
N -1.11937 -0.06434 -1.97451
C 1.33636 -2.47168 -1.94110
N 3.71445 -1.68564 -1.40104
C 2.36233 -1.59096 -1.30224
C 5.59645 -0.23400 -0.45598
N 0.07595 -2.37795 -1.14044
C 4.27003 -0.61055 -0.68233
N 1.99789 -0.52450 -0.56232
C 5.79751 0.90562 0.32579
C 3.18023 0.11809 -0.15391
C 0.08710 -3.27679 0.05484
C 4.71281 1.63879 0.85901
C 3.38991 1.25796 0.62945
C -0.66016 -2.60497 1.16197
N -0.80170 -1.26511 1.19974
N -1.21955 -3.19243 2.25233
C -1.24962 -4.62156 2.59009
C -1.49530 -0.95661 2.38380
C -1.91206 0.26696 2.91833
C -1.76063 -2.17129 3.05574
C -2.59189 0.23124 4.13683
C -2.44019 -2.21337 4.27578
C -2.85160 -0.98775 4.80400
H -3.62625 0.77189 -5.55619
H -3.47315 3.24112 -5.28798
H -2.19477 4.24721 -3.42917
H -1.01216 2.81149 -1.75824
H -4.49562 -2.94722 -4.35643
H -3.97904 -1.96817 -4.39914
H -2.67999 -1.68870 -5.59067
H -1.96759 -2.88198 -1.32911
H -1.00997 -3.30926 -2.74680
H 1.12546 -2.10968 -2.95329
H 1.67239 -3.51052 -2.03123
H 3.84086 -3.47097 -2.51045
H 5.02402 -2.22637 -2.96102
H 5.22265 -3.14806 -1.44529
H 6.43049 -0.79193 -0.86373
H 6.81002 1.23609 0.52825
H 4.91549 2.51798 1.46026
H 2.55498 1.81632 1.03314
H 1.12813 -3.42866 0.36023
H -0.32500 -4.26280 -0.18603
H -0.89343 -5.21013 1.74659
H -0.61024 -4.81336 3.45475
H -2.27493 -4.91759 2.81906
H -2.63989 -3.14483 4.79130
H -3.38263 -0.97097 5.74903
H -2.92915 1.15941 4.58430
H -1.70738 1.19706 2.40339
H -0.03294 2.44426 0.69750
```

1_{Oh} without substrate

```
69
Oh with Def2-TZVPP (2/3)
Fe 0.64923 -0.39730 0.91870
O 0.68961 1.08441 1.58448
C -2.43806 1.97592 -2.94069
C -2.43178 3.25775 -2.41262
C -2.06959 -1.08362 -3.62063
C -1.73647 1.00527 -2.23334
C -1.74898 3.55722 -1.22261
N -1.54442 -0.34851 -2.47701
C 4.48856 -2.36681 -2.24418
C -1.05096 1.29619 -1.04129
C -1.05059 2.58808 -0.51979
C -0.78178 -0.82332 -1.47325
C -0.32086 -2.22952 -1.30359
N -0.46707 0.11551 -0.60112
C 1.92619 -2.73859 -0.41649
N 3.75758 -1.33465 -1.51967
C 2.65723 -1.47793 -0.75434
C 5.14333 0.71229 -2.08537
N 0.52514 -2.36537 -0.07158
C 4.10177 0.01089 -1.48548
N 2.26086 -0.32438 -0.23615
C 5.19498 2.07613 -1.84316
C 3.14610 0.64502 -0.67296
C -0.11031 -3.28196 0.91666
C 4.24332 2.71661 -1.03110
C 3.20725 2.01668 -0.43497
C -1.10110 -2.47898 1.69889
N -0.93241 -1.17166 1.83617
N -2.18665 -2.91972 2.36562
C -2.68874 -4.28490 2.46288
C -1.95965 -0.70977 2.63970
C -2.26890 0.56765 3.10262
C -2.75841 -1.81428 2.98310
C -3.38823 0.69488 3.90862
C -3.88345 -1.68844 3.79252
C -4.18267 -0.41380 4.24759
H -2.96371 1.74646 -3.85629
H -2.96456 4.04430 -2.92887
H -1.76933 4.57052 -0.84571
H -0.52465 2.81442 0.39460
H -1.80376 -2.13208 -3.53761
H -3.15373 -0.99641 -3.64629
H -1.65007 -0.68357 -4.54170
H -1.17870 -2.89749 -1.23248
H 0.24802 -2.54793 -2.17649
H 1.95804 -3.47241 -1.22054
H 2.39061 -3.19497 0.45670
H 3.94216 -3.30241 -2.20282
H 4.59933 -2.06864 -3.28429
H 5.47154 -2.50893 -1.79912
H 5.87864 0.22317 -2.70771
H 5.98774 2.66119 -2.28834
H 4.32463 3.78245 -0.86809
H 2.47560 2.50297 0.19274
H 0.65805 -3.65658 1.59213
H -0.56067 -4.14420 0.42703
H -2.09152 -4.94196 1.84076
H -2.63204 -4.62669 3.49451
H -3.72207 -4.31842 2.12434
H -4.49591 -2.53833 4.05692
H -5.04774 -0.26921 4.87982
H -3.65897 1.67046 4.28827
H -1.65362 1.41566 2.84150
N 1.79527 -1.16451 2.37468
C 2.44724 -1.48323 3.25982
C 3.26809 -1.88804 4.37845
H 3.61665 -2.90831 4.22389
H 4.12572 -1.22173 4.46062
H 2.68240 -1.84082 5.29549

69
Oh with Def2-TZVPP (2/5)
Fe 0.59201 -0.30366 0.88133
O 0.65630 1.14987 1.59086
C -2.57591 1.95388 -3.17932
C -2.60085 3.25446 -2.69628
C -2.13674 -1.12370 -3.73310
C -1.86167 1.02586 -2.42990
C -1.93727 3.61217 -1.51158
N -1.63411 -0.33408 -2.61621
C 4.45643 -2.34703 -2.26331
C -1.19584 1.37460 -1.24388
C -1.22625 2.68268 -0.76770
C -0.87152 -0.74725 -1.58421
C -0.38648 -2.14271 -1.37093
N -0.58756 0.23128 -0.74492
C 1.86572 -2.65727 -0.47806
N 3.76648 -1.30751 -1.50891
C 2.64924 -1.41977 -0.76920
C 5.27365 0.68073 -1.96974
N 0.46422 -2.26512 -0.13421
C 4.18536 0.01669 -1.41419
N 2.30603 -0.26735 -0.20482
C 5.39592 2.02930 -1.67025
C 3.25328 0.66783 -0.59040
C -0.15329 -3.21158 0.84465
C 4.46680 2.68825 -0.84811
C 3.38317 2.02304 -0.29689
C -1.12367 -2.45144 1.68817
N -0.94806 -1.15087 1.89564
N -2.17904 -2.93356 2.36768
C -2.67608 -4.30386 2.40759
C -1.94671 -0.74335 2.76582
C -2.24022 0.50347 3.31238
C -2.72997 -1.86735 3.07328
C -3.32855 0.57872 4.16702
C -3.82346 -1.79577 3.92951
C -4.10699 -0.55064 4.47028
H -3.08753 1.68221 -4.09131
H -3.14425 4.01060 -3.24586
H -1.98323 4.63806 -1.17290
H -0.71404 2.95273 0.14392
H -1.84191 -2.16083 -3.61452
H -3.22298 -1.06767 -3.76241
H -1.72788 -0.74358 -4.66733
H -1.23711 -2.81807 -1.28752
H 0.18659 -2.47255 -2.23667
H 1.88458 -3.37307 -1.29780
H 2.30756 -3.14558 0.38939
H 3.86565 -3.25600 -2.26381
H 4.59574 -2.01519 -3.28957
H 5.42503 -2.55154 -1.81134
H 5.99123 0.17671 -2.60071
H 6.22722 2.58683 -2.07883
H 4.60288 3.74070 -0.64094
H 2.66717 2.52561 0.33640
H 0.63189 -3.60309 1.49024
H -0.60833 -4.05933 0.33569
H -2.11483 -4.91971 1.71412
H -2.56399 -4.70730 3.41194
H -3.72621 -4.31713 2.12448
H -4.42416 -2.66216 4.16536
H -4.94777 -0.44676 5.14198
H -3.58675 1.52937 4.61276
H -1.63881 1.36900 3.07687
N 1.91282 -1.33227 2.49672
C 2.56332 -1.58220 3.40817
C 3.38256 -1.89925 4.55853
H 2.79675 -2.46529 5.28128
H 4.24047 -2.49264 4.24573
H 3.73272 -0.97785 5.02196

69
```

Oh with LACVP (2/3)
Fe 0.65349 -0.46844 0.90550
O 0.70207 1.03383 1.59776
C -2.39615 2.00293 -2.92517
C -2.37296 3.28729 -2.37938
C -2.08138 -1.07894 -3.63883
C -1.70722 1.00913 -2.22366
C -1.68596 3.56650 -1.17556
N -1.52820 -0.35848 -2.48555
C 4.52891 -2.34801 -2.27493
C -1.01806 1.28110 -1.01682
C -0.99964 2.57268 -0.47706
C -0.76996 -0.86870 -1.47456
C -0.32496 -2.28084 -1.30614
N -0.44724 0.07384 -0.58499
C 1.95996 -2.78193 -0.40997
N 3.77031 -1.32928 -1.53863
C 2.66896 -1.51176 -0.75573
C 5.10293 0.77411 -2.11882
N 0.53840 -2.40659 -0.05967
C 4.08212 0.03990 -1.50662
N 2.24927 -0.35202 -0.22890
C 5.11972 2.14810 -1.87491
C 3.11127 0.65414 -0.67806
C -0.09728 -3.33603 0.94844
C 4.15351 2.76677 -1.04686
C 3.13658 2.03299 -0.43681
C -1.09305 -2.52204 1.71150
N -0.91836 -1.19733 1.82750
N -2.20312 -2.93545 2.38678
C -2.72377 -4.30259 2.51102
C -1.96118 -0.69980 2.61614
C -2.26355 0.59758 3.04662
C -2.77848 -1.79867 2.97816
C -3.39842 0.75553 3.84160
C -3.91659 -1.64219 3.77579
C -4.21171 -0.34559 4.19944
H -2.92490 1.79122 -3.84664
H -2.89440 4.08913 -2.89001
H -1.69354 4.57868 -0.78671
H -0.47163 2.77994 0.44416
H -1.69382 -2.09667 -3.65870
H -3.17127 -1.11331 -3.57243
H -1.78657 -0.57370 -4.56075
H -1.18682 -2.94868 -1.21363
H 0.24543 -2.61758 -2.17704
H 1.98611 -3.52140 -1.21511
H 2.42251 -3.23744 0.47019
H 3.97292 -3.28411 -2.28834
H 4.67842 -2.01420 -3.30334
H 5.49824 -2.51387 -1.79896
H 5.84788 0.30506 -2.74999
H 5.89381 2.75633 -2.32923
H 4.20810 3.83727 -0.88323
H 2.39691 2.49788 0.20231
H 0.68272 -3.70084 1.62283
H -0.54154 -4.20534 0.45562
H -2.14939 -4.97541 1.87644
H -2.64621 -4.63913 3.54738
H -3.76882 -4.32582 2.19557
H -4.54118 -2.48189 4.05553
H -5.08508 -0.17800 4.81968
H -3.66555 1.74481 4.19616
H -1.63365 1.43405 2.77210
N 1.80043 -1.24126 2.36001
C 2.46141 -1.53941 3.27100
C 3.28237 -1.91376 4.40835
H 3.58353 -2.96241 4.32770
H 4.18105 -1.29118 4.44495
H 2.72103 -1.77899 5.33761

69
Oh with LACVP (2/5)
Fe 0.57050 -0.38406 0.86123
O 0.64527 1.09115 1.60340
C -2.49013 1.97693 -3.25028
C -2.48713 3.28627 -2.76331
C -2.14134 -1.13987 -3.79507
C -1.81671 1.02215 -2.48325
C -1.83608 3.62740 -1.55535
N -1.61834 -0.35808 -2.66802
C 4.47173 -2.28442 -2.30820
C -1.16442 1.35665 -1.27287
C -1.16526 2.67036 -0.79231
C -0.88465 -0.80517 -1.60718
C -0.45293 -2.21344 -1.36160
N -0.59525 0.18309 -0.75601
C 1.86563 -2.69436 -0.50822
N 3.74969 -1.27171 -1.52659
C 2.62467 -1.43824 -0.78200
C 5.21520 0.78195 -1.94905
N 0.44631 -2.31452 -0.13251
C 4.14061 0.07501 -1.40298
N 2.25768 -0.28774 -0.18792
C 5.30455 2.13605 -1.62023
C 3.18928 0.69208 -0.55697
C -0.14606 -3.27207 0.88364
C 4.35572 2.75885 -0.77653
C 3.28396 2.04967 -0.23299
C -1.11486 -2.49772 1.71548
N -0.93650 -1.17431 1.88985
N -2.17975 -2.94956 2.42860
C -2.69075 -4.32433 2.51315
C -1.93624 -0.72683 2.76395
C -2.21936 0.54460 3.27401
C -2.72759 -1.84691 3.11175
C -3.30894 0.65331 4.13882
C -3.82025 -1.74153 3.97669
C -4.09594 -0.46997 4.48353
H -2.99225 1.72165 -4.17563
H -2.99746 4.06020 -3.32574
H -1.86002 4.65708 -1.21620
H -0.66361 2.92182 0.13391
H -1.73961 -2.15178 -3.76356
H -3.23176 -1.18764 -3.74493
H -1.83910 -0.67262 -4.73447
H -1.32821 -2.85116 -1.20511
H 0.08036 -2.61544 -2.22807
H 1.87207 -3.39180 -1.34964
H 2.31752 -3.20553 0.34647
H 3.85339 -3.17312 -2.42307
H 4.69433 -1.88194 -3.29782
H 5.40237 -2.55528 -1.80434
H 5.94619 0.30872 -2.59308
H 6.12261 2.72415 -2.02053
H 4.46628 3.81275 -0.54726
H 2.55462 2.51849 0.41540
H 0.66356 -3.63933 1.51992
H -0.59636 -4.13504 0.38647
H -2.15663 -4.96070 1.80989
H -2.54855 -4.71215 3.52418
H -3.75312 -4.33323 2.26221
H -4.42592 -2.59849 4.24501
H -4.93413 -0.34083 5.15889
H -3.56006 1.62115 4.55799
H -1.61091 1.39917 3.00623
N 1.92127 -1.45528 2.47170
C 2.59191 -1.69513 3.39689
C 3.42431 -1.99424 4.55014
H 2.85040 -2.54919 5.29800
H 4.28615 -2.59727 4.24986
H 3.78685 -1.06696 5.00371

70
FeOH Oh with LACVP (2/2)
Fe 0.65360 -0.48042 0.88543
O 0.66416 1.19159 1.58145
C -2.38086 2.01394 -2.98291
C -2.34903 3.30543 -2.45432
C -2.09296 -1.07845 -3.65275
C -1.70210 1.02408 -2.26548
C -1.66366 3.59404 -1.25158
N -1.53382 -0.34727 -2.51032
C 4.50735 -2.36715 -2.32438
C -1.01374 1.30437 -1.05880
C -0.98767 2.60455 -0.53673
C -0.78118 -0.84789 -1.48679
C -0.35256 -2.26377 -1.30395
N -0.45217 0.09865 -0.60645
C 1.94303 -2.78421 -0.43788
N 3.76601 -1.34735 -1.57309
C 2.66557 -1.52450 -0.78578
C 5.11990 0.74907 -2.13149
N 0.52885 -2.38915 -0.06704
C 4.09380 0.01751 -1.52466
N 2.26212 -0.36940 -0.24244
C 5.15357 2.11927 -1.86763
C 3.13426 0.63195 -0.68230
C -0.09092 -3.33478 0.94069
C 4.19865 2.73728 -1.02572
C 3.17636 2.00679 -0.42060
C -1.08618 -2.53444 1.71522
N -0.90659 -1.21297 1.83514
N -2.19237 -2.95080 2.39688
C -2.71317 -4.31775 2.51777
C -1.94196 -0.71655 2.63410
C -2.23612 0.58040 3.07192
C -2.75976 -1.81507 2.99785
C -3.36432 0.73873 3.87624
C -3.89104 -1.65757 3.80518
C -4.17825 -0.36145 4.23624
H -2.90843 1.79426 -3.90341
H -2.86226 4.10470 -2.97766
H -1.66482 4.61183 -0.87656
H -0.45876 2.80555 0.38431
H -1.70550 -2.09652 -3.66591
H -3.18285 -1.11320 -3.58185
H -1.80395 -0.58271 -4.58185
H -1.22230 -2.91745 -1.18736
H 0.19942 -2.62321 -2.17756
H 1.94558 -3.52294 -1.24395
H 2.40866 -3.24842 0.43627
H 3.94205 -3.29779 -2.33842
H 4.64982 -2.02799 -3.35213
H 5.48003 -2.54624 -1.86002
H 5.85645 0.28097 -2.77329
H 5.93266 2.72490 -2.31708
H 4.26714 3.80474 -0.84730
H 2.44093 2.46282 0.22973
H 0.69904 -3.69351 1.60674
H -0.52711 -4.20535 0.44316
H -2.14499 -4.98675 1.87339
H -2.62663 -4.66144 3.55115
H -3.76115 -4.33876 2.21181
H -4.51654 -2.49610 4.08664
H -5.04622 -0.19363 4.86411
H -3.62598 1.72739 4.23687
H -1.60166 1.41103 2.79032
N 1.79950 -1.14444 2.38000
C 2.47060 -1.45661 3.28014
C 3.30591 -1.84791 4.40200
H 3.47626 -2.92848 4.38566
H 4.27250 -1.33858 4.34887
H 2.81872 -1.58325 5.34500
H 1.12387 1.24514 2.44663

70
FeOH Oh with LACVP (2/6)
Fe 0.60919 -0.17453 0.95063
O 0.66944 1.46942 1.71757
C -2.50235 1.99279 -3.18799
C -2.51437 3.30468 -2.70802
C -2.11356 -1.11459 -3.72290
C -1.80566 1.05280 -2.42357
C -1.85494 3.66090 -1.50932
N -1.58964 -0.32428 -2.60258
C 4.45798 -2.41678 -2.31535
C -1.14503 1.40193 -1.22325
C -1.16070 2.71821 -0.74877
C -0.83810 -0.76223 -1.54908
C -0.39715 -2.17949 -1.34298
N -0.55195 0.23699 -0.70593
C 1.88406 -2.71719 -0.47668
N 3.77454 -1.36196 -1.55739
C 2.65512 -1.47174 -0.78263
C 5.27724 0.64071 -2.08594
N 0.47515 -2.34599 -0.12604
C 4.19801 -0.02330 -1.49527
N 2.32503 -0.29595 -0.22901
C 5.40073 2.00403 -1.80900
C 3.27480 0.64406 -0.65665
C -0.14105 -3.26246 0.88703
C 4.48065 2.67761 -0.97226
C 3.40508 2.01070 -0.38446
C -1.11470 -2.48081 1.71227
N -0.95813 -1.16291 1.90749
N -2.19191 -2.96265 2.39954
C -2.68423 -4.34432 2.45778
C -1.98418 -0.74770 2.76965
C -2.29193 0.51260 3.29456
C -2.76799 -1.88133 3.08829
C -3.39772 0.59721 4.14141
C -3.87672 -1.80125 3.93610
C -4.17700 -0.54036 4.45620
H -3.01085 1.72435 -4.10612
H -3.04308 4.06774 -3.26843
H -1.89083 4.69175 -1.17445
H -0.65141 2.97692 0.17118
H -1.69180 -2.11825 -3.70072
H -3.20211 -1.18379 -3.65736
H -1.83470 -0.63944 -4.66563
H -1.27772 -2.82353 -1.24124
H 0.14477 -2.53323 -2.22718
H 1.91286 -3.43414 -1.30407
H 2.33507 -3.20883 0.39087
H 3.85150 -3.32069 -2.32422
H 4.60796 -2.08473 -3.34451
H 5.42511 -2.64120 -1.85915
H 5.98716 0.12972 -2.72504
H 6.22334 2.55958 -2.24532
H 4.61730 3.73676 -0.78407
H 2.69557 2.51619 0.25944
H 0.65343 -3.64183 1.53728
H -0.60763 -4.12975 0.40763
H -2.14148 -4.96225 1.74475
H -2.54085 -4.75109 3.46160
H -3.74603 -4.36397 2.20390
H -4.47598 -2.66931 4.18290
H -5.02823 -0.43113 5.11892
H -3.66768 1.55591 4.57023
H -1.68653 1.37662 3.04860
N 1.89994 -1.15938 2.53122
C 2.57771 -1.50813 3.41452
C 3.42127 -1.94116 4.51509
H 3.57172 -3.02389 4.47244
H 4.39658 -1.44882 4.46020
H 2.95319 -1.68937 5.47124
H 1.02128 1.95828 2.48155

1$_{Oh}$ with cyclohexene

85
MECP (2/3 and 2/5)
Fe 0.54878 -0.91167 0.03400
O 0.93609 0.39525 0.96716
C -3.12565 2.37573 -2.65336
C -2.88841 3.55306 -1.93981
C -3.18505 -0.57005 -3.87021
C -2.37248 1.25753 -2.28409
C -1.93483 3.60845 -0.89739
N -2.34727 -0.05937 -2.77867
C 3.42944 -2.52617 -4.22380
C -1.41786 1.30646 -1.24009
C -1.18544 2.48959 -0.53055
C -1.42023 -0.74650 -2.05099
C -1.04440 -2.18130 -2.22643
N -0.84556 0.02965 -1.12852
C 1.28365 -3.05270 -1.90707
N 2.99602 -1.60149 -3.16819
C 2.07756 -1.82139 -2.18942
C 4.44986 0.43385 -3.69828
N 0.01178 -2.61220 -1.21260
C 3.50206 -0.30219 -2.98237
N 1.95676 -0.75282 -1.38123
C 4.70970 1.72748 -3.24338
C 2.83848 0.22883 -1.85073
C -0.52219 -3.67955 -0.28011
C 4.05035 2.26351 -2.11257
C 3.10647 1.52539 -1.39830
C -1.23265 -2.98318 0.83189
N -0.86066 -1.74110 1.18912
N -2.23483 -3.44864 1.62437
C -2.88870 -4.76307 1.57429
C -1.66349 -1.35964 2.27204
C -1.71265 -0.17697 3.01773
C -2.53695 -2.43704 2.55386
C -2.65941 -0.11028 4.03998
C -3.48400 -2.37479 3.57926
C -3.53076 -1.18976 4.31522
H -3.85828 2.33913 -3.45085
H -3.44962 4.44588 -2.19255
H -1.78077 4.54329 -0.37038
H -0.45375 2.53097 0.26692
H -2.87669 -1.58198 -4.12959
H -4.23363 -0.58514 -3.56316
H -3.06778 0.06670 -4.74934
H -1.92208 -2.82454 -2.11849
H -0.65218 -2.34848 -3.23370
H 1.05732 -3.63591 -2.80385
H 1.84048 -3.69869 -1.22248
H 2.78605 -3.40463 -4.23399
H 3.36152 -2.02826 -5.19285
H 4.46034 -2.83949 -4.04338
H 4.95885 0.02723 -4.56344
H 5.43604 2.33617 -3.76953
H 4.28463 3.27363 -1.79635
H 2.59934 1.92718 -0.53014
H 0.32797 -4.23799 0.12189
H -1.15896 -4.38657 -0.81896
H -2.50429 -5.33568 0.73198
H -2.68576 -5.31043 2.49752
H -3.96602 -4.63293 1.45370
H -4.15262 -3.19934 3.79386
H -4.25281 -1.09496 5.11807
H -2.73193 0.79108 4.63804
H -1.03916 0.64351 2.80466
N 2.00562 -2.27745 1.10734
C 2.81032 -2.74731 1.80934
C 3.81327 -3.32487 2.68703
H 4.73122 -3.53169 2.12897
H 4.04541 -2.62984 3.49968
H 3.44549 -4.25987 3.11946
H 2.80893 3.47954 3.30908
C 1.71661 3.47626 3.18350
C 1.03046 3.81373 4.52374
C -0.45621 4.15928 4.31229
C -0.61195 5.38382 3.38699
C 0.30034 5.30404 2.18173
C 1.32901 4.44441 2.08587
H 1.45787 2.45039 2.87396
H 1.53541 4.67611 4.98294
H -0.94828 4.34875 5.27431
H -1.65609 5.47753 3.05687
H -0.39687 6.30684 3.95030
H 0.09605 5.99406 1.36378
H 1.93868 4.43232 1.18293
H -0.96527 3.29588 3.85877
H 1.13550 2.97487 5.22301

85
H^{1}AT Reactant Complex (2/3)
Fe 0.53982 -0.97667 -0.00173
O 0.89207 0.36088 0.90766
C -3.00859 2.34939 -2.54033
C -2.74336 3.50401 -1.80231
C -3.15174 -0.55320 -3.83044
C -2.27692 1.20652 -2.20445
C -1.78136 3.51339 -0.76646
N -2.29040 -0.09340 -2.73452
C 3.49114 -2.52824 -4.19409
C -1.31305 1.20802 -1.16653
C -1.05320 2.37126 -0.43210
C -1.37716 -0.82488 -2.03615
C -1.03414 -2.26089 -2.23512
N -0.77616 -0.08752 -1.09900
C 1.30021 -3.10212 -1.92464
N 3.00201 -1.60576 -3.16207
C 2.06170 -1.84597 -2.20432
C 4.40912 0.46855 -3.66728
N 0.02453 -2.68738 -1.22895
C 3.45638 -0.28922 -2.97875
N 1.87927 -0.77216 -1.42160
C 4.61833 1.77241 -3.21587
C 2.73765 0.23445 -1.87624
C -0.51021 -3.73692 -0.28254
C 3.90438 2.30008 -2.11415
C 2.95526 1.54285 -1.42806
C -1.23210 -3.00788 0.80512
N -0.88882 -1.74588 1.10198
N -2.22315 -3.45746 1.62637
C -2.85823 -4.78114 1.63017
C -1.68962 -1.32964 2.17122
C -1.75155 -0.11852 2.87057
C -2.53644 -2.41288 2.51149
C -2.67867 -0.03010 3.90870
C -3.46623 -2.32639 3.55248
C -3.52239 -1.11528 4.24365
H -3.74680 2.34394 -3.33313
H -3.28760 4.41402 -2.02904
H -1.60218 4.43082 -0.21689
H -0.31722 2.38010 0.36083
H -2.87108 -1.56496 -4.12053
H -4.19721 -0.54974 -3.51334
H -3.02846 0.10493 -4.69284
H -1.91970 -2.89244 -2.11732
H -0.65655 -2.43090 -3.24806
H 1.08557 -3.68502 -2.82472
H 1.87149 -3.74229 -1.24663
H 2.86932 -3.42185 -4.21508
H 3.44044 -2.04156 -5.16991
H 4.52344 -2.81631 -3.98175
H 4.96254 0.06788 -4.50782
H 5.34800 2.39586 -3.72029
H 4.10278 3.31779 -1.79687
H 2.40879 1.93717 -0.58077
H 0.33627 -4.28856 0.13602
H -1.14397 -4.45579 -0.80925
H -2.48406 -5.37265 0.79624
H -2.63057 -5.30060 2.56376
H -3.93948 -4.66912 1.52756
H -4.11216 -3.15559 3.81447
H -4.22888 -1.00372 5.05850
H -2.75552 0.89139 4.47504
H -1.09920 0.70567 2.61181
N 1.86293 -2.09016 1.02027
C 2.66072 -2.59229 1.70380
C 3.65495 -3.21641 2.55784
H 4.56626 -3.42295 1.98923
H 3.90219 -2.55070 3.39030
H 3.26951 -4.15684 2.96238
H 2.81084 3.48481 3.32091
C 1.71886 3.48195 3.19263
C 1.02928 3.81764 4.53154
C -0.45696 4.16286 4.31645
C -0.61065 5.38913 3.39312
C 0.30628 5.31285 2.19114
C 1.33461 4.45264 2.09588
H 1.46076 2.45646 2.88172
H 1.53279 4.67971 4.99288
H -0.95207 4.35012 5.27728
H -1.65361 5.48194 3.05893
H -0.39919 6.31133 3.95902

H 0.10559 6.00586 1.37482
H 1.94694 4.44282 1.19477
H -0.96394 3.29998 3.85968
H 1.13283 2.97798 5.22998

85
H[1]AT Transition State (2/3)
Fe 0.85639 -0.43269 0.74018
O 0.84410 1.18411 1.43726
C -3.00565 1.80523 -2.50379
C -3.01883 3.08110 -1.93768
C -2.50572 -1.21655 -3.34269
C -2.11536 0.88039 -1.94965
C -2.17093 3.41814 -0.85746
N -1.85198 -0.45964 -2.26955
C 4.43197 -2.07869 -2.90895
C -1.26226 1.20938 -0.86737
C -1.28269 2.49337 -0.30701
C -0.88310 -0.89554 -1.41043
C -0.26620 -2.25349 -1.38329
N -0.50753 0.06427 -0.56297
C 2.12090 -2.65643 -0.76114
N 3.69353 -1.10398 -2.09721
C 2.71036 -1.34916 -1.18200
C 4.77616 1.08155 -2.86470
N 0.73368 -2.35629 -0.24174
C 3.90053 0.28453 -2.12001
N 2.27605 -0.21623 -0.61404
C 4.70805 2.45890 -2.64882
C 2.99248 0.84062 -1.18563
C 0.27510 -3.34422 0.80557
C 3.79625 3.02079 -1.72405
C 2.92597 2.22383 -0.98031
C -0.65534 -2.61107 1.71635
N -0.53622 -1.28436 1.85520
N -1.65538 -3.10814 2.50243
C -2.08025 -4.50576 2.64250
C -1.50771 -0.87026 2.77273
C -1.83617 0.39812 3.26537
C -2.21650 -2.02257 3.19328
C -2.87956 0.47273 4.18788
C -3.26156 -1.95050 4.12011
C -3.57991 -0.68245 4.60902
H -3.65499 1.54957 -3.33257
H -3.69394 3.83043 -2.33621
H -2.21303 4.42176 -0.44828
H -0.62680 2.73553 0.51784
H -2.15872 -2.24898 -3.33137
H -3.58774 -1.20838 -3.19387
H -2.26780 -0.77374 -4.31285
H -1.02938 -3.02919 -1.26577
H 0.24865 -2.45745 -2.32776
H 2.08594 -3.39122 -1.57099
H 2.70806 -3.09043 0.05295
H 4.01126 -3.07268 -2.76539
H 4.35438 -1.81091 -3.96465
H 5.48316 -2.09283 -2.61151
H 5.47368 0.65618 -3.57614
H 5.36829 3.11476 -3.20529
H 3.77483 4.09714 -1.59351
H 2.22153 2.64039 -0.27230
H 1.15153 -3.68701 1.36267
H -0.18331 -4.22309 0.34302
H -1.57802 -5.12057 1.89729
H -1.82863 -4.87776 3.63856
H -3.15871 -4.57668 2.48772
H -3.80108 -2.83178 4.44550
H -4.38426 -0.58001 5.32897
H -3.16292 1.43749 4.59398
H -1.29165 1.27182 2.93211
N 2.23870 -1.11262 2.01897
C 3.02295 -1.48609 2.79577
C 4.00287 -1.95372 3.76118
H 4.93048 -2.23340 3.25338
H 4.22358 -1.16467 4.48610
H 3.61793 -2.82530 4.29846
H 3.49156 1.47128 2.81277
C 2.63302 2.10224 3.06683
C 2.08053 1.87336 4.47479
C 0.98686 2.90370 4.81864
C 1.50688 4.34794 4.67102
C 2.30381 4.54101 3.40574
C 2.81133 3.50817 2.68426
H 1.76573 1.61881 2.25690
H 2.90702 1.96145 5.19841
H 0.61494 2.73859 5.83639
H 0.66961 5.05869 4.69703
H 2.14043 4.61087 5.53512
H 2.49968 5.56366 3.08959
H 3.38369 3.71529 1.78280
H 0.13627 2.75838 4.13949
H 1.68801 0.85400 4.57234

85
H[1]AT Intermediate (2/3)
Fe 0.27180 -0.58417 0.06051
O 0.26958 1.02801 0.87909
C -3.60077 1.86439 -3.01151
C -3.58007 3.11587 -2.39369
C -3.18260 -1.12899 -3.97693
C -2.72207 0.90042 -2.50810
C -2.71091 3.39047 -1.31270
N -2.49055 -0.42946 -2.88915
C 3.71189 -1.92391 -3.82828
C -1.84848 1.16616 -1.42435
C -1.83490 2.42650 -0.81209
C -1.52055 -0.92021 -2.06221
C -0.94173 -2.29364 -2.08608
N -1.11502 -0.00709 -1.17870
C 1.49237 -2.67943 -1.63447
N 3.01783 -1.02354 -2.90002
C 2.06114 -1.34238 -1.98048
C 4.12043 1.20794 -3.48278
N 0.13385 -2.42972 -1.01561
C 3.25011 0.35725 -2.79356
N 1.66380 -0.26362 -1.29411
C 4.09964 2.55504 -3.11788
C 2.38733 0.83314 -1.77532
C -0.24424 -3.49032 -0.00368
C 3.24286 3.03483 -2.09900
C 2.37545 2.18544 -1.41243
C -1.15995 -2.83336 0.97581
N -1.05923 -1.51354 1.17768
N -2.11605 -3.38898 1.77541
C -2.51350 -4.79951 1.85541
C -1.99344 -1.16478 2.15864
C -2.31197 0.06847 2.74002
C -2.66463 -2.35103 2.54593
C -3.31286 0.07358 3.71146
C -3.66799 -2.34744 3.52050
C -3.97971 -1.11421 4.09502
H -4.26623 1.65507 -3.84052
H -4.24492 3.89443 -2.75142
H -2.72715 4.37715 -0.86232
H -1.16320 2.61724 0.01285
H -2.83033 -2.15777 -4.03846
H -4.25837 -1.13650 -3.78726
H -2.98380 -0.62969 -4.92811
H -1.71838 -3.04426 -1.90894
H -0.50387 -2.51549 -3.06409
H 1.41228 -3.35171 -2.49311
H 2.12548 -3.16984 -0.88894
H 3.31169 -2.93223 -3.73378
H 3.56616 -1.57912 -4.85417
H 4.77951 -1.94439 -3.59769
H 4.78122 0.84425 -4.26047
H 4.75841 3.25066 -3.62574
H 3.26501 4.08918 -1.84622
H 1.72185 2.53660 -0.62450
H 0.66641 -3.82290 0.50239
H -0.68674 -4.36122 -0.49507
H -2.00843 -5.36912 1.07692
H -2.24126 -5.21118 2.83003
H -3.59239 -4.88451 1.71098
H -4.18074 -3.25382 3.81907
H -4.75176 -1.06518 4.85483
H -3.58874 1.00877 4.18612
H -1.79115 0.96728 2.43605
N 1.69942 -1.25512 1.28370
C 2.54210 -1.58295 2.01885
C 3.59557 -1.99295 2.93094
H 4.23206 -2.74629 2.45750
H 4.21364 -1.13176 3.20171
H 3.16435 -2.41751 3.84212
H 1.92431 0.99542 4.20553
C 1.77252 1.99806 3.81436
C 0.58594 2.79346 4.29853
C 0.21751 3.92190 3.30854
C 1.45461 4.75812 2.90939
C 2.60775 3.88085 2.49289
C 2.71062 2.56497 2.94813
H 0.90997 1.11894 1.62106
H 0.81345 3.23208 5.28648
H -0.55444 4.56890 3.74066
H 1.19445 5.45678 2.10330
H 1.75910 5.39033 3.76263
H 3.37976 4.29770 1.85195
H 3.56479 1.96732 2.63550
H -0.20725 3.46757 2.40313
H -0.27725 2.13422 4.45971

85
H[2]AT Reactant Complex (2/3)
Fe 0.18927 -0.40512 -0.21156
O 0.16847 1.18596 0.24654
C -3.58514 1.17527 -3.86302
C -3.65504 2.51793 -3.48846
C -2.97816 -1.91745 -4.23592
C -2.68772 0.37108 -3.15442
C -2.85645 3.03569 -2.44289
N -2.37380 -0.99238 -3.26948
C 3.96734 -2.44930 -3.41142
C -1.88398 0.88254 -2.10675
C -1.96165 2.23078 -1.73706
C -1.42572 -1.27033 -2.33043
C -0.76205 -2.58061 -2.07592
N -1.10909 -0.18282 -1.62250
C 1.59537 -2.78272 -1.27662
N 3.16650 -1.39149 -2.78280
C 2.15248 -1.53447 -1.88252
C 4.22569 0.69277 -3.81839
N 0.17177 -2.46527 -0.88009
C 3.33660 -0.01462 -3.00296
N 1.65759 -0.34364 -1.51373
C 4.11761 2.08412 -3.80422
C 2.37385 0.64321 -2.19863
C -0.31884 -3.28392 0.29116
C 3.15791 2.74633 -3.00263
C 2.27277 2.03941 -2.18915
C -1.30574 -2.43827 1.03073
N -1.21883 -1.10189 0.96252
N -2.31885 -2.82632 1.85683
C -2.72319 -4.19416 2.20493
C -2.21979 -0.56930 1.78179
C -2.57245 0.75253 2.07918
C -2.91993 -1.65874 2.35547
C -3.63899 0.94389 2.95727
C -3.98954 -1.46867 3.23626
C -4.33678 -0.14811 3.52504
H -4.19781 0.78017 -4.66422
H -4.33734 3.17886 -4.01115
H -2.94248 4.08519 -2.18411
H -1.34842 2.62266 -0.93652
H -2.54686 -2.91031 -4.11705
H -4.05567 -1.97690 -4.06749
H -2.78541 -1.56819 -5.25262
H -1.49827 -3.36782 -1.88862
H -0.18191 -2.89032 -2.95101
H 1.63441 -3.64467 -1.94895
H 2.15421 -3.04197 -0.37326
H 3.54528 -3.42357 -3.17034
H 3.95719 -2.31859 -4.49521
H 4.99611 -2.40710 -3.04635
H 4.96504 0.19170 -4.43131
H 4.78714 2.67257 -4.42149
H 3.11247 3.82949 -3.02239
H 1.53846 2.53702 -1.56861
H 0.53583 -3.50598 0.93696
H -0.73646 -4.23801 -0.04223
H -2.18345 -4.90836 1.58512
H -2.50090 -4.39428 3.25568
H -3.79397 -4.31308 2.02834
H -4.52438 -2.30103 3.67732
H -5.16010 0.04596 4.20329
H -3.94171 1.95302 3.21377
H -2.02910 1.58219 1.64558
N 1.52996 -0.85776 1.21069
C 2.29020 -0.93318 2.08966
C 3.23476 -1.00435 3.18885
H 4.21851 -1.31482 2.82468
H 3.32380 -0.01591 3.65486
H 2.89168 -1.72213 3.93954
H 1.36692 2.74052 2.15948
C 1.64840 3.29658 3.06481
C 0.57749 3.10166 4.15828
C 1.09331 3.58166 5.52844
C 2.34581 2.78818 5.95645
C 3.32836 2.61933 4.81669
C 3.02147 2.86164 3.53001
H 1.68479 4.35652 2.76291
H 0.31758 2.03494 4.22605
H 0.30983 3.48816 6.29051
H 2.84179 3.29149 6.79840
H 2.04935 1.79782 6.33878
H 4.33615 2.29971 5.07968
H 3.78868 2.75368 2.76389
H 1.34674 4.64967 5.46111
H -0.34120 3.63518 3.88454

85
H[2]AT Transition State (2/3)
Fe 0.66691 -0.14565 0.70682
O 0.52651 1.54440 1.17171
C -2.94890 1.48899 -3.13226
C -3.06938 2.82076 -2.73218
C -2.25508 -1.57974 -3.53957
C -2.07903 0.68526 -2.38910
C -2.34590 3.32742 -1.62809
N -1.73108 -0.66722 -2.51751
C 4.63390 -2.06772 -2.35409
C -1.34954 1.18403 -1.28155
C -1.47873 2.52271 -0.88808
C -0.83623 -0.94846 -1.52407
C -0.17817 -2.26246 -1.26926
N -0.58216 0.12312 -0.77061
C 2.14362 -2.48091 -0.37569
N 3.79150 -1.03453 -1.74052
C 2.72777 -1.21049 -0.90290
C 4.89687 1.08892 -2.63971
N 0.70281 -2.18210 -0.03260
C 3.96658 0.34918 -1.90235
N 2.20796 -0.03708 -0.51890
C 4.77886 2.47868 -2.58448
C 2.95513 0.97403 -1.13190
C 0.17123 -3.05244 1.08199
C 3.76766 3.10813 -1.82059
C 2.84164 2.36883 -1.08471
C -0.86006 -2.25053 1.80832
N -0.79346 -0.91311 1.79068
N -1.90975 -2.68779 2.56478
C -2.30307 -4.07343 2.84636
C -1.85199 -0.42899 2.56695
C -2.25344 0.87584 2.87819
C -2.56160 -1.54950 3.06520
C -3.37438 1.01889 3.69577
C -3.68522 -1.40791 3.88606
C -4.07852 -0.10387 4.19131
H -3.50493 1.10161 -3.97759
H -3.73295 3.48073 -3.28008
H -2.46938 4.36870 -1.35065
H -0.91888 2.89643 -0.04209
H -1.77010 -2.55107 -3.45261
H -3.33232 -1.70846 -3.41029
H -2.05322 -1.17527 -4.53394
H -0.92232 -3.05311 -1.13217
H 0.43736 -2.55321 -2.12660
H 2.21632 -3.31440 -1.08072
H 2.66120 -2.77849 0.54045
H 4.19329 -3.04970 -2.18859
H 4.70320 -1.89030 -3.42909
H 5.63410 -2.04746 -1.91477
H 5.67378 0.61261 -3.22546
H 5.47957 3.09122 -3.14086
H 3.71377 4.19113 -1.80906
H 2.06150 2.83608 -0.49774
H 0.99860 -3.29490 1.75530
H -0.22013 -3.99594 0.69061
H -1.68041 -4.75830 2.27295
H -2.17846 -4.28801 3.91040
H -3.34695 -4.22347 2.56316
H -4.22772 -2.26385 4.26912
H -4.94499 0.05248 4.82426
H -3.71642 2.01341 3.96031
H -1.70361 1.72530 2.49441
N 1.93869 -0.58719 2.18220
C 2.66920 -0.83665 3.05474
C 3.58304 -1.16074 4.13579
H 4.14088 -2.07153 3.89854
H 4.29151 -0.34028 4.28086
H 3.02972 -1.31894 5.06606
H 1.26018 2.13249 2.04545
C 1.79068 2.99970 2.84886
C 0.97515 2.93531 4.14300
C 1.79174 3.45992 5.34623
C 3.10638 2.66726 5.50142
C 3.83312 2.53201 4.18392
C 3.22700 2.72803 2.98501
H 1.57216 3.86726 2.21176
H 0.69004 1.89279 4.34660
H 1.19481 3.39096 6.26320
H 3.76302 3.15548 6.23356
H 2.88996 1.66913 5.91724
H 4.90232 2.33106 4.21775
H 3.82227 2.71025 2.07398
H 2.02647 4.52187 5.19115
H 0.04343 3.50060 4.03249

85
H[2]AT Intermediate (2/3)
Fe 0.24768 -0.44439 -0.09494
O 0.19886 1.29148 0.41171
C -3.47403 1.34038 -3.74995
C -3.53028 2.67300 -3.33845
C -2.90554 -1.74732 -4.20293
C -2.59646 0.50399 -3.05320
C -2.73727 3.14899 -2.26881
N -2.30179 -0.85942 -3.20335
C 4.00648 -2.45445 -3.34742
C -1.79716 0.97267 -1.98090
C -1.86215 2.31248 -1.57488
C -1.36714 -1.17411 -2.25812
C -0.72935 -2.50443 -2.03983
N -1.04134 -0.11579 -1.51435
C 1.61482 -2.79989 -1.22350
N 3.23557 -1.40161 -2.67552
C 2.21193 -1.55180 -1.78559
C 4.35907 0.69519 -3.61388
N 0.19489 -2.45146 -0.82921
C 3.44503 -0.02204 -2.83523
N 1.74826 -0.36677 -1.36863
C 4.29166 2.08722 -3.53703
C 2.49639 0.62759 -2.00701
C -0.31927 -3.31975 0.29910
C 3.34676 2.74072 -2.71079
C 2.43627 2.02453 -1.93421
C -1.29259 -2.49340 1.07394
N -1.17848 -1.15985 1.05672
N -2.31300 -2.89589 1.88599
C -2.73800 -4.26909 2.18257
C -2.16986 -0.63992 1.89538
C -2.49953 0.67738 2.23727
C -2.89086 -1.73663 2.42923
C -3.56289 0.85713 3.12191
C -3.95671 -1.55749 3.31720
C -4.27954 -0.24153 3.65249
H -4.08200 0.97683 -4.56977
H -4.19694 3.35802 -3.85076
H -2.81249 4.19238 -1.98193
H -1.24800 2.65889 -0.75562
H -2.51048 -2.75599 -4.08958
H -3.98906 -1.77601 -4.06705
H -2.67390 -1.38856 -5.20850
H -1.48139 -3.28402 -1.88655
H -0.14492 -2.79606 -2.91836
H 1.63395 -3.64528 -1.91694
H 2.15623 -3.09742 -0.32104
H 3.57124 -3.42761 -3.12576
H 3.98173 -2.29401 -4.42718
H 5.04176 -2.44100 -2.99877
H 5.08708 0.20067 -4.24551
H 4.98222 2.68279 -4.12371
H 3.33387 3.82468 -2.68176
H 1.71030 2.50819 -1.29324
H 0.52782 -3.59173 0.93608
H -0.75227 -4.24676 -0.08668
H -2.21990 -4.96568 1.52509
H -2.50564 -4.51871 3.22064
H -3.81304 -4.36178 2.01621
H -4.50755 -2.39449 3.72904
H -5.09923 -0.05666 4.33783
H -3.84890 1.86202 3.41240
H -1.94026 1.50680 1.82387
N 1.55851 -0.86320 1.34855
C 2.31899 -1.02259 2.21701
C 3.26765 -1.20977 3.29995
H 4.21706 -1.58948 2.91129
H 3.44670 -0.25150 3.79842
H 2.87421 -1.92132 4.03167
H 0.77877 1.50640 1.17620
C 1.41619 3.41214 2.72628
C 0.33906 3.54345 3.77547
C 0.94241 3.68737 5.19143
C 2.00901 2.60363 5.46967
C 3.01433 2.51783 4.34814
C 2.68438 2.92886 3.05529
H 1.20146 3.73581 1.71105
H -0.32264 2.65979 3.74989
H 0.15013 3.64225 5.94746
H 2.51683 2.80789 6.42135
H 1.50996 1.62742 5.60288
H 4.01252 2.14579 4.56461
H 3.44299 2.87341 2.27709
H 1.41373 4.67612 5.27546
H -0.30660 4.40253 3.55090

85
Rebound Transition State (2/3)
Fe 0.37891 -0.55141 0.19538
O 0.50522 1.20744 1.02242
C -3.30323 1.82936 -3.17659
C -3.31144 3.08717 -2.57045
C -2.84849 -1.18292 -4.07251
C -2.45957 0.86566 -2.61506
C -2.50598 3.36797 -1.44272
N -2.21897 -0.47148 -2.95564
C 3.97359 -2.51945 -3.39881
C -1.64319 1.14060 -1.49107
C -1.66378 2.40377 -0.88724
C -1.29420 -0.95679 -2.06797
C -0.75027 -2.35076 -2.07269
N -0.92363 -0.02664 -1.18349
C 1.56406 -2.92253 -1.35681
N 3.29161 -1.48736 -2.61088
C 2.25140 -1.64695 -1.73212
C 4.60570 0.59421 -3.30396

N 0.17612 -2.58357 -0.91188
C 3.62989 -0.12692 -2.60739
N 1.89830 -0.48529 -1.17002
C 4.66034 1.96887 -3.06603
C 2.74116 0.49916 -1.69938
C -0.38392 -3.53238 0.09996
C 3.77242 2.60152 -2.16410
C 2.80263 1.87867 -1.46956
C -1.27612 -2.76682 1.02773
N -1.08989 -1.46002 1.24670
N -2.31241 -3.25874 1.77817
C -2.80681 -4.63849 1.83889
C -2.04861 -1.05757 2.18402
C -2.30510 0.19272 2.75814
C -2.82333 -2.19120 2.52992
C -3.34834 0.27100 3.68042
C -3.86957 -2.11712 3.45553
C -4.11794 -0.86590 4.02336
H -3.92322 1.61596 -4.03930
H -3.95129 3.86499 -2.97286
H -2.54644 4.35742 -0.99979
H -1.04588 2.59554 -0.02202
H -2.57496 -2.23669 -4.04206
H -3.93508 -1.10209 -3.99528
H -2.51968 -0.75885 -5.02475
H -1.56992 -3.07781 -2.03896
H -0.20836 -2.53688 -3.00735
H 1.55541 -3.64587 -2.18008
H 2.09012 -3.38959 -0.51847
H 3.40705 -3.44867 -3.36258
H 4.04650 -2.19482 -4.43876
H 4.97622 -2.69880 -3.00231
H 5.28948 0.11611 -3.99519
H 5.40178 2.56629 -3.58509
H 3.85089 3.67240 -2.01128
H 2.11695 2.34260 -0.77351
H 0.44797 -3.96102 0.66795
H -0.90833 -4.36568 -0.38118
H -2.34157 -5.23366 1.05481
H -2.57026 -5.08265 2.80905
H -3.88852 -4.64648 1.68932
H -4.46109 -2.98436 3.72369
H -4.92016 -0.76307 4.74583
H -3.57694 1.22268 4.14767
H -1.70318 1.04873 2.48194
N 1.67754 -1.23133 1.53934
C 2.43483 -1.61229 2.34050
C 3.37766 -2.09002 3.33828
H 4.13607 -2.72397 2.86943
H 3.87800 -1.24501 3.82057
H 2.85676 -2.67265 4.10371
H 1.00235 1.10863 1.86150
C 0.98770 3.53324 1.71636
C -0.16505 3.91607 2.60512
C 0.31580 4.55206 3.92944
C 1.40795 3.69250 4.60000
C 2.48736 3.31436 3.62546
C 2.26512 3.28073 2.26500
H 0.87764 3.63380 0.64544
H -0.75575 3.01701 2.83394
H -0.53356 4.68612 4.60713
H 1.84398 4.21911 5.45749
H 0.95846 2.77243 5.01376
H 3.47215 3.07079 4.01507
H 3.08313 3.04024 1.59301
H 0.72618 5.54884 3.72158
H -0.84202 4.59385 2.07245

85
Rebound Product (2/3)
Fe 0.22543 -0.45525 0.24171
O 0.23185 1.36093 1.70337
C -3.43007 1.93669 -3.16428
C -3.52747 3.15456 -2.48867
C -2.79746 -0.99352 -4.20388
C -2.56907 0.98003 -2.61779
C -2.79370 3.40185 -1.30610
N -2.25569 -0.32466 -3.01667
C 3.97790 -2.34069 -3.26674
C -1.81756 1.22314 -1.44289
C -1.93393 2.44380 -0.76735
C -1.35009 -0.82318 -2.11605
C -0.76470 -2.20274 -2.18079
N -1.05617 0.07396 -1.16707
C 1.50364 -2.78715 -1.34682
N 3.25242 -1.31839 -2.50484
C 2.18590 -1.48985 -1.65931
C 4.55603 0.77038 -3.17811
N 0.08635 -2.50598 -0.99229
C 3.57053 0.04482 -2.50067
N 1.79762 -0.33043 -1.10990
C 4.57827 2.14985 -2.96719
C 2.64109 0.66411 -1.62943
C -0.52072 -3.47627 -0.04388
C 3.64431 2.78088 -2.11351
C 2.66600 2.05129 -1.43804
C -1.44206 -2.75811 0.89781
N -1.29257 -1.46395 1.20791
N -2.50024 -3.31911 1.56761
C -2.96677 -4.70901 1.52187
C -2.31190 -1.14413 2.12020
C -2.64612 0.06157 2.75143
C -3.07143 -2.31528 2.35903
C -3.73547 0.05165 3.62299
C -4.16295 -2.33039 3.23357
C -4.48096 -1.12570 3.86288
H -3.99841 1.74708 -4.06709
H -4.18384 3.92552 -2.87697
H -2.90538 4.35734 -0.80529
H -1.38803 2.62440 0.14761
H -2.54753 -2.05320 -4.17931
H -3.88473 -0.89275 -4.21523
H -2.38216 -0.55079 -5.11299
H -1.56871 -2.94510 -2.26116
H -0.16221 -2.30422 -3.09168
H 1.57972 -3.49084 -2.18484
H 1.98729 -3.25897 -0.48590
H 3.41429 -3.27211 -3.27311
H 4.10425 -2.00293 -4.29730
H 4.95903 -2.52212 -2.82040
H 5.26945 0.29129 -3.83786
H 5.32523 2.75174 -3.47277
H 3.68964 3.85663 -1.98422
H 1.94545 2.53954 -0.79632
H 0.28298 -3.94863 0.53070
H -1.04543 -4.27936 -0.57581
H -2.44790 -5.25121 0.73327
H -2.77348 -5.20375 2.47715
H -4.03861 -4.72842 1.31320
H -4.73802 -3.23002 3.41776
H -5.32005 -1.09129 4.54901
H -4.01980 0.96814 4.12851
H -2.07941 0.96366 2.56109
N 1.50264 -1.14404 1.60006
C 2.25944 -1.55425 2.38795
C 3.20258 -2.06270 3.37012
H 3.95330 -2.69234 2.88330
H 3.71266 -1.23317 3.86895
H 2.68077 -2.65844 4.12481
H 0.33602 0.90513 2.56446
C 0.79207 2.74655 1.82962
C -0.02760 3.55124 2.84541
C 0.68934 4.87312 3.18373
C 2.07433 4.60534 3.80834
C 2.81951 3.50554 3.08859
C 2.25211 2.67891 2.19494
H 0.65193 3.14810 0.82127
H -0.13742 2.95497 3.76288
H 0.07238 5.46744 3.86654
H 2.67750 5.52304 3.80333
H 1.96288 4.33027 4.86945
H 3.87854 3.39820 3.31571
H 2.84307 1.92522 1.68114
H 0.81001 5.46626 2.26652
H -1.03379 3.73615 2.45404

85
Desaturation Transition State (2/3)
Fe -0.07149 -0.04963 0.03189
O -0.11322 -0.09726 2.00123
C 5.44051 -0.10460 0.59459
C 5.47290 -0.21351 1.98617
C 4.71131 0.13077 -2.48086
C 4.17748 -0.04834 -0.00308
C 4.28355 -0.26596 2.74886
N 3.78889 0.04907 -1.34415
C -0.32072 -4.41344 -3.24434
C 2.98076 -0.09281 0.75250
C 3.02569 -0.20772 2.14707
C 2.41748 0.06414 -1.37052
C 1.59359 0.16561 -2.61573
N 1.89787 -0.01268 -0.14131
C -0.44193 -1.26815 -2.81293
N -0.18530 -3.68581 -1.97847
C -0.21518 -2.32818 -1.77703
C 0.06207 -5.62773 -0.33111
N 0.12992 0.02217 -2.32566
C -0.02512 -4.28729 -0.72203
N -0.08118 -2.02257 -0.48330
C 0.21657 -5.87444 1.03479
C 0.04098 -3.22880 0.21667
C -0.64746 1.23243 -2.72957
C 0.27884 -4.82100 1.97765
C 0.19217 -3.48504 1.58519
C -0.44962 2.28631 -1.68216
N -0.19598 1.95740 -0.41107
N -0.53867 3.64663 -1.84376
C -0.81163 4.39657 -3.07405
C -0.11429 3.15248 0.31375
C 0.12629 3.38912 1.67315
C -0.33160 4.22621 -0.58445
C 0.14505 4.71806 2.09729
C -0.31429 5.55996 -0.16212
C -0.07088 5.78582 1.19414
H 6.35242 -0.06693 0.01049
H 6.43108 -0.26070 2.49221
H 4.35321 -0.35460 3.82786
H 2.10751 -0.25294 2.71330
H 4.15185 0.12495 -3.41514
H 5.29603 1.05257 -2.42562
H 5.38687 -0.72781 -2.47149
H 1.77081 1.13493 -3.09661
H 1.90319 -0.59825 -3.33882
H -0.01931 -1.55070 -3.78419
H -1.51901 -1.13556 -2.95892
H -0.35809 -3.70941 -4.07406
H 0.53679 -5.07573 -3.38356
H -1.23969 -5.00494 -3.24201
H 0.01005 -6.43963 -1.04684
H 0.28744 -6.89954 1.38186
H 0.39447 -5.06166 3.02895
H 0.22943 -2.66440 2.29155
H -1.70669 0.96087 -2.77734
H -0.35650 1.58411 -3.72656
H -0.85313 3.71535 -3.92226
H -1.76920 4.91687 -2.99258
H -0.01595 5.12497 -3.24621
H -0.48243 6.38194 -0.84793
H -0.04899 6.80477 1.56494
H 0.32698 4.94148 3.14297
H 0.28147 2.56116 2.35346
N -2.05473 -0.10944 0.03484
C -3.22047 -0.15473 0.04963
C -4.67309 -0.21200 0.06673
H -5.09323 0.65358 -0.45395
H -5.02280 -1.12310 -0.42759
H -5.03930 -0.21103 1.09767
H -1.04529 -0.26954 2.25705
C 0.57996 -0.69299 5.63216
C 0.28412 0.48004 4.81603
C -1.04896 1.16427 5.18660
C -2.18660 0.13923 5.38663
C -1.75063 -1.04897 6.19125
C -0.42415 -1.41497 6.30401
H 1.60472 -1.05299 5.67847
H 0.23685 0.15099 3.71026
H -1.32890 1.88847 4.41532
H -3.05541 0.61321 5.85941
H -2.55550 -0.22773 4.41198
H -2.51741 -1.65631 6.66484
H -0.15158 -2.28943 6.88501
H -0.90855 1.72574 6.11992
H 1.12332 1.18747 4.81477

85
Desaturation Product (2/3)
Fe -0.53167 -0.15046 -0.40929
O -0.81745 -0.32546 1.75151
C 4.98307 -0.17452 0.25492
C 4.99732 -0.44412 1.62427
C 4.30957 0.37298 -2.78660
C 3.72946 -0.08673 -0.35787
C 3.79816 -0.62802 2.34869
N 3.36492 0.14100 -1.68894
C -0.48846 -4.33114 -3.94529
C 2.51938 -0.24675 0.36018
C 2.55048 -0.53547 1.73052
C 1.99511 0.12555 -1.74783
C 1.20738 0.32414 -3.00730
N 1.45095 -0.08857 -0.54300
C -0.71150 -1.23433 -3.36919
N -0.45426 -3.67504 -2.63425
C -0.53058 -2.33130 -2.35898
C -0.27471 -5.70702 -1.09273
N -0.24584 0.06047 -2.80785
C -0.36679 -4.34713 -1.40790
N -0.49247 -2.09921 -1.04273
C -0.20433 -6.03452 0.26280
C -0.38840 -3.34487 -0.40790
C -1.09425 1.23557 -3.14081
C -0.22646 -5.03918 1.26766
C -0.31762 -3.68380 0.94952
C -0.96476 2.24514 -2.03932
N -0.69144 1.88788 -0.77772
N -1.12165 3.60360 -2.15846
C -1.45592 4.37282 -3.36160
C -0.66269 3.06779 -0.01981
C -0.40915 3.28713 1.34038
C -0.93996 4.15529 -0.88434
C -0.44579 4.60403 1.79899
C -0.98329 5.47700 -0.42819
C -0.73040 5.68221 0.92898
H 5.90274 -0.04290 -0.30259
H 5.94749 -0.52119 2.14106
H 3.84956 -0.85120 3.40872
H 1.64199 -0.70397 2.28979
H 3.78292 0.36852 -3.73963
H 4.80659 1.33842 -2.66100
H 5.05861 -0.42180 -2.79885
H 1.34006 1.35298 -3.36265
H 1.59909 -0.32647 -3.79922
H -0.19411 -1.47049 -4.30714
H -1.77665 -1.14650 -3.61010
H -0.40897 -3.58684 -4.73595
H 0.35302 -5.02217 -4.03069
H -1.42451 -4.88184 -4.06997
H -0.26152 -6.47425 -1.85772
H -0.13318 -7.07727 0.55232
H -0.17250 -5.33952 2.30848
H -0.33962 -2.91653 1.71365
H -2.13443 0.90201 -3.21055
H -0.82815 1.66807 -4.11361
H -1.28037 3.76914 -4.25072
H -2.50476 4.68012 -3.33978
H -0.81920 5.25814 -3.41187
H -1.20256 6.30593 -1.09064
H -0.75212 6.69123 1.32563
H -0.25127 4.80965 2.84605
H -0.19395 2.46296 2.00816
N -2.51274 -0.24806 -0.43182
C -3.67716 -0.31910 -0.46584
C -5.12755 -0.40866 -0.51052
H -5.54342 0.44229 -1.05808
H -5.43546 -1.33217 -1.00966
H -5.53816 -0.40547 0.50358
H -1.73099 -0.57333 1.98536
C 0.07607 -0.38280 4.93342
C 0.25013 0.95002 4.76410
C -0.79922 1.92808 5.25461
C -2.22166 1.32209 5.24208
C -2.23485 -0.12100 5.70499
C -1.15544 -0.91281 5.53612
H 0.86385 -1.08479 4.67192
H -0.35158 -0.01204 2.55707
H -0.78265 2.85075 4.66408
H -2.88984 1.93144 5.86087
H -2.63496 1.36739 4.21906
H -3.15598 -0.51764 6.12427
H -1.17713 -1.95910 5.82611
H -0.53199 2.22347 6.28404
H 1.18748 1.34494 4.37897

85
H[1]AT Reactant Complex (2/5)
Fe 0.29845 -0.47364 -0.13264
O 0.50015 1.01837 0.54957
C -3.68581 1.71522 -3.47454
C -3.65598 3.02062 -2.97811
C -3.25122 -1.36561 -4.15618
C -2.79241 0.80655 -2.90064
C -2.76644 3.40281 -1.94762
N -2.55674 -0.55822 -3.14607
C 3.78159 -2.55711 -3.65600
C -1.89831 1.18291 -1.87025
C -1.87530 2.49211 -1.37781
C -1.56454 -0.95484 -2.29695
C -0.95427 -2.31556 -2.22446
N -1.14649 0.05046 -1.52248
C 1.39349 -2.84927 -1.55337
N 3.14891 -1.49683 -2.86027
C 2.11679 -1.61650 -1.98479
C 4.54319 0.52697 -3.57196
N 0.02504 -2.42398 -1.05919
C 3.54288 -0.14512 -2.86441
N 1.81258 -0.43152 -1.42231
C 4.66126 1.89838 -3.33735
C 2.69089 0.52303 -1.95342
C -0.49690 -3.34539 0.02564
C 3.81190 2.57179 -2.42924
C 2.81385 1.89766 -1.72460
C -1.30594 -2.52962 0.97939
N -1.05198 -1.21642 1.12835
N -2.27861 -2.94430 1.83373
C -2.82182 -4.29975 1.99330
C -1.90207 -0.73515 2.13409
C -2.06132 0.54229 2.68213
C -2.68081 -1.82598 2.58792
C -3.01457 0.68524 3.69154
C -3.63624 -1.68595 3.59814
C -3.78909 -0.40887 4.14144
H -4.36867 1.42975 -4.26560
H -4.33174 3.75945 -3.39432
H -2.77849 4.42787 -1.59415
H -1.19009 2.77547 -0.58850
H -2.97478 -2.41343 -4.04643
H -4.33035 -1.27194 -4.01934
H -2.97909 -1.02840 -5.15928
H -1.72262 -3.08696 -2.11857
H -0.41482 -2.52992 -3.15253
H 1.30510 -3.59707 -2.34587
H 1.93096 -3.30858 -0.71934
H 3.20466 -3.47624 -3.57080
H 3.81174 -2.25469 -4.70432
H 4.79688 -2.73769 -3.29597
H 5.19793 0.01690 -4.26783
H 5.42412 2.46058 -3.86391
H 3.94161 3.63751 -2.27800
H 2.16127 2.40588 -1.02602
H 0.36144 -3.76953 0.55452
H -1.05874 -4.17567 -0.40936
H -2.46129 -4.94013 1.19010
H -2.50831 -4.71760 2.95265
H -3.91168 -4.25900 1.94933
H -4.22997 -2.52183 3.94747
H -4.51844 -0.25293 4.92828
H -3.16555 1.65945 4.14284
H -1.46368 1.37840 2.34160
N 1.84488 -1.52569 1.29896
C 2.61639 -1.73613 2.14977
C 3.57628 -1.99477 3.21005
H 4.58900 -2.04884 2.80022
H 3.54055 -1.19213 3.95281
H 3.34677 -2.94199 3.70688
H 1.93747 5.01609 2.20944
C 1.50931 4.06693 2.56169
C 2.40650 3.45290 3.65663
C 1.67618 2.30784 4.38461
C 0.39401 2.82108 5.07267
C -0.39608 3.75327 4.17890
C 0.09546 4.29593 3.05201
H 1.48828 3.40239 1.68264
H 2.67152 4.23066 4.38757
H 2.33671 1.83572 5.12259
H -0.23826 1.97332 5.37224
H 0.65414 3.34171 6.00900
H -1.41469 3.98443 4.48891
H -0.53554 4.94624 2.44721
H 1.40793 1.53298 3.65167
H 3.34592 3.09429 3.21775

85
H[1]AT Transition State (2/5)
Fe 0.92257 -0.26730 0.63306
O 1.08853 1.28131 1.31746
C -3.01781 1.86052 -2.76396
C -2.99595 3.16308 -2.26004
C -2.57780 -1.21191 -3.45647
C -2.13255 0.94867 -2.18226
C -2.12134 3.53846 -1.21462
N -1.89383 -0.41355 -2.43224
C 4.36943 -2.50224 -2.98246
C -1.25306 1.31767 -1.13766
C -1.23833 2.62432 -0.63762
C -0.91269 -0.82027 -1.57348
C -0.32283 -2.19394 -1.51960
N -0.50517 0.18202 -0.78576
C 2.01529 -2.74746 -0.85883
N 3.76274 -1.42290 -2.19385
C 2.74008 -1.51406 -1.29498
C 5.17158 0.57275 -2.95613
N 0.64917 -2.34872 -0.37103
C 4.17471 -0.07919 -2.22416
N 2.46093 -0.32148 -0.74555
C 5.30758 1.94616 -2.74333
C 3.34391 0.61038 -1.30936
C 0.12621 -3.26849 0.69830
C 4.47864 2.64193 -1.83274
C 3.48513 1.98747 -1.10370
C -0.70540 -2.47870 1.65911
N -0.48958 -1.16804 1.84811
N -1.68746 -2.94704 2.48391
C -2.19455 -4.31987 2.59798
C -1.37577 -0.74246 2.84822
C -1.57998 0.51643 3.42435
C -2.13477 -1.86348 3.25931
C -2.55523 0.61171 4.41800
C -3.11326 -1.77223 4.25366
C -3.30930 -0.51328 4.82545
H -3.68857 1.57922 -3.56682
H -3.66565 3.90432 -2.68182
H -2.13832 4.56130 -0.85476
H -0.56433 2.90081 0.16298
H -2.31641 -2.26304 -3.34327
H -3.65817 -1.10591 -3.33964
H -2.28362 -0.87662 -4.45407

H -1.11233 -2.94767 -1.43048
H 0.20325 -2.40197 -2.45796
H 1.94741 -3.49574 -1.65508
H 2.55686 -3.20481 -0.02549
H 3.76162 -3.40232 -2.90743
H 4.42182 -2.20047 -4.03025
H 5.37479 -2.71850 -2.61323
H 5.81117 0.04608 -3.65401
H 6.06847 2.49258 -3.28936
H 4.62116 3.70862 -1.69976
H 2.84573 2.51086 -0.40365
H 0.98117 -3.69387 1.23273
H -0.42880 -4.10376 0.25978
H -1.80769 -4.92789 1.78207
H -1.88214 -4.75852 3.54871
H -3.28482 -4.30954 2.54164
H -3.69271 -2.63105 4.57032
H -4.05767 -0.39576 5.60126
H -2.74037 1.57025 4.89020
H -0.99803 1.37353 3.10958
N 2.42689 -1.26752 2.03101
C 3.18960 -1.57543 2.85873
C 4.13786 -1.95804 3.89099
H 5.14951 -2.00650 3.47783
H 4.12497 -1.22500 4.70307
H 3.87734 -2.93857 4.30013
H 2.13084 4.20622 2.03830
C 1.71284 3.52581 2.79264
C 2.78034 3.02681 3.77982
C 2.12820 2.26024 4.94602
C 1.12253 3.15143 5.70371
C 0.24873 3.95221 4.77110
C 0.51507 4.11105 3.45258
H 1.37387 2.61953 2.16107
H 3.33656 3.89106 4.17381
H 2.89313 1.88590 5.63648
H 0.49346 2.54076 6.36625
H 1.66038 3.84563 6.37135
H -0.62222 4.44043 5.20470
H -0.16407 4.69435 2.83394
H 1.60178 1.38366 4.54317
H 3.50759 2.39249 3.25952

85
H^{1}AT Intermediate (2/5)
Fe 0.29336 -0.14680 -0.00063
O 0.41721 1.51398 0.67227
C -3.69720 1.68362 -3.51404
C -3.71371 3.00460 -3.06012
C -3.17148 -1.39592 -4.08755
C -2.78968 0.81974 -2.89467
C -2.85458 3.44309 -2.02650
N -2.51092 -0.54273 -3.09299
C 3.78055 -2.48559 -3.59030
C -1.92633 1.25130 -1.86097
C -1.94951 2.57638 -1.41129
C -1.52353 -0.89124 -2.21413
C -0.90887 -2.25384 -2.11518
N -1.14851 0.14991 -1.46257
C 1.44383 -2.72588 -1.45523
N 3.14855 -1.39680 -2.83597
C 2.13213 -1.48350 -1.92699
C 4.50361 0.60685 -3.67167
N 0.07073 -2.36436 -0.97740
C 3.52715 -0.04577 -2.91315
N 1.82658 -0.28212 -1.41580
C 4.60734 1.98931 -3.50300
C 2.68447 0.65177 -2.01576
C -0.42299 -3.25107 0.12398
C 3.76741 2.69310 -2.60880
C 2.79429 2.03773 -1.85338
C -1.27264 -2.45126 1.06208
N -1.10006 -1.13049 1.21123
N -2.24107 -2.92698 1.90112
C -2.70130 -4.31170 2.05838
C -2.00169 -0.70485 2.19861
C -2.24779 0.56395 2.73642
C -2.72443 -1.83663 2.64373
C -3.22709 0.65787 3.72654
C -3.70608 -1.74710 3.63527
C -3.94414 -0.47835 4.16815
H -4.35627 1.35246 -4.30756
H -4.40167 3.71056 -3.51209
H -2.90126 4.47812 -1.70606
H -1.28622 2.90033 -0.61911
H -2.82928 -2.42430 -3.98185
H -4.25258 -1.36827 -3.93520
H -2.93631 -1.04634 -5.09575
H -1.69083 -3.01229 -1.99701
H -0.39175 -2.48544 -3.05363
H 1.40577 -3.49606 -2.23337
H 2.00215 -3.14448 -0.61233
H 3.19206 -3.39608 -3.49082
H 3.82987 -2.21396 -4.64653
H 4.78941 -2.66965 -3.21299
H 5.15228 0.07400 -4.35645
H 5.35154 2.53651 -4.07091
H 3.88509 3.76650 -2.50957
H 2.14683 2.56635 -1.16428
H 0.44322 -3.63711 0.67059
H -0.96138 -4.11696 -0.27631
H -2.30893 -4.92839 1.25166
H -2.36054 -4.71618 3.01470
H -3.79203 -4.33763 2.01982
H -4.25680 -2.61443 3.97898
H -4.69679 -0.36175 4.93998
H -3.44531 1.62373 4.16866
H -1.69224 1.42885 2.39499
N 1.82220 -1.08335 1.40738
C 2.59980 -1.41183 2.21299
C 3.56605 -1.82015 3.21824
H 4.58434 -1.68979 2.84071
H 3.44600 -1.21535 4.12196
H 3.41953 -2.87244 3.47887
H 2.42849 3.88143 1.72890
C 1.83513 3.56549 2.58351
C 2.45297 2.63220 3.59489
C 1.37311 1.90761 4.42942
C 0.33421 2.89633 5.00440
C -0.17081 3.85291 3.95551
C 0.57678 4.13593 2.81303
H 0.74765 2.21311 1.27946
H 3.11139 3.20954 4.26775
H 1.84035 1.33676 5.23987
H -0.50412 2.34573 5.45087
H 0.78858 3.46763 5.83308
H -1.12372 4.34936 4.11680
H 0.17798 4.83761 2.08369
H 0.85498 1.18615 3.78301
H 3.10432 1.90248 3.09733

85
H^{2}AT Reactant Complex (2/5)
Fe -0.18809 -0.39683 -0.10802
O -0.30870 1.13674 0.49858
C -3.67512 1.12944 -4.27043
C -3.86706 2.45747 -3.88188
C -2.83989 -1.92475 -4.60414
C -2.83277 0.35740 -3.46581
C -3.24114 2.99233 -2.73238
N -2.42232 -0.98485 -3.55670
C 3.99317 -2.06879 -3.04080
C -2.20319 0.88628 -2.31416
C -2.40088 2.21726 -1.93141
C -1.59117 -1.22440 -2.50102
C -0.91251 -2.51752 -2.18725
N -1.43490 -0.13792 -1.73959
C 1.41241 -2.63655 -1.24917
N 3.12499 -1.08685 -2.37745
C 2.00952 -1.32507 -1.63846
C 4.33074 1.08896 -2.97468
N -0.05170 -2.40638 -0.93153
C 3.33840 0.30470 -2.38048
N 1.48204 -0.17994 -1.16677
C 4.24040 2.46816 -2.77606
C 2.29278 0.87195 -1.61451
C -0.54704 -3.34212 0.15402
C 3.19756 3.04108 -2.01188
C 2.20743 2.25490 -1.42101
C -1.60683 -2.62502 0.92355
N -1.58875 -1.28094 0.99404
N -2.61399 -3.14434 1.67434
C -2.95613 -4.55906 1.87262
C -2.63886 -0.88929 1.83531
C -3.07451 0.37491 2.24658
C -3.29223 -2.06539 2.27289
C -4.17277 0.41912 3.10618
C -4.39292 -2.02490 3.13296
C -4.82094 -0.76002 3.54131
H -4.15836 0.72534 -5.15177
H -4.51269 3.09381 -4.47684
H -3.41982 4.02895 -2.46907
H -1.91774 2.61830 -1.04901
H -2.32124 -2.87404 -4.47761
H -3.91687 -2.09776 -4.54300
H -2.59025 -1.51580 -5.58549
H -1.65219 -3.31001 -2.03883
H -0.27737 -2.82808 -3.02224
H 1.52793 -3.40466 -2.01796
H 1.90526 -2.99844 -0.34242
H 3.50397 -3.04125 -3.06160
H 4.17980 -1.74779 -4.06700
H 4.94107 -2.15405 -2.50452
H 5.13342 0.65527 -3.55850
H 4.98955 3.11568 -3.21747
H 3.16891 4.11717 -1.88284
H 1.40705 2.68521 -0.83268
H 0.29132 -3.56556 0.81996
H -0.89086 -4.28666 -0.27531
H -2.36854 -5.17984 1.19872
H -2.74620 -4.85227 2.90373
H -4.01552 -4.70866 1.65663
H -4.89250 -2.92480 3.47032
H -5.67114 -0.68003 4.20921
H -4.53972 1.37956 3.45031
H -2.57207 1.27293 1.91001
N 1.27498 -1.13515 1.58078
C 1.97659 -1.11211 2.51411
C 2.85132 -1.05907 3.67282
H 3.73681 -1.68071 3.51074
H 3.17132 -0.02459 3.84179
H 2.32703 -1.41852 4.56306
H 1.27938 2.75042 2.07693
C 1.92163 3.40553 2.68248
C 1.24505 3.70945 4.03532
C 2.24719 4.33345 5.02564
C 3.42387 3.37340 5.29925
C 3.94496 2.73737 4.02758
C 3.28244 2.76657 2.85787
H 2.02787 4.33613 2.10055
H 0.85296 2.77499 4.46322
H 1.74786 4.59503 5.96670
H 4.23958 3.91065 5.80339
H 3.10899 2.58697 6.00436
H 4.91789 2.25038 4.08422
H 3.73121 2.31906 1.97160
H 2.63541 5.27008 4.59962
H 0.38635 4.37552 3.88561

85
H^{2}AT Transition State (2/5)
Fe 0.69648 -0.18255 0.71291
O 0.75455 1.39512 1.37210
C -2.87822 1.74452 -3.16629
C -2.92093 3.06772 -2.72064
C -2.36690 -1.35393 -3.65403
C -2.06997 0.86513 -2.44055
C -2.18362 3.49349 -1.59194
N -1.79731 -0.50391 -2.60182
C 4.37610 -2.33019 -2.74280
C -1.32957 1.28404 -1.31068
C -1.37788 2.61114 -0.87026
C -0.93600 -0.86937 -1.60673
C -0.39852 -2.25050 -1.39533
N -0.63302 0.16844 -0.81748
C 1.96856 -2.64811 -0.69190
N 3.69713 -1.26732 -1.99202
C 2.64941 -1.38879 -1.12468
C 5.04321 0.77587 -2.74132
N 0.57383 -2.31481 -0.23994
C 4.05148 0.09216 -2.03152
N 2.30195 -0.20224 -0.60463
C 5.11206 2.15722 -2.54812
C 3.16100 0.75847 -1.15659
C 0.08773 -3.22780 0.85109
C 4.22208 2.83023 -1.67904
C 3.23369 2.14399 -0.97243
C -0.84804 -2.46370 1.73368
N -0.73998 -1.13264 1.86704
N -1.84055 -2.96590 2.52537
C -2.25594 -4.36554 2.67761
C -1.71429 -0.72933 2.79102
C -2.04976 0.53743 3.28201
C -2.41188 -1.88404 3.21704
C -3.08992 0.60661 4.20967
C -3.45423 -1.81961 4.14655
C -3.77992 -0.55252 4.63496
H -3.44632 1.42283 -4.03084
H -3.53519 3.78537 -3.25307
H -2.24745 4.53049 -1.28119
H -0.80958 2.92535 -0.00404
H -1.94637 -2.35634 -3.59022
H -3.45127 -1.41612 -3.53659
H -2.12950 -0.93460 -4.63414
H -1.22642 -2.94261 -1.20571
H 0.09900 -2.60377 -2.30494
H 1.95790 -3.40787 -1.48024
H 2.51091 -3.07045 0.15949
H 3.80716 -3.25568 -2.67204
H 4.44856 -2.04256 -3.79345
H 5.37789 -2.49538 -2.33901
H 5.72837 0.26685 -3.40841
H 5.86667 2.72796 -3.07777
H 4.31194 3.90445 -1.56139
H 2.54527 2.65084 -0.30774
H 0.95235 -3.55096 1.43864
H -0.37673 -4.12739 0.43428
H -1.75572 -4.98416 1.93469
H -1.99618 -4.72754 3.67526
H -3.33502 -4.44271 2.53051
H -3.98655 -2.70391 4.47545
H -4.58222 -0.45479 5.35779
H -3.37826 1.57003 4.61529
H -1.51648 1.41876 2.94826
N 2.18735 -1.05856 2.19512
C 2.97276 -1.20947 3.04482
C 3.95238 -1.37848 4.10410
H 4.86094 -1.84403 3.71128
H 4.21191 -0.40302 4.52738
H 3.54827 -2.01060 4.90003
H 1.23619 2.59148 2.21367
C 1.63672 3.45757 2.88510
C 0.65546 3.64215 4.05513
C 1.34433 4.28918 5.27540
C 2.54340 3.43667 5.73932
C 3.42776 3.04557 4.58095
C 3.01933 3.09884 3.29089
H 1.62893 4.30146 2.17825
H 0.26413 2.66052 4.35862
H 0.62431 4.41018 6.09331
H 3.13587 3.98117 6.48641
H 2.18049 2.53002 6.25192
H 4.45345 2.75999 4.80690
H 3.72747 2.87805 2.49431
H 1.69867 5.29375 5.00559
H -0.20475 4.24044 3.73427

85
H^{2}AT Intermediate (2/5)
Fe 0.14905 -0.17553 0.04907
O 0.16614 1.50985 0.68664
C -3.46224 1.45983 -3.92957
C -3.54166 2.79596 -3.52951
C -2.85977 -1.63392 -4.31561
C -2.62990 0.62880 -3.17468
C -2.81640 3.28043 -2.41679
N -2.31778 -0.73609 -3.28937
C 3.90351 -2.43871 -3.31545
C -1.90231 1.10622 -2.06031
C -1.98669 2.44602 -1.66556
C -1.44649 -1.04391 -2.28205
C -0.86845 -2.40486 -2.03723
N -1.17412 0.02762 -1.52892
C 1.48641 -2.73697 -1.28063
N 3.19775 -1.36388 -2.60770
C 2.14478 -1.47541 -1.74397
C 4.51225 0.67688 -3.41758
N 0.07944 -2.42983 -0.86770
C 3.52754 -0.00054 -2.69208
N 1.77061 -0.27868 -1.26925
C 4.55445 2.06508 -3.27118
C 2.61783 0.67830 -1.84749
C -0.41274 -3.30374 0.24478
C 3.64616 2.75054 -2.43127
C 2.66501 2.07040 -1.70885
C -1.36341 -2.52045 1.09602
N -1.27751 -1.18576 1.19145
N -2.35284 -3.01569 1.89786
C -2.74600 -4.41650 2.09073
C -2.26194 -0.77194 2.10111
C -2.61557 0.50296 2.55783
C -2.94413 -1.92433 2.55663
C -3.66001 0.58268 3.47991
C -3.99037 -1.84937 3.48095
C -4.33559 -0.57409 3.93375
H -4.02108 1.09288 -4.78206
H -4.17553 3.47757 -4.08589
H -2.90862 4.32554 -2.14221
H -1.42513 2.80287 -0.81116
H -2.41002 -2.62100 -4.22164
H -3.94215 -1.72481 -4.19783
H -2.63326 -1.23766 -5.30791
H -1.67893 -3.12127 -1.86013
H -0.34310 -2.75092 -2.93464
H 1.51598 -3.52116 -2.04503
H 2.02498 -3.11743 -0.40722
H 3.34195 -3.36787 -3.23438
H 3.99622 -2.17693 -4.37123
H 4.89802 -2.58379 -2.88647
H 5.21214 0.15798 -4.06138
H 5.30262 2.63137 -3.81459
H 3.71607 3.82952 -2.34879
H 1.96392 2.58628 -1.06435
H 0.44591 -3.60507 0.85286
H -0.87054 -4.22032 -0.14280
H -2.24170 -5.04818 1.36167
H -2.47537 -4.74774 3.09630
H -3.82474 -4.51328 1.95284
H -4.51086 -2.73178 3.83309
H -5.14158 -0.46824 4.65135
H -3.96247 1.55248 3.85927
H -2.09138 1.38182 2.20230
N 1.62495 -0.99585 1.56791
C 2.38962 -1.24125 2.41429
C 3.34061 -1.54373 3.46993
H 4.27124 -1.92892 3.04311
H 3.56503 -0.63841 4.04179
H 2.92690 -2.29484 4.14916
H 0.56299 2.18763 1.27620
C 1.11378 3.96188 2.48878
C 0.21524 3.96387 3.70300
C 1.03015 3.84495 5.01104
C 2.05122 2.68660 4.94191
C 2.87458 2.75191 3.68111
C 2.38856 3.38883 2.53842
H 0.78404 4.48101 1.59179
H -0.50169 3.12642 3.64494
H 0.35698 3.70714 5.86472
H 2.70423 2.70252 5.82409
H 1.51332 1.72292 4.98702
H 3.86031 2.29484 3.67150
H 3.02059 3.43714 1.65414
H 1.57363 4.78522 5.17562
H -0.39590 4.87534 3.71822

85
Rebound Transition State (2/5)
Fe 0.20338 -0.26956 0.20668
O 0.24535 1.44975 0.97888
C -3.75271 1.63434 -3.36557
C -3.81935 2.93139 -2.85050
C -3.12914 -1.40517 -4.05387
C -2.84382 0.76384 -2.75647
C -3.00712 3.34171 -1.76799
N -2.52008 -0.57876 -3.00630
C 3.78328 -2.19530 -3.55914
C -2.02843 1.16703 -1.67315
C -2.10112 2.46856 -1.16338
C -1.55390 -0.94107 -2.10268
C -0.92812 -2.30311 -2.03735
N -1.23548 0.07146 -1.29222
C 1.46395 -2.68533 -1.44970
N 3.10893 -1.19143 -2.72841
C 2.10009 -1.38146 -1.82174
C 4.37407 0.91992 -3.42874
N 0.08306 -2.43399 -0.93367
C 3.43150 0.17494 -2.71301
N 1.75346 -0.23428 -1.22390
C 4.41912 2.29100 -3.16599
C 2.56713 0.77171 -1.76533
C -0.33890 -3.40988 0.11729
C 3.55420 2.89498 -2.22358
C 2.61629 2.14722 -1.51031
C -1.26329 -2.73417 1.08199
N -1.19442 -1.41796 1.32328
N -2.22269 -3.33849 1.84963
C -2.58897 -4.75864 1.89232
C -2.16593 -1.13115 2.29491
C -2.54157 0.07712 2.89425
C -2.81480 -2.34091 2.63894
C -3.56290 0.03305 3.84376
C -3.83850 -2.39138 3.59025
C -4.19963 -1.18199 4.18756
H -4.37703 1.32583 -4.19572
H -4.51068 3.64077 -3.29226
H -3.09218 4.35910 -1.40165
H -1.46823 2.76655 -0.33619
H -2.70654 -2.40855 -4.03017
H -4.20775 -1.47413 -3.89332
H -2.93559 -0.96556 -5.03537
H -1.70946 -3.06029 -1.90149
H -0.44488 -2.52811 -2.99562
H 1.45272 -3.38740 -2.29127
H 2.05055 -3.15073 -0.65099
H 3.27065 -3.15217 -3.47768
H 3.76739 -1.87604 -4.60337
H 4.81866 -2.31921 -3.23217
H 5.03945 0.46392 -4.15201
H 5.13486 2.90782 -3.69822
H 3.62454 3.96384 -2.05354
H 1.94831 2.59463 -0.78447
H 0.55424 -3.74329 0.65491
H -0.79849 -4.30049 -0.32641
H -2.31884 -5.18701 2.86062
H -3.66455 -4.86378 1.73517
H -2.06535 -5.30243 1.10812
H -4.33200 -3.31876 3.85534
H -4.98891 -1.17371 4.93108
H -3.87862 0.95000 4.32904
H -2.05951 1.00770 2.62154
N 1.76541 -1.18240 1.61643
C 2.57034 -1.57311 2.36627
C 3.57392 -2.05772 3.29964
H 4.44149 -2.44352 2.75636
H 3.90359 -1.24580 3.95460

H 3.16112 -2.86052 3.91739
H 0.07681 1.79441 1.87471
C 2.20650 2.54336 2.62381
C 2.17136 3.93797 2.06736
C 2.02831 5.00026 3.17908
C 0.89023 4.64434 4.16030
C 0.97255 3.21505 4.61435
C 1.63037 2.24711 3.86840
H 2.73120 1.77134 2.07428
H 1.31931 4.01463 1.37031
H 1.85204 5.98599 2.73619
H 0.90303 5.31587 5.02768
H -0.08809 4.80974 3.67457
H 0.49639 2.94040 5.55157
H 1.68645 1.23084 4.24735
H 2.97163 5.06040 3.73775
H 3.06713 4.12631 1.46354

85
Rebound Product (2/5)
Fe 0.21206 -0.20985 0.18754
O 0.15421 1.70177 1.15914
C -3.22979 1.78671 -3.93573
C -3.13946 3.14418 -3.62078
C -3.03060 -1.36984 -4.12888
C -2.52519 0.90156 -3.11380
C -2.36827 3.59874 -2.52672
N -2.37798 -0.49155 -3.15222
C 3.50757 -2.17559 -3.81395
C -1.76276 1.34357 -2.00625
C -1.67009 2.70913 -1.70917
C -1.56844 -0.84487 -2.09983
C -1.19294 -2.25636 -1.76110
N -1.18966 0.22084 -1.38420
C 1.28519 -2.59203 -1.63728
N 2.95827 -1.15490 -2.91530
C 1.98576 -1.30604 -1.95867
C 4.34524 0.88034 -3.60421
N 0.02048 -2.33872 -0.88328
C 3.38680 0.17925 -2.86559
N 1.76053 -0.16570 -1.29691
C 4.50770 2.23331 -3.29799
C 2.61950 0.79753 -1.84976
C -0.18596 -3.29716 0.24560
C 3.73827 2.86230 -2.29215
C 2.78512 2.15632 -1.55702
C -1.10997 -2.67434 1.24472
N -1.15801 -1.34767 1.43591
N -1.96967 -3.34311 2.07697
C -2.19055 -4.78964 2.18307
C -2.10514 -1.12660 2.45102
C -2.56936 0.05573 3.04231
C -2.61563 -2.38113 2.86500
C -3.53488 -0.05661 4.04304
C -3.58161 -2.50097 3.86940
C -4.03322 -1.31524 4.45102
H -3.81848 1.44415 -4.77839
H -3.66956 3.86644 -4.23180
H -2.31683 4.66247 -2.32194
H -1.06409 3.06411 -0.88492
H -2.59018 -2.36481 -4.09110
H -4.10048 -1.44642 -3.91725
H -2.88789 -0.96495 -5.13281
H -2.03212 -2.72411 -1.23341
H -1.03497 -2.84376 -2.67311
H 1.08479 -3.16639 -2.54956
H 1.94382 -3.21073 -1.01780
H 2.88441 -3.06820 -3.78955
H 3.52451 -1.79038 -4.83556
H 4.52302 -2.44271 -3.50968
H 4.93680 0.40486 -4.37754
H 5.24005 2.81582 -3.84609
H 3.89352 3.91652 -2.09040
H 2.18693 2.63662 -0.79267
H 0.78506 -3.47882 0.71626
H -0.56448 -4.26353 -0.10901
H -1.73380 -5.17811 3.09691
H -3.26352 -4.99070 2.19899
H -1.75511 -5.29803 1.32446
H -3.96444 -3.46370 4.18657
H -4.78238 -1.36024 5.23372
H -3.91166 0.84083 4.52120
H -2.18575 1.02174 2.74206
N 1.83823 -0.87147 1.63776
C 2.69283 -1.25087 2.33725
C 3.75827 -1.71970 3.20855
H 4.66735 -1.90524 2.62894
H 3.97821 -0.97021 3.97456
H 3.46244 -2.64927 3.70362
H -0.69848 2.17914 1.14650
C 1.08842 2.31502 2.17091
C 1.15222 3.83207 1.96444
C 1.86983 4.49956 3.15502
C 1.11306 4.23739 4.47305
C 0.65360 2.80261 4.58668
C 0.65040 1.93662 3.56004
H 2.03877 1.84168 1.91028
H 0.12858 4.22883 1.89669
H 1.96212 5.57616 2.97571
H 1.74869 4.48979 5.33212
H 0.23873 4.90385 4.54528
H 0.31888 2.46802 5.56671
H 0.34208 0.90464 3.70133
H 2.89063 4.10069 3.23353
H 1.65663 4.06529 1.02111

85
Desaturation Transition State (2/5)
Fe 0.40351 -0.40340 0.16143
O 0.64829 1.25052 1.04854
C -3.59566 1.86750 -3.14093
C -3.55777 3.14572 -2.57832
C -3.19268 -1.17084 -3.96882
C -2.71478 0.92169 -2.60784
C -2.67152 3.46472 -1.52367
N -2.48780 -0.42703 -2.91958
C 3.70198 -2.51251 -3.77740
C -1.82576 1.23275 -1.55289
C -1.79371 2.51620 -0.99562
C -1.50338 -0.88189 -2.07861
C -0.96510 -2.28286 -2.10282
N -1.08405 0.07840 -1.24943
C 1.40397 -2.88227 -1.62590
N 3.13929 -1.48522 -2.89407
C 2.13647 -1.62171 -1.96975
C 4.57922 0.53253 -3.53509
N 0.06911 -2.54234 -1.04758
C 3.58648 -0.15574 -2.83034
N 1.90705 -0.47438 -1.32022
C 4.75943 1.87901 -3.20985
C 2.80143 0.47426 -1.83605
C -0.39507 -3.51430 -0.01235
C 3.97912 2.51415 -2.21531
C 2.98983 1.82354 -1.51417
C -1.19300 -2.79468 1.03151
N -0.98021 -1.50411 1.31425
N -2.14764 -3.33817 1.85090
C -2.63860 -4.72023 1.87641
C -1.83430 -1.17007 2.37466
C -2.01926 0.03886 3.05590
C -2.57485 -2.32417 2.72305
C -2.96018 0.05304 4.08626
C -3.51827 -2.31481 3.75546
C -3.69770 -1.10453 4.42931
H -4.27588 1.62856 -3.94983
H -4.22378 3.91172 -2.96039
H -2.67589 4.47074 -1.11812
H -1.10874 2.74729 -0.18951
H -2.86729 -2.20995 -3.97210
H -4.26901 -1.14096 -3.78384
H -2.98028 -0.73172 -4.94680
H -1.79052 -2.99450 -1.98144
H -0.52865 -2.48436 -3.08835
H 1.30723 -3.54408 -2.49462
H 1.97745 -3.42796 -0.86961
H 3.08631 -3.40980 -3.74371
H 3.72259 -2.13993 -4.80365
H 4.71720 -2.76648 -3.46203
H 5.18422 0.05249 -4.29501
H 5.51867 2.45130 -3.73157
H 4.15776 3.56087 -1.99440
H 2.38694 2.29097 -0.74452
H 0.48627 -3.95662 0.46344
H -0.96389 -4.33718 -0.46099
H -2.29185 -5.25531 0.99399
H -2.27562 -5.23471 2.76984
H -3.73056 -4.71804 1.87714
H -4.08363 -3.19857 4.02620
H -4.41912 -1.05149 5.23731
H -3.13113 0.97005 4.63961
H -1.44165 0.91455 2.78346
N 2.00148 -1.41503 1.51696
C 2.82232 -1.84227 2.22899
C 3.84542 -2.37150 3.11651
H 4.68546 -2.76389 2.53598
H 4.21584 -1.58334 3.77869
H 3.43536 -3.17922 3.72969
H 1.32697 1.40270 1.73523
C 2.11374 4.10210 2.57096
C 0.77638 4.30110 1.95367
C -0.26876 4.82234 2.96331
C -0.22035 4.04038 4.29390
C 1.17944 3.86490 4.79683
C 2.27675 3.91363 3.94698
H 2.98575 4.07112 1.92289
H 0.45530 3.31815 1.53282
H -1.27262 4.76544 2.53077
H -0.83654 4.53122 5.05702
H -0.66607 3.03723 4.16214
H 1.32759 3.65820 5.85324
H 3.27387 3.77080 4.35065
H -0.06532 5.88157 3.16896
H 0.85371 4.96729 1.08483

85
Desaturation Product (2/5)
Fe 0.42713 -0.42827 0.12464
O 0.86163 1.28692 1.28709
C -4.03627 1.87015 -2.64635
C -4.16782 3.02183 -1.86793
C -3.22927 -0.87308 -4.00762
C -2.99318 1.00059 -2.31200
C -3.29030 3.29024 -0.79230
N -2.59286 -0.22769 -2.85458
C 3.89269 -2.67518 -3.56115
C -2.09926 1.26621 -1.24717
C -2.24980 2.41903 -0.46691
C -1.50051 -0.65227 -2.13791
C -0.72853 -1.90318 -2.42558
N -1.16764 0.21671 -1.17503
C 1.40252 -2.84809 -1.60728
N 3.32971 -1.59706 -2.74083
C 2.24973 -1.64744 -1.89806
C 4.93523 0.30737 -3.31494
N 0.03240 -2.38712 -1.22984
C 3.84811 -0.29587 -2.67425
N 2.03168 -0.46831 -1.29864
C 5.17138 1.65107 -3.01834
C 3.02244 0.40928 -1.76591
C -0.72142 -3.37944 -0.40716
C 4.35214 2.36428 -2.11248
C 3.26976 1.75676 -1.47564
C -1.38058 -2.72243 0.77043
N -1.01150 -1.52838 1.24492
N -2.38180 -3.28006 1.52609
C -3.03364 -4.58104 1.34233
C -1.80936 -1.27505 2.37185
C -1.84795 -0.17797 3.24076
C -2.67504 -2.37858 2.55980
C -2.76677 -0.22248 4.29032
C -3.59760 -2.42873 3.60963
C -3.62731 -1.32995 4.47158
H -4.71307 1.66681 -3.46773
H -4.96284 3.72481 -2.09117
H -3.43217 4.19260 -0.20756
H -1.58720 2.62279 0.36464
H -2.91218 -1.91233 -4.07814
H -4.31342 -0.84941 -3.88130
H -2.96060 -0.35506 -4.93217
H -1.38832 -2.69479 -2.79944
H -0.00953 -1.69223 -3.22531
H 1.37710 -3.54184 -2.45670
H 1.82433 -3.38969 -0.75497
H 3.22071 -3.53165 -3.56312
H 4.01613 -2.32489 -4.58806
H 4.86229 -2.98525 -3.16344
H 5.56860 -0.23528 -4.00654
H 6.00372 2.15965 -3.49218
H 4.57331 3.40636 -1.90928
H 2.64521 2.29928 -0.77716
H -0.02168 -4.13935 -0.04106
H -1.46064 -3.90697 -1.02154
H -2.70165 -5.03437 0.40979
H -2.78191 -5.24983 2.16935
H -4.11686 -4.44696 1.30073
H -4.25874 -3.27488 3.75450
H -4.32697 -1.32627 5.30021
H -2.82383 0.60917 4.98412
H -1.18650 0.66805 3.09676
N 1.98229 -1.34714 1.59787
C 2.72801 -1.88217 2.32041
C 3.65436 -2.55106 3.22006
H 4.57849 -2.80557 2.69296
H 3.90090 -1.89928 4.06342
H 3.20736 -3.47101 3.60838
H 1.44546 1.13619 2.05264
C 1.64834 4.45141 1.58000
C 0.33154 4.67597 1.35416
C -0.60529 4.96896 2.50967
C -0.14454 4.29780 3.82415
C 1.35707 4.37266 4.01177
C 2.18618 4.42540 2.94815
H 2.34105 4.33331 0.75069
H 0.71375 2.24962 1.16022
H -1.62974 4.66080 2.27253
H -0.66284 4.75322 4.67530
H -0.44556 3.23510 3.82285
H 1.75183 4.32472 5.02337
H 3.26434 4.43420 3.07755
H -0.64270 6.06361 2.64673
H -0.05270 4.76036 0.34047

85
OAT Reactant Complex (2/3)
Fe -0.24407 -0.26348 -0.63232
O -0.31065 -0.41429 1.01426
C 5.18184 -0.13102 0.15719
C 5.17026 -0.25376 1.54745
C 4.55058 0.12421 -2.94608
C 3.93924 -0.11545 -0.48290
C 3.95941 -0.35606 2.27023
N 3.59504 -0.00687 -1.83954
C -0.49238 -4.45174 -3.96041
C 2.72244 -0.21767 0.23417
C 2.72035 -0.33994 1.62891
C 2.23488 -0.04244 -1.91635
C 1.39841 0.05110 -3.14624
N 1.68239 -0.16735 -0.70691
C -0.69139 -1.30850 -3.36939
N -0.30975 -3.76455 -2.67588
C -0.38177 -2.42635 -2.42577
C 0.14286 -5.75100 -1.13203
N -0.07530 -0.05952 -2.78180
C -0.03345 -4.40191 -1.45518
N -0.17055 -2.16134 -1.12817
C 0.41454 -6.04495 0.20495
C 0.05656 -3.37958 -0.47878
C -0.82237 1.20362 -3.14421
C 0.50463 -5.02824 1.18476
C 0.32789 -3.68326 0.86067
C -0.62601 2.15958 -2.01104
N -0.36727 1.68918 -0.78191
N -0.71265 3.52015 -2.01198
C -0.99255 4.40431 -3.15028
C -0.27400 2.78677 0.08049
C -0.02373 2.87094 1.45556
C -0.49563 3.95214 -0.69339
C -0.00148 4.14606 2.02119
C -0.47398 5.23114 -0.12815
C -0.22217 5.30663 1.24239
H 6.11056 -0.05074 -0.39455
H 6.11147 -0.26999 2.08548
H 3.99622 -0.44874 3.34998
H 1.79069 -0.41681 2.17692
H 4.01686 0.13648 -3.89546
H 5.11421 1.05431 -2.84363
H 5.23907 -0.72345 -2.94004
H 1.57171 1.00245 -3.65852
H 1.65475 -0.74104 -3.85615
H -0.32282 -1.48906 -4.38274
H -1.77342 -1.16241 -3.43239
H -0.66785 -3.72126 -4.74844
H 0.40435 -5.02648 -4.20164
H -1.35265 -5.12224 -3.90265
H 0.07251 -6.53310 -1.87815
H 0.55885 -7.07810 0.50052
H 0.71548 -5.30403 2.21201
H 0.39116 -2.90042 1.60556
H -1.88320 0.95934 -3.24887
H -0.48039 1.60107 -4.10401
H -1.08112 3.81556 -4.06189
H -1.92994 4.93929 -2.98236
H -0.17754 5.12143 -3.26846
H -0.64477 6.12210 -0.72000
H -0.19613 6.27829 1.72270
H 0.18927 4.25255 3.08323
H 0.13983 1.97860 2.04601
N -2.24422 -0.35364 -0.78025
C -3.40333 -0.43012 -0.70028
C -4.84874 -0.52627 -0.60452
H -5.13031 -0.99693 0.34220
H -5.29765 0.47016 -0.65017
H -5.24268 -1.12982 -1.42749
H -1.00729 -0.65485 5.65951
C -1.92064 -0.04580 5.71584
C -1.55589 1.45223 5.77278
C -2.79493 2.33110 5.51398
C -3.38788 2.04991 4.11758
C -3.46485 0.56677 3.82269
C -2.82270 -0.36779 4.54352
H -2.41687 -0.34546 6.65363
H -0.79615 1.67022 5.00765
H -2.54039 3.39401 5.60856
H -4.38952 2.49551 4.03617
H -2.77820 2.54896 3.34655
H -4.08971 0.26454 2.98284
H -2.94583 -1.42101 4.29352
H -3.55367 2.11526 6.28028
H -1.10733 1.69430 6.74418

85
OAT Transition State 1 (2/3)
Fe -0.03517 -0.00468 0.05305
O -0.02058 -0.00795 1.81946
C 5.44254 0.04546 0.78370
C 5.45231 0.01537 2.17930
C 4.76327 0.09491 -2.31750
C 4.18943 0.04606 0.16324
C 4.25139 -0.01330 2.92530
N 3.82480 0.06987 -1.19051
C -0.46721 -4.34111 -3.09390
C 2.98119 0.01798 0.90270
C 3.00217 -0.01282 2.30329
C 2.45822 0.05671 -1.23999
C 1.62066 0.06513 -2.47643
N 1.92097 0.02638 -0.01880
C -0.54353 -1.17911 -2.63229
N -0.23298 -3.61174 -1.84240
C -0.27547 -2.26175 -1.63746
C 0.26858 -5.54455 -0.24776
N 0.14547 0.06165 -2.12107
C 0.08448 -4.20686 -0.61238
N -0.02110 -1.94859 -0.35928
C 0.62002 -5.79031 1.08059
C 0.23143 -3.14802 0.31730
C -0.53363 1.33454 -2.56131
C 0.78828 -4.73659 2.00948
C 0.59968 -3.40396 1.64308
C -0.27465 2.35395 -1.49969
N -0.04267 1.96102 -0.24049
N -0.23892 3.71501 -1.61617
C -0.45936 4.52161 -2.82171
C 0.17981 3.11535 0.51977
C 0.50160 3.28735 1.87168
C 0.04549 4.23109 -0.34305
C 0.66455 4.59524 2.32834
C 0.20473 5.54387 0.11289
C 0.51487 5.70549 1.46425
H 6.36362 0.06689 0.21349
H 6.40229 0.01371 2.70251
H 4.30495 -0.03646 4.00844
H 2.07388 -0.03427 2.85773
H 4.21258 0.11103 -3.25706
H 5.38960 0.98825 -2.26084
H 5.39603 -0.79550 -2.29538
H 1.84293 0.94575 -3.08806
H 1.84279 -0.81038 -3.09535
H -0.19943 -1.43591 -3.63891
H -1.61658 -0.97823 -2.69332
H -0.69445 -3.63835 -3.89388
H 0.42383 -4.91264 -3.36338
H -1.31404 -5.02054 -2.97352
H 0.15132 -6.35376 -0.95849
H 0.77491 -6.81285 1.40653
H 1.07448 -4.97311 3.02843
H 0.73903 -2.58883 2.33998
H -1.60692 1.14237 -2.64421
H -0.18010 1.65031 -3.54768
H -0.62450 3.86842 -3.67704
H -1.33812 5.15702 -2.68931
H 0.41628 5.14525 -3.01493
H 0.09752 6.39685 -0.54648
H 0.64832 6.70602 1.86045
H 0.91273 4.76804 3.36980
H 0.61691 2.42787 2.51858
N -2.03437 -0.02567 -0.11724
C -3.19670 -0.02091 -0.20402
C -4.64543 -0.01898 -0.31641
H -5.08707 -0.61578 0.48714
H -5.02927 1.00294 -0.24797
H -4.94986 -0.44582 -1.27667
H 0.50843 -0.38045 5.52281
C -0.56400 -0.25171 5.30816
C -0.93160 1.24351 5.23709
C -2.30073 1.42620 4.55871
C -2.27198 0.91473 3.10106
C -1.55832 -0.42588 2.95609
C -0.92420 -1.00418 4.06226
H -1.08084 -0.72338 6.16189
H -0.16740 1.78654 4.66506
H -2.60015 2.48093 4.56951
H -3.29902 0.81211 2.72702
H -1.78260 1.65570 2.46084
H -1.96058 -1.11091 2.21765
H -0.63374 -2.05028 4.01283
H -3.06049 0.87395 5.13048
H -0.93791 1.67365 6.24531

85
OAT Intermediate (2/3)
Fe -0.40246 0.04688 -0.29914
O -0.32083 0.15134 1.51061
C 5.10928 0.14135 0.15552
C 5.19698 0.22033 1.54621
C 4.26628 -0.02845 -2.89659

C 3.82383 0.08586 -0.39173
C 4.03910 0.24436 2.35711
N 3.38797 0.01217 -1.72232
C -1.13596 -4.40811 -3.19428
C 2.65725 0.10430 0.41269
C 2.75794 0.18750 1.80744
C 2.02250 -0.01252 -1.69638
C 1.11684 -0.08860 -2.87831
N 1.54913 0.03610 -0.44929
C -1.10414 -1.22993 -2.86003
N -0.81600 -3.63469 -1.98871
C -0.81121 -2.27910 -1.83974
C -0.29905 -5.51664 -0.34430
N -0.33669 0.00111 -2.43574
C -0.45564 -4.18793 -0.75120
N -0.47975 -1.91840 -0.59073
C 0.09777 -5.72512 0.97706
C -0.23336 -3.09815 0.12731
C -0.98345 1.28005 -2.92033
C 0.32915 -4.64334 1.85809
C 0.17005 -3.31895 1.44994
C -0.62950 2.34069 -1.93176
N -0.35741 1.99599 -0.66674
N -0.54368 3.69057 -2.11496
C -0.79342 4.44939 -3.34583
C -0.05671 3.17296 0.03017
C 0.32828 3.39513 1.35800
C -0.18458 4.25199 -0.87971
C 0.56110 4.71535 1.74274
C 0.04435 5.57717 -0.49500
C 0.41827 5.78922 0.83278
H 5.99662 0.12556 -0.46592
H 6.17425 0.26602 2.01409
H 4.15146 0.30945 3.43396
H 1.86423 0.21196 2.41309
H 3.66813 -0.08023 -3.80530
H 4.88287 0.87274 -2.93067
H 4.91064 -0.90935 -2.84909
H 1.32788 0.71731 -3.58769
H 1.26720 -1.03035 -3.41582
H -0.83000 -1.53191 -3.87498
H -2.17011 -0.98921 -2.86488
H -1.32391 -3.73289 -4.02736
H -0.29661 -5.05924 -3.44731
H -2.02929 -5.01295 -3.02243
H -0.47320 -6.34645 -1.01866
H 0.23336 -6.73930 1.33592
H 0.63836 -4.85048 2.87672
H 0.33870 -2.49259 2.12829
H -2.06646 1.13110 -2.94049
H -0.66403 1.51730 -3.93904
H -0.92583 3.76373 -4.18147
H -1.69622 5.05530 -3.23752
H 0.05927 5.09863 -3.55436
H -0.06033 6.40210 -1.18941
H 0.60665 6.80101 1.17431
H 0.85972 4.92674 2.76367
H 0.43717 2.56435 2.04145
N -2.40627 0.07449 -0.36001
C -3.57132 0.09981 -0.36640
C -5.02324 0.12933 -0.36414
H -5.41659 -0.74339 0.16549
H -5.38096 1.03532 0.13379
H -5.40362 0.11868 -1.38975
H -1.16905 -1.52660 5.68018
C -1.71218 -1.15659 4.80384
C -2.58764 0.07454 5.18887
C -3.24150 0.69791 3.93985
C -2.19521 1.06133 2.86414
C -1.37027 -0.19501 2.45837
C -0.76753 -0.80350 3.69188
H -2.39241 -1.96462 4.48337
H -1.95311 0.82446 5.68124
H -3.80546 1.59680 4.21920
H -2.67732 1.49222 1.97978
H -1.50160 1.81393 3.25950
H -2.06372 -0.91538 1.99307
H 0.29292 -0.66357 3.88077
H -3.96936 -0.01113 3.51669
H -3.35459 -0.22777 5.91322

85
OAT Transition State 2 (2/3)
Fe -0.51267 -0.08348 -0.25436
O -0.54789 -0.17779 1.65179
C 4.98802 0.01992 0.43723
C 5.00663 -0.01560 1.83263
C 4.28990 0.07557 -2.65714
C 3.73128 0.00586 -0.17588
C 3.81028 -0.06358 2.58471
N 3.35792 0.03511 -1.52568
C -1.01953 -4.31903 -3.58873
C 2.52727 -0.04423 0.56881
C 2.55809 -0.07861 1.96894
C 1.98971 0.00049 -1.56865
C 1.16771 0.00379 -2.81934
N 1.45778 -0.04759 -0.34379
C -1.01825 -1.18267 -3.02815
N -0.76966 -3.64015 -2.31230
C -0.77543 -2.29599 -2.05801
C -0.33665 -5.64398 -0.78768
N -0.30645 0.03025 -2.50517
C -0.47749 -4.28899 -1.10445
N -0.51699 -2.03672 -0.76885
C -0.00370 -5.94867 0.53327
C -0.30539 -3.26887 -0.13688
C -0.95400 1.32677 -2.89609
C 0.18816 -4.93498 1.50114
C 0.04253 -3.58521 1.18159
C -0.69219 2.31390 -1.80244
N -0.50252 1.90177 -0.54215
N -0.60781 3.67631 -1.90281
C -0.78646 4.50393 -3.10101
C -0.26069 3.04161 0.23387
C 0.04267 3.18727 1.59316
C -0.34139 4.17048 -0.61779
C 0.23794 4.48366 2.06945
C -0.15240 5.47234 -0.14178
C 0.13705 5.60835 1.21693
H 5.90544 0.05578 -0.13823
H 5.95955 -0.00635 2.35047
H 3.86973 -0.08969 3.66754
H 1.63369 -0.11596 2.52761
H 3.73608 0.17575 -3.58961
H 4.95902 0.93280 -2.55399
H 4.87956 -0.84387 -2.69268
H 1.42292 0.86741 -3.44362
H 1.39152 -0.88708 -3.41662
H -0.68460 -1.43609 -4.04029
H -2.08765 -0.95983 -3.08425
H -1.19253 -3.58316 -4.37213
H -0.15499 -4.92945 -3.85930
H -1.90311 -4.95597 -3.50394
H -0.47337 -6.42293 -1.52816
H 0.11718 -6.98663 0.82286
H 0.45812 -5.21640 2.51307
H 0.20550 -2.80091 1.90787
H -2.03043 1.15986 -2.99610
H -0.58895 1.67751 -3.86734
H -0.70761 3.88636 -3.99464
H -1.76523 4.99004 -3.08671
H -0.00344 5.26370 -3.13307
H -0.22359 6.33645 -0.79141
H 0.29264 6.59963 1.62809
H 0.47383 4.63628 3.11697
H 0.12133 2.31580 2.22936
N -2.49932 -0.11682 -0.40112
C -3.65955 -0.14801 -0.51114
C -5.10602 -0.18785 -0.64580
H -5.38483 -0.32431 -1.69494
H -5.51653 -1.01844 -0.06398
H -5.54585 0.74650 -0.28475
H 0.37304 0.34929 5.00639
C -0.69449 0.10808 4.87822
C -1.55822 1.38525 4.82934
C -2.91386 1.09180 4.16572
C -2.72176 0.66180 2.69594
C -1.71778 -0.50284 2.52551
C -0.89174 -0.80601 3.71906
H -0.94871 -0.47480 5.78300
H -1.04208 2.16915 4.26005
H -3.55818 1.97835 4.20061
H -3.68942 0.37965 2.26801
H -2.35211 1.51685 2.11955
H -2.20741 -1.39793 2.12728
H -0.34969 -1.74713 3.72055
H -3.43364 0.30061 4.72596
H -1.69510 1.77199 5.84540

85
OAT Product (2/3)
Fe -0.44481 -0.05608 -0.22328
O -0.86902 0.00450 2.05360
C 5.05847 0.03003 0.47152
C 5.06205 0.03855 1.86751
C 4.39565 0.00725 -2.62704
C 3.80887 0.00498 -0.15531
C 3.85755 0.02425 2.60691
N 3.44842 0.00104 -1.50732
C -1.05160 -4.25260 -3.68119
C 2.59624 -0.01642 0.57488
C 2.61389 -0.00236 1.97453
C 2.07866 -0.02714 -1.56744
C 1.29456 -0.04455 -2.84680
N 1.53267 -0.04217 -0.34456
C -0.92434 -1.14453 -3.09209
N -0.78961 -3.60511 -2.39136
C -0.73465 -2.26315 -2.11155
C -0.50352 -5.65559 -0.89638
N -0.17558 0.04635 -2.60884
C -0.56135 -4.28961 -1.19160
N -0.49039 -2.03899 -0.81304
C -0.22472 -6.00192 0.42692
C -0.36012 -3.29541 -0.20349
C -0.76667 1.35615 -2.99270
C -0.00529 -5.01723 1.41787
C -0.06717 -3.65660 1.11715
C -0.55990 2.34173 -1.88088
N -0.43697 1.96305 -0.60299
N -0.49830 3.70714 -2.01020
C -0.63418 4.50280 -3.23469
C -0.27492 3.13117 0.15467
C -0.07266 3.31614 1.52769
C -0.32307 4.23870 -0.72603
C 0.06397 4.62652 1.98629
C -0.19195 5.55490 -0.26985
C 0.00235 5.72867 1.10161
H 5.98256 0.04261 -0.09409
H 6.00893 0.05815 2.39570
H 3.90248 0.03558 3.69044
H 1.69474 -0.00605 2.54178
H 3.85879 0.12132 -3.56754
H 5.08899 0.84410 -2.51741
H 4.95791 -0.92967 -2.65147
H 1.61537 0.78239 -3.49237
H 1.51617 -0.96633 -3.39859
H -0.60892 -1.44066 -4.10041
H -1.98600 -0.88484 -3.15113
H -1.07116 -3.50805 -4.47496
H -0.26048 -4.97421 -3.89629
H -2.01567 -4.76661 -3.65504
H -0.66476 -6.41337 -1.65381
H -0.16987 -7.04980 0.70037
H 0.21945 -5.32880 2.43196
H 0.12071 -2.90353 1.87074
H -1.84010 1.21744 -3.15801
H -0.34562 1.72662 -3.93560
H -0.43624 3.88239 -4.10772
H -1.64168 4.92006 -3.31247
H 0.09402 5.31565 -3.21670
H -0.23725 6.40302 -0.94254
H 0.11004 6.73237 1.49795
H 0.22040 4.80740 3.04418
H -0.02935 2.46542 2.19448
N -2.42434 -0.05144 -0.31815
C -3.58668 -0.04395 -0.41881
C -5.03522 -0.03579 -0.54490
H -5.34241 -0.61410 -1.42136
H -5.49542 -0.47793 0.34376
H -5.40078 0.98933 -0.65521
H 0.51740 0.83504 4.50005
C -0.47112 0.36642 4.58483
C -1.58036 1.43054 4.71526
C -2.97308 0.78875 4.59456
C -3.17773 0.14508 3.20632
C -2.00489 -0.71730 2.77841
C -0.68550 -0.59941 3.44396
H -0.44552 -0.24296 5.50040
H -1.46340 2.19802 3.93996
H -3.75616 1.53580 4.76670
H -4.08411 -0.47123 3.20455
H -3.32637 0.92920 2.45327
H -2.23928 -1.65660 2.28725
H -0.02496 -1.46141 3.42839
H -3.08723 0.02237 5.37437
H -1.47460 1.93677 5.68141

85
OAT Reactant Complex (2/5)
Fe 0.20502 -0.73771 -0.13406
O 0.36055 0.73335 0.60271
C -3.55264 1.54793 -3.67172
C -3.55006 2.84217 -3.14629
C -3.09718 -1.51877 -4.38620
C -2.70327 0.62227 -3.05945
C -2.72958 3.19608 -2.05061
N -2.45932 -0.73820 -3.31907
C 3.86722 -2.69252 -3.54696
C -1.87731 0.97056 -1.96430
C -1.88213 2.26859 -1.44212
C -1.52788 -1.16024 -2.41490
C -0.94135 -2.53093 -2.32698
N -1.15593 -0.17466 -1.59299
C 1.38391 -3.06477 -1.56923
N 3.19567 -1.66413 -2.74128
C 2.12243 -1.81612 -1.92191
C 4.62217 0.38298 -3.30635
N -0.00915 -2.66288 -1.12572
C 3.58799 -0.31360 -2.67533
N 1.78964 -0.65255 -1.33153
C 4.72859 1.74413 -3.01361
C 2.69196 0.32054 -1.78268
C -0.56909 -3.61769 -0.08934
C 3.83540 2.38367 -2.12315
C 2.80378 1.68499 -1.49496
C -1.43301 -2.83453 0.84365
N -1.20851 -1.52035 1.02624
N -2.43662 -3.27919 1.64546
C -2.96296 -4.64597 1.75785
C -2.11369 -1.06931 1.99630
C -2.32350 0.19815 2.54993
C -2.89407 -2.17959 2.39613
C -3.32724 0.31172 3.51278
C -3.90043 -2.06933 3.35941
C -4.10209 -0.80234 3.91065
H -4.18288 1.28276 -4.51205
H -4.19330 3.59387 -3.59012
H -2.76107 4.21323 -1.67590
H -1.25458 2.53427 -0.60023
H -2.80685 -2.56536 -4.30449
H -4.18277 -1.44747 -4.29307
H -2.78832 -1.13983 -5.36331
H -1.72752 -3.28796 -2.25102
H -0.37310 -2.75341 -3.23585
H 1.33782 -3.78603 -2.38921
H 1.88341 -3.55037 -0.72660
H 3.28384 -3.61142 -3.53368
H 3.95417 -2.34454 -4.57773
H 4.86129 -2.89385 -3.14155
H 5.31066 -0.10206 -3.98742
H 5.51668 2.32468 -3.47963
H 3.95779 3.44245 -1.92442
H 2.11838 2.16695 -0.80936
H 0.26895 -4.04463 0.46858
H -1.09959 -4.44311 -0.57078
H -2.51973 -5.27711 0.98957
H -2.72240 -5.05774 2.74048
H -4.04593 -4.63035 1.62153
H -4.49703 -2.91952 3.66682
H -4.87222 -0.66948 4.66206
H -3.51962 1.27684 3.96796
H -1.72892 1.04744 2.23765
N 1.67650 -1.83030 1.35292
C 2.39946 -2.09125 2.23185
C 3.29747 -2.41682 3.32729
H 4.24329 -2.80642 2.93963
H 3.50464 -1.52274 3.92286
H 2.84526 -3.17274 3.97594
H 3.01567 5.31167 0.99263
C -2.29108 5.52980 1.79000
C -2.80331 4.97854 3.13656
C -1.68000 4.97121 4.19112
C -0.50532 4.07796 3.74035
C -0.14994 4.29842 2.28524
C -0.93808 4.95991 1.42052
H -2.22637 6.62934 1.83661
H -3.16789 3.95064 2.99263
H -2.06307 4.62952 5.16061
H 0.37649 4.26879 4.36835
H -0.75830 3.01723 3.90342
H 0.80677 3.90168 1.94779
H -0.60408 5.11188 0.39470
H -1.31841 5.99967 4.33582
H -3.65686 5.57207 3.48650

85
OAT Transition State (2/5)
Fe -0.15605 -0.22378 -0.06625
O -0.26503 1.36990 0.49390
C -3.88735 1.06153 -4.06966
C -4.12257 2.38053 -3.67499
C -2.90674 -1.93595 -4.46027
C -2.95359 0.34042 -3.32025
C -3.44870 2.95557 -2.57295
N -2.48680 -0.98053 -3.42847
C 4.08891 -2.27191 -2.85797
C -2.27357 0.90992 -2.21844
C -2.51635 2.23147 -1.82825
C -1.56858 -1.17120 -2.43477
C -0.78422 -2.42410 -2.20548
N -1.41356 -0.06770 -1.69318
C 1.44667 -2.64503 -1.12536
N 3.22473 -1.22032 -2.30866
C 2.08366 -1.36885 -1.57469
C 4.47814 0.87274 -3.08000
N -0.01788 -2.38332 -0.90218
C 3.46271 0.15889 -2.43653
N 1.56824 -0.18119 -1.21949
C 4.39890 2.26570 -3.02014
C 2.40793 0.80722 -1.75168
C -0.61169 -3.28835 0.14227
C 3.34296 2.92052 -2.34428
C 2.33241 2.20369 -1.70254
C -1.67178 -2.54416 0.89060
N -1.63907 -1.20738 0.99725
N -2.72236 -3.07569 1.58302
C -3.08389 -4.49041 1.73390
C -2.72955 -0.83030 1.79339
C -3.17875 0.43028 2.20162
C -3.41687 -2.00671 2.17431
C -4.31978 0.47223 3.00380
C -4.55966 -1.97001 2.97903
C -4.99781 -0.70837 3.38714
H -4.40494 0.62628 -4.91605
H -4.83885 2.97810 -4.22788
H -3.66286 3.98366 -2.30236
H -1.99477 2.66073 -0.98234
H -2.55030 -2.93411 -4.20983
H -3.99693 -1.95734 -4.51154
H -2.50123 -1.64471 -5.43247
H -1.44036 -3.30054 -2.21599
H -0.07120 -2.55747 -3.02656
H 1.59960 -3.46219 -1.83833
H 1.88846 -2.95382 -0.17366
H 3.59209 -3.23780 -2.78255
H 4.28999 -2.06227 -3.91026
H 5.03146 -2.31071 -2.30659
H 5.28896 0.37683 -3.59981
H 5.16523 2.86003 -3.50509
H 3.32048 4.00449 -2.32687
H 1.51669 2.69390 -1.18632
H 0.18229 -3.57572 0.83843
H -0.99404 -4.20902 -0.30995
H -2.48198 -5.10118 1.06334
H -2.91035 -4.81459 2.76281
H -4.13740 -4.62523 1.48124
H -5.08417 -2.87067 3.27449
H -5.88046 -0.63190 4.01226
H -4.69772 1.43066 3.34207
H -2.65388 1.32746 1.89901
N 1.22171 -0.92925 1.61438
C 1.88549 -1.09549 2.55963
C 2.71099 -1.30286 3.73734
H 3.61897 -1.85219 3.47181
H 2.99774 -0.33995 4.17036
H 2.16054 -1.87570 4.48936
H -2.33521 4.03327 1.64945
C -1.41332 4.35157 2.15596
C -1.37420 3.81038 3.60063
C 0.03681 3.94259 4.20428
C 1.06813 3.15444 3.37017
C 0.90165 3.38454 1.89052
C -0.21562 3.93101 1.34375
H -1.45798 5.45363 2.17017
H -1.66575 2.75079 3.60224
H 0.04561 3.58873 5.24185
H 2.09067 3.42196 3.66989
H 0.97386 2.07570 3.57867
H 1.73373 3.11391 1.24683
H -0.24935 4.12212 0.27431
H 0.32369 5.00363 4.22621
H -2.10832 4.34243 4.21699

85
OAT Product (2/5)
Fe -0.13247 -0.06769 0.10564
O -0.23783 1.82695 1.18697
C -4.06090 1.07691 -3.90643
C -4.38415 2.37308 -3.49919
C -2.88365 -1.83289 -4.33540
C -3.06760 0.41733 -3.17589
C -3.73696 2.98536 -2.40157
N -2.51424 -0.86394 -3.29824
C 4.12743 -2.24467 -2.68948
C -2.40930 1.02222 -2.07890
C -2.74536 2.32071 -1.67871
C -1.56516 -0.99415 -2.31266
C -0.70736 -2.21402 -2.14204
N -1.46959 0.11210 -1.56539
C 1.47375 -2.50030 -0.99611
N 3.28041 -1.15223 -2.19869
C 2.12799 -1.23715 -1.46176
C 4.58633 0.86326 -3.06555
N 0.00996 -2.25479 -0.82511
C 3.54962 0.20905 -2.39267
N 1.63436 -0.02618 -1.16336
C 4.53983 2.25830 -3.08661
C 2.50212 0.91164 -1.74928
C -0.62005 -3.18480 0.16065
C 3.49138 2.97093 -2.46106
C 2.46184 2.31119 -1.78920
C -1.69918 -2.47736 0.92043
N -1.67112 -1.15659 1.13564
N -2.78539 -3.06699 1.51595
C -3.14865 -4.48776 1.53750

C -2.80413 -0.85016 1.90481
C -3.28138 0.37355 2.38875
C -3.50865 -2.05135 2.15744
C -4.46174 0.35475 3.13266
C -4.69026 -2.07725 2.90522
C -5.15381 -0.85189 3.38876
H -4.55896 0.61234 -4.74918
H -5.14897 2.92238 -4.03719
H -4.01886 3.99322 -2.11699
H -2.25297 2.78873 -0.83650
H -2.44231 -2.80382 -4.11649
H -3.96992 -1.94253 -4.36169
H -2.52941 -1.49551 -5.31315
H -1.30979 -3.12211 -2.26149
H 0.03846 -2.23141 -2.94562
H 1.66477 -3.33203 -1.68509
H 1.88698 -2.78335 -0.02326
H 3.61182 -3.19671 -2.57646
H 4.34467 -2.08838 -3.74810
H 5.06401 -2.27898 -2.12715
H 5.38916 0.32006 -3.54954
H 5.32289 2.80760 -3.59735
H 3.48731 4.05432 -2.50786
H 1.65417 2.86355 -1.32624
H 0.15172 -3.51216 0.86505
H -1.00123 -4.08547 -0.33441
H -2.55834 -5.03569 0.80492
H -2.96761 -4.91149 2.52874
H -4.20537 -4.59549 1.28461
H -5.22540 -2.99843 3.10284
H -6.06685 -0.82467 3.97332
H -4.85960 1.28448 3.52461
H -2.74635 1.29223 2.18570
N 1.27522 -0.63434 1.81187
C 1.97254 -0.93907 2.69751
C 2.84028 -1.31374 3.80258
H 3.83269 -1.58471 3.43053
H 2.94434 -0.47829 4.50122
H 2.42179 -2.16949 4.34032
H -2.20782 3.98867 1.22845
C -1.23165 4.14858 1.70299
C -1.30321 3.88143 3.22085
C 0.10175 3.87784 3.84682
C 0.98020 2.74962 3.26447
C 0.91002 2.66676 1.75282
C -0.17591 3.33656 0.99344
H -0.97340 5.20397 1.53144
H -1.79251 2.91830 3.41369
H 0.03592 3.76014 4.93425
H 2.02640 2.89529 3.55645
H 0.67024 1.78137 3.67757
H 1.83641 2.45382 1.22899
H 0.00827 3.59965 -0.04400
H 0.58263 4.84863 3.66075
H -1.92692 4.65215 3.68739

$\mathbf{1}_{TBP}$ with cyclohexene

79
HAT Reactant Complex (2/5)
Fe 0.12713 -0.41570 -0.48390
O 0.14600 1.14543 0.04970
C -2.87386 1.13466 -4.88643
C -2.70366 2.51492 -4.75903
C -2.88747 -2.03148 -4.62345
C -2.24321 0.33707 -3.92848
C -1.93319 3.07477 -3.71406
N -2.20015 -1.06190 -3.75910
C 4.53158 -2.91018 -2.28054
C -1.47182 0.89118 -2.88103
C -1.30394 2.27408 -2.75985
C -1.44254 -1.31662 -2.66514
C -1.14233 -2.62731 -2.01652
N -0.98508 -0.17497 -2.10861
C 1.35872 -2.66206 -2.00145
N 3.76730 -1.87151 -1.57520
C 2.42258 -1.77869 -1.43896
C 5.66756 -0.36655 -0.75528
N 0.10591 -2.44539 -1.17885
C 4.33746 -0.75948 -0.92259
N 2.07537 -0.67780 -0.73859
C 5.88449 0.81119 -0.03683
C 3.26111 -0.00896 -0.39581
C 0.08904 -3.34045 0.04203
C 4.81241 1.56553 0.49276
C 3.48511 1.16874 0.32403
C -0.64978 -2.61796 1.11906
N -0.74313 -1.27154 1.08113
N -1.23418 -3.12111 2.23294
C -1.32020 -4.52868 2.64665
C -1.43079 -0.86759 2.23667
C -1.80916 0.39800 2.69522
C -1.74296 -2.03414 2.97245
C -2.49955 0.45272 3.90690
C -2.43297 -1.98386 4.18609
C -2.80580 -0.71678 4.63965
H -3.46619 0.71181 -5.68844
H -3.17494 3.17373 -5.47946
H -1.83040 4.15231 -3.65421
H -0.71495 2.69499 -1.95483
H -2.61578 -3.04427 -4.33089
H -3.96855 -1.90999 -4.52810
H -2.58815 -1.86878 -5.66044
H -1.96317 -2.90682 -1.34787
H -1.00573 -3.44265 -2.73273
H 1.14210 -2.37144 -3.03467
H 1.63183 -3.72127 -2.00693
H 3.85760 -3.68932 -2.63224
H 5.04698 -2.47099 -3.13732
H 5.26035 -3.35120 -1.59815
H 6.49256 -0.94004 -1.15952
H 6.90059 1.15570 0.11809
H 5.02874 2.47425 1.04296
H 2.65921 1.74271 0.72474
H 1.12529 -3.51112 0.35157
H -0.34741 -4.31299 -0.20303
H -0.95388 -5.17111 1.84784
H -0.71447 -4.68946 3.54102
H -2.36106 -4.78155 2.85590
H -2.66966 -2.87717 4.75080
H -3.34378 -0.62840 5.57665
H -2.80737 1.41754 4.29359
H -1.57231 1.29341 2.13501
H -0.44817 5.25446 1.04920
C -0.41876 4.48495 1.83409
C 0.71810 4.79171 2.83183
C 0.56528 3.95623 4.11794
C -0.76953 4.27228 4.82329
C -1.92576 4.32788 3.84776
C -1.76845 4.40519 2.51517
H -0.21229 3.53710 1.30997
H 0.69251 5.85937 3.09448
H 1.40507 4.14003 4.79936
H -0.97396 3.52024 5.59837
H -0.69178 5.23335 5.35775
H -2.92904 4.30665 4.27195
H -2.64576 4.42595 1.86958
H 0.59240 2.88790 3.85759
H 1.69193 4.60333 2.36273

79
HAT Transition State (2/5)
Fe -0.02747 0.20466 0.05368
O -0.04558 1.80579 0.63881
C -3.05253 1.69586 -4.38967
C -2.92841 3.07703 -4.22497
C -2.95604 -1.47174 -4.21579
C -2.40609 0.89328 -3.44594
C -2.18611 3.63270 -3.15765
N -2.31472 -0.50542 -3.31433
C 4.43368 -2.31057 -1.78368
C -1.66511 1.44208 -2.37454
C -1.54259 2.82646 -2.21782
C -1.56010 -0.76531 -2.21481
C -1.22522 -2.09986 -1.62982
N -1.14972 0.37373 -1.62128
C 1.26799 -2.05774 -1.59627
N 3.65734 -1.30296 -1.04854
C 2.30648 -1.19901 -0.94909
C 5.54906 0.12213 -0.08056
N 0.00782 -1.94706 -0.78821
C 4.22030 -0.24183 -0.31456
N 1.95032 -0.13925 -0.19396
C 5.75657 1.24822 0.71886
C 3.13581 0.48772 0.22352
C 0.01247 -2.86918 0.39545
C 4.67632 1.98061 1.26281
C 3.35138 1.61261 1.02548
C -0.72724 -2.20650 1.51265
N -0.86296 -0.86573 1.55906
N -1.28699 -2.79866 2.59996
C -1.32230 -4.22987 2.92869
C -1.55656 -0.56203 2.74318
C -1.97623 0.65914 3.28001
C -1.82449 -1.77991 3.40878
C -2.65867 0.61801 4.49690
C -2.50623 -1.82679 4.62764
C -2.91839 -0.60328 5.15997
H -3.62285 1.27558 -5.20894
H -3.41322 3.73942 -4.93319
H -2.11666 4.71107 -3.06905
H -0.97243 3.24243 -1.39732
H -2.60365 -2.47723 -3.99265
H -4.04056 -1.43609 -4.09044
H -2.69769 -1.22862 -5.24804
H -2.04374 -2.42958 -0.98089
H -1.08626 -2.86989 -2.39623
H 1.05981 -1.68439 -2.60471
H 1.58229 -3.10239 -1.69301
H 3.76787 -3.07439 -2.18118
H 4.96629 -1.83695 -2.61136
H 5.14990 -2.78102 -1.10739
H 6.38000 -0.43568 -0.49476
H 6.77109 1.56836 0.92777
H 4.88473 2.84849 1.87837
H 2.51723 2.16688 1.43571
H 1.05291 -3.03605 0.69429
H -0.41054 -3.84489 0.13404
H -0.95665 -4.81355 2.08577
H -0.69241 -4.42695 3.79906
H -2.35021 -4.52676 3.14467
H -2.70823 -2.76046 5.13823
H -3.45155 -0.59024 6.10389
H -2.99912 1.54482 4.94507
H -1.77583 1.59285 2.77068
H -0.30931 4.93851 0.61574
C -0.34355 4.38000 1.56097
C 0.85109 4.70137 2.47212
C 0.66361 4.06803 3.86349
C -0.63052 4.57555 4.53269
C -1.79527 4.61788 3.57722
C -1.66075 4.51781 2.23094
H -0.23765 3.27795 1.20097
H 0.93516 5.79415 2.57478
H 1.52656 4.28336 4.50385
H -0.88606 3.94877 5.39832
H -0.47279 5.58737 4.94309
H -2.78453 4.76387 4.00690
H -2.54617 4.54457 1.59931
H 0.60984 2.97553 3.75443
H 1.78444 4.35850 2.01095

79
HAT Intermediate (2/5)
Fe 0.03227 -0.12493 -0.25392
O 0.00225 1.54691 0.37146
C -3.03942 1.20934 -4.72217
C -2.93692 2.59373 -4.56982
C -2.89491 -1.95313 -4.52060
C -2.37562 0.42521 -3.77503
C -2.19919 3.16974 -3.51033
N -2.26204 -0.97018 -3.63150
C 4.49703 -2.68762 -2.16011
C -1.63797 0.99355 -2.71187
C -1.53844 2.38144 -2.56707
C -1.49865 -1.20962 -2.53211
C -1.14817 -2.53953 -1.94475
N -1.10172 -0.06080 -1.95068
C 1.34030 -2.47816 -1.92487
N 3.72149 -1.68121 -1.42310
C 2.37030 -1.59080 -1.30173
C 5.61374 -0.21986 -0.51387
N 0.08636 -2.38105 -1.11717
C 4.28522 -0.60263 -0.71681
N 2.01427 -0.52387 -0.55875
C 5.82319 0.92303 0.26092
C 3.20159 0.12322 -0.17247
C 0.10228 -3.27493 0.08020
C 4.74447 1.65350 0.80991
C 3.41971 1.26635 0.60332
C -0.65761 -2.60623 1.18058
N -0.80747 -1.26740 1.21728
N -1.23096 -3.19901 2.26128
C -1.25999 -4.62885 2.59532
C -1.52490 -0.96557 2.38921
C -1.96678 0.25334 2.91446
C -1.79190 -2.18273 3.05635
C -2.66957 0.21005 4.11985
C -2.49313 -2.23187 4.26393
C -2.92747 -1.01082 4.78404
H -3.60750 0.77277 -5.53448
H -3.43585 3.24235 -5.28099
H -2.14716 4.24975 -3.43005
H -0.97344 2.81549 -1.75215
H -2.50230 -2.94729 -4.31444
H -3.97654 -1.95535 -4.36723
H -2.67242 -1.69559 -5.55764
H -1.96117 -2.87126 -1.28965
H -1.01690 -3.31019 -2.71263
H 1.12212 -2.12515 -2.93874
H 1.67853 -3.51696 -2.00948
H 3.83605 -3.47045 -2.52735
H 5.00061 -2.21994 -3.00921
H 5.23829 -3.13349 -1.49421
H 6.44321 -0.77556 -0.93389
H 6.83762 1.25830 0.44522
H 4.95342 2.53565 1.40474
H 2.58762 1.82156 1.01671
H 1.14372 -3.41489 0.38991
H -0.29922 -4.26636 -0.15719
H -0.89147 -5.21418 1.75489
H -0.63069 -4.82085 3.46733
H -2.28701 -4.92904 2.81097
H -2.69293 -3.16551 4.77550
H -3.47635 -0.99937 5.71892
H -3.02748 1.13484 4.55842
H -1.76646 1.18783 2.40566
H 0.32136 4.83535 0.37649
C 0.05190 4.55544 1.39204
C 1.12692 4.52393 2.45043
C 0.70718 3.65403 3.65645
C -0.69803 4.03680 4.17263
C -1.69928 4.13678 3.05042
C -1.29303 4.37621 1.73725
H -0.08896 2.46168 0.71510
H 1.32942 5.55362 2.79433
H 1.44388 3.74215 4.46263
H -1.03713 3.30936 4.92173
H -0.64402 5.00406 4.70296
H -2.75697 4.05140 3.28407
H -2.04852 4.44713 0.95773
H 0.69433 2.60035 3.34444
H 2.07386 4.16230 2.02926

79
Rebound Transition State (2/5)
Fe 0.18357 -0.19243 -0.02472
O 0.33051 1.48332 0.73145
C -2.51705 1.66070 -4.58550
C -2.20422 3.01077 -4.41117
C -2.83707 -1.49384 -4.44124
C -1.99409 0.77013 -3.64351
C -1.39552 3.45201 -3.33834
N -2.08739 -0.62734 -3.52341
C 4.42668 -2.95290 -2.21621
C -1.19480 1.20498 -2.56180
C -0.87769 2.55811 -2.39965
C -1.37616 -0.99195 -2.41845
C -1.18747 -2.37735 -1.88310
N -0.83330 0.07655 -1.80790
C 1.29815 -2.52423 -1.90617
N 3.74269 -1.94133 -1.40163
C 2.40021 -1.75633 -1.24431
C 5.75309 -0.67749 -0.44748
N 0.06530 -2.40320 -1.07344
C 4.39678 -0.95301 -0.64508
N 2.13928 -0.71738 -0.43213
C 6.05681 0.40120 0.38602
C 3.37793 -0.18436 -0.03687
C 0.02434 -3.39443 0.03795
C 5.04290 1.17596 0.99584
C 3.69032 0.89653 0.79557
C -0.64922 -2.77482 1.22043
N -0.68012 -1.44235 1.40608
N -1.24448 -3.43903 2.25217
C -1.39333 -4.88919 2.42563
C -1.33083 -1.22045 2.63372
C -1.64197 -0.03819 3.31386
C -1.68673 -2.47727 3.17494
C -2.30597 -0.15410 4.53554
C -2.35157 -2.60144 4.39822
C -2.65499 -1.41541 5.06975
H -3.13177 1.32778 -5.41295
H -2.58726 3.73780 -5.11851
H -1.17220 4.50914 -3.24664
H -0.25015 2.88109 -1.57835
H -2.73582 -2.53351 -4.13553
H -3.89511 -1.22300 -4.42346
H -2.44779 -1.38111 -5.45546
H -2.02525 -2.63600 -1.22589
H -1.16242 -3.12575 -2.68457
H 1.09345 -2.08511 -2.88881
H 1.56598 -3.57390 -2.07331
H 3.70478 -3.67185 -2.59949
H 4.93382 -2.47550 -3.05803
H 5.15815 -3.48131 -1.60149
H 6.53418 -1.26463 -0.91517
H 7.09587 0.65235 0.56799
H 5.32609 2.00735 1.63195
H 2.90341 1.48831 1.24712
H 1.05577 -3.64970 0.30606
H -0.46420 -4.32550 -0.27296
H -1.16856 -5.40086 1.49150
H -0.71423 -5.24784 3.20294
H -2.42330 -5.11365 2.70872
H -2.61950 -3.56638 4.81121
H -3.16997 -1.46320 6.02265
H -2.56050 0.74343 5.08819
H -1.37915 0.92746 2.90422
H -1.84382 3.37410 0.27265
C -1.50042 3.82591 1.19745
C -0.36420 4.80567 1.14322
C 0.29736 5.00485 2.52387
C -0.75078 5.24533 3.63071
C -1.88583 4.26829 3.55974
C -2.20399 3.59558 2.38509
H 0.03791 2.06274 1.45681
H -0.75754 5.76988 0.77353
H 1.00405 5.83973 2.48538
H -0.28275 5.20970 4.62232
H -1.16411 6.26625 3.53979
H -2.49694 4.11955 4.44564
H -3.04419 2.90777 2.37673
H 0.87856 4.10660 2.77459
H 0.37865 4.48805 0.40171

79
Rebound Product (2/5)
Fe -0.08919 -0.07924 0.10236
O -0.23060 1.61403 1.38280
C -2.74489 1.57692 -4.67512
C -2.47345 2.94391 -4.59320
C -2.94846 -1.56326 -4.35281
C -2.19718 0.76684 -3.67616
C -1.67434 3.47580 -3.55594
N -2.24027 -0.62083 -3.47887
C 4.34247 -2.36065 -2.25723
C -1.41635 1.29002 -2.61838
C -1.13365 2.66038 -2.56063
C -1.51977 -0.89526 -2.35074
C -1.26213 -2.25652 -1.78086
N -1.02271 0.22220 -1.78921
C 1.22531 -2.21676 -1.80642
N 3.61997 -1.44114 -1.37070
C 2.27193 -1.36737 -1.15270
C 5.56169 -0.05016 -0.45880
N -0.01098 -2.20090 -0.97374
C 4.22384 -0.42733 -0.61121
N 1.96044 -0.37622 -0.30078
C 5.81764 1.01912 0.40183
C 3.17200 0.23617 0.06301
C 0.02461 -3.20943 0.11971
C 4.77393 1.68560 1.08421
C 3.44118 1.30460 0.92616
C -0.82139 -2.72553 1.25394
N -1.05025 -1.41843 1.46724
N -1.42651 -3.50913 2.19648
C -1.38948 -4.97098 2.31965
C -1.85841 -1.33956 2.61772
C -2.40807 -0.24132 3.28984
C -2.09311 -2.65434 3.08559
C -3.17914 -0.49698 4.42413
C -2.86296 -2.91839 4.22255
C -3.40332 -1.81458 4.88432
H -3.34533 1.16959 -5.47963
H -2.87609 3.61082 -5.34737
H -1.47221 4.54100 -3.53803
H -0.50009 3.07131 -1.78553
H -2.82072 -2.57935 -3.98430
H -4.01487 -1.32650 -4.36448
H -2.54936 -1.49951 -5.36770
H -2.08294 -2.54612 -1.11564
H -1.19901 -3.01765 -2.56884
H 0.98377 -1.79740 -2.78913
H 1.57720 -3.24176 -1.97471
H 3.69228 -3.18215 -2.55336
H 4.68356 -1.83442 -3.15235
H 5.20330 -2.77173 -1.72654
H 6.36508 -0.55644 -0.98032
H 6.84070 1.34635 0.55023
H 5.01687 2.51108 1.74409
H 2.64108 1.81354 1.44741
H 1.06330 -3.30673 0.45492
H -0.29447 -4.19702 -0.23610
H -0.95492 -5.41043 1.42355
H -0.78825 -5.26066 3.18504
H -2.40602 -5.35104 2.43889
H -3.03460 -3.92723 4.57822
H -4.00787 -1.97116 5.77077
H -3.61724 0.33355 4.96671
H -2.23663 0.76712 2.94096
H -1.42928 2.83975 0.27236
C -0.78495 3.01169 1.13588
C 0.35794 3.97215 0.79081
C 1.08604 4.47973 2.04977
C 0.10452 5.19130 2.99921
C -1.19225 4.43595 3.14960
C -1.59047 3.45084 2.32519
H 0.13656 1.54387 2.28629
H -0.07523 4.82737 0.25335
H 1.89969 5.15527 1.76562
H 0.56286 5.33757 3.98577

H -0.11748 6.20320 2.62311
H -1.84222 4.73516 3.96946
H -2.54660 2.95837 2.47885
H 1.55114 3.63496 2.57797
H 1.05435 3.47940 0.10356

79
OAT Reactant Complex (2/5)
Fe 0.41235 -0.58773 -0.85344
O 0.63779 -0.69019 0.77667
C 5.84758 -1.40128 -1.60393
C 6.16148 -1.81238 -0.30683
C 4.51523 -0.40936 -4.31213
C 4.50969 -1.08473 -1.85169
C 5.17526 -1.90256 0.70225
N 3.85413 -0.65048 -3.02187
C -2.23569 -4.30790 -3.67712
C 3.51923 -1.17145 -0.84631
C 3.83966 -1.58596 0.45016
C 2.54432 -0.48549 -2.71753
C 1.43860 0.02307 -3.58119
N 2.29883 -0.78875 -1.42519
C -0.23182 -1.83320 -3.47519
N -1.81318 -3.58820 -2.46720
C -0.97822 -2.52456 -2.38313
C -3.05844 -4.91853 -0.67178
N 0.13336 -0.45069 -2.97662
C -2.21225 -3.91809 -1.15607
N -0.80649 -2.13499 -1.10206
C -3.24674 -4.96069 0.71127
C -1.57344 -2.99341 -0.29746
C -0.98343 0.54031 -3.23022
C -2.61395 -4.03682 1.57407
C -1.76955 -3.03794 1.08669
C -0.95751 1.54271 -2.12415
N -0.40134 1.21757 -0.93778
N -1.49413 2.78637 -2.09146
C -2.20062 3.48926 -3.17134
C -0.58759 2.30904 -0.07503
C -0.21366 2.51044 1.25734
C -1.28074 3.30656 -0.79865
C -0.55960 3.73322 1.83448
C -1.62750 4.53245 -0.22530
C -1.25325 4.72672 1.10599
H 6.60683 -1.33238 -2.37316
H 7.18741 -2.06805 -0.06754
H 5.46588 -2.22543 1.69553
H 3.07930 -1.65043 1.21809
H 3.76727 -0.23670 -5.08418
H 5.16505 0.46548 -4.23970
H 5.10643 -1.28576 -4.58282
H 1.43768 1.11792 -3.57785
H 1.51879 -0.30466 -4.62183
H 0.69600 -2.37306 -3.69103
H -0.79823 -1.76310 -4.40839
H -1.87351 -3.78743 -4.56204
H -1.82814 -5.32100 -3.66630
H -3.32574 -4.34961 -3.71116
H -3.54631 -5.62781 -1.32892
H -3.89491 -5.72034 1.13320
H -2.78999 -4.10650 2.64163
H -1.28697 -2.32909 1.74838
H -1.93347 -0.00370 -3.21262
H -0.87884 0.98776 -4.22285
H -2.08211 2.94367 -4.10588
H -3.26351 3.56701 -2.93234
H -1.77560 4.48742 -3.28860
H -2.16089 5.29622 -0.77772
H -1.50197 5.66255 1.59326
H -0.29094 3.92785 2.86655
H 0.31538 1.74434 1.80988
H -3.31902 -0.84837 5.14553
C -2.28950 -0.74274 5.51586
C -1.89038 -1.98655 6.33636
C -0.37065 -2.01382 6.58873
C 0.40935 -2.06519 5.25827
C -0.15379 -1.10743 4.22965
C -1.35004 -0.50663 4.35243
H -2.30043 0.14658 6.16746
H -2.17933 -2.89332 5.78477
H -0.09932 -2.87051 7.21800
H 1.47030 -1.83711 5.43425
H 0.39195 -3.09082 4.85436
H 0.45950 -0.90806 3.35183
H -1.68199 0.19202 3.58501
H -0.08391 -1.10818 7.14301
H -2.43909 -2.00376 7.28614

79
OAT Transition State (2/5)
Fe 0.15683 -0.61778 -0.37159
O 0.16695 -0.66565 1.34049
C 5.68485 -1.39752 -0.85887
C 5.92638 -1.75452 0.46932
C 4.50729 -0.52308 -3.67027
C 4.35993 -1.11077 -1.19839
C 4.88188 -1.82023 1.41982
N 3.76992 -0.73145 -2.41723
C -2.30889 -4.37187 -3.47778
C 3.31038 -1.17327 -0.25375
C 3.56112 -1.53202 1.07394
C 2.43691 -0.57533 -2.19679
C 1.40961 -0.11755 -3.18173
N 2.11634 -0.83103 -0.91191
C -0.25616 -1.97002 -3.14204
N -2.02054 -3.60619 -2.25796
C -1.14881 -2.57368 -2.10570
C -3.57535 -4.77642 -0.59668
N 0.06384 -0.57211 -2.71276
C -2.61547 -3.84663 -1.00585
N -1.13492 -2.12493 -0.83431
C -3.96091 -4.72738 0.74460
C -2.05367 -2.90545 -0.11382
C -1.02168 0.39886 -3.06405
C -3.40790 -3.78373 1.64083
C -2.44821 -2.85906 1.22638
C -1.03589 1.47505 -2.02609
N -0.54809 1.25443 -0.78958
N -1.53778 2.73375 -2.14472
C -2.17099 3.34494 -3.32024
C -0.73359 2.43884 -0.05780
C -0.39188 2.77387 1.25635
C -1.36400 3.37749 -0.90603
C -0.71246 4.06053 1.69120
C -1.68863 4.66709 -0.47646
C -1.35228 4.99061 0.83980
H 6.48842 -1.34558 -1.58328
H 6.93933 -1.98575 0.77904
H 5.11488 -2.10066 2.44097
H 2.75602 -1.57696 1.79415
H 3.80919 -0.37465 -4.49216
H 5.14893 0.35687 -3.58391
H 5.11806 -1.40279 -3.88122
H 1.40703 0.97718 -3.21937
H 1.61669 -0.47552 -4.19607
H 0.68090 -2.53483 -3.19590
H -0.70324 -1.98596 -4.14203
H -1.80021 -3.92146 -4.32813
H -1.96275 -5.40119 -3.36040
H -3.38442 -4.36596 -3.66495
H -4.00293 -5.50040 -1.27952
H -4.70341 -5.42926 1.10720
H -3.73900 -3.78056 2.67333
H -2.01443 -2.13216 1.90034
H -1.97803 -0.13525 -3.05373
H -0.88324 0.79715 -4.07530
H -2.07985 2.68086 -4.17795
H -3.22967 3.52538 -3.12060
H -1.67523 4.29007 -3.54975
H -2.17495 5.38423 -1.12642
H -1.58466 5.98010 1.21709
H -0.46464 4.35687 2.70433
H 0.10335 2.05665 1.89755
H -2.57797 -1.08372 4.11613
C -1.62018 -1.06681 4.65581
C -1.09478 -2.49818 4.89431
C 0.39159 -2.48281 5.29529
C 1.24945 -1.83442 4.18737
C 0.66169 -0.53358 3.70066
C -0.64326 -0.18737 3.92894
H -1.85182 -0.58609 5.62214
H -1.21059 -3.09078 3.97673
H 0.74745 -3.50071 5.49086
H 2.27386 -1.66326 4.54222
H 1.33475 -2.53048 3.33891
H 1.33500 0.19152 3.25717
H -1.00106 0.78548 3.60317
H 0.51282 -1.91555 6.22866
H -1.69793 -2.98863 5.66670

79
OAT Product (2/5)
Fe 0.00979 -0.74166 -0.15630
O -0.22136 -1.07171 1.97052
C 5.59994 -1.46721 -0.92018
C 5.89710 -1.95233 0.35494
C 4.30196 -0.34449 -3.58501
C 4.25962 -1.16599 -1.18046
C 4.88977 -2.13302 1.33056
N 3.61888 -0.68179 -2.33076
C -2.25347 -4.39073 -3.62237
C 3.24531 -1.33387 -0.20847
C 3.55416 -1.83024 1.06325
C 2.28733 -0.56844 -2.03931
C 1.22747 -0.04527 -2.96013
N 2.02042 -0.94355 -0.77665
C -0.40940 -1.90531 -3.05769
N -1.97884 -3.77207 -2.32037
C -1.19554 -2.68456 -2.05137
C -3.31558 -5.31857 -0.78908
N -0.10259 -0.55385 -2.51385
C -2.47706 -4.24287 -1.09719
N -1.15330 -2.41327 -0.73581
C -3.62079 -5.50884 0.55990
C -1.95531 -3.38234 -0.10364
C -1.20747 0.42333 -2.72861
C -3.10273 -4.65539 1.56098
C -2.26600 -3.58448 1.24539
C -1.07830 1.50943 -1.70529
N -0.44576 1.31296 -0.53316
N -1.52108 2.79464 -1.83558
C -2.26792 3.38598 -2.95204
C -0.44804 2.55513 0.13042
C 0.11923 2.96007 1.34565
C -1.14027 3.48833 -0.67787
C -0.05491 4.29006 1.73134
C -1.32221 4.82097 -0.29704
C -0.77049 5.20493 0.92637
H 6.37432 -1.33343 -1.66599
H 6.92374 -2.19885 0.60203
H 5.16336 -2.51743 2.30693
H 2.78198 -1.97899 1.80715
H 3.57018 -0.10155 -4.35352
H 4.95750 0.51699 -3.43531
H 4.89394 -1.19856 -3.92078
H 1.21304 1.04865 -2.91098
H 1.42586 -0.31544 -4.00395
H 0.53880 -2.42096 -3.24634
H -0.93188 -1.83575 -4.01957
H -1.84317 -3.77612 -4.42147
H -1.79823 -5.38307 -3.66914
H -3.33273 -4.47821 -3.76458
H -3.70994 -5.97672 -1.55390
H -4.26718 -6.33105 0.84636
H -3.36065 -4.84086 2.59797
H -1.85481 -2.93388 2.00353
H -2.15764 -0.10714 -2.60215
H -1.19398 0.82915 -3.74809
H -2.38414 2.65509 -3.75010
H -3.25891 3.69642 -2.61252
H -1.72707 4.25192 -3.33977
H -1.85815 5.52763 -0.91918
H -0.88481 6.22957 1.26184
H 0.37378 4.63195 2.66676
H 0.69274 2.27562 1.95767
H -2.77133 -0.96133 3.38986
C -1.85660 -0.73292 3.95043
C -1.35529 -1.96268 4.73727
C 0.05881 -1.72445 5.29407
C 1.08180 -1.50314 4.15890
C 0.60496 -0.49397 3.13252
C -0.82964 -0.13547 3.02255
H -2.12065 0.06546 4.65959
H -1.34651 -2.85256 4.09507
H 0.37749 -2.57525 5.90633
H 2.03724 -1.15806 4.56926
H 1.28146 -2.45499 3.64938
H 1.33987 0.21440 2.76353
H -1.08694 0.82500 2.58820
H 0.04733 -0.84441 5.95230
H -2.05687 -2.17060 5.55268

2_{TBP} without substrate

60
TBP with Def2-TZVPP (2/3)
Fe -0.96189 1.56443 -0.30670
N 0.74895 0.57654 -0.13507
N 0.07035 3.26065 -0.87603
N -2.12820 -0.12638 -0.34931
N -0.82728 1.10847 -2.30518
O -1.68649 2.17114 0.96979
C 0.26230 0.09603 -2.46173
C 1.16679 0.02754 -1.27023
C 2.38873 -0.65361 -1.37120
C 3.17812 -0.77126 -0.26348
C 2.76261 -0.20894 0.95990
C 3.54467 -0.31468 2.13251
C 3.11765 0.24000 3.30968
C 1.88929 0.92499 3.35237
C 1.10616 1.04900 2.23075
C 1.51712 0.48562 1.00930
C -0.53970 2.36682 -3.03902
C 0.25616 3.31540 -2.19331
C 1.08933 4.25770 -2.81250
C 1.74506 5.17412 -2.03980
C 1.53835 5.18810 -0.64761
C 2.16087 6.14940 0.18230
C 1.90929 6.17668 1.52773
C 1.01246 5.24601 2.08540
C 0.40414 4.28814 1.31124
C 0.66203 4.21733 -0.07235
C -2.14550 0.52968 -2.66830
C -2.60318 -0.37877 -1.56632
C -3.51238 -1.41096 -1.83379
C -3.94451 -2.19656 -0.80184
C -3.46196 -1.96884 0.50123
C -3.87129 -2.76575 1.59546
C -3.38066 -2.52929 2.85174
C -2.46005 -1.48352 3.05561
C -2.04367 -0.68938 2.01528
C -2.53064 -0.90745 0.71263
H 0.83540 0.30458 -3.36375
H -0.18831 -0.88720 -2.59868
H 2.67891 -1.07304 -2.32286
H 4.12427 -1.29264 -0.31388
H 4.48497 -0.84610 2.07750
H 3.71760 0.15432 4.20442
H 1.55258 1.36268 4.28172
H 0.17120 1.58081 2.28805
H -1.48918 2.84973 -3.27156
H -0.04250 2.15852 -3.98486
H 1.20657 4.23453 -3.88539
H 2.41371 5.89753 -2.48661
H 2.82956 6.86715 -0.27336
H 2.38259 6.91525 2.15926
H 0.79107 5.28672 3.14309
H -0.30313 3.61067 1.75367
H -2.09428 0.00667 -3.62382
H -2.86059 1.34532 -2.77782
H -3.85134 -1.56688 -2.84686
H -4.64763 -2.99990 -0.97560
H -4.57796 -3.56447 1.41526
H -3.69493 -3.14016 3.68620
H -2.07248 -1.29955 4.04813
H -1.34787 0.10767 2.19952

60
TBP with Def2-TZVPP (2/5)
Fe -0.04874 1.16282 0.02705
N 1.65677 -0.03750 -0.08161
N 0.03827 3.11647 -0.69846
N -1.87812 0.16511 -0.16503
N -0.03266 0.78838 -1.98730
O -0.07395 1.47717 1.62113
C 0.54857 -0.56605 -2.16947
C 1.65874 -0.79006 -1.18256
C 2.62216 -1.77692 -1.42638
C 3.60643 -1.98497 -0.49912
C 3.66439 -1.18565 0.65907
C 4.69262 -1.33639 1.61812
C 4.74751 -0.51439 2.71220
C 3.77746 0.49279 2.87940
C 2.75990 0.66202 1.97145
C 2.66891 -0.18100 0.84735
C 0.80184 1.84626 -2.61155
C 0.56002 3.16072 -1.92461
C 0.90349 4.36041 -2.56006
C 0.70566 5.54095 -1.89668
C 0.11993 5.54127 -0.61536
C -0.14482 6.74113 0.08473
C -0.75714 6.70944 1.30957
C -1.13590 5.47444 1.87060
C -0.88620 4.28898 1.22193
C -0.23571 4.29144 -0.02682
C -1.44490 0.85306 -2.44284
C -2.34352 0.23156 -1.41216
C -3.61732 -0.22478 -1.77350
C -4.42558 -0.76184 -0.80894
C -3.95788 -0.88673 0.51409
C -4.74246 -1.48063 1.52969
C -4.24316 -1.62622 2.79672
C -2.93698 -1.18787 3.08886
C -2.14981 -0.59925 2.12856
C -2.64454 -0.42191 0.82200
H 0.90040 -0.69863 -3.19299
H -0.23575 -1.30427 -2.00022
H 2.57247 -2.35302 -2.33805
H 4.35790 -2.74693 -0.65665
H 5.43604 -2.10652 1.46281
H 5.53590 -0.62863 3.44280
H 3.83455 1.14953 3.73659
H 2.02717 1.43833 2.11355
H 0.59681 1.91794 -3.68039
H 1.85077 1.57003 -2.50155
H 1.32011 4.33416 -3.55590
H 0.97639 6.48177 -2.35685
H 0.13790 7.67998 -0.37186
H -0.96103 7.62728 1.84286
H -1.63717 5.45653 2.82863
H -1.18503 3.35325 1.66320
H -1.55966 0.36407 -3.41098
H -1.71857 1.90028 -2.57364
H -3.93762 -0.14625 -2.80166
H -5.41823 -1.11353 -1.05629
H -5.73768 -1.82345 1.28085
H -4.84267 -2.08357 3.57120
H -2.54229 -1.31981 4.08693
H -1.15273 -0.27023 2.36839

60
TBP with LACVP (2/5)
Fe -0.08005 1.14994 -0.02514
N 1.61929 -0.03191 -0.09604
N 0.07321 3.09607 -0.70123
N -1.89833 0.17086 -0.18939
N -0.05533 0.78024 -2.00650
O -0.10729 1.46093 1.60569
C 0.50005 -0.60728 -2.17735
C 1.62224 -0.81591 -1.19680
C 2.60507 -1.79748 -1.42182
C 3.60616 -1.97005 -0.48780
C 3.65797 -1.14562 0.66356
C 4.69647 -1.26782 1.62727
C 4.73848 -0.42761 2.72085
C 3.74319 0.56781 2.88461
C 2.71472 0.71246 1.96920
C 2.64083 -0.14624 0.84649
C 0.82594 1.82514 -2.63360
C 0.60278 3.14358 -1.94353
C 0.95426 4.35482 -2.56761
C 0.75437 5.54060 -1.89047
C 0.16454 5.53633 -0.60164
C -0.09748 6.74032 0.10827
C -0.70919 6.70458 1.34464
C -1.08695 5.46102 1.90924
C -0.84203 4.26882 1.24936
C -0.19687 4.27706 -0.01025
C -1.48134 0.88311 -2.47431
C -2.38061 0.24659 -1.44919
C -3.65932 -0.22624 -1.79714
C -4.45378 -0.79023 -0.81952
C -3.97091 -0.91966 0.50666
C -4.74381 -1.53313 1.53068
C -4.23189 -1.67374 2.80425
C -2.92528 -1.20849 3.09544
C -2.14606 -0.60248 2.12492
C -2.65351 -0.43353 0.81442
H 0.83597 -0.75754 -3.20828
H -0.30526 -1.32326 -1.98505
H 2.56337 -2.39682 -2.32183
H 4.37115 -2.72405 -0.63577
H 5.45498 -2.02892 1.47977
H 5.53224 -0.52048 3.45284
H 3.78857 1.23124 3.74095
H 1.95948 1.47208 2.10926
H 0.62512 1.89648 -3.70748
H 1.86734 1.51002 -2.51357
H 1.37423 4.33846 -3.56499
H 1.02785 6.48576 -2.34613
H 0.18617 7.68343 -0.34607
H -0.91033 7.62325 1.88323
H -1.58130 5.44159 2.87403
H -1.13455 3.32782 1.69178
H -1.59506 0.41213 -3.45611
H -1.72731 1.94414 -2.58503
H -3.99739 -0.14453 -2.82200
H -5.44546 -1.15622 -1.06117
H -5.73768 -1.89229 1.28662
H -4.82131 -2.14399 3.58266
H -2.52588 -1.33232 4.09576
H -1.15321 -0.24824 2.36121

61
FeOH TBP with LACVP (2/6)
Fe -0.00920 -0.61025 -0.30034
N -1.10812 -0.36420 -2.12262
N -0.96130 -1.85741 1.19208
N 2.10692 -0.87093 -0.63429
N 0.12010 -2.58233 -1.17579
O -0.00489 1.01754 0.43139
C 0.17148 -2.37464 -2.65503
C -0.78755 -1.28092 -3.05617
C -1.30404 -1.23466 -4.36757
C -2.17387 -0.22206 -4.71350
C -2.56106 0.74401 -3.75006
C -3.48480 1.78217 -4.05132
C -3.85926 2.68842 -3.08028
C -3.32128 2.58637 -1.77283
C -2.41622 1.59151 -1.44583
C -2.01131 0.65279 -2.42596
C -1.10437 -3.32412 -0.75239

C -1.43416 -3.01091 0.68452
C -2.22258 -3.90456 1.43958
C -2.52400 -3.59496 2.74852
C -2.01618 -2.40633 3.33273
C -2.26680 -2.06667 4.69044
C -1.72790 -0.91887 5.23544
C -0.91428 -0.07380 4.43997
C -0.65520 -0.37145 3.11343
C -1.20760 -1.53514 2.52610
C 1.37219 -3.19357 -0.63613
C 2.47507 -2.16477 -0.60440
C 3.82678 -2.56414 -0.54229
C 4.81147 -1.59915 -0.51572
C 4.46609 -0.22541 -0.60155
C 5.44949 0.80102 -0.63725
C 5.07604 2.12314 -0.77124
C 3.70463 2.46258 -0.88457
C 2.72117 1.48947 -0.84325
C 3.07672 0.12824 -0.68200
H -0.05854 -3.30467 -3.18732
H 1.19239 -2.08669 -2.92605
H -1.01584 -1.99774 -5.07928
H -2.58284 -0.16570 -5.71634
H -3.89032 1.84210 -5.05560
H -4.56618 3.47700 -3.31082
H -3.62543 3.29913 -1.01439
H -2.00581 1.52671 -0.44806
H -0.97204 -4.40326 -0.89158
H -1.93361 -3.01344 -1.39655
H -2.57498 -4.81979 0.98074
H -3.13322 -4.26315 3.34728
H -2.88319 -2.73060 5.28708
H -1.91829 -0.66294 6.27134
H -0.48479 0.82000 4.87880
H -0.03549 0.27722 2.51190
H 1.67209 -4.06058 -1.23637
H 1.16836 -3.55517 0.37720
H 4.06975 -3.61888 -0.51698
H 5.85703 -1.88043 -0.45410
H 6.49550 0.52245 -0.56695
H 5.82717 2.90396 -0.80152
H 3.42084 3.50141 -1.01159
H 1.67939 1.75779 -0.93978
H 0.11589 1.90535 0.80441

2_{Oh} without substrate

66
Oh with Def2-TZVPP (2/3)
Fe -0.04346 -0.04170 0.03252
N 1.99941 -0.26783 -0.27333
N -0.00578 1.98912 -0.30600
N -2.08506 0.04299 -0.31667
N 0.04484 -0.16670 -2.03747
O 0.01338 -0.03487 1.66241
N -0.22298 -2.02588 0.12125
C 1.12144 -1.13661 -2.35069
C 2.27077 -0.89380 -1.41575
C 3.55769 -1.32680 -1.76773
C 4.59258 -1.10109 -0.90549
C 4.36054 -0.40007 0.29374
C 5.41387 -0.09588 1.18765
C 5.17543 0.62527 2.32652
C 3.86937 1.07072 2.60674
C 2.82159 0.78266 1.76688
C 3.03196 0.03165 0.59281
C 0.41160 1.17717 -2.55851
C 0.12618 2.28412 -1.59389
C 0.08108 3.59332 -2.10229
C -0.09255 4.63509 -1.24206
C -0.22756 4.37960 0.13600
C -0.40352 5.43820 1.05657
C -0.53689 5.18728 2.39559
C -0.50161 3.85817 2.85250
C -0.33681 2.80656 1.98336
C -0.19026 3.02774 0.59926
C -1.28663 -0.60479 -2.51294
C -2.37792 -0.11759 -1.60486
C -3.66689 0.06679 -2.12885
C -4.68470 0.41188 -1.28703
C -4.43436 0.53373 0.09281
C -5.47174 0.83453 1.00622
C -5.22171 0.89619 2.35053
C -3.91966 0.64930 2.82579
C -2.88530 0.37400 1.96542
C -3.10508 0.32340 0.57384
H 1.44116 -1.04632 -3.39002
H 0.74234 -2.14698 -2.21623
H 3.70493 -1.82775 -2.71300
H 5.59440 -1.43326 -1.14257
H 6.41075 -0.43809 0.94440
H 5.98299 0.86050 3.00551
H 3.68493 1.65369 3.49876
H 1.83326 1.12967 2.00410
H -0.08665 1.36085 -3.50965
H 1.48226 1.19366 -2.76391
H 0.18697 3.74733 -3.16575
H -0.13152 5.65430 -1.60212
H -0.42755 6.44994 0.67456
H -0.66864 5.99902 3.09712
H -0.60620 3.65349 3.90925
H -0.31438 1.80206 2.36372
H -1.31338 -1.69473 -2.50468
H -1.45929 -0.28985 -3.54126
H -3.82728 -0.06089 -3.18883
H -5.68478 0.57839 -1.66418
H -6.46708 1.00095 0.61661
H -6.01781 1.11935 3.04691
H -3.72766 0.67177 3.88988
H -1.90042 0.17137 2.34765
C -0.37115 -3.13811 0.34600
C -0.55559 -4.54349 0.62526
H 0.40696 -4.99870 0.85430
H -1.22323 -4.65808 1.47833
H -0.99140 -5.03389 -0.24416

66
Oh with Def2-TZVPP (2/5)
Fe 0.01765 -0.00112 0.10429
N 2.11549 -0.29245 -0.24763
N -0.00998 2.14974 -0.28402
N -2.11978 0.04086 -0.30230
N 0.08836 -0.08952 -1.97690
O 0.04255 0.02217 1.72636
N -0.20966 -2.17605 0.14549
C 1.16358 -1.05301 -2.33555
C 2.34493 -0.85484 -1.43151
C 3.61503 -1.28743 -1.84014
C 4.67290 -1.13386 -0.98792
C 4.48193 -0.51528 0.26348
C 5.55436 -0.29952 1.15986
C 5.34506 0.33677 2.35439
C 4.05251 0.78414 2.69042
C 2.98736 0.58419 1.84635
C 3.16939 -0.07905 0.61647
C 0.44972 1.26542 -2.49532
C 0.06677 2.39374 -1.58577
C -0.09774 3.67327 -2.14270
C -0.32968 4.73238 -1.31231
C -0.39454 4.52761 0.08004
C -0.61311 5.59804 0.97797
C -0.66437 5.37486 2.32811
C -0.50146 4.06724 2.82415
C -0.29503 3.00433 1.97875
C -0.23328 3.20141 0.58399
C -1.23676 -0.54177 -2.47986
C -2.36685 -0.09122 -1.60088
C -3.64274 0.08076 -2.16120
C -4.69271 0.38237 -1.33971
C -4.48514 0.49174 0.04912
C -5.54708 0.76631 0.94225
C -5.32099 0.83670 2.29092
C -4.02060 0.63181 2.79262
C -2.96456 0.37644 1.95266
C -3.16410 0.30620 0.55851
H 1.44799 -0.93946 -3.38273
H 0.78216 -2.06417 -2.20932
H 3.73515 -1.73203 -2.81682
H 5.66282 -1.46605 -1.27097
H 6.54087 -0.64156 0.87708
H 6.16660 0.50318 3.03695
H 3.89367 1.29704 3.62915
H 2.00631 0.93042 2.12066
H 0.02241 1.40439 -3.48721
H 1.53302 1.30470 -2.61332
H -0.03590 3.79888 -3.21339
H -0.46282 5.72926 -1.71090
H -0.73380 6.59428 0.57393
H -0.82768 6.19505 3.01311
H -0.53912 3.89365 3.89094
H -0.17755 2.01132 2.37693
H -1.24126 -1.63194 -2.48460
H -1.38431 -0.21768 -3.50897
H -3.77304 -0.02473 -3.22788
H -5.68548 0.53087 -1.74307
H -6.53936 0.91040 0.53608
H -6.13492 1.04148 2.97225
H -3.84924 0.67361 3.85964
H -1.97707 0.21461 2.35064
C -0.36985 -3.27672 0.42329
C -0.56964 -4.66516 0.77065
H 0.29851 -5.24644 0.46287
H -0.70096 -4.75436 1.84826
H -1.45676 -5.04415 0.26511

66
Oh with LACVP (2/3)
Fe -0.03714 -0.05204 -0.02931
N 1.98900 -0.27076 -0.29604
N 0.00007 1.95283 -0.33249
N -2.06596 0.03735 -0.33426
N 0.05032 -0.18875 -2.06641
O 0.02343 -0.06332 1.63395
N -0.22750 -2.04422 0.06990
C 1.12890 -1.18836 -2.37163
C 2.27721 -0.92729 -1.43748
C 3.58018 -1.35186 -1.76763
C 4.61337 -1.08704 -0.89654
C 4.36375 -0.35926 0.29352
C 5.41301 -0.02188 1.19272
C 5.15494 0.71851 2.32723
C 3.83290 1.15005 2.59775
C 2.78702 0.83286 1.74943
C 3.01912 0.06382 0.58278
C 0.44170 1.16257 -2.60232
C 0.15865 2.26676 -1.63077
C 0.12952 3.59226 -2.11664
C -0.05822 4.62892 -1.23564
C -0.22564 4.35379 0.14394
C -0.42039 5.40556 1.08077
C -0.58501 5.13408 2.42260
C -0.56140 3.79109 2.86669
C -0.37901 2.74393 1.97997
C -0.20186 2.98721 0.59587
C -1.30042 -0.62196 -2.54837
C -2.37770 -0.10432 -1.63769
C -3.67311 0.13009 -2.14383
C -4.67727 0.50161 -1.27841
C -4.41192 0.59089 0.11020
C -5.43802 0.90528 1.04403
C -5.17488 0.92409 2.39745
C -3.87238 0.61565 2.86220
C -2.84584 0.32717 1.98101
C -3.07836 0.32759 0.58339
H 1.44426 -1.11028 -3.41784
H 0.73135 -2.19378 -2.22193
H 3.74578 -1.87365 -2.70153
H 5.62388 -1.41010 -1.12085
H 6.41940 -0.35367 0.96100
H 5.95719 0.97728 3.00852
H 3.63548 1.74305 3.48389
H 1.78907 1.16752 1.97578
H -0.06169 1.34562 -3.55607
H 1.51666 1.15542 -2.81039
H 0.25709 3.76657 -3.17729
H -0.08486 5.65601 -1.58197
H -0.43415 6.42581 0.71258
H -0.73119 5.93843 3.13408
H -0.68949 3.57345 3.92122
H -0.36529 1.73050 2.34675
H -1.33295 -1.71632 -2.53085
H -1.46285 -0.30864 -3.58334
H -3.85336 0.02160 -3.20548
H -5.67644 0.70969 -1.64472
H -6.43339 1.11390 0.66655
H -5.96052 1.15687 3.10692
H -3.67606 0.59919 3.92857
H -1.86365 0.07258 2.34933
C -0.39463 -3.16494 0.33681
C -0.60025 -4.56397 0.66363
H 0.35574 -5.04012 0.90021
H -1.26254 -4.65212 1.52997
H -1.05551 -5.08674 -0.18265

66
Oh with LACVP (2/5)
Fe 0.03915 -0.00450 0.01701
N 2.09837 -0.29523 -0.27629
N -0.00408 2.14168 -0.33404
N -2.06560 0.03554 -0.30903
N 0.10622 -0.09115 -2.02736
O 0.07154 -0.00749 1.67533
N -0.21267 -2.23415 0.04628
C 1.17969 -1.09015 -2.37853
C 2.35128 -0.89126 -1.46011
C 3.63679 -1.33598 -1.82686
C 4.68362 -1.16073 -0.94674
C 4.46899 -0.50469 0.29138
C 5.53073 -0.26464 1.20656
C 5.29880 0.41016 2.38743
C 3.99417 0.87318 2.68986
C 2.93634 0.65104 1.82550
C 3.14291 -0.05273 0.61468
C 0.49715 1.27274 -2.55627
C 0.10167 2.40140 -1.64764
C -0.05437 3.69745 -2.18707
C -0.30810 4.75167 -1.33778
C -0.40780 4.52762 0.05884
C -0.65434 5.58861 0.97315
C -0.74230 5.34060 2.32762
C -0.58871 4.01805 2.81264
C -0.35410 2.96195 1.95000
C -0.25505 3.18696 0.55470
C -1.24421 -0.53176 -2.52841
C -2.34967 -0.07124 -1.62176
C -3.64356 0.14083 -2.14107
C -4.67174 0.45304 -1.27793
C -4.42771 0.52832 0.11583
C -5.46837 0.80689 1.04470
C -5.20885 0.83940 2.39902
C -3.89603 0.58778 2.87045
C -2.85744 0.32707 1.99443
C -3.09160 0.30128 0.59765
H 1.47137 -0.97956 -3.42846
H 0.77091 -2.09444 -2.24931
H 3.78181 -1.80595 -2.79108
H 5.68072 -1.50337 -1.20034
H 6.52467 -0.61636 0.95172
H 6.11007 0.59455 3.08200
H 3.82084 1.41492 3.61298
H 1.94863 1.00898 2.07014
H 0.07797 1.40760 -3.55723
H 1.58709 1.28883 -2.66085
H 0.03065 3.84353 -3.25634
H -0.43312 5.75650 -1.72600
H -0.76811 6.59428 0.58245
H -0.92735 6.15142 3.02274
H -0.65641 3.82928 3.87831
H -0.24315 1.95773 2.33163
H -1.25284 -1.62637 -2.54734
H -1.39678 -0.18827 -3.55511
H -3.80858 0.05887 -3.20760
H -5.67284 0.63344 -1.65376
H -6.46884 0.98355 0.66435
H -6.00440 1.04730 3.10519
H -3.70181 0.59639 3.93727
H -1.86302 0.12603 2.36563
C -0.42094 -3.33694 0.36484
C -0.68140 -4.70968 0.75963
H 0.25900 -5.26018 0.85580
H -1.20132 -4.73100 1.72204
H -1.30577 -5.20662 0.01137

67
FeOH Oh with LACVP (2/2)
Fe 0.03598 -0.30633 -0.76462
N 2.06991 -0.47604 -1.05476
N -0.03684 1.71581 -1.17834
N -2.01963 -0.29062 -1.05076
N 0.09188 -0.54018 -2.77715
O 0.11242 -0.15124 1.04582
N -0.04257 -2.27544 -0.48301
C 1.19556 -1.52315 -3.05457
C 2.35854 -1.17238 -2.17188
C 3.66998 -1.55006 -2.52401
C 4.71477 -1.19151 -1.70144
C 4.46477 -0.41592 -0.54214
C 5.52261 0.02092 0.30261
C 5.26189 0.80832 1.40448
C 3.92817 1.18723 1.69675
C 2.87302 0.77307 0.90335
C 3.10974 -0.04487 -0.22952
C 0.42723 0.79235 -3.39115
C 0.05895 1.94051 -2.50086
C -0.10185 3.21403 -3.09084
C -0.35824 4.29992 -2.28946
C -0.45354 4.12478 -0.88700
C -0.70699 5.22735 -0.02517
C -0.79119 5.04904 1.33965
C -0.62400 3.75286 1.88380
C -0.38231 2.65606 1.07445
C -0.28983 2.80621 -0.33219
C -1.24477 -1.05473 -3.22317
C -2.33788 -0.53650 -2.33571
C -3.64776 -0.40741 -2.84422
C -4.66435 -0.03059 -1.99664
C -4.38913 0.18555 -0.62400
C -5.42018 0.52634 0.29492
C -5.14115 0.68704 1.63596
C -3.81554 0.50557 2.10232
C -2.78489 0.19049 1.23486
C -3.03811 0.03551 -0.15048
H 1.47640 -1.49725 -4.11310
H 0.83246 -2.52902 -2.83493
H 3.83346 -2.10792 -3.43720
H 5.73301 -1.47540 -1.94340
H 6.53714 -0.27279 0.05524
H 6.07079 1.14285 2.04380
H 3.72890 1.81512 2.55830
H 1.85999 1.05032 1.14464
H -0.05429 0.88325 -4.36888
H 1.50783 0.82587 -3.56453
H -0.02026 3.31122 -4.16599
H -0.48953 5.28856 -2.71520
H -0.82863 6.21045 -0.46781
H -0.98162 5.89220 1.99393
H -0.68618 3.61351 2.95779
H -0.25340 1.67259 1.49874
H -1.22839 -2.14712 -3.15074
H -1.42226 -0.80195 -4.27220
H -3.82900 -0.60310 -3.89328
H -5.67768 0.09079 -2.36323
H -6.43022 0.64445 -0.08317
H -5.93045 0.94057 2.33448
H -3.60380 0.61278 3.16075
H -1.77470 0.04746 1.58957
C -0.16173 -3.39536 -0.18368
C -0.30830 -4.79199 0.18322
H -1.36043 -5.02198 0.37516
H 0.05203 -5.43402 -0.62597
H 0.27087 -5.00559 1.08647
H 0.44836 -0.96144 1.48418

67
FeOH Oh with LACVP (2/6)
Fe 0.05116 -0.38111 -0.59437
N 2.21366 -0.48761 -1.10843
N -0.10156 1.72758 -0.98364
N -2.11711 -0.47652 -1.04282
N 0.07210 -0.49233 -2.77919
O 0.16203 -0.55625 1.21405
N -0.01028 -2.64189 -0.67817
C 1.24270 -1.33847 -3.17402
C 2.44303 -0.98861 -2.33376
C 3.74516 -1.21408 -2.83372
C 4.83175 -0.90735 -2.04417
C 4.63504 -0.35824 -0.75098
C 5.72392 -0.00195 0.09144
C 5.49530 0.54263 1.33876
C 4.16622 0.74709 1.78735
C 3.08376 0.41049 0.99402
C 3.28982 -0.14964 -0.29123
C 0.25175 0.91516 -3.28270
C -0.10758 2.00056 -2.29811
C -0.35263 3.29978 -2.79954
C -0.57323 4.33501 -1.91898
C -0.55154 4.09321 -0.52159
C -0.75738 5.13207 0.42695
C -0.72754 4.86064 1.77988
C -0.49271 3.53718 2.22842
C -0.29258 2.50118 1.33239
C -0.31489 2.75397 -0.06149
C -1.22196 -1.09639 -3.22538
C -2.37342 -0.68880 -2.34327
C -3.67808 -0.62182 -2.88236
C -4.73844 -0.33830 -2.04930
C -4.51462 -0.13578 -0.66349
C -5.57649 0.13609 0.24282
C -5.32196 0.30572 1.58856
C -3.99412 0.20380 2.07526
C -2.93643 -0.05053 1.22053
C -3.16864 -0.21757 -0.16751
H 1.46683 -1.21638 -4.23990
H 0.97728 -2.38645 -3.01251
H 3.86877 -1.61663 -3.83128
H 5.84155 -1.06861 -2.40559
H 6.73435 -0.16547 -0.26813
H 6.32712 0.81475 1.97836
H 3.99470 1.17348 2.76963
H 2.07408 0.55152 1.35093
H -0.31598 1.04800 -4.20924
H 1.30813 1.04849 -3.54119
H -0.35885 3.46256 -3.86994
H -0.76356 5.33875 -2.28287
H -0.93464 6.13917 0.06453
H -0.88217 5.65459 2.50150
H -0.46927 3.33148 3.29300
H -0.11849 1.49286 1.68359
H -1.11919 -2.18499 -3.17017
H -1.42470 -0.84214 -4.27119
H -3.82428 -0.79012 -3.94187
H -5.74757 -0.27118 -2.44105
H -6.58754 0.20065 -0.14546
H -6.13347 0.50983 2.27776
H -3.80508 0.32378 3.13645
H -1.92636 -0.14255 1.59690
C -0.07925 -3.78493 -0.45357
C -0.16273 -5.20817 -0.17892
H 0.83602 -5.65440 -0.19595
H -0.60637 -5.37598 0.80690
H -0.78249 -5.70280 -0.93258
H 0.38687 -1.24951 1.86122

2_{Oh} with cyclohexene

82
H¹AT Reactant Complex (2/3)
Fe -0.20354 -0.16979 -0.73389
N 1.80595 -0.56910 -0.89637
N 0.00047 1.78566 -1.23359
N -2.20702 0.04147 -1.12794
N -0.06016 -0.52024 -2.74219
O -0.19845 -0.01205 0.92379
N -0.54758 -2.11977 -0.44055
C 0.94241 -1.62644 -2.90283
C 2.07751 -1.35942 -1.95402
C 3.35238 -1.91399 -2.18697
C 4.37402 -1.64246 -1.30438
C 4.14443 -0.78117 -0.20260
C 5.18656 -0.43789 0.70269
C 4.95193 0.43206 1.74676
C 3.66157 0.99238 1.91682
C 2.62231 0.67337 1.06064
C 2.82996 -0.22698 -0.01337
C 0.46109 0.73465 -3.38974
C 0.22519 1.95154 -2.54946
C 0.30910 3.21807 -3.16765
C 0.16728 4.35114 -2.40439
C -0.06722 4.23289 -1.01234
C -0.21889 5.38684 -0.19550
C -0.45112 5.26753 1.15843
C -0.54070 3.97921 1.73633
C -0.40207 2.83576 0.96852
C -0.15808 2.92204 -0.42409
C -1.42494 -0.89203 -3.23495
C -2.48573 -0.20280 -2.42368
C -3.73977 0.08256 -3.00279
C -4.73689 0.61930 -2.21967
C -4.51128 0.82410 -0.83629
C -5.53738 1.31272 0.01935
C -5.31968 1.44286 1.37470
C -4.06550 1.07399 1.92110
C -3.03822 0.61677 1.11533
C -3.22175 0.50053 -0.28484
H 1.29611 -1.68128 -3.93807
H 0.45966 -2.57708 -2.66894
H 3.50682 -2.53880 -3.05736
H 5.36195 -2.06346 -1.45448
H 6.16949 -0.86962 0.54770
H 5.74903 0.69478 2.43252
H 3.48422 1.68759 2.72987
H 1.64781 1.10580 1.21123
H 0.01729 0.85472 -4.38234
H 1.54010 0.62472 -3.53903
H 0.48509 3.27195 -4.23436
H 0.22745 5.33598 -2.85382
H -0.14600 6.36221 -0.66454
H -0.56479 6.14936 1.77806
H -0.72315 3.88132 2.80071
H -0.47700 1.86665 1.43464
H -1.54759 -1.97312 -3.11210
H -1.52685 -0.67162 -4.30119
H -3.89396 -0.11745 -4.05526
H -5.70202 0.87047 -2.64541
H -6.49780 1.56410 -0.41784
H -6.10587 1.80861 2.02502
H -3.90803 1.14496 2.99168
H -2.09533 0.31839 1.54808
C -0.79190 -3.18610 -0.04175
C -1.08639 -4.51178 0.46791
H -2.15435 -4.72682 0.36827
H -0.52002 -5.26591 -0.08649
H -0.80867 -4.56521 1.52739
H -0.29639 -1.51396 4.93296
C 0.19782 -2.11345 4.15510
C 1.72779 -2.08118 4.35460
C 2.41745 -3.17083 3.51098
C 1.92489 -4.57584 3.91517
C 0.42188 -4.62275 4.08841
C -0.34909 -3.52475 4.18072
H -0.06310 -1.63023 3.19931
H 1.96013 -2.24961 5.41621
H 3.50741 -3.10827 3.61771
H 2.23550 -5.31642 3.16481
H 2.41140 -4.88605 4.85446
H -0.03579 -5.60961 4.14807
H -1.42725 -3.63206 4.29466
H 2.19123 -2.99815 2.44834
H 2.11975 -1.09006 4.09546

82
H¹AT Transition State (2/3)
Fe -0.15711 0.01260 0.16559
N 1.87590 -0.34460 -0.10930
N 0.00714 2.02599 -0.33030
N -2.19087 0.22442 -0.18865
N -0.08254 -0.29975 -1.85990
O -0.06293 0.24441 1.91348
N -0.47717 -1.92797 0.44584
C 0.93405 -1.38142 -2.08619
C 2.11135 -1.10501 -1.19561
C 3.38803 -1.60850 -1.52245
C 4.45766 -1.30390 -0.71134
C 4.27027 -0.45754 0.41001
C 5.36053 -0.06313 1.23435
C 5.16473 0.79934 2.29264
C 3.86492 1.29512 2.56262
C 2.77931 0.92105 1.79041
C 2.94883 0.03309 0.69955
C 0.37818 0.97476 -2.50872
C 0.12771 2.18542 -1.65979
C 0.10220 3.44489 -2.30201
C -0.03841 4.58438 -1.54866
C -0.15131 4.47835 -0.14039
C -0.28544 5.63567 0.67520
C -0.38711 5.52393 2.04597
C -0.35809 4.24071 2.64335
C -0.23615 3.09420 1.87780
C -0.12938 3.17347 0.46684
C -1.45042 -0.70886 -2.31104
C -2.50899 -0.06346 -1.46473
C -3.79836 0.14030 -2.00307
C -4.79519 0.63867 -1.19655
C -4.52031 0.91841 0.16482
C -5.53061 1.40072 1.04245
C -5.25206 1.63933 2.37202
C -3.94701 1.39849 2.86795
C -2.93846 0.94124 2.03904
C -3.19027 0.69624 0.66719
H 1.23554 -1.41374 -3.13924
H 0.48408 -2.34601 -1.84560
H 3.50535 -2.21583 -2.41100
H 5.44948 -1.68107 -0.93503
H 6.34858 -0.44758 1.00435
H 5.99877 1.10348 2.91469
H 3.71678 1.98032 3.39020
H 1.79040 1.28135 2.01835
H -0.08977 1.08550 -3.49144
H 1.45698 0.90045 -2.68111
H 0.19410 3.48808 -3.38003
H -0.06477 5.56286 -2.01547
H -0.30233 6.60716 0.19239
H -0.48633 6.40859 2.66462
H -0.43299 4.15195 3.72186
H -0.21244 2.11954 2.34125
H -1.53510 -1.79483 -2.20209
H -1.59286 -0.48049 -3.37163
H -3.97932 -0.09782 -3.04347
H -5.79169 0.81345 -1.58690
H -6.52513 1.56781 0.64239
H -6.02568 2.00263 3.03885
H -3.73360 1.57413 3.91674
H -1.94614 0.75662 2.41812
C -0.73516 -3.05057 0.61972
C -1.05709 -4.45716 0.78560
H -1.97708 -4.56927 1.36592
H -1.19970 -4.92467 -0.19353
H -0.24621 -4.97173 1.30793
H -0.93193 -0.47649 4.45071
C -0.25655 -1.22491 4.01838
C 1.16522 -1.16586 4.57855
C 2.01421 -2.34169 4.06006
C 1.35974 -3.69565 4.40254
C -0.12377 -3.69803 4.13876
C -0.84851 -2.56258 3.94733
H -0.18238 -0.69839 2.85344
H 1.11052 -1.20745 5.67845
H 3.02592 -2.29591 4.47866
H 1.83891 -4.50722 3.83779
H 1.52998 -3.94065 5.46471
H -0.62944 -4.66159 4.14263
H -1.91887 -2.63370 3.76625
H 2.11502 -2.25392 2.96950
H 1.63425 -0.20937 4.32455

82
H¹AT Intermediate (2/3)
Fe -0.14218 -0.25444 -0.68684
N 1.87843 -0.60365 -0.91113
N -0.00993 1.75709 -1.13906
N -2.17858 -0.05427 -1.04678
N -0.04559 -0.53668 -2.69398
O -0.11138 -0.07180 1.12054
N -0.41088 -2.19979 -0.38016
C 0.97763 -1.61546 -2.91707
C 2.14055 -1.34126 -2.00794
C 3.42789 -1.82227 -2.32134
C 4.47837 -1.52211 -1.48304
C 4.26015 -0.70644 -0.34497
C 5.32965 -0.32604 0.51239
C 5.10380 0.50131 1.59237
C 3.79359 0.97539 1.85137
C 2.72696 0.61727 1.04534
C 2.92866 -0.23486 -0.06893
C 0.41885 0.74849 -3.32396
C 0.14553 1.94408 -2.46157
C 0.13335 3.21559 -3.07812
C -0.03186 4.33821 -2.30410
C -0.18673 4.20207 -0.90258
C -0.35298 5.34156 -0.06807
C -0.50047 5.19982 1.29572
C -0.48655 3.90425 1.86631
C -0.33177 2.77296 1.08357
C -0.17751 2.88507 -0.32108
C -1.40779 -0.94618 -3.16967
C -2.47595 -0.30077 -2.33674
C -3.74946 -0.05967 -2.89438
C -4.75286 0.43362 -2.09181
C -4.50391 0.65728 -0.71541
C -5.52723 1.11860 0.15854
C -5.27839 1.28777 1.50439
C -3.99216 0.99406 2.02135
C -2.96860 0.55948 1.19833
C -3.18983 0.39156 -0.19109
H 1.29007 -1.63831 -3.96666
H 0.52553 -2.58184 -2.68624
H 3.56926 -2.40930 -3.21983
H 5.47864 -1.88224 -1.69677
H 6.32570 -0.69472 0.29175
H 5.92192 0.79378 2.24050
H 3.62192 1.63292 2.69661
H 1.72992 0.96330 1.26330
H -0.03704 0.86591 -4.31120
H 1.50015 0.68054 -3.48190
H 0.25509 3.28224 -4.15192
H -0.04732 5.32632 -2.75058
H -0.35861 6.32298 -0.53065
H -0.62474 6.07084 1.92908
H -0.59911 3.79317 2.93953
H -0.31731 1.78937 1.52656
H -1.49283 -2.03215 -3.05997
H -1.52853 -0.71676 -4.23212
H -3.91427 -0.26370 -3.94458
H -5.73710 0.64144 -2.49684
H -6.50845 1.32193 -0.25731
H -6.06231 1.63370 2.16851
H -3.80581 1.10971 3.08365
H -1.98845 0.33237 1.59133
C -0.64434 -3.29779 -0.06721
C -0.93447 -4.66285 0.32920
H -1.96734 -4.91859 0.07471
H -0.26056 -5.35789 -0.18001
H -0.79868 -4.76415 1.41150
H 0.21446 -0.70906 3.95905
C 0.51659 -1.75322 3.97322
C 1.97330 -2.08522 4.17696
C 2.30762 -3.50737 3.67360
C 1.30975 -4.55418 4.21818
C -0.11946 -4.11486 4.02364
C -0.44625 -2.76280 3.90183
H 0.09638 -0.89904 1.61001
H 2.22146 -2.00975 5.25075
H 3.33163 -3.77820 3.95524
H 1.48078 -5.52672 3.73804
H 1.50247 -4.71750 5.29357
H -0.90451 -4.86679 4.03306
H -1.49077 -2.48439 3.77735
H 2.26306 -3.51300 2.57550
H 2.60867 -1.34542 3.67349

82
H²AT Reactant Complex (2/3)
Fe 0.02770 -0.02072 0.26909
N 0.22681 -0.21388 2.30421
N 2.02853 -0.00604 -0.06997
N -0.21166 -0.41264 -1.73053
N 0.24610 -2.04689 0.42732
O -0.23863 1.62251 0.29662
N -1.95302 -0.24143 0.45649
C -0.48466 -2.44711 1.67709
C -0.17823 -1.42485 2.73596
C -0.30965 -1.74440 4.10253
C -0.01413 -0.78678 5.04713
C 0.45799 0.48547 4.63874
C 0.82149 1.48308 5.58526
C 1.31646 2.70054 5.16729
C 1.46935 2.95793 3.78240
C 1.11733 2.01411 2.83404
C 0.59225 0.76024 3.23267
C 1.71473 -2.33859 0.58278
C 2.57447 -1.22819 0.06282
C 3.93240 -1.50411 -0.20789
C 4.75760 -0.48628 -0.61954
C 4.23394 0.82118 -0.77232
C 5.06262 1.89594 -1.19669
C 4.54834 3.16630 -1.34819
C 3.17874 3.39741 -1.07890
C 2.34389 2.37252 -0.66805
C 2.84040 1.05684 -0.49755
C -0.32995 -2.66341 -0.81040
C -0.18082 -1.73602 -1.98347
C -0.10368 -2.26298 -3.28958
C -0.07852 -1.40141 -4.36311
C -0.18662 -0.00555 -4.14732
C -0.23590 0.91241 -5.23304
C -0.40892 2.26135 -5.00563
C -0.54989 2.73542 -3.67781
C -0.48353 1.87391 -2.59746
C -0.27879 0.48616 -2.79777
H -0.18377 -3.45076 1.99701
H -1.55519 -2.47581 1.46567
H -0.63629 -2.73702 4.38515
H -0.11617 -1.00207 6.10496
H 0.70771 1.26020 6.64075
H 1.59587 3.45761 5.89081
H 1.87285 3.91067 3.45779
H 1.23735 2.23144 1.78623
H 1.96165 -3.28499 0.09284
H 1.92978 -2.47027 1.64807
H 4.29808 -2.51548 -0.08527
H 5.80419 -0.67045 -0.83474
H 6.10900 1.69101 -1.39617
H 5.18331 3.98339 -1.67026
H 2.77089 4.39520 -1.19660
H 1.30418 2.57692 -0.46992
H -1.39820 -2.83253 -0.64006
H 0.12446 -3.63819 -1.00778
H -0.05820 -3.33589 -3.42480
H 0.00332 -1.77963 -5.37602
H -0.15082 0.52355 -6.24214
H -0.45409 2.95725 -5.83538
H -0.71955 3.79213 -3.50317
H -0.61394 2.24643 -1.59269
C -3.11298 -0.14793 0.49361
C -4.55702 -0.02152 0.54487
H -5.00099 -0.37544 -0.39021
H -4.95966 -0.61123 1.37372
H -4.82651 1.03088 0.69296
H -2.21152 3.65368 0.79798
C -3.06324 4.34767 0.76253
C -3.39328 4.70494 -0.70202
C -4.77196 5.38504 -0.80814
C -5.88866 4.45348 -0.29235
C -5.50509 3.77260 1.00439
C -4.24837 3.74015 1.48180
H -2.73318 5.25045 1.30255
H -3.39844 3.78653 -1.30738
H -4.97724 5.68148 -1.84412
H -6.81817 5.02219 -0.14888
H -6.12315 3.69267 -1.05453
H -6.30959 3.30621 1.57200
H -4.04860 3.26302 2.44079
H -4.76360 6.30667 -0.20824
H -2.61136 5.35374 -1.11598

82
H²AT Transition State (2/3)
Fe -0.01012 0.06387 0.22684
N 2.02466 -0.16415 -0.01982
N -0.01957 2.06922 -0.30492
N -2.05844 0.11749 -0.12055
N 0.09334 -0.26985 -1.78916
O 0.02510 0.32775 1.97498
N -0.19107 -1.89225 0.55109
C 1.16854 -1.30144 -1.98117
C 2.31599 -0.94665 -1.07668
C 3.62227 -1.39649 -1.36079
C 4.65801 -1.01356 -0.53801
C 4.40845 -0.13434 0.54591
C 5.45998 0.34549 1.37515
C 5.20006 1.24314 2.38971
C 3.87389 1.69298 2.60789
C 2.82430 1.23551 1.83082
C 3.06003 0.30428 0.78866
C 0.49941 1.01803 -2.44864
C 0.13153 2.22055 -1.63250
C 0.02552 3.46517 -2.29371
C -0.23554 4.59797 -1.56207
C -0.39221 4.49957 -0.15751
C -0.65705 5.65026 0.63516
C -0.80451 5.54536 2.00230
C -0.69034 4.27627 2.61945
C -0.43818 3.13575 1.87700
C -0.28242 3.20880 0.47029
C -1.24941 -0.74763 -2.24801
C -2.34688 -0.16122 -1.40580
C -3.63867 -0.01090 -1.95541
C -4.66839 0.41845 -1.14986
C -4.42655 0.66665 0.22392
C -5.47285 1.05961 1.10409
C -5.22623 1.25080 2.44753
C -3.91906 1.04854 2.95596
C -2.87462 0.68288 2.12583
C -3.09356 0.49576 0.73850
H 1.48988 -1.33600 -3.02846
H 0.76372 -2.28327 -1.73009
H 3.78913 -2.02677 -2.22512
H 5.67078 -1.35184 -0.72733
H 6.46971 -0.00157 1.18334
H 6.00468 1.61205 3.01539
H 3.67705 2.41053 3.39691
H 1.81664 1.57143 2.01371
H 0.06542 1.07937 -3.45113
H 1.58694 1.00971 -2.57502
H 0.15071 3.50289 -3.36844
H -0.32589 5.56510 -2.04423
H -0.73731 6.61130 0.13805
H -1.00424 6.42511 2.60343
H -0.80204 4.19381 3.69526
H -0.34709 2.17239 2.35639
H -1.27807 -1.83681 -2.13786
H -1.39734 -0.52722 -3.30929
H -3.79613 -0.23381 -3.00299
H -5.66714 0.55584 -1.54944
H -6.46895 1.19304 0.69534
H -6.02732 1.54397 3.11653
H -3.73351 1.17942 4.01659
H -1.87981 0.52318 2.51447
C -0.42740 -3.00386 0.80618
C -0.72546 -4.39415 1.09852
H -1.62183 -4.46435 1.72160
H -0.89910 -4.94513 0.16935
H 0.11221 -4.85232 1.63137
H 0.53685 -0.55410 2.81169
C 0.99467 -1.13365 3.85928
C -0.21965 -1.33989 4.77074
C 0.02138 -2.48863 5.77631
C 0.36566 -3.79744 5.03561
C 1.42592 -3.57725 3.98414
C 1.72744 -2.34883 3.48758
H 1.65451 -0.30617 4.15153
H -1.09743 -1.59597 4.15967
H -0.86604 -2.62805 6.40449
H 0.70667 -4.56205 5.74564
H -0.54455 -4.21026 4.56956
H 2.00785 -4.44057 3.66722
H 2.56716 -2.24137 2.80420
H 0.85249 -2.22120 6.44294
H -0.46045 -0.40921 5.29568

82
H²AT Intermediate (2/3)
Fe 0.03413 -0.31051 -0.76331
N 2.06808 -0.47667 -1.05799
N -0.03729 1.71377 -1.17531
N -2.02261 -0.29188 -1.05036
N 0.08759 -0.54239 -2.77775
O 0.11048 -0.16074 1.04601
N -0.04596 -2.27819 -0.49139
C 1.19302 -1.52237 -3.05813
C 2.35618 -1.17256 -2.17535
C 3.66756 -1.55094 -2.52757
C 4.71257 -1.19345 -1.70488
C 4.46307 -0.41634 -0.54636
C 5.52113 0.02174 0.29772
C 5.26110 0.81313 1.39682
C 3.92779 1.19568 1.68687
C 2.87225 0.77917 0.89461
C 3.10847 -0.04377 -0.23491
C 0.41742 0.79145 -3.39133
C 0.05243 1.93878 -2.49815
C -0.11087 3.21272 -3.08687
C -0.36286 4.29854 -2.28398
C -0.45079 4.12308 -0.88104
C -0.69838 5.22537 -0.01714
C -0.77458 5.04634 1.34809
C -0.60530 3.74970 1.89064
C -0.36948 2.65318 1.07923
C -0.28505 2.80420 -0.32784
C -1.24807 -1.06105 -3.22126
C -2.34163 -0.54380 -2.33380
C -3.65269 -0.42101 -2.84129
C -4.66955 -0.04380 -1.99427
C -4.39289 0.18133 -0.62332

C -5.42316 0.52553 0.29522
C -5.14176 0.69779 1.63437
C -3.81440 0.52523 2.09920
C -2.78476 0.20623 1.23198
C -3.04066 0.03845 -0.15129
H 1.47343 -1.49337 -4.11676
H 0.83198 -2.52948 -2.84103
H 3.83069 -2.10886 -3.44082
H 5.73054 -1.47863 -1.94643
H 6.53543 -0.27374 0.05153
H 6.07019 1.14894 2.03520
H 3.72919 1.82869 2.54481
H 1.85964 1.05993 1.13313
H -0.06929 0.88300 -4.36649
H 1.49706 0.82708 -3.57043
H -0.03430 3.31039 -4.16238
H -0.49578 5.28735 -2.70883
H -0.82175 6.20887 -0.45843
H -0.96038 5.88932 2.00394
H -0.66130 3.60998 2.96494
H -0.23957 1.66859 1.50113
H -1.22882 -2.15322 -3.14694
H -1.42756 -0.81056 -4.27059
H -3.83460 -0.62213 -3.88924
H -5.68384 0.07194 -2.35999
H -6.43435 0.63772 -0.08161
H -5.93044 0.95421 2.33255
H -3.60046 0.64242 3.15612
H -1.77295 0.06926 1.58457
C -0.16281 -3.39857 -0.19315
C -0.30180 -4.79265 0.18354
H -1.34179 -5.11304 0.07304
H 0.33245 -5.42109 -0.44857
H 0.00091 -4.92001 1.22827
H 0.44479 -0.96525 1.50189
C 1.26005 -1.79982 3.73819
C 0.08233 -1.52627 4.64263
C -0.24424 -2.74735 5.53230
C -0.33337 -4.04905 4.70335
C 0.86682 -4.21369 3.80460
C 1.60271 -3.10575 3.38037
H 1.87093 -0.96531 3.40337
H -0.80570 -1.26940 4.03867
H -1.18072 -2.57973 6.07655
H -0.43221 -4.91603 5.36937
H -1.25679 -4.03238 4.09774
H 1.16556 -5.21493 3.50479
H 2.47616 -3.26520 2.75125
H 0.55019 -2.86028 6.28261
H 0.28014 -0.64530 5.26704

82
Rebound Transition State (2/3)
Fe 0.03897 -0.53340 -0.70113
N 2.19626 -0.61744 -1.19128
N 0.02080 1.51662 -1.00389
N -2.12215 -0.50536 -1.06557
N 0.00766 -0.64252 -2.81337
O 0.13118 -0.55603 1.20269
N -0.00083 -2.51409 -0.58737
C 1.18804 -1.46617 -3.22777
C 2.40451 -1.05311 -2.44191
C 3.69466 -1.15082 -3.01501
C 4.79304 -0.78588 -2.26812
C 4.61761 -0.31979 -0.93950
C 5.71209 0.07702 -0.12170
C 5.49818 0.52175 1.16717
C 4.17937 0.57869 1.68791
C 3.09152 0.20221 0.92084
C 3.28373 -0.24729 -0.41012
C 0.11461 0.75259 -3.35118
C -0.00827 1.83155 -2.30924
C -0.10539 3.16245 -2.78752
C -0.16124 4.20335 -1.89553
C -0.12115 3.92941 -0.50482
C -0.16885 4.97507 0.45735
C -0.12901 4.69112 1.80705
C -0.04098 3.34398 2.23377
C 0.00616 2.30204 1.32302
C -0.03175 2.56255 -0.06907
C -1.28094 -1.29787 -3.20002
C -2.41470 -0.81053 -2.33761
C -3.72863 -0.74220 -2.85861
C -4.76162 -0.35449 -2.03402
C -4.49742 -0.03726 -0.67667
C -5.52299 0.36171 0.22505
C -5.22421 0.65211 1.54086
C -3.88707 0.54804 2.00421
C -2.86413 0.16686 1.15486
C -3.14356 -0.12538 -0.20388
H 1.36698 -1.37218 -4.30516
H 0.95947 -2.51598 -3.02496
H 3.79785 -1.50100 -4.03470
H 5.79247 -0.84353 -2.68592
H 6.71520 0.02091 -0.53180
H 6.33501 0.82378 1.78710
H 4.02405 0.92083 2.70573
H 2.08216 0.20886 1.31129
H -0.64009 0.90736 -4.12994
H 1.08726 0.86621 -3.84305
H -0.13131 3.33509 -3.85661
H -0.23525 5.22991 -2.23766
H -0.23639 5.99919 0.10464
H -0.16478 5.49096 2.53836
H -0.01072 3.12305 3.29572
H 0.07004 1.27385 1.64962
H -1.16589 -2.37629 -3.05406
H -1.49638 -1.13400 -4.26194
H -3.90092 -0.99020 -3.89871
H -5.77691 -0.28659 -2.40978
H -6.54166 0.42975 -0.14283
H -6.00869 0.95534 2.22533
H -3.66623 0.76935 3.04312
H -1.84103 0.06261 1.49443
C -0.02957 -3.66917 -0.42671
C -0.06073 -5.10853 -0.23159
H -1.09411 -5.46680 -0.21425
H 0.47271 -5.61147 -1.04371
H 0.41819 -5.36978 0.71677
H 0.18145 -1.47639 1.53100
C 0.55395 -0.82957 3.98901
C -0.81435 -0.98307 4.57937
C -0.91687 -2.22154 5.49616
C -0.31654 -3.47482 4.82555
C 1.02506 -3.19959 4.22072
C 1.42149 -1.92133 3.85639
H 0.89187 0.15894 3.70292
H -1.54215 -1.07036 3.75465
H -1.96163 -2.40100 5.76752
H -0.24346 -4.30401 5.53943
H -0.98962 -3.83646 4.02647
H 1.69790 -4.03622 4.05309
H 2.40861 -1.76472 3.43429
H -0.36994 -2.02147 6.42650
H -1.09305 -0.07086 5.12001

82
Rebound Product (2/3)
Fe -0.09519 -0.42075 -1.19279
N 1.95214 -0.53327 -1.54442
N -0.01327 1.61617 -1.31269
N -2.15956 -0.44564 -1.43109
N -0.16184 -0.27738 -3.36909
O 0.04274 -0.96301 2.64034
N -0.17342 -2.38134 -0.94084
C 1.06315 -1.01295 -3.77994
C 2.22039 -0.70491 -2.85271
C 3.53621 -0.66185 -3.36653
C 4.59250 -0.44317 -2.51010
C 4.35386 -0.29736 -1.12002
C 5.41296 -0.09930 -0.19103
C 5.14973 0.00236 1.15907
C 3.81569 -0.10553 1.62686
C 2.75926 -0.28847 0.75187
C 2.99935 -0.36708 -0.64419
C -0.12632 1.16362 -3.73800
C -0.01824 2.10458 -2.56097
C 0.06478 3.49123 -2.84100
C 0.14704 4.38858 -1.80509
C 0.14570 3.91778 -0.46585
C 0.22118 4.81210 0.63621
C 0.21304 4.33388 1.93047
C 0.12968 2.93951 2.15956
C 0.05756 2.03995 1.10879
C 0.06347 2.50290 -0.23198
C -1.44400 -0.93776 -3.72217
C -2.52314 -0.59181 -2.71873
C -3.86840 -0.49325 -3.14044
C -4.85532 -0.24998 -2.21093
C -4.51776 -0.13876 -0.83827
C -5.50328 0.07043 0.16592
C -5.14574 0.12849 1.49693
C -3.78748 -0.03424 1.86921
C -2.80084 -0.22526 0.91845
C -3.13696 -0.26178 -0.45899
H 1.33882 -0.78712 -4.81700
H 0.85032 -2.08640 -3.72682
H 3.69197 -0.79129 -4.43018
H 5.60854 -0.38723 -2.88535
H 6.42898 -0.03907 -0.56689
H 5.95789 0.15158 1.86607
H 3.61952 -0.04948 2.69203
H 1.76063 -0.40193 1.15464
H -1.03171 1.41716 -4.30230
H 0.71424 1.34908 -4.41732
H 0.06036 3.82099 -3.87290
H 0.21114 5.45456 -1.99470
H 0.28347 5.87663 0.43590
H 0.26915 5.01758 2.76988
H 0.12201 2.56478 3.17731
H -0.00256 0.98581 1.34421
H -1.28641 -2.02167 -3.70021
H -1.76953 -0.67757 -4.73657
H -4.10067 -0.60137 -4.19249
H -5.89176 -0.15165 -2.51500
H -6.54008 0.17158 -0.13728
H -5.89881 0.28347 2.26118
H -3.51685 -0.01825 2.91926
H -1.78165 -0.37963 1.24732
C -0.21683 -3.53444 -0.77015
C -0.27292 -4.97075 -0.56156
H -1.18712 -5.23981 -0.02429
H -0.26539 -5.49160 -1.52394
H 0.59049 -5.30223 0.02281
H -0.13364 -1.88495 2.35781
C 0.27447 -0.93888 4.10673
C -1.02211 -1.23619 4.87145
C -0.72745 -1.46002 6.36755
C 0.21436 -2.66545 6.57041
C 1.34467 -2.67815 5.56698
C 1.37912 -1.89836 4.47436
H 0.58758 0.09739 4.27887
H -1.47710 -2.14440 4.45003
H -1.66289 -1.61218 6.91761
H 0.62515 -2.65964 7.58916
H -0.35402 -3.60574 6.48616
H 2.16921 -3.36146 5.76304
H 2.23035 -1.92894 3.79775
H -0.25778 -0.55722 6.78282
H -1.73403 -0.41590 4.72730

82
Desaturation Transition State (2/3)
Fe 0.03498 -0.54534 -0.81269
N 2.20962 -0.52202 -1.26188
N -0.07931 1.52530 -0.92852
N -2.12239 -0.57617 -1.21251
N 0.06090 -0.46270 -2.90877
O 0.11010 -0.70971 1.07032
N 0.05518 -2.53179 -0.86387
C 1.25701 -1.24228 -3.37008
C 2.45321 -0.88408 -2.52903
C 3.75890 -0.94913 -3.07048
C 4.83470 -0.62707 -2.27254
C 4.62073 -0.23119 -0.92671
C 5.68990 0.12802 -0.05970
C 5.43708 0.51098 1.24199
C 4.10351 0.54206 1.72627
C 3.03951 0.19925 0.91182
C 3.27208 -0.18803 -0.43215
C 0.18526 0.97662 -3.31494
C -0.07734 1.95258 -2.20191
C -0.25238 3.30957 -2.57004
C -0.42014 4.26128 -1.59549
C -0.41647 3.86863 -0.23313
C -0.57859 4.81911 0.81180
C -0.57171 4.42030 2.13262
C -0.40369 3.04964 2.44646
C -0.24664 2.09767 1.45348
C -0.24709 2.47742 0.08845
C -1.21198 -1.08015 -3.40299
C -2.37632 -0.71702 -2.52065
C -3.67855 -0.60901 -3.06347
C -4.74053 -0.36253 -2.22124
C -4.51841 -0.23512 -0.82549
C -5.57788 -0.00544 0.09590
C -5.32053 0.09099 1.44852
C -3.99217 -0.04208 1.92925
C -2.93624 -0.25722 1.06240
C -3.17351 -0.35156 -0.33255
H 1.45290 -1.05431 -4.43203
H 1.03388 -2.30674 -3.26168
H 3.89193 -1.24002 -4.10527
H 5.84584 -0.66240 -2.66376
H 6.70457 0.09521 -0.44314
H 6.25467 0.78548 1.89932
H 3.91761 0.83705 2.75371
H 2.02042 0.18571 1.27424
H -0.48131 1.18351 -4.15886
H 1.20470 1.14777 -3.67841
H -0.24809 3.57347 -3.62066
H -0.55572 5.30652 -1.85172
H -0.70639 5.86321 0.54509
H -0.69393 5.14818 2.92706
H -0.39841 2.73798 3.48589
H -0.12171 1.05138 1.69257
H -1.08547 -2.16729 -3.38042
H -1.39925 -0.79461 -4.44392
H -3.82006 -0.71903 -4.13158
H -5.74801 -0.26785 -2.61199
H -6.58958 0.08553 -0.28609
H -6.13117 0.26261 2.14806
H -3.80388 0.02417 2.99571
H -1.91791 -0.37112 1.41425
C 0.04009 -3.69679 -0.80575
C 0.02161 -5.14810 -0.74021
H -0.89499 -5.53550 -1.19471
H 0.88202 -5.56204 -1.27425
H 0.06349 -5.47889 0.30171
H 0.14360 -1.65351 1.32887
C 1.76580 -1.88321 4.53055
C 0.81301 -0.76475 4.31611
C -0.51981 -0.97376 5.06673
C -1.07188 -2.40056 4.86127
C -0.01549 -3.44742 5.03274
C 1.33688 -3.16264 4.89269
H 2.82328 -1.70619 4.35345
H 0.61957 -0.67930 3.22094
H -1.25705 -0.23423 4.73884
H -1.90859 -2.59762 5.54280
H -1.49607 -2.50296 3.84576
H -0.32886 -4.46646 5.24316
H 2.06808 -3.95293 5.02630
H -0.35172 -0.80943 6.13907
H 1.27756 0.19067 4.59077

82
Desaturation Product (2/3)
Fe -0.05202 -0.45427 -0.73975
N 2.19842 -0.42594 -1.21032
N -0.16209 1.57344 -0.78811
N -2.18359 -0.52309 -1.27384
N 0.11567 -0.26083 -2.90005
O 0.30147 -0.93350 1.32634
N -0.05384 -2.43426 -0.84747
C 1.23157 -1.15926 -3.32153
C 2.41466 -1.01708 -2.39015
C 3.69050 -1.49231 -2.78493
C 4.75792 -1.34282 -1.92740
C 4.58384 -0.65683 -0.69432
C 5.65990 -0.39546 0.19839
C 5.45254 0.34232 1.34726
C 4.16262 0.85644 1.64004
C 3.09157 0.60000 0.80296
C 3.27193 -0.17666 -0.36925
C 0.46186 1.17421 -3.13936
C 0.08620 2.08982 -2.00462
C 0.06466 3.48188 -2.26708
C -0.20643 4.36386 -1.24996
C -0.49821 3.86620 0.04614
C -0.81251 4.73590 1.12582
C -1.12679 4.22870 2.37011
C -1.14634 2.82734 2.56871
C -0.83750 1.95501 1.53912
C -0.49234 2.44551 0.25537
C -1.19146 -0.64897 -3.50464
C -2.37268 -0.39759 -2.59234
C -3.64871 -0.14372 -3.15344
C -4.74456 -0.04091 -2.32450
C -4.59102 -0.22665 -0.92513
C -5.68718 -0.18460 -0.01946
C -5.49125 -0.41510 1.32768
C -4.19142 -0.70392 1.81852
C -3.10270 -0.73682 0.96679
C -3.27404 -0.48437 -0.41811
H 1.54393 -0.93884 -4.35182
H 0.86729 -2.18954 -3.31039
H 3.80796 -1.96749 -3.75161
H 5.74093 -1.71559 -2.19502
H 6.64719 -0.77227 -0.04843
H 6.27660 0.54688 2.02144
H 4.01940 1.46586 2.52580
H 2.11619 1.02069 1.00780
H -0.00539 1.52678 -4.06669
H 1.54372 1.25086 -3.28929
H 0.27155 3.82937 -3.27178
H -0.21412 5.43386 -1.42628
H -0.80582 5.80599 0.94683
H -1.36764 4.89472 3.19068
H -1.41342 2.42879 3.54121
H -0.88438 0.89264 1.71101
H -1.16070 -1.72504 -3.70977
H -1.34021 -0.14592 -4.46711
H -3.74446 -0.03125 -4.22653
H -5.72883 0.16770 -2.72998
H -6.67859 0.02092 -0.40974
H -6.32993 -0.38788 2.01422
H -4.05265 -0.90633 2.87496
H -2.11447 -0.97638 1.33890
C -0.12922 -3.59812 -0.89311
C -0.22347 -5.04650 -0.95759
H -1.13804 -5.34246 -1.47995
H 0.63737 -5.45870 -1.49232
H -0.24377 -5.46827 0.05169
H 0.35115 -1.89813 1.46209
C 1.90979 -1.14126 4.15161
C 1.13069 -0.10660 4.54682
C -0.11961 -0.35640 5.36663
C -0.75311 -1.73556 5.06972
C 0.28959 -2.82235 4.90000
C 1.52869 -2.52963 4.45185
H 2.84793 -0.96333 3.63339
H 0.70727 -0.48528 2.10128
H -0.85844 0.43610 5.20372
H -1.45830 -1.99933 5.86575
H -1.35249 -1.67668 4.14404
H -0.00348 -3.85077 5.09512
H 2.26466 -3.31177 4.28988
H 0.15578 -0.29845 6.43398
H 1.43787 0.92173 4.37150

82
H^{1}AT Reactant Complex (2/5)
Fe 0.24085 -0.29088 -0.84782
N 2.28024 -0.36775 -1.33563
N -0.07697 1.82902 -1.22636
N -1.87289 -0.48828 -0.97078
N 0.12673 -0.41718 -2.89012
O 0.43610 -0.24798 0.79971
N 0.23764 -2.53798 -0.76691
C 1.25912 -1.31272 -3.32498
C 2.48405 -0.97229 -2.52468
C 3.77024 -1.29576 -2.99999
C 4.86886 -0.98708 -2.22573
C 4.70103 -0.31487 -0.98906
C 5.81079 0.06507 -0.18499
C 5.61807 0.75623 0.99346
C 4.30531 1.09667 1.40434
C 3.20201 0.73646 0.65029
C 3.37015 0.01163 -0.55407
C 0.32960 0.96666 -3.46818
C -0.11655 2.06643 -2.54775
C -0.47093 3.32142 -3.08976
C -0.77289 4.35977 -2.23648
C -0.72398 4.16061 -0.83355
C -1.01438 5.20753 0.08411
C -0.95652 4.98355 1.44430
C -0.60786 3.69961 1.93248
C -0.32511 2.65734 1.06747
C -0.37250 2.85908 -0.33410
C -1.21339 -0.99814 -3.25622
C -2.26856 -0.63424 -2.25077
C -3.62053 -0.55536 -2.64313
C -4.58814 -0.34266 -1.68431
C -4.22169 -0.23933 -0.31963
C -5.19184 -0.07032 0.70694
C -4.80923 -0.01402 2.03103
C -3.43844 -0.12875 2.37333
C -2.46726 -0.27667 1.39911
C -2.82930 -0.32572 0.03084
H 1.44122 -1.20070 -4.39895
H 0.96822 -2.34927 -3.14216
H 3.87576 -1.77715 -3.96373
H 5.86890 -1.23484 -2.56416
H 6.80870 -0.19218 -0.52335
H 6.46552 1.04784 1.60288
H 4.16143 1.65329 2.32365
H 2.20875 1.00256 0.97645
H -0.17417 1.03220 -4.43660
H 1.40127 1.09420 -3.65279
H -0.49813 3.44969 -4.16429
H -1.04998 5.33285 -2.62689
H -1.27874 6.18363 -0.30867
H -1.17564 5.78383 2.14172
H -0.56223 3.53004 3.00256
H -0.06403 1.68214 1.45144
H -1.11363 -2.08837 -3.26372
H -1.49613 -0.68988 -4.26649
H -3.87753 -0.66063 -3.68929
H -5.63346 -0.26533 -1.96247
H -6.23690 0.00154 0.42511
H -5.55141 0.10746 2.81164
H -3.14001 -0.10924 3.41583
H -1.42709 -0.37389 1.67377
C 0.18366 -3.65454 -0.43314
C 0.11667 -5.04533 -0.02134
H 1.07912 -5.53661 -0.19222
H -0.12745 -5.10994 1.04315
H -0.65406 -5.57186 -0.59182
H 1.82969 -0.92811 4.90548
C 0.91887 -1.31702 4.42812
C 0.93962 -2.85996 4.42727
C -0.45068 -3.42890 4.08383
C -1.50169 -2.98008 5.12035
C -1.37187 -1.51041 5.45947

C -0.30022 -0.76609 5.13676
H 0.94390 -0.94315 3.39147
H 1.23759 -3.22010 5.42277
H -0.41734 -4.52442 4.03161
H -2.51401 -3.18595 4.74493
H -1.39990 -3.58039 6.03934
H -2.20232 -1.05539 5.99823
H -0.28027 0.29115 5.39862
H -0.74955 -3.06885 3.08801
H 1.69242 -3.22637 3.71817

82
H^{1}AT Transition State (2/5)
Fe 0.24581 -0.04859 0.08134
N 2.35890 -0.10707 -0.47518
N -0.04002 2.06998 -0.32462
N -1.92702 -0.22208 -0.21420
N 0.17766 -0.16479 -2.06426
O 0.42399 -0.07979 1.77525
N 0.23439 -2.29142 0.05964
C 1.33347 -1.02141 -2.48750
C 2.55575 -0.67338 -1.67889
C 3.84408 -0.96162 -2.18164
C 4.94896 -0.65370 -1.41812
C 4.78639 -0.02403 -0.15720
C 5.89661 0.35170 0.64830
C 5.70133 0.99312 1.85453
C 4.38561 1.28271 2.29601
C 3.28298 0.92461 1.54068
C 3.45472 0.25759 0.30271
C 0.35018 1.23208 -2.59629
C -0.08704 2.31404 -1.64493
C -0.44255 3.57604 -2.17423
C -0.73544 4.61131 -1.31542
C -0.67354 4.40525 0.08607
C -0.94994 5.44820 1.01247
C -0.87638 5.21707 2.37084
C -0.52481 3.92966 2.84771
C -0.25599 2.89140 1.97356
C -0.32135 3.10030 0.57379
C -1.13533 -0.76885 -2.45794
C -2.24511 -0.40250 -1.50717
C -3.57709 -0.35192 -1.97700
C -4.60076 -0.12857 -1.08211
C -4.31180 0.02872 0.29730
C -5.33377 0.22824 1.26651
C -5.01682 0.35217 2.60388
C -3.66272 0.27952 3.01827
C -2.64359 0.09882 2.10093
C -2.93973 -0.02559 0.72080
H 1.53184 -0.90225 -3.55909
H 1.06625 -2.06726 -2.31771
H 3.94350 -1.41489 -3.15993
H 5.94842 -0.87030 -1.77938
H 6.89671 0.13003 0.29109
H 6.54938 1.28148 2.46504
H 4.24072 1.79476 3.24095
H 2.28341 1.13591 1.88868
H -0.17136 1.32977 -3.55402
H 1.41609 1.38362 -2.79880
H -0.47722 3.71001 -3.24804
H -1.01350 5.58688 -1.69913
H -1.21564 6.42725 0.62780
H -1.08481 6.01451 3.07490
H -0.46591 3.75418 3.91637
H 0.00780 1.91129 2.34296
H -1.02140 -1.85776 -2.43833
H -1.39347 -0.48934 -3.48468
H -3.77260 -0.48842 -3.03315
H -5.62995 -0.07744 -1.42054
H -6.36502 0.27281 0.93227
H -5.79844 0.49882 3.34063
H -3.41943 0.36306 4.07199
H -1.61358 0.03621 2.42031
C 0.18867 -3.42747 0.32094
C 0.13181 -4.84274 0.64108
H 1.05186 -5.34007 0.32023
H 0.01615 -4.97968 1.72021
H -0.71686 -5.31108 0.13399
H 1.93111 -0.24118 4.56992
C 0.94498 -0.70951 4.44601
C 1.01792 -2.24463 4.49575
C -0.39277 -2.85989 4.56088
C -1.16674 -2.34704 5.79265
C -1.01085 -0.86245 5.99185
C -0.05644 -0.12315 5.36987
H 0.66701 -0.40636 3.36626
H 1.59137 -2.54619 5.38556
H -0.33347 -3.95428 4.58538
H -2.23296 -2.59925 5.70984
H -0.81615 -2.86423 6.70214
H -1.68603 -0.38093 6.69662
H -0.00580 0.94827 5.55241
H -0.94400 -2.58865 3.64944
H 1.56453 -2.62354 3.62438

82
H^{1}AT Intermediate (2/5)
Fe 0.05792 -0.29601 -0.51611
N 2.22460 -0.36909 -1.03337
N -0.16983 1.80085 -1.05426
N -2.10924 -0.46622 -0.97565
N 0.09912 -0.51479 -2.70672
O 0.16745 -0.30525 1.29049
N 0.02263 -2.56110 -0.48947
C 1.27627 -1.37706 -3.03985
C 2.46674 -0.98041 -2.20418
C 3.77475 -1.27148 -2.65505
C 4.85150 -0.91445 -1.87331
C 4.64090 -0.23655 -0.64435
C 5.71855 0.18944 0.18012
C 5.47406 0.87181 1.35469
C 4.14029 1.15297 1.74506
C 3.06832 0.74754 0.96921
C 3.29148 0.03988 -0.23840
C 0.28499 0.86204 -3.28100
C -0.15695 1.99000 -2.38259
C -0.45555 3.23976 -2.97443
C -0.75316 4.31634 -2.16966
C -0.75508 4.16544 -0.75927
C -1.04056 5.24931 0.11571
C -1.02860 5.06663 1.48370
C -0.73217 3.78951 2.02207
C -0.45563 2.71156 1.19921
C -0.45900 2.87270 -0.20870
C -1.18897 -1.14175 -3.13506
C -2.35139 -0.72476 -2.26975
C -3.65430 -0.70207 -2.81882
C -4.72669 -0.41836 -2.00174
C -4.51699 -0.16930 -0.62108
C -5.58995 0.10424 0.27159
C -5.34636 0.32184 1.61249
C -4.01858 0.26989 2.10810
C -2.95048 0.01532 1.26662
C -3.17243 -0.20289 -0.11643
H 1.51793 -1.31166 -4.10763
H 1.01092 -2.41602 -2.82907
H 3.91047 -1.76468 -3.60957
H 5.86461 -1.12979 -2.19534
H 6.73336 -0.02774 -0.13613
H 6.29735 1.19816 1.97985
H 3.95734 1.69576 2.66597
H 2.05383 0.95427 1.27750
H -0.22354 0.93039 -4.24853
H 1.35377 1.00277 -3.47695
H -0.44296 3.33189 -4.05326
H -0.98676 5.28284 -2.60288
H -1.26383 6.21997 -0.31455
H -1.24382 5.89513 2.14890
H -0.72224 3.65427 3.09817
H -0.23460 1.73678 1.61383
H -1.07756 -2.22772 -3.05074
H -1.39392 -0.92004 -4.18805
H -3.78985 -0.90499 -3.87381
H -5.73435 -0.38636 -2.40182
H -6.60041 0.13211 -0.12270
H -6.16635 0.52694 2.29139
H -3.83843 0.42958 3.16566
H -1.93809 -0.03526 1.64560
C -0.07213 -3.70606 -0.28507
C -0.19065 -5.13329 -0.04324
H 0.79520 -5.60600 -0.08327
H -0.62801 -5.31470 0.94283
H -0.83171 -5.59193 -0.80187
H 2.45511 -1.42119 3.21181
C 1.56081 -1.77963 3.71556
C 1.24746 -3.25291 3.68216
C -0.23909 -3.52581 4.00269
C -0.68984 -2.79018 5.28462
C -0.26664 -1.34541 5.28088
C 0.80853 -0.90649 4.51108
H 0.48624 -0.80181 2.08082
H 1.88335 -3.77319 4.42040
H -0.41324 -4.60271 4.10416
H -1.77812 -2.86742 5.40532
H -0.25854 -3.29248 6.16877
H -0.79804 -0.64436 5.91842
H 1.08622 0.14442 4.54493
H -0.85322 -3.17682 3.16094
H 1.51585 -3.68155 2.70862

82
H^{2}AT Reactant Complex (2/5)
Fe 0.19693 -0.12973 -0.78721
N 2.25101 -0.30652 -1.20038
N -0.02476 1.96999 -1.30233
N -1.92130 -0.25993 -0.97188
N 0.14239 -0.38150 -2.82007
O 0.33482 0.00843 0.86071
N 0.10990 -2.35805 -0.57006
C 1.25934 -1.33435 -3.16340
C 2.47059 -0.97890 -2.34948
C 3.75990 -1.35907 -2.77166
C 4.84596 -1.03511 -1.98616
C 4.66301 -0.29626 -0.79046
C 5.76107 0.09638 0.02356
C 5.55549 0.84628 1.16321
C 4.24111 1.23367 1.52421
C 3.14901 0.86452 0.75838
C 3.32975 0.08213 -0.40760
C 0.40229 0.95668 -3.47791
C -0.02029 2.12665 -2.63633
C -0.30986 3.35827 -3.26375
C -0.59403 4.45801 -2.48467
C -0.59153 4.34398 -1.07143
C -0.86757 5.45574 -0.22874
C -0.85481 5.31531 1.14377
C -0.56644 4.05304 1.71953
C -0.29944 2.94945 0.92866
C -0.30319 3.06419 -0.48340
C -1.20172 -0.94982 -3.19141
C -2.27836 -0.48950 -2.25062
C -3.61383 -0.40387 -2.69563
C -4.60545 -0.08962 -1.79117
C -4.28101 0.11072 -0.42649
C -5.27840 0.39314 0.54766
C -4.93806 0.54575 1.87568
C -3.58434 0.41451 2.27480
C -2.58694 0.15476 1.35176
C -2.90508 0.00846 -0.02068
H 1.47398 -1.29806 -4.23663
H 0.93198 -2.34802 -2.92297
H 3.87743 -1.89496 -3.70476
H 5.84786 -1.32370 -2.28435
H 6.76068 -0.19969 -0.27582
H 6.39408 1.14701 1.78041
H 4.08720 1.83369 2.41414
H 2.15430 1.16590 1.04719
H -0.08408 0.98000 -4.45708
H 1.48036 1.03653 -3.65224
H -0.30290 3.42005 -4.34446
H -0.82191 5.41477 -2.94153
H -1.08484 6.41405 -0.68843
H -1.06292 6.16484 1.78398
H -0.55473 3.94902 2.79886
H -0.08417 1.99209 1.37983
H -1.13247 -2.04009 -3.12227
H -1.44267 -0.70332 -4.22905
H -3.83853 -0.58231 -3.73930
H -5.63805 -0.00396 -2.11112
H -6.31037 0.47553 0.22358
H -5.70054 0.75567 2.61687
H -3.32478 0.51478 3.32288
H -1.56042 0.04424 1.66932
C 0.01835 -3.42893 -0.11562
C -0.09194 -4.75494 0.46373
H 0.65456 -5.42378 0.02521
H 0.07459 -4.69801 1.54569
H -1.08775 -5.16801 0.27820
H 0.86878 -1.45223 3.17287
C 0.74349 -2.00089 4.11718
C -0.70859 -1.85964 4.61982
C -1.01015 -2.87962 5.73486
C -0.83270 -4.32436 5.22319
C 0.43140 -4.48486 4.40532
C 1.14183 -3.44842 3.92639
H 1.43457 -1.52373 4.83160
H -1.40097 -2.02906 3.78209
H -2.02696 -2.73909 6.12171
H -0.81511 -5.02508 6.06978
H -1.70544 -4.61648 4.61669
H 0.77274 -5.50303 4.22183
H 2.06267 -3.63562 3.37482
H -0.32218 -2.70560 6.57495
H -0.88516 -0.83690 4.97580

82
H^{2}AT Transition State (2/5)
Fe 0.11833 0.04962 0.13622
N 2.25989 -0.12842 -0.33639
N 0.00308 2.16423 -0.31712
N -2.05021 0.01118 -0.26575
N 0.12846 -0.12322 -2.01087
O 0.20666 0.02467 1.84577
N -0.00293 -2.19159 0.16188
C 1.26876 -1.02691 -2.37210
C 2.47654 -0.69601 -1.53572
C 3.77127 -1.00783 -2.00773
C 4.86291 -0.72361 -1.21679
C 4.68039 -0.10304 0.04577
C 5.77674 0.23898 0.88465
C 5.56320 0.86390 2.09639
C 4.24215 1.16882 2.51089
C 3.15274 0.84613 1.72131
C 3.34301 0.20025 0.47462
C 0.35842 1.25335 -2.57392
C -0.00046 2.38256 -1.64270
C -0.23982 3.65931 -2.20227
C -0.45887 4.73313 -1.36959
C -0.43818 4.55233 0.03674
C -0.64058 5.63436 0.93686
C -0.60832 5.42706 2.30074
C -0.37443 4.12525 2.80925
C -0.18012 3.04943 1.96087
C -0.20506 3.23343 0.55634
C -1.18610 -0.70335 -2.43302
C -2.32063 -0.24253 -1.55674
C -3.62830 -0.17155 -2.08901
C -4.67783 0.15830 -1.25986
C -4.43926 0.41099 0.11507
C -5.48903 0.73842 1.01729
C -5.22063 0.96356 2.35206
C -3.88972 0.86586 2.83149
C -2.84438 0.55716 1.97981
C -3.09062 0.32797 0.60352
H 1.50164 -0.94836 -3.44042
H 0.96239 -2.05793 -2.17776
H 3.88572 -1.45946 -2.98516
H 5.86690 -0.95510 -1.55560
H 6.78113 0.00257 0.54950
H 6.40080 1.12554 2.73283
H 4.08260 1.66339 3.46277
H 2.14831 1.06749 2.04873
H -0.17964 1.35849 -3.52167
H 1.42526 1.34761 -2.80584
H -0.24367 3.77371 -3.27894
H -0.64613 5.72045 -1.77750
H -0.81647 6.62370 0.52792
H -0.75984 6.25413 2.98488
H -0.34800 3.96843 3.88204
H -0.00904 2.05792 2.35471
H -1.11206 -1.79242 -2.34846
H -1.38790 -0.47210 -3.48427
H -3.78497 -0.37517 -3.14083
H -5.68899 0.22596 -1.64624
H -6.50204 0.80274 0.63411
H -6.02308 1.21030 3.03792
H -3.68836 1.03316 3.88394
H -1.83152 0.47169 2.34625
C -0.06132 -3.29504 0.53632
C -0.12607 -4.66232 1.01901
H 0.56729 -5.29688 0.45938
H 0.14665 -4.69040 2.07896
H -1.13882 -5.05911 0.90367
H 0.47796 -0.53918 3.29372
C 0.65431 -0.94442 4.37239
C -0.70770 -1.00724 5.08510
C -0.70875 -2.05182 6.22117
C -0.34042 -3.44735 5.67655
C 0.88642 -3.39604 4.80234
C 1.35131 -2.24437 4.25120
H 1.32150 -0.16719 4.77630
H -1.48459 -1.28525 4.35855
H -1.69202 -2.08036 6.70475
H -0.17431 -4.15299 6.50087
H -1.18705 -3.85823 5.10079
H 1.44686 -4.31879 4.66563
H 2.28895 -2.25579 3.69900
H 0.02124 -1.76006 6.98876
H -0.97545 -0.01708 5.47045

82
H^{2}AT Intermediate (2/5)
Fe 0.08169 -0.38524 -0.56971
N 2.24521 -0.48285 -1.09787
N -0.09451 1.73836 -0.98128
N -2.09455 -0.47935 -1.02478
N 0.09878 -0.48618 -2.76768
O 0.18168 -0.51999 1.24354
N -0.00504 -2.64845 -0.66471
C 1.26404 -1.34047 -3.15786
C 2.46807 -0.99828 -2.31784
C 3.76834 -1.24400 -2.81537
C 4.85860 -0.94299 -2.02888
C 4.66840 -0.37426 -0.74276
C 5.76013 -0.01679 0.09567
C 5.53572 0.55275 1.33266
C 4.20841 0.78351 1.77461
C 3.12324 0.44467 0.98552
C 3.32567 -0.14300 -0.28838
C 0.29006 0.91790 -3.26975
C -0.09972 2.00310 -2.29672
C -0.36989 3.29371 -2.80949
C -0.61786 4.33041 -1.93834
C -0.59802 4.09844 -0.53910
C -0.83133 5.13816 0.40231
C -0.80104 4.87558 1.75697
C -0.53816 3.56030 2.21490
C -0.31161 2.52380 1.32607
C -0.33415 2.76748 -0.06964
C -1.19870 -1.07952 -3.21507
C -2.34980 -0.68147 -2.32627
C -3.65579 -0.61493 -2.86449
C -4.71739 -0.34417 -2.02901
C -4.49368 -0.15097 -0.64152
C -5.55504 0.10912 0.26899
C -5.29797 0.27250 1.61512
C -3.96797 0.17773 2.09823
C -2.91090 -0.06584 1.23964
C -3.14670 -0.22887 -0.14859
H 1.49271 -1.22362 -4.22380
H 0.99145 -2.38631 -2.99433
H 3.88750 -1.65803 -3.80886
H 5.86639 -1.12178 -2.38779
H 6.76936 -0.19783 -0.25893
H 6.36971 0.82627 1.96890
H 4.04085 1.23289 2.74731
H 2.11371 0.60680 1.33454
H -0.25032 1.04903 -4.21321
H 1.35364 1.05260 -3.49641
H -0.37384 3.44831 -3.88120
H -0.82827 5.32721 -2.31041
H -1.02972 6.13895 0.03321
H -0.97660 5.67035 2.47303
H -0.51439 3.36214 3.28099
H -0.11619 1.52011 1.68014
H -1.09997 -2.16922 -3.17440
H -1.40545 -0.81262 -4.25733
H -3.80175 -0.77475 -3.92547
H -5.72711 -0.27954 -2.41986
H -6.56757 0.17037 -0.11618
H -6.10920 0.46760 2.30738
H -3.77718 0.29540 3.15950
H -1.89728 -0.15158 1.60912
C -0.13865 -3.79349 -0.48360
C -0.30871 -5.21881 -0.26392
H 0.65282 -5.73291 -0.35371
H -0.71230 -5.39951 0.73677
H -1.00040 -5.63456 -1.00247
H 0.46648 -1.18487 1.91347
C 1.44181 -2.01324 3.67603
C 0.91813 -0.98272 4.64526
C -0.03300 -1.61099 5.68832
C -1.09651 -2.51315 5.02268
C -0.47072 -3.48581 4.05932
C 0.75388 -3.21066 3.45196
H 2.40136 -1.84016 3.19549
H 0.38389 -0.18904 4.09271
H -0.51805 -0.82524 6.27784
H -1.67159 -3.05183 5.78636
H -1.83052 -1.88474 4.48706
H -0.99303 -4.41125 3.83344
H 1.18666 -3.94514 2.77726
H 0.55926 -2.21932 6.38495
H 1.75465 -0.47892 5.14590

82
Rebound Transition State (2/5)
Fe 0.08056 -0.38389 -0.56521
N 2.24593 -0.48352 -1.09149
N -0.09553 1.74142 -0.98257
N -2.09721 -0.47667 -1.02449
N 0.09869 -0.48635 -2.76485
O 0.17392 -0.51072 1.25288
N -0.00770 -2.64811 -0.65411
C 1.26487 -1.34045 -3.15216
C 2.46881 -0.99542 -2.31291
C 3.76927 -1.23561 -2.81292
C 4.85975 -0.93280 -2.02743
C 4.66947 -0.36890 -0.73920
C 5.76104 -0.01092 0.09926
C 5.53618 0.55244 1.33900
C 4.20859 0.77605 1.78394
C 3.12356 0.43697 0.99477
C 3.32657 -0.14386 -0.28229
C 0.28895 0.91672 -3.26940
C -0.10157 2.00355 -2.29836
C -0.37334 3.29295 -2.81379
C -0.62177 4.33126 -1.94478
C -0.60085 4.10216 -0.54501
C -0.83436 5.14342 0.39465
C -0.80286 4.88328 1.74978
C -0.53864 3.56900 2.20998
C -0.31183 2.53104 1.32292
C -0.33556 2.77234 -0.07322

C -1.19786 -1.08160 -3.21198
C -2.35043 -0.68143 -2.32582
C -3.65561 -0.61510 -2.86639
C -4.71838 -0.34165 -2.03332
C -4.49671 -0.14501 -0.64593
C -5.55902 0.11861 0.26246
C -5.30346 0.28568 1.60844
C -3.97412 0.19131 2.09360
C -2.91613 -0.05573 1.23714
C -3.15052 -0.22276 -0.15090
H 1.49389 -1.22676 -4.21840
H 0.99308 -2.38605 -2.98549
H 3.88835 -1.64681 -3.80760
H 5.86761 -1.10693 -2.38845
H 6.77047 -0.18691 -0.25737
H 6.37006 0.82622 1.97530
H 4.04083 1.21990 2.75915
H 2.11356 0.59252 1.34584
H -0.25141 1.04598 -4.21319
H 1.35247 1.05177 -3.49630
H -0.37806 3.44526 -3.88585
H -0.83330 5.32712 -2.31880
H -1.03386 6.14341 0.02394
H -0.97854 5.67924 2.46451
H -0.51405 3.37294 3.27646
H -0.11535 1.52788 1.67821
H -1.09861 -2.17115 -3.16804
H -1.40375 -0.81795 -4.25530
H -3.79999 -0.77718 -3.92726
H -5.72745 -0.27729 -2.42591
H -6.57102 0.17974 -0.12415
H -6.11542 0.48354 2.29908
H -3.78471 0.31218 3.15477
H -1.90263 -0.14101 1.60736
C -0.14269 -3.79339 -0.47537
C -0.31464 -5.21896 -0.25850
H 0.64706 -5.73349 -0.34374
H -0.72381 -5.40088 0.73970
H -1.00251 -5.63336 -1.00137
H 0.45308 -1.18786 1.91236
C 1.44448 -2.02715 3.66767
C 0.92224 -0.99324 4.63289
C -0.02144 -1.61780 5.68473
C -1.08354 -2.52965 5.03052
C -0.45866 -3.50483 4.07005
C 0.76112 -3.22898 3.45402
H 2.39920 -1.85159 3.17861
H 0.38282 -0.20554 4.07656
H -0.50756 -0.82978 6.27013
H -1.65243 -3.06646 5.80002
H -1.82343 -1.90902 4.49382
H -0.97882 -4.43330 3.85181
H 1.19282 -3.96514 2.78076
H 0.57653 -2.21799 6.38348
H 1.75955 -0.48265 5.12513

82
Rebound Product (2/5)
Fe -0.09217 -0.52653 -0.39874
N 2.17649 -0.57250 -0.83695
N -0.10070 1.64626 -0.86058
N -2.28710 -0.40849 -1.05524
N 0.10007 -0.60792 -2.59754
O -0.36807 -1.11409 1.67003
N -0.27772 -2.84321 -0.52276
C 1.23910 -1.53556 -2.87756
C 2.41141 -1.25495 -1.96526
C 3.70274 -1.71659 -2.32430
C 4.76637 -1.46092 -1.48784
C 4.57218 -0.68050 -0.31608
C 5.64196 -0.31942 0.54883
C 5.41622 0.49937 1.63764
C 4.11409 1.00166 1.89013
C 3.05028 0.65526 1.07621
C 3.24680 -0.21400 -0.02725
C 0.39945 0.77350 -3.10422
C 0.02691 1.89986 -2.16648
C -0.09684 3.20993 -2.69896
C -0.33685 4.26716 -1.85091
C -0.46295 4.03806 -0.45410
C -0.69990 5.08499 0.47866
C -0.81490 4.80926 1.82723
C -0.70266 3.47405 2.29176
C -0.47666 2.43424 1.40806
C -0.34709 2.69065 0.02002
C -1.19300 -1.14110 -3.12263
C -2.39816 -0.61599 -2.37523
C -3.61475 -0.43020 -3.07809
C -4.74130 -0.03433 -2.39197
C -4.67044 0.18698 -0.99193
C -5.79777 0.59260 -0.22505
C -5.68246 0.79745 1.13512
C -4.43238 0.60511 1.77780
C -3.31751 0.21411 1.05942
C -3.40662 -0.00529 -0.33883
H 1.55849 -1.45709 -3.92565
H 0.89073 -2.55963 -2.72398
H 3.83367 -2.26723 -3.24814
H 5.76041 -1.82325 -1.72769
H 6.63864 -0.68765 0.32866
H 6.23461 0.77675 2.29236
H 3.95377 1.67401 2.72582
H 2.06921 1.07842 1.25068
H -0.08607 0.92416 -4.07553
H 1.47833 0.84226 -3.28216
H 0.00319 3.36062 -3.76707
H -0.43239 5.27653 -2.23656
H -0.78622 6.10230 0.11097
H -0.99261 5.61042 2.53570
H -0.79738 3.26707 3.35207
H -0.40488 1.41558 1.76662
H -1.17261 -2.22990 -3.01159
H -1.29199 -0.92679 -4.19356
H -3.64116 -0.60189 -4.14727
H -5.68303 0.11485 -2.90947
H -6.74757 0.73548 -0.73003
H -6.54395 1.10484 1.71727
H -4.35172 0.76740 2.84716
H -2.36755 0.06827 1.55426
C -0.43905 -3.99802 -0.45022
C -0.63775 -5.43450 -0.36028
H -0.10390 -5.94128 -1.16966
H -0.26034 -5.80785 0.59632
H -1.70218 -5.67517 -0.43695
H -1.05220 -1.81409 1.71700
C 0.54361 -1.23100 2.87558
C -0.27422 -0.99526 4.14852
C 0.54992 -1.40134 5.38703
C 0.92241 -2.89710 5.33408
C 1.39020 -3.31669 3.96027
C 1.23064 -2.56870 2.85600
H 1.25224 -0.41857 2.70364
H -1.18608 -1.60802 4.10821
H -0.01774 -1.18142 6.29751
H 1.70390 -3.12063 6.07211
H 0.05577 -3.51248 5.62393
H 1.89542 -4.27740 3.88296
H 1.62307 -2.89701 1.89744
H 1.46669 -0.79734 5.42896
H -0.58555 0.05280 4.20581

82
OAT Reactant Complex (2/3)
Fe -0.12803 -0.11455 -0.81624
N 1.91624 -0.34190 -0.78986
N -0.04505 1.82441 -1.40818
N -2.10235 -0.10689 -1.38132
N 0.21471 -0.55135 -2.78242
O -0.28122 0.12597 0.82402
N -0.32420 -2.07180 -0.43788
C 1.32180 -1.56550 -2.79974
C 2.34467 -1.15061 -1.77964
C 3.67790 -1.59787 -1.87936
C 4.59260 -1.19837 -0.93077
C 4.19586 -0.31530 0.10412
C 5.12267 0.15716 1.07426
C 4.72507 1.04524 2.05155
C 3.38177 1.49431 2.08687
C 2.45201 1.04896 1.16414
C 2.82741 0.12695 0.15655
C 0.67213 0.71154 -3.46153
C 0.26983 1.94289 -2.71043
C 0.29602 3.17875 -3.39270
C -0.00199 4.33200 -2.70911
C -0.33436 4.26454 -1.33366
C -0.64487 5.44135 -0.59850
C -0.96923 5.37249 0.73986
C -0.99355 4.11303 1.38370
C -0.70116 2.94796 0.69567
C -0.36012 2.98265 -0.67875
C -1.06440 -1.07663 -3.35773
C -2.24764 -0.45050 -2.67616
C -3.46958 -0.32433 -3.36903
C -4.57572 0.15245 -2.70266
C -4.48741 0.45717 -1.32200
C -5.62364 0.88779 -0.58235
C -5.53301 1.11953 0.77393
C -4.29856 0.91457 1.43842
C -3.16870 0.51658 0.74653
C -3.22321 0.29811 -0.65228
H 1.76453 -1.63732 -3.79887
H 0.90700 -2.54436 -2.55234
H 3.95956 -2.24356 -2.70139
H 5.62239 -1.53462 -0.97736
H 6.14841 -0.19182 1.02153
H 5.43433 1.40610 2.78738
H 3.07523 2.20261 2.84855
H 1.43474 1.39794 1.21166
H 0.29366 0.74151 -4.48738
H 1.76475 0.69193 -3.52953
H 0.55126 3.19296 -4.44453
H 0.00976 5.29407 -3.20894
H -0.61795 6.39375 -1.11709
H -1.20355 6.27175 1.29750
H -1.24709 4.05459 2.43637
H -0.72849 2.00274 1.21296
H -1.09798 -2.15688 -3.18219
H -1.09600 -0.92191 -4.43995
H -3.51331 -0.59798 -4.41535
H -5.52100 0.28148 -3.21810
H -6.56421 1.01373 -1.10781
H -6.40227 1.44087 1.33600
H -4.23787 1.06590 2.51053
H -2.24086 0.34070 1.26918
C -0.49359 -3.13332 0.00944
C -0.68709 -4.45175 0.58285
H -0.26183 -5.21762 -0.07238
H -0.18744 -4.49834 1.55718
H -1.75384 -4.65307 0.71705
H 0.26383 -1.15538 3.18695
C 0.73545 -1.72699 3.99844
C -0.32432 -2.16881 5.02898
C 0.24629 -3.23713 5.98168
C 0.68875 -4.49345 5.20233
C 1.45562 -4.14141 3.94531
C 1.48968 -2.90450 3.41900
H 1.45020 -1.03331 4.47165
H -1.19326 -2.58725 4.50010
H -0.49344 -3.50854 6.74481
H 1.30803 -5.13636 5.84372
H -0.19262 -5.10099 4.93987
H 2.01520 -4.94583 3.46918
H 2.09151 -2.71248 2.53109
H 1.11251 -2.81612 6.51250
H -0.68425 -1.30083 5.59513

82
OAT Transition State 1 (2/3)
Fe 0.14317 -0.60991 -0.50907
N 2.20539 -0.70735 -0.76479
N 0.07341 1.43539 -0.92500
N -1.92025 -0.58976 -0.91724
N 0.26673 -0.83084 -2.55527
O 0.08828 -0.46097 1.26541
N 0.06487 -2.60184 -0.37308
C 1.42595 -1.74774 -2.81379
C 2.54477 -1.37532 -1.88355
C 3.87806 -1.70412 -2.21098
C 4.89423 -1.31083 -1.37047
C 4.59312 -0.53754 -0.22100
C 5.61653 -0.03498 0.62918
C 5.30345 0.76896 1.70571
C 3.94968 1.09375 1.96918
C 2.92778 0.60352 1.17476
C 3.21828 -0.22730 0.06598
C 0.53238 0.51948 -3.15429
C 0.15460 1.65564 -2.24886
C -0.02361 2.92743 -2.84202
C -0.27579 4.01644 -2.04493
C -0.34551 3.84861 -0.63980
C -0.58258 4.95511 0.22178
C -0.63474 4.78484 1.58935
C -0.45309 3.49187 2.13666
C -0.22960 2.39293 1.32565
C -0.16812 2.53326 -0.08353
C -1.02498 -1.41982 -3.02598
C -2.17295 -0.92336 -2.19639
C -3.46488 -0.88596 -2.76730
C -4.53430 -0.50044 -1.99403
C -4.32464 -0.15118 -0.63710
C -5.40194 0.24876 0.20115
C -5.17999 0.58093 1.52119
C -3.86591 0.51836 2.04680
C -2.79506 0.13548 1.25875
C -2.98938 -0.20301 -0.10282
H 1.74882 -1.67941 -3.85928
H 1.10755 -2.77701 -2.64165
H 4.07859 -2.25113 -3.12366
H 5.92670 -1.55611 -1.59383
H 6.64733 -0.28655 0.40317
H 6.08658 1.15879 2.34581
H 3.70856 1.73714 2.80842
H 1.89918 0.83756 1.39178
H 0.02039 0.60787 -4.11761
H 1.60528 0.59821 -3.36097
H 0.04405 3.01975 -3.91876
H -0.41930 5.00180 -2.47448
H -0.71572 5.93572 -0.22322
H -0.81117 5.63148 2.24310
H -0.49053 3.35726 3.21243
H -0.10106 1.40757 1.74928
H -0.96158 -2.50751 -2.92466
H -1.18411 -1.20505 -4.08737
H -3.59001 -1.15867 -3.80760
H -5.53540 -0.45750 -2.40881
H -6.40025 0.28415 -0.22224
H -6.00353 0.88513 2.15720
H -3.69631 0.77367 3.08737
H -1.79563 0.07044 1.66124
C -0.06378 -3.75469 -0.26234
C -0.21661 -5.19373 -0.13690
H -0.11604 -5.66918 -1.11733
H 0.55066 -5.59888 0.52945
H -1.20266 -5.43500 0.27070
H 0.50069 0.48429 4.89038
C 0.43475 -0.61171 4.80304
C -1.03382 -1.07839 4.82490
C -1.14049 -2.52115 4.30151
C -0.67354 -2.61532 2.83179
C 0.61825 -1.84807 2.56791
C 1.17999 -1.06185 3.58412
H 0.96393 -0.99572 5.69232
H -1.64376 -0.41712 4.19499
H -2.17081 -2.88694 4.37956
H -0.51890 -3.66885 2.56645
H -1.46406 -2.24325 2.17232
H 1.31123 -2.28827 1.85934
H 2.20360 -0.71766 3.47223
H -0.52060 -3.17724 4.92908
H -1.43308 -1.00378 5.84269

82
OAT Intermediate (2/3)
Fe 0.09794 -0.58168 -0.57148
N 2.14665 -0.70770 -0.78839
N 0.04504 1.47093 -0.93290
N -1.95940 -0.52428 -1.00297
N 0.26193 -0.75089 -2.59506
O 0.03703 -0.50014 1.25412
N -0.01859 -2.57068 -0.47684
C 1.38553 -1.71887 -2.85088
C 2.49179 -1.41038 -1.88459
C 3.81737 -1.80656 -2.15746
C 4.81961 -1.44147 -1.28656
C 4.51793 -0.61695 -0.17335
C 5.53594 -0.12313 0.68768
C 5.22613 0.74865 1.71184
C 3.88335 1.15211 1.90984
C 2.86349 0.66722 1.10925
C 3.15039 -0.23313 0.05594
C 0.62184 0.60251 -3.14481
C 0.19701 1.72375 -2.24517
C 0.04946 3.00807 -2.81662
C -0.25026 4.07677 -2.00746
C -0.39985 3.87377 -0.61359
C -0.69131 4.95718 0.26061
C -0.82169 4.75158 1.61809
C -0.66511 3.44591 2.14250
C -0.38991 2.36822 1.31887
C -0.24917 2.54561 -0.07995
C -1.04045 -1.25732 -3.13698
C -2.19222 -0.77902 -2.30395
C -3.47085 -0.68519 -2.89653
C -4.54964 -0.33069 -2.12115
C -4.36345 -0.07613 -0.74014
C -5.45386 0.27438 0.10320
C -5.25673 0.50322 1.44898
C -3.95494 0.38598 1.99523
C -2.87116 0.05425 1.20191
C -3.04004 -0.18066 -0.18377
H 1.73614 -1.63282 -3.88567
H 1.01545 -2.73572 -2.71762
H 4.02531 -2.38047 -3.05165
H 5.84608 -1.74231 -1.46478
H 6.56056 -0.43093 0.50838
H 6.00608 1.13409 2.35846
H 3.64710 1.85068 2.70476
H 1.84460 0.97484 1.27162
H 0.19759 0.72136 -4.14591
H 1.71034 0.64864 -3.25410
H 0.17647 3.12715 -3.88522
H -0.37208 5.07233 -2.41972
H -0.80336 5.94821 -0.16659
H -1.03983 5.58059 2.28168
H -0.76301 3.28443 3.21070
H -0.27432 1.37488 1.72312
H -1.01881 -2.35126 -3.11201
H -1.15893 -0.96273 -4.18391
H -3.57903 -0.89269 -3.95357
H -5.54119 -0.24547 -2.55192
H -6.44263 0.35205 -0.33654
H -6.09083 0.76710 2.08921
H -3.80401 0.55699 3.05571
H -1.88206 -0.04579 1.61846
C -0.17685 -3.71980 -0.36771
C -0.36512 -5.15280 -0.23203
H -0.05465 -5.66248 -1.14902
H 0.23318 -5.53240 0.60156
H -1.41871 -5.37828 -0.04267
H 2.26616 -1.13513 5.21287
C 1.79919 -1.71326 4.40820
C 0.67407 -2.62772 4.98356
C -0.10032 -3.32920 3.84960
C -0.64710 -2.32093 2.81474
C 0.52615 -1.48729 2.21306
C 1.24523 -0.81089 3.34461
H 2.58087 -2.36581 3.98412
H -0.02015 -2.01221 5.57213
H -0.93304 -3.90968 4.26577
H -1.19752 -2.83561 2.02027
H -1.34736 -1.63278 3.30474
H 1.20890 -2.18543 1.70420
H 1.01138 0.22678 3.56407
H 0.56259 -4.04724 3.34377
H 1.10925 -3.36902 5.66570

82
OAT Transition State 2 (2/3)
Fe 0.12005 -0.56556 -0.51365
N 2.23382 -0.65193 -0.84804
N 0.05262 1.48006 -0.93215
N -1.95107 -0.54072 -0.94216
N 0.23689 -0.78517 -2.60407
O 0.16097 -0.47568 1.37698
N 0.07987 -2.54745 -0.38600
C 1.39875 -1.68593 -2.88370
C 2.53795 -1.32460 -1.97138
C 3.85993 -1.68056 -2.32157
C 4.89750 -1.31783 -1.49339
C 4.63218 -0.54239 -0.33591
C 5.67597 -0.07013 0.50703
C 5.39319 0.73995 1.58758
C 4.05153 1.10705 1.85980
C 3.01072 0.64702 1.07238
C 3.26984 -0.19662 -0.03469
C 0.47089 0.57516 -3.18443
C 0.10855 1.70266 -2.25740
C -0.08270 2.97777 -2.84143
C -0.32010 4.06497 -2.03717
C -0.35881 3.89375 -0.63121
C -0.57573 4.99502 0.24215
C -0.59302 4.81601 1.60977
C -0.39455 3.52049 2.14562
C -0.19108 2.42602 1.32305
C -0.16768 2.57687 -0.08560
C -1.05572 -1.38857 -3.04742
C -2.20360 -0.88855 -2.21651
C -3.49819 -0.85353 -2.78262
C -4.56358 -0.45114 -2.01144
C -4.34779 -0.07538 -0.66227
C -5.41512 0.35652 0.17271
C -5.17854 0.72435 1.48090
C -3.86106 0.66475 1.99931
C -2.80003 0.24590 1.21607
C -3.01126 -0.12713 -0.13361
H 1.70645 -1.60682 -3.93367
H 1.09182 -2.72023 -2.71841
H 4.03447 -2.22795 -3.23955
H 5.92005 -1.58936 -1.73191
H 6.69802 -0.34853 0.27263
H 6.19186 1.10573 2.22276
H 3.83740 1.76191 2.69765
H 1.99051 0.91603 1.28931
H -0.06754 0.67472 -4.13274
H 1.53688 0.66897 -3.41963
H -0.03688 3.07402 -3.91908
H -0.47396 5.05094 -2.46189
H -0.72061 5.97836 -0.19307
H -0.75405 5.65868 2.27265
H -0.40273 3.38128 3.22146
H -0.04574 1.43851 1.73533
H -0.98357 -2.47410 -2.93017
H -1.23048 -1.19146 -4.11045
H -3.62858 -1.13966 -3.81873
H -5.56573 -0.41059 -2.42396
H -6.41649 0.39026 -0.24347
H -5.99392 1.05549 2.11395
H -3.68192 0.95155 3.02996
H -1.79830 0.17853 1.61308
C 0.00402 -3.70786 -0.30955
C -0.08732 -5.15481 -0.22156
H 0.00877 -5.59952 -1.21666
H 0.71080 -5.54601 0.41628
H -1.05312 -5.44673 0.20144
H -0.14710 0.74691 4.74011

C 0.03676 -0.33845 4.67881
C -1.28130 -1.13597 4.72805
C -1.06117 -2.55339 4.17719
C -0.67405 -2.50659 2.68387
C 0.50396 -1.54487 2.37703
C 0.89214 -0.65479 3.50133
H 0.63679 -0.56007 5.58093
H -2.05090 -0.63283 4.12832
H -1.96850 -3.15808 4.29235
H -0.41952 -3.51683 2.34774
H -1.54353 -2.18406 2.10172
H 1.36949 -2.09241 1.98887
H 1.85110 -0.15293 3.42004
H -0.27183 -3.05349 4.75727
H -1.65345 -1.16782 5.75808

82
OAT Product (2/3)
Fe 0.07365 -0.51861 -0.55394
N 2.26725 -0.58855 -0.91537
N 0.04215 1.47886 -0.92946
N -2.02703 -0.55055 -1.09302
N 0.27141 -0.68356 -2.72948
O 0.21904 -0.80802 1.81421
N -0.03596 -2.48669 -0.41064
C 1.40611 -1.62126 -2.95341
C 2.54861 -1.29662 -2.01816
C 3.86120 -1.71938 -2.34121
C 4.90348 -1.38509 -1.50606
C 4.66043 -0.56538 -0.37190
C 5.70602 -0.10856 0.47713
C 5.43428 0.74993 1.52374
C 4.10525 1.18810 1.75436
C 3.06326 0.74325 0.95993
C 3.31097 -0.15455 -0.10806
C 0.58770 0.69569 -3.20459
C 0.20788 1.78180 -2.22911
C 0.09636 3.10437 -2.72471
C -0.18443 4.13689 -1.86226
C -0.36018 3.86527 -0.48112
C -0.64880 4.89323 0.45795
C -0.81220 4.59746 1.79619
C -0.69097 3.25752 2.23922
C -0.41286 2.23454 1.34944
C -0.24305 2.50843 -0.02961
C -1.02614 -1.19499 -3.24115
C -2.20659 -0.74700 -2.40719
C -3.47487 -0.63044 -3.02686
C -4.57832 -0.32193 -2.26409
C -4.43678 -0.14474 -0.86336
C -5.54384 0.14325 -0.01803
C -5.36782 0.28258 1.34367
C -4.07561 0.13466 1.90884
C -2.97642 -0.13517 1.11366
C -3.12711 -0.27204 -0.28947
H 1.75962 -1.57782 -3.99267
H 1.05264 -2.64032 -2.77790
H 4.02542 -2.29616 -3.24348
H 5.91530 -1.71059 -1.72253
H 6.72101 -0.43515 0.27597
H 6.23485 1.10340 2.16360
H 3.90484 1.88438 2.56136
H 2.05430 1.09158 1.12889
H 0.10795 0.88269 -4.17267
H 1.66759 0.76539 -3.37646
H 0.23386 3.28016 -3.78445
H -0.27633 5.15541 -2.22326
H -0.73585 5.91341 0.09896
H -1.03134 5.38389 2.50933
H -0.81958 3.03006 3.29192
H -0.32017 1.21766 1.70094
H -0.99353 -2.28977 -3.21459
H -1.17649 -0.90658 -4.28853
H -3.55640 -0.78343 -4.09604
H -5.55730 -0.21820 -2.71938
H -6.52762 0.24315 -0.46478
H -6.21413 0.49797 1.98608
H -3.95022 0.23181 2.98179
H -1.99524 -0.25950 1.55440
C -0.18243 -3.64212 -0.34402
C -0.36298 -5.08200 -0.26479
H -0.35499 -5.51897 -1.26788
H 0.44320 -5.53391 0.32057
H -1.31878 -5.31735 0.21253
H 0.64111 0.96998 4.13484
C 0.54892 -0.11199 4.28899
C -0.89329 -0.50756 4.66155
C -1.05461 -2.03873 4.67954
C -0.78167 -2.67222 3.29625
C 0.44349 -2.09777 2.61131
C 1.08102 -0.85050 3.08728
H 1.22172 -0.36148 5.12314
H -1.60032 -0.06380 3.94903
H -2.06251 -2.31339 5.01032
H -0.64372 -3.75454 3.40181
H -1.64808 -2.53264 2.63752
H 1.06596 -2.78955 2.05503
H 2.12904 -0.69940 2.85600
H -0.35432 -2.45944 5.41493
H -1.13594 -0.09068 5.64541

82
OAT Reactant Complex (2/5)
Fe 0.23375 -0.52452 -1.02937
N 2.29536 -0.74879 -1.36406
N 0.13456 1.63872 -1.24088
N -1.87265 -0.51965 -1.32865
N 0.27969 -0.47744 -3.07630
O 0.28880 -0.63477 0.62416
N 0.04062 -2.75971 -1.14556
C 1.36843 -1.42970 -3.50204
C 2.54643 -1.26620 -2.58467
C 3.83567 -1.66494 -2.98933
C 4.88759 -1.52751 -2.10851
C 4.67401 -0.95266 -0.83045
C 5.73993 -0.75247 0.08952
C 5.50817 -0.15457 1.31113
C 4.19970 0.27075 1.65080
C 3.13780 0.08548 0.78248
C 3.34423 -0.54243 -0.46956
C 0.64071 0.92585 -3.51581
C 0.21985 1.98378 -2.53625
C 0.02083 3.30591 -2.99097
C -0.25394 4.29653 -2.07417
C -0.33283 3.98198 -0.69388
C -0.60162 4.97539 0.28755
C -0.67096 4.63979 1.62404
C -0.47448 3.29428 2.02276
C -0.21605 2.30207 1.09359
C -0.13725 2.61750 -0.28544
C -1.06716 -0.90889 -3.59370
C -2.17196 -0.54805 -2.64189
C -3.48019 -0.34831 -3.12957
C -4.50590 -0.13301 -2.23474
C -4.24399 -0.14172 -0.84223
C -5.28070 0.03590 0.11532
C -5.00266 -0.00826 1.46557
C -3.67428 -0.23768 1.90304
C -2.63957 -0.40306 0.99957
C -2.89337 -0.34947 -0.39310
H 1.64533 -1.24748 -4.54572
H 0.98102 -2.44826 -3.43281
H 3.97959 -2.07147 -3.98209
H 5.88752 -1.83780 -2.39096
H 6.73681 -1.07228 -0.19428
H 6.32258 -0.00052 2.00941
H 4.02677 0.75471 2.60554
H 2.14751 0.41565 1.05411
H 0.21916 1.11541 -4.50681
H 1.73013 0.97249 -3.61572
H 0.08955 3.52137 -4.04961
H -0.41180 5.31976 -2.39692
H -0.74818 5.99983 -0.03783
H -0.87381 5.39904 2.37054
H -0.52775 3.03641 3.07477
H -0.06940 1.28059 1.41228
H -1.05208 -1.99834 -3.70061
H -1.24181 -0.48833 -4.58775
H -3.65802 -0.36493 -4.19707
H -5.51834 0.03501 -2.58490
H -6.29272 0.19732 -0.24054
H -5.79486 0.12294 2.19362
H -3.46439 -0.28799 2.96584
H -1.63364 -0.58892 1.34690
C -0.11842 -3.89097 -0.90904
C -0.31322 -5.29982 -0.61681
H 0.54102 -5.88158 -0.97536
H -0.41202 -5.44929 0.46245
H -1.21971 -5.66625 -1.10737
H -1.68095 0.73205 5.31708
C -0.96923 -0.00431 5.71675
C -1.66211 -1.37166 5.89043
C -0.62632 -2.48657 6.13128
C 0.34496 -2.60541 4.93796
C 0.81492 -1.25148 4.44989
C 0.23910 -0.09183 4.80928
H -0.66300 0.38665 6.70103
H -2.23627 -1.60673 4.98188
H -1.12669 -3.44680 6.30725
H 1.21328 -3.21859 5.21816
H -0.14322 -3.14684 4.11093
H 1.67296 -1.24176 3.77872
H 0.64908 0.84920 4.44382
H -0.05518 -2.25302 7.04160
H -2.38087 -1.32793 6.71793

82
OAT Transition State (2/5)
Fe 0.17349 -0.52139 -0.55103
N 2.31780 -0.72882 -0.98109
N 0.09059 1.60158 -1.01380
N -1.98510 -0.51873 -0.99565
N 0.23112 -0.69110 -2.69271
O 0.23084 -0.51775 1.14644
N 0.00317 -2.75553 -0.53090
C 1.35299 -1.62759 -3.02865
C 2.54765 -1.32952 -2.16174
C 3.84366 -1.69299 -2.59144
C 4.92328 -1.42045 -1.78015
C 4.72867 -0.75389 -0.54294
C 5.81384 -0.40933 0.30939
C 5.58902 0.26915 1.48993
C 4.26775 0.62698 1.85912
C 3.18854 0.30013 1.05699
C 3.39072 -0.40116 -0.15722
C 0.51869 0.67780 -3.24893
C 0.13516 1.81534 -2.33912
C -0.07505 3.09134 -2.91229
C -0.31657 4.17000 -2.09212
C -0.34818 3.99409 -0.68532
C -0.57626 5.08027 0.20378
C -0.59429 4.87710 1.56856
C -0.38668 3.57549 2.08926
C -0.16891 2.49588 1.25163
C -0.14211 2.67554 -0.15343
C -1.08934 -1.22785 -3.15266
C -2.23020 -0.74423 -2.29720
C -3.51975 -0.61896 -2.86258
C -4.57800 -0.25921 -2.05747
C -4.36700 -0.03330 -0.67349
C -5.42732 0.32630 0.20373
C -5.18667 0.52531 1.54766
C -3.87500 0.36445 2.06192
C -2.81951 0.02051 1.23636
C -3.03668 -0.17734 -0.14986
H 1.61585 -1.55190 -4.09056
H 1.01233 -2.64998 -2.84835
H 3.96872 -2.17333 -3.55379
H 5.92772 -1.69266 -2.08574
H 6.81916 -0.68446 0.00834
H 6.41834 0.53413 2.13573
H 4.10055 1.16631 2.78501
H 2.18223 0.56170 1.34761
H 0.03248 0.78929 -4.22362
H 1.59773 0.74883 -3.42513
H -0.03971 3.20126 -3.98888
H -0.48236 5.15700 -2.51000
H -0.73139 6.06943 -0.21408
H -0.76517 5.70738 2.24424
H -0.39961 3.42192 3.16282
H -0.01767 1.50430 1.65341
H -1.04910 -2.31967 -3.08283
H -1.25961 -0.97699 -4.20494
H -3.65551 -0.80285 -3.92094
H -5.57489 -0.14713 -2.46974
H -6.42589 0.43661 -0.20592
H -5.99639 0.79864 2.21462
H -3.69853 0.51205 3.12170
H -1.82110 -0.11493 1.62893
C -0.12786 -3.89164 -0.30024
C -0.28975 -5.30777 -0.02177
H 0.02435 -5.90106 -0.88551
H 0.31779 -5.59437 0.84162
H -1.33832 -5.53132 0.19595
H -1.17870 0.63452 4.56958
C -0.62431 -0.27030 4.85687
C -1.54343 -1.50903 4.82811
C -0.72033 -2.80951 4.88379
C 0.24283 -2.90162 3.68169
C 0.97367 -1.60917 3.43191
C 0.58680 -0.42117 3.97777
H -0.28302 -0.07973 5.88892
H -2.13909 -1.50187 3.90467
H -1.38230 -3.68300 4.89855
H 0.97125 -3.71018 3.82987
H -0.31904 -3.17236 2.77362
H 1.87520 -1.64914 2.82936
H 1.19009 0.46691 3.80607
H -0.13996 -2.83236 5.81696
H -2.25164 -1.46529 5.66350

82
OAT Product (2/5)
Fe 0.15492 -0.58390 -0.32911
N 2.40302 -0.64512 -0.78082
N 0.02405 1.58716 -0.81700
N -2.01221 -0.60676 -0.96092
N 0.32563 -0.68592 -2.54105
O 0.27777 -0.87878 1.85121
N -0.06631 -2.84192 -0.30334
C 1.44550 -1.64065 -2.79692
C 2.62365 -1.35877 -1.89378
C 3.90819 -1.83974 -2.25007
C 4.98284 -1.56046 -1.43576
C 4.80700 -0.73171 -0.29498
C 5.89272 -0.32849 0.53028
C 5.68783 0.54582 1.57920
C 4.39016 1.05933 1.83080
C 3.30940 0.66859 1.05926
C 3.48626 -0.25388 -0.00330
C 0.66295 0.69309 -3.01946
C 0.17272 1.81370 -2.12819
C -0.03585 3.09368 -2.70356
C -0.38521 4.15325 -1.89639
C -0.53484 3.95602 -0.49794
C -0.88262 5.00772 0.39407
C -1.01246 4.76346 1.74701
C -0.80131 3.45656 2.25709
C -0.46589 2.41239 1.41443
C -0.32493 2.63647 0.02189
C -0.96725 -1.18083 -3.09749
C -2.16624 -0.75236 -2.28355
C -3.42062 -0.59917 -2.92440
C -4.53484 -0.30326 -2.17063
C -4.41772 -0.16690 -0.76238
C -5.53200 0.11801 0.07443
C -5.37040 0.22687 1.44108
C -4.08718 0.05293 2.02071
C -2.98211 -0.21758 1.23424
C -3.12005 -0.32863 -0.17225
H 1.77060 -1.59814 -3.84571
H 1.07534 -2.65291 -2.61521
H 4.02568 -2.42052 -3.15701
H 5.97234 -1.93572 -1.67415
H 6.88529 -0.70673 0.30866
H 6.51863 0.85808 2.20171
H 4.24527 1.77460 2.63300
H 2.33125 1.09473 1.23770
H 0.28593 0.83796 -4.03890
H 1.75391 0.77417 -3.07442
H 0.08483 3.22134 -3.77253
H -0.54893 5.13989 -2.31659
H -1.04104 6.00290 -0.00860
H -1.27571 5.56769 2.42478
H -0.90617 3.27652 3.32152
H -0.30892 1.41442 1.80229
H -0.93765 -2.27594 -3.09788
H -1.08731 -0.86601 -4.14117
H -3.48520 -0.71429 -3.99950
H -5.50414 -0.17451 -2.64034
H -6.50873 0.24264 -0.38160
H -6.22195 0.44106 2.07706
H -3.97489 0.13190 3.09665
H -2.00462 -0.35807 1.67823
C -0.30476 -3.98517 -0.29768
C -0.60005 -5.40814 -0.29246
H 0.14338 -5.95158 -0.88297
H -0.58543 -5.79350 0.73123
H -1.59008 -5.58964 -0.72108
H 0.57849 0.89922 4.17677
C 0.56382 -0.18675 4.32888
C -0.84469 -0.68463 4.70903
C -0.90379 -2.22333 4.70771
C -0.59877 -2.81720 3.31343
C 0.58964 -2.16362 2.63777
C 1.14430 -0.88142 3.12514
H 1.25813 -0.39023 5.15792
H -1.58718 -0.28089 4.00931
H -1.88973 -2.56804 5.03870
H -0.39984 -3.89169 3.39850
H -1.47244 -2.71373 2.65782
H 1.24907 -2.80561 2.06466
H 2.17880 -0.65813 2.89187
H -0.17330 -2.60805 5.43321
H -1.10432 -0.29735 5.70051

2_{TBP} with cyclohexene

76
HAT Reactant Complex (2/5)
Fe -0.22761 -0.78967 -0.67760
N -1.21000 -0.81471 -2.49256
N -1.15766 -1.76841 0.88721
N 1.83505 -0.67193 -0.72057
N 0.18266 -2.68732 -1.22210
O -0.56129 0.77865 -0.24500
C 0.33873 -2.67473 -2.71830
C -0.69749 -1.75873 -3.31243
C -1.08795 -1.88048 -4.65882
C -2.02726 -1.00538 -5.16583
C -2.61644 -0.02556 -4.32818
C -3.61882 0.86447 -4.80294
C -4.19988 1.78176 -3.95154
C -3.80171 1.83475 -2.59250
C -2.82507 0.98777 -2.09697
C -2.20033 0.05097 -2.95447
C -0.98276 -3.52929 -0.78107
C -1.46867 -3.04125 0.55640
C -2.22759 -3.87564 1.39787
C -2.67467 -3.38144 2.60634
C -2.33979 -2.06387 3.00617
C -2.74744 -1.53373 4.26106
C -2.37395 -0.25969 4.63700
C -1.57303 0.52645 3.77142
C -1.16271 0.04362 2.54025
C -1.54740 -1.25249 2.12290
C 1.45714 -3.06445 -0.51809
C 2.39520 -1.88756 -0.53702
C 3.78073 -2.06030 -0.36325
C 4.60249 -0.95172 -0.38735
C 4.05854 0.33562 -0.62462
C 4.87905 1.49371 -0.71188
C 4.32268 2.72596 -0.98760
C 2.92416 2.84059 -1.18840
C 2.09338 1.73606 -1.10198
C 2.63851 0.46364 -0.80745
H 0.25243 -3.69002 -3.11805
H 1.34366 -2.31094 -2.95442
H -0.64968 -2.65595 -5.27355
H -2.33719 -1.07252 -6.20272
H -3.91996 0.80046 -5.84293
H -4.96543 2.45755 -4.31445
H -4.27294 2.54868 -1.92631
H -2.52856 1.04053 -1.05953
H -0.69655 -4.58548 -0.74279
H -1.77764 -3.43172 -1.52745
H -2.44667 -4.88882 1.08669
H -3.26845 -4.00198 3.26830
H -3.35027 -2.15432 4.91514
H -2.68418 0.14145 5.59493
H -1.27195 1.52379 4.07437
H -0.55404 0.65326 1.88858
H 1.90944 -3.94199 -0.99233
H 1.21030 -3.33747 0.51282
H 4.18000 -3.05569 -0.21830
H 5.67248 -1.05830 -0.24804
H 5.94845 1.38500 -0.56756
H 4.95023 3.60651 -1.05976
H 2.49655 3.80956 -1.42014
H 1.02863 1.83736 -1.25419
H 0.05682 5.18625 1.45543
C 0.38177 4.37157 2.11825
C 1.87954 4.52913 2.45451
C 2.27822 3.62475 3.63670
C 1.47682 3.98893 4.90352
C 0.00820 4.20058 4.60420
C -0.48135 4.35482 3.36189
H 0.22242 3.44409 1.54346
H 2.08334 5.57663 2.72031
H 3.35417 3.70258 3.83582
H 1.59077 3.20203 5.66237
H 1.89409 4.90157 5.35995
H -0.66824 4.23017 5.45757
H -1.55274 4.48897 3.21770
H 2.07818 2.57649 3.36988
H 2.48926 4.30015 1.57207

76
HAT Transition state (2/5)
Fe -0.09953 0.17291 0.14986
N -1.18683 0.41398 -1.67436
N -1.03469 -0.99582 1.68016
N 1.99593 -0.06109 -0.17626
N 0.00967 -1.79109 -0.67261
O -0.14556 1.74724 0.81598
C 0.06060 -1.62952 -2.15780
C -0.86413 -0.51941 -2.59076
C -1.34635 -0.47479 -3.91605
C -2.18170 0.55434 -4.29505
C -2.57819 1.53341 -3.34843
C -3.47644 2.58489 -3.67959
C -3.87128 3.49556 -2.72075
C -3.38311 3.38254 -1.39461
C -2.50096 2.37672 -1.04017
C -2.07022 1.43807 -2.00849
C -1.21613 -2.51430 -0.22106
C -1.52936 -2.15707 1.20938
C -2.31893 -3.01853 1.99962
C -2.59691 -2.67005 3.30414
C -2.06258 -1.47506 3.84981
C -2.28244 -1.09941 5.20348
C -1.71506 0.05182 5.71061

C -0.90550 0.86594 4.87934
C -0.67706 0.53469 3.55507
C -1.25579 -0.63574 3.00829
C 1.26484 -2.38449 -0.11649
C 2.36778 -1.35611 -0.15466
C 3.72100 -1.75249 -0.17160
C 4.70412 -0.78673 -0.22562
C 4.35149 0.58495 -0.30286
C 5.32931 1.61064 -0.42234
C 4.94653 2.93103 -0.54119
C 3.57005 3.27054 -0.54494
C 2.59163 2.29968 -0.41684
C 2.95931 0.93832 -0.28565
H -0.19889 -2.56811 -2.66103
H 1.08881 -1.38280 -2.44149
H -1.05676 -1.25102 -4.61298
H -2.55924 0.61287 -5.31003
H -3.84902 2.64938 -4.69629
H -4.55937 4.29375 -2.97425
H -3.70897 4.09428 -0.64416
H -2.12782 2.29614 -0.02968
H -1.09266 -3.59802 -0.33095
H -2.04747 -2.21475 -0.86796
H -2.68920 -3.94153 1.57156
H -3.20648 -3.31352 3.92905
H -2.89634 -1.73993 5.82761
H -1.88016 0.33448 6.74393
H -0.45554 1.76301 5.28941
H -0.06728 1.16275 2.92147
H 1.55284 -3.28350 -0.67342
H 1.07075 -2.68873 0.91747
H 3.96672 -2.80661 -0.15082
H 5.75171 -1.06712 -0.23476
H 6.37757 1.33181 -0.42873
H 5.69280 3.71095 -0.63914
H 3.27867 4.30937 -0.65444
H 1.54432 2.56655 -0.40985
H -0.86137 4.73446 0.66345
C -0.51423 4.36144 1.63701
C 0.82466 4.98485 2.06117
C 1.15807 4.64876 3.52653
C 0.03833 5.12379 4.47431
C -1.33413 4.79714 3.95263
C -1.57568 4.44100 2.66135
H -0.33953 3.23151 1.38996
H 0.75822 6.07711 1.94094
H 2.11165 5.10493 3.81524
H 0.16773 4.69077 5.47583
H 0.10597 6.21555 4.62208
H -2.16751 4.88813 4.64612
H -2.59308 4.21028 2.35303
H 1.28258 3.56126 3.62630
H 1.62780 4.64457 1.39871

76
HAT Intermediate (2/5)
Fe -0.00658 -0.58152 -0.29623
N -1.12870 -0.36330 -2.12735
N -0.96755 -1.83550 1.19744
N 2.11346 -0.86892 -0.60780
N 0.11065 -2.56433 -1.17114
O -0.03268 1.04217 0.44185
C 0.17393 -2.36132 -2.64946
C -0.77541 -1.26372 -3.06349
C -1.25279 -1.20064 -4.38998
C -2.11674 -0.18743 -4.74739
C -2.54567 0.75652 -3.77890
C -3.47361 1.78888 -4.08735
C -3.89736 2.66404 -3.10784
C -3.40896 2.53402 -1.78338
C -2.49827 1.54618 -1.45103
C -2.03900 0.64312 -2.44022
C -1.12028 -3.29566 -0.75103
C -1.44180 -2.98768 0.68932
C -2.21875 -3.88846 1.44868
C -2.50237 -3.58979 2.76401
C -1.99116 -2.40289 3.34896
C -2.22115 -2.07397 4.71299
C -1.68128 -0.92577 5.25626
C -0.88999 -0.06789 4.45185
C -0.65040 -0.35507 3.11942
C -1.20042 -1.52172 2.53551
C 1.35428 -3.18409 -0.62312
C 2.46772 -2.16673 -0.59359
C 3.81591 -2.58152 -0.55307
C 4.81221 -1.62851 -0.53699
C 4.48088 -0.25049 -0.60684
C 5.47481 0.76531 -0.65568
C 5.11320 2.09206 -0.77412
C 3.74320 2.44732 -0.85342
C 2.74957 1.48547 -0.79576
C 3.09426 0.11887 -0.65799
H -0.05826 -3.29113 -3.18201
H 1.19890 -2.08182 -2.91426
H -0.93753 -1.95052 -5.10445
H -2.49210 -0.11521 -5.76230
H -3.84542 1.86769 -5.10331
H -4.60836 3.44729 -3.34395
H -3.75764 3.21722 -1.01694
H -2.13082 1.45332 -0.43939
H -1.00025 -4.37567 -0.89599
H -1.94748 -2.97227 -1.39148
H -2.57368 -4.80210 0.98851
H -3.09933 -4.26518 3.36709
H -2.82281 -2.74607 5.31555
H -1.85540 -0.67829 6.29714
H -0.46437 0.82935 4.88735
H -0.05197 0.30551 2.50857
H 1.64816 -4.05841 -1.21593
H 1.14328 -3.53648 0.39201
H 4.04711 -3.63914 -0.53921
H 5.85536 -1.92236 -0.49658
H 6.51895 0.47492 -0.60855
H 5.87211 2.86479 -0.81674
H 3.46959 3.49046 -0.96727
H 1.70745 1.76369 -0.85514
H -0.81899 4.15469 -0.01007
C -0.46780 4.13919 1.01881
C 0.87823 4.73962 1.33872
C 1.42592 4.22099 2.68689
C 0.37516 4.34082 3.81325
C -0.96464 3.79840 3.39078
C -1.32061 3.71491 2.04485
H -0.13862 1.96949 0.75151
H 0.78272 5.83912 1.37941
H 2.33644 4.76578 2.95980
H 0.72668 3.82714 4.71753
H 0.26433 5.40164 4.10041
H -1.67366 3.49987 4.15784
H -2.30470 3.32992 1.78601
H 1.70564 3.16449 2.57168
H 1.59416 4.53500 0.53291

76
HAT Intermediate (prior to ET) (2/5)
Fe 0.02128 -0.60328 -0.27777
N -1.16062 -0.38421 -2.07456
N -0.98877 -1.86755 1.15412
N 2.15840 -0.90795 -0.51941
N 0.14097 -2.55843 -1.21423
O -0.06794 1.02561 0.44654
C 0.21665 -2.29969 -2.68420
C -0.74028 -1.19476 -3.06199
C -1.16509 -1.03552 -4.39854
C -2.04574 -0.01996 -4.70714
C -2.55702 0.81744 -3.68101
C -3.51586 1.83582 -3.93689
C -4.02803 2.58978 -2.90000
C -3.60590 2.34498 -1.56862
C -2.66347 1.37116 -1.28613
C -2.10728 0.60066 -2.33572
C -1.09852 -3.29478 -0.82542
C -1.44667 -3.01273 0.61508
C -2.24104 -3.92536 1.34161
C -2.56137 -3.64498 2.65276
C -2.07323 -2.46305 3.26685
C -2.34805 -2.14860 4.62606
C -1.83486 -1.00101 5.19596
C -1.02613 -0.12930 4.42438
C -0.74126 -0.40298 3.09806
C -1.26294 -1.56928 2.48754
C 1.37198 -3.21155 -0.68049
C 2.49411 -2.20966 -0.57749
C 3.83454 -2.64933 -0.53509
C 4.84543 -1.71770 -0.43679
C 4.53671 -0.33307 -0.41980
C 5.54796 0.66552 -0.37417
C 5.21108 2.00361 -0.40324
C 3.84900 2.38766 -0.48263
C 2.83900 1.44182 -0.51783
C 3.15746 0.06295 -0.47647
H -0.00625 -3.21007 -3.25389
H 1.24277 -2.00597 -2.92865
H -0.79502 -1.71138 -5.15912
H -2.37581 0.13107 -5.72911
H -3.84313 1.99896 -4.95814
H -4.76277 3.36200 -3.09652
H -4.03352 2.92521 -0.75851
H -2.35242 1.18108 -0.26845
H -0.97764 -4.37212 -0.98822
H -1.91595 -2.95886 -1.47137
H -2.58210 -4.83300 0.85978
H -3.17291 -4.33007 3.22973
H -2.96394 -2.82996 5.20330
H -2.04430 -0.76386 6.23272
H -0.62369 0.76880 4.87982
H -0.13126 0.27006 2.51229
H 1.66860 -4.05910 -1.30970
H 1.14230 -3.61159 0.31303
H 4.04785 -3.70969 -0.58309
H 5.88257 -2.03162 -0.39400
H 6.58577 0.35329 -0.32567
H 5.98333 2.76361 -0.37324
H 3.59421 3.44096 -0.52004
H 1.80228 1.74032 -0.57288
H -1.26712 4.00533 0.06729
C -0.68994 4.10163 0.98365
C 0.61369 4.85842 0.94618
C 1.51335 4.50212 2.15098
C 0.74149 4.59440 3.48646
C -0.58435 3.88397 3.41868
C -1.22767 3.66585 2.20044
H -0.24134 1.95003 0.73401
H 0.40240 5.94242 0.95411
H 2.39037 5.15850 2.17558
H 1.34974 4.18923 4.30560
H 0.57338 5.65609 3.74083
H -1.05840 3.57195 4.34515
H -2.19126 3.16094 2.19858
H 1.88367 3.47546 2.02471
H 1.14296 4.66913 0.00341

76
Rebound Transition State 1 (2/5)
Fe 0.04216 -0.59658 -0.23938
N -1.17078 -0.36348 -2.02830
N -0.98569 -1.89427 1.17218
N 2.18726 -0.91447 -0.50222
N 0.15066 -2.54753 -1.20999
O -0.02931 1.02023 0.54958
C 0.21235 -2.26248 -2.67442
C -0.76211 -1.16400 -3.02755
C -1.21298 -1.00216 -4.35630
C -2.10793 0.00647 -4.64442
C -2.60272 0.83838 -3.60554
C -3.57019 1.85432 -3.83796
C -4.05908 2.60678 -2.78880
C -3.60278 2.36455 -1.46798
C -2.65232 1.39229 -1.20880
C -2.12290 0.61989 -2.27126
C -1.08326 -3.29410 -0.82695
C -1.42841 -3.03757 0.61915
C -2.20757 -3.97416 1.33363
C -2.52840 -3.72011 2.64944
C -2.05925 -2.53824 3.27880
C -2.33732 -2.24667 4.64251
C -1.84660 -1.09598 5.22577
C -1.05906 -0.19719 4.46300
C -0.77071 -0.44861 3.13309
C -1.26744 -1.61969 2.50944
C 1.38399 -3.21003 -0.69718
C 2.51299 -2.21642 -0.58689
C 3.85098 -2.66777 -0.56433
C 4.87058 -1.74709 -0.45761
C 4.57253 -0.36047 -0.41285
C 5.59101 0.63040 -0.35920
C 5.26301 1.97105 -0.36314
C 3.90286 2.36576 -0.42361
C 2.88632 1.42735 -0.46439
C 3.19585 0.04557 -0.45021
H -0.00084 -3.16511 -3.26052
H 1.23245 -1.94887 -2.91973
H -0.85148 -1.67164 -5.12673
H -2.46009 0.15789 -5.65899
H -3.92162 2.01787 -4.85115
H -4.80012 3.37742 -2.96746
H -4.00979 2.94646 -0.64841
H -2.30982 1.20501 -0.20060
H -0.96051 -4.36864 -1.00851
H -1.90511 -2.95044 -1.46325
H -2.53592 -4.87930 0.83828
H -3.12649 -4.42394 3.21802
H -2.93833 -2.94746 5.21231
H -2.05864 -0.87630 6.26596
H -0.67621 0.70402 4.92951
H -0.18135 0.24557 2.54954
H 1.67370 -4.05089 -1.33931
H 1.16068 -3.62283 0.29277
H 4.05495 -3.72887 -0.63360
H 5.90554 -2.06990 -0.42934
H 6.62721 0.31066 -0.32561
H 6.04079 2.72526 -0.32788
H 3.65588 3.42144 -0.44207
H 1.85045 1.73177 -0.50170
H -1.15638 4.10269 -0.14727
C -0.64086 4.19333 0.80509
C 0.67706 4.91687 0.85148
C 1.49547 4.54024 2.10632
C 0.64346 4.62988 3.39122
C -0.68767 3.95285 3.23394
C -1.26284 3.75590 1.97916
H -0.20290 1.95939 0.76448
H 0.48160 6.00422 0.84949
H 2.37491 5.18711 2.19126
H 1.18742 4.20462 4.24406
H 0.47352 5.69039 3.65086
H -1.22600 3.64759 4.12676
H -2.23604 3.27609 1.91628
H 1.86276 3.51112 1.99499
H 1.25438 4.72226 -0.06079

76
Rebound Intermediate (2/5)
Fe 0.18733 -0.59039 -0.27033
N -1.12876 -0.38175 -2.10528
N -0.75687 -1.88499 1.26638
N 2.40308 -1.15782 -0.51121
N 0.12285 -2.64274 -1.21351
O 0.28153 1.20653 0.45249
C 0.04004 -2.43771 -2.68447
C -0.93837 -1.33827 -3.02355
C -1.60437 -1.33794 -4.27404
C -2.48934 -0.32324 -4.56653
C -2.73768 0.69708 -3.60999
C -3.66219 1.75340 -3.83898
C -3.88185 2.71179 -2.86953
C -3.18296 2.64931 -1.63602
C -2.27460 1.63770 -1.38105
C -2.03243 0.64139 -2.36156
C -1.08482 -3.32530 -0.66745
C -1.23797 -3.04912 0.81067
C -1.89036 -3.98175 1.65388
C -2.03848 -3.69207 2.99338
C -1.53577 -2.46968 3.51451
C -1.64363 -2.11613 4.88805
C -1.13326 -0.91594 5.34173
C -0.50065 -0.02216 4.43812
C -0.37851 -0.33195 3.09494
C -0.88926 -1.56367 2.60971
C 1.37297 -3.34675 -0.81893
C 2.57542 -2.43577 -0.87821
C 3.83491 -2.95908 -1.26211
C 4.94074 -2.13736 -1.25728
C 4.80907 -0.78460 -0.84911
C 5.91429 0.11010 -0.79984
C 5.74281 1.41058 -0.36990
C 4.45924 1.86122 0.03503
C 3.36158 1.02135 -0.00954
C 3.50788 -0.31492 -0.46363
H -0.23646 -3.36605 -3.20282
H 1.03846 -2.15613 -3.03909
H -1.41387 -2.13837 -4.97869
H -3.01256 -0.30120 -5.51668
H -4.19128 1.78886 -4.78585
H -4.58872 3.51497 -3.04603
H -3.36435 3.40901 -0.88327
H -1.71910 1.59333 -0.45060
H -1.04912 -4.40685 -0.85448
H -1.96073 -2.93483 -1.19729
H -2.25604 -4.91212 1.23648
H -2.52936 -4.39307 3.66027
H -2.13182 -2.80588 5.56894
H -1.21529 -0.64992 6.38988
H -0.10821 0.91873 4.80975
H 0.07929 0.35736 2.39192
H 1.53577 -4.23778 -1.43978
H 1.24758 -3.69136 0.21371
H 3.90867 -3.99743 -1.56175
H 5.91298 -2.51256 -1.55907
H 6.89259 -0.25214 -1.09927
H 6.58800 2.08904 -0.33090
H 4.34108 2.87995 0.38947
H 2.37902 1.34087 0.32001
H -0.06940 6.53940 0.26982
C -0.37594 5.83924 1.04393
C 0.67832 5.22432 1.87969
C 0.19786 3.98097 2.65065
C -1.19616 4.19953 3.26665
C -2.14149 4.87901 2.35410
C -1.73559 5.62155 1.24859
H 0.41786 1.95747 -0.15849
H 1.02268 6.02327 2.56834
H 0.91626 3.72993 3.43515
H -1.63802 3.25885 3.61942
H -1.14582 4.83164 4.17701
H -3.20141 4.83849 2.59582
H -2.46814 6.10592 0.61585
H 0.15538 3.12648 1.96331
H 1.55891 5.00781 1.26177

76
Rebound Transition State 2 (2/5)
Fe 0.14992 -0.48935 -0.22240
N -1.25332 -0.33554 -2.00963
N -0.64653 -1.87322 1.32738
N 2.37305 -0.92963 -0.58534
N 0.15665 -2.52744 -1.20165
O 0.16430 1.30587 0.51552
C 0.01883 -2.30573 -2.66539
C -1.02130 -1.25101 -2.95924
C -1.70098 -1.24963 -4.20267
C -2.64386 -0.27739 -4.45464
C -2.94130 0.69419 -3.46184
C -3.92965 1.70023 -3.64598
C -4.20083 2.60576 -2.63949
C -3.49253 2.53814 -1.41181
C -2.52023 1.57671 -1.20190
C -2.22181 0.63721 -2.22175
C -0.99668 -3.27793 -0.62923
C -1.10436 -3.04217 0.85980
C -1.68748 -4.02003 1.70248
C -1.78668 -3.77293 3.05476
C -1.30133 -2.54940 3.58942
C -1.35569 -2.24141 4.97683
C -0.86274 -1.03930 5.44428
C -0.30329 -0.09801 4.54104
C -0.23582 -0.36242 3.18446
C -0.72832 -1.59544 2.68426
C 1.45262 -3.17121 -0.85628
C 2.60301 -2.19875 -0.95144
C 3.87636 -2.65612 -1.37187
C 4.93563 -1.77621 -1.40641
C 4.74237 -0.42836 -1.00651
C 5.79683 0.52672 -1.00390
C 5.56587 1.82196 -0.58646
C 4.27200 2.20658 -0.14785
C 3.22211 1.30649 -0.14451
C 3.43014 -0.02639 -0.58400
H -0.22835 -3.23928 -3.18964
H 0.99094 -1.97139 -3.04579
H -1.47436 -2.01591 -4.93410
H -3.17712 -0.25403 -5.39917
H -4.46754 1.73855 -4.58775
H -4.95725 3.36967 -2.78137
H -3.72022 3.25225 -0.62777
H -1.96097 1.52875 -0.27447
H -0.91685 -4.35242 -0.84225
H -1.90908 -2.91890 -1.11812
H -2.03809 -4.95118 1.27409
H -2.22366 -4.50886 3.72148
H -1.78864 -2.96749 5.65728
H -0.90307 -0.80782 6.50295
H 0.07446 0.84380 4.92473
H 0.16266 0.36502 2.48433
H 1.63864 -4.04848 -1.49028
H 1.38142 -3.52854 0.17706
H 3.99668 -3.69104 -1.66818
H 5.91713 -2.10089 -1.73552
H 6.78399 0.21527 -1.33019
H 6.37216 2.54725 -0.58376
H 4.11022 3.22373 0.19376
H 2.23319 1.57324 0.21377
H 1.99188 4.51079 1.53500
C 0.91686 4.53087 1.69810
C 0.39221 3.96320 2.95976
C -1.11091 3.64544 2.88734
C -1.89731 4.80298 2.24704
C -1.23937 5.35475 1.04129
C 0.10885 5.16205 0.75492
H 0.13711 2.05824 -0.10811
H 0.61192 4.71220 3.74803
H -1.50209 3.42920 3.88406
H -2.92831 4.51553 2.00513
H -2.01320 5.65302 2.95018
H -1.83109 5.98134 0.37758
H 0.54316 5.58320 -0.14272
H -1.23089 2.74524 2.27371
H 0.98336 3.08540 3.24284

76
Rebound Product (2/5)
Fe 0.22320 -0.40617 -0.08503
N -1.30740 -0.30044 -1.69723
N -0.53947 -1.84527 1.43861
N 2.36455 -0.63955 -0.76182
N 0.29106 -2.37110 -1.09261
O 0.04247 1.66328 0.46483
C 0.16782 -2.05554 -2.54120
C -0.89762 -1.00429 -2.76426
C -1.43458 -0.79897 -4.05827
C -2.41563 0.15161 -4.23792
C -2.92730 0.86468 -3.11981
C -3.99210 1.80030 -3.22844
C -4.50091 2.41499 -2.10097
C -3.97302 2.10400 -0.82224

C -2.92322 1.21145 -0.68409
C -2.36389 0.59218 -1.83034
C -0.85233 -3.17663 -0.58769
C -1.06859 -2.94890 0.88894
C -1.82488 -3.88484 1.63613
C -2.03348 -3.66805 2.97971
C -1.44792 -2.53865 3.61160
C -1.57700 -2.28872 5.00534
C -0.94654 -1.20471 5.58413
C -0.15609 -0.33623 4.78963
C -0.02358 -0.54797 3.42891
C -0.67548 -1.63825 2.80669
C 1.60158 -2.96410 -0.72341
C 2.70629 -1.93756 -0.79637
C 4.05011 -2.36968 -0.90383
C 5.05713 -1.43450 -0.98633
C 4.73410 -0.05230 -1.02423
C 5.72201 0.95691 -1.18972
C 5.35640 2.28441 -1.28975
C 3.98697 2.64803 -1.23204
C 3.00396 1.69131 -1.04991
C 3.35325 0.32478 -0.92822
H -0.06884 -2.95429 -3.12742
H 1.13410 -1.68488 -2.89689
H -1.06448 -1.38857 -4.88813
H -2.82670 0.34278 -5.22333
H -4.40546 2.00989 -4.20940
H -5.31726 3.12300 -2.18606
H -4.40608 2.56288 0.05957
H -2.55112 0.94683 0.29833
H -0.69831 -4.24613 -0.78399
H -1.75212 -2.87812 -1.13448
H -2.23045 -4.75665 1.13724
H -2.62217 -4.36282 3.56901
H -2.17035 -2.97131 5.60461
H -1.04353 -1.01933 6.64776
H 0.35302 0.50011 5.25551
H 0.59625 0.10175 2.82787
H 1.84675 -3.82017 -1.36733
H 1.52231 -3.34550 0.30049
H 4.26553 -3.43109 -0.92048
H 6.09513 -1.74199 -1.05333
H 6.76416 0.66117 -1.25079
H 6.11067 3.05116 -1.42500
H 3.70791 3.69067 -1.33953
H 1.96096 1.97086 -1.00994
H 1.19492 1.97544 2.13339
C 0.43883 2.57887 1.62840
C -0.77385 2.83185 2.53042
C -1.68657 3.94254 1.97822
C -0.90851 5.25982 1.81034
C 0.44347 5.03988 1.18064
C 1.04435 3.84060 1.08250
H -0.45609 2.18328 -0.19819
H -0.39320 3.13038 3.51730
H -2.54252 4.08722 2.64596
H -1.48527 5.97306 1.20749
H -0.76859 5.74493 2.79003
H 0.95994 5.92067 0.80416
H 2.02565 3.75398 0.62843
H -2.09628 3.63731 1.00572
H -1.32601 1.89821 2.67335

76
OAT Reactant Complex (2/5)
Fe 0.14693 -0.92220 -0.99783
N 2.19313 -0.91012 -1.32072
N -0.73934 0.95505 -0.95610
N -0.93974 -2.56276 -1.62979
N 0.15254 -0.54585 -2.97787
O 0.15497 -1.24886 0.63075
C 1.31524 -1.31137 -3.55017
C 2.48343 -1.20418 -2.60676
C 3.80145 -1.41636 -3.05153
C 4.83781 -1.32248 -2.14448
C 4.57706 -0.97797 -0.79430
C 5.62118 -0.82672 0.15935
C 5.33500 -0.45338 1.45651
C 3.99276 -0.21277 1.84298
C 2.95020 -0.35640 0.94335
C 3.21654 -0.75453 -0.38848
C 0.32176 0.93931 -3.14506
C -0.45310 1.65693 -2.07393
C -0.83152 3.00290 -2.23719
C -1.52244 3.63287 -1.22264
C -1.87571 2.91984 -0.04966
C -2.62673 3.52207 0.99684
C -2.98947 2.78964 2.10856
C -2.61472 1.42656 2.20857
C -1.87632 0.80973 1.21293
C -1.48068 1.54276 0.06854
C -1.16867 -1.03232 -3.50587
C -1.52819 -2.32467 -2.82288
C -2.44685 -3.21947 -3.40172
C -2.76024 -4.38474 -2.73161
C -2.13377 -4.69002 -1.49758
C -2.39711 -5.90172 -0.80132
C -1.74270 -6.18618 0.37965
C -0.79702 -5.26868 0.90142
C -0.51990 -4.07679 0.25391
C -1.19014 -3.75398 -0.95009
H 1.56794 -0.92987 -4.54460
H 1.01422 -2.35766 -3.66388
H 3.98267 -1.64669 -4.09342
H 5.86118 -1.49110 -2.46083
H 6.64349 -1.00297 -0.15708
H 6.13229 -0.33538 2.18099
H 3.77812 0.09279 2.86096
H 1.93056 -0.17357 1.25066
H 0.00052 1.24744 -4.14553
H 1.38715 1.17326 -3.05516
H -0.57793 3.52089 -3.15301
H -1.81808 4.67140 -1.32154
H -2.91322 4.56345 0.89746
H -3.56585 3.24892 2.90314
H -2.91450 0.85356 3.07889
H -1.59263 -0.22858 1.30449
H -1.12343 -1.15343 -4.59310
H -1.92274 -0.26873 -3.28948
H -2.89005 -2.98260 -4.36014
H -3.47233 -5.08568 -3.15260
H -3.11470 -6.59747 -1.22248
H -1.94220 -7.11146 0.90743
H -0.27689 -5.50534 1.82284
H 0.20058 -3.38468 0.66490
H -0.89004 1.73530 5.10354
C -0.29318 0.98040 5.63469
C -1.22139 -0.04980 6.31048
C -0.42673 -1.28637 6.77281
C 0.25113 -1.98592 5.57598
C 0.90395 -0.99669 4.63426
C 0.67392 0.32659 4.67096
H 0.27048 1.53609 6.40205
H -1.99335 -0.36808 5.59432
H -1.08203 -1.99124 7.29926
H 1.00148 -2.70481 5.93469
H -0.49115 -2.58586 5.02416
H 1.59957 -1.40370 3.90133
H 1.19889 0.98601 3.98053
H 0.34304 -0.96942 7.49146
H -1.74410 0.41176 7.15729

76
OAT Transition State (2/5)
Fe 0.20523 -0.74638 -0.40645
N 2.29208 -0.81377 -1.01038
N -0.78762 1.16314 -0.67616
N -0.87710 -2.50329 -1.02906
N 0.10451 -0.54026 -2.56633
O 0.24392 -0.93592 1.31462
C 1.20692 -1.37252 -3.12679
C 2.44646 -1.24133 -2.27663
C 3.71030 -1.57035 -2.81570
C 4.83353 -1.44758 -2.02687
C 4.71817 -0.95473 -0.70108
C 5.84888 -0.75749 0.13817
C 5.69539 -0.23614 1.40711
C 4.40419 0.11024 1.87987
C 3.28242 -0.07961 1.09212
C 3.41224 -0.62451 -0.20717
C 0.28437 0.91053 -2.85425
C -0.48872 1.73591 -1.85682
C -0.87544 3.05498 -2.17966
C -1.60138 3.78705 -1.26561
C -1.98517 3.20023 -0.03216
C -2.79248 3.88984 0.91337
C -3.19011 3.26606 2.07814
C -2.78650 1.93231 2.33975
C -1.98275 1.23809 1.45178
C -1.56504 1.85587 0.24819
C -1.24649 -1.04454 -2.94935
C -1.56153 -2.29815 -2.17009
C -2.52894 -3.21030 -2.64478
C -2.77508 -4.36377 -1.93106
C -2.02483 -4.64850 -0.76064
C -2.18440 -5.85936 -0.03266
C -1.39331 -6.12254 1.06748
C -0.41481 -5.18224 1.47800
C -0.24530 -3.98586 0.80262
C -1.05018 -3.68974 -0.32313
H 1.42364 -1.09076 -4.16476
H 0.87912 -2.41705 -3.13911
H 3.77748 -1.91141 -3.84117
H 5.81277 -1.70355 -2.41648
H 6.83134 -1.01620 -0.24222
H 6.55928 -0.08235 2.04344
H 4.29770 0.53234 2.87317
H 2.29452 0.17684 1.44731
H -0.02969 1.15255 -3.87713
H 1.35184 1.14384 -2.77936
H -0.60404 3.46610 -3.14385
H -1.90800 4.80300 -1.48938
H -3.09748 4.90743 0.69365
H -3.81444 3.78851 2.79382
H -3.11821 1.44888 3.25179
H -1.65362 0.22837 1.66077
H -1.30523 -1.24083 -4.02718
H -1.98257 -0.26645 -2.72203
H -3.05704 -2.99384 -3.56490
H -3.51960 -5.07503 -2.27172
H -2.92855 -6.57426 -0.36728
H -1.51070 -7.04972 1.61660
H 0.21122 -5.40583 2.33462
H 0.49258 -3.26338 1.12238
H -0.64641 1.46598 4.33102
C -0.26578 0.52714 4.75771
C -1.41558 -0.45102 5.07251
C -0.88220 -1.87873 5.28582
C -0.15795 -2.38545 4.01929
C 0.82120 -1.37651 3.47800
O 0.77668 -0.04604 3.85122
H 0.23889 0.83023 5.69215
H -2.13165 -0.46085 4.23941
H -1.70102 -2.56164 5.53754
H 0.36803 -3.32610 4.22351
H -0.89689 -2.61604 3.23972
H 1.69527 -1.74331 2.95320
H 1.55328 0.62993 3.50517
H -0.18531 -1.88664 6.13524
H -1.96175 -0.10509 5.95682

76
OAT Product (2/5)
Fe 0.28773 -0.71572 -0.20328
N 2.45305 -0.74798 -0.88927
N -0.90255 1.12690 -0.52743
N -0.93142 -2.42161 -0.92969
N 0.20394 -0.44916 -2.39430
O 0.30107 -0.80250 1.96435
C 1.28710 -1.28242 -2.97434
C 2.53808 -1.24723 -2.13145
C 3.74996 -1.74405 -2.67291
C 4.89302 -1.72576 -1.90608
C 4.86284 -1.14044 -0.61199
C 6.02136 -1.01711 0.20306
C 5.95510 -0.37226 1.42300
C 4.73002 0.19038 1.86279
C 3.58420 0.06849 1.09715
C 3.61515 -0.62100 -0.13633
C 0.40920 1.01296 -2.58332
C -0.46120 1.78259 -1.61376
C -0.82111 3.12337 -1.88746
C -1.68365 3.77761 -1.03476
C -2.24472 3.08735 0.07282
C -3.21857 3.67405 0.92668
C -3.78933 2.93667 1.94513
C -3.40313 1.58709 2.14874
C -2.43919 0.99468 1.35146
C -1.83673 1.73161 0.30291
C -1.14212 -0.90702 -2.83688
C -1.55614 -2.15131 -2.08618
C -2.57474 -2.98257 -2.61191
C -2.94222 -4.11820 -1.92509
C -2.26205 -4.47269 -0.72966
C -2.54612 -5.66798 -0.01384
C -1.81570 -6.00068 1.10971
C -0.76958 -5.15212 1.55306
C -0.48133 -3.97350 0.88752
C -1.22788 -3.60003 -0.25553
H 1.52353 -0.96504 -3.99988
H 0.92416 -2.31371 -3.03838
H 3.75579 -2.14081 -3.68090
H 5.82524 -2.12689 -2.28890
H 6.95951 -1.42458 -0.15894
H 6.84163 -0.27560 2.03920
H 4.69534 0.73043 2.80245
H 2.65808 0.53479 1.39932
H 0.18165 1.32134 -3.61306
H 1.46623 1.23499 -2.40440
H -0.42480 3.61105 -2.76964
H -1.97036 4.80708 -1.22077
H -3.51533 4.70280 0.75132
H -4.54099 3.38165 2.58711
H -3.87106 1.01313 2.94094
H -2.13926 -0.03285 1.51453
H -1.15836 -1.09903 -3.91799
H -1.86349 -0.10744 -2.64482
H -3.04883 -2.71321 -3.54774
H -3.72918 -4.76276 -2.30139
H -3.33640 -6.31768 -0.37522
H -2.02909 -6.91597 1.64988
H -0.18535 -5.43587 2.42148
H 0.32831 -3.33801 1.22010
H -0.95807 1.31329 3.61182
C -0.35811 0.53734 4.09658
C -1.23850 -0.59776 4.65187
C -0.36546 -1.75687 5.16166
C 0.46380 -2.38493 4.02008
C 1.14331 -1.35675 3.13569
C 0.72235 0.06356 3.16022
H 0.16929 1.02642 4.92981
H -1.92175 -0.96340 3.87373
H -0.98617 -2.53375 5.62159
H 1.23490 -3.04778 4.42870
H -0.18820 -3.00839 3.39922
H 2.15011 -1.58073 2.79887
H 1.44123 0.82073 2.86836
H 0.30833 -1.38279 5.94509
H -1.86144 -0.20352 5.46238

3_{TBP} without substrate

42
TBP with Def2-TZVPP (2/3)
Fe 0.30808 7.23587 4.24781
O -0.08863 7.08361 2.70097
N 0.59729 7.32062 6.31203
N 2.05069 8.03598 4.12442
N -0.56007 8.99487 4.56985
N 1.06994 5.40998 4.50615
C 2.63423 8.35018 2.95129
H 2.07661 8.12374 2.05760
C 3.88405 8.93105 2.91421
H 4.32647 9.17028 1.95921
C 4.54283 9.19371 4.10988
H 5.52308 9.64829 4.10791
C 3.92913 8.86742 5.30686
H 4.41199 9.05817 6.25428
C 2.67080 8.28251 5.28928
C -0.88436 9.87081 3.60775
H -0.67199 9.56928 2.59337
C -1.46351 11.08914 3.90738
H -1.71453 11.77040 3.10866
C -1.70209 11.40933 5.23774
H -2.14383 12.35955 5.50215
C -1.36436 10.49796 6.22852
H -1.53625 10.71656 7.27209
C -0.79907 9.28735 5.86420
C 1.52537 4.62656 3.51849
C 2.05361 3.37565 3.77652
H 2.40913 2.76815 2.95822
C 2.11961 2.93363 5.09159
H 2.53735 1.96431 5.32369
C 1.64781 3.75099 6.10952
H 1.68738 3.43820 7.14250
C 1.11651 4.98794 5.78559
C 1.96010 7.89600 6.55608
H 2.56552 7.16725 7.09373
H 1.87613 8.76699 7.20419
C -0.48460 8.19541 6.84954
H -1.37708 7.58277 6.97725
H -0.22218 8.59666 7.82762
C 0.49933 5.91404 6.79712
H -0.55725 5.66501 6.89557
H 0.95509 5.80039 7.77997
H 1.45220 5.02490 2.51798

42
TBP with Def2-TZVPP (2/5)
Fe 1.06808 7.56994 4.03226
O 0.94888 7.52775 2.41405
N 1.21963 7.61957 6.11232
N 2.89160 8.45381 4.17333
N -0.58566 8.69007 4.42961
N 0.89330 5.57759 4.38394
C 3.52375 9.07049 3.16259
H 3.03333 9.03658 2.20146
C 4.73285 9.70990 3.35550
H 5.21906 10.19689 2.52397
C 5.29264 9.71450 4.62748
H 6.23364 10.21419 4.80891
C 4.63240 9.07640 5.66932
H 5.04171 9.06743 6.66866
C 3.42895 8.44405 5.41104
C -1.56408 8.94850 3.54822
H -1.41857 8.56831 2.54829
C -2.68888 9.66262 3.91260
H -3.45904 9.85722 3.18187
C -2.80197 10.11001 5.22343
H -3.67478 10.66426 5.53820
C -1.78676 9.83738 6.13121
H -1.84924 10.17011 7.15671
C -0.67896 9.12739 5.70248
C 0.98901 4.62699 3.44084
C 0.94454 3.28555 3.76616
H 1.02299 2.54314 2.98660
C 0.80528 2.92477 5.10106
H 0.77590 1.88239 5.38517
C 0.70749 3.91297 6.07182
H 0.60038 3.66147 7.11664
C 0.74805 5.24036 5.68206
C 2.67408 7.65759 6.44599
H 3.04662 6.63248 6.44596
H 2.82814 8.05807 7.44745
C 0.51373 8.85113 6.57549
H 0.23529 8.76079 7.62518
H 1.20677 9.68921 6.49472
C 0.56534 6.38505 6.63903
H -0.50165 6.58606 6.74031
H 0.94385 6.14550 7.63226
H 1.10285 4.97302 2.42456

42
TBP with LACVP (2/5)
Fe 1.05987 7.57375 4.08262
O 0.93686 7.53430 2.43254
N 1.21248 7.62022 6.12616
N 2.87060 8.45434 4.18647
N -0.58854 8.68193 4.44553
N 0.91538 5.58711 4.39493
C 3.48787 9.07906 3.15175
H 2.97553 9.05314 2.19992
C 4.71378 9.71223 3.33158
H 5.19116 10.20489 2.49496
C 5.30465 9.70128 4.60144
H 6.25518 10.19398 4.76621
C 4.65998 9.05348 5.66206
H 5.09622 9.03456 6.65261
C 3.43852 8.42645 5.42786
C -1.57115 8.92582 3.54190
H -1.42163 8.52477 2.54893
C -2.70058 9.65646 3.89769
H -3.47320 9.84169 3.16337
C -2.81413 10.13598 5.20873
H -3.68770 10.70139 5.50969
C -1.79436 9.87975 6.13344
H -1.86164 10.23921 7.15232
C -0.67945 9.15178 5.72447
C 1.03942 4.64219 3.42852
C 0.99278 3.28842 3.74605
H 1.09345 2.54948 2.96223
C 0.81950 2.90977 5.08338
H 0.78740 1.86152 5.35464
C 0.69044 3.89218 6.07259
H 0.55686 3.62240 7.11248
C 0.73496 5.23409 5.70148
C 2.68671 7.63550 6.46505
H 3.03975 6.59877 6.46178
H 2.83882 8.03213 7.47299
C 0.51689 8.87873 6.59753
H 0.24529 8.78660 7.65342
H 1.22896 9.70613 6.51028
C 0.53040 6.37879 6.65788
H -0.53927 6.59759 6.74149
H 0.89797 6.14678 7.66169
H 1.17447 5.00290 2.41814

43
FeOH TBP with LACVP (2/6)
Fe 0.01570 0.30514 0.22961
O -0.17170 0.34075 -1.54110
N 0.21988 0.26886 2.45174
N 1.89767 1.15592 0.49548
N -1.66052 1.38851 0.84208
N -0.03039 -1.73915 0.63501
C 2.54405 1.81076 -0.50468
H 2.04455 1.83285 -1.46340
C 3.77936 2.41349 -0.28920
H 4.27600 2.92885 -1.10079
C 4.35351 2.34314 0.98664
H 5.31101 2.81067 1.18264
C 3.68053 1.66852 2.01072
H 4.10142 1.60323 3.00633
C 2.44904 1.07262 1.73746
C -2.69498 1.66108 0.00486
H -2.59637 1.30246 -1.01036
C -3.81067 2.36582 0.44603
H -4.62290 2.57192 -0.23862
C -3.85783 2.79206 1.77953
H -4.71757 3.33752 2.14980
C -2.78866 2.50488 2.63525
H -2.80350 2.81951 3.67129

C -1.69035 1.80290 2.13846
C 0.13632 -2.67864 -0.33202
C 0.12639 -4.03583 -0.02526
H 0.26219 -4.76683 -0.81147
C -0.05752 -4.42721 1.30707
H -0.06378 -5.47743 1.57317
C -0.22898 -3.45284 2.29645
H -0.36918 -3.73031 3.33375
C -0.21774 -2.10612 1.93301
C 1.68772 0.25931 2.75478
H 2.03147 -0.77991 2.70911
H 1.87908 0.61868 3.77169
C -0.46017 1.50451 2.96012
H -0.70674 1.40699 4.02326
H 0.24600 2.33695 2.86424
C -0.45969 -0.98502 2.91439
H -1.53479 -0.78186 2.97123
H -0.12800 -1.26188 3.92120
H 0.27395 -2.31043 -1.33938
H -0.28806 0.36340 -2.50363

3_{Oh} without substrate

48
Oh with Def2-TZVPP (2/3)
Fe 0.16946 7.19135 4.24258
O -0.01000 7.14552 2.62217
N 0.52995 7.30966 6.31565
N 1.97264 8.00041 4.12552
N -0.62396 8.99354 4.58026
N 0.99189 5.38944 4.50582
C 2.56764 8.29424 2.95639
H 2.00290 8.06183 2.06715
C 3.82582 8.85844 2.90589
H 4.27121 9.08010 1.94787
C 4.49005 9.12693 4.09724
H 5.47690 9.56749 4.09001
C 3.87035 8.82271 5.29698
H 4.35591 9.01759 6.24230
C 2.60242 8.25595 5.28042
C -0.91876 9.88631 3.62711
H -0.72075 9.58189 2.61060
C -1.44912 11.12568 3.93704
H -1.67688 11.82138 3.14367
C -1.66949 11.44633 5.26978
H -2.07438 12.41053 5.54267
C -1.35911 10.51644 6.25256
H -1.51344 10.73601 7.29878
C -0.84266 9.28700 5.87721
C 1.45389 4.61129 3.51935
C 2.03398 3.38279 3.77989
H 2.39417 2.77908 2.96066
C 2.14524 2.95961 5.09750
H 2.60278 2.00893 5.33185
C 1.66738 3.77383 6.11512
H 1.74312 3.47770 7.15108
C 1.08336 4.98677 5.78845
C 1.88413 7.90576 6.55132
H 2.49051 7.20673 7.12628
H 1.78282 8.79904 7.16624
C -0.54869 8.18171 6.85665
H -1.44572 7.57617 6.97969
H -0.28723 8.57689 7.83776
C 0.46443 5.90601 6.80745
H -0.58393 5.63714 6.92954
H 0.94197 5.80196 7.78103
H 1.34549 4.99679 2.51696
N -1.62770 6.38049 4.52645
C -2.67194 5.91237 4.54565
C -3.98941 5.32034 4.57178
H -4.19089 4.92343 5.56587
H -4.73334 6.07666 4.32539
H -4.03763 4.51232 3.84286

48
Oh with Def2-TZVPP (2/5)
Fe 0.23797 7.11654 4.15158
O 0.06220 7.03657 2.54099
N 0.62191 7.25695 6.23442
N 2.11811 8.07456 4.06323
N -0.63941 8.96857 4.52005
N 0.98581 5.21886 4.51599
C 2.68601 8.52447 2.93440
H 2.17909 8.27244 2.01450
C 3.84737 9.27205 2.95488
H 4.28131 9.61715 2.02854
C 4.42583 9.57104 4.18376
H 5.32865 10.16323 4.23480
C 3.83274 9.10498 5.34729
H 4.26033 9.31891 6.31618
C 2.67393 8.34683 5.25114
C -1.00965 9.84427 3.57658
H -0.91137 9.51390 2.55289
C -1.48672 11.10054 3.90183
H -1.78040 11.78228 3.11804
C -1.56628 11.45720 5.24217
H -1.92437 12.43619 5.52795
C -1.17712 10.54674 6.21573
H -1.22585 10.79749 7.26518
C -0.72323 9.29793 5.82239
C 1.42569 4.37282 3.57528
C 1.94865 3.13542 3.90321
H 2.29338 2.47523 3.12180
C 2.02218 2.77514 5.24272
H 2.43356 1.81791 5.53031
C 1.56860 3.65815 6.21435
H 1.61963 3.40796 7.26392
C 1.04508 4.87773 5.81877
C 2.03311 7.72504 6.45991
H 2.63310 6.85986 6.74176
H 2.05965 8.40977 7.30593
C -0.38126 8.20792 6.80192
H -1.29131 7.64582 7.00971
H -0.03171 8.61891 7.74807
C 0.45658 5.87526 6.77925
H -0.60896 5.67573 6.88054
H 0.90283 5.78995 7.76954
H 1.34820 4.71242 2.55294
N -1.77793 6.26516 4.56591
C -2.84360 5.84186 4.55254
C -4.18750 5.30897 4.54155
H -4.34637 4.70073 5.43098
H -4.90436 6.12897 4.53141
H -4.32872 4.69418 3.65365

48
Oh with LACVP (2/3)
Fe 0.17782 7.19406 4.29508
O -0.02541 7.13888 2.64669
N 0.52158 7.30589 6.33365
N 1.95467 7.99233 4.14224
N -0.60740 8.98479 4.59051
N 0.99612 5.40742 4.51802
C 2.53655 8.28146 2.94861
H 1.95888 8.04274 2.06707
C 3.80278 8.85093 2.88447
H 4.24134 9.07035 1.91982
C 4.48578 9.12831 4.07542
H 5.47414 9.57111 4.05253
C 3.87866 8.82832 5.29577
H 4.38066 9.03086 6.23387
C 2.60322 8.25688 5.30340
C -0.87834 9.87655 3.60866
H -0.66506 9.55746 2.59811
C -1.40728 11.13081 3.90520
H -1.61729 11.82599 3.10292
C -1.65180 11.46746 5.24124
H -2.05484 12.43988 5.49721
C -1.36725 10.53851 6.24820
H -1.54222 10.77353 7.29057
C -0.85003 9.29268 5.89587
C 1.47160 4.64843 3.50296
C 2.06053 3.41010 3.74920
H 2.43146 2.82009 2.92134
C 2.16488 2.95663 5.06891
H 2.62675 2.00099 5.28563
C 1.67224 3.75040 6.11055
H 1.74381 3.42732 7.14154
C 1.08098 4.97628 5.80801
C 1.89140 7.90937 6.58102
H 2.49323 7.20191 7.15951
H 1.77992 8.80446 7.20011
C -0.57455 8.18594 6.88096
H -1.47186 7.57159 6.99812
H -0.30990 8.57568 7.86817
C 0.45145 5.88412 6.83292
H -0.60326 5.62135 6.95340
H 0.92971 5.78722 7.81177
H 1.36427 5.05639 2.50770
N -1.62254 6.38141 4.58504
C -2.68430 5.90372 4.57680
C -4.00700 5.30653 4.56973
H -4.23937 4.89156 5.55492
H -4.75896 6.05984 4.31754
H -4.05039 4.50207 3.82953

48
Oh with LACVP (2/5)
Fe 0.25677 7.12542 4.21457
O 0.05188 7.03592 2.57390
N 0.62558 7.25860 6.25935
N 2.12641 8.08028 4.09189
N -0.61799 8.94297 4.51769
N 0.98483 5.25192 4.51553
C 2.68789 8.53031 2.94208
H 2.16767 8.28139 2.02692
C 3.86291 9.27548 2.95912
H 4.29562 9.62276 2.02989
C 4.45958 9.56869 4.19291
H 5.36964 10.15508 4.23549
C 3.87225 9.10158 5.37241
H 4.31600 9.31296 6.33763
C 2.69897 8.34720 5.29070
C -0.97895 9.80151 3.53347
H -0.85701 9.44724 2.51887
C -1.47312 11.06813 3.83330
H -1.75841 11.73721 3.03214
C -1.58263 11.45254 5.17531
H -1.95436 12.43667 5.43410
C -1.20537 10.55903 6.18452
H -1.27922 10.83450 7.22899
C -0.73056 9.29712 5.82883
C 1.43189 4.42970 3.53586
C 1.96258 3.17838 3.83901
H 2.31299 2.53629 3.04167
C 2.03511 2.77861 5.17879
H 2.45090 1.81289 5.43976
C 1.57287 3.63643 6.18440
H 1.62483 3.35160 7.22769
C 1.04153 4.87390 5.82589
C 2.05497 7.72614 6.50172
H 2.64411 6.85051 6.79335
H 2.06876 8.41545 7.35023
C -0.39597 8.22092 6.82758
H -1.30372 7.64888 7.04233
H -0.04026 8.64131 7.77226
C 0.44710 5.85482 6.80150
H -0.62524 5.66630 6.89632
H 0.89306 5.76616 7.79625
H 1.35190 4.80129 2.52336
N -1.79808 6.26021 4.65896
C -2.88425 5.83522 4.62493
C -4.23613 5.30600 4.58724
H -4.42529 4.68953 5.47100
H -4.96142 6.12477 4.56738
H -4.37524 4.69078 3.69341

49
FeOH Oh with LACVP (2/2)
Fe 0.17770 7.18259 4.32372
O 0.01538 7.14915 2.51348
N 0.52780 7.30100 6.33849
N 1.95239 7.98467 4.14268
N -0.61004 8.97368 4.61338
N 0.98813 5.39208 4.55173
C 2.51878 8.27753 2.94517
H 1.92242 8.02688 2.07942
C 3.78041 8.86005 2.87032
H 4.21092 9.08354 1.90267
C 4.46970 9.14671 4.05533
H 5.45304 9.60066 4.02412
C 3.87623 8.84186 5.28231
H 4.38438 9.05147 6.21575
C 2.60759 8.25601 5.29702
C -0.87908 9.85700 3.62422
H -0.66889 9.51923 2.61898
C -1.39599 11.11850 3.91349
H -1.60631 11.80869 3.10683
C -1.62678 11.47011 5.24829
H -2.01953 12.44848 5.49776
C -1.34085 10.54927 6.26289
H -1.50434 10.79655 7.30435
C -0.83735 9.29633 5.91658
C 1.46723 4.63536 3.53760
C 2.05973 3.39870 3.78728
H 2.43414 2.80796 2.96138
C 2.16474 2.94783 5.10792
H 2.62984 1.99409 5.32641
C 1.66976 3.74190 6.14891
H 1.74300 3.42111 7.18054
C 1.07484 4.96450 5.84178
C 1.90851 7.88912 6.57806
H 2.50998 7.16119 7.13101
H 1.81379 8.76959 7.22027
C -0.55781 8.18999 6.89905
H -1.45701 7.57988 7.02546
H -0.27812 8.57453 7.88405
C 0.44170 5.88290 6.85325
H -0.61713 5.63106 6.96174
H 0.90740 5.79522 7.83901
H 1.35858 5.04995 2.54506
N -1.62800 6.37112 4.51666
C -2.69234 5.89620 4.52572
C -4.01933 5.30700 4.54172
H -4.14663 4.68851 5.43506
H -4.78065 6.09260 4.54478
H -4.16283 4.67992 3.65686
H -0.83114 6.77296 2.19279

49
FeOH Oh with LACVP (2/6)
Fe 0.20009 7.11326 4.05848
O -0.01164 7.02790 2.27015
N 0.59329 7.25430 6.28454
N 2.07950 8.06306 4.04748
N -0.65549 9.00411 4.55019
N 1.00185 5.19980 4.53725
C 2.65316 8.50108 2.89630
H 2.12932 8.24931 1.98419
C 3.83596 9.23229 2.91243
H 4.27604 9.56901 1.98270
C 4.43106 9.52497 4.14729
H 5.34820 10.10038 4.19123
C 3.83185 9.07111 5.32496
H 4.27361 9.28315 6.29120
C 2.64848 8.32941 5.24731
C -1.00217 9.91278 3.60499
H -0.89937 9.59575 2.57570
C -1.45840 11.18135 3.95427
H -1.73136 11.88857 3.18173
C -1.54484 11.51727 5.31106
H -1.88660 12.50070 5.61145
C -1.18169 10.57487 6.27913
H -1.23664 10.81167 7.33459
C -0.74489 9.31316 5.86955
C 1.48006 4.34935 3.59526
C 2.02940 3.11797 3.94473
H 2.40445 2.45641 3.17460
C 2.08921 2.76480 5.29842
H 2.51844 1.81638 5.59894
C 1.59676 3.64938 6.26433
H 1.63767 3.40274 7.31823
C 1.04843 4.86599 5.85456
C 2.00714 7.74180 6.48281
H 2.61653 6.88971 6.80396
H 2.03472 8.46903 7.30100
C -0.42818 8.20137 6.84134
H -1.34529 7.63087 7.02127
H -0.10338 8.60665 7.80606
C 0.43128 5.85736 6.81156
H -0.64018 5.65264 6.89545
H 0.86460 5.75773 7.81298
H 1.41039 4.68327 2.56858
N -1.80710 6.25210 4.52665
C -2.88783 5.81442 4.56422
C -4.23304 5.27056 4.61083
H -4.36249 4.65799 5.50792
H -4.96711 6.08157 4.62894
H -4.41742 4.64787 3.73036
H -0.51842 6.77804 1.48019

3_{Oh} with cyclohexene

64
MECP (2/3 or 2/5)
Fe 0.06032 0.15129 0.57875
O -0.31232 0.39330 -1.01521
N 0.62881 -0.10637 2.56517
N 1.91819 1.13603 0.45821
N -0.82124 1.83108 1.33389
N 0.87558 -1.70840 0.40753
C 2.39747 1.73907 -0.65891
H 1.78519 1.65186 -1.54645
C 3.60603 2.42619 -0.64183
H 3.97274 2.89684 -1.54467
C 4.32560 2.49611 0.55972
H 5.26789 3.02906 0.60196
C 3.82185 1.87359 1.70471
H 4.36206 1.91204 2.64303
C 2.60586 1.18836 1.62257
C -1.27130 2.87087 0.59076
H -1.22303 2.75019 -0.48312
C -1.76221 4.02443 1.19653
H -2.11551 4.84422 0.58472
C -1.78226 4.09986 2.59452
H -2.15185 4.99047 3.08851
C -1.31859 3.01862 3.35375
H -1.32711 3.05443 4.43571
C -0.84244 1.88502 2.69625
C 1.23614 -2.29124 -0.76154
C 1.86717 -3.53288 -0.77645
H 2.14806 -3.98122 -1.72027
C 2.12902 -4.17528 0.43957
H 2.62550 -5.13814 0.45273
C 1.75007 -3.56594 1.64204
H 1.94328 -4.04567 2.59345
C 1.11635 -2.32517 1.60084
C 2.03475 0.43698 2.79840
H 2.69071 -0.40929 3.02621
H 2.02351 1.07517 3.68651
C -0.40095 0.62843 3.39889
H -1.26494 -0.03276 3.51216
H -0.00790 0.83516 4.39780
C 0.58988 -1.60147 2.81232
H -0.45405 -1.88509 2.97008
H 1.14621 -1.85614 3.71855
H 1.00733 -1.74110 -1.66413
N -1.92707 -0.90883 1.03013
C -2.99050 -1.38738 0.98022
C -4.31300 -1.98549 0.92452
H -4.95083 -1.56682 1.70854
H -4.77581 -1.78802 -0.04686
H -4.24433 -3.06806 1.06679
H -2.17010 1.31649 -4.50339
C -1.68407 0.37584 -4.20535
C -2.64521 -0.80885 -4.44039
C -1.89510 -2.15508 -4.39999
C -0.79661 -2.21135 -5.48178
C 0.00801 -0.93104 -5.53927
C -0.38152 0.21622 -4.95836
H -1.47001 0.47796 -3.12958
H -3.12689 -0.69737 -5.42270
H -2.59603 -2.98857 -4.53117
H -0.12618 -3.06229 -5.29513
H -1.25112 -2.40858 -6.46653
H 0.94955 -0.96747 -6.08562
H 0.25828 1.09625 -5.02283
H -1.43276 -2.27974 -3.40950
H -3.44632 -0.79515 -3.69025

64
HAT Reactant Complex (2/3)
Fe 0.05074 0.13612 0.61198
O -0.31269 0.38314 -0.99112
N 0.58987 -0.12099 2.59304
N 1.77474 1.04125 0.45407
N -0.76477 1.79250 1.32052
N 0.95333 -1.61162 0.40799
C 2.22914 1.57251 -0.71115
H 1.57456 1.47601 -1.56552
C 3.46728 2.20014 -0.78125
H 3.80331 2.61442 -1.72278
C 4.25582 2.28172 0.37350
H 5.22501 2.76475 0.34510
C 3.77922 1.73302 1.56503
H 4.36457 1.77968 2.47511
C 2.52647 1.11398 1.58027
C -1.16134 2.83944 0.55930
H -1.03292 2.73292 -0.50871
C -1.70880 3.98130 1.13995
H -2.02030 4.80465 0.51054
C -1.84038 4.04049 2.53182
H -2.25626 4.92080 3.00679
C -1.42555 2.95357 3.30916
H -1.51150 2.97403 4.38834
C -0.89394 1.83038 2.67682
C 1.35119 -2.13675 -0.77458
C 2.00557 -3.36543 -0.82921
H 2.31214 -3.76642 -1.78645
C 2.25746 -4.05534 0.36187
H 2.77144 -5.00879 0.34546
C 1.84427 -3.50194 1.57865
H 2.03006 -4.01180 2.51565
C 1.18359 -2.27409 1.57635
C 1.94997 0.50834 2.82928
H 2.63130 -0.25071 3.22444
H 1.85627 1.27702 3.60209
C -0.47919 0.57415 3.39940
H -1.33587 -0.10088 3.47860
H -0.12943 0.78455 4.41433
C 0.62867 -1.61335 2.81190
H -0.39638 -1.95672 2.97788
H 1.20996 -1.86452 3.70387
H 1.12904 -1.55381 -1.65732
N -1.68095 -0.81447 0.90065
C -2.71963 -1.34053 0.89507
C -4.01301 -1.99891 0.89051
H -4.77150 -1.34453 1.32977
H -4.30591 -2.23895 -0.13607
H -3.96685 -2.92579 1.46960
H -3.53773 0.90147 -3.90425
C -2.67176 0.22396 -3.90185
C -3.14222 -1.23699 -4.05999
C -1.95611 -2.16403 -4.38980
C -1.28112 -1.74674 -5.71321
C -1.09568 -0.24741 -5.80903
C -1.70487 0.62923 -4.99387
H -2.19032 0.35724 -2.91938
H -3.87986 -1.29606 -4.87356

H -2.28694 -3.20841 -4.44826
H -0.30810 -2.24809 -5.81506
H -1.88399 -2.09830 -6.56672
H -0.42704 0.11532 -6.58882
H -1.51183 1.69539 -5.10816
H -1.22066 -2.10761 -3.57354
H -3.64952 -1.57115 -3.14597

64
HAT Transition State (2/3)
Fe 0.09717 7.32501 4.21990
O -0.08934 7.46587 2.47254
N 0.51177 7.24836 6.24533
N 1.87206 8.15764 4.08049
N -0.69702 9.07005 4.71958
N 0.94840 5.53463 4.24970
C 2.42009 8.56086 2.90556
H 1.81086 8.39175 2.02876
C 3.67989 9.14869 2.85932
H 4.09138 9.46003 1.90779
C 4.39232 9.32550 4.05216
H 5.37562 9.78052 4.04442
C 3.82111 8.90753 5.25546
H 4.34673 9.02969 6.19481
C 2.55117 8.32309 5.24160
C -0.99506 10.05565 3.84122
H -0.80093 9.83717 2.80066
C -1.51898 11.27135 4.27660
H -1.75185 12.04364 3.55502
C -1.72759 11.47068 5.64600
H -2.12637 12.41017 6.00952
C -1.40973 10.44768 6.54637
H -1.55347 10.57678 7.61191
C -0.89850 9.24684 6.05497
C 1.40363 4.88490 3.15347
C 2.02494 3.64209 3.26178
H 2.37922 3.14073 2.37042
C 2.18361 3.06875 4.52850
H 2.67070 2.10733 4.63891
C 1.71265 3.75101 5.65599
H 1.82643 3.33453 6.64905
C 1.08876 4.98688 5.48879
C 1.87925 7.85103 6.50300
H 2.50884 7.10661 7.00001
H 1.77398 8.68636 7.20203
C -0.57705 8.05059 6.91335
H -1.46219 7.41345 6.99631
H -0.28424 8.34380 7.92601
C 0.48087 5.78586 6.61294
H -0.56480 5.49289 6.74385
H 0.99440 5.60881 7.56291
H 1.25284 5.38745 2.20838
N -1.68339 6.46556 4.44322
C -2.72329 5.94449 4.51130
C -4.01794 5.29168 4.59917
H -4.80166 6.02954 4.79348
H -4.24357 4.77623 3.66094
H -4.01568 4.55804 5.41075
H -3.05257 7.10124 1.80467
C -2.23549 7.05065 1.07707
C -2.01884 5.66068 0.47400
C -0.94414 5.70579 -0.63018
C -1.31930 6.71231 -1.73739
C -1.83926 8.01267 -1.17835
C -2.25357 8.15534 0.10668
H -1.23907 7.25680 1.81341
H -2.97045 5.30349 0.04883
H -0.79604 4.70912 -1.06147
H -0.45368 6.90606 -2.38566
H -2.08731 6.27682 -2.39893
H -1.90599 8.85761 -1.86088
H -2.61723 9.12202 0.44890
H 0.01128 6.00796 -0.17957
H -1.73661 4.94482 1.25537

64
HAT Intermediate (2/3)
Fe 0.07283 -0.23306 0.44051
O -0.06114 -0.38173 -1.36380
N 0.39623 0.01025 2.44984
N 1.86732 0.52418 0.23777
N -0.72171 1.57002 0.61516
N 0.88444 -2.00568 0.77894
C 2.47297 0.69624 -0.96379
H 1.88816 0.39487 -1.82117
C 3.75698 1.22576 -1.05262
H 4.21804 1.35307 -2.02366
C 4.42946 1.58305 0.12280
H 5.43023 1.99624 0.08094
C 3.79641 1.40061 1.35431
H 4.29028 1.66700 2.28100
C 2.50570 0.86586 1.38284
C -0.97305 2.39991 -0.42382
H -0.74167 2.01349 -1.40659
C -1.50773 3.66950 -0.21183
H -1.70373 4.31564 -1.05766
C -1.77721 4.08542 1.09687
H -2.18557 5.07084 1.28635
C -1.50999 3.21948 2.16365
H -1.70400 3.51633 3.18679
C -0.98551 1.95637 1.89427
C 1.36401 -2.82216 -0.18701
C 1.96606 -4.03655 0.13814
H 2.34122 -4.67632 -0.65009
C 2.07999 -4.40110 1.48451
H 2.55263 -5.33576 1.76155
C 1.58302 -3.54589 2.47496
H 1.66192 -3.80120 3.52439
C 0.97851 -2.34901 2.09320
C 1.75595 0.65126 2.66966
H 2.34276 0.02231 3.34576
H 1.61376 1.60970 3.17810
C -0.71502 0.90738 2.94081
H -1.60766 0.29084 3.07983
H -0.46302 1.34953 3.90915
C 0.33559 -1.37658 3.04741
H -0.71866 -1.63885 3.17574
H 0.80494 -1.39726 4.03512
H 1.24751 -2.47043 -1.20267
N -1.73874 -1.01938 0.67481
C -2.80000 -1.49841 0.72251
C -4.12280 -2.09418 0.78514
H -4.88609 -1.31309 0.84817
H -4.30652 -2.69565 -0.11005
H -4.20465 -2.73961 1.66464
H -2.91183 -2.10076 -2.84398
C -2.56042 -1.25616 -3.43133
C -1.59994 -1.50917 -4.56715
C -0.81216 -0.23217 -4.93792
C -1.75042 0.98140 -5.12749
C -2.71177 1.12537 -3.97491
C -3.06183 0.02562 -3.18948
H -0.95058 -0.61592 -1.71358
H -2.15922 -1.86536 -5.45061
H -0.22161 -0.40053 -5.84572
H -1.16129 1.89968 -5.25148
H -2.31644 0.86324 -6.06880
H -3.15698 2.09741 -3.78083
H -3.76812 0.16744 -2.37386
H -0.10801 -0.01001 -4.12519
H -0.90632 -2.32037 -4.30953

64
Rebound Transition State (2/3)
Fe 0.04215 0.27365 0.26582
O -0.11125 0.56293 -1.64418
N 0.36634 0.07395 2.41035
N 1.85634 1.03752 0.30919
N -0.71757 2.05707 0.89713
N 0.81805 -1.60219 0.31543
C 2.48576 1.48177 -0.80873
H 1.92601 1.37315 -1.72507
C 3.76235 2.03266 -0.75708
H 4.23628 2.37732 -1.66737
C 4.40951 2.12932 0.48130
H 5.40340 2.55522 0.55279
C 3.75785 1.66722 1.62608
H 4.23226 1.72512 2.59858
C 2.47484 1.12058 1.51331
C -0.94727 3.11101 0.08049
H -0.74634 2.94369 -0.96892
C -1.41479 4.32555 0.58076
H -1.59211 5.15349 -0.09383
C -1.63926 4.44981 1.95679
H -1.99413 5.38509 2.37344
C -1.39544 3.35514 2.79364
H -1.55520 3.42388 3.86293
C -0.93895 2.15991 2.23463
C 1.30314 -2.25163 -0.76766
C 1.86453 -3.52304 -0.65925
H 2.24340 -4.02132 -1.54247
C 1.93191 -4.12779 0.60113
H 2.37095 -5.11178 0.71583
C 1.43162 -3.44665 1.71622
H 1.47552 -3.88754 2.70473
C 0.86937 -2.18021 1.54574
C 1.74053 0.59530 2.72423
H 2.33147 -0.20511 3.18337
H 1.66352 1.38898 3.47546
C -0.71462 0.89911 3.03716
H -1.63429 0.30536 3.02955
H -0.48402 1.13440 4.08244
C 0.23898 -1.39433 2.67264
H -0.82800 -1.63393 2.71992
H 0.68030 -1.66990 3.63749
H 1.22635 -1.72539 -1.70968
N -1.77880 -0.50235 0.27918
C -2.85521 -0.94943 0.23272
C -4.19614 -1.50656 0.17613
H -4.55344 -1.73591 1.18448
H -4.88345 -0.79118 -0.28503
H -4.19845 -2.42731 -0.41457
H -0.95393 0.18362 -1.97117
C 0.01630 1.32983 -3.88002
C 0.87799 0.27669 -4.52536
C 0.26095 -0.24634 -5.84248
C -1.22160 -0.63236 -5.65426
C -1.99050 0.45929 -4.96224
C -1.37123 1.39130 -4.15998
H 0.48981 2.16555 -3.38303
H 0.99524 -0.56184 -3.82287
H 0.83527 -1.10452 -6.20695
H -1.68610 -0.86422 -6.62042
H -1.29376 -1.55991 -5.05941
H -3.06486 0.51160 -5.11737
H -1.95653 2.18998 -3.71386
H 0.32852 0.53787 -6.60799
H 1.88647 0.66924 -4.70002

64
Rebound Product (2/3)
Fe -0.17678 -0.21851 0.35978
O -0.48354 -0.42791 -1.87038
N 0.16259 -0.17278 2.59000
N 1.65955 0.52826 0.35323
N -0.98379 1.63283 0.85213
N 0.64895 -2.09486 0.63974
C 2.35140 0.75700 -0.79459
H 1.83756 0.52576 -1.71460
C 3.65354 1.24450 -0.79084
H 4.16662 1.41484 -1.72865
C 4.27521 1.49752 0.43794
H 5.29014 1.87506 0.47632
C 3.57063 1.24666 1.61570
H 4.02704 1.42094 2.58311
C 2.25946 0.75999 1.55054
C -1.23055 2.63635 -0.02446
H -0.99900 2.44190 -1.06257
C -1.75240 3.86165 0.38618
H -1.93634 4.64032 -0.34303
C -2.02033 4.05904 1.74512
H -2.41961 5.00308 2.09665
C -1.75733 3.02464 2.64833
H -1.94460 3.15036 3.70806
C -1.24290 1.81431 2.17609
C 1.13830 -2.87358 -0.35611
C 1.76171 -4.09195 -0.09383
H 2.13929 -4.69132 -0.91251
C 1.89378 -4.51015 1.23517
H 2.38213 -5.44830 1.47120
C 1.39466 -3.69875 2.25855
H 1.48857 -3.99204 3.29734
C 0.76671 -2.49295 1.93447
C 1.47813 0.49284 2.81862
H 2.08961 -0.11399 3.49719
H 1.30877 1.44632 3.33262
C -0.98351 0.63501 3.09026
H -1.86907 -0.00860 3.10233
H -0.81937 0.98301 4.11826
C 0.13636 -1.60567 2.98920
H -0.91196 -1.90059 3.10886
H 0.62894 -1.76469 3.95702
H 1.02122 -2.49387 -1.36253
N -1.98798 -1.01182 0.42863
C -3.05919 -1.47410 0.46238
C -4.39290 -2.04980 0.50676
H -4.86991 -1.82389 1.46521
H -5.01027 -1.63744 -0.29684
H -4.34122 -3.13611 0.38804
H -1.13239 -1.15430 -1.97277
C -0.43664 0.35879 -3.15127
C 0.29972 -0.44186 -4.23113
C 0.10534 0.22043 -5.60967
C -1.38769 0.26447 -5.99495
C -2.26314 0.67297 -4.83364
C -1.83845 0.72761 -3.56069
H 0.13712 1.24656 -2.86493
H -0.11122 -1.46086 -4.25495
H 0.67805 -0.32396 -6.36827
H -1.54401 0.95552 -6.83385
H -1.71260 -0.72287 -6.36007
H -3.29225 0.94258 -5.06284
H -2.50311 1.06049 -2.76679
H 0.50625 1.24317 -5.58149
H 1.36271 -0.52531 -3.98002

64
Desaturation Transition State (2/3)
Fe -0.26588 -0.02774 0.59233
O -0.78247 -0.13258 -1.30034
N 0.54675 0.08876 2.66630
N 1.58485 0.47073 0.12657
N -0.62886 1.98553 1.05389
N 0.29940 -2.02600 0.96479
C 1.96808 0.70854 -1.15495
H 1.19635 0.56644 -1.89625
C 3.26022 1.11783 -1.47032
H 3.53048 1.29626 -2.50356
C 4.18640 1.29757 -0.43544
H 5.19869 1.62028 -0.64933
C 3.78544 1.06044 0.88042
H 4.47535 1.19516 1.70532
C 2.47447 0.64296 1.13763
C -0.93717 2.91980 0.12466
H -1.06780 2.55357 -0.88566
C -1.07209 4.26604 0.46313
H -1.32150 4.99336 -0.29928
C -0.87039 4.65014 1.79439
H -0.95768 5.69053 2.08531
C -0.54946 3.67799 2.74801
H -0.38491 3.94759 3.78464
C -0.44261 2.34271 2.34948
C 0.45782 -2.95650 -0.00368
C 0.85883 -4.25879 0.29513
H 0.97771 -4.98439 -0.49984
C 1.10658 -4.59858 1.63050
H 1.42690 -5.60034 1.89241
C 0.94221 -3.62968 2.62673
H 1.13201 -3.86315 3.66789
C 0.52803 -2.34533 2.26414
C 2.02000 0.34331 2.54689
H 2.55913 -0.54084 2.90640
H 2.30906 1.16772 3.20916
C -0.18714 1.21199 3.32200
H -1.15236 0.82261 3.66342
H 0.34764 1.57783 4.20732
C 0.25957 -1.24764 3.27000
H -0.79979 -1.26788 3.54528
H 0.84040 -1.41067 4.18663
H 0.25014 -2.62451 -1.01288
N -2.11020 -0.47583 1.11934
C -3.21492 -0.73480 1.39313
C -4.59068 -1.05698 1.73631
H -5.05121 -0.22611 2.27897
H -5.17227 -1.24704 0.82923
H -4.62569 -1.95015 2.36714
H -0.13105 -2.75956 -4.10581
C -0.76303 -1.96760 -4.50206
C -0.46114 -0.59709 -4.11954
C -1.44419 0.45923 -4.67356
C -2.01427 0.09380 -6.05657
C -2.41796 -1.34399 -6.13802
C -1.82250 -2.31634 -5.35938
H -1.74530 -0.29994 -1.37996
H 0.60009 -0.37458 -4.32539
H -0.95903 1.43871 -4.71354
H -2.86565 0.73849 -6.30506
H -1.27287 0.27570 -6.85587
H -3.14546 -1.63473 -6.89147
H -2.08320 -3.35970 -5.49634
H -2.28168 0.55006 -3.96961
H -0.48462 -0.52965 -2.97220

64
Desaturation Product (2/3)
Fe -0.20467 -0.04945 0.49215
O -0.91555 -0.22143 -1.54951
N 0.55839 0.13222 2.61743
N 1.67884 0.42798 0.08024
N -0.58811 1.95402 0.86194
N 0.33774 -2.01741 0.90278
C 2.13307 0.61311 -1.18829
H 1.42004 0.46351 -1.98399
C 3.44381 0.98674 -1.46266
H 3.76050 1.12062 -2.48908
C 4.32576 1.18690 -0.39395
H 5.35308 1.48170 -0.57226
C 3.85868 1.00543 0.90761
H 4.51267 1.15715 1.75833
C 2.52904 0.62284 1.12308
C -0.87436 2.86152 -0.10271
H -0.96623 2.47641 -1.11013
C -1.03958 4.21396 0.19168
H -1.26875 4.91488 -0.60097
C -0.89502 4.63783 1.51774
H -1.00729 5.68422 1.77636
C -0.59859 3.69599 2.50800
H -0.47796 3.99571 3.54228
C -0.45735 2.35115 2.15498
C 0.52092 -2.97655 -0.03632
C 0.91461 -4.26994 0.30352
H 1.05228 -5.01306 -0.47169
C 1.13102 -4.57683 1.65164
H 1.44532 -5.57121 1.94630
C 0.94297 -3.58248 2.61694
H 1.10834 -3.78876 3.66780
C 0.53688 -2.30676 2.21659
C 2.02324 0.39870 2.53131
H 2.56606 -0.45052 2.96349
H 2.28004 1.26847 3.14795
C -0.22024 1.26530 3.18554
H -1.19158 0.87537 3.50878
H 0.26857 1.68877 4.07248
C 0.24874 -1.19836 3.20841
H -0.81749 -1.21493 3.45702
H 0.80310 -1.37052 4.14001
H 0.34387 -2.68512 -1.06311
N -2.07337 -0.48282 0.96400
C -3.18060 -0.73770 1.23169
C -4.55859 -1.05526 1.56758
H -5.02220 -0.21799 2.09754
H -5.13287 -1.25488 0.65790
H -4.59802 -1.94169 2.20757
H 0.66966 -1.94922 -4.21446
C -0.16641 -1.30547 -4.47530
C 0.02395 0.01378 -4.71784
C -1.14666 0.91469 -5.06501
C -2.28916 0.14402 -5.76732
C -2.51669 -1.22778 -5.16423
C -1.50739 -1.90452 -4.57703
H -1.87833 -0.35601 -1.61745
H 1.01509 0.45588 -4.65069
H -0.81219 1.74529 -5.69585
H -3.20987 0.73702 -5.73472
H -2.04945 0.01730 -6.83709
H -3.49810 -1.68147 -5.27648
H -1.65442 -2.91024 -4.19465
H -1.52688 1.37639 -4.13712
H -0.49792 -0.37643 -2.42705

64
HAT Reactant Complex (2/5)
Fe -0.30757 0.15525 0.51717
O -0.64234 0.37557 -1.09004
N 0.21227 -0.09261 2.51637
N 1.54502 1.15708 0.44484
N -1.14724 1.87769 1.21629
N 0.42470 -1.73545 0.40737
C 2.00949 1.84610 -0.62665
H 1.43528 1.75610 -1.53885
C 3.15720 2.62841 -0.53636
H 3.51255 3.16776 -1.40478
C 3.82595 2.70883 0.69245
H 4.71460 3.32041 0.79321
C 3.33851 1.99544 1.79201
H 3.83901 2.03858 2.75160
C 2.19163 1.21387 1.63496
C -1.57654 2.90062 0.43810
H -1.53499 2.74097 -0.63081
C -2.03806 4.08616 1.00374
H -2.37897 4.88993 0.36449
C -2.04346 4.21447 2.39818
H -2.38886 5.13044 2.86222
C -1.59633 3.15270 3.19288
H -1.59050 3.22881 4.27294
C -1.15659 1.98264 2.57471
C 0.78831 -2.36116 -0.73854
C 1.31534 -3.65015 -0.71180
H 1.59865 -4.13148 -1.63862
C 1.47127 -4.29650 0.51987
H 1.88455 -5.29689 0.56494
C 1.09588 -3.64017 1.69843
H 1.21273 -4.11649 2.66367
C 0.56588 -2.35404 1.61677
C 1.66064 0.32636 2.72827
H 2.26577 -0.58585 2.75113
H 1.76029 0.80039 3.70822
C -0.75160 0.74474 3.33027
H -1.64405 0.13785 3.51102
H -0.31668 0.99001 4.30314
C 0.06428 -1.57299 2.80271
H -0.99786 -1.78110 2.95351
H 0.59310 -1.84186 3.72170
H 0.64916 -1.81283 -1.66156
N -2.33175 -0.79106 0.95064
C -3.42473 -1.19728 0.90528
C -4.78522 -1.70229 0.84861
H -5.12111 -1.99881 1.84662
H -5.45805 -0.92892 0.46638
H -4.83721 -2.57203 0.18711
H 0.62797 0.93238 -5.30730
C 0.13059 0.14718 -4.72048
C -1.16924 -0.29808 -5.42319
C -1.70459 -1.60653 -4.81024
C -0.67907 -2.74834 -4.96656

C 0.72644 -2.29931 -4.62885
C 1.08418 -1.00903 -4.50596
H -0.11052 0.60606 -3.74793
H -0.96782 -0.45921 -6.49228
H -2.65705 -1.88910 -5.27527
H -0.96003 -3.59878 -4.32946
H -0.70267 -3.13318 -5.99936
H 1.47263 -3.08126 -4.49148
H 2.11274 -0.75738 -4.24967
H -1.90663 -1.44402 -3.74121
H -1.92381 0.49556 -5.35752

64
HAT Transition State (2/5)
Fe 0.28476 7.40883 4.23433
O 0.17914 7.64122 2.54725
N 0.60030 7.14875 6.40410
N 2.14975 8.38120 4.43980
N -0.60842 9.17696 4.96332
N 1.06854 5.45221 4.32401
C 2.74537 9.05722 3.42464
H 2.27260 8.96870 2.45632
C 3.88827 9.82189 3.63664
H 4.34629 10.34925 2.80978
C 4.41745 9.90018 4.93169
H 5.29953 10.49790 5.12885
C 3.79677 9.20227 5.97122
H 4.18640 9.24553 6.98103
C 2.66036 8.43605 5.69470
C -0.93047 10.23678 4.18218
H -0.79550 10.10456 3.11702
C -1.40137 11.42561 4.73470
H -1.65468 12.25717 4.08988
C -1.52783 11.52014 6.12605
H -1.88137 12.43655 6.58350
C -1.18902 10.42278 6.92517
H -1.27468 10.47159 8.00379
C -0.73600 9.25151 6.31506
C 1.58251 4.79166 3.25839
C 2.11844 3.51225 3.39161
H 2.52194 3.00431 2.52518
C 2.12690 2.91048 4.65554
H 2.54379 1.91920 4.78810
C 1.59864 3.60162 5.75192
H 1.60020 3.16161 6.74156
C 1.06648 4.87696 5.55826
C 2.00693 7.57678 6.74849
H 2.61303 6.67189 6.86716
H 2.01249 8.08764 7.71682
C -0.44302 7.98797 7.08746
H -1.36219 7.39531 7.13924
H -0.14630 8.21800 8.11629
C 0.41551 5.67810 6.66003
H -0.65865 5.47267 6.66370
H 0.81056 5.39445 7.64178
H 1.55055 5.30924 2.30800
N -1.74180 6.48374 4.44584
C -2.82791 6.07076 4.34173
C -4.18022 5.55756 4.21395
H -4.57290 5.27737 5.19583
H -4.83264 6.32053 3.77910
H -4.18948 4.67595 3.56644
H 0.20814 8.53952 -0.49292
C 0.08153 7.50053 -0.16078
C -1.30425 6.93236 -0.50094
C -1.36698 5.42381 -0.19392
C -0.28764 4.64973 -0.97855
C 1.04974 5.34392 -0.95620
C 1.21070 6.63874 -0.58249
H 0.14242 7.59823 1.00234
H -1.50658 7.09959 -1.57014
H -2.36036 5.02506 -0.42968
H -0.18265 3.63019 -0.58272
H -0.60178 4.52276 -2.02854
H 1.91272 4.77191 -1.29164
H 2.20597 7.07829 -0.58566
H -1.20848 5.27475 0.88330
H -2.08017 7.47181 0.05492

64
HAT Intermediate (2/5)
Fe -0.09965 0.22484 0.16665
O -0.14382 0.52921 -1.59658
N 0.13103 -0.13111 2.39825
N 1.77501 1.15136 0.52632
N -0.99309 1.97696 0.99713
N 0.68091 -1.76273 0.27918
C 2.42816 1.84526 -0.44174
H 1.98902 1.80204 -1.42887
C 3.58291 2.56806 -0.16057
H 4.08645 3.11089 -0.95013
C 4.06543 2.58323 1.15511
H 4.95663 3.14622 1.40628
C 3.38604 1.86767 2.14425
H 3.73845 1.86263 3.16867
C 2.23800 1.14688 1.79907
C -1.26480 3.07965 0.25614
H -1.08969 2.99610 -0.80834
C -1.73659 4.25016 0.84584
H -1.94885 5.11641 0.23254
C -1.91740 4.28067 2.23418
H -2.27276 5.18109 2.72115
C -1.63056 3.13988 2.99145
H -1.75857 3.13854 4.06704
C -1.17422 1.99019 2.34307
C 1.23846 -2.39597 -0.78251
C 1.76731 -3.67962 -0.66429
H 2.20630 -4.16349 -1.52727
C 1.72266 -4.31695 0.58145
H 2.13306 -5.31235 0.70337
C 1.14910 -3.65560 1.67298
H 1.10801 -4.12310 2.64920
C 0.62689 -2.37352 1.49286
C 1.52116 0.28128 2.80817
H 2.11496 -0.62855 2.95092
H 1.48707 0.78620 3.77954
C -0.93418 0.68647 3.06598
H -1.86169 0.10488 3.04232
H -0.69004 0.86542 4.11908
C -0.06821 -1.60586 2.59187
H -1.14229 -1.80811 2.54333
H 0.28318 -1.92995 3.57805
H 1.24510 -1.85353 -1.71903
N -2.13570 -0.69427 0.29881
C -3.21984 -1.10653 0.17363
C -4.56944 -1.61915 0.01947
H -4.96491 -1.93993 0.98772
H -5.22308 -0.84195 -0.38740
H -4.57225 -2.47435 -0.66263
H -0.80901 1.24372 -4.74178
C -0.77021 0.16088 -4.65001
C -2.06448 -0.61312 -4.61319
C -1.86681 -2.02213 -4.01032
C -0.67781 -2.76209 -4.66390
C 0.55390 -1.89617 -4.72764
C 0.46011 -0.50448 -4.71573
H -0.25017 0.40886 -2.56620
H -2.46171 -0.70517 -5.63951
H -2.78415 -2.61166 -4.11729
H -0.46321 -3.69075 -4.11933
H -0.95696 -3.07546 -5.68549
H 1.52488 -2.37383 -4.82597
H 1.37238 0.08465 -4.77935
H -1.67187 -1.92039 -2.93384
H -2.82714 -0.06120 -4.04900

64
Rebound Transition State (2/5)
Fe -0.09507 0.16248 0.16582
O -0.11216 0.47164 -1.67727
N 0.17687 -0.12003 2.42229
N 1.78312 1.14447 0.48381
N -0.98750 1.94750 0.97546
N 0.67711 -1.84105 0.33885
C 2.40466 1.84849 -0.49592
H 1.95674 1.77226 -1.47797
C 3.53355 2.61987 -0.23320
H 4.01285 3.16983 -1.03319
C 4.02046 2.67468 1.07958
H 4.89010 3.27599 1.31808
C 3.37280 1.94905 2.08328
H 3.72958 1.97526 3.10607
C 2.25246 1.17806 1.75366
C -1.28135 3.02742 0.21093
H -1.13588 2.90940 -0.85501
C -1.73663 4.21700 0.77598
H -1.96716 5.06402 0.14245
C -1.87667 4.29124 2.16749
H -2.21820 5.20655 2.63657
C -1.56601 3.17451 2.95047
H -1.66165 3.20680 4.02914
C -1.12775 2.00459 2.32414
C 1.22587 -2.52016 -0.69790
C 1.76520 -3.79459 -0.53187
H 2.19627 -4.31388 -1.37824
C 1.74184 -4.37514 0.74175
H 2.16023 -5.36168 0.90304
C 1.18056 -3.66669 1.80994
H 1.15823 -4.08867 2.80744
C 0.64661 -2.39694 1.57925
C 1.57788 0.29257 2.77838
H 2.18049 -0.61765 2.87704
H 1.58681 0.78022 3.76003
C -0.86385 0.72582 3.08581
H -1.79360 0.14727 3.11248
H -0.59115 0.94649 4.12478
C -0.03222 -1.58469 2.65794
H -1.10906 -1.77656 2.62048
H 0.32127 -1.88792 3.65097
H 1.22279 -2.01590 -1.65543
N -2.16017 -0.75095 0.27402
C -3.24422 -1.17857 0.20751
C -4.59401 -1.71042 0.12724
H -4.78298 -2.39083 0.96276
H -5.32367 -0.89616 0.16506
H -4.72879 -2.25937 -0.80941
H -0.43708 -0.01131 -2.46027
C -2.33730 0.74594 -3.50216
C -1.71618 1.89324 -4.24386
C -1.64624 1.63227 -5.76415
C -1.08021 0.23017 -6.07724
C -1.73886 -0.83601 -5.25245
C -2.34881 -0.54865 -4.03693
H -2.81460 0.93764 -2.54715
H -0.70108 2.05445 -3.84049
H -1.03829 2.40217 -6.25000
H -1.18516 -0.00080 -7.14436
H 0.00662 0.21089 -5.87871
H -1.72130 -1.85962 -5.61605
H -2.82612 -1.34792 -3.47780
H -2.65804 1.70637 -6.18382
H -2.26661 2.81838 -4.03347

64
Rebound Product (2/5)
Fe -0.27005 -0.16742 0.21936
O -0.97230 -0.11905 -1.81086
N 0.35232 -0.42024 2.38574
N 1.55031 1.07062 0.26208
N -1.30568 1.49098 1.16188
N 0.77355 -2.07366 0.21713
C 1.96958 1.90328 -0.72370
H 1.48710 1.79182 -1.68416
C 2.96604 2.85602 -0.52429
H 3.27151 3.49920 -1.33985
C 3.54586 2.96294 0.74516
H 4.31480 3.70140 0.94000
C 3.11977 2.10391 1.76122
H 3.55240 2.16017 2.75316
C 2.12535 1.15685 1.49033
C -1.87002 2.52340 0.48902
H -1.92345 2.42383 -0.58726
C -2.35322 3.65317 1.14645
H -2.80079 4.45988 0.57997
C -2.23699 3.71979 2.53993
H -2.59256 4.58951 3.07999
C -1.65354 2.65288 3.23088
H -1.55107 2.67903 4.30914
C -1.20123 1.54035 2.51537
C 1.25596 -2.70050 -0.88322
C 1.92959 -3.91787 -0.79976
H 2.30199 -4.39316 -1.69831
C 2.11488 -4.49920 0.46004
H 2.64076 -5.44164 0.55860
C 1.62139 -3.84704 1.59479
H 1.75825 -4.26981 2.58293
C 0.94598 -2.63283 1.44487
C 1.73666 0.13315 2.53427
H 2.43927 -0.70400 2.44760
H 1.87271 0.55274 3.53839
C -0.66083 0.30782 3.20744
H -1.49957 -0.37581 3.38036
H -0.25455 0.57240 4.19162
C 0.33254 -1.89795 2.61645
H -0.71358 -2.20423 2.71805
H 0.84574 -2.16979 3.54775
H 1.08980 -2.20546 -1.83083
N -2.21290 -1.37297 0.41819
C -3.21460 -1.95306 0.57512
C -4.45988 -2.67557 0.77419
H -4.36890 -3.35874 1.62381
H -5.27631 -1.97514 0.97282
H -4.70657 -3.25787 -0.11848
H -1.66906 -0.79719 -1.92187
C -0.72814 0.58320 -3.11812
C 0.21101 -0.25027 -3.99617
C 0.21625 0.29295 -5.43918
C -1.19445 0.22250 -6.05825
C -2.26207 0.68074 -5.09261
C -2.05406 0.85530 -3.77727
H -0.25241 1.51672 -2.80326
H -0.14400 -1.29011 -4.00141
H 0.92820 -0.27525 -6.04747
H -1.24006 0.83028 -6.97151
H -1.41582 -0.80857 -6.37707
H -3.24702 0.88629 -5.50694
H -2.84702 1.22593 -3.13150
H 0.56239 1.33584 -5.43516
H 1.22130 -0.24840 -3.57223

64
OAT Reactant Complex (2/3)
Fe -0.13444 -0.21256 0.93091
O -0.61195 -1.30305 -0.22877
N 0.55125 1.15195 2.32955
N 1.56631 0.13553 0.03599
N -0.90416 1.40974 0.10231
N 0.75545 -1.50147 2.13896
C 1.92666 -0.46476 -1.12847
H 1.21477 -1.16359 -1.54377
C 3.14399 -0.18339 -1.73718
H 3.40387 -0.67759 -2.66410
C 4.00966 0.73824 -1.13449
H 4.96362 0.97580 -1.58938
C 3.62989 1.34882 0.06177
H 4.27648 2.06509 0.55363
C 2.39505 1.02782 0.63224
C -1.36982 1.47932 -1.16726
H -1.33628 0.56911 -1.75048
C -1.87452 2.67235 -1.68032
H -2.24320 2.70066 -2.69735
C -1.89056 3.81138 -0.86814
H -2.27094 4.75181 -1.24837
C -1.40745 3.72795 0.44230
H -1.40580 4.59320 1.09324
C -0.92360 2.50718 0.91087
C 1.06686 -2.77627 1.80655
C 1.71903 -3.61357 2.70900
H 1.95550 -4.62956 2.42095
C 2.05943 -3.11851 3.97271
H 2.57406 -3.74815 4.68840
C 1.73317 -1.79912 4.30562
H 1.98720 -1.38811 5.27466
C 1.06996 -1.00704 3.36931
C 1.92931 1.63914 1.92394
H 2.63921 1.40110 2.72183
H 1.91212 2.72952 1.83594
C -0.45203 2.27801 2.32400
H -1.30008 1.97781 2.94586
H -0.02634 3.18515 2.76261
C 0.60203 0.40026 3.63648
H -0.40941 0.37556 4.05175
H 1.24408 0.91234 4.35887
H 0.77865 -3.09838 0.81573
N -1.83570 -0.47525 1.94082
C -2.86838 -0.73491 2.41166
C -4.15312 -1.05281 3.00721
H -4.96417 -0.71657 2.35480
H -4.24200 -2.13321 3.15396
H -4.25161 -0.55604 3.97703
H -0.47534 0.37980 -5.58974
C -1.10507 -0.51985 -5.54338
C -0.27345 -1.72525 -5.05838
C -1.18582 -2.90435 -4.66941
C -2.14344 -2.50886 -3.52586
C -2.75662 -1.14199 -3.74596
C -2.30234 -0.26102 -4.65413
H -1.44705 -0.69377 -6.57689
H 0.32038 -1.42621 -4.18187
H -0.58616 -3.77462 -4.37504
H -2.94100 -3.25880 -3.42568
H -1.60515 -2.51657 -2.56436
H -3.61885 -0.88566 -3.13121
H -2.81188 0.69355 -4.78176
H -1.77446 -3.20566 -5.54812
H 0.43872 -2.02880 -5.83553

64
OAT Transition State 1 (2/3)
Fe 0.06030 6.84865 4.52560
O -0.09280 6.09397 2.92998
N 0.47663 7.74568 6.35494
N 1.93146 7.31215 4.10192
N -0.53332 8.69189 4.07502
N 0.74147 5.23262 5.46396
C 2.53415 6.99744 2.92674
H 1.90680 6.48194 2.21320
C 3.86539 7.32140 2.68539
H 4.31783 7.05757 1.73805
C 4.59610 7.98232 3.68080
H 5.63537 8.24373 3.52057
C 3.96900 8.30059 4.88683
H 4.50560 8.81131 5.67732
C 2.62712 7.95438 5.07167
C -0.69511 9.16963 2.81904
H -0.50722 8.46943 2.01841
C -1.07675 10.49049 2.59062
H -1.20219 10.84445 1.57550
C -1.28287 11.33675 3.68553
H -1.57311 12.36969 3.53519
C -1.09845 10.84015 4.98066
H -1.23657 11.47582 5.84654
C -0.72620 9.50673 5.15069
C 1.14893 4.09820 4.84921
C 1.67185 3.03096 5.57747
H 1.98898 2.13376 5.06167
C 1.78430 3.14708 6.96747
H 2.19466 2.33475 7.55534
C 1.37091 4.32833 7.59352
H 1.45603 4.45052 8.66628
C 0.84525 5.36046 6.81602
C 1.88804 8.29374 6.33837
H 2.43439 7.91099 7.20588
H 1.84550 9.38155 6.45278
C -0.53526 8.85273 6.49619
H -1.47810 8.40931 6.82746
H -0.22666 9.57702 7.25666
C 0.31743 6.65448 7.38225
H -0.74946 6.54931 7.59925
H 0.81831 6.91939 8.31864
H 1.04474 4.08279 3.77350
N -1.80299 6.40716 5.08660
C -2.88922 6.10229 5.37907
C -4.24385 5.72566 5.74390
H -4.96617 6.28718 5.14421
H -4.39759 4.65643 5.57124
H -4.42297 5.94024 6.80165
H 0.14582 5.47568 -0.67216
C -0.79270 5.05360 -0.28102
C -0.55138 3.66419 0.34093
C -1.77249 3.23685 1.17483
C -2.00469 4.20384 2.35775
C -1.79237 5.66404 1.98171
C -1.41115 6.01813 0.68653
H -1.45212 4.96113 -1.16136
H 0.33603 3.70043 0.98711
H -1.64600 2.21634 1.55466
H -3.02900 4.08585 2.73688
H -1.33937 3.94440 3.18800
H -2.36195 6.39445 2.54570
H -1.50139 7.05530 0.37127
H -2.66046 3.22670 0.52654
H -0.34529 2.93225 -0.44839

64
OAT Intermediate (2/3)
Fe -0.16363 0.12722 0.24645
O -0.39741 -0.63038 -1.39197
N 0.30304 1.01458 2.04836
N 1.69777 0.55031 -0.23278
N -0.74761 1.98021 -0.18509
N 0.53391 -1.49618 1.15941
C 2.26814 0.20108 -1.41318
H 1.61138 -0.30322 -2.10762
C 3.60546 0.48011 -1.67920
H 4.03410 0.19078 -2.63016
C 4.37333 1.12765 -0.70354
H 5.41815 1.35154 -0.88323
C 3.77728 1.48205 0.50877
H 4.34337 1.98446 1.28381
C 2.42818 1.18348 0.71757
C -0.91396 2.47299 -1.43517
H -0.72607 1.78748 -2.24868
C -1.29739 3.79639 -1.64530
H -1.42693 4.16205 -2.65567
C -1.49838 4.62990 -0.53995
H -1.79043 5.66411 -0.67698
C -1.30242 4.11985 0.74826
H -1.43063 4.74647 1.62209
C -0.92876 2.78523 0.90040
C 0.91537 -2.63072 0.52882
C 1.45925 -3.70040 1.23778
H 1.75417 -4.59835 0.71037
C 1.62208 -3.58577 2.62287
H 2.04993 -4.40024 3.19499
C 1.23714 -2.40317 3.26430
H 1.36191 -2.28149 4.33314
C 0.68780 -1.36925 2.50650
C 1.71007 1.57726 1.98026
H 2.27419 1.25180 2.85913
H 1.64977 2.66888 2.03315
C -0.70842 2.11828 2.23338
H -1.64056 1.66884 2.58491
H -0.37724 2.83163 2.99441
C 0.18489 -0.07385 3.08735
H -0.87265 -0.17679 3.34685
H 0.72279 0.19847 4.00043
H 0.77526 -2.64444 -0.54235
N -2.01680 -0.29633 0.84625
C -3.10137 -0.58854 1.15670
C -4.45397 -0.95167 1.54039
H -5.17742 -0.32822 1.00690
H -4.64487 -2.00103 1.29703
H -4.59248 -0.80917 2.61619
H 0.27612 -1.18116 -4.73269

C -0.69502 -1.59880 -4.41493
C -0.49094 -2.95208 -3.70073
C -1.78467 -3.35157 -2.96812
C -2.14602 -2.35222 -1.83979
C -1.68950 -0.88887 -2.11433
C -1.43832 -0.61852 -3.55953
H -1.25403 -1.76020 -5.35287
H 0.33333 -2.87302 -2.97985
H -1.69711 -4.36062 -2.54747
H -3.23238 -2.35622 -1.68534
H -1.69299 -2.67119 -0.89520
H -2.42864 -0.18641 -1.71807
H -1.70775 0.34985 -3.97498
H -2.60116 -3.38810 -3.70331
H -0.20702 -3.72056 -4.42929

64
OAT Transition State 2 (2/3)
Fe -0.18148 0.15197 0.20527
O -0.47673 -0.49708 -1.57945
N 0.34796 0.98788 2.12169
N 1.68043 0.62975 -0.25799
N -0.76552 2.06886 -0.08737
N 0.52682 -1.51270 1.08559
C 2.23154 0.37368 -1.47273
H 1.57057 -0.09462 -2.18780
C 3.55476 0.69894 -1.75529
H 3.96373 0.48107 -2.73371
C 4.33315 1.30301 -0.76013
H 5.36699 1.56568 -0.95111
C 3.75993 1.56283 0.48595
H 4.33467 2.02903 1.27750
C 2.42419 1.21582 0.71347
C -0.98732 2.62302 -1.30211
H -0.85650 1.96897 -2.15208
C -1.35157 3.96196 -1.43404
H -1.52494 4.37719 -2.41853
C -1.47596 4.74684 -0.28225
H -1.75007 5.79248 -0.35622
C -1.22985 4.17090 0.96879
H -1.30323 4.75694 1.87678
C -0.87979 2.82178 1.04122
C 0.91137 -2.62535 0.41721
C 1.45608 -3.72043 1.08532
H 1.75195 -4.59835 0.52553
C 1.61816 -3.65501 2.47368
H 2.04552 -4.48921 3.01718
C 1.23511 -2.49439 3.15447
H 1.36299 -2.40922 4.22671
C 0.68510 -1.43197 2.43547
C 1.76253 1.49402 2.04256
H 2.35460 1.04595 2.84784
H 1.76446 2.57436 2.22372
C -0.63736 2.09481 2.34250
H -1.57429 1.64798 2.68815
H -0.29675 2.78484 3.12265
C 0.19951 -0.15560 3.07997
H -0.86334 -0.25590 3.32059
H 0.73123 0.03863 4.01813
H 0.77518 -2.60413 -0.65449
N -2.03344 -0.29674 0.76236
C -3.12650 -0.55941 1.07195
C -4.48865 -0.88920 1.45531
H -4.63035 -0.72443 2.52750
H -5.19794 -0.26214 0.90724
H -4.70001 -1.93896 1.23082
H 0.53082 -1.58759 -4.60367
C -0.50745 -1.84974 -4.34830
C -0.58844 -3.21179 -3.63212
C -1.97203 -3.38560 -2.98319
C -2.21416 -2.33850 -1.87231
C -1.75009 -0.91339 -2.24521
C -1.15337 -0.74398 -3.58974
H -1.02272 -1.91704 -5.32490
H 0.19219 -3.27469 -2.86241
H -2.07703 -4.39168 -2.56057
H -3.28066 -2.31635 -1.61888
H -1.68111 -2.63906 -0.96387
H -2.52024 -0.16863 -2.02632
H -1.10394 0.26243 -3.99637
H -2.74400 -3.28865 -3.76030
H -0.39154 -4.01588 -4.34978

64
OAT Product (2/3)
Fe -0.20196 0.16170 0.23405
O -0.72345 -0.83574 -1.70984
N 0.46253 1.06821 2.19446
N 1.65916 0.60527 -0.27702
N -0.77384 2.14136 -0.02394
N 0.50751 -1.51842 1.20325
C 2.17399 0.29446 -1.49647
H 1.50110 -0.19541 -2.18300
C 3.49156 0.57959 -1.83778
H 3.86156 0.31589 -2.82036
C 4.31424 1.20198 -0.89097
H 5.34649 1.43511 -1.12406
C 3.78607 1.51477 0.36188
H 4.39733 1.99278 1.11849
C 2.45059 1.20782 0.64877
C -1.06867 2.71443 -1.21547
H -1.01636 2.07456 -2.08514
C -1.41615 4.05996 -1.32020
H -1.64605 4.48337 -2.28965
C -1.45100 4.83923 -0.15854
H -1.71009 5.89023 -0.20771
C -1.13763 4.24676 1.06867
H -1.14560 4.82590 1.98426
C -0.80732 2.88980 1.11209
C 0.79194 -2.68954 0.58407
C 1.34410 -3.76729 1.27394
H 1.55861 -4.68997 0.74976
C 1.61811 -3.62576 2.63897
H 2.05525 -4.44299 3.20053
C 1.32787 -2.41265 3.27112
H 1.53504 -2.27108 4.32518
C 0.76388 -1.37051 2.53028
C 1.85821 1.55780 1.99741
H 2.50560 1.15917 2.78777
H 1.87420 2.64812 2.11337
C -0.51386 2.17020 2.41171
H -1.44156 1.72691 2.78833
H -0.16301 2.88344 3.16879
C 0.35745 -0.05596 3.16371
H -0.68896 -0.12966 3.47888
H 0.95490 0.13004 4.06542
H 0.56715 -2.73587 -0.47283
N -2.03565 -0.27955 0.80721
C -3.12159 -0.54930 1.13841
C -4.47449 -0.88678 1.54926
H -4.58774 -0.75089 2.62893
H -5.19745 -0.24438 1.03792
H -4.69552 -1.92961 1.30285
H 0.81096 -1.40829 -4.16103
C -0.24457 -1.69961 -4.09235
C -0.38885 -3.16596 -3.64017
C -1.86360 -3.51372 -3.36860
C -2.46545 -2.65649 -2.23222
C -2.08005 -1.19301 -2.31736
C -0.99297 -0.72928 -3.21330
H -0.66154 -1.58521 -5.10402
H 0.21000 -3.33944 -2.73677
H -1.96607 -4.57456 -3.11404
H -3.55913 -2.72762 -2.24819
H -2.14336 -3.04004 -1.25527
H -2.83380 -0.46901 -2.02516
H -1.01119 0.30406 -3.54770
H -2.44134 -3.35188 -4.28958
H 0.01751 -3.82158 -4.41845

64
OAT Reactant Complex (2/5)
Fe -0.46325 -0.39755 0.58459
O -1.01055 -0.39714 -0.97892
N 0.32518 -0.37254 2.50927
N 1.22781 0.78636 0.16958
N -1.41508 1.29000 1.22811
N 0.45420 -2.21085 0.56316
C 1.46511 1.41044 -1.01069
H 0.80520 1.16477 -1.83246
C 2.50540 2.32634 -1.14242
H 2.67849 2.80930 -2.09536
C 3.30320 2.61145 -0.02680
H 4.11101 3.32990 -0.09960
C 3.05012 1.96270 1.18620
H 3.65416 2.16296 2.06258
C 2.00353 1.04071 1.25280
C -2.06284 2.16842 0.42496
H -2.13640 1.89980 -0.62012
C -2.59315 3.34990 0.93614
H -3.10928 4.03648 0.27798
C -2.43820 3.62815 2.29972
H -2.83346 4.54534 2.71955
C -1.76559 2.71558 3.12035
H -1.63245 2.90986 4.17727
C -1.26552 1.54096 2.55887
C 0.73040 -2.92386 -0.55554
C 1.39305 -4.14630 -0.47992
H 1.60248 -4.70052 -1.38536
C 1.77968 -4.63190 0.77496
H 2.30255 -5.57698 0.85849
C 1.49218 -3.88688 1.92507
H 1.78593 -4.23936 2.90571
C 0.81789 -2.67430 1.79471
C 1.73034 0.21171 2.47835
H 2.43320 -0.62764 2.48529
H 1.90669 0.78294 3.39358
C -0.61875 0.44544 3.36431
H -1.40074 -0.22805 3.72764
H -0.09457 0.84334 4.23750
C 0.38785 -1.81849 2.95710
H -0.61426 -2.11546 3.27630
H 1.05850 -1.92577 3.81483
H 0.40814 -2.49152 -1.49293
N -2.29643 -1.49594 1.37220
C -3.32608 -2.02531 1.51798
C -4.60658 -2.68591 1.70065
H -4.45906 -3.69025 2.10832
H -5.23237 -2.11389 2.39188
H -5.12690 -2.76880 0.74184
H 1.69676 -0.78009 -4.65083
C 0.89509 -0.26316 -5.19715
C -0.46872 -0.90823 -4.87408
C -1.62786 -0.01303 -5.35364
C -1.58805 1.36054 -4.65195
C -0.18724 1.93297 -4.60410
C 0.91819 1.21278 -4.86187
H 1.13058 -0.40033 -6.26539
H -0.55479 -1.04861 -3.78659
H -2.59322 -0.50145 -5.17182
H -2.25814 2.06613 -5.16305
H -1.98284 1.26669 -3.62689
H -0.09638 2.99010 -4.35717
H 1.89403 1.69678 -4.84122
H -1.54351 0.13208 -6.44053
H -0.53342 -1.90264 -5.33274

64
OAT Transition State 1 (2/5)
Fe 0.50686 7.16994 4.17045
O 0.48821 7.38131 2.49256
N 0.70504 6.97314 6.34825
N 2.20206 8.38700 4.47198
N -0.67345 8.80067 4.80333
N 1.54156 5.34885 4.33201
C 2.77197 9.12046 3.48237
H 2.37861 8.95689 2.48850
C 3.79115 10.02884 3.75070
H 4.23169 10.60040 2.94398
C 4.22008 10.19028 5.07492
H 5.00427 10.89848 5.31514
C 3.62756 9.43067 6.08724
H 3.94330 9.53434 7.11826
C 2.61822 8.52183 5.75515
C -1.08608 9.80059 3.98714
H -0.85916 9.68349 2.93612
C -1.75734 10.91358 4.48840
H -2.07934 11.69785 3.81555
C -1.99347 10.99586 5.86612
H -2.50404 11.85503 6.28470
C -1.56032 9.96119 6.70243
H -1.72769 10.00225 7.77176
C -0.90502 8.86314 6.14188
C 2.21041 4.76226 3.30981
C 2.91167 3.57253 3.49302
H 3.43725 3.12271 2.66064
C 2.92492 2.98461 4.76353
H 3.46878 2.06338 4.93554
C 2.23649 3.59945 5.81555
H 2.23892 3.16903 6.80934
C 1.54246 4.78540 5.57182
C 2.01059 7.59893 6.78220
H 2.72432 6.78900 6.96978
H 1.87192 8.12207 7.73399
C -0.49051 7.65773 6.95028
H -1.31749 6.94025 6.94969
H -0.29884 7.93297 7.99285
C 0.71548 5.49240 6.61806
H -0.31647 5.13497 6.56106
H 1.08463 5.27818 7.62691
H 2.16615 5.27013 2.35600
N -1.38077 5.96982 4.24951
C -2.38216 5.39365 4.08704
C -3.62878 4.67664 3.88458
H -3.47109 3.60143 4.00992
H -4.37833 5.00934 4.60855
H -4.00856 4.86092 2.87535
H 0.28955 5.12356 0.35050
C -0.06480 5.90014 -0.34032
C -1.59674 6.04823 -0.24628
C -2.07199 7.33088 -0.95530
C -1.43183 8.58322 -0.32023
C 0.03827 8.40314 -0.04973
C 0.65565 7.19191 -0.05696
H 0.21783 5.54975 -1.34722
H -1.88860 6.09190 0.81238
H -3.16480 7.41018 -0.91722
H -1.58283 9.46150 -0.96312
H -1.94261 8.82508 0.62741
H 0.62056 9.29750 0.16003
H 1.72997 7.13980 0.09828
H -1.79286 7.28028 -2.01745
H -2.08510 5.16671 -0.67805

64
OAT Intermediate (2/5)
Fe 0.03396 -0.08244 -0.06016
O 0.09692 0.07680 -1.86355
N 0.15513 -0.32668 2.20065
N 1.78227 1.06830 0.38546
N -1.07099 1.63688 0.65451
N 1.02295 -1.98078 0.20712
C 2.41955 1.81697 -0.55079
H 2.08115 1.69460 -1.56976
C 3.44230 2.69656 -0.20951
H 3.93405 3.27862 -0.97833
C 3.80642 2.81566 1.13798
H 4.59053 3.50133 1.43682
C 3.14735 2.04200 2.09646
H 3.41016 2.11278 3.14510
C 2.13850 1.16230 1.68989
C -1.38996 2.70195 -0.12026
H -1.15135 2.61930 -1.17188
C -1.98780 3.84226 0.41227
H -2.23360 4.67541 -0.23368
C -2.24934 3.88583 1.78673
H -2.70433 4.76261 2.23226
C -1.91111 2.78746 2.58376
H -2.09724 2.79616 3.65094
C -1.32609 1.66681 1.98883
C 1.74197 -2.59588 -0.76372
C 2.38891 -3.80889 -0.53674
H 2.95538 -4.27555 -1.33237
C 2.29461 -4.39699 0.73000
H 2.79178 -5.33715 0.93761
C 1.56069 -3.75358 1.73207
H 1.48139 -4.17947 2.72493
C 0.92842 -2.54255 1.44241
C 1.47266 0.22649 2.67040
H 2.15147 -0.61804 2.83487
H 1.34752 0.72096 3.64011
C -1.01738 0.41110 2.76831
H -1.88609 -0.25285 2.71042
H -0.85915 0.64528 3.82744
C 0.07825 -1.80339 2.44766
H -0.96549 -2.10815 2.32896
H 0.38016 -2.05372 3.47161
H 1.78596 -2.09144 -1.71866
N -1.91718 -1.18605 0.01859
C -2.95335 -1.71027 -0.09555
C -4.24263 -2.36346 -0.23620
H -4.13388 -3.44482 -0.11107
H -4.93992 -1.98965 0.51933
H -4.65898 -2.16419 -1.22801
H 0.65578 -1.75833 -3.68425
C -0.07467 -1.03848 -4.07024
C -1.50736 -1.59433 -3.97584
C -2.53329 -0.56550 -4.48818
C -2.43427 0.76935 -3.70796
C -1.02481 1.25320 -3.57985
C 0.09180 0.29835 -3.33324
H 0.17938 -0.86265 -5.12550
H -1.73212 -1.85523 -2.93336
H -3.55167 -0.96317 -4.40546
H -3.05461 1.54256 -4.17758
H -2.86517 0.61721 -2.70004
H -0.82239 2.31852 -3.50437
H 1.06349 0.74469 -3.57196
H -2.34943 -0.37230 -5.55434
H -1.57963 -2.52059 -4.55870

64
OAT Transition State 2 (2/5)
Fe -0.02341 -0.00730 -0.06448
O 0.04641 0.22268 -1.87873
N 0.12636 -0.29141 2.19200
N 1.77421 1.08444 0.37802
N -1.04852 1.74867 0.69960
N 0.89335 -1.95371 0.15685
C 2.41945 1.83672 -0.54968
H 2.06338 1.74614 -1.56592
C 3.47033 2.68107 -0.20398
H 3.96726 3.26666 -0.96686
C 3.85571 2.76071 1.14046
H 4.66233 3.41806 1.44311
C 3.18762 1.98493 2.09094
H 3.46507 2.02627 3.13741
C 2.14950 1.14225 1.67911
C -1.32999 2.84549 -0.04481
H -1.11213 2.77717 -1.10153
C -1.86489 4.00037 0.52227
H -2.08176 4.85834 -0.10117
C -2.10137 4.02524 1.90168
H -2.50742 4.91195 2.37409
C -1.80080 2.89491 2.66838
H -1.96688 2.88861 3.73892
C -1.27877 1.76195 2.03881
C 1.56777 -2.58678 -0.83379
C 2.17688 -3.82364 -0.63096
H 2.70814 -4.30333 -1.44303
C 2.09126 -4.41814 0.63317
H 2.56016 -5.37647 0.82279
C 1.40211 -3.75778 1.65582
H 1.32940 -4.18871 2.64704
C 0.80575 -2.52344 1.38914
C 1.46904 0.20662 2.65004
H 2.12124 -0.66396 2.78324
H 1.37810 0.68198 3.63322
C -1.01147 0.47786 2.78689
H -1.90555 -0.15106 2.72206
H -0.83570 0.68203 3.84962
C 0.00075 -1.76745 2.41887
H -1.05509 -2.03351 2.31468
H 0.31036 -2.04467 3.43369
H 1.60691 -2.07760 -1.78612
N -2.00575 -1.06247 0.00421
C -3.04214 -1.59354 -0.07035
C -4.33231 -2.25437 -0.16052
H -4.21208 -3.33527 -0.04250
H -5.00052 -1.88648 0.62364
H -4.79043 -2.05594 -1.13395
H 1.08553 -1.31442 -3.79257
C 0.17715 -0.80542 -4.13452
C -1.05434 -1.72550 -4.04961
C -2.32055 -0.98618 -4.52395
C -2.57301 0.29891 -3.69876
C -1.34128 1.12051 -3.50875
C -0.00394 0.49095 -3.33682
H 0.35040 -0.52404 -5.18327
H -1.18909 -2.06932 -3.01520
H -3.19714 -1.64084 -4.45727
H -3.35859 0.91221 -4.15844
H -2.97231 0.01406 -2.70770
H -1.43565 2.18716 -3.32321
H 0.80814 1.19331 -3.55277
H -2.20282 -0.71505 -5.58235
H -0.88883 -2.61867 -4.66380

64
OAT Product (2/5)
Fe -0.33994 0.03910 0.08761
O -0.44201 -0.18299 -2.07079
N 0.11363 -0.21287 2.30940
N 1.61462 1.00212 0.20688
N -1.11210 1.90827 0.95644
N 0.41903 -2.00819 0.23416
C 2.18933 1.72173 -0.78955
H 1.72233 1.65120 -1.76214
C 3.31483 2.51491 -0.58037
H 3.74604 3.07256 -1.40214
C 3.85845 2.57914 0.70838
H 4.72612 3.19648 0.91020
C 3.26655 1.83957 1.73535
H 3.66667 1.87077 2.74204
C 2.14636 1.04770 1.45513
C -1.44376 3.01131 0.24060
H -1.42549 2.91517 -0.83723
C -1.78889 4.21389 0.85426
H -2.05130 5.07367 0.25097
C -1.77777 4.28224 2.25242
H -2.03073 5.20557 2.76034
C -1.43172 3.14548 2.98877
H -1.41167 3.16900 4.07181
C -1.10998 1.96406 2.31345
C 0.89048 -2.73944 -0.80500
C 1.41593 -4.01886 -0.62603
H 1.78349 -4.57629 -1.47836
C 1.46194 -4.55366 0.66611
H 1.87148 -5.54215 0.83858
C 0.98150 -3.79381 1.73821
H 1.01358 -4.17767 2.75090
C 0.45776 -2.52202 1.49258
C 1.55285 0.14891 2.51944
H 2.13295 -0.78136 2.52262
H 1.68799 0.60367 3.50815
C -0.82635 0.67616 3.05222
H -1.77245 0.13525 3.16718
H -0.45505 0.89196 4.06224
C -0.13036 -1.66176 2.58658
H -1.21425 -1.81374 2.61344
H 0.26863 -1.95952 3.56481
H 0.83148 -2.27015 -1.77743
N -2.43838 -0.74704 0.18828
C -3.51802 -1.18700 0.25220
C -4.86041 -1.73916 0.33059

H -4.83379 -2.82032 0.16533
H -5.29273 -1.54610 1.31671
H -5.50279 -1.28432 -0.42909
H 1.47539 0.63180 -4.12287
C 0.44780 0.37988 -4.41321
C 0.34274 -1.09229 -4.85867
C -1.12672 -1.50045 -5.06855
C -1.95306 -1.39097 -3.76695
C -1.67143 -0.12365 -2.98673
C -0.49955 0.73159 -3.29477
H 0.19230 1.03866 -5.25622
H 0.80910 -1.74446 -4.10895
H -1.18810 -2.52561 -5.45034
H -3.02414 -1.42343 -3.99749
H -1.74978 -2.24919 -3.11335
H -2.50836 0.33575 -2.47163
H -0.54612 1.77914 -3.01125
H -1.57011 -0.84954 -5.83528
H 0.90852 -1.22496 -5.78761

3_{TBP} with cyclohexene

58
HAT Reactant Complex (2/5)
Fe 0.20530 0.42595 0.40881
O 0.19180 0.57920 -1.23939
N 0.22681 0.24484 2.45053
N 1.98588 1.31862 0.73330
N -1.47574 1.47775 0.78168
N 0.13448 -1.58898 0.49390
C 2.65471 2.06445 -0.18229
H 2.20284 2.14123 -1.16161
C 3.85563 2.68585 0.14542
H 4.37458 3.27650 -0.59777
C 4.36772 2.53418 1.44037
H 5.29799 3.01379 1.71953
C 3.67053 1.76201 2.37731
H 4.04591 1.63260 3.38447
C 2.47620 1.15433 1.99681
C -2.39842 1.81774 -0.15344
H -2.17686 1.53255 -1.17258
C -3.55883 2.49654 0.20528
H -4.28306 2.75989 -0.55408
C -3.76689 2.82217 1.55158
H -4.66629 3.34430 1.85460
C -2.80822 2.46771 2.50854
H -2.94850 2.70783 3.55476
C -1.65891 1.79726 2.09655
C 0.37035 -2.41852 -0.55424
C 0.35959 -3.79990 -0.38376
H 0.54984 -4.44497 -1.23127
C 0.10409 -4.32745 0.88789
H 0.09824 -5.39931 1.04416
C -0.14275 -3.46278 1.96133
H -0.34237 -3.84751 2.95330
C -0.13016 -2.08825 1.73752
C 1.67489 0.24168 2.88668
H 2.04880 -0.78317 2.79190
H 1.75127 0.52477 3.94066
C -0.52138 1.43324 3.01331
H -0.86295 1.21771 4.03038
H 0.18279 2.27025 3.07062
C -0.45778 -1.06078 2.78807
H -1.53755 -0.87775 2.79646
H -0.17031 -1.39079 3.79068
H 0.55614 -1.95352 -1.51374
H 0.49494 0.26456 -5.65034
C -0.01360 -0.23006 -4.81065
C -1.52821 -0.32542 -5.08936
C -2.20852 -1.29485 -4.10325
C -1.62261 -2.71607 -4.23461
C -0.11179 -2.70109 -4.32924
C 0.60597 -1.59021 -4.57097
H 0.16401 0.41079 -3.93221
H -1.68786 -0.68737 -6.11557
H -3.29261 -1.31747 -4.26950
H -1.93399 -3.33344 -3.38005
H -2.04138 -3.21256 -5.12530
H 0.39836 -3.65495 -4.19842
H 1.69298 -1.64977 -4.61302
H -2.04940 -0.93069 -3.07760
H -1.98598 0.66983 -5.02873

58
HAT Transition State (2/5)
Fe 1.08281 7.66369 3.89827
O 1.00760 7.70577 2.19675
N 1.18419 7.59886 6.06969
N 2.92297 8.54631 4.20156
N -0.60615 8.75076 4.37488
N 1.02640 5.61822 4.20895
C 3.59228 9.22746 3.23620
H 3.12919 9.24931 2.25944
C 4.80410 9.85486 3.50868
H 5.32036 10.39225 2.72406
C 5.32914 9.77952 4.80509
H 6.26724 10.26561 5.04474
C 4.63255 9.07581 5.79366
H 5.01614 9.00628 6.80393
C 3.42628 8.45725 5.46507
C -1.58239 9.04789 3.47948
H -1.41532 8.71740 2.46362
C -2.72520 9.74094 3.86709
H -3.49072 9.96792 3.13677
C -2.86080 10.12778 5.20637
H -3.74419 10.66216 5.53472
C -1.84933 9.81719 6.12221
H -1.93264 10.10323 7.16324
C -0.71947 9.12975 5.67932
C 1.23653 4.70034 3.23204
C 1.23917 3.33738 3.51511
H 1.40953 2.62357 2.71982
C 1.02318 2.91850 4.83368
H 1.02684 1.86371 5.08112
C 0.80560 3.87193 5.83477
H 0.63872 3.57288 6.86207
C 0.80483 5.22473 5.49581
C 2.63993 7.61420 6.43885
H 3.00587 6.58236 6.39688
H 2.77684 7.96453 7.46750
C 0.45983 8.81687 6.56755
H 0.15111 8.68831 7.61077
H 1.16276 9.65692 6.53720
C 0.50745 6.32444 6.48596
H -0.57227 6.51092 6.50232
H 0.80339 6.03776 7.50089
H 1.39697 5.08540 2.23342
H 1.63509 8.06896 -0.89470
C 1.04635 7.24131 -0.47777
C -0.42643 7.27492 -0.91129
C -1.15994 6.00268 -0.44505
C -0.48669 4.73352 -1.00681
C 1.01551 4.78715 -0.91322
C 1.70709 5.93188 -0.67076
H 1.06975 7.47019 0.67071
H -0.47527 7.34934 -2.00862
H -2.21298 6.03333 -0.74707
H -0.85832 3.83894 -0.48839
H -0.76720 4.59269 -2.06467
H 1.55876 3.86014 -1.08594
H 2.79294 5.89990 -0.61198
H -1.14162 5.96627 0.65329
H -0.91659 8.17097 -0.51276

58
HAT Intermediate (2/5)
Fe 0.00133 0.31206 0.22149
O -0.18368 0.33792 -1.55098
N 0.21836 0.26759 2.45121
N 1.88801 1.16815 0.49229
N -1.66646 1.39579 0.84324
N -0.04282 -1.74103 0.63130
C 2.53131 1.83070 -0.50461
H 2.02899 1.86043 -1.46163
C 3.76715 2.43265 -0.28952
H 4.26067 2.95411 -1.09917
C 4.34597 2.35303 0.98362
H 5.30424 2.81900 1.17965
C 3.67624 1.67118 2.00489
H 4.10035 1.59898 2.99871
C 2.44362 1.07698 1.73156
C -2.70192 1.67320 0.00903
H -2.60322 1.31868 -1.00788
C -3.81583 2.37760 0.45562
H -4.62922 2.58831 -0.22628
C -3.85962 2.79776 1.79120
H -4.71783 3.34281 2.16570
C -2.78899 2.50565 2.64350
H -2.80138 2.81616 3.68085
C -1.69236 1.80460 2.14152
C 0.11899 -2.68329 -0.33355
C 0.11081 -4.04009 -0.02362
H 0.24251 -4.77233 -0.80947
C -0.06635 -4.42923 1.31000
H -0.07163 -5.47890 1.57847
C -0.23256 -3.45230 2.29755
H -0.36763 -3.72696 3.33635
C -0.22310 -2.10625 1.93088
C 1.68625 0.25796 2.74779
H 2.03038 -0.78087 2.69500
H 1.88313 0.61224 3.76569
C -0.46023 1.50309 2.96014
H -0.70547 1.40681 4.02386
H 0.24628 2.33522 2.86317
C -0.45989 -0.98535 2.91400
H -1.53472 -0.78146 2.97500
H -0.12558 -1.26512 3.91934
H 0.25088 -2.32223 -1.34507
H 0.70857 0.94325 -4.68241
C 0.17093 0.00076 -4.61174
C -1.29293 -0.03327 -4.97748
C -1.99708 -1.27144 -4.37777
C -1.21825 -2.57167 -4.67857
C 0.24802 -2.43287 -4.36053
C 0.86723 -1.18334 -4.33702
H -0.02923 0.20456 -2.51434
H -1.39144 -0.05044 -6.07717
H -3.02150 -1.34653 -4.75860
H -1.65159 -3.41173 -4.12061
H -1.33682 -2.83238 -5.74522
H 0.83364 -3.33175 -4.18817
H 1.93056 -1.12680 -4.11521
H -2.06559 -1.14368 -3.28848
H -1.79365 0.88657 -4.64929

58
Rebound Transition State (2/5)
Fe -0.07656 0.21777 0.22738
O -0.40461 0.25327 -1.56035
N 0.24975 0.24396 2.46556
N 1.74827 1.27199 0.43084
N -1.73786 1.30259 0.91746
N -0.12016 -1.83879 0.71740
C 2.28258 2.00882 -0.57630
H 1.73048 2.01688 -1.50660
C 3.47463 2.70815 -0.40806
H 3.88076 3.28832 -1.22649
C 4.12332 2.64724 0.83174
H 5.04870 3.18740 0.99305
C 3.56560 1.88753 1.86583
H 4.04590 1.82946 2.83481
C 2.37310 1.19868 1.63704
C -2.81607 1.54469 0.12896
H -2.74704 1.18645 -0.88957
C -3.93162 2.21824 0.61923
H -4.78024 2.40009 -0.02743
C -3.93063 2.64509 1.95342
H -4.78852 3.16538 2.36264
C -2.81467 2.39230 2.75873
H -2.79089 2.70985 3.79397
C -1.72012 1.72076 2.21169
C -0.04118 -2.81615 -0.22189
C -0.00547 -4.16189 0.13218
H 0.05788 -4.92054 -0.63709
C -0.04894 -4.50440 1.48940
H -0.01554 -5.54368 1.79412
C -0.13389 -3.49308 2.45187
H -0.16809 -3.73069 3.50806
C -0.17660 -2.16024 2.03859
C 1.73006 0.30059 2.66748
H 2.11907 -0.71683 2.54657
H 1.97999 0.62658 3.68413
C -0.44276 1.46825 2.97754
H -0.63712 1.39347 4.05382
H 0.23255 2.31838 2.82895
C -0.35120 -1.01369 3.00589
H -1.42273 -0.83428 3.14950
H 0.06876 -1.26255 3.98746
H -0.01070 -2.49077 -1.25303
H 1.51541 0.30233 -4.17161
C 0.69415 -0.38646 -4.35331
C -0.57956 0.14701 -4.94810
C -1.76550 -0.81454 -4.71613
C -1.40474 -2.26514 -5.10067
C -0.08043 -2.68822 -4.53787
C 0.89254 -1.76106 -4.17622
H -0.04198 -0.03834 -2.42674
H -0.42124 0.29670 -6.03127
H -2.64005 -0.47946 -5.28246
H -2.19116 -2.95894 -4.77842
H -1.36302 -2.36141 -6.20082
H 0.13077 -3.75023 -4.44951
H 1.84118 -2.11159 -3.78037
H -2.03623 -0.78513 -3.65228
H -0.80258 1.14238 -4.54448

58
Rebound Product (2/5)
Fe -0.16007 -0.06858 0.15107
O -0.15522 -0.76842 -1.86064
N 0.24578 0.30844 2.34115
N 1.85674 0.66570 0.14736
N -1.54186 1.52450 0.61891
N -0.53339 -1.98711 1.02622
C 2.50328 1.14944 -0.94385
H 1.94476 1.15933 -1.87107
C 3.81473 1.61341 -0.87475
H 4.30275 1.99078 -1.76420
C 4.47363 1.58591 0.36032
H 5.49241 1.94478 0.44728
C 3.80069 1.10138 1.48642
H 4.28277 1.08240 2.45637
C 2.48797 0.64175 1.35281
C -2.59367 1.89172 -0.15750
H -2.69234 1.39068 -1.11044
C -3.50848 2.86156 0.24569
H -4.33485 3.12610 -0.40148
C -3.33713 3.47130 1.49366
H -4.03551 4.22433 1.83922
C -2.25581 3.09320 2.29477
H -2.10077 3.54363 3.26776
C -1.36648 2.12001 1.83153
C -0.61598 -3.14710 0.32680
C -0.80898 -4.37343 0.95894
H -0.87184 -5.27994 0.37068
C -0.91148 -4.40343 2.35443
H -1.05508 -5.34270 2.87542
C -0.81926 -3.20724 3.07328
H -0.88720 -3.20130 4.15442
C -0.63640 -2.00655 2.38337
C 1.70767 0.06815 2.51435
H 1.86310 -1.01616 2.55030
H 2.07256 0.47935 3.46432
C -0.13963 1.72137 2.61908
H -0.29727 1.88959 3.69171
H 0.69741 2.35960 2.31411
C -0.59361 -0.67030 3.08854
H -1.60996 -0.26240 3.13608
H -0.24449 -0.79018 4.12233
H -0.52193 -3.06330 -0.74695
H -2.03320 -0.26722 -2.48918
C -1.12334 -0.55602 -3.01821
C -1.33609 -1.87020 -3.77629
C -0.19434 -2.15185 -4.77101
C -0.06386 -1.00169 -5.78728
C -0.13739 0.35306 -5.12631
C -0.60298 0.55741 -3.88135
H 0.70479 -1.08933 -2.19922
H -2.28380 -1.78470 -4.32561
H -0.37447 -3.10002 -5.28842
H 0.87672 -1.08840 -6.34605
H -0.86477 -1.07497 -6.54089
H 0.19882 1.20526 -5.71352
H -0.62663 1.55706 -3.45551
H 0.75615 -2.27044 -4.22961
H -1.45831 -2.69042 -3.06114

58
OAT Reactant Complex (2/5)
Fe 1.67021 7.50749 4.20159
O 1.99983 7.41417 2.58134
N 1.27549 7.62381 6.20980
N 3.37299 8.43878 4.75848
N -0.02147 8.60149 4.07323
N 1.49859 5.52772 4.55581
C 4.22972 9.05504 3.90509
H 3.98700 8.99415 2.85317
C 5.35322 9.72270 4.38247
H 6.02474 10.20824 3.68689
C 5.58931 9.75423 5.76262
H 6.45413 10.27348 6.15742
C 4.70009 9.11423 6.63451
H 4.86154 9.12792 7.70480
C 3.59427 8.45270 6.10568
C -0.74084 8.78839 2.93775
H -0.34556 8.35330 2.02884
C -1.93389 9.50503 2.96245
H -2.49350 9.64268 2.04674
C -2.38871 10.02988 4.17813
H -3.31789 10.58507 4.22083
C -1.63923 9.83013 5.34409
H -1.97272 10.22381 6.29586
C -0.44781 9.11330 5.26607
C 1.91201 4.55265 3.70734
C 1.80958 3.21066 4.06040
H 2.14440 2.44707 3.37093
C 1.27529 2.87633 5.31111
H 1.19263 1.83852 5.61022
C 0.85040 3.88976 6.17893
H 0.43731 3.65388 7.15138
C 0.96622 5.21762 5.77449
C 2.60587 7.66843 6.92724
H 2.95825 6.63763 7.03965
H 2.47976 8.08628 7.93044
C 0.47993 8.89083 6.43095
H -0.05797 8.83707 7.38217
H 1.19060 9.72142 6.49787
C 0.48201 6.39211 6.58291
H -0.56957 6.58996 6.34877
H 0.55198 6.20890 7.65904
H 2.31767 4.88003 2.76008
H 0.11482 10.16418 -1.01873
C 0.17726 9.17754 -1.49910
C 1.60485 8.60898 -1.36041
C 1.63839 7.11142 -1.72297
C 0.72121 6.29700 -0.78660
C -0.61615 6.97322 -0.57284
C -0.86273 8.25286 -0.90374
H -0.05395 9.35237 -2.56274
H 1.94558 8.73265 -0.32199
H 2.66431 6.72588 -1.67403
H 0.56393 5.28847 -1.19458
H 1.21750 6.15196 0.18674
H -1.40971 6.36690 -0.13735
H -1.85934 8.66643 -0.75268
H 1.30022 6.98614 -2.76198
H 2.29877 9.17502 -1.99399

58
OAT Transition State (2/5)
Fe 1.02189 7.69524 3.93452
O 0.85718 7.70360 2.24914
N 1.22489 7.68447 6.09523
N 2.87384 8.57892 4.12302
N -0.66458 8.76569 4.47120
N 0.96184 5.66275 4.29712
C 3.49738 9.23785 3.11328
H 2.99161 9.23457 2.15799
C 4.71711 9.87663 3.31483
H 5.19502 10.39546 2.49426
C 5.29939 9.83756 4.58791
H 6.24454 10.33357 4.77343
C 4.64997 9.15741 5.62379
H 5.07740 9.11650 6.61786
C 3.43363 8.52559 5.36511
C -1.69987 9.01033 3.62836
H -1.58610 8.64868 2.61600
C -2.83515 9.68881 4.06193
H -3.64886 9.87245 3.37264
C -2.90011 10.11734 5.39369
H -3.77548 10.64155 5.75797
C -1.82862 9.85970 6.25628
H -1.85756 10.17651 7.29136
C -0.71093 9.18335 5.76790
C 1.11507 4.72120 3.33181
C 1.12305 3.36496 3.64382
H 1.24791 2.63221 2.85740
C 0.97198 2.97736 4.98106
H 0.98129 1.92826 5.25145
C 0.81287 3.95426 5.97023
H 0.69742 3.67936 7.01125
C 0.80454 5.29949 5.60182
C 2.69581 7.70701 6.39495
H 3.05921 6.67405 6.35826
H 2.88204 8.08014 7.40769
C 0.52273 8.91496 6.59442
H 0.27897 8.82142 7.65836
H 1.21522 9.75777 6.49085
C 0.57034 6.42331 6.58125
H -0.50567 6.61422 6.65934
H 0.92668 6.15979 7.58292
H 1.22864 5.08841 2.32143
H 1.91961 9.76211 0.03114
C 1.61990 8.98322 -0.68339
C 2.77558 7.99397 -0.93606
C 2.27474 6.74643 -1.68917
C 1.18575 6.01186 -0.87947
C 0.18033 6.95341 -0.27544
C 0.37517 8.29891 -0.18784
H 1.37845 9.52341 -1.61427
H 3.20511 7.68407 0.02708
H 3.10624 6.06405 -1.89975
H 0.66591 5.27622 -1.50873
H 1.65400 5.42164 -0.07321
H -0.74488 6.52398 0.10066
H -0.41628 8.92920 0.20765
H 1.86008 7.05291 -2.65995
H 3.57492 8.48900 -1.49943

58
OAT Product (2/5)
Fe 1.09671 7.64384 3.70825
O 1.06740 7.70899 1.59809
N 1.20022 7.68057 5.95783
N 3.03974 8.45236 4.04737
N -0.72736 8.64140 4.23824
N 1.10065 5.56663 4.20574
C 3.78931 9.03591 3.07809
H 3.38407 9.00448 2.07624
C 5.01284 9.63862 3.35937
H 5.58688 10.09425 2.56280
C 5.47222 9.64372 4.68200

H 6.41706 10.11085 4.93370
C 4.69800 9.04201 5.67869
H 5.02817 9.03318 6.71044
C 3.48362 8.44318 5.33321
C -1.80915 8.80307 3.43500
H -1.74736 8.37438 2.44414
C -2.95120 9.47678 3.86115
H -3.79366 9.58907 3.19099
C -2.98244 9.99038 5.16263
H -3.85766 10.51595 5.52571
C -1.87530 9.80649 5.99666
H -1.87756 10.17801 7.01417
C -0.75390 9.13112 5.50908
C 1.35683 4.55957 3.33282
C 1.32956 3.22266 3.72190
H 1.53573 2.44428 2.99851
C 1.03886 2.91680 5.05700
H 1.01563 1.88650 5.39205
C 0.78731 3.95523 5.95885
H 0.57030 3.74769 6.99981
C 0.81867 5.27701 5.50613
C 2.64118 7.69681 6.34322
H 2.98621 6.65707 6.38350
H 2.77961 8.11649 7.34742
C 0.49062 8.93279 6.34461
H 0.23926 8.93947 7.41319
H 1.17890 9.76770 6.16825
C 0.50019 6.44523 6.41379
H -0.57777 6.63950 6.37905
H 0.74846 6.20300 7.45492
H 1.58650 4.85117 2.31684
H 2.16196 10.01688 0.16388
C 1.64295 9.22724 -0.39363
C 2.63301 8.18889 -0.95841
C 1.87864 6.99576 -1.57165
C 1.03398 6.24314 -0.51984
C 0.26643 7.16594 0.40460
C 0.57191 8.61764 0.47272
H 1.12242 9.72719 -1.22371
H 3.30470 7.83578 -0.16474
H 2.58114 6.29538 -2.03642
H 0.31659 5.57911 -1.01504
H 1.68142 5.59965 0.09019
H -0.71743 6.83527 0.72270
H -0.20543 9.29146 0.82001
H 1.22017 7.36247 -2.37147
H 3.26166 8.67032 -1.71540