Electronic Supplementary Material (ESI) for Chemical Communications

Nonheme iron-oxo and –superoxo reactivities: O_2 binding and spin inversion probability matter

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Electronic Supplementary Information

Contents

I. Clarifications to main text

Computational details

By default, every single calculation was done using the CPCM scheme to account for solvation (acetonitrile) effects as implemented in Gaussian 09.[S1] The reason for including solvent effects in even geometry optimizations was to avoid artificial effects such as self interaction errors (SIE) that is occurring in highly charged species (in our case, 2+) during a DFT run[S2]. Geometry optimizations and frequency calculations were done at B3LYP/LACVP level,[S3] and single-point calculations on the obtained geometry were done using larger basis set (B3LYP/LACV3P^{*+}//LACVP)[S3] in order to extract more accurate energies as well as Mulliken spin density distribution. Certain other functionals were also used here in order to gauge the reliability of B3LYP (see Figure S1). Dispersion was included using DFT-D3 program[S4] on the obtained geometry. The free energies could then be calculated as the LACV3P^{*+} obtained energy (ΔE) with addition of zero-point vibrational energy (ΔZ_0), enthalpy ($\Delta E_{thermal}$) and entropy ($-\Delta TS$, T=298K) contributions from the frequency calculations (at LACVP level) as well as the dispersion correction (ΔD). However, since the geometry optimizations were done in solvent, the obtained geometry is not suitable for gas-phase frequency calculations where it may not be a stationary point. Aggravating the situation, extracting thermal energy contributions from frequency calculations on a dielectric medium solvated model is not theoretically correct either due to several reasons,[S5] one of the reasons being "double counting" of energies because the solvent model is parameterized to fit to experimental free energies, i.e. including ΔZ_0, $\Delta E_{thermal}$, $-\Delta TS$ and ΔD. Hence, one has to review the results from the frequency calculations carefully in order to assess their reliability. The same situation holds for the dispersion corrections as well; the DFT-D3 parametrization may not be optimal for use on a geometry obtained under solvent parametrization. In the current study, all these effects are in many cases unreasonably large, and the final free energies obtained are many times not reasonable, as can be seen in the energy tables below. Hence, we chose to use our common sense judgment in this case and not include these "additives" in our conclusions based on their unreasonable effects as well as theoretical incorrectness. The energies discussed in the main text are, unless otherwise specified, including substrate in the model even if it is not influencing directly the specific energy discussed.

Choice of TMC stereoisomer

To decide on which TMC structure to calculate on is not an easy task, given the huge number of combinatorial possibilities. For every C-H activation reaction, one has to calculate the reactant, transition state and products (intermediates), hence a minimum of three structures. The reaction could be done with oxo or super-oxo group bound *syn* or *anti* relative to the TMC methyl groups doubling the number of structures to six. For each of these structures, there may or may not be a sixth (solvent) axial ligand present, doubling again the number of structures to 12. There is also the issue of the two $-CH_2CH_2-$ bridges present in the TMC ligand itself. If these two bridges are projected onto the same plane, they could be parallel to each other in direction, or cross, hence

now we have 24 structures to calculate. For **3**, we have two spin states, hence 24*2=48 calculations. For **4**, we found at least 12 different electronic configurations, leading to 24*12=288 structures. Hence, for TMC, we would need at least 48+288=336 structural calculations for a complete and full investigation. Since this is not feasible, we used common sense, combined with a smaller number of trial calculations as described below, to sort out the most likely stereo-/electroisomers to calculate.

The strongest clue to the structure of the active stereoisomer of **3** comes from the crystal structure, which shows that the oxo is *anti* to the TMC methyls, has an axial CH_3CN ligand and the -CH_3CH_3- bridge is parallel to each other. As we deem the -CH_3CH_3- bridge orientation not to be relevant to reactivity issues, we reduce the number of possible conformations by keeping this orientation as is in the crystal structure. Despite this, we find that the *syn* structure has a smaller barrier (i.e. relative to the *syn* reactant complex, 10.0 kcal/mol) than the *anti* structure (10.6 kcal/mol), as also found by others previously.[S6] However, comparing the reactants to each other, the *anti* structure is 1.9 kcal/mol more stable. Hence, the reason why the *syn* structure has a lower barrier may be because it is already higher up in energy from the beginning. Without the axial ligands, the barriers were found to be low (maximum 8.9 and 7.8 kcal/mol for *syn* and *anti* relative to their reactant complexes, respectively, Table SIV-4). While these barriers are low, no CH_3CN ligand binding means missing out on the binding energy (2.5 and 5.4 kcal/mol for the *syn* and *anti* conformations, respectively), which makes it more likely that the reaction occurs with an axial ligand.

For **4**, the closest available crystal structure is on the $[(TMC)Fe^{III}O_2]^+$ peroxo species.[S7] This structure features the O_2 moiety bound side-on *syn* to the TMC methyl groups, with no axial ligand and the -CH_3CH_3- bridge cross to each other. We tried many possible stereoisomers for **4**, and always found that the CH_3CN and/or O_2 binding was endothermic, except in the case where CH_3CN binds *syn* to the methyl groups (in which case the subsequent O_2-binding on the opposite side becomes prohibitively expensive). Hence, the least endothermic configuration was found to be when O_2 binds *syn* with respect to the methyl groups without CH_3CN binding, as found in all available metal(III)peroxo crystal structures.[S8] Therefore, we limit our superoxo reactivity study to this species.

Independent verification of $[(N4Py)Fe^{IV}O]^{2+}$ versus $[(TMC)Fe^{IV}O]^{2+}$ barriers

The barrier calculations of **1** vs. **3** was independently reproduced, using Jaguar[S9] gas-phase calculations and its Poisson-Boltzmann solver for single-point solvation (acetonitrile) effects, and Gaussian 03 for frequency calculations and thermal corrections. The models include counter ions which should remove self-interaction errors.[S10] It is confirmed that **3** has a lower calculated barrier than **1**.

Table SI-1. Calculated barriers (kcal/mol).[a]

	LACV3P^{*+} gas	LACV3P^{*+} + solv	LACV3P^{*+} + solv + G
Quintet			
1 + counter ions + CHD	14.1	15.0	20.6
3 + counter ions + CHD	13.1	14.1	18.4
Triplet			
1 + counter ions + CHD	17.6	18.1	25.6
3 + counter ions + CHD	21.6	22.3	29.0

[a] Relative to triplet reactant state with substrate separated. The results hold with energies relative to complexed reactants as well. Values for **1** was published in reference [S10].

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II. $[(N4Py)Fe^{IV}O]^{2+}$ (1)

$[(N4Py)Fe^{IV}O]^{2+}$ (1) with no substrates

Table SII-1. Relative energies (kcal/mol)

These energies are not used in the main text, but rather, the energies in Table SII-4 is used.

	Δlacvp	Δlacv3p^{*+}	**ΔE**[a]	ΔZ_0	$\Delta E_{thermal}$[b]	$-T\Delta S$[b]	Δ_{Disp}	**ΔG**[c]
$^3[Fe^{IV}O(N4Py)]^{2+}$	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
$^5[Fe^{IV}O(N4Py)]^{2+}$	14.05	-5.64	**8.41**	-1.55	+0.68	-2.68	+2.01	**6.87**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] ΔG=Sum of the previous five columns.

Table SII-2. Mulliken spin density distribution

	Fe	O	5 x ligated N	Rest
$^3[Fe^{IV}O(N4Py)]^{2+}$	1.30	0.91	-0.14	-0.07
$^5[Fe^{IV}O(N4Py)]^{2+}$	3.08	0.72	0.12	0.09

Table SII-3. Geometries (Å and °)

	D_{Fe-O}	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	$D_{Fe-N(ax)}$	$A_{N(eq)-Fe-N(eq)}$[a]
$^3[Fe^{IV}O(N4Py)]^{2+}$	1.66	1.99	1.99	1.97	1.97	2.06	90.72
$^5[Fe^{IV}O(N4Py)]^{2+}$	1.65	2.13	2.13	2.08	2.09	2.08	90.95

[a] The largest angle of the four possible ones.

Reactivity with 1,4-cyclohexadiene

Table SII-4. Relative energies (kcal/mol)

	Δlacvp	Δlacv3p^{*+}	**ΔE**[a]	ΔZ_0	$\Delta E_{thermal}$[b]	$-T\Delta S$[b]	Δ_{Disp}	**ΔG**[c]
Triplet (S=1)								
Reactants, complexed	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Transition state	10.10	+3.33	**13.43**	-3.42	-0.64	+3.87	-4.57	**8.67**
Intermediate	-13.49	-0.99	**-14.48**	-1.66	+0.13	-0.33	-1.94	**-18.28**
Quintet (S=2)								
Reactants, complexed	13.88	-5.75	**8.14**	-1.46	+0.69	-2.80	+2.01	**6.57**
Transition state	17.19	-4.85	**12.34**	-3.65	+0.26	-0.44	+1.39	**9.90**
Intermediate	-7.62	-7.11	**-14.73**	-4.08	+1.09	-2.41	-0.74	**-20.88**
Triplet (S=1) with two counter ions $[ClO_4]^-$								
Reactants, complexed	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Transition state	10.57	+3.18	**13.75**	-3.69	-0.55	+3.98	-4.44	**9.05**
Intermediate	-13.30	-0.30	**-13.59**	-1.83	+0.13	+1.03	-1.79	**-16.05**
Quintet (S=2) with two counter ions $[ClO_4]^-$								
Reactants, complexed	13.85	-4.13	**9.71**	-1.60	+0.68	-1.49	+0.45	**7.76**
Transition state	17.32	-3.69	**13.63**	-3.58	+0.23	+1.33	+1.10	**12.71**
Intermediate	-10.66	-5.18	**-15.85**	-3.67	+0.79	-0.09	-1.49	**-20.30**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] ΔG=Sum of the previous five columns. This value is however deemed unreliable and is not used.

Table SII-5. Mulliken spin density distribution

	Fe	O	5 x ligated N	Substrate	Rest
Triplet (S=1)					
Reactants, complexed	1.21	0.91	-0.10	0.00	-0.03
Transition state	0.99	0.71	-0.10	0.40	-0.01
Intermediate	0.99	0.16	-0.15	0.98	0.02
Quintet (S=2)					
Reactants, complexed	3.10	0.71	0.12	0.00	0.07
Transition state	3.57	0.41	0.17	-0.23	0.07
Intermediate	4.07	0.40	0.35	-0.97	0.14
Triplet (S=1) with two counter ions $[ClO_4]^-$					
Reactants, complexed	1.18	0.94	-0.08	0.00	-0.05
Transition state	0.99	0.73	-0.08	0.39	-0.03
Intermediate	0.98	0.17	-0.14	0.98	0.01
Quintet (S=2) with two counter ions $[ClO_4]^-$					
Reactants, complexed	3.12	0.74	0.10	0.00	0.04
Transition state	3.57	0.44	0.17	-0.21	0.03
Intermediate	4.20	0.45	0.25	-0.97	0.08

Table SII-6. Geometries (Å and °)

	D_{Fe-O}	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	$D_{Fe-N(ax)}$	D_{O-H}	$D_{FeOH-C(subs)}$	A_{Fe-O-H}
Triplet (S=1)									
Reactants, complexed	1.66	1.99	1.99	1.97	1.97	2.06	2.65	1.10	153.55
Transition state	1.75	1.99	1.99	1.98	1.98	2.05	1.39	1.25	124.46
Intermediate	1.82	1.99	1.99	1.98	1.97	2.03	0.98	2.47	116.55
Quintet (S=2)									
Reactants, complexed	1.65	2.14	2.13	2.08	2.09	2.08	2.57	1.10	151.37
Transition state	1.69	2.15	2.16	2.12	2.11	2.18	1.65	1.15	165.73
Intermediate	1.79	2.18	2.18	2.15	2.13	2.27	0.98	2.18	160.81
Triplet (S=1) with two counter ions $[ClO_4]^-$									
Reactants, complexed	1.65	1.99	1.99	1.97	1.97	2.06	2.69	1.10	171.63
Transition state	1.75	1.99	1.99	1.98	1.98	2.05	1.39	1.24	124.70
Intermediate	1.81	1.99	1.99	1.98	1.97	2.03	0.98	2.40	117.74
Quintet (S=2) with two counter ions $[ClO_4]^-$									
Reactants, complexed	1.65	2.14	2.12	2.08	2.09	2.08	2.60	1.10	151.49
Transition state	1.69	2.16	2.15	2.12	2.11	2.18	1.67	1.15	170.72
Intermediate	1.78	2.18	2.17	2.16	2.14	2.27	0.99	3.18	155.14

III. $[(N4Py)Fe^{III}O_2]^{2+}$ (2)

$[(N4Py)Fe^{III}O_2]^{2+}$ (2) with no substrates

Table SIII-1. Valence electron configurations

	d_{xy}	d_{xz}	d_{yz}	d_{z^2}	$d_{x^2-y^2}$	$^{OO}\pi^*_{xy}$	$^{OO}\pi^*_{xz}$
Singlet	↑↓	↑↓	↑	----	----	↓	↑↓
Triplet	↑	↑↓	↑↓	----	----	↑	↑↓
Quintet (QI)	↑	↑	↑	----	----	↑	↑↓
Quintet (QII)[a]	↑	↑	↑	↑	↑	↓	↑↓
Quintet (QIII)	↑	↑	↑	↑	↑	↑↓	↓
Quintet sideon (QSI)	↑↓	↑	↑	↑	----	↑	↑↓
Quintet sideon (QSII)	↑	↑	↑	↑	↑	↓	↑↓
Septet endon	↑	↑	↑	↑	↑	↑	↑
Septet sideon	↑	↑	↑	↑	↑	↑	↑↓
Septet O_2-unbound[b]	↑	↑	↑↓	↑	↑	↑	↑

[a] As the Fe-O-O angle is linear, the choice of x and y is arbitrary. [b] O_2 was placed approximately 20 Å from the iron.

Table SIII-2. Relative energies (kcal/mol)

These energies are not used in the main text, but rather, the energies in Table SIII-5 is used.

	Δlacvp	$\Delta lacv3p^{*+}$	**ΔE^a**	ΔZ_0	$\Delta E_{thermal}{}^b$	$-T\Delta S^b$	Δ_{Disp}	**ΔG^c**
Singlet	-8.19	+8.06	**-0.13**	+1.91	-0.78	+3.23	-2.59	**1.65**
Triplet	-4.63	+8.86	**4.23**	+1.72	-0.64	+2.07	-2.62	**4.76**
Quintet (QI)	10.25	+4.49	**14.74**	-0.06	+0.12	-0.60	-0.56	**13.64**
Quintet (QII)	8.66	-0.16	**8.50**	-0.90	-0.59	+0.85	-1.12	**6.74**
Quintet (QIII)	7.59	+0.15	**7.74**	-0.52	+0.30	-1.29	-1.57	**4.66**
Quintet sideon (QSI)	7.39	+6.24	**13.64**	+0.85	-0.30	+1.26	-1.77	**13.67**
Quintet sideon (QSII)	5.43	-0.30	**5.13**	-0.05	+0.04	+0.11	-0.08	**5.15**
Septet endon	6.97	+0.09	**7.06**	-1.13	+0.73	-3.52	-0.38	**2.75**
Septet sideon	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Septet O_2-unbound[d]	6.82	-5.14	**1.68**	-1.98	+0.22	-4.85	+3.34	**0.30**

[a] Sum of the previous two columns. [b] T=298.15 K. [c] ΔG=Sum of the previous five columns. [d] O_2 was placed approximately 20 Å from the iron.

Table SIII-3. Mulliken spin density distribution

	Fe	O_{inner}	O_{outer}	N_{ax}	4 x N_{eq}	Rest
Singlet	1.17	-0.30	-0.67	-0.08	-0.14	0.01
Triplet	1.11	0.36	0.61	-0.08	-0.11	0.11
Quintet (QI)	3.10	0.26	0.60	-0.14	0.07	0.10
Quintet (QII)	4.02	-0.06	-0.55	0.03	0.44	0.13
Quintet (QIII)	3.98	0.02	-0.54	-0.03	0.38	0.19
Quintet sideon (QSI)	2.63	0.68	0.68	0.00	-0.05	0.07
Quintet sideon (QSII)	4.24	-0.33	-0.33	-0.01	0.33	0.10
Septet endon	3.99	0.72	0.98	-0.03	0.22	0.12
Septet sideon	4.09	0.71	0.71	-0.02	0.39	0.12
Septet O_2-unbound[a]	3.57	1.00	1.00	-0.06	0.22	0.27

[a] O_2 was placed approximately 20 Å from the iron.

Table SIII-4. Geometries (Å and °)

	D(Fe-O)	D(O-O)	D(Fe-N_{ax})	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{eq4})	A(Fe-O-O)
Singlet	1.85	1.36	2.02	1.99	1.99	1.98	1.98	118.37
Triplet	1.91	1.37	2.02	1.98	1.98	1.97	1.97	113.17
Quintet (QI)	1.93	1.36	2.07	2.01	2.21	2.17	2.00	108.88
Quintet (QII)	1.86	1.32	2.21	2.16	2.17	2.13	2.13	179.17
Quintet (QIII)	1.90	1.33	2.20	2.16	2.16	2.13	2.12	138.54
Quintet sideon (QSI)	2.21	1.36	2.22	2.04	2.04	2.03	2.03	71.94
Quintet sideon (QSII)	2.17	1.37	2.22	2.17	2.17	2.14	2.14	70.99
Septet endon	2.04	1.28	2.19	2.18	2.18	2.14	2.14	177.61
Septet sideon	2.17	1.36	2.21	2.17	2.18	2.14	2.14	71.37
Septet O_2-unbound[a]	19.88	1.25	2.20	2.21	2.21	2.16	2.16	178.29

[a] O_2 was placed approximately 20 Å from the iron.

Reactivity with 1,4-cyclohexadiene

Table SIII-5. Relative energies (kcal/mol)

	Δlacvp	Δlacv3p^{*+}	**ΔE**^{a}	ΔZ_0	$\Delta E_{Thermal}$ ^{b}	$-T\Delta S^{b}$	Δ_{Disp}	**ΔG**^{c}
Singlet								
Reactants, complexed	-8.04	+8.62	**0.57**	+1.92	-0.81	+3.53	-2.89	**2.32**
Transition state	**0.66**	**+13.60**	**14.26**	**-1.15**	**-1.67**	**+7.36**	**-5.69**	**13.12**
Intermediate	-14.94	+10.47	**-4.47**	+0.80	-0.92	+4.42	-3.50	**-3.66**
Triplet								
Reactants, complexed	-4.94	+9.54	**4.60**	+1.91	-0.76	+1.98	-2.57	**5.17**
Transition state	1.85	+13.49	**15.34**	-0.87	-1.59	+6.03	-4.27	**14.64**
Intermediate	-14.93	10.46	**-4.47**	0.77	-0.89	-3.48	3.11	**-4.96**
Quintet								
Reactants, complexed, QI	9.89	+4.58	**14.47**	+0.11	-0.01	-0.19	-0.45	**13.93**
Transition state, QI	14.69	+8.98	**23.67**	-2.85	-0.84	+3.30	-2.39	**20.90**
Intermediate, QI	-0.74	+5.91	**5.17**	-0.79	-0.21	+0.94	-1.34	**3.78**
Reactants, complexed, QIII	6.65	+0.62	**7.27**	-0.14	+0.08	+0.04	-2.62	**4.64**
Transition state, QIII	10.53	+4.74	**15.27**	-3.42	-0.43	+1.19	-1.30	**11.30**
Intermediate, QIII	-47.35	+5.48	**-41.88**	+0.05	+0.31	-0.51	-2.82	**-44.85**
Reactants, complexed, QSII	5.50	-0.52	**4.97**	+0.07	-0.05	+0.03	+0.75	**5.79**
Transition state, QSII	10.48	+4.96	**15.44**	-2.84	-0.66	+2.84	-1.62	**13.17**
Intermediate, QSII	-47.27	+5.39	**-41.88**	+0.12	+0.29	-0.45	-2.30	**-44.23**
Septet								
Reactants, complexed	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Transition state	9.56	+5.96	**15.52**	-3.35	-0.75	+3.51	-5.32	**9.61**
Intermediate	-1.73	+2.29	**0.56**	-1.09	-0.07	+0.58	-4.53	**-4.55**
With 2x $[ClO_4]^-$								
Septet Reactants, complexed	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Singlet Reactants, complexed	-8.63	+8.66	**0.03**	+1.85	-0.79	+2.93	-2.31	**1.72**
Singlet Transition state	0.56	+13.93	**14.49**	-1.27	-1.65	+8.17	-5.44	**14.30**
Singlet Intermediate	-15.42	+10.86	**-4.56**	+0.64	-0.86	+4.08	-3.31	**-4.01**

[a] Sum of the previous two columns. [b] T=298.15 K. [c] ΔG= Sum of the previous five columns. This value is however deemed unreliable and is not used.

Table SIII-6. Mulliken spin density distribution

	Fe	O_{inner}	O_{outer}	N_{ax}	4 x N_{eq}	Substrate	Rest
Singlet							
Reactants, complexed	1.17	-0.34	-0.64	-0.08	-0.15	0.00	0.04
Transition state	0.97	0.06	-0.38	-0.07	-0.08	-0.49	0.01
Intermediate	0.93	0.18	0.01	-0.07	-0.06	-1.00	0.01
Triplet							
Reactants, complexed	1.19	0.35	0.62	-0.08	-0.16	0.00	0.09
Transition state	0.90	0.27	0.48	-0.07	-0.06	0.45	0.02
Intermediate	0.93	0.18	0.01	-0.07	-0.06	1.00	0.01
Quintet							
Reactants, complexed, QI	3.13	0.29	0.56	-0.16	0.05	0.01	0.13
Transition state, QI	3.14	0.04	0.33	-0.16	0.07	0.48	0.10
Intermediate, QI	3.00	0.04	-0.03	-0.16	0.07	0.99	0.09
Reactants, complexed, QIII	3.96	0.02	-0.52	-0.04	0.39	-0.01	0.19
Transition state, QIII	4.01	0.33	-0.23	-0.06	0.30	-0.50	0.16
Intermediate, QIII	3.83	0.02	-0.01	-0.08	0.08	0.01[a]	0.16
Reactants, complexed, QSII	4.22	-0.32	-0.32	-0.02	0.35	0.00	0.10
Transition state, QSII	4.13	0.13	-0.18	-0.04	0.33	-0.51	0.13
Intermediate, QSII	3.81	0.02	-0.01	-0.09	0.11	0.01[a]	0.16
Septet							
Reactants, complexed	4.17	0.71	0.70	-0.03	0.35	0.01	0.09
Transition state	4.21	0.39	0.42	-0.05	0.31	0.63	0.08
Intermediate	4.19	0.29	0.04	-0.03	0.37	1.01	0.13
With 2x $[ClO_4]^-$							
Septet Reactants, complexed	4.20	0.69	0.69	-0.07	0.39	0.00	0.09
Singlet Reactants, complexed	1.15	-0.34	-0.64	-0.08	-0.16	0.00	0.07
Singlet Transition state	0.96	0.06	-0.39	-0.07	-0.07	-0.48	0.00
Singlet Intermediate	0.93	0.19	0.02	-0.07	-0.07	-1.00	0.01

[a] No spin on the substrate after the reaction indicate that a hydride, rather than a hydrogen atom, transfer has occurred, and we obtain here H_2O_2 formation by automatic transfer of one more proton from the substrate. This could be self-interaction errors within DFT, or a real effect due to the specific substrate used. As the spin density distribution at the transition states are characteristic of hydrogen atom transfers, the state of the intermediates are immaterial for the barrier discussions.

Table SIII-7. Geometries (Å)

	D_{Fe-O}	D_{O-O}	$D_{Fe-N(ax)}$	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	D_{O-H}	D_{H-C}	A_{O-O-H}
Singlet										
Reactants, complexed	1.87	1.36	2.02	1.99	1.98	1.98	1.98	2.54	1.10	110.25
Transition state	1.82	1.44	2.03	2.00	1.99	1.98	1.99	1.39	1.25	106.97
Intermediate	1.81	1.51	2.02	2.00	2.00	1.98	1.98	0.99	2.18	100.86
Triplet										
Reactants, complexed	1.92	1.37	2.01	1.99	1.97	1.98	1.97	2.57	1.10	117.62
Transition state	1.83	1.44	2.02	2.00	2.00	1.99	1.98	1.47	1.21	104.64
Intermediate	1.81	1.51	2.02	2.00	2.00	1.98	1.98	0.99	2.18	100.97
Quintet										
Reactants, compl, QI	1.94	1.36	2.07	2.03	2.22	2.16	2.00	2.54	1.10	108.37
Transition state, QI	1.87	1.42	2.10	2.09	2.24	2.16	2.04	1.45	1.22	107.05
Intermediate, QI	1.83	1.49	2.07	2.07	2.23	2.16	2.03	1.00	2.16	102.56
Reactants, compl, QIII	1.89	1.33	2.20	2.16	2.16	2.13	2.12	2.55	1.10	92.14
Transition state, QIII	1.89	1.40	2.24	2.17	2.18	2.15	2.13	1.43	1.23	104.59
Intermediate, QIII	2.13	1.52	2.23	2.19	2.27	2.20	2.16	0.99	3.21	101.26
Reactants, compl, QSII	2.15	1.37	2.22	2.17	2.17	2.14	2.14	2.71	1.10	95.10
Transition state, QSII	2.00	1.46	2.27	2.19	2.17	2.14	2.19	1.47	1.22	104.69
Intermediate, QSII	2.13	1.52	2.23	2.23	2.22	2.18	2.20	0.99	2.99	101.09
Septet										
Reactants, complexed	2.17	1.36	2.22	2.17	2.17	2.14	2.15	2.74	1.10	90.49
Transition state	1.99	1.47	2.27	2.20	2.16	2.13	2.21	1.36	1.29	106.01
Intermediate	1.94	1.52	2.26	2.18	2.16	2.12	2.19	1.00	2.11	103.26
With 2x $[ClO_4]^-$										
Septet React, compl	2.17	1.36	2.22	2.18	2.17	2.14	2.14	2.89	1.10	91.47
Singlet React, compl	1.87	1.36	2.02	2.00	1.99	1.98	1.97	2.55	1.10	107.76
Singlet Transition state	1.81	1.44	2.03	2.00	1.99	1.98	1.99	1.38	1.25	106.73
Singlet Intermediate	1.80	1.51	2.02	2.00	2.00	1.98	1.98	0.99	2.19	100.56

IV. $[(TMC)Fe^{IV}O]^{2+}$ (3)

$[(TMC)Fe^{IV}O]^{2+}$ (3) with no substrates

Table SIV-1. Relative energies (kcal/mol)

These energies are not used in the main text, but rather, the energies in Table SIV-4 is used.

	Δlacvp	Δlacv3p^{*+}	**ΔE**[a]	ΔZ_0	$\Delta E_{thermal}$[b]	$-T\Delta S$[b]	Δ_{Disp}	Δ_{phase}[c]	**ΔG**[d]
***Syn* to methyls**									
$^3[Fe^{IV}O(TMC)]^{2+}$	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**		**0.00**
$^5[Fe^{IV}O(TMC)]^{2+}$	6.57	-2.42	**4.14**	-1.77	+0.57	-1.88	+1.45		**2.52**
***Anti* to methyls**									
$^3[Fe^{IV}O(TMC)]^{2+}$	0.16	+0.98	**1.15**	+0.45	-0.22	+0.60	-1.19		**0.79**
$^5[Fe^{IV}O(TMC)]^{2+}$	10.06	-1.11	**8.95**	-1.45	+0.29	-0.89	-0.10		**6.80**
***Syn* to methyls, with $CNCH_3$**									
$^3[Fe^{IV}O(TMC)]^{2+} + CNCH_3$	8.57	-4.02	**4.55**	-1.64	-0.48	-2.44	+5.13	+1.75	**6.87**
$^3[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.30	+0.73	**2.03**	+0.08	+0.04	-0.02	-0.39		**1.74**
$^5[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	10.10	-2.30	**7.80**	-1.75	+0.62	-1.67	-2.36		**2.63**
***Anti* to methyls, with $CNCH_3$**									
$^3[Fe^{IV}O(TMC)]^{2+} + CNCH_3$	8.39	-2.95	**5.44**	-1.18	-0.19	-3.15	+3.86	+1.75	**6.52**
$^3[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**		**0.00**
$^5[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	7.57	-3.03	**4.54**	-1.81	+0.56	-1.63	-1.91		**-0.26**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] Free energy correction in solution phase due to complexation. [d] ΔG=Sum of the previous six columns.

Table SIV-2. Mulliken spin density distribution

	Fe	O	4 x N_{eq}	$CNCH_3$	Rest
***Syn* to methyls**					
$^3[Fe^{IV}O(TMC)]^{2+}$	1.35	0.73	-0.07	----	-0.01
$^5[Fe^{IV}O(TMC)]^{2+}$	3.19	0.60	0.15	----	0.07
***Anti* to methyls**					
$^3[Fe^{IV}O(TMC)]^{2+}$	1.39	0.72	-0.10	----	0.00
$^5[Fe^{IV}O(TMC)]^{2+}$	3.17	0.66	0.11	----	0.06
***Syn* to methyls, with $CNCH_3$**					
$^3[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.42	0.80	-0.17	-0.01	-0.03
$^5[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	3.25	0.55	0.14	-0.01	0.07
***Anti* to methyls, with $CNCH_3$**					
$^3[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.34	0.76	-0.07	-0.04	0.00
$^5[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	3.23	0.57	0.19	-0.06	0.07

Table SIV-3. Geometries (Å and °)

	D_{Fe-O}	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	$D_{Fe-N(ax)}$
***Syn* to methyls**						
$^{3}[Fe^{IV}O(TMC)]^{2+}$	1.62	2.08	2.13	2.12	2.08	----
$^{5}[Fe^{IV}O(TMC)]^{2+}$	1.65	2.21	2.13	2.13	2.22	----
***Anti* to methyls**						
$^{3}[Fe^{IV}O(TMC)]^{2+}$	1.62	2.08	2.07	2.08	2.08	----
$^{5}[Fe^{IV}O(TMC)]^{2+}$	1.67	2.07	2.21	2.22	2.06	----
***Syn* to methyls, with $CNCH_3$**						
$^{3}[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.63	2.10	2.13	2.13	2.10	2.14
$^{5}[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.63	2.21	2.20	2.20	2.21	2.13
***Anti* to methyls, with $CNCH_3$**						
$^{3}[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.64	2.11	2.13	2.13	2.11	2.07
$^{5}[Fe^{IV}O(TMC)(CNCH_3)]^{2+}$	1.65	2.16	2.26	2.26	2.16	2.06

Reactivity with 1,4-cyclohexadiene

Table SIV-4. Relative energies (kcal/mol)

	Δlacvp	Δlacv3p^{*+}	**ΔE**[a]	ΔZ_0	$\Delta E_{thermal}$[b]	$-T\Delta S$[b]	Δ_{Disp}	Δ_{phase}[c]	**ΔG**[d]
***Syn* to methyls**									
Triplet									
Reactant	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**		**0.00**
Transition state	5.65	+3.22	**8.87**	-3.21	-0.43	+2.86	-1.95		**6.14**
Intermediate	-16.05	+0.04	**-16.01**	-2.91	+0.49	+0.04	-1.80		**-20.18**
Quintet									
Reactant (20Å separated)	7.43	-2.99	**4.44**	-1.44	-0.67	+1.33	+5.58	+1.89	**11.14**
Transition state[e]	----	----	----	----	----	----	----		----
Intermediate	-22.58	-2.59	**-25.17**	-4.16	+0.83	-1.07	+0.36		**-29.21**
***Anti* to methyls**									
Triplet									
Reactant	-0.30	+1.45	**1.15**	+0.86	-0.40	+2.19	-2.30		**1.50**
Transition state	12.13	+5.94	**18.07**	-3.38	-0.69	+4.01	-5.69		**12.32**
Intermediate	-6.59	+1.76	**-4.84**	-1.37	-0.12	+2.26	-3.89		**-7.96**
Quintet									
Reactant	9.28	-0.77	**8.51**	-0.89	+0.07	+1.08	-2.24		**6.53**
Transition state	9.78	-0.87	**8.91**	-2.05	-2.16	+0.61	-0.98		**6.37**
Intermediate	-16.54	-0.83	**-17.37**	-3.79	0.57	-0.18	-1.77		**-22.53**
***Syn* to methyls, with $CNCH_3$**									
Triplet									
Reactant	1.38	+0.55	**1.93**	+0.30	-0.03	+0.05	+0.78		3.03
Transition state	18.44	+3.97	**22.41**	-3.68	-0.55	+3.41	-3.36		**18.23**
Intermediate	-6.10	-0.54	**-6.65**	-1.57	+0.12	+0.31	-1.55		**-9.33**
Quintet									
Reactant	10.28	-2.58	**7.70**	-1.92	+0.09	-0.38	-1.47		**4.01**
Transition state	12.65	-0.76	**11.89**	-4.06	+0.24	+0.05	-2.53		**5.58**
Intermediate	-17.70	-4.56	**-22.27**	-5.80	+1.97	-6.89	+4.31		**-28.67**
***Anti* to methyls, with $CNCH_3$**									
Triplet									
Reactant	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**		**0.00**
Transition state	15.75	+3.91	**19.66**	-3.43	-0.66	+3.51	-4.04		**15.05**
Intermediate	-8.84	-0.29	**-9.12**	-1.35	+0.02	+0.85	-2.46		**-12.06**
Quintet									
Reactant	7.33	-3.01	**4.32**	-2.17	+0.69	-2.47	-2.23		**-1.86**
Transition state	11.08	-0.48	**10.60**	-4.37	+0.09	+1.01	-3.79		**3.54**
Intermediate	-9.91	-2.44	**-12.35**	-4.39	+0.92	-2.28	-3.26		**-21.37**
***Anti* to methyls, with $CNCH_3$ and 2x$[CF_3SO_3]^-$**									
Triplet									
Reactant	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**		**0.00**
Transition state	17.51	+2.69	**20.21**	-3.91	-0.44	+2.04	-5.65		**12.25**
Intermediate	-7.38	-1.38	**-8.76**	-1.44	+0.08	+0.85	-2.80		**-12.07**
Quintet									
Reactant	8.57	-4.12	**4.45**	-2.28	+0.68	-2.65	-4.39		**-4.19**
Transition state	12.24	-1.33	**10.91**	-4.48	+0.16	+0.51	-6.58		**0.52**
Intermediate	-8.96	-3.05	**-12.01**	-4.61	+0.97	-1.92	-6.08		**-23.65**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] Free energy correction in solution phase due to complexation. [d] ΔG=Sum of the previous six columns. This value is however deemed unreliable and is not used. [e] Does not exist, but it is a downhill reaction at LACVP level.

Table SIV-5. Mulliken spin density distribution

	Fe	O	4 x N_{eq}	$CNCH_3$	Substrate	Rest
***Syn* to methyls**						
Triplet						
Reactant	1.33	0.73	-0.06	----	0.00	-0.01
Transition state	1.97	0.30	0.00	----	-0.32	0.04
Intermediate	2.97	0.34	-0.32	----	-0.98	0.00
Quintet						
Reactant (20Å separated)	3.19	0.60	0.14	----	0.00	0.07
Intermediate	4.05	0.42	0.37	----	-0.94	0.10
***Anti* to methyls**						
Triplet						
Reactant	1.41	0.72	-0.11	----	0.00	-0.02
Transition state	1.12	0.57	-0.07	----	0.36	0.02
Intermediate	1.13	0.04	-0.17	----	1.00	0.00
Quintet						
Reactant	3.14	0.62	0.16	----	0.00	0.09
Transition state	3.13	0.51	0.28	----	-0.06	0.14
Intermediate	3.65	0.41	0.64	----	-0.97	0.26
***Syn* to methyls, with $CNCH_3$**						
Triplet						
Reactant	1.33	0.81	-0.12	-0.01	0.00	-0.01
Transition state	1.04	0.65	-0.09	-0.02	0.42	0.01
Intermediate	1.06	0.10	-0.14	-0.02	0.98	0.02
Quintet						
Reactant	3.24	0.55	0.15	-0.01	0.00	0.07
Transition state	3.70	0.30	0.09	0.08	-0.24	0.08
Intermediate	4.04	0.42	0.36	0.00	-0.95	0.13
***Anti* to methyls, with $CNCH_3$**						
Triplet						
Reactant	1.36	0.79	-0.10	-0.04	0.00	-0.01
Transition state	1.06	0.66	-0.10	-0.04	0.42	0.00
Intermediate	1.08	0.09	-0.14	-0.04	1.00	0.01
Quintet						
Reactant	3.21	0.59	0.18	-0.06	0.00	0.07
Transition state	3.72	0.29	0.12	0.09	-0.32	0.10
Intermediate	4.10	0.39	0.23	0.11	-0.98	0.15
***Anti* to methyls, with $CNCH_3$ and 2x$[CF_3SO_3]^-$**						
Triplet						
Reactant	1.36	0.77	-0.09	-0.04	0.00	0.00
Transition state	1.05	0.66	-0.11	-0.03	0.42	0.01
Intermediate	1.09	0.10	-0.15	-0.04	0.99	0.01
Quintet						
Reactant	3.20	0.59	0.16	-0.05	0.00	0.11
Transition state	3.68	0.30	0.10	0.09	-0.30	0.13
Intermediate	4.09	0.45	0.22	0.09	-1.02	0.16

Table SIV-6. Geometries (Å and °)

	D_{Fe-O}	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	$D_{Fe-N(ax)}$	D_{O-H}	D_{C-H}	A_{Fe-O-H}
***Syn* to methyls**									
Triplet									
Reactant	1.62	2.08	2.12	2.11	2.08	----	2.54	1.10	174.79
Transition state	1.69	2.11	2.12	2.12	2.13	----	1.49	1.18	175.98
Intermediate	1.82	2.13	2.13	2.12	2.16	----	0.98	2.30	141.28
Quintet									
Reactant (20Å separated)	1.65	2.22	2.13	2.13	2.21	----	19.71	1.10	178.45
Intermediate	1.78	2.20	2.25	2.25	2.20	----	0.98	2.14	155.69
***Anti* to methyls**									
Triplet									
Reactant	1.62	2.08	2.07	2.08	2.09	----	2.53	1.10	169.06
Transition state	1.72	2.08	2.08	2.09	2.07	----	1.35	1.26	150.82
Intermediate	1.80	2.09	2.07	2.09	2.07	----	0.98	2.54	121.96
Quintet									
Reactant	1.66	2.09	2.22	2.22	2.08	----	2.56	1.10	160.89
Transition state	1.66	2.10	2.21	2.21	2.10	----	2.05	1.11	176.34
Intermediate	1.78	2.19	2.18	2.18	2.19	----	0.98	2.11	172.49
***Syn* to methyls, with $CNCH_3$**									
Triplet									
Reactant	1.63	2.10	2.13	2.13	2.10	2.14	3.27	1.10	152.08
Transition state	1.73	2.12	2.12	2.15	2.10	2.16	1.33	1.29	145.78
Intermediate	1.80	2.11	2.13	2.14	2.10	2.08	0.98	2.66	118.98
Quintet									
Reactant	1.64	2.21	2.20	2.20	2.20	2.13	2.60	1.10	161.87
Transition state	1.68	2.21	2.22	2.22	2.21	2.31	1.66	1.15	176.45
Intermediate	1.77	2.19	2.26	2.26	2.19	4.54	0.98	2.10	160.66
***Anti* to methyls, with $CNCH_3$**									
Triplet									
Reactant	1.64	2.11	2.13	2.13	2.11	2.07	2.63	1.10	179.40
Transition state	1.75	2.12	2.13	2.16	2.10	2.08	1.35	1.28	145.65
Intermediate	1.82	2.11	2.14	2.15	2.10	2.02	0.98	3.42	120.84
Quintet									
Reactant	1.65	2.16	2.26	2.26	2.16	2.07	2.62	1.10	176.65
Transition state	1.71	2.20	2.25	2.25	2.20	2.20	1.57	1.17	177.50
Intermediate	1.80	2.21	2.24	2.24	2.21	2.25	0.98	2.20	179.46
***Anti* to methyls, with $CNCH_3$ and 2x$[CF_3SO_3]^-$**									
Triplet									
Reactant	1.64	2.11	2.14	2.13	2.11	2.08	5.21	1.10	138.04
Transition state	1.75	2.12	2.14	2.15	2.10	2.08	1.35	1.28	145.29
Intermediate	1.82	2.11	2.14	2.15	2.10	2.02	0.98	2.95	120.49
Quintet									
Reactant	1.65	2.16	2.27	2.27	2.15	2.07	2.57	1.10	169.42
Transition state	1.70	2.20	2.26	2.25	2.19	2.20	1.59	1.17	174.78
Intermediate	1.80	2.22	2.25	2.25	2.20	2.25	0.98	2.20	173.05

V. $[(TMC)Fe^{III}O_2]^{2+}$ (4)

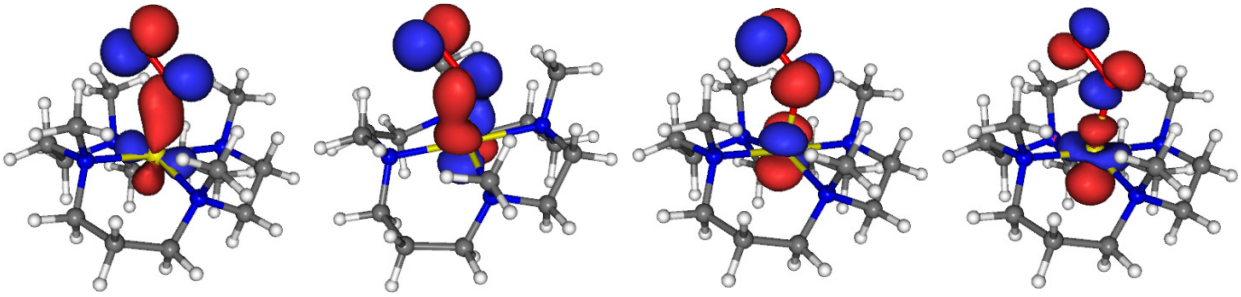
$[(TMC)Fe^{III}O_2]^{2+}$ (4) with no substrates

Table SV-1. Valence electron configurations

	d_{xy}	d_{xz}	d_{yz}	d_{z^2}	$d_{x^2-y^2}$	$^{OO}\pi^*_{xy}$	$^{OO}\pi^*_{xz}$
Singlet endon	↑↓	↑↓	↑	↑	----	↓	↓
Triplet endon I	↑↓	↑	↑	↑	----	↓	↑↓
Triplet endon II	↑↓	↑	↑	↑	----	↑↓	↓
Triplet sideon	↑↓	↑	↑	↑	----	↓	↑↓
Quintet endon I	↑	↑	↑	↑	↑	↓	↑↓
Quintet endon II	↑	↑	↑	↑	↑	↑↓	↓
Quintet endon III	↑↓	↑	↑	↑	----	↑	↑↓
Quintet sideon I	↑	↑	↑	↑	↑	↓	↑↓
Quintet sideon II	↑	↑	↑	↑	↑	↑↓	↓
Quintet sideon III	↑↓	↑	↑	↑	----	↑	↑↓
Septet sideon	↑	↑	↑	↑	↑	↑	↑↓
Septet O_2-unbound	↑	↑	↑↓	↑	↑	↑	↑

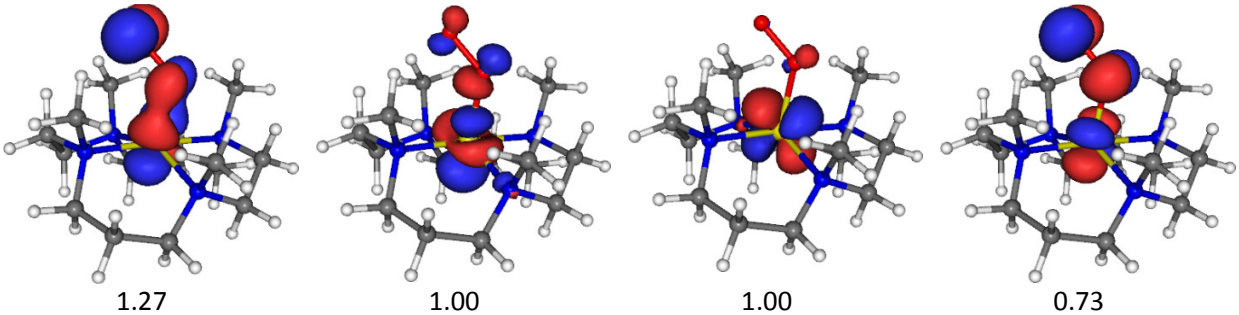
Table SV-2. Valence orbitals (natural orbitals and their occupation numbers)

Singlet



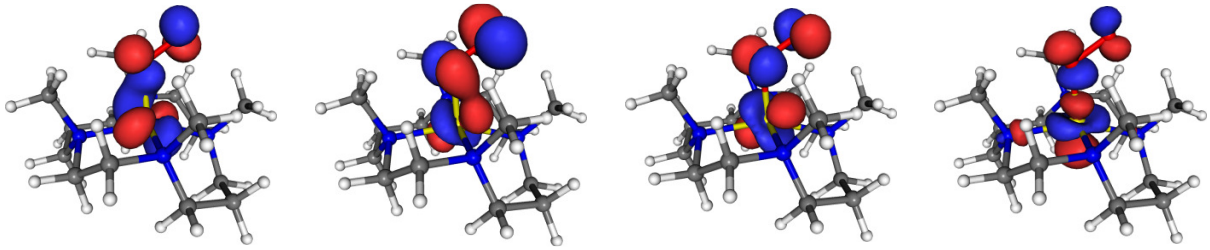
1.58 1.20 0.80 0.42

Triplet I



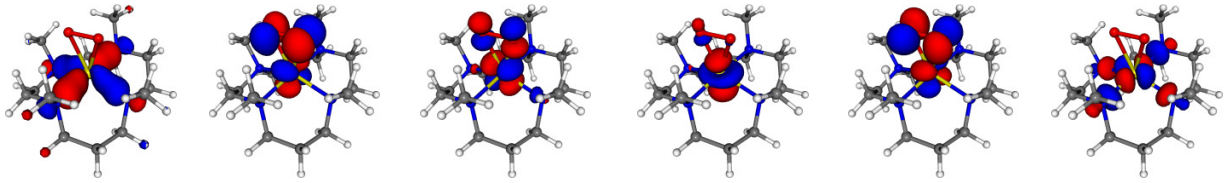
1.27 1.00 1.00 0.73

Triplet II



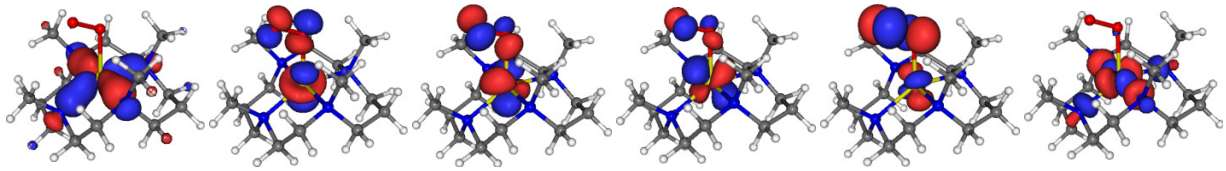
1.89 1.00 1.00 0.11

Triplet sideon



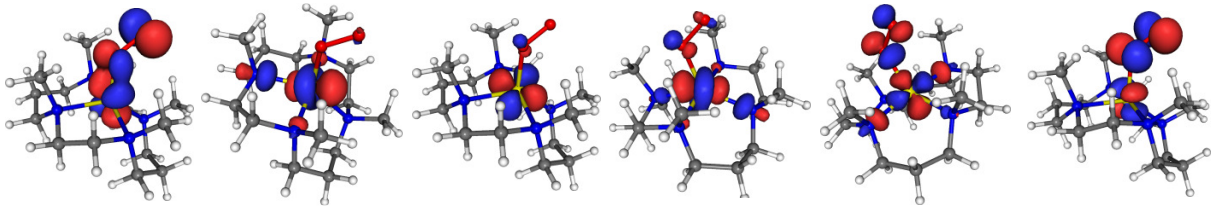
1.94 1.01 1.00 1.00 0.99 0.06

Quintet I



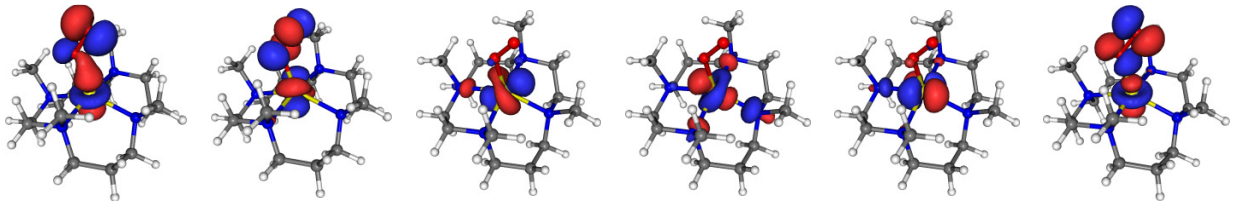
1.95 1.00 1.00 1.00 1.00 0.05

Quintet II



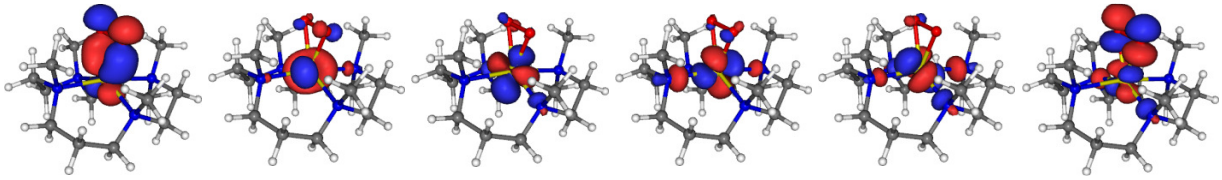
1.26 1.00 1.00 1.00 1.00 0.74

Quintet III



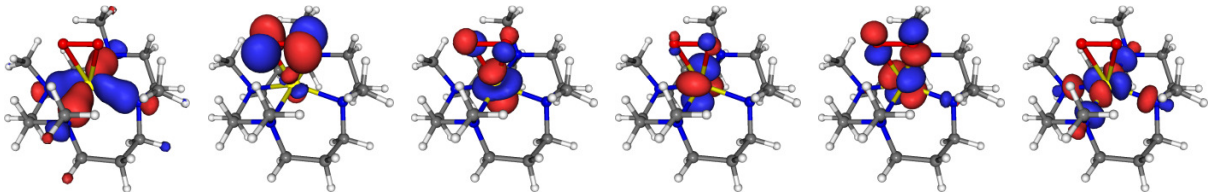
1.35 1.00 1.00 1.00 1.00 0.65

Quintet-sideon I



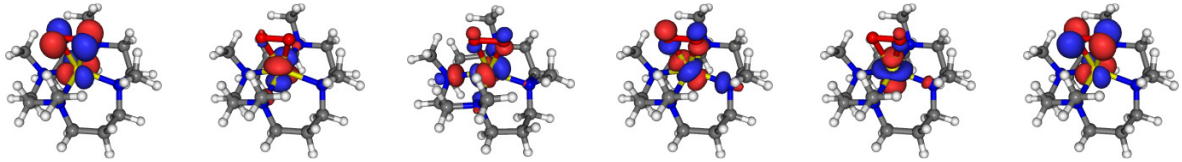
1.72 1.00 1.00 1.00 1.00 0.28

Quintet-sideon II



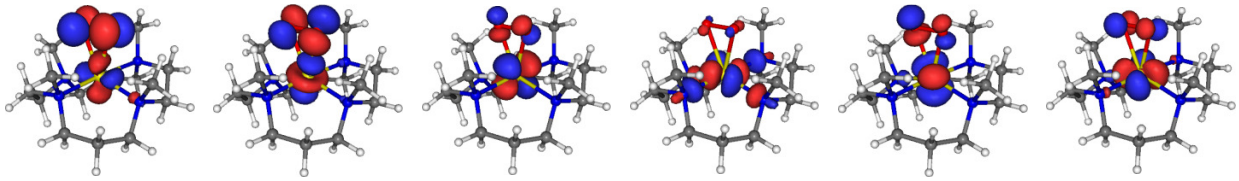
1.94 1.00 1.00 1.00 1.00 0.06

Quintet-sideon III



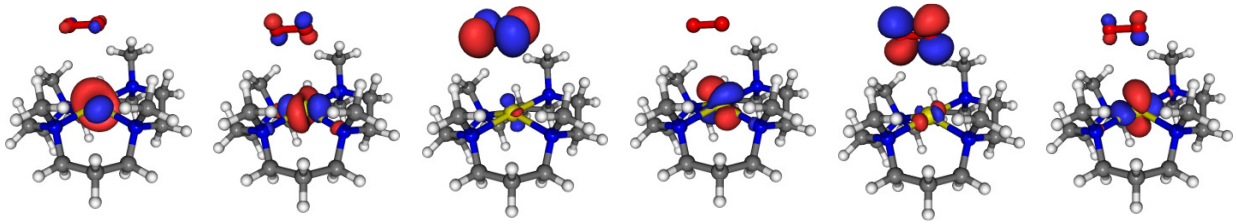
1.13 1.00 1.00 1.00 1.00 0.87

Septet O_2-bound



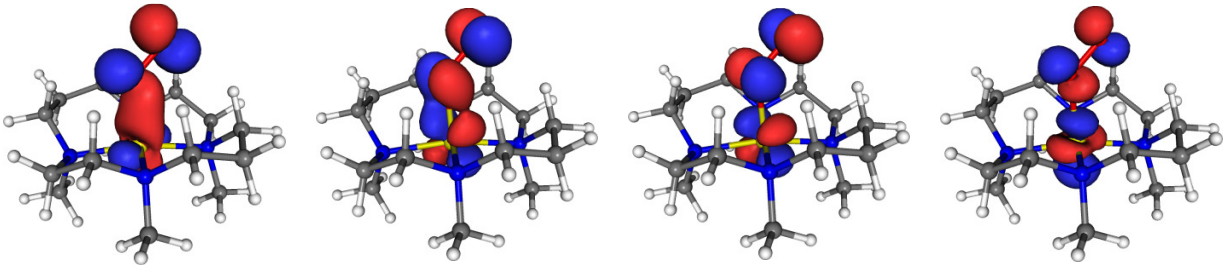
1.00 1.00 1.00 1.00 1.00 1.00

Septet O_2-unbound



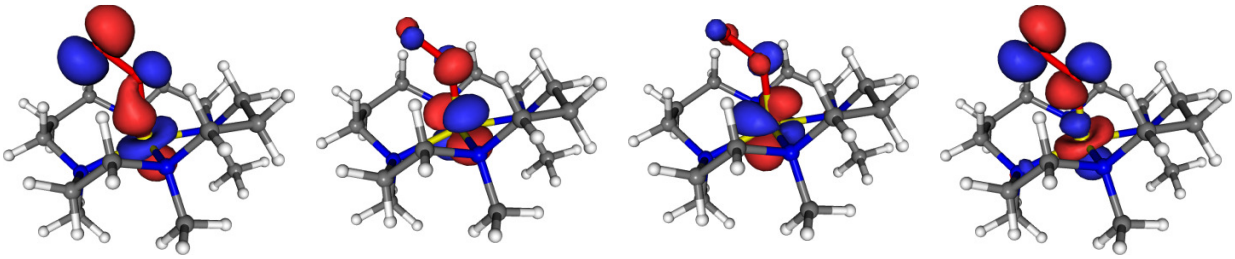
1.00 1.00 1.00 1.00 1.00 1.00

Singlet-inverted



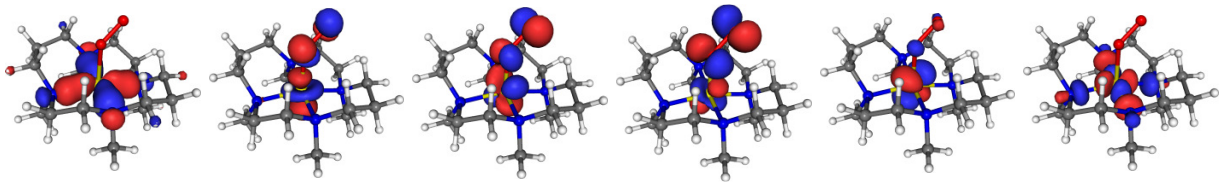
1.57 1.15 0.85 0.43

Triplet-inverted



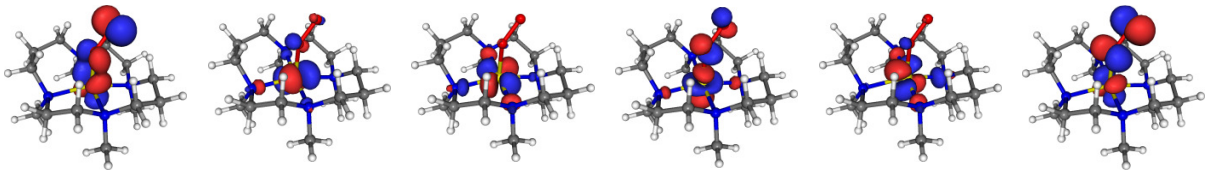
1.42 1.00 1.00 0.58

Quintet-inverted I



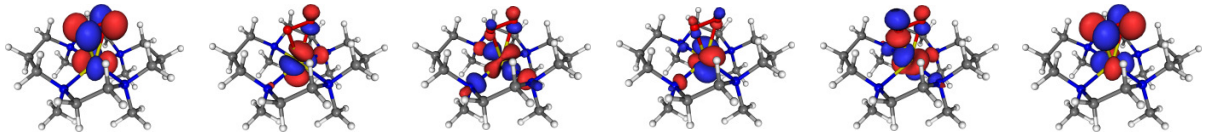
1.96 1.00 1.00 1.00 1.00 0.04

Quintet-inverted II



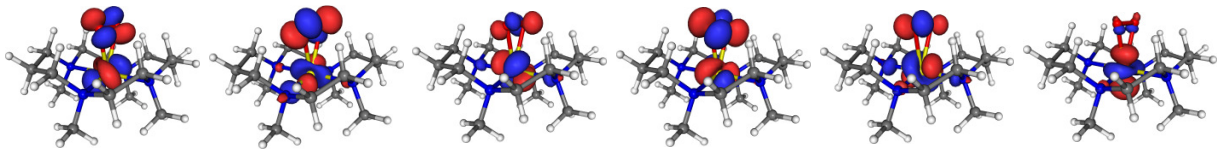
1.27 1.00 1.00 1.00 1.00 0.73

Quintet-inverted-sideon



1.10 1.00 1.00 1.00 1.00 0.90

Septet-inverted-sideon



1.00 1.00 1.00 1.00 1.00 1.00

Table SV-3. Relative energies (kcal/mol)

These energies are not used in the main text, but rather, the energies in Table SV-6 is used.

	Δlacvp	Δlacv3p^{*+}	**ΔE**[a]	ΔZ_0	$\Delta E_{thermal}$[b]	$-T\Delta S$[b]	Dispersion	**ΔG**[c]
Singlet	11.27	+6.00	**17.27**	+2.18	-0.92	+4.72	-4.59	**18.67**
Triplet I	12.02	+7.26	**19.28**	+1.76	-0.78	+3.64	-4.77	**19.14**
Triplet II	18.17	+7.33	**25.50**	+2.23	-0.98	+4.19	-5.49	**25.44**
Triplet sideon	14.63	+7.18	**21.81**	+2.58	-1.23	+5.05	-5.38	**22.84**
Quintet I	11.28	+7.22	**18.50**	+2.47	-1.10	+4.30	-4.27	**19.90**
Quintet II	12.15	+1.44	**13.59**	+0.63	-0.49	+2.38	-2.12	**14.00**
Quintet III	12.18	+1.37	**13.54**	+0.67	-0.57	+2.70	-2.06	**14.28**
Quintet sideon I	20.90	+0.87	**21.76**	+0.82	-0.63	+3.25	-4.28	**20.93**
Quintet sideon II	9.76	+7.14	**16.91**	+2.04	-1.00	+4.25	-5.35	**16.84**
Quintet sideon III	12.43	+1.82	**14.24**	+0.94	-0.67	+3.38	-3.63	**14.26**
Septet O_2-bound	7.34	+2.24	**9.58**	+0.97	-0.69	+3.22	-3.53	**9.54**
Septet O_2-unbound	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Singlet-inverted[d]	13.63	+7.52	**21.15**	+2.27	-0.90	+4.68	-6.23	**20.96**
Triplet-inverted[d]	15.85	+9.11	**24.96**	+2.51	-1.09	+4.38	-6.45	**24.31**
Quintet-inverted I[d]	12.67	+9.32	**21.99**	+2.26	-0.97	+4.08	-6.35	**21.01**
Quintet-inverted II[d]	18.60	+4.03	**22.63**	+0.67	-0.54	+2.91	-4.62	**21.06**
Quintet-inv-sideon[d]	22.69	+3.55	**26.24**	+0.82	-0.55	+2.78	-4.60	**24.69**
Septet-inv-sideon[d]	17.39	+3.67	**21.06**	+0.97	-0.66	+3.10	-4.50	**19.97**

[a] Sum of the previous two columns. [b] T=298.15 K. [c] ΔG=Sum of the previous five columns. [d] The four ligand methyl groups are pointing in the opposite direction as the Fe-O vector.

Table SV-4. Mulliken spin density distribution

	Fe	O_{inner}	O_{outer}	4 x ligated N	Rest
Singlet	1.76	-0.80	-0.91	-0.10	0.05
Triplet I	3.15	-0.18	-0.59	-0.41	0.04
Triplet II	1.40	0.17	0.58	-0.17	0.01
Triplet sideon	3.18	-0.36	-0.38	-0.44	0.01
Quintet I	3.04	0.56	0.80	-0.42	0.02
Quintet II	4.28	-0.09	-0.54	0.23	0.12
Quintet III	4.08	0.01	-0.46	0.27	0.10
Quintet sideon I	4.11	-0.27	-0.26	0.35	0.07
Quintet sideon II	3.12	0.67	0.67	-0.42	-0.04
Quintet sideon III	4.27	-0.32	-0.32	0.27	0.10
Septet O_2-bound	4.23	0.73	0.73	0.22	0.08
Septet O_2-unbound	3.73	1.00	1.00	0.07	0.20
Singlet-inverted[a]	1.78	-0.80	-0.90	-0.13	0.05
Triplet-inverted[a]	2.95	-0.10	-0.55	-0.30	0.00
Quintet-inverted I[a]	3.19	0.60	0.75	-0.50	-0.04
Quintet-inverted II[a]	4.25	-0.10	-0.55	0.29	0.11
Quintet-inv-sideon[a]	4.18	-0.33	-0.31	0.38	0.08
Septet-inv-sideon[a]	4.16	0.74	0.74	0.24	0.13

[a] The four ligand methyl groups are pointing in the opposite direction as the Fe-O vector.

Table SV-5. Geometries (Å and °)

	D(Fe-O)	D(O-O)	D(Fe-N_{eq1})	D(Fe-N_{eq2})	D(Fe-N_{eq3})	D(Fe-N_{eq4})	A(Fe-O-O)
Singlet	2.07	1.28	2.10	2.13	2.12	2.10	125.73
Triplet I	1.97	1.36	2.12	2.14	2.12	2.13	123.57
Triplet II	1.91	1.34	2.11	2.10	2.12	2.09	114.68
Triplet sideon	2.17	1.38	2.14	2.14	2.12	2.15	71.96
Quintet I	2.13	1.34	2.12	2.12	2.13	2.15	113.24
Quintet II	2.02	1.34	2.20	2.23	2.25	2.22	119.29
Quintet III	1.95	1.32	2.22	2.23	2.25	2.19	131.69
Quintet sideon I	2.00	1.41	2.19	2.24	2.22	2.19	69.13
Quintet sideon II	2.16	1.37	2.14	2.14	2.12	2.14	71.78
Quintet sideon III	2.15	1.37	2.19	2.23	2.20	2.20	71.66
Septet O_2-bound	2.18	1.35	2.20	2.23	2.20	2.20	72.10
Septet O_2-unbound	3.61	1.25	2.19	2.22	2.24	2.19	79.59
Singlet-inverted[a]	2.14	1.29	2.08	2.08	2.09	2.08	127.62
Triplet-inverted[a]	1.93	1.36	2.09	2.10	2.12	2.08	134.47
Quintet-inverted I[a]	2.15	1.34	2.07	2.09	2.11	2.07	128.45
Quintet-inverted II[a]	2.00	1.34	2.17	2.16	2.17	2.18	135.41
Quintet-inv-sideon[a]	2.20	1.36	2.16	2.18	2.21	2.15	70.36
Septet-inv-sideon[a]	2.23	1.34	2.16	2.18	2.20	2.16	72.08

[a] The four ligand methyl groups are pointing in the opposite direction as the Fe-O vector.

Reactivity with 1,4-cyclohexadiene

Table SV-6. Relative energies (kcal/mol)

	Δlacvp	Δlacv3p^{*+}	**ΔE**^{a}	ΔZ_0	$\Delta E_{Thermal}$ ^{b}	$-T\Delta S^{b}$	Δ_{Disp}	**ΔG**^{c}
Singlet								
Reactants, complexed	10.98	+6.28	**17.26**	+2.43	-1.04	+6.16	-6.05	**18.75**
Transition state	21.78	+13.42	**35.20**	-1.55	-1.62	+8.52	-7.23	**33.30**
Intermediate	9.08	+10.70	**19.78**	+2.54	-1.68	+8.49	-7.99	**21.14**
Triplet								
Reactants, complexed, TI	11.32	+7.65	**18.98**	+2.54	-1.15	+5.41	-6.04	**19.74**
Transition state, TI	17.94	+12.30	**30.24**	-0.43	-1.93	+8.72	-8.00	**28.60**
Intermediate, TI	3.74	+9.47	**13.21**	+1.37	-1.23	+6.40	-7.18	**12.57**
Quintet								
Reactants, complexed, QI	10.86	+7.93	**18.79**	+2.48	-1.08	+4.63	-5.50	**19.31**
Transition state, QI	19.58	+12.47	**32.05**	-0.67	-1.88	+8.24	-7.82	**29.91**
Intermediate, QI	-14.87	+10.46	**-4.41**	+0.04	-0.60	+5.05	-3.74	**-3.67**
Reactants, complexed, QII	11.59	+1.61	**13.19**	+1.54	-0.98	+4.36	-2.12	**15.99**
Reactants, complexed, QIII	11.69	+4.02	**15.72**	-0.07	-0.88	+5.65	-4.00	**16.41**
Transition state, QIII	12.24	+7.64	**19.88**	-1.94	-1.53	+7.37	-4.66	**19.12**
Intermediate, QIII	-13.00	+9.47	**-3.53**	+0.48	-0.71	+5.01	-4.11	**-2.86**
Reactants, complexed, QSIII	12.23	+1.41	**13.64**	+1.48	-0.95	+4.55	-3.18	**15.54**
Transition state, QSIII	**14.14**	**+5.56**	**19.70**	**-0.06**	**-1.61**	**+7.96**	**-6.38**	**19.59**
Intermediate, QSIII	-15.84	+10.70	**-5.14**	+0.32	-0.66	+4.95	-4.64	**-5.17**
Septet								
Reactants, comp, O_2-bound	7.04	+2.12	**9.16**	+1.67	-1.01	+4.83	-4.42	**10.24**
Transition state, O_2-bound	14.02	+8.32	**22.34**	-1.63	-1.75	+7.91	-6.56	**20.31**
Intermediate, O_2-bound	1.30	+4.47	**5.77**	-0.01	-0.81	+4.38	-4.14	**5.19**
Reactants, comp, O_2-unb	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
Transition state, O_2-unb	15.74	+10.26	**26.00**	-2.86	-1.29	+6.13	-3.55	**24.43**
Intermediate, O_2-unb	0.48	+4.30	**4.78**	+0.34	-1.07	+5.47	-4.59	**4.93**
With 2x[CF_3SO_3]$^-$								
Reactants, complxd, Septet O_2-unb	**0.00**	**+0.00**	**0.00**	**+0.00**	**+0.00**	**+0.00**	**+0.00**	**0.00**
Reactants, complxd, Septet O_2-bound	6.28	+1.69	**7.97**	+0.85	-0.59	+2.44	-3.09	**7.59**
Reactants, complexed, QSIII	11.41	+1.21	**12.61**	+1.04	-1.30	+5.58	-3.85	**14.08**
Transition state, QSIII	15.04	+4.86	**19.90**	-0.67	-1.22	+4.61	-6.85	**15.76**
Intermediate, QSIII	-20.25	+11.15	**-9.10**	-0.50	-0.63	+3.58	-4.11	**-10.76**

[a] Sum of the previous two columns. [b] T=298.15 K. [c] ΔG= Sum of the previous five columns. This value is however deemed unreliable and is not used.

Table SV-7. Mulliken spin density distribution

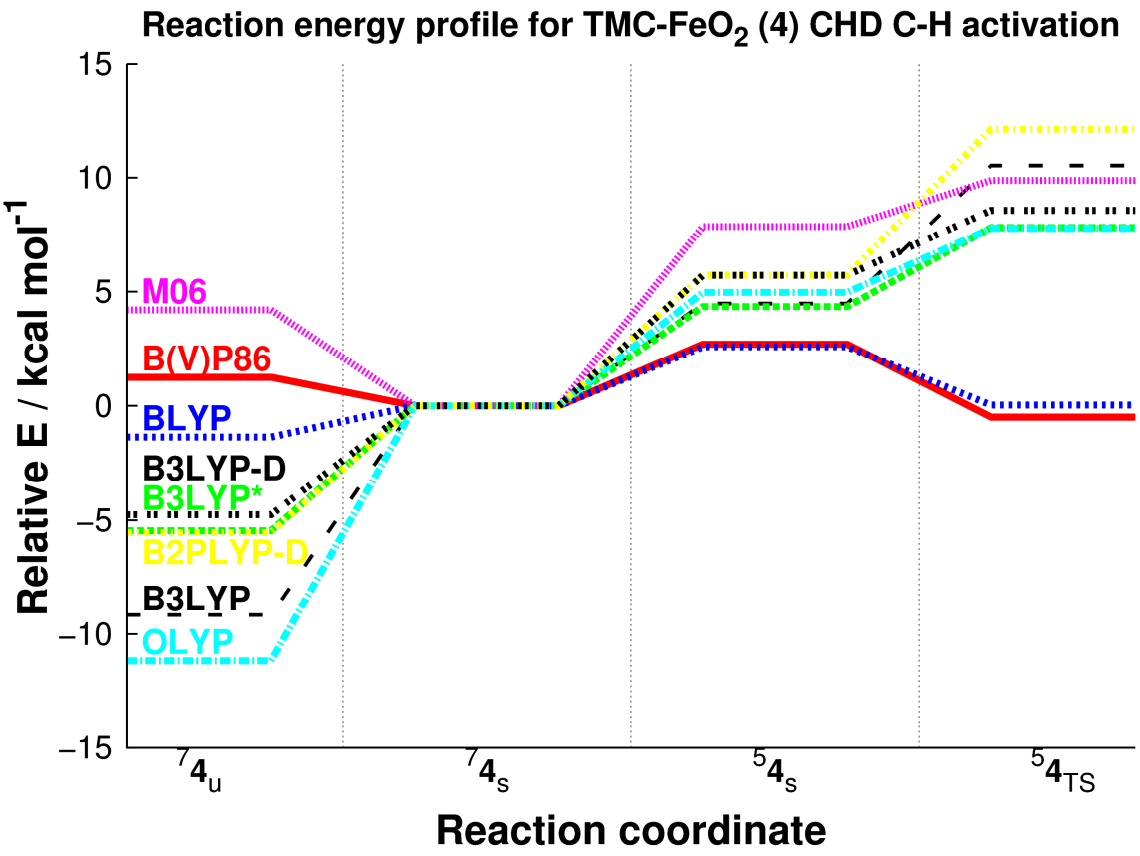
	Fe	O_{inner}	O_{outer}	4 x ligated N	Substrate	Rest
Singlet						
Reactants, complexed	1.65	-0.78	-0.90	-0.06	-0.01	0.09
Transition state	1.91	-0.55	-0.59	-0.10	-0.72	0.06
Intermediate	1.02	0.07	0.00	-0.11	-0.99	0.02
Triplet						
Reactants, complexed, TI	3.18	-0.19	-0.59	-0.43	0.00	0.03
Transition state, TI	2.90	0.20	-0.32	-0.34	-0.46	0.01
Intermediate, TI	3.00	0.27	0.04	-0.36	-0.98	0.02
Quintet						
Reactants, complexed, QI	3.08	0.60	0.76	-0.48	0.00	0.04
Transition state, QI	2.87	0.40	0.54	-0.31	0.49	0.01
Intermediate, QI	3.85	0.10	0.02	-0.04	0.00[a]	0.06
Reactants, complexed, QII	4.29	-0.09	-0.56	0.24	0.00	0.12
Reactants, complexed, QIII	4.06	0.10	-0.29	0.19	-0.16	0.09
Transition state, QIII	4.07	0.35	-0.09	0.14	-0.54	0.08
Intermediate, QIII	3.83	0.09	0.03	-0.03	0.01[a]	0.07
Reactants, complexed, QSIII	4.30	-0.32	-0.33	0.27	0.00	0.09
Transition state, QSIII	4.26	-0.04	-0.17	0.22	-0.33	0.07
Intermediate, QSIII	3.82	0.10	0.03	-0.02	0.00[a]	0.07
Septet						
Reactants, comp, O_2-bound	4.24	0.74	0.73	0.21	0.00	0.07
Transition state, O_2-bound	4.26	0.41	0.45	0.18	0.64	0.06
Intermediate, O_2-bound	4.22	0.35	0.09	0.26	0.99	0.10
Reactants, comp, O_2-unb	3.69	1.00	0.99	0.10	0.01	0.21
Transition state, O_2-unb	3.83	0.59	0.66	0.05	0.74	0.13
Intermediate, O_2-unb	4.21	0.36	0.11	0.24	0.99	0.09
With 2x$[CF_3SO_3]^-$						
Reactants, complxd, Septet O_2-unb	3.53	1.00	1.01	0.21	0.00	0.24
Reactants, complxd, Septet O_2-bound	4.36	0.72	0.73	0.13	0.00	0.06
Reactants, complexed, QSIII	4.38	-0.31	-0.34	0.19	0.00	0.08
Transition state, QSIII	4.28	-0.03	-0.21	0.19	-0.32	0.09
Intermediate, QSIII	3.88	0.13	0.03	-0.10	0.00[a]	0.06

[a] No spin on the substrate after the reaction indicate that a hydride, rather than a hydrogen atom, transfer has occurred. This could be self-interaction errors within DFT, or a real effect due to the specific substrate used. As the spin density distribution at the transition states are characteristic of hydrogen atom transfers, the state of the intermediates are immaterial for the barrier discussions.

Table SV-8. Geometries (Å and °)

	D_{Fe-O}	D_{O-O}	$D_{Fe-N(eq1)}$	$D_{Fe-N(eq2)}$	$D_{Fe-N(eq3)}$	$D_{Fe-N(eq4)}$	D_{O-H}	D_{H-C}	A_{O-O-H}
Singlet									
Reactants, complexed	2.05	1.29	2.10	2.13	2.12	2.10	2.76	1.10	116.05
Transition state	2.10	1.37	2.13	2.12	2.11	2.12	1.27	1.37	108.57
Intermediate	1.78	1.50	2.10	2.12	2.10	2.11	1.00	2.15	101.36
Triplet									
Reactants, complexed, TI	1.96	1.36	2.14	2.14	2.12	2.11	2.69	1.10	93.43
Transition state, TI	1.88	1.43	2.13	2.12	2.12	2.14	1.42	1.23	104.96
Intermediate, TI	1.89	1.50	2.13	2.12	2.12	2.15	1.00	2.12	101.13
Quintet									
Reactants, complexed, QI	2.10	1.34	2.10	2.13	2.12	2.10	2.68	1.10	97.15
Transition state, QI	1.91	1.41	2.14	2.12	2.11	2.14	1.44	1.22	103.47
Intermediate, QI	1.98	1.54	2.24	2.31	2.30	2.24	0.98	4.67	100.90
Reactants, complexed, QII	1.99	1.35	2.20	2.26	2.22	2.21	2.63	1.10	106.85
Reactants, complexed, QIII	2.00	1.33	2.22	2.24	2.25	2.19	1.87	1.13	107.04
Transition state, QIII	1.96	1.38	2.23	2.25	2.26	2.20	1.46	1.23	105.48
Intermediate, QIII	1.97	1.52	2.23	2.31	2.30	2.25	0.98	2.87	100.71
Reactants, complexed, QSIII	2.15	1.37	2.22	2.22	2.21	2.20	2.75	1.10	104.75
Transition state, QSIII	2.04	1.43	2.23	2.22	2.23	2.21	1.77	1.14	106.12
Intermediate, QSIII	1.99	1.54	2.25	2.29	2.29	2.25	0.98	3.68	101.37
Septet									
Reactants, comp, O_2-bound	2.17	1.35	2.21	2.21	2.21	2.21	3.11	1.10	73.48
Transition state, O_2-bound	1.96	1.47	2.23	2.24	2.25	2.25	1.41	1.26	108.44
Intermediate, O_2-bound	1.88	1.48	2.20	2.25	2.24	2.18	1.00	2.10	102.53
Reactants, comp, O_2-unb	3.57	1.26	2.19	2.23	2.23	2.18	2.77	1.10	91.23
Transition state, O_2-unb	2.23	1.36	2.23	2.21	2.22	2.23	1.28	1.36	105.89
Intermediate, O_2-unb	1.88	1.47	2.19	2.26	2.25	2.18	1.00	2.10	101.49
With 2x$[CF_3SO_3]^-$									
Reactants, cmpl, Septet O_2-unb	3.60	1.25	2.19	2.22	2.23	2.20	2.80	1.10	119.03
Reactants, cmpl, Septet O_2-bound	2.16	1.36	2.21	2.21	2.21	2.22	4.39	1.10	106.75
Reactants, complexed, QSIII	2.13	1.37	2.21	2.22	2.21	2.20	3.38	1.10	112.39
Transition state, QSIII	2.02	1.43	2.22	2.22	2.24	2.22	1.77	1.14	111.85
Intermediate, QSIII	1.94	1.53	2.24	2.32	2.33	2.25	0.99	4.99	99.30

Figure S1. Functional dependence on the CHD C-H activation by 4.



Coordinates

The coordinates are in xyz-file format, with a comment field in the second line, with charge/multiplicity in parenthesis.

[(N4Py)FeO]$^{2+}$ (1)

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C 6.72510 1.85406 5.48665
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C 7.27012 1.89743 8.02254
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C 6.74266 1.93777 5.48832
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FeO + CHD Reactant (2/3)
Fe 6.13239 4.06953 4.65836
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O 6.92110 5.52522 4.60961
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C 7.11731 3.91529 8.83311
C 7.07553 2.53447 9.04788
C 6.78323 1.67438 7.97867
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C 2.54311 6.34151 5.78867
C 1.63009 5.30135 6.00038
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65
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Fe 6.34876 4.06505 4.66101
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H 5.81588 0.41340 5.63827
H 8.00604 -0.68980 4.80759
H 10.11324 -0.40421 3.48393
H 10.71106 1.86670 2.61025
H 9.16147 3.78918 3.08318
H 5.15567 6.89978 5.10739
H 2.89376 7.81312 5.71886
H 1.04330 6.19082 6.21403
H 1.51201 3.74069 6.11163
H 3.63821 2.02451 0.90021
H 3.83602 3.92452 -0.70905
H 5.22241 5.92028 -0.08138
H 6.33758 5.94456 2.17179
H 3.15268 1.94575 5.19303
H 4.15032 2.25272 6.60461
H 3.95556 1.29667 3.36238
H 5.67657 1.11871 3.06248
H 8.06201 7.67063 5.55827
C 8.61143 8.25911 6.31201
C 7.96349 8.08240 7.66525
C 8.61302 7.62042 8.74553
C 10.07182 7.22637 8.73748
C 10.71834 7.39862 7.38271
C 10.06887 7.86131 6.30427
H 8.50584 9.30632 5.98071
H 6.91315 8.35854 7.74178
H 8.08788 7.52358 9.69418
H 10.62110 7.81480 9.49222
H 10.17999 6.18194 9.07547
H 11.77042 7.12943 7.30892
H 10.59639 7.96712 5.35790

65
FeO + CHD TS (2/5)
Fe 6.36017 4.18402 4.87789
N 5.20713 2.33427 4.79944
N 6.65995 3.37869 6.85107
N 7.86177 2.71970 4.34720
N 4.44697 4.90682 5.44399
N 5.72420 4.24453 2.87050
O 7.23549 5.62671 4.95025
C 6.97860 4.05216 7.97702
C 7.10970 3.38650 9.19844
C 6.90348 2.00402 9.24448
C 6.57630 1.31166 8.06921
C 6.46383 2.03291 6.88435
C 6.19381 1.42495 5.51428
C 7.50042 1.46657 4.73336
C 8.30848 0.36328 4.47417
C 9.52177 0.56720 3.80069
C 9.88679 1.85956 3.40951
C 9.02813 2.92319 3.69757
C 4.14429 6.22499 5.54345
C 2.84302 6.65242 5.79366
C 1.83244 5.69244 5.93264
C 2.15249 4.33536 5.82740
C 3.47872 3.96551 5.58885
C 3.91546 2.51960 5.55228
C 4.98082 1.95956 3.35733
C 5.03269 3.15804 2.43757
C 4.45611 3.14135 1.16485
C 4.61273 4.25261 0.33072
C 5.33877 5.36073 0.78595
C 5.87926 5.32718 2.06841
H 7.13130 5.12027 7.88083
H 7.36734 3.94397 10.08969
H 6.99538 1.46723 10.18104
H 6.41242 0.24128 8.07724
H 5.81513 0.40295 5.59987
H 8.00076 -0.62684 4.78695
H 10.16947 -0.27394 3.58478
H 10.81769 2.04523 2.88952
H 9.25685 3.94282 3.41695
H 4.96800 6.91378 5.41273
H 2.62705 7.71026 5.87028
H 0.80887 5.99630 6.11738
H 1.38841 3.57430 5.93034
H 3.89818 2.27313 0.83564
H 4.17222 4.25471 -0.65923
H 5.47796 6.23543 0.16384
H 6.43905 6.15237 2.48768
H 3.13329 1.89158 5.11616
H 4.05848 2.17238 6.58041
H 4.02670 1.43541 3.25141
H 5.76023 1.25400 3.05334
H 8.05771 6.97295 5.42431
C 8.59415 7.86021 5.92575
C 8.04831 7.98370 7.31054
C 8.78124 7.72137 8.41209
C 10.23293 7.32572 8.35518
C 10.80666 7.35199 6.96331
C 10.06545 7.61284 5.86808
H 8.28976 8.70136 5.28427
H 7.00789 8.28487 7.40870
H 8.33586 7.81609 9.39970
H 10.82408 7.98303 9.01551
H 10.36574 6.32182 8.79734
H 11.87412 7.16727 6.86899
H 10.53382 7.63432 4.88688

65
FeO+CHD Intermediate (2/5)
Fe 6.50284 4.19892 4.86463
N 5.22400 2.32366 4.81271
N 6.73861 3.33371 6.85046
N 7.90007 2.61860 4.32894
N 4.57791 4.94513 5.44858
N 5.78622 4.21097 2.85430
O 7.50762 5.67568 4.92036
C 7.07872 3.99440 7.97916
C 7.18648 3.32507 9.20039
C 6.93274 1.95030 9.24540
C 6.57969 1.27219 8.06983
C 6.49268 1.99767 6.88467
C 6.18824 1.39520 5.51886
C 7.48893 1.38544 4.72567
C 8.24737 0.24698 4.46577
C 9.46138 0.39312 3.77939
C 9.87768 1.66619 3.37594
C 9.06841 2.76679 3.66628
C 4.31800 6.27386 5.54500
C 3.03623 6.74662 5.81167
C 1.99667 5.82133 5.97122
C 2.27145 4.45480 5.86793
C 3.58159 4.03892 5.61206
C 3.95761 2.57413 5.57633
C 4.96971 1.95713 3.38008
C 5.04036 3.15085 2.45302
C 4.42211 3.14698 1.19926
C 4.59384 4.24407 0.34992
C 5.37763 5.32604 0.77129
C 5.95730 5.28023 2.03612
H 7.26232 5.05751 7.88517
H 7.46195 3.87317 10.09214
H 7.00607 1.40979 10.18150
H 6.37564 0.20865 8.07689
H 5.78515 0.38325 5.61855
H 7.90006 -0.72685 4.78819
H 10.06985 -0.47671 3.56287
H 10.81023 1.80884 2.84539
H 9.33872 3.77429 3.37864
H 5.16010 6.93638 5.39767
H 2.85710 7.81157 5.88496
H 0.98647 6.15944 6.16973
H 1.48467 3.71937 5.98538
H 3.82050 2.29843 0.89639
H 4.12109 4.25584 -0.62506
H 5.53071 6.18985 0.13725
H 6.56225 6.08671 2.42884
H 3.13800 1.98293 5.15580
H 4.09303 2.22765 6.60602
H 4.00068 1.45770 3.28301
H 5.72578 1.23155 3.06338
H 7.92774 6.49667 5.25003
C 8.55596 8.41224 6.07096
C 7.91149 8.22312 7.33082
C 8.57557 7.66946 8.39644
C 10.01640 7.23971 8.30481
C 10.63298 7.48149 6.95241
C 9.92462 8.03899 5.91738
H 8.02954 8.90207 5.25814
H 6.87578 8.53175 7.44246
H 8.07361 7.54241 9.35160
H 10.61203 7.74956 9.08687
H 10.11160 6.17087 8.57799
H 11.67497 7.20512 6.81936
H 10.41089 8.20722 4.96049

75
FeO+CHD+counterions React(0/3)
Fe 6.26457 3.85591 4.74299
N 5.16152 2.11928 4.76875
N 6.53674 3.37768 6.65357
N 7.73617 2.58082 4.33699
N 4.53653 4.70398 5.17847
N 5.76640 3.89863 2.83746
O 7.16399 5.24433 4.74634
C 6.82182 4.21197 7.67500
C 6.96040 3.71811 8.97455
C 6.79651 2.34929 9.20898
C 6.50419 1.49143 8.13805
C 6.38407 2.04046 6.86689
C 6.15186 1.27904 5.57109
C 7.45957 1.32795 4.79708
C 8.34126 0.27218 4.60091
C 9.53867 0.52436 3.91417
C 9.81131 1.81475 3.45076
C 8.88390 2.83672 3.67393
C 4.33039 6.04407 5.18210
C 3.07158 6.57932 5.44520
C 2.00462 5.70946 5.69813
C 2.22632 4.32892 5.69070
C 3.51066 3.84699 5.43455
C 3.85631 2.37914 5.48098
C 4.95972 1.65124 3.34804
C 5.09883 2.80337 2.38275
C 4.63290 2.74880 1.06827
C 4.87755 3.82704 0.21221
C 5.58387 4.93648 0.69027
C 6.01407 4.94749 2.01502
H 6.94630 5.25955 7.43328
H 7.19329 4.40001 9.78188
H 6.89465 1.94949 10.21087
H 6.37329 0.42762 8.29002
H 5.79860 0.25976 5.73740
H 8.10177 -0.71726 4.96953
H 10.24488 -0.27944 3.74511
H 10.72848 2.03664 2.92081
H 9.04733 3.85266 3.33533
H 5.18504 6.67130 4.97235
H 2.94424 7.65504 5.44343
H 1.01306 6.09890 5.89635
H 1.41930 3.63246 5.88279
H 4.09459 1.87416 0.72435
H 4.52388 3.79940 -0.81146
H 5.80181 5.78406 0.05378
H 6.57146 5.77365 2.43431
H 3.06117 1.77306 5.04003
H 3.95285 2.06134 6.52364
H 3.98577 1.16617 3.24728
H 5.71469 0.89414 3.11491
H 8.44499 7.58906 5.08909
C 8.95366 8.13560 5.89871
C 8.07663 8.15214 7.12854
C 8.47338 7.70061 8.32888
C 9.84623 7.12544 8.59337
C 10.70822 7.07221 7.35304
C 10.31092 7.52395 6.15415
H 9.07189 9.16236 5.51124
H 7.07602 8.56037 7.00043
H 7.79402 7.74808 9.17848
H 10.35360 7.71396 9.37738
H 9.75287 6.11628 9.02887
H 11.70176 6.64288 7.46994
H 10.98285 7.45840 5.30004
Cl 4.46897 10.32576 4.66448
O 5.38901 9.11635 4.81476
O 4.21920 10.59296 3.18774
O 3.14113 10.03981 5.36102
O 5.12256 11.54124 5.30256
Cl 9.67019 6.70248 1.39666
O 10.73395 7.78274 1.29869
O 9.52185 6.00508 0.05275
O 10.08363 5.68224 2.45507
O 8.33822 7.33397 1.79220

75
FeO+CHD+counterions TS (0/3)
Fe 6.24550 4.08406 4.83126
N 5.35075 2.24143 4.81894
N 6.54682 3.61976 6.74434
N 7.86656 2.99666 4.42703
N 4.41808 4.73605 5.22888
N 5.75123 4.10814 2.91524
O 6.93702 5.68623 4.82538
C 6.67312 4.45995 7.79239
C 6.80868 3.96415 9.09149
C 6.80887 2.58142 9.29971
C 6.67236 1.71553 8.20455
C 6.54218 2.27095 6.93672
C 6.42175 1.50865 5.62772
C 7.72403 1.71532 4.86997
C 8.70542 0.75486 4.65227
C 9.86418 1.13197 3.95766
C 9.99630 2.44618 3.49932
C 8.97200 3.36567 3.74374
C 4.05674 6.04130 5.22275
C 2.73139 6.42375 5.42391
C 1.76332 5.43367 5.62734
C 2.14702 4.08823 5.63516
C 3.49056 3.76374 5.43993
C 4.01246 2.34809 5.50966
C 5.22244 1.77371 3.38981
C 5.21821 2.94980 2.44166
C 4.75753 2.86026 1.12699
C 4.86745 3.97488 0.28923
C 5.43482 5.15366 0.78649
C 5.86559 5.19248 2.11137
H 6.66587 5.51736 7.56745
H 6.91097 4.65337 9.91958
H 6.90831 2.17783 10.30003
H 6.66013 0.64096 8.33581
H 6.18858 0.45231 5.77744
H 8.56799 -0.25901 5.00673
H 10.64548 0.40487 3.77207
H 10.87626 2.76211 2.95403
H 9.01955 4.38891 3.39289
H 4.84954 6.75786 5.05614
H 2.47724 7.47653 5.40699
H 0.72392 5.70240 5.77538
H 1.41891 3.30142 5.79131
H 4.32653 1.93344 0.76838
H 4.51622 3.92234 -0.73445
H 5.54419 6.03241 0.16430
H 6.31710 6.06952 2.55448
H 3.30355 1.64225 5.06962
H 4.13588 2.06022 6.55814
H 4.32206 1.16581 3.27059
H 6.07317 1.12713 3.15395
H 8.16362 6.01907 5.38169
C 9.22833 6.55250 5.74461
C 8.82050 7.82564 6.38253
C 8.97837 8.06177 7.70319
C 9.63012 7.07620 8.63728
C 10.15212 5.84774 7.94029
C 9.97980 5.62547 6.61868
H 9.66227 6.67351 4.74379
H 8.35653 8.57596 5.74715
H 8.65052 9.00517 8.13311
H 10.44961 7.56860 9.18907
H 8.91925 6.78531 9.43204
H 10.70912 5.13694 8.54602
H 10.40127 4.73339 6.16176
Cl 4.36960 10.12192 4.45281
O 5.22170 9.16090 5.27807
O 4.59149 9.85226 2.97155
O 2.89787 9.91149 4.79482
O 4.76397 11.55435 4.77647
Cl 9.30628 7.25427 1.29416
O 10.34630 8.35091 1.13405
O 9.00051 6.63631 -0.06169
O 9.85265 6.17558 2.23081
O 8.03030 7.84213 1.88604

75
FeO+CHD+counterions Int (0/3)
Fe 6.17455 4.00290 4.78361
N 5.25602 2.19460 4.77353
N 6.47363 3.56016 6.70018
N 7.79125 2.89717 4.42405
N 4.36561 4.70219 5.15853
N 5.68954 4.04583 2.87003
O 6.93659 5.64533 4.75618
C 6.63837 4.40658 7.73839
C 6.77185 3.91895 9.04070
C 6.72349 2.53905 9.26312
C 6.54794 1.66715 8.17824
C 6.42820 2.21340 6.90555
C 6.29928 1.44162 5.60161
C 7.61672 1.61758 4.86238
C 8.58812 0.64251 4.67064
C 9.77233 1.00391 4.01034
C 9.94133 2.31858 3.56654
C 8.92522 3.25401 3.78325
C 4.04234 6.01623 5.14964
C 2.72556 6.43289 5.34077
C 1.73047 5.46782 5.53460
C 2.07755 4.11201 5.54709
C 3.41366 3.75335 5.36415
C 3.90697 2.32812 5.44509
C 5.13718 1.72087 3.34231
C 5.14188 2.89627 2.39318
C 4.67685 2.81929 1.07976
C 4.79720 3.93948 0.24999
C 5.37798 5.10953 0.75273
C 5.81426 5.13486 2.07647
H 6.66776 5.46272 7.50626
H 6.90896 4.61270 9.85991
H 6.81818 2.14219 10.26654
H 6.50256 0.59493 8.32080
H 6.03831 0.39279 5.75527
H 8.42659 -0.36911 5.02127
H 10.54693 0.26492 3.84468
H 10.84466 2.62490 3.05518
H 9.01027 4.28169 3.45236
H 4.86091 6.70529 4.99449
H 2.49846 7.49179 5.32567
H 0.69729 5.76384 5.67394
H 1.32735 3.34539 5.69882
H 4.23400 1.90029 0.71569
H 4.44224 3.89796 -0.77290
H 5.49180 5.99076 0.13477
H 6.27501 5.99935 2.53493
H 3.19432 1.63270 4.99545
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H 4.01214 2.04072 6.49567
H 4.23737 1.11319 3.22078
H 5.99024 1.07378 3.11719
H 7.79292 5.75964 5.22287
C 9.46617 7.38880 5.78094
C 8.55695 7.98595 6.70338
C 8.71931 7.84504 8.05955
C 9.86482 7.06539 8.65290
C 10.77764 6.45900 7.61807
C 10.56755 6.62990 6.27240
H 9.33337 7.52373 4.71319
H 7.71711 8.55892 6.31858
H 8.01954 8.31000 8.74890
H 10.44762 7.71279 9.33800
H 9.47829 6.27559 9.32631
H 11.62431 5.87871 7.97477
H 11.25289 6.18179 5.55784
Cl 4.47544 10.13963 4.68893
O 5.15289 9.13950 5.62409
O 4.93961 9.89233 3.26081
O 2.96315 9.96113 4.77235
O 4.84176 11.55462 5.10858
Cl 9.59796 6.93456 1.41954
O 10.71862 7.84601 0.94350
O 9.10439 6.08130 0.26004
O 10.12599 6.02381 2.52883
O 8.44773 7.77696 1.95802

75
FeO+CHD+counterions React(0/5)
Fe 6.33037 4.10438 4.77539
N 5.22401 2.34531 4.84062
N 6.71896 3.45629 6.77865
N 7.82554 2.68344 4.27120
N 4.51506 4.93356 5.36685
N 5.61000 4.14068 2.81481
O 7.21872 5.49233 4.74198
C 7.07410 4.19393 7.85224
C 7.26126 3.59434 9.10077
C 7.07283 2.21475 9.22997
C 6.70625 1.45588 8.10826
C 6.53917 2.11214 6.89360
C 6.22319 1.44217 5.56522
C 7.49980 1.44654 4.73827
C 8.31900 0.34562 4.51504
C 9.50704 0.53572 3.79249
C 9.83420 1.81071 3.32144
C 8.96653 2.87728 3.57472
C 4.24698 6.26250 5.38833
C 2.97094 6.73135 5.69171
C 1.95518 5.80597 5.96339
C 2.24042 4.43684 5.92713
C 3.53999 4.02309 5.62905
C 3.95287 2.57217 5.63600
C 4.93351 1.87966 3.42751
C 4.89621 3.03754 2.46205
C 4.22609 2.98128 1.23948
C 4.30591 4.07617 0.37106
C 5.04752 5.20272 0.74550
C 5.68883 5.20792 1.98279
H 7.21033 5.25697 7.69909
H 7.54792 4.20186 9.94912
H 7.20824 1.73068 10.18944
H 6.55510 0.38616 8.17979
H 5.82454 0.43385 5.69827
H 8.04106 -0.63047 4.89126
H 10.16399 -0.30384 3.60148
H 10.74591 1.98420 2.76383
H 9.17294 3.88206 3.23238
H 5.06447 6.92487 5.13673
H 2.77953 7.79689 5.70348
H 0.95215 6.14466 6.19335
H 1.46906 3.70274 6.12565
H 3.65356 2.10078 0.97481
H 3.78972 4.05054 -0.58124
H 5.12345 6.07323 0.10776
H 6.25939 6.05744 2.32920
H 3.15511 1.93705 5.24287
H 4.12985 2.25545 6.66841
H 3.99688 1.31671 3.40804
H 5.72599 1.18989 3.12392
H 8.11464 7.66128 5.86630
C 8.80938 8.11516 6.59157
C 8.24278 8.00106 7.98716
C 8.89296 7.41899 9.00734
C 10.27066 6.81062 8.88110
C 10.81966 6.89046 7.47529
C 10.17018 7.47280 6.45621
H 8.86450 9.17746 6.29681
H 7.25526 8.43023 8.14913
H 8.43087 7.37746 9.99225
H 10.96267 7.30560 9.58432
H 10.24792 5.75982 9.21597
H 11.79877 6.44382 7.31036
H 10.61568 7.49056 5.46389
Cl 5.56380 9.24221 2.16756
O 5.86030 8.54695 3.49276
O 6.12174 8.40726 1.01805
O 4.05796 9.39198 2.00099
O 6.21788 10.61470 2.15935
Cl 10.17726 6.57678 2.03544
O 9.69862 7.86606 2.69174
O 11.19905 6.90369 0.95498
O 10.82374 5.67694 3.08525
O 8.99119 5.84824 1.41092

75
FeO+CHD+counterions TS (0/5)
Fe 6.30016 4.09569 5.03662
N 5.16078 2.25028 4.84297
N 6.61351 3.15505 6.95158
N 7.80284 2.69393 4.39560
N 4.40044 4.76190 5.69977
N 5.60443 4.31343 3.05868
O 7.17668 5.52262 5.22382
C 6.92656 3.75291 8.12072
C 7.07348 3.00578 9.29192
C 6.88843 1.62011 9.24065
C 6.56487 1.00714 8.02120
C 6.43596 1.80855 6.89031
C 6.16144 1.29884 5.48156
C 7.46035 1.41155 4.69496
C 8.27835 0.34044 4.34908
C 9.48353 0.60814 3.68219
C 9.82879 1.92955 3.38399
C 8.96069 2.96121 3.75267
C 4.09797 6.06606 5.91589
C 2.80300 6.46536 6.23557
C 1.79896 5.49240 6.32248
C 2.11881 4.15036 6.09549
C 3.43885 3.80749 5.79021
C 3.87417 2.37040 5.61735
C 4.92589 1.98036 3.37929
C 4.91835 3.25025 2.55998
C 4.29554 3.32375 1.31232
C 4.39839 4.50408 0.56814
C 5.11664 5.58705 1.08806
C 5.70597 5.46262 2.34498
H 7.05717 4.82721 8.09661
H 7.32639 3.50271 10.21959
H 6.99301 1.02037 10.13682
H 6.41514 -0.06334 7.95520
H 5.79256 0.26957 5.49473
H 7.98492 -0.67381 4.58999
H 10.13860 -0.20751 3.40023
H 10.75218 2.16810 2.87214
H 9.17948 3.99709 3.53374
H 4.91623 6.76693 5.81957
H 2.58680 7.51237 6.40472
H 0.78030 5.77537 6.56020
H 1.35996 3.37948 6.15527
H 3.74386 2.47201 0.93292
H 3.92149 4.57623 -0.40241
H 5.22374 6.51761 0.54595
H 6.26083 6.27189 2.79957
H 3.08767 1.78710 5.12991
H 4.02165 1.92945 6.60822
H 3.99113 1.42851 3.24407
H 5.72812 1.33273 3.01223
H 8.07570 6.85772 5.66587
C 8.66133 7.76810 6.04488
C 8.04439 8.20875 7.33217
C 8.68876 8.14773 8.51444
C 10.11060 7.66910 8.65045
C 10.75532 7.32894 7.33214
C 10.10237 7.39012 6.15461
H 8.48296 8.48852 5.23207
H 7.02298 8.58087 7.28991
H 8.19121 8.47343 9.42521
H 10.71179 8.43217 9.17491
H 10.15002 6.79512 9.32520
H 11.80366 7.03986 7.36019
H 10.61617 7.14168 5.22948
Cl 6.39931 9.54217 1.94513
O 6.58580 8.74388 3.23390
O 6.53874 8.60965 0.74552
O 5.01418 10.17312 1.93708
O 7.45699 10.63132 1.86670
Cl 10.37506 6.34895 1.95307
O 10.25293 7.78426 2.44811
O 11.18326 6.31992 0.66304
O 11.08266 5.50287 3.01012
O 8.98495 5.77486 1.69664

75
FeO+CHD+counterions Int (0/5)
Fe 6.12316 4.34462 4.78727
N 5.14078 2.29411 4.84755
N 6.54592 3.61764 6.79487
N 7.72618 2.98141 4.26850
N 4.10483 4.80698 5.39940
N 5.35389 4.15806 2.79511
O 6.82970 5.98334 4.77570
C 6.82175 4.36959 7.88332
C 7.05688 3.77788 9.12680
C 6.99987 2.38466 9.23719
C 6.71738 1.61130 8.10212
C 6.49745 2.26301 6.89135
C 6.25679 1.56085 5.56097
C 7.52247 1.71776 4.72735
C 8.44037 0.69961 4.48558
C 9.60049 1.00207 3.75690
C 9.80344 2.30515 3.29322
C 8.83881 3.28017 3.56126
C 3.63782 6.08099 5.44811
C 2.30241 6.35518 5.73156
C 1.42713 5.28572 5.95924
C 1.91434 3.97692 5.90398
C 3.26825 3.76361 5.62710
C 3.87112 2.37628 5.63902
C 4.91554 1.82901 3.43980
C 4.77962 2.97469 2.46058
C 4.14333 2.81098 1.22661
C 4.11716 3.87918 0.32532
C 4.72128 5.09192 0.67889
C 5.32813 5.20289 1.92782
H 6.86142 5.44121 7.73767
H 7.27867 4.39918 9.98489
H 7.17340 1.90279 10.19195
H 6.66908 0.53090 8.15885
H 6.02217 0.50333 5.71537
H 8.25607 -0.30192 4.85447
H 10.33104 0.22734 3.55638
H 10.68869 2.57725 2.73358
H 8.94679 4.29845 3.21258
H 4.35643 6.86525 5.24949
H 1.95748 7.38071 5.76533
H 0.38050 5.46840 6.17265
H 1.25857 3.13127 6.07367
H 3.68024 1.86303 0.97988
H 3.62919 3.76808 -0.63592
H 4.71666 5.93940 0.00543
H 5.79368 6.12226 2.25942
H 3.14499 1.64461 5.27033
H 4.08675 2.10336 6.67716
H 4.03314 1.18306 3.39086
H 5.76732 1.21338 3.13327
H 6.80331 6.96853 4.76105
C 9.43120 7.98918 6.23128
C 8.64066 8.11384 7.40938
C 9.04471 7.57471 8.60571
C 10.34506 6.82413 8.74531
C 11.12446 6.73225 7.45792
C 10.67083 7.29118 6.28872
H 9.08978 8.42578 5.30022
H 7.69783 8.65108 7.35013
H 8.43190 7.68637 9.49645
H 10.96878 7.29077 9.53362
H 10.15512 5.80894 9.14671
H 12.07363 6.20347 7.48412
H 11.26205 7.20185 5.38119
Cl 6.43142 9.45952 3.38299
O 6.32019 8.67993 4.71184
O 6.12309 8.51504 2.23094
O 5.42932 10.59516 3.40913
O 7.83958 10.00671 3.24453
Cl 10.68859 6.45574 1.87303
O 10.92874 7.79348 2.56020
O 11.31766 6.47107 0.48710
O 11.31558 5.33841 2.70104
O 9.18649 6.20955 1.74413
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[(N4Py)FeOO]$^{2+}$ (2)

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52
FeOO Singlet (2/1)
Fe 6.15249 4.39428 4.91064
N 5.51737 2.47566 4.83830
N 6.70302 3.87059 6.75245
N 7.86988 3.57949 4.31625
N 4.30755 4.79296 5.49622
N 5.47445 4.50048 3.05754
O 6.65335 6.17766 4.93884
C 6.84849 4.65566 7.84110
C 7.19480 4.10429 9.07669
C 7.38209 2.72284 9.18175
C 7.22473 1.91376 8.04668
C 6.88632 2.52243 6.84446
C 6.73830 1.83374 5.49818
C 7.93221 2.26177 4.66161
C 9.01813 1.46810 4.31349
C 10.06811 2.05559 3.59231
C 9.99550 3.40767 3.24407
C 8.87366 4.15112 3.61734
C 3.78000 6.03580 5.60762
C 2.44646 6.22189 5.96210
C 1.64239 5.09983 6.19318
C 2.19505 3.82117 6.07105
C 3.54104 3.69222 5.72682
C 4.24247 2.35809 5.64541
C 5.31901 2.08867 3.38877
C 5.05652 3.31137 2.54407
C 4.47068 3.24781 1.27936
C 4.33278 4.42215 0.53279
C 4.77995 5.63504 1.06929
C 5.34373 5.64377 2.34242
H 6.69128 5.71642 7.70866
H 7.31133 4.75166 9.93582
H 7.64422 2.27608 10.13296
H 7.35937 0.84099 8.09852
H 6.64534 0.74972 5.58265
H 9.04444 0.42281 4.59354
H 10.92722 1.46143 3.30583
H 10.79168 3.88601 2.68898
H 8.76884 5.19778 3.37020
H 4.44919 6.86093 5.40521
H 2.04958 7.22506 6.04657
H 0.59935 5.21732 6.46102
H 1.59497 2.93595 6.24145
H 4.13222 2.29589 0.88932
H 3.88056 4.39058 -0.45108
H 4.68778 6.56162 0.51793
H 5.69619 6.54974 2.81641
H 3.59410 1.59506 5.20891
H 4.49658 2.01852 6.65389
H 4.50578 1.36438 3.30380
H 6.22600 1.59088 3.03332
O 7.86107 6.50198 5.47777

52
FeOO Triplet (2/3)
Fe 6.13884 4.37302 4.90493
N 5.50661 2.45959 4.83288
N 6.65711 3.86788 6.75052
N 7.84116 3.57168 4.28190
N 4.31530 4.79176 5.51974
N 5.49554 4.49490 3.04737
O 6.60398 6.22702 4.90409
C 6.79044 4.66000 7.83547
C 7.14868 4.11747 9.07142
C 7.36329 2.73996 9.17690
C 7.22090 1.92407 8.04341
C 6.86811 2.52301 6.84153
C 6.72921 1.83017 5.49398
C 7.91993 2.26031 4.65015
C 9.01570 1.47692 4.31374
C 10.05711 2.06916 3.58197
C 9.96756 3.41464 3.21258
C 8.83660 4.14900 3.57592
C 3.79568 6.03728 5.64633
C 2.47178 6.22612 6.03085
C 1.66890 5.10476 6.27377
C 2.21212 3.82417 6.13196
C 3.54972 3.69017 5.75816
C 4.23308 2.34734 5.64110
C 5.31550 2.07727 3.38235
C 5.08646 3.30294 2.52926
C 4.52674 3.23899 1.25283
C 4.40429 4.41287 0.50294
C 4.83851 5.62802 1.04691
C 5.37599 5.63913 2.33042
H 6.61448 5.71667 7.69544
H 7.25441 4.76736 9.92992
H 7.63666 2.30000 10.12815
H 7.37807 0.85460 8.09853
H 6.64475 0.74560 5.58256
H 9.05804 0.43653 4.60937
H 10.92421 1.48226 3.30463
H 10.75782 3.89403 2.65015
H 8.71484 5.19122 3.31845
H 4.46739 6.85760 5.43357
H 2.08000 7.22986 6.13040
H 0.63238 5.22496 6.56487
H 1.61030 2.94147 6.30881
H 4.19468 2.28736 0.85668
H 3.97212 4.37993 -0.48988
H 4.75653 6.55317 0.49166
H 5.71994 6.54320 2.81406
H 3.56788 1.60853 5.18848
H 4.48056 1.97679 6.64045
H 4.48657 1.37216 3.28752
H 6.21328 1.55754 3.03460
O 7.82787 6.47629 5.46865

52
FeOO Quintet QI (2/5)
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Fe 6.18317 4.53519 4.95890
N 5.53005 2.57113 4.87071
N 6.79019 3.96815 6.79298
N 8.00854 3.49785 4.26794
N 4.13293 4.81295 5.61339
N 5.53692 4.65758 3.06686
O 6.56459 6.40636 5.25267
C 7.00089 4.74925 7.87415
C 7.37405 4.18675 9.09600
C 7.52359 2.79931 9.18876
C 7.30218 1.99650 8.05909
C 6.93549 2.61130 6.86787
C 6.73717 1.90388 5.53295
C 7.95518 2.20214 4.67121
C 8.95716 1.29168 4.35317
C 10.04950 1.74558 3.59789
C 10.10035 3.08178 3.18842
C 9.05439 3.94086 3.53770
C 3.49913 6.00371 5.73993
C 2.13273 6.07012 6.00379
C 1.40935 4.87668 6.12406
C 2.07110 3.65144 5.98903
C 3.44509 3.65186 5.74076
C 4.26361 2.38509 5.67756
C 5.33442 2.22751 3.40936
C 5.10640 3.46165 2.56718
C 4.53007 3.39254 1.29815
C 4.41212 4.55858 0.53517
C 4.86943 5.77460 1.05682
C 5.42455 5.79269 2.33242
H 6.86413 5.81384 7.73765
H 7.54096 4.82686 9.95217
H 7.80726 2.34155 10.12855
H 7.41034 0.92058 8.10778
H 6.58113 0.83007 5.65823
H 8.89016 0.26158 4.68000
H 10.84625 1.06086 3.33359
H 10.93225 3.45682 2.60642
H 9.03451 4.98314 3.24874
H 4.10988 6.88929 5.62123
H 1.64790 7.03267 6.10358
H 0.34344 4.89926 6.31710
H 1.53394 2.71505 6.07714
H 4.18293 2.44088 0.91521
H 3.96698 4.51829 -0.45162
H 4.79244 6.69393 0.49150
H 5.78542 6.70332 2.78849
H 3.68395 1.55702 5.26198
H 4.54618 2.09709 6.69466
H 4.50069 1.52953 3.30336
H 6.22746 1.70957 3.04831
O 7.63399 6.76358 4.48834

52
FeOO Quintet QII (2/5)
Fe 6.23520 4.66040 4.92990
N 5.54221 2.56186 4.84241
N 6.78783 3.89504 6.87416
N 8.01680 3.59623 4.30843
N 4.21781 4.89110 5.57512
N 5.49623 4.58116 2.93701
O 7.27043 7.66512 5.11119
C 6.96927 4.59388 8.01725
C 7.30347 3.94911 9.20990
C 7.44488 2.55771 9.21308
C 7.25217 1.83889 8.02439
C 6.92491 2.54160 6.86865
C 6.75115 1.91317 5.49229
C 7.97381 2.28365 4.66284
C 9.00145 1.40605 4.33042
C 10.10080 1.90252 3.61502
C 10.13838 3.25370 3.25606
C 9.07277 4.08086 3.61741
C 3.60056 6.09247 5.71491
C 2.24466 6.18346 6.01461
C 1.50629 5.00251 6.16198
C 2.14693 3.76879 6.01523
C 3.51425 3.73888 5.72835
C 4.28165 2.43767 5.65175
C 5.34741 2.17328 3.40358
C 5.06822 3.36358 2.51304
C 4.45385 3.21638 1.26640
C 4.29781 4.33618 0.44493
C 4.75510 5.58395 0.88740
C 5.34605 5.67352 2.14387
H 6.84319 5.66698 7.95988
H 7.44685 4.52891 10.11239
H 7.69922 2.03491 10.12715
H 7.35257 0.76102 7.99984
H 6.63783 0.82837 5.56716
H 8.94574 0.36369 4.61824
H 10.91341 1.24019 3.34207
H 10.97437 3.66390 2.70462
H 9.04776 5.13181 3.36118
H 4.21587 6.97166 5.57730
H 1.77983 7.15491 6.12204
H 0.44674 5.04200 6.38489
H 1.59806 2.84133 6.12356
H 4.10785 2.24071 0.94766
H 3.82418 4.23768 -0.52455
H 4.65045 6.47069 0.27589
H 5.70488 6.61417 2.53991
H 3.64947 1.64327 5.24450
H 4.54834 2.13398 6.66883
H 4.54278 1.43690 3.31925
H 6.25801 1.68138 3.04742
O 6.84682 6.41834 5.02645

52
FeOO Quintet QIII (2/5)
Fe 6.25007 4.64595 4.89494
N 5.54512 2.56032 4.83366
N 6.81028 3.91256 6.84635
N 8.01789 3.57565 4.27040
N 4.24385 4.89766 5.57446
N 5.51014 4.57078 2.91298
O 6.66598 7.48149 5.86538
C 7.00971 4.62489 7.97725
C 7.34672 3.99252 9.17578
C 7.47177 2.59968 9.19641
C 7.26361 1.86715 8.01863
C 6.93512 2.55762 6.85589
C 6.75282 1.91361 5.48711
C 7.97523 2.26990 4.65099
C 9.00535 1.38797 4.33848
C 10.10656 1.87211 3.61772
C 10.14381 3.21616 3.23244
C 9.07551 4.04818 3.57277
C 3.63927 6.10474 5.71587
C 2.28081 6.20771 6.00167
C 1.52841 5.03428 6.13377
C 2.15786 3.79431 5.98917
C 3.52732 3.75100 5.71663
C 4.28512 2.44464 5.64500
C 5.34620 2.16620 3.39551
C 5.06951 3.35384 2.49918
C 4.44372 3.20651 1.25860
C 4.28966 4.32480 0.43407
C 4.75869 5.57145 0.86749
C 5.36087 5.66213 2.11866
H 6.89921 5.69962 7.90592
H 7.50491 4.58261 10.06905
H 7.72664 2.08623 10.11559
H 7.35417 0.78822 8.00755
H 6.63574 0.83026 5.57510
H 8.95026 0.35136 4.64632
H 10.92106 1.20578 3.36070
H 10.98137 3.61678 2.67647
H 9.05019 5.09370 3.29442
H 4.26482 6.98046 5.59841
H 1.82535 7.18348 6.10974
H 0.46679 5.08382 6.34441
H 1.59837 2.87223 6.08823
H 4.08676 2.23266 0.94657
H 3.80746 4.22580 -0.53111
H 4.65409 6.45628 0.25325
H 5.72918 6.60061 2.51193
H 3.64826 1.65206 5.24198
H 4.55240 2.14399 6.66293
H 4.53831 1.43298 3.31634
H 6.25413 1.66859 3.04057
O 6.83008 6.44617 5.04566

52
FeOO Quintet QSI (2/5)
Fe 6.23800 4.55553 4.91997
N 5.52349 2.45466 4.83406
N 6.71711 3.90901 6.79099
N 7.92295 3.59812 4.28876
N 4.32438 4.83899 5.53546
N 5.52077 4.53017 3.01833
O 6.70291 6.59291 5.64528
C 6.84152 4.65928 7.90874
C 7.15316 4.07105 9.13603
C 7.33018 2.68636 9.20499
C 7.19243 1.91512 8.04241
C 6.88647 2.55827 6.84811
C 6.74779 1.87247 5.49792
C 7.94646 2.28692 4.65870
C 9.00539 1.45415 4.31389
C 10.06659 1.98917 3.57029
C 10.03147 3.33431 3.19274
C 8.93881 4.11983 3.56487
C 3.76358 6.06746 5.68537
C 2.42975 6.21908 6.05035
C 1.64911 5.07609 6.25716
C 2.23145 3.81710 6.09917
C 3.57934 3.71945 5.74299
C 4.26392 2.37419 5.63139
C 5.34544 2.10033 3.39532
C 5.10524 3.32557 2.54080
C 4.52254 3.22341 1.27457
C 4.37985 4.36741 0.48704
C 4.82218 5.59792 0.98562
C 5.38401 5.64736 2.25728
H 6.69498 5.72410 7.80252
H 7.25220 4.69373 10.01543
H 7.56780 2.20920 10.14789
H 7.31501 0.83972 8.06495
H 6.69191 0.78605 5.60577
H 8.99943 0.41398 4.61394
H 10.90327 1.36139 3.28909
H 10.83430 3.77679 2.61776
H 8.86535 5.16389 3.29830
H 4.40413 6.92018 5.51274
H 2.01630 7.21281 6.16252
H 0.60527 5.16411 6.53316
H 1.65379 2.91342 6.25068
H 4.18992 2.25641 0.91732
H 3.92952 4.30115 -0.49600
H 4.73027 6.50740 0.40644
H 5.73762 6.57429 2.68526
H 3.58129 1.64100 5.19147
H 4.49707 2.01270 6.63816
H 4.52229 1.38936 3.27656
H 6.24634 1.59283 3.03593
O 7.29222 6.43328 4.42878

52
FeOO Quintet QSII (2/5)
Fe 6.25472 4.70186 4.94172
N 5.55199 2.59468 4.86008
N 6.80491 3.91662 6.88394
N 8.02270 3.60259 4.31593
N 4.21678 4.91473 5.55086
N 5.50404 4.59764 2.94524
O 6.72062 6.68759 5.68802
C 6.99678 4.61650 8.02488
C 7.33455 3.97188 9.21669
C 7.47035 2.58018 9.22213
C 7.26796 1.86035 8.03562
C 6.93711 2.56265 6.88106
C 6.75444 1.93368 5.50787
C 7.97478 2.29119 4.67317
C 8.99309 1.40564 4.33458
C 10.08980 1.89282 3.60877
C 10.13287 3.24279 3.24681
C 9.07636 4.07858 3.61534
C 3.59462 6.11687 5.65905
C 2.23507 6.20854 5.94142
C 1.49931 5.02813 6.10512
C 2.14555 3.79396 5.99005
C 3.51557 3.76374 5.71794
C 4.29309 2.47022 5.67239
C 5.35013 2.19695 3.42389
C 5.06393 3.38154 2.53141
C 4.43227 3.23298 1.29389
C 4.26891 4.35139 0.47178
C 4.73750 5.59826 0.90452
C 5.34723 5.68855 2.15217
H 6.87831 5.68983 7.96499
H 7.48580 4.55315 10.11693
H 7.72800 2.05798 10.13557
H 7.36431 0.78214 8.01157
H 6.62732 0.85064 5.58375
H 8.93182 0.36441 4.62514
H 10.89538 1.22440 3.33003
H 10.96649 3.64658 2.68717
H 9.05834 5.12911 3.35881
H 4.20920 6.99527 5.51227
H 1.76584 7.18027 6.02384
H 0.43743 5.06837 6.31633
H 1.59942 2.86665 6.11175
H 4.07822 2.25771 0.98302
H 3.78092 4.25233 -0.49046
H 4.62750 6.48406 0.29262
H 5.71901 6.62740 2.54087
H 3.67199 1.65919 5.28150
H 4.56401 2.19306 6.69563
H 4.54672 1.45836 3.34993
H 6.25990 1.70532 3.06577
O 7.31359 6.52017 4.46394

52
FeOO Septet endon (2/7)
Fe 6.23014 4.63912 4.92527
N 5.53567 2.56404 4.84520
N 6.79757 3.89948 6.89850
N 8.03231 3.58792 4.29488
N 4.22006 4.92009 5.60000
N 5.49829 4.59912 2.91591
O 6.92439 6.55595 5.06324
C 6.98950 4.57514 8.05430
C 7.32645 3.91233 9.23612
C 7.45904 2.52022 9.21813
C 7.25425 1.82247 8.01970
C 6.92507 2.54458 6.87515
C 6.74344 1.92025 5.49539
C 7.97177 2.27984 4.66627
C 8.99129 1.38461 4.35254
C 10.10224 1.85512 3.63876
C 10.15896 3.20037 3.26039
C 9.10039 4.04440 3.60222
C 3.59647 6.11796 5.73739
C 2.23442 6.20696 6.01077
C 1.49422 5.02472 6.13349
C 2.13929 3.79312 5.98823
C 3.51253 3.76588 5.72851
C 4.27492 2.45813 5.65350
C 5.33837 2.18749 3.40539
C 5.04935 3.37995 2.51489
C 4.40039 3.22454 1.28642
C 4.22922 4.33642 0.45709
C 4.70473 5.58548 0.87509
C 5.33010 5.68236 2.11499
H 6.86799 5.64985 8.01707
H 7.47788 4.47819 10.14627
H 7.71477 1.98166 10.12271
H 7.34677 0.74427 7.97823
H 6.63319 0.83491 5.57507
H 8.91953 0.34707 4.65442
H 10.90797 1.17824 3.38121
H 11.00344 3.59221 2.70835
H 9.09202 5.09090 3.32647
H 4.21117 7.00026 5.61717
H 1.76670 7.17738 6.11571
H 0.43019 5.06138 6.33490
H 1.58834 2.86453 6.07563
H 4.03788 2.24828 0.98777
H 3.72886 4.23076 -0.49820
H 4.58748 6.46722 0.25848
H 5.70218 6.62595 2.49201
H 3.63343 1.66860 5.25035
H 4.53906 2.15598 6.67183
H 4.53656 1.44804 3.31618
H 6.25056 1.70208 3.04409
O 7.40678 7.74092 5.16901

52
FeOO Septet sideon (2/7)
Fe 6.25379 4.69902 4.94169
N 5.55412 2.59903 4.86096
N 6.81078 3.92213 6.89059
N 8.03150 3.60811 4.31550
N 4.21445 4.92333 5.55280
N 5.50347 4.60623 2.94057
O 6.73252 6.68023 5.68884
C 7.00100 4.61507 8.03645
C 7.33524 3.96476 9.22607
C 7.46946 2.57295 9.22554
C 7.26801 1.85956 8.03524
C 6.94043 2.56771 6.88303
C 6.75742 1.94046 5.50865
C 7.97855 2.29685 4.67382
C 8.99244 1.40595 4.33514
C 10.09076 1.88616 3.60753
C 10.13920 3.23521 3.24306
C 9.08707 4.07630 3.61183
C 3.58514 6.12227 5.66033
C 2.22499 6.20831 5.94131
C 1.49397 5.02495 6.10435
C 2.14604 3.79404 5.98937
C 3.51673 3.76961 5.71878
C 4.29587 2.47614 5.67308
C 5.35278 2.20326 3.42502
C 5.06526 3.38751 2.53105
C 4.43212 3.23245 1.29479
C 4.26468 4.34649 0.46793
C 4.73033 5.59619 0.89545
C 5.34125 5.69293 2.14199
H 6.88325 5.68869 7.98341
H 7.48499 4.54185 10.12928
H 7.72458 2.04604 10.13701
H 7.36201 0.78122 8.00629
H 6.63258 0.85709 5.58519
H 8.92595 0.36533 4.62691
H 10.89281 1.21340 3.32900
H 10.97364 3.63430 2.68120
H 9.07440 5.12580 3.35135
H 4.19415 7.00418 5.51289
H 1.75162 7.17813 6.02304
H 0.43169 5.06046 6.31447
H 1.60384 2.86419 6.10964
H 4.07985 2.25493 0.98879
H 3.77578 4.24207 -0.49331
H 4.61708 6.47941 0.28036
H 5.70878 6.63540 2.52524
H 3.67363 1.66515 5.28354
H 4.56672 2.19968 6.69657
H 4.54990 1.46407 3.34934
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H 6.26286 1.71252 3.06635
O 7.31706 6.52235 4.46991

52
FeOO Septet O2-unbound (2/7)
Fe 6.22438 4.66340 5.00289
N 5.54837 2.57327 4.81655
N 6.78632 3.83409 6.97488
N 8.07672 3.64877 4.36045
N 4.18212 4.89919 5.66445
N 5.53416 4.70240 2.95527
O 13.05745 23.30950 5.83139
C 6.96277 4.43673 8.17213
C 7.27832 3.70583 9.31987
C 7.40407 2.31628 9.22258
C 7.21501 1.69255 7.98196
C 6.90810 2.48257 6.87488
C 6.75235 1.92589 5.46040
C 7.99835 2.32665 4.67252
C 9.01843 1.43575 4.34185
C 10.14886 1.92446 3.67320
C 10.22461 3.28420 3.35437
C 9.16436 4.12088 3.71068
C 3.52918 6.07538 5.83762
C 2.15369 6.12887 6.05332
C 1.43142 4.92971 6.07946
C 2.10649 3.71895 5.89839
C 3.49101 3.72879 5.69942
C 4.27601 2.43295 5.59228
C 5.38231 2.26985 3.36001
C 5.08437 3.49753 2.51555
C 4.42640 3.38381 1.28605
C 4.24559 4.52395 0.49769
C 4.72147 5.75868 0.95567
C 5.35733 5.81101 2.19409
H 6.84604 5.51267 8.19501
H 7.41807 4.21653 10.26414
H 7.64238 1.72369 10.09788
H 7.30167 0.61767 7.87903
H 6.66294 0.83505 5.49400
H 8.93102 0.38662 4.59692
H 10.95426 1.25144 3.40404
H 11.08418 3.69172 2.83764
H 9.17012 5.17850 3.47987
H 4.13386 6.97236 5.79428
H 1.66303 7.08433 6.18872
H 0.35880 4.93732 6.23421
H 1.56984 2.77767 5.91148
H 4.06379 2.41790 0.95459
H 3.73764 4.45084 -0.45687
H 4.59666 6.66144 0.37136
H 5.73286 6.74035 2.60332
H 3.64644 1.65170 5.15315
H 4.52232 2.09993 6.60581
H 4.59621 1.52097 3.21589
H 6.30985 1.82040 2.99060
O 13.51757 24.47547 5.86240

66
FeOO + CHD React (2/1)
Fe 6.21526 4.36853 4.71321
N 5.47366 2.50270 4.91922
N 6.69592 4.10201 6.62880
N 7.86279 3.37690 4.22184
N 4.40350 4.96484 5.25352
N 5.59859 4.22677 2.83893
O 7.04679 6.01136 4.39430
C 6.85753 5.02659 7.59848
C 7.18380 4.64184 8.90179
C 7.32991 3.28408 9.19881
C 7.15355 2.32890 8.18511
C 6.84038 2.77364 6.90766
C 6.66291 1.90462 5.67316
C 7.87276 2.13447 4.78171
C 8.92517 1.25313 4.56966
C 9.99401 1.67561 3.76394
C 9.97495 2.95541 3.20049
C 8.88446 3.79306 3.44569
C 3.93062 6.23457 5.19697
C 2.61534 6.53331 5.54108
C 1.76502 5.49688 5.94277
C 2.25674 4.18963 5.99356
C 3.58671 3.94743 5.64743
C 4.20260 2.57226 5.73238
C 5.25665 1.91083 3.54458
C 5.12150 2.99646 2.50413
C 4.58457 2.76056 1.23762
C 4.55472 3.80187 0.30544
C 5.05991 5.05832 0.66084
C 5.57276 5.24236 1.94157
H 6.72811 6.05925 7.30368
H 7.31904 5.39983 9.66183
H 7.57395 2.96591 10.20504
H 7.25350 1.27015 8.38753
H 6.51020 0.85198 5.91694
H 8.91341 0.26680 5.01533
H 10.82831 1.00968 3.58053
H 10.78873 3.30508 2.57895
H 8.81189 4.79374 3.04208
H 4.62662 6.99992 4.88763
H 2.26885 7.55714 5.48921
H 0.73488 5.70195 6.20782
H 1.62217 3.36597 6.29656
H 4.20077 1.77873 0.98928
H 4.14224 3.63543 -0.68232
H 5.05467 5.88449 -0.03803
H 5.97770 6.18830 2.27316
H 3.50087 1.80721 5.39252
H 4.43811 2.34309 6.77583
H 4.37698 1.26357 3.55488
H 6.11219 1.27559 3.29622
H 9.16197 7.72916 6.20250
C 10.12990 7.67800 6.72836
C 9.92471 7.90389 8.20778
C 10.32369 7.04012 9.15342
C 11.02620 5.73685 8.85127
C 11.20515 5.49675 7.37035
C 10.80692 6.36193 6.42517
H 10.71862 8.50834 6.30140
H 9.42683 8.82876 8.49376
H 10.14885 7.26621 10.20378
H 12.00767 5.71459 9.35531
H 10.46950 4.89784 9.30170
H 11.69342 4.56692 7.08394
H 10.97362 6.13081 5.37443
O 6.90033 7.03470 5.28031

FeOO + CHD TS (2/1)
Fe 6.31850 4.35650 4.90260
N 5.48273 2.50427 4.99118
N 6.68814 3.97927 6.82964
N 7.94789 3.30084 4.45723
N 4.49791 4.98902 5.37300
N 5.78298 4.28511 2.98959
O 7.15745 5.94978 4.66290
C 6.82284 4.85017 7.85127
C 7.04515 4.39387 9.15384
C 7.12002 3.01948 9.39556
C 6.97093 2.12040 8.32846
C 6.75640 2.63553 7.05605
C 6.60695 1.82689 5.77826
C 7.86903 2.03610 4.95708
C 8.88143 1.10712 4.74676
C 10.00397 1.50334 4.00432
C 10.07583 2.80568 3.49978
C 9.02246 3.69084 3.74213
C 4.08276 6.27911 5.33516
C 2.75587 6.61968 5.58824
C 1.83555 5.60582 5.87633
C 2.27040 4.27763 5.91101
C 3.61382 3.99417 5.66039
C 4.17675 2.59670 5.74286
C 5.30889 1.96779 3.58997
C 5.26483 3.09427 2.58624
C 4.77200 2.93037 1.29034
C 4.82849 4.00591 0.39892
C 5.37502 5.22238 0.82470
C 5.84157 5.33247 2.13221
H 6.75933 5.89750 7.58942
H 7.15516 5.11020 9.95744
H 7.28575 2.64631 10.39893
H 7.01393 1.05011 8.48573
H 6.40101 0.77240 5.97182
H 8.79713 0.10390 5.14492
H 10.80782 0.80047 3.82226
H 10.93117 3.13562 2.92469
H 9.01695 4.71006 3.38159
H 4.83838 7.01971 5.11623
H 2.45460 7.65870 5.55350
H 0.79596 5.84381 6.06727
H 1.58186 3.47040 6.12890
H 4.35464 1.97757 0.98834
H 4.45055 3.89628 -0.61052
H 5.43618 6.07408 0.15966
H 6.27404 6.24132 2.52735
H 3.46709 1.86170 5.35565
H 4.35534 2.34110 6.79151
H 4.40651 1.35425 3.53381
H 6.15151 1.30954 3.35690
H 8.27709 7.27548 6.13160
C 9.41844 7.60796 6.51295
C 9.37103 7.71111 7.98452
C 9.97138 6.80474 8.79039
C 10.77222 5.64984 8.25654
C 10.93210 5.66375 6.76218
C 10.32888 6.58326 5.97084
H 9.45882 8.57274 5.99231
H 8.81854 8.54215 8.41450
H 9.90820 6.90557 9.87065
H 11.76529 5.62863 8.73777
H 10.31186 4.69619 8.57475
H 11.58654 4.91280 6.32749
H 10.49902 6.57484 4.89811
O 7.00843 6.98753 5.65358

FeOO + CHD Intermediate (2/1)
Fe 6.31948 4.23142 4.96362
N 5.41566 2.41974 4.95252
N 6.66299 3.74037 6.87436
N 7.91607 3.13317 4.48442
N 4.52282 4.91592 5.43763
N 5.80594 4.28143 3.04894
O 7.26427 5.76579 4.82823
C 6.84730 4.55007 7.93896
C 7.05821 4.01636 9.21386
C 7.06739 2.62901 9.38394
C 6.87014 1.79474 8.27317
C 6.67333 2.38488 7.03069
C 6.49869 1.65096 5.71134
C 7.77805 1.84800 4.91412
C 8.75462 0.88988 4.66796
C 9.90486 1.27867 3.96508
C 10.03977 2.60311 3.53664
C 9.01951 3.51735 3.81099
C 4.15792 6.22178 5.44279
C 2.83935 6.60189 5.68454
C 1.87541 5.61404 5.91309
C 2.25900 4.26949 5.90222
C 3.59545 3.94499 5.66646
C 4.10588 2.52603 5.69868
C 5.23261 1.95922 3.52391
C 5.24813 3.13443 2.57775
C 4.76931 3.05732 1.26879
C 4.88019 4.17485 0.43600
C 5.46527 5.34590 0.93228
C 5.91632 5.36989 2.24953
H 6.83281 5.61149 7.73280
H 7.20674 4.68440 10.05285
H 7.22156 2.19639 10.36502
H 6.86551 0.71685 8.37427
H 6.24280 0.59811 5.84488
H 8.62376 -0.12867 5.01076
H 10.68225 0.55375 3.75648
H 10.91894 2.92835 2.99587
H 9.06503 4.55461 3.50933
H 4.94693 6.93954 5.27196
H 2.57834 7.65241 5.68673
H 0.84184 5.88425 6.09344
H 1.53540 3.48178 6.07264
H 4.32069 2.13832 0.91205
H 4.51375 4.13240 -0.58265
H 5.56801 6.22820 0.31391
H 6.37551 6.24011 2.69754
H 3.37568 1.83210 5.27608
H 4.26855 2.22261 6.73697
H 4.30499 1.38963 3.43110
H 6.04912 1.27797 3.26676
H 7.95623 7.19015 5.97515
C 9.91138 8.09767 6.31826
C 9.62993 8.33749 7.69705
C 9.98013 7.43073 8.66569
C 10.68097 6.13883 8.33637
C 10.95922 5.96188 6.86670
C 10.58980 6.90128 5.93653
H 9.67674 8.85263 5.57477
H 9.13171 9.26115 7.97835
H 9.76079 7.63032 9.71074
H 11.62472 6.06400 8.91094
H 10.09075 5.28169 8.71556
H 11.47792 5.05808 6.55931
H 10.82036 6.74007 4.88711
O 7.04584 6.79493 5.90601

66
FeOO + CHD React (2/3)
Fe 6.17369 4.30206 4.73268
N 5.43039 2.43742 4.87214
N 6.63358 3.98118 6.64398
N 7.83251 3.34205 4.25983
N 4.36312 4.90317 5.24448
N 5.59223 4.23301 2.84883
O 6.96511 6.02216 4.41847
C 6.78231 4.87781 7.64237
C 7.06773 4.45291 8.94274
C 7.19226 3.08606 9.20550
C 7.03429 2.16073 8.16105
C 6.75694 2.64365 6.88996
C 6.60211 1.81285 5.62678
C 7.83055 2.07675 4.76851
C 8.88901 1.20718 4.54272
C 9.97457 1.66531 3.77867
C 9.96710 2.96780 3.26932
C 8.87010 3.79337 3.52460
C 3.89894 6.17749 5.21174
C 2.57756 6.47216 5.53282
C 1.71373 5.42825 5.88550
C 2.19740 4.11717 5.91282
C 3.53416 3.87755 5.59277
C 4.14308 2.49701 5.66031
C 5.23544 1.89328 3.47453
C 5.11752 3.01382 2.46847
C 4.59795 2.82204 1.18772
C 4.58475 3.89413 0.29035
C 5.08704 5.13766 0.69351
C 5.58094 5.27893 1.98668
H 6.68022 5.91881 7.36657
H 7.19135 5.18820 9.72662
H 7.40710 2.73765 10.20837
H 7.12025 1.09598 8.33613
H 6.44842 0.75269 5.83472
H 8.87091 0.20301 4.94617
H 10.81381 1.00825 3.58593
H 10.79461 3.34351 2.68221
H 8.80131 4.80982 3.16157
H 4.60737 6.94453 4.93777
H 2.23579 7.49838 5.50208
H 0.67860 5.63138 6.13196
H 1.55165 3.28943 6.17856
H 4.21461 1.85069 0.90087
H 4.18606 3.76121 -0.70811
H 5.09219 5.98594 0.02174
H 5.98221 6.21023 2.36157
H 3.44402 1.74273 5.29214
H 4.35632 2.24704 6.70380
H 4.35565 1.24647 3.44724
H 6.09492 1.26640 3.21794
H 9.13814 7.87877 6.30361
C 10.05435 7.81216 6.91315
C 9.70004 7.86837 8.38064
C 10.05091 6.92390 9.26627
C 10.84457 5.69062 8.90203
C 11.17300 5.61889 7.42884
C 10.82274 6.56465 6.54399
H 10.63783 8.70677 6.63481
H 9.13115 8.73595 8.71043
H 9.76694 7.02810 10.31202
H 11.77476 5.65522 9.49482
H 10.29245 4.78595 9.20735
H 11.73145 4.74534 7.09702
H 11.09896 6.45566 5.49655
O 6.91353 6.94769 5.42865

66
FeOO + CHD TS (2/3)
Fe 6.30998 4.28436 4.92941
N 5.43821 2.45792 4.93928
N 6.66423 3.81804 6.84114
N 7.92300 3.20858 4.45351
N 4.49694 4.94914 5.39594
N 5.79543 4.31586 3.01824
O 7.28984 5.83179 4.83700
C 6.84009 4.64460 7.89330
C 7.07177 4.13115 9.17276
C 7.10842 2.74645 9.35974
C 6.91965 1.89439 8.26102
C 6.70279 2.46530 7.01277
C 6.53584 1.71453 5.70141
C 7.80863 1.92571 4.89695
C 8.79867 0.98037 4.65426
C 9.93761 1.37907 3.93880
C 10.04789 2.70045 3.49419
C 9.01503 3.60093 3.76650
C 4.09999 6.24594 5.38730
C 2.77374 6.59990 5.62489
C 1.83267 5.59281 5.86547
C 2.24703 4.25766 5.86892
C 3.59088 3.96099 5.63611
C 4.12965 2.55248 5.68686
C 5.25741 1.98813 3.51385
C 5.25310 3.15708 2.55823
C 4.77322 3.06203 1.25064
C 4.86838 4.17347 0.40776
C 5.44000 5.35633 0.89198
C 5.89236 5.39767 2.20835
H 6.80396 5.70331 7.67343
H 7.21628 4.81119 10.00218
H 7.27779 2.32951 10.34512
H 6.93732 0.81803 8.37592
H 6.29957 0.65860 5.84741
H 8.68568 -0.03651 5.00828
H 10.72467 0.66410 3.73207
H 10.91741 3.03351 2.94257
H 9.04149 4.63542 3.45342
H 4.87098 6.98066 5.20317
H 2.48899 7.64414 5.61482
H 0.79319 5.84130 6.04325
H 1.54193 3.45534 6.04883
H 4.33632 2.13420 0.90224
H 4.50108 4.11724 -0.60993
H 5.53172 6.23364 0.26481
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H 6.34357 6.27793 2.64515
H 3.41039 1.83851 5.27853
H 4.30087 2.26863 6.72936
H 4.33763 1.40483 3.42673
H 6.08235 1.31673 3.25738
H 8.31852 7.38785 6.18283
C 9.41488 7.77456 6.51468
C 9.37994 7.93293 7.98684
C 10.01517 7.07763 8.81944
C 10.84603 5.92816 8.32164
C 11.01159 5.90243 6.82818
C 10.37247 6.76831 6.00694
H 9.43703 8.72524 5.96617
H 8.80120 8.75957 8.38995
H 9.95631 7.21530 9.89591
H 11.83644 5.94257 8.80782
H 10.40451 4.97359 8.66418
H 11.69737 5.16507 6.41918
H 10.54103 6.72906 4.93457
O 7.00117 6.86641 5.78993

66
FeOO + CHD Inter (2/3)
Fe 6.31804 4.23898 4.97164
N 5.41808 2.42572 4.93656
N 6.65198 3.72847 6.87917
N 7.92040 3.14898 4.49189
N 4.51494 4.91524 5.43722
N 5.82053 4.30640 3.05371
O 7.26233 5.77584 4.86187
C 6.83357 4.52715 7.95251
C 7.04286 3.97969 9.22175
C 7.05241 2.59091 9.37766
C 6.85843 1.76822 8.25782
C 6.66435 2.37138 7.02121
C 6.49801 1.65094 5.69345
C 7.78171 1.85879 4.90592
C 8.76126 0.90509 4.65446
C 9.91502 1.30360 3.96288
C 10.05064 2.63310 3.55079
C 9.02728 3.54235 3.82957
C 4.14492 6.21990 5.44748
C 2.82254 6.59325 5.67807
C 1.86038 5.60015 5.89084
C 2.24892 4.25715 5.87470
C 3.58887 3.93936 5.65002
C 4.10412 2.52225 5.67654
C 5.24358 1.97965 3.50239
C 5.26908 3.16302 2.56677
C 4.80484 3.09662 1.25195
C 4.92387 4.22126 0.43002
C 5.50234 5.38856 0.94264
C 5.93880 5.40174 2.26489
H 6.81933 5.59079 7.75786
H 7.19112 4.63798 10.06789
H 7.20507 2.14863 10.35463
H 6.85499 0.68935 8.34748
H 6.24334 0.59631 5.81462
H 8.62991 -0.11757 4.98452
H 10.69459 0.58221 3.75033
H 10.93258 2.96612 3.01937
H 9.07336 4.58333 3.54087
H 4.93287 6.94139 5.28859
H 2.55720 7.64260 5.68370
H 0.82392 5.86521 6.06220
H 1.52661 3.46558 6.03238
H 4.36125 2.18024 0.88236
H 4.56891 4.18714 -0.59301
H 5.61133 6.27613 0.33294
H 6.39257 6.26833 2.72529
H 3.37878 1.82772 5.24652
H 4.26296 2.21340 6.71388
H 4.31462 1.41423 3.39787
H 6.05938 1.29789 3.24436
H 7.92366 7.20190 6.02694
C 9.82759 8.17342 6.47961
C 9.53301 8.19834 7.87624
C 9.94481 7.19012 8.71108
C 10.73168 6.00746 8.21017
C 11.01986 6.05794 6.73255
C 10.58468 7.09071 5.93981
H 9.54094 9.00732 5.84690
H 8.97412 9.03795 8.28018
H 9.71395 7.22588 9.77199
H 11.67877 5.91646 8.77683
H 10.20114 5.06795 8.46062
H 11.59849 5.24350 6.30595
H 10.82338 7.09365 4.87986
O 7.01970 6.79557 5.94360

66
FeOO + CHD React QI (2/5)
Fe 6.19231 4.46371 4.76574
N 5.41279 2.54667 4.88493
N 6.73292 4.06000 6.67952
N 7.96413 3.22850 4.24257
N 4.16880 4.96342 5.33960
N 5.63211 4.38537 2.84960
O 7.09422 6.16373 4.50071
C 6.96698 4.92995 7.68461
C 7.26900 4.47342 8.96953
C 7.31987 3.09727 9.20847
C 7.07299 2.19942 8.15837
C 6.78247 2.71091 6.89925
C 6.56113 1.87831 5.64388
C 7.81166 1.99419 4.78617
C 8.75472 0.98819 4.60205
C 9.89348 1.28028 3.83612
C 10.04725 2.55561 3.28264
C 9.05469 3.51527 3.50079
C 3.60921 6.19902 5.33270
C 2.24918 6.38027 5.57157
C 1.44959 5.25626 5.81355
C 2.03301 3.98524 5.82158
C 3.40478 3.86995 5.58857
C 4.12955 2.54822 5.68276
C 5.21036 2.04238 3.47104
C 5.12891 3.17409 2.47283
C 4.61759 2.99377 1.18697
C 4.64213 4.06226 0.28476
C 5.17595 5.29379 0.68410
C 5.66258 5.42591 1.98073
H 6.90304 5.98147 7.43574
H 7.46061 5.18904 9.75773
H 7.54483 2.72104 10.19901
H 7.10192 1.12945 8.32004
H 6.32891 0.83768 5.88005
H 8.60807 0.00855 5.03959
H 10.64665 0.51867 3.67432
H 10.91686 2.80607 2.68898
H 9.11698 4.51440 3.08962
H 4.27257 7.03035 5.13479
H 1.82808 7.37722 5.56172
H 0.38669 5.36728 5.99178
H 1.43777 3.09975 6.00815
H 4.21182 2.03227 0.89795
H 4.24908 3.93463 -0.71664
H 5.21127 6.13759 0.00775
H 6.08521 6.34961 2.35306
H 3.49126 1.72338 5.35639
H 4.37941 2.36125 6.73147
H 4.30998 1.42501 3.42702
H 6.04997 1.39258 3.20679
H 8.98650 7.92399 6.44913
C 9.96051 7.87753 6.96500
C 9.74975 7.84492 8.46035
C 10.22691 6.87612 9.25639
C 11.03143 5.70081 8.75198
C 11.22500 5.72258 7.25371
C 10.74982 6.69333 6.45853
H 10.46723 8.81527 6.67879
H 9.18045 8.66764 8.88926
H 10.04441 6.91598 10.32885
H 12.01292 5.67500 9.25572
H 10.54591 4.75741 9.05379
H 11.79185 4.89831 6.82450
H 10.93406 6.65435 5.38626
O 6.80370 7.08125 5.45969

66
FeOO + CHD TS QI (2/5)
Fe 6.29706 4.53512 4.99788
N 5.47100 2.60891 4.99965
N 6.70564 4.00466 6.97381
N 8.07605 3.25366 4.55836
N 4.23487 5.03149 5.41852
N 5.85259 4.48081 3.00266
O 6.98766 6.25810 4.80930
C 6.88413 4.80201 8.04797
C 7.07578 4.26252 9.32274
C 7.07329 2.87392 9.48080
C 6.88052 2.05013 8.36158
C 6.69977 2.64709 7.11814
C 6.54645 1.88640 5.80782
C 7.85606 2.00520 5.04404
C 8.78087 0.97745 4.88151
C 9.97011 1.25744 4.19249
C 10.19092 2.54436 3.69089
C 9.21632 3.52660 3.88954
C 3.69732 6.27517 5.38534
C 2.32464 6.47577 5.51673
C 1.49099 5.36105 5.67267
C 2.05237 4.08017 5.70459
C 3.43727 3.94634 5.58283
C 4.13684 2.61414 5.70677
C 5.35611 2.13935 3.56618
C 5.35408 3.28706 2.58074
C 4.91370 3.12940 1.26436
C 5.00551 4.20902 0.38011
C 5.53085 5.42767 0.82854
C 5.94182 5.53245 2.15455
H 6.87005 5.86605 7.85127
H 7.22107 4.92229 10.16815
H 7.21433 2.43221 10.45992
H 6.86769 0.97165 8.45723
H 6.27884 0.84100 5.98070
H 8.58016 -0.01123 5.27543
H 10.70894 0.47841 4.04763
H 11.09819 2.78661 3.15244
H 9.33270 4.53621 3.51869
H 4.39170 7.09450 5.25460
H 1.91984 7.47934 5.49051
H 0.41875 5.48671 5.76577
H 1.43022 3.20148 5.82428
H 4.50908 2.17854 0.93957
H 4.66862 4.10115 -0.64406
H 5.61418 6.28074 0.16777
H 6.34460 6.44495 2.57605
H 3.50987 1.80212 5.32850
H 4.31228 2.41103 6.76763
H 4.45395 1.53369 3.44674
H 6.20351 1.48402 3.34347
H 8.28004 7.41318 6.34078
C 9.42283 7.74014 6.61566
C 9.56536 7.61003 8.08136
C 10.29121 6.61898 8.64893
C 11.04774 5.60456 7.83957
C 11.02477 5.86688 6.36097
C 10.29563 6.86588 5.80739
H 9.37638 8.77778 6.26086
H 9.04722 8.33387 8.70426
H 10.36510 6.54402 9.73046
H 12.09167 5.54591 8.19252
H 10.65102 4.59258 8.04490
H 11.64696 5.23202 5.73606
H 10.32843 7.03740 4.73523
O 6.91577 7.08396 5.96728

66
FeOO + CHD Interm QI (2/5)
Fe 6.26398 4.48048 5.01262
N 5.44790 2.57355 4.96944
N 6.66774 3.91613 6.96721
N 8.04850 3.22255 4.54848
N 4.20890 4.96873 5.44583
N 5.82544 4.48585 3.03289
O 6.92247 6.17525 4.83733
C 6.84060 4.69074 8.06082
C 7.03119 4.12304 9.32323
C 7.03644 2.73157 9.45211
C 6.85146 1.93185 8.31462
C 6.66966 2.55472 7.08461
C 6.52194 1.82402 5.75899
C 7.83334 1.96201 5.00247
C 8.76562 0.94441 4.82200
C 9.95828 1.25048 4.14969
C 10.17497 2.55134 3.68314
C 9.19184 3.52203 3.89692
C 3.67938 6.21572 5.43994
C 2.31000 6.41983 5.59744
C 1.47405 5.30593 5.74909
C 2.02825 4.02131 5.74790
C 3.41018 3.88424 5.60070
C 4.11132 2.55016 5.67940
C 5.33266 2.13258 3.52420
C 5.33342 3.30367 2.57081
C 4.90285 3.18556 1.24771
C 4.99701 4.29254 0.39824
C 5.51399 5.49860 0.88833
C 5.91571 5.56469 2.21938
H 6.82822 5.75792 7.88684
H 7.16930 4.76555 10.18304
H 7.17776 2.26976 10.42181
H 6.84497 0.85148 8.38571
H 6.24825 0.77608 5.90197
H 8.56937 -0.05503 5.19016
H 10.70380 0.48050 3.99154
H 11.08563 2.81289 3.15975
H 9.30244 4.54176 3.55266
H 4.37675 7.03172 5.30363
H 1.90880 7.42515 5.59336
H 0.40422 5.43521 5.86252
H 1.40295 3.14397 5.86057
H 4.50396 2.24389 0.89112
H 4.66785 4.21533 -0.63113
H 5.59800 6.37233 0.25536
H 6.30982 6.46533 2.67296
H 3.48927 1.74917 5.27168
H 4.28899 2.30967 6.73183
H 4.43005 1.53080 3.39282
H 6.18029 1.48214 3.28926
H 8.05426 7.15137 6.11522
C 10.00117 8.02731 6.44618
C 9.84497 8.03033 7.86547
C 10.26781 6.97377 8.63153
C 10.91921 5.75789 8.02767
C 11.07347 5.83587 6.53189
C 10.63395 6.91768 5.80957
H 9.70993 8.89581 5.86442
H 9.38428 8.89155 8.34106
H 10.14364 6.99240 9.71047
H 11.90510 5.58302 8.50023
H 10.34783 4.84942 8.30211
H 11.55715 5.00134 6.03254
H 10.77479 6.94048 4.73251
O 7.07591 6.96253 6.09574

66
FeOO + CHD React QIII (2/5)
Fe 6.39675 4.16188 5.85118
N 5.49751 2.37312 4.92814
N 5.92592 2.93833 7.56767
N 8.08529 2.82383 5.69385
N 4.35514 4.76973 5.72836
N 6.61744 4.66245 3.80722
O 7.05913 5.68380 6.76157
C 5.71119 3.33999 8.83995
C 5.40115 2.41861 9.84243
C 5.30657 1.06274 9.51250
C 5.52978 0.65382 8.18967
C 5.84125 1.62084 7.23871
C 6.18787 1.32719 5.78468
C 7.69074 1.52282 5.62746
C 8.61282 0.48958 5.49028
C 9.97610 0.81255 5.42511
C 10.37311 2.15136 5.49859
C 9.39814 3.14249 5.62989
C 3.92944 6.03677 5.96587
C 2.61016 6.41480 5.73342
C 1.71317 5.46240 5.23440
C 2.15781 4.15917 4.99373
C 3.49010 3.83247 5.25879
C 4.00688 2.41943 5.11339
C 5.89961 2.33417 3.47974
C 6.22212 3.70547 2.92682
C 6.18373 3.96956 1.55534
C 6.57435 5.22894 1.09070
C 6.99396 6.20155 2.00693
C 6.99920 5.88811 3.36300
H 5.79507 4.40092 9.03972
H 5.23702 2.76132 10.85575
H 5.06153 0.32993 10.27173
H 5.46164 -0.38938 7.90772
H 5.89059 0.31238 5.50667
H 8.27786 -0.53868 5.43441
H 10.71427 0.02709 5.31692
H 11.41820 2.42890 5.45305
H 9.65302 4.19386 5.68612
H 4.66376 6.73464 6.34698
H 2.29794 7.43176 5.93262
H 0.68279 5.73103 5.03411
H 1.48382 3.40356 4.60900
H 5.85475 3.20090 0.86681
H 6.54937 5.44874 0.03004
H 7.30439 7.18563 1.68049
H 7.30642 6.60541 4.11390
H 3.50706 1.91206 4.28325
H 3.75042 1.86234 6.02005
H 5.11414 1.85937 2.88506
H 6.78868 1.70354 3.38163
H 8.80033 7.93476 7.43219
C 9.65954 8.28092 6.83457
C 10.62649 7.14221 6.61409
C 11.06185 6.76274 5.40182
C 10.63187 7.42714 4.11498
C 9.60710 8.51619 4.33136
C 9.17302 8.89551 5.54359
H 10.13313 9.05581 7.46191
H 10.98506 6.62846 7.50410
H 11.77594 5.94580 5.31288
H 11.51316 7.84123 3.59555
H 10.23516 6.67152 3.41679
H 9.22598 9.01014 3.43936
H 8.43955 9.69486 5.63132
O 6.69515 6.52121 7.73147

66
FeOO + CHD TS QIII (2/5)
Fe 6.52197 4.15136 5.50789
N 5.36733 2.34701 4.86745
N 6.25067 3.06664 7.37132
N 8.08164 2.66002 5.18980
N 4.49847 4.87087 5.67061
N 6.43284 4.47666 3.40567
O 7.43768 5.69186 6.10875
C 6.25699 3.56595 8.62660
C 6.03453 2.73992 9.73098
C 5.79494 1.37782 9.52133
C 5.78861 0.86791 8.21489
C 6.02336 1.74356 7.15793
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C 6.12090 1.32617 5.69428
C 7.59135 1.39557 5.29729
C 8.40533 0.28062 5.11249
C 9.76048 0.47998 4.81450
C 10.25863 1.78268 4.70950
C 9.38755 2.85715 4.90024
C 4.18175 6.17250 5.88730
C 2.86550 6.62228 5.81510
C 1.85513 5.70415 5.50319
C 2.18789 4.36336 5.28834
C 3.52486 3.96759 5.38758
C 3.93227 2.51453 5.26675
C 5.53823 2.18386 3.38567
C 5.84920 3.48811 2.68005
C 5.60856 3.65331 1.31273
C 5.99078 4.84518 0.69040
C 6.60313 5.85226 1.44737
C 6.80510 5.63732 2.80768
H 6.44494 4.62872 8.72300
H 6.04712 3.15890 10.72890
H 5.61306 0.71794 10.36117
H 5.60355 -0.18213 8.02549
H 5.73006 0.31414 5.55318
H 7.99230 -0.71698 5.19607
H 10.41389 -0.37113 4.66487
H 11.30044 1.96754 4.48158
H 9.71935 3.88452 4.82407
H 5.00535 6.83167 6.13060
H 2.64059 7.66610 5.99305
H 0.82332 6.02701 5.42881
H 1.42436 3.63220 5.05103
H 5.13230 2.85998 0.74920
H 5.81128 4.98738 -0.36872
H 6.91130 6.78629 0.99551
H 7.26279 6.38050 3.44782
H 3.27814 1.99538 4.55927
H 3.78077 2.03521 6.23955
H 4.64416 1.72573 2.95126
H 6.36332 1.48846 3.20096
H 8.11089 7.57563 7.11260
C 8.95975 8.44914 6.94347
C 10.15364 8.00219 7.68611
C 11.25173 7.51899 7.05779
C 11.36448 7.45445 5.56170
C 10.19970 8.06163 4.83538
C 9.10805 8.54354 5.48088
H 8.42157 9.28709 7.40351
H 10.11995 8.04740 8.77096
H 12.10866 7.18068 7.63385
H 12.30084 7.94018 5.23561
H 11.49897 6.40450 5.24065
H 10.27150 8.13197 3.75346
H 8.29656 8.99621 4.91804
O 7.14375 6.52512 7.19290

66
FeOO + CHD Interm QIII (2/5)
Fe 6.63105 4.18726 5.61937
N 5.47383 2.42242 4.91209
N 6.47977 2.99637 7.45249
N 8.25043 2.66093 5.15755
N 4.57851 4.96210 5.77511
N 6.49395 4.63708 3.50731
O 7.68702 5.92757 6.26133
C 6.53333 3.39213 8.74458
C 6.33041 2.48915 9.79126
C 6.06121 1.15072 9.48838
C 6.00326 0.74541 8.14780
C 6.21869 1.69580 7.15144
C 6.25074 1.36442 5.66143
C 7.70596 1.41476 5.20417
C 8.44806 0.27436 4.89864
C 9.79213 0.42275 4.53211
C 10.34823 1.70408 4.47800
C 9.54563 2.80296 4.79498
C 4.21402 6.25567 5.95789
C 2.88977 6.67473 5.84978
C 1.90982 5.72734 5.53086
C 2.28511 4.39444 5.34149
C 3.63020 4.03430 5.47774
C 4.06233 2.58420 5.37577
C 5.59056 2.33854 3.42362
C 5.89488 3.67173 2.76348
C 5.62151 3.87725 1.40620
C 5.98539 5.08690 0.80926
C 6.61196 6.07249 1.58259
C 6.84509 5.81488 2.93089
H 6.74005 4.44033 8.91921
H 6.38067 2.83193 10.81692
H 5.89570 0.43050 10.28087
H 5.79268 -0.28398 7.88422
H 5.84008 0.36312 5.49314
H 7.98646 -0.70477 4.94118
H 10.38954 -0.44782 4.28860
H 11.38189 1.85539 4.19377
H 9.93372 3.81182 4.75655
H 5.00941 6.94721 6.19735
H 2.63656 7.71589 6.00486
H 0.87178 6.02175 5.42869
H 1.54752 3.64039 5.09313
H 5.13288 3.09955 0.83106
H 5.78068 5.25976 -0.24086
H 6.90713 7.02132 1.15282
H 7.31437 6.54467 3.57843
H 3.37765 2.03545 4.71939
H 3.96984 2.13351 6.36920
H 4.67507 1.91526 2.99557
H 6.39753 1.64267 3.17237
H 7.18703 7.48170 7.36047
C 9.37639 9.23374 5.79445
C 9.60160 8.85773 7.12711
C 10.29404 7.67136 7.41419
C 10.76098 6.86031 6.36538
C 10.53916 7.24348 5.02989
C 9.84495 8.42808 4.74646
H 8.84324 10.15273 5.57447
H 9.25065 9.48953 7.93671
H 10.47402 7.38222 8.44409
H 11.31814 5.95524 6.58578
H 8.67492 6.02470 6.31754
H 10.91305 6.62554 4.22014
H 9.67652 8.72468 3.71659
O 7.20484 6.51521 7.57573

66
FeOO + CHD React QSII (2/5)
Fe 6.34246 4.61763 5.39724
N 5.39744 2.61866 5.15136
N 6.28199 3.83987 7.42308
N 8.03960 3.27624 5.24243
N 4.27410 5.12197 5.56456
N 6.05598 4.54800 3.27891
O 6.88861 6.54918 6.21552
C 6.27167 4.55120 8.57241
C 6.19929 3.91373 9.81287
C 6.13179 2.51770 9.85676
C 6.14031 1.78639 8.66015
C 6.21714 2.48189 7.45743
C 6.30061 1.83202 6.08419
C 7.72736 1.99690 5.58331
C 8.66990 0.97553 5.52034
C 9.97013 1.28981 5.09841
C 10.28464 2.60833 4.75589
C 9.29129 3.58685 4.83700
C 3.81798 6.40119 5.57885
C 2.45648 6.68776 5.56835
C 1.54431 5.62557 5.53104
C 2.02040 4.31166 5.51597
C 3.39905 4.08410 5.54143
C 3.96935 2.68716 5.61777
C 5.51238 2.19843 3.71267
C 5.57787 3.38059 2.77567
C 5.23255 3.27091 1.42636
C 5.39870 4.37607 0.58682
C 5.90413 5.57094 1.11439
C 6.21849 5.62582 2.46900
H 6.32375 5.62759 8.48092
H 6.19450 4.50388 10.71998
H 6.07056 2.00149 10.80717
H 6.08585 0.70496 8.66405
H 6.01565 0.77763 6.12803
H 8.39838 -0.03709 5.79113
H 10.72294 0.51311 5.03885
H 11.28045 2.88068 4.43112
H 9.48319 4.62221 4.59130
H 4.56713 7.18161 5.59616
H 2.12206 7.71695 5.58181
H 0.47831 5.81813 5.51151
H 1.33616 3.47243 5.48790
H 4.84371 2.33506 1.04420
H 5.13581 4.30687 -0.46194
H 6.04633 6.44503 0.49230
H 6.60288 6.52548 2.93081
H 3.35355 1.99282 5.03906
H 3.92412 2.35015 6.65806
H 4.68074 1.54027 3.44540
H 6.42720 1.61039 3.59175
H 8.92438 7.22951 7.86555
C 9.99692 7.48661 7.88061
C 10.80116 6.35452 7.28702
C 11.63480 6.50196 6.24567
C 11.87024 7.81942 5.54497
C 11.04988 8.94739 6.12576
C 10.21739 8.79951 7.16683
H 10.23837 7.59622 8.95185
H 10.68235 5.37728 7.75191
H 12.19003 5.64444 5.86960
H 12.94253 8.07741 5.58475
H 11.65603 7.71517 4.46793
H 11.16404 9.92281 5.65639
H 9.65797 9.65558 7.53976
O 7.69179 6.27598 5.13721

66
FeOO + CHD TS QSII (2/5)
Fe 6.60569 4.57803 5.42260
N 5.45871 2.63490 5.22447
N 6.46679 3.81598 7.47511
N 8.14775 3.06263 5.26463
N 4.58714 5.26217 5.56148
N 6.20267 4.43885 3.27076
O 7.30497 6.49459 6.24843
C 6.50158 4.53612 8.61833
C 6.36310 3.92375 9.86597
C 6.18067 2.53855 9.92556
C 6.13778 1.79685 8.73668
C 6.28361 2.47003 7.52648
C 6.29966 1.79508 6.16359
C 7.73007 1.82599 5.64302
C 8.57732 0.72276 5.58557
C 9.88870 0.90856 5.12509
C 10.30934 2.18411 4.73473
C 9.40870 3.24861 4.81441
C 4.25298 6.57716 5.52248
C 2.92377 6.98853 5.48202
C 1.91677 6.01506 5.47424
C 2.26837 4.66289 5.51718
C 3.62009 4.30950 5.56749
C 4.05589 2.86703 5.70455
C 5.50185 2.15699 3.80445
C 5.61707 3.29955 2.82440
C 5.20231 3.17476 1.49521
C 5.41024 4.23921 0.61343
C 6.02354 5.40767 1.08186
C 6.40259 5.47726 2.42043
H 6.63895 5.60320 8.51323
H 6.39584 4.52391 10.76610
H 6.06763 2.04028 10.88092
H 5.98934 0.72420 8.75091
H 5.93168 0.76726 6.23377
H 8.22335 -0.25545 5.88641
H 10.56763 0.06614 5.06894
H 11.31489 2.35535 4.37278
H 9.67313 4.25787 4.52895
H 5.07660 7.27883 5.52968
H 2.68565 8.04402 5.45198
H 0.87336 6.30475 5.43367
H 1.50895 3.89024 5.51344
H 4.72744 2.25979 1.16199
H 5.09526 4.15968 -0.42039
H 6.19867 6.25171 0.42697
H 6.86943 6.35420 2.84839
H 3.36129 2.21055 5.17128
H 3.99483 2.58949 6.76157
H 4.62147 1.54576 3.58108
H 6.37299 1.50642 3.68026
H 8.51331 6.78465 7.03895
C 9.57774 7.07489 7.54803
C 10.57630 6.34299 6.75068
C 11.38543 6.97076 5.85876
C 11.36900 8.45689 5.66463
C 10.46322 9.18969 6.61013
C 9.66096 8.54860 7.49313
H 9.41113 6.66677 8.55273
H 10.63667 5.26647 6.87913
H 12.10066 6.40080 5.27221
H 12.39625 8.85362 5.74521
H 11.09047 8.69249 4.62006
H 10.48850 10.27530 6.57908
H 9.03028 9.11537 8.17189
O 7.80809 6.09838 4.93365

66
FeOO + CHD Interm QSII (2/5)
Fe 6.65963 4.50966 5.61536
N 5.45941 2.72985 5.02653
N 6.33303 3.48022 7.56816
N 8.21401 2.93397 5.42418
N 4.65292 5.34920 5.75099
N 6.49079 4.81800 3.44800
O 7.34958 6.97576 7.37951
C 6.29221 3.98111 8.82277
C 5.96651 3.18095 9.92079
C 5.66829 1.83133 9.70881
C 5.70171 1.31580 8.40582
C 6.03881 2.16979 7.35682
C 6.16001 1.71754 5.90417
C 7.64329 1.70459 5.54460
C 8.38783 0.53421 5.40772
C 9.76002 0.63540 5.14164
C 10.34321 1.90030 5.02036
C 9.53758 3.03233 5.16596
C 4.34539 6.66017 5.92113
C 3.03664 7.12758 5.82596
C 2.01613 6.21336 5.53629
C 2.33529 4.86394 5.36349
C 3.66779 4.45273 5.48411
C 4.03174 2.98035 5.39581
C 5.65067 2.50232 3.56222
C 5.89937 3.78447 2.79238
C 5.58624 3.87806 1.43179
C 5.89805 5.04823 0.73475
C 6.50913 6.10772 1.41620
C 6.78336 5.95858 2.77354
H 6.51724 5.03398 8.92759
H 5.94441 3.61064 10.91423
H 5.40779 1.18858 10.54137
H 5.46681 0.27655 8.21026
H 5.73757 0.71409 5.78588
H 7.90763 -0.43198 5.50370
H 10.35985 -0.25997 5.02960
H 11.40025 2.01301 4.81559
H 9.94356 4.03158 5.08075
H 5.17441 7.32040 6.14004
H 2.82489 8.17971 5.96886
H 0.98875 6.54629 5.44469
H 1.56394 4.13618 5.13989
H 5.10599 3.04553 0.93129
H 5.66286 5.13453 -0.31963
H 6.76089 7.03151 0.91099
H 7.23684 6.75622 3.34665
H 3.36485 2.47848 4.68613
H 3.83821 2.52657 6.37341
H 4.78870 1.97441 3.13882
H 6.51631 1.84719 3.42167
H 8.03929 6.90816 8.08618
C 10.56456 8.40709 7.53901
C 11.45229 7.32854 7.41128
C 11.62735 6.70398 6.16852
C 10.91431 7.15791 5.04919
C 10.02056 8.23701 5.17540
C 9.84863 8.86272 6.42234
H 10.43735 8.89470 8.50005
H 12.00672 6.97896 8.27596
H 12.31944 5.87424 6.07031
H 11.05919 6.68578 4.08284
H 8.53185 6.68190 5.79856
H 9.48976 8.60783 4.30399
H 9.16682 9.70097 6.51789
O 7.93665 6.07168 6.31101

66
FeOO + CHD React sideon (2/7)
Fe 6.22825 4.86851 5.24405
N 5.51217 2.77732 5.05687
N 6.45478 4.08558 7.25992
N 8.06188 3.75236 4.91442
N 4.13338 5.12920 5.58375
N 5.77640 4.77592 3.14860
O 6.60415 6.84187 6.05530
C 6.45767 4.77856 8.42099
C 6.56739 4.12557 9.65047
C 6.67068 2.73128 9.67293
C 6.66357 2.01808 8.46559
C 6.55504 2.72921 7.27432
C 6.58880 2.10376 5.88797
C 7.93164 2.44233 5.25840
C 8.97198 1.53489 5.08465
C 10.17965 1.99640 4.54176
C 10.30726 3.34422 4.19227
C 9.22399 4.20357 4.39055
C 3.52108 6.34095 5.63594
C 2.13829 6.45413 5.74169
C 1.36709 5.28574 5.78414
C 2.00219 4.04214 5.72866
C 3.39559 3.98977 5.63492
C 4.13931 2.67427 5.65864
C 5.53868 2.37702 3.60899
C 5.39777 3.55916 2.67897
C 4.96079 3.40419 1.36065
C 4.93058 4.51661 0.51533
C 5.33395 5.76461 1.00676
C 5.74617 5.86137 2.33227
H 6.37108 5.85398 8.34846
H 6.56931 4.70251 10.56608
H 6.75221 2.20247 10.61485
H 6.73539 0.93768 8.45257
H 6.44135 1.02180 5.94099
H 8.84272 0.49608 5.36127
H 11.00479 1.31047 4.39328
H 11.22675 3.72887 3.77054
H 9.27399 5.25478 4.14311
H 4.16269 7.21045 5.58850
H 1.67910 7.43328 5.78282
H 0.28754 5.34272 5.85640
H 1.42925 3.12339 5.75874
H 4.65315 2.42804 1.00621
H 4.59497 4.41245 -0.50954
H 5.32320 6.64651 0.37958
H 6.05562 6.80268 2.76614
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H 3.56101 1.90091 5.14480
H 4.23663 2.35060 6.69956
H 4.75737 1.63809 3.40854
H 6.49369 1.88517 3.39993
H 8.77165 7.79048 7.43006
C 9.86171 7.89548 7.55841
C 10.37090 6.84439 8.51677
C 11.35148 5.97974 8.21661
C 12.06271 5.95340 6.88398
C 11.52432 6.97607 5.91097
C 10.54308 7.84087 6.21154
H 9.98893 8.89857 8.00111
H 9.90254 6.81405 9.49891
H 11.67598 5.24920 8.95541
H 13.14460 6.11220 7.03336
H 11.99462 4.94474 6.44297
H 11.98050 6.99501 4.92280
H 10.20555 8.55848 5.46613
O 7.36776 6.68391 4.93727

66
FeOO + CHD TS sideon (2/7)
Fe 6.48232 4.92540 5.28482
N 5.66039 2.82271 5.08384
N 6.64094 4.07324 7.30335
N 8.22920 3.71226 4.90556
N 4.40784 5.25746 5.64780
N 5.87785 4.79027 3.16540
O 6.98466 6.91253 6.16831
C 6.62501 4.74029 8.47857
C 6.69531 4.06358 9.69834
C 6.78014 2.66775 9.69589
C 6.78246 1.97935 8.47474
C 6.70818 2.71599 7.29522
C 6.71793 2.10960 5.90090
C 8.06499 2.40942 5.25781
C 9.07449 1.47056 5.06427
C 10.28079 1.89264 4.48747
C 10.43895 3.23359 4.12165
C 9.38756 4.12578 4.34470
C 3.86049 6.49740 5.72336
C 2.48597 6.67904 5.84660
C 1.65753 5.55021 5.88377
C 2.22850 4.27683 5.80634
C 3.61704 4.15517 5.69511
C 4.29009 2.79881 5.69531
C 5.64802 2.40579 3.64485
C 5.44855 3.58251 2.72121
C 4.90628 3.43472 1.44120
C 4.82255 4.55078 0.60373
C 5.27698 5.79128 1.06755
C 5.79354 5.87761 2.35857
H 6.54655 5.81703 8.42167
H 6.68103 4.62246 10.62516
H 6.83457 2.11932 10.62862
H 6.83065 0.89793 8.44155
H 6.54176 1.03083 5.94607
H 8.92109 0.43702 5.34876
H 11.08091 1.18122 4.32213
H 11.35670 3.58569 3.66848
H 9.45086 5.17477 4.08919
H 4.55192 7.32869 5.68700
H 2.07627 7.67912 5.90607
H 0.58298 5.66021 5.96979
H 1.61005 3.38775 5.83362
H 4.55882 2.46318 1.11085
H 4.40547 4.45495 -0.39188
H 5.22518 6.67667 0.44679
H 6.14475 6.80889 2.78215
H 3.66070 2.06904 5.17655
H 4.37107 2.45501 6.73126
H 4.87973 1.64468 3.47365
H 6.60863 1.93814 3.40798
H 8.18568 7.15669 6.75323
C 9.28065 7.62499 7.23752
C 9.71649 6.73146 8.31594
C 10.79591 5.91897 8.18406
C 11.65085 5.91227 6.95153
C 11.25189 6.92840 5.92298
C 10.16604 7.73275 6.07464
H 8.82781 8.56782 7.56830
H 9.14352 6.72916 9.23848
H 11.09036 5.26128 8.99691
H 12.70965 6.05956 7.22986
H 11.64988 4.90226 6.50017
H 11.88734 7.02571 5.04722
H 9.92694 8.47460 5.31899
O 7.26889 6.66795 4.74333

66
FeOO + CHD Interm sideon (2/7)
Fe 6.44701 4.87239 5.24010
N 5.62621 2.77689 5.03754
N 6.64767 4.02667 7.24419
N 8.18822 3.66885 4.82969
N 4.39902 5.21011 5.65583
N 5.83167 4.75120 3.14037
O 7.00534 6.97059 6.21261
C 6.67118 4.69510 8.41925
C 6.77132 4.01648 9.63558
C 6.84282 2.62011 9.63110
C 6.80808 1.93150 8.41037
C 6.70888 2.66792 7.23325
C 6.69544 2.06172 5.83880
C 8.03422 2.36454 5.18015
C 9.05083 1.43477 4.98327
C 10.25507 1.87054 4.41163
C 10.40503 3.21508 4.05584
C 9.34549 4.09758 4.27734
C 3.86600 6.45467 5.76047
C 2.49707 6.64454 5.92350
C 1.66084 5.52170 5.96848
C 2.21788 4.24444 5.85867
C 3.60149 4.11246 5.70919
C 4.26392 2.75154 5.67063
C 5.59643 2.36388 3.59673
C 5.40549 3.54766 2.68167
C 4.87239 3.41466 1.39666
C 4.79526 4.54007 0.57115
C 5.24584 5.77581 1.05150
C 5.75290 5.84925 2.34653
H 6.60325 5.77251 8.36471
H 6.78972 4.57552 10.56212
H 6.91785 2.07111 10.56199
H 6.84945 0.84991 8.37597
H 6.51762 0.98356 5.88406
H 8.90653 0.39905 5.26417
H 11.06162 1.16672 4.24537
H 11.32338 3.57796 3.61282
H 9.40314 5.14866 4.02869
H 4.56198 7.28153 5.71361
H 2.09714 7.64681 6.00630
H 0.59001 5.63929 6.08475
H 1.59230 3.36059 5.89008
H 4.52672 2.44711 1.05337
H 4.38539 4.45524 -0.42834
H 5.19781 6.66791 0.44032
H 6.09840 6.77641 2.78357
H 3.62244 2.03778 5.14534
H 4.35851 2.38444 6.69744
H 4.81609 1.61462 3.43031
H 6.54852 1.88356 3.35097
H 7.93887 7.17685 6.50640
C 9.66974 8.07215 7.31830
C 9.83620 7.19995 8.43720
C 10.71306 6.14589 8.39596
C 11.55846 5.85584 7.18419
C 11.33599 6.81914 6.04821
C 10.44353 7.85826 6.13758
H 9.03401 8.94852 7.40157
H 9.25754 7.38544 9.33783
H 10.82939 5.49334 9.25652
H 12.62955 5.84822 7.46624
H 11.38603 4.81758 6.84058
H 11.92351 6.67557 5.14586
H 10.32561 8.54134 5.30105
O 7.17466 6.60013 4.74634

76
FeOO+CHD+CI React sideon(0/7)
Fe 6.18330 5.07857 5.34505
N 5.55198 2.97061 5.05345
N 6.54526 4.16248 7.28876
N 8.03478 4.06678 4.82375
N 4.09139 5.21981 5.76034
N 5.60423 5.11759 3.28918
O 6.49978 6.98009 6.31333
C 6.57563 4.77058 8.49628
C 6.79188 4.04113 9.66736
C 6.97656 2.65769 9.58204
C 6.93856 2.03188 8.32796
C 6.71952 2.81661 7.19956
C 6.70086 2.29075 5.77266
C 7.98862 2.73397 5.09421
C 9.05566 1.89126 4.79983
C 10.20050 2.44294 4.20616
C 10.23770 3.81151 3.92483
C 9.13265 4.60555 4.24512
C 3.42278 6.39718 5.86721
C 2.03776 6.43659 6.00708
C 1.32648 5.23107 6.02974
C 2.02015 4.02288 5.91164
C 3.41103 4.04375 5.78086
C 4.22040 2.76893 5.71893
C 5.51016 2.68026 3.58044
C 5.24585 3.91922 2.75595
C 4.71063 3.83905 1.46832
C 4.55835 5.00876 0.71722
C 4.94052 6.23509 1.27214
C 5.45614 6.25834 2.56593
H 6.42551 5.84126 8.50702
H 6.81281 4.55140 10.62159
H 7.14354 2.07003 10.47667
H 7.07012 0.96129 8.23169
H 6.60236 1.20198 5.75581
H 8.99368 0.83293 5.02055
H 11.04441 1.80864 3.96279
H 11.10199 4.26601 3.45806
H 9.11913 5.66654 4.03237
H 4.01160 7.30295 5.81644
H 1.53971 7.39435 6.07802
H 0.24740 5.23074 6.12889
H 1.49394 3.07591 5.91774
H 4.42024 2.87683 1.06407
H 4.14419 4.96290 -0.28303
H 4.83479 7.16084 0.72179
H 5.74171 7.18452 3.04605
H 3.65765 1.98471 5.20370
H 4.38997 2.41317 6.73975
H 4.75875 1.91356 3.36956
H 6.47575 2.26242 3.27996
H 8.79897 7.68454 7.91714
C 9.87187 7.67621 8.17216
C 10.23195 6.36748 8.83585
C 11.19556 5.54856 8.38778
C 12.03839 5.83905 7.16797
C 11.65951 7.13417 6.48865
C 10.69424 7.95176 6.93544
H 9.98805 8.50500 8.89163
H 9.66610 6.10190 9.72698
H 11.40819 4.62098 8.91643
H 13.10586 5.86069 7.44733
H 11.96121 5.00436 6.45122
H 12.21834 7.39490 5.59173
H 10.47403 8.87355 6.40012
O 7.25443 6.95343 5.18001
Cl 3.67344 9.88642 4.07176
O 4.97458 9.12215 4.31889
O 3.00180 9.35324 2.81433
O 2.74620 9.69390 5.26727
O 3.98065 11.36515 3.90043
Cl 9.25570 7.72036 1.56876
O 10.20732 8.44390 0.62865
O 8.92633 6.34633 1.00243
O 9.92229 7.55547 2.93396
O 7.97608 8.53171 1.72296

76
FeOO+CHD+CI R sideon(0/1)
Fe 6.18532 4.39734 4.80328
N 5.36360 2.55777 4.94481
N 6.59625 4.06647 6.72811
N 7.80392 3.34773 4.33439
N 4.37811 5.05130 5.28137
N 5.61523 4.32692 2.91386
O 7.08500 6.01611 4.56051
C 6.76616 4.95922 7.72601
C 7.04179 4.52999 9.02722
C 7.12891 3.16074 9.29281
C 6.94266 2.23914 8.25060
C 6.68080 2.72721 6.97726
C 6.50374 1.89464 5.71815
C 7.74686 2.09346 4.86662
C 8.76452 1.17155 4.66148
C 9.87375 1.56534 3.89582
C 9.92490 2.85627 3.36330
C 8.86304 3.73597 3.59407
C 3.95189 6.33526 5.19558
C 2.62946 6.67709 5.46773
C 1.72610 5.67138 5.82752
C 2.17044 4.34762 5.90282
C 3.50734 4.06061 5.62583
C 4.07293 2.66458 5.72300
C 5.16471 2.00859 3.54961
C 5.10036 3.12494 2.53413
C 4.58372 2.94531 1.25044
C 4.60836 4.01507 0.34987
C 5.14393 5.24263 0.75544
C 5.63874 5.37165 2.05096
H 6.68587 6.00298 7.45418
H 7.18298 5.26280 9.81067
H 7.33434 2.80848 10.29632
H 6.99627 1.17254 8.42782
H 6.30202 0.84384 5.93363
H 8.69671 0.17646 5.08245
H 10.68372 0.86758 3.72086
H 10.76781 3.19844 2.77823
H 8.85104 4.74106 3.19376
H 4.67476 7.08349 4.90714
H 2.32458 7.71158 5.38241
H 0.69016 5.91010 6.03634
H 1.49248 3.54552 6.16757
H 4.17030 1.98582 0.96496
H 4.21033 3.89222 -0.65024
H 5.17269 6.09514 0.08976
H 6.05125 6.30320 2.41313
H 3.35645 1.92403 5.36014
H 4.27329 2.42397 6.77110
H 4.26066 1.39616 3.51811
H 6.00272 1.34730 3.30977
H 9.28150 7.75700 6.17691
C 10.24987 7.62161 6.68637
C 10.07228 7.78502 8.17750
C 10.42351 6.85123 9.07404
C 11.04169 5.52434 8.69925
C 11.19533 5.35041 7.20580
C 10.84219 6.28393 6.30868
H 10.88400 8.43498 6.29314
H 9.63421 8.72271 8.51528
H 10.27011 7.03353 10.13632
H 12.02319 5.41562 9.19229
H 10.43661 4.69970 9.11245
H 11.62415 4.40837 6.86790
H 10.98401 6.09805 5.24556
O 6.94589 7.01163 5.47855
Cl 4.51008 9.35279 2.44488
O 4.40566 9.33116 3.96877
O 5.79836 8.65458 2.01722
O 3.31570 8.62630 1.84451
O 4.52975 10.79243 1.95955
Cl 10.74665 6.74905 1.68087
O 10.83883 8.08126 2.40836
O 11.42806 6.85543 0.32533
O 11.43508 5.66645 2.51129
O 9.27976 6.37469 1.48359

76
FeOO+CHD+CI TS sideon(0/1)
Fe 6.33100 4.38588 4.86760
N 5.42435 2.56777 4.96800
N 6.72428 3.98610 6.79135
N 7.90515 3.26432 4.38499
N 4.54800 5.08673 5.36793
N 5.74817 4.34895 2.97036
O 7.21932 5.94905 4.61997
C 6.91176 4.84349 7.81663
C 7.12920 4.37038 9.11411
C 7.14619 2.99264 9.34818
C 6.94483 2.10788 8.27812
C 6.73625 2.63964 7.01121
C 6.53338 1.84361 5.73313
C 7.78836 2.00441 4.89083
C 8.76062 1.03724 4.66586
C 9.88563 1.38973 3.90412
C 9.99598 2.68623 3.39342
C 8.97905 3.61124 3.64659
C 4.18460 6.39148 5.31481
C 2.87461 6.78703 5.57831
C 1.92031 5.81486 5.89626
C 2.30210 4.47004 5.94169
C 3.62887 4.12984 5.67423
C 4.13599 2.70967 5.74298
C 5.20794 2.04498 3.56754
C 5.18019 3.17906 2.57118
C 4.64571 3.04383 1.28893
C 4.70634 4.12845 0.40778
C 5.29568 5.32425 0.83237
C 5.80717 5.40664 2.12611
H 6.89418 5.89396 7.56029
H 7.27856 5.07677 9.92040
H 7.30741 2.60664 10.34747
H 6.94308 1.03573 8.42882
H 6.28902 0.79715 5.92694
H 8.64478 0.03892 5.06876
H 10.66004 0.65665 3.71279
H 10.85050 2.99353 2.80530
H 9.01044 4.62167 3.26488
H 4.95462 7.10501 5.06133
H 2.61842 7.83651 5.51777
H 0.89316 6.09566 6.09687
H 1.58355 3.69396 6.17591
H 4.19042 2.10749 0.99003
H 4.29464 4.04146 -0.59073
H 5.35310 6.18799 0.18295
H 6.26269 6.30791 2.51127
H 3.39070 2.00662 5.36318
H 4.32268 2.43967 6.78658
H 4.28532 1.46089 3.52505
H 6.02527 1.36213 3.31676
H 8.47834 7.16779 6.05783
C 9.65021 7.44227 6.39691
C 9.59708 7.81516 7.82418
C 10.09543 7.01706 8.79662
C 10.78740 5.71479 8.50200
C 10.96246 5.44233 7.03400
C 10.46041 6.25418 6.07218
H 9.79075 8.28543 5.70941
H 9.12274 8.75822 8.08236
H 10.02811 7.31656 9.83930
H 11.76936 5.69087 9.00573
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H 10.23508 4.88169 8.97453
H 11.54769 4.56811 6.75996
H 10.64422 6.03737 5.02388
O 7.17510 6.96083 5.64694
Cl 4.73027 9.44276 2.57159
O 4.63663 9.44763 4.09574
O 6.01411 8.73711 2.14469
O 3.52996 8.70841 1.99205
O 4.74660 10.87469 2.06120
Cl 10.66535 6.76680 1.72320
O 10.60477 8.07128 2.50470
O 11.44019 6.97751 0.43181
O 11.36705 5.70103 2.56607
O 9.25056 6.29850 1.39750

76
FeOO+CHD+CI Interm sideon(0/1)
Fe 6.31545 4.21070 4.91372
N 5.32846 2.44397 4.88611
N 6.68047 3.66036 6.80591
N 7.84319 3.04764 4.36569
N 4.56699 4.96924 5.44218
N 5.75347 4.33347 3.01839
O 7.33436 5.69616 4.80013
C 6.92751 4.43505 7.88402
C 7.14059 3.86165 9.14110
C 7.08828 2.47205 9.28036
C 6.82648 1.67472 8.15622
C 6.62949 2.30287 6.93249
C 6.39046 1.60851 5.60257
C 7.65904 1.76264 4.77949
C 8.58614 0.76683 4.49651
C 9.73717 1.11640 3.77326
C 9.91835 2.43922 3.35942
C 8.94427 3.39327 3.66741
C 4.26266 6.29015 5.46270
C 2.96690 6.72770 5.73146
C 1.96512 5.78302 5.97696
C 2.28609 4.42186 5.94691
C 3.60028 4.03865 5.67742
C 4.04192 2.59585 5.66480
C 5.09454 2.02543 3.45190
C 5.14021 3.22099 2.53223
C 4.62594 3.19653 1.23507
C 4.75290 4.33387 0.43085
C 5.38588 5.47056 0.94570
C 5.87534 5.44266 2.25014
H 6.95969 5.50053 7.70161
H 7.33969 4.50093 9.99151
H 7.24434 2.01032 10.24783
H 6.77322 0.59606 8.23251
H 6.08800 0.56599 5.72021
H 8.41756 -0.25028 4.82722
H 10.47761 0.36134 3.53798
H 10.79540 2.74531 2.80470
H 9.03272 4.42584 3.36092
H 5.07111 6.97958 5.27145
H 2.75934 7.78960 5.73127
H 0.94823 6.09747 6.17995
H 1.52985 3.66677 6.12406
H 4.13522 2.30411 0.86606
H 4.35817 4.33288 -0.57820
H 5.49423 6.37216 0.35710
H 6.36226 6.29443 2.70310
H 3.26910 1.94991 5.24111
H 4.21166 2.25645 6.69079
H 4.14000 1.50041 3.36804
H 5.87370 1.31450 3.16191
H 8.09941 7.11081 5.90489
C 10.11801 7.94315 6.02002
C 9.75842 8.60003 7.23497
C 9.96954 8.00975 8.45634
C 10.59584 6.64597 8.58789
C 10.96495 6.02316 7.26667
C 10.73237 6.65533 6.07078
H 9.98975 8.44059 5.06429
H 9.31022 9.58876 7.18544
H 9.68953 8.52393 9.37150
H 11.48784 6.70169 9.24221
H 9.91933 5.97118 9.14852
H 11.43710 5.04467 7.28889
H 11.01923 6.17704 5.13850
O 7.19129 6.70558 5.90905
Cl 4.99707 9.49955 2.98868
O 4.82659 9.44085 4.50469
O 6.26790 8.75376 2.59226
O 3.79601 8.84912 2.31733
O 5.10433 10.95062 2.54775
Cl 10.74524 6.49831 1.75207
O 10.83922 7.85320 2.44021
O 11.46066 6.55419 0.41085
O 11.40179 5.43295 2.63054
O 9.27934 6.13753 1.53243
```

[(TMC)FeO]$^{2+}$ (3)

```
52
FeO syn (2/3)
Fe -0.06375 0.08747 -0.04494
H 1.70767 -1.60981 -3.71189
H -0.66835 -1.29297 -3.69455
H -1.53514 0.98066 -3.64663
H 1.44204 0.10664 -3.59275
C 1.33748 -0.82895 -3.03634
H -0.04632 1.59601 -2.89806
C -0.12218 -1.15953 -2.75225
C -1.02324 1.16989 -2.69694
H -2.86898 -0.62383 -2.60437
H 1.74471 1.75706 -2.27454
H -0.18454 -2.10154 -2.19751
H 3.28175 -0.73916 -2.09702
H -1.59096 1.88569 -2.10671
N -0.88937 -0.12402 -1.93958
H 3.35500 1.60156 -1.55157
C 2.23216 -0.85817 -1.80071
C -2.27039 -0.70241 -1.69030
H -2.14984 -1.76392 -1.46379
C 2.27859 1.57301 -1.34829
H 2.13684 -1.82658 -1.30156
H -3.08095 1.08131 -0.78536
N 1.92655 0.22168 -0.77904
H 2.01172 2.34254 -0.62751
C -2.92774 0.02791 -0.54756
H -3.90785 -0.40535 -0.32022
H 3.80322 -0.31016 0.11790
O -0.09680 1.69445 0.14777
C 2.80795 0.01647 0.43900
H -2.14306 -2.16646 0.69599
N -2.04632 -0.04193 0.68516
H 2.08852 -1.97207 0.87537
H 2.92243 0.98258 0.93191
H -2.23163 2.04621 1.04763
C 2.18122 -0.99823 1.36109
C -2.29663 -1.35346 1.41096
H 0.17525 -2.55559 1.57060
H -3.35294 -1.36344 1.70725
C -2.44530 1.11508 1.56747
H -3.51673 1.04111 1.78492
N 0.78675 -0.53941 1.74936
H 2.78518 -1.13406 2.26523
C 0.06517 -1.75720 2.31124
H 1.39020 1.41812 2.36445
C -1.41176 -1.56785 2.63595
H -1.89684 1.10187 2.50287
H -1.74742 -2.49875 3.10893
C 0.89132 0.54832 2.78628
H 0.61107 -2.06330 3.21250
H -0.09605 0.85040 3.11957
H -1.56707 -0.79078 3.38959
H 1.45812 0.17305 3.64515

52
FeO syn (2/5)
Fe -0.06126 0.24043 -0.02970
H 1.73722 -1.62793 -3.66587
H -0.64758 -1.36856 -3.75437
H -1.57321 0.88780 -3.75068
H 1.42109 0.08040 -3.58454
C 1.31811 -0.84891 -3.01714
H -0.08285 1.51550 -3.01606
C -0.14842 -1.21456 -2.78802
C -1.06121 1.09473 -2.80338
H -2.94150 -0.66001 -2.58482
H 1.75408 1.80172 -2.28865
H -0.21116 -2.15233 -2.22690
H 3.24086 -0.77666 -2.03813
H -1.62727 1.83091 -2.23586
N -0.92910 -0.18085 -2.01439
H 3.38169 1.62339 -1.60105
C 2.18235 -0.84167 -1.75688
C -2.30063 -0.71846 -1.69644
H -2.19745 -1.77435 -1.43818
C 2.31021 1.62318 -1.37286
H 2.04104 -1.78056 -1.21640
H -3.05481 1.12140 -0.83145
N 1.93436 0.29599 -0.77094
H 2.08014 2.41242 -0.65892
C -2.92296 0.07299 -0.56107
H -3.91099 -0.33084 -0.31346
H 3.80708 -0.19910 0.13656
O -0.08510 1.87828 0.18844
C 2.79800 0.07877 0.46156
H -2.09770 -2.09310 0.64381
N -2.05550 0.03421 0.68746
H 2.15031 -1.95484 0.85814
H 2.87060 1.03752 0.97672
H -2.29302 2.11106 1.07390
C 2.21971 -0.99242 1.36845
C -2.25883 -1.30798 1.38646
H 0.19377 -2.59129 1.53871
H -3.31601 -1.34049 1.67919
C -2.47916 1.16719 1.58331
H -3.54633 1.06579 1.80929
N 0.83466 -0.60125 1.81889
H 2.87150 -1.13114 2.23992
C 0.09532 -1.82149 2.31046
H 1.46415 1.31661 2.53084
C -1.38458 -1.57942 2.61067
H -1.91699 1.14932 2.51226
H -1.76930 -2.50610 3.05410
C 0.93012 0.44227 2.89850
H 0.60055 -2.18772 3.21482
H -0.06004 0.75987 3.21304
H -1.52199 -0.81562 3.38148
H 1.46076 0.02608 3.76329

52
FeO anti (2/3)
Fe -0.04663 -0.33300 -0.09426
H 1.80965 -1.17477 -3.95299
H -0.58740 -0.84754 -3.98682
H -1.89098 1.20913 -3.26033
H 1.48656 0.47657 -3.51503
C 1.38538 -0.55230 -3.15527
H -0.21593 1.64554 -2.89449
C -0.07845 -0.96415 -3.02155
C -1.12649 1.22404 -2.47677
H -2.79914 -0.81366 -2.71024
H 1.46129 1.82726 -1.86145
H -0.13779 -2.01316 -2.72706
H 3.29564 -0.58009 -2.16068
H -1.46145 1.86292 -1.65981
N -0.87645 -0.18428 -1.99316
H 3.13223 1.70855 -1.27562
C 2.24765 -0.79312 -1.91673
C -2.19891 -0.89840 -1.79699
H -1.97785 -1.95090 -1.62165
C 2.08194 1.52669 -1.02445
H 2.17301 -1.83462 -1.59632
H -3.28401 0.71672 -0.86277
N 1.89148 0.05965 -0.70974
H 1.81248 2.12675 -0.15433
C -2.92796 -0.28602 -0.62250
H -3.80325 -0.88555 -0.35741
H 3.72511 -0.78156 0.04292
O -0.01506 -1.94534 -0.28646
C 2.83180 -0.29390 0.44241
H -2.19955 -2.23832 1.00463
N -2.00245 -0.17858 0.58940
H 1.95019 -2.18134 1.01290
H 3.15475 0.63618 0.91183
H -1.98551 1.96223 0.55041
C 2.13483 -1.19463 1.43690
C -2.31538 -1.30504 1.55984
H 0.12243 -2.57966 2.06513
H -3.36940 -1.19825 1.84489
C -2.26379 1.16274 1.23860
H -3.32961 1.24543 1.47525
N 0.78701 -0.59984 1.79468
H 2.73875 -1.30941 2.34468
C 0.02382 -1.63449 2.60123
H 1.36505 1.46569 1.99302
C -1.45460 -1.32423 2.82265
H -1.69104 1.27457 2.15259
H -1.84826 -2.13157 3.45287
C 0.98624 0.65271 2.61072
H 0.53180 -1.73229 3.56887
H 0.04568 0.96669 3.05418
H -1.59326 -0.41291 3.41278
H 1.69947 0.45173 3.41703

52
FeO anti (2/5)
Fe -0.04427 -0.41110 -0.10067
H 1.80045 -1.18370 -3.94516
H -0.59029 -0.91678 -3.95982
H -1.83539 1.21796 -3.21584
H 1.43951 0.46196 -3.52523
C 1.37918 -0.56254 -3.14470
H -0.16084 1.60335 -2.78152
C -0.07822 -1.01586 -2.99421
C -1.09304 1.18782 -2.41161
H -2.82191 -0.84811 -2.67841
H 1.67514 1.88685 -1.93609
H -0.11776 -2.06271 -2.68805
H 3.33396 -0.55201 -2.23951
H -1.43869 1.80047 -1.57951
N -0.89291 -0.23968 -1.97612
H 3.31451 1.74341 -1.27651
C 2.29913 -0.75387 -1.93121
C -2.23288 -0.91788 -1.75646
H -2.03100 -1.96925 -1.55054
C 2.25031 1.58402 -1.06551
H 2.24437 -1.78662 -1.57977
H -3.31364 0.74712 -0.89671
N 2.00091 0.13778 -0.73792
H 1.95249 2.20606 -0.22064
C -2.98092 -0.25108 -0.60830
H -3.87846 -0.83051 -0.36724
H 3.79743 -0.73423 0.06549
O -0.01192 -2.06507 -0.30214
C 2.88372 -0.25835 0.43690
H -2.27270 -2.18690 0.99427
N -2.11436 -0.10933 0.63474
H 2.00851 -2.18376 0.95365
H 3.18654 0.65598 0.94888
H -2.15791 2.02347 0.62397
C 2.17006 -1.20145 1.39855
C -2.36815 -1.27068 1.58102
H 0.10252 -2.61835 2.00771
H -3.40825 -1.19126 1.92540
C -2.42913 1.20583 1.29295
H -3.50006 1.26359 1.52168
N 0.80463 -0.64831 1.76602
H 2.76206 -1.32439 2.31314
C 0.02439 -1.68010 2.56020
H 1.33255 1.43332 1.90065
C -1.44910 -1.33489 2.80851
H -1.87033 1.31743 2.21789
H -1.83957 -2.14620 3.43601
C 0.94794 0.63791 2.53666
H 0.53683 -1.80150 3.52271
H -0.01319 0.94682 2.93535
H -1.54893 -0.43437 3.42219
H 1.64029 0.47857 3.37039

58
FeO+CNCH3 syn (2/3)
Fe -0.05445 -0.14195 -0.07022
H 1.77202 -1.21491 -3.96101
H -0.59574 -0.75834 -3.99935
H -1.72309 1.19698 -3.43607
H 1.52007 0.44744 -3.51535
C 1.37985 -0.57702 -3.15876
H -0.19015 1.74604 -2.72283
C -0.10297 -0.92345 -3.03257
C -1.13667 1.25525 -2.51232
H -2.82825 -0.72649 -2.70423
H 1.64971 1.81440 -1.95758
H -0.21166 -1.98002 -2.79200
H 3.29812 -0.71253 -2.19003
H -1.66791 1.84646 -1.77191
N -0.89135 -0.13950 -1.99346
H 3.33269 1.52857 -1.45720
C 2.24214 -0.85102 -1.92392
C -2.21943 -0.84500 -1.79952
H -2.01966 -1.90718 -1.67398
C 2.28370 1.48187 -1.14301
H 2.12262 -1.88074 -1.58574
H -3.33251 0.71875 -0.82193
N 1.95219 0.06122 -0.74802
H 2.11987 2.13957 -0.29328
C -2.96016 -0.28278 -0.60431
H -3.83038 -0.90719 -0.37639
H 3.74986 -0.80498 0.05935
O -0.08646 1.47942 0.12726
C 2.85625 -0.29066 0.42741
H -2.16192 -2.27282 0.98917
N -2.06746 -0.18344 0.62752
H 1.98129 -2.15930 1.06459
H 3.18774 0.64415 0.88050
H -2.31701 1.93545 0.67091
C 2.14397 -1.15361 1.44702
C -2.31620 -1.35511 1.55727
H 0.18320 -2.56332 2.13848
H -3.37433 -1.32061 1.84764
C -2.45541 1.09127 1.34127
H -3.50600 1.02206 1.64596
N 0.79208 -0.56301 1.79975
H 2.75078 -1.23808 2.35702
C 0.03879 -1.59818 2.62180
H 1.47977 1.45187 2.04901
C -1.45484 -1.34452 2.82267
H -1.83771 1.24891 2.21854
H -1.81774 -2.16568 3.45394
C 0.98835 0.67848 2.63233
H 0.53111 -1.64846 3.60142
H 0.02478 1.06061 2.95731
H -1.62886 -0.43729 3.40857
H 1.59223 0.43046 3.51228
N -0.01932 -2.26510 -0.32822
C -0.00513 -3.42342 -0.46859
C 0.01226 -4.86294 -0.64083
H 0.91996 -5.16698 -1.17090
H -0.01048 -5.35832 0.33480
H -0.85942 -5.18269 -1.21989

58
FeO+CNCH3 syn (2/5)
```

```
Fe -0.05579 -0.10812 -0.06827
H 1.78015 -1.14194 -3.98817
H -0.57268 -0.79584 -4.07116
H -1.78687 1.17946 -3.53596
H 1.48107 0.49606 -3.49249
C 1.36667 -0.54220 -3.16700
H -0.26475 1.74082 -2.80450
C -0.11606 -0.92958 -3.08080
C -1.20849 1.23667 -2.60568
H -2.90354 -0.77436 -2.70962
H 1.73134 1.84631 -1.92894
H -0.20641 -1.98564 -2.82736
H 3.30713 -0.70977 -2.24689
H -1.75488 1.82168 -1.86926
N -0.95074 -0.14842 -2.08469
H 3.41711 1.54588 -1.44097
C 2.25708 -0.83132 -1.94684
C -2.25311 -0.86623 -1.82957
H -2.03193 -1.92358 -1.69697
C 2.36897 1.49515 -1.12267
H 2.13249 -1.86170 -1.61187
H -3.39585 0.68119 -0.84577
N 2.02632 0.07559 -0.75306
H 2.21179 2.14036 -0.26091
C -2.99875 -0.30857 -0.61641
H -3.85595 -0.95555 -0.39869
H 3.77193 -0.87039 0.06506
O -0.08668 1.51481 0.12713
C 2.89438 -0.32490 0.42923
H -2.17241 -2.25884 1.00801
N -2.14267 -0.17034 0.63314
H 1.99359 -2.18494 1.09123
H 3.25835 0.59497 0.88890
H -2.40473 1.94396 0.64385
C 2.17612 -1.18175 1.47219
C -2.33441 -1.34249 1.57664
H 0.17416 -2.57910 2.16773
H -3.38685 -1.33510 1.89260
C -2.53557 1.10761 1.32726
H -3.58396 1.04415 1.64267
N 0.84814 -0.59222 1.88436
H 2.82576 -1.27711 2.35237
C 0.04713 -1.61713 2.66355
H 1.58383 1.39887 2.14949
C -1.44868 -1.31647 2.83337
H -1.90888 1.28082 2.19759
H -1.83446 -2.10872 3.48806
C 1.05567 0.63817 2.71994
H 0.50307 -1.70510 3.65939
H 0.09342 1.04833 3.01880
H -1.59991 -0.39000 3.39548
H 1.63200 0.38201 3.61742
N -0.01750 -2.22245 -0.32376
C -0.00050 -3.38095 -0.46012
C 0.02041 -4.82028 -0.62690
H 0.92890 -5.12339 -1.15630
H -0.00036 -5.31162 0.35096
H -0.85083 -5.14414 -1.20443

58
FeO+CNCH3 anti (2/3)
Fe -0.00228 -0.37066 0.01591
H -2.07113 0.08401 3.85242
H -3.47118 0.18380 1.89888
H -3.86585 -1.53731 0.36307
H -2.01777 -1.47866 3.08823
C -1.69863 -0.43949 2.96270
H -2.45001 -2.39079 1.00519
C -2.38193 0.22149 1.76803
C -2.78692 -1.68918 0.24628
H -3.68031 0.59910 -0.64316
H -0.80892 -2.84182 2.00724
H -2.07999 1.26798 1.72181
H 0.19762 -0.66386 3.96607
H -2.59079 -2.11637 -0.73434
N -2.07657 -0.37436 0.40242
H 0.45421 -2.82057 3.25295
C -0.17373 -0.31841 2.99253
C -2.58366 0.61504 -0.63007
H -2.25833 1.60586 -0.31385
C 0.23188 -2.60503 2.20168
H 0.12981 0.71998 2.85454
H -2.43851 -0.67279 -2.35120
N 0.52666 -1.14747 1.92971
H 0.86025 -3.23187 1.57598
C -2.03936 0.27910 -1.99830
H -2.33863 1.04347 -2.72396
H 2.30174 -0.80882 3.09328
O -0.05797 1.18132 0.55285
C 2.03444 -0.97626 2.04414
H -0.25446 2.22444 -1.55172
N -0.52167 0.16535 -1.98373
H 2.13492 1.11759 1.54414
H 2.49905 -1.91532 1.74066
H -0.71868 -1.71110 -2.99449
C 2.52709 0.16563 1.18767
C 0.10696 1.51263 -2.29456
H 1.93812 2.09621 -0.27693
H -0.26161 1.81966 -3.28200
C -0.14583 -0.79360 -3.08972
H -0.38050 -0.32985 -4.05460
N 2.05977 -0.00651 -0.24531
H 3.62260 0.21284 1.21120
C 2.30255 1.31889 -0.94881
H 2.70151 -2.04413 -0.40539
C 1.63721 1.49089 -2.31243
H 0.91212 -1.03194 -3.06193
H 1.95915 2.47162 -2.68512
C 2.85073 -1.09502 -0.91489
H 3.38946 1.43423 -1.05171
H 2.53922 -1.20463 -1.95078
H 2.01758 0.76942 -3.04227
H 3.91589 -0.83862 -0.89277
N 0.06653 -2.32863 -0.66256
C 0.10730 -3.43256 -1.03433
C 0.15912 -4.80691 -1.49318
H 0.52773 -5.45657 -0.69338
H -0.83956 -5.14273 -1.78851
H 0.82931 -4.89142 -2.35392

58
FeO+CNCH3 anti (2/5)
Fe -0.13238 -0.29239 0.03312
H -1.64618 -0.25257 4.15429
H -3.31429 -0.27240 2.46845
H -3.69016 -2.07785 0.98777
H -1.45081 -1.75010 3.29418
C -1.31898 -0.66827 3.19245
H -2.04849 -2.67841 1.30941
C -2.28011 -0.08627 2.14896
C -2.64428 -2.03861 0.66128
H -4.00527 0.10081 -0.05239
H -0.07220 -2.90743 2.19918
H -2.13446 0.99293 2.08669
H 0.68660 -0.56625 3.98724
H -2.57587 -2.41554 -0.35682
N -2.14752 -0.62505 0.73344
H 1.38981 -2.66173 3.17672
C 0.16791 -0.30146 3.05488
C -2.93212 0.27518 -0.20098
H -2.71137 1.30362 0.08571
C 0.92869 -2.48220 2.19711
H 0.27604 0.77333 2.89851
H -2.91140 -0.96213 -1.97292
N 0.88525 -1.00553 1.92137
H 1.51967 -2.98338 1.43379
C -2.58597 0.03349 -1.66633
H -3.13527 0.75424 -2.28485
H 2.70860 -0.23809 2.75644
O -0.35815 1.23545 0.60096
C 2.30830 -0.50794 1.77120
H -1.06339 2.20652 -1.51029
N -1.10445 0.13603 -1.96230
H 1.92867 1.56155 1.25568
H 2.90844 -1.34121 1.40157
H -1.17407 -1.76598 -2.92857
C 2.43642 0.69153 0.83926
C -0.70251 1.55526 -2.30814
H 1.27899 2.46609 -0.53155
H -1.22482 1.82836 -3.23618
C -0.78767 -0.76760 -3.12079
H -1.25659 -0.37751 -4.03305
N 1.82667 0.42964 -0.52375
H 3.49820 0.94030 0.71671
C 1.68558 1.75574 -1.25255
H 2.78147 -1.46537 -0.78334
C 0.80846 1.75443 -2.51069
H 0.28590 -0.83376 -3.27919
H 0.92717 2.75324 -2.95024
C 2.67513 -0.52155 -1.31417
H 2.69869 2.08481 -1.52013
H 2.21837 -0.71665 -2.28261
H 1.19858 1.06573 -3.26675
H 3.66843 -0.08461 -1.47169
N 0.14458 -2.21064 -0.67853
C 0.30094 -3.29450 -1.07824
C 0.49737 -4.64313 -1.57107
H 1.55052 -4.80038 -1.82302
H 0.20456 -5.36844 -0.80584
H -0.10882 -4.80929 -2.46672

66
FeO+CHD syn React (2/3)
Fe -0.18684 -0.21182 -0.01303
H 2.20510 -1.25958 -3.57862
H -0.18393 -1.17356 -3.86590
H -1.39988 0.89470 -3.65205
H 1.71983 0.39199 -3.32113
C 1.65835 -0.60901 -2.88504
H -0.06636 1.59430 -2.71201
C 0.22507 -1.12655 -2.84874
C -0.99452 1.03649 -2.64449
H -2.56274 -0.98495 -2.96356
H 1.58746 1.89026 -1.83978
H 0.21755 -2.14213 -2.44080
H 3.44248 -0.43378 -1.67704
H -1.69391 1.61017 -2.04059
N -0.75600 -0.31233 -2.01566
H 3.13112 1.85330 -0.96913
C 2.38360 -0.68839 -1.54399
C -2.06261 -1.08647 -1.99401
H -1.82170 -2.14263 -1.85483
C 2.05309 1.67503 -0.88433
H 2.33359 -1.71027 -1.15683
H -3.19570 0.47594 -1.02821
N 1.82706 0.23925 -0.47886
H 1.62283 2.32794 -0.12851
C -2.93497 -0.57216 -0.87780
H -3.86999 -1.14030 -0.82020
H 3.64887 -0.11749 0.59908
O -0.46375 1.34611 0.32593
C 2.58599 0.03211 0.81751
H -1.98584 -2.77806 0.21731
N -2.19805 -0.67561 0.44404
H 2.12703 -2.07009 0.98261
H 2.49522 0.94791 1.40259
H -2.71640 1.31324 1.00763
C 2.01653 -1.14916 1.55931
C -2.33760 -2.08569 0.98713
H 0.24679 -2.97397 1.34658
H -3.40807 -2.27188 1.13937
C -2.85814 0.30255 1.38371
H -3.92713 0.06856 1.44163
N 0.53429 -0.92946 1.80278
H 2.52467 -1.29558 2.51880
C -0.06151 -2.28901 2.14291
H 0.78693 1.00023 2.68792
C -1.57806 -2.33360 2.28875
H -2.43349 0.23640 2.37964
H -1.82818 -3.35197 2.61052
C 0.35877 0.03441 2.94704
H 0.41632 -2.62311 3.07253
H -0.69436 0.17705 3.16459
H -1.92962 -1.68300 3.09450
H 0.85686 -0.36905 3.83539
H -0.78099 3.84549 0.66655
C -1.22541 4.64867 1.27802
C -2.72774 4.49107 1.30626
C -3.43869 4.34778 2.43510
C -2.82188 4.33363 3.81445
C -1.31955 4.49419 3.78661
C -0.60965 4.63736 2.65754
H -0.95546 5.58137 0.75394
H -3.23615 4.50184 0.34358
H -4.52081 4.24107 2.38520
H -3.27154 5.12921 4.43290
H -3.09052 3.39960 4.33638
H -0.81309 4.49633 4.75016
H 0.47131 4.75660 2.70851

FeO+CHD syn TS (2/3)
Fe -0.25872 -0.06932 0.04272
H 2.18721 -1.12047 -3.51324
H -0.19804 -1.10034 -3.83115
H -1.44302 0.95646 -3.63741
H 1.65348 0.51863 -3.26848
C 1.61464 -0.48219 -2.82901
H -0.14948 1.68273 -2.66033
C 0.19373 -1.03636 -2.80730
C -1.06478 1.10166 -2.61897
H -2.61954 -0.90741 -2.93630
H 1.50252 2.03228 -1.79947
H 0.20791 -2.04873 -2.39162
H 3.38559 -0.26898 -1.60898
H -1.79122 1.65491 -2.02793
N -0.80956 -0.24232 -1.98926
H 3.04475 2.01653 -0.92447
C 2.32850 -0.53542 -1.47965
C -2.10499 -1.02998 -1.97607
H -1.85316 -2.08699 -1.87102
C 1.96788 1.82717 -0.84118
H 2.28972 -1.55495 -1.08627
H -3.24019 0.49373 -0.95431
N 1.75464 0.39343 -0.42665
H 1.52608 2.47648 -0.09039
C -2.97452 -0.55774 -0.83717
H -3.90665 -1.13335 -0.79350
H 3.58101 0.12718 0.66745
O -0.61042 1.53747 0.42856
C 2.50764 0.20735 0.87523
H -1.87724 -2.76005 0.14625
N -2.23544 -0.68990 0.47942
H 2.17672 -1.92169 1.01062
H 2.35314 1.10740 1.47206
H -2.88261 1.22448 1.13510
C 2.00720 -1.01764 1.59875
C -2.28341 -2.13386 0.94516
H 0.33572 -2.92549 1.30289
H -3.34123 -2.39918 1.07082
C -2.95607 0.19179 1.46619
H -4.00644 -0.11896 1.51673
N 0.51760 -0.89384 1.84378
H 2.52829 -1.14422 2.55506
C -0.01117 -2.28877 2.12276
H 0.66448 1.00947 2.80318
C -1.52654 -2.40854 2.24337
H -2.52083 0.11015 2.45668
H -1.73530 -3.45117 2.51330
C 0.28696 0.01297 3.02213
H 0.46612 -2.64367 3.04601
H -0.77347 0.09547 3.23705
H -1.91655 -1.81304 3.07354
H 0.79927 -0.39688 3.90066
H -0.88250 2.94093 0.86564
C -1.06620 4.05956 1.21065
C -2.53024 4.31362 1.15179
C -3.28346 4.48612 2.25839
C -2.70639 4.48410 3.64843
C -1.20537 4.38016 3.67517
C -0.46265 4.20868 2.56161
H -0.50738 4.59546 0.43010
H -2.99243 4.34346 0.16815
H -4.35318 4.65914 2.16977
H -3.02732 5.39220 4.18682
H -3.15017 3.66107 4.23755
H -0.72284 4.47290 4.64509
H 0.62121 4.15909 2.63224

FeO+CHD  Intermediate (2/3)
Fe -0.26321 0.07771 -0.10246
H 2.32177 -1.61573 -3.33668
H -0.04418 -1.61922 -3.76173
H -1.15618 0.53141 -3.96355
H 1.81046 0.04753 -3.38426
C 1.73291 -0.86811 -2.79118
H 0.07512 1.35268 -2.97901
C 0.30100 -1.39070 -2.74430
C -0.85925 0.80295 -2.94395
H -2.50043 -1.15616 -3.06876
H 1.77457 1.77667 -2.16974
H 0.26763 -2.31751 -2.16290
H 3.45557 -0.48957 -1.54488
H -1.61235 1.44879 -2.49786
N -0.70736 -0.44984 -2.12066
H 3.17130 1.91410 -1.08965
C 2.38866 -0.71580 -1.42068
C -2.04007 -1.16781 -2.07385
H -1.84975 -2.21041 -1.81308
C 2.09154 1.73032 -1.13200
H 2.31078 -1.66088 -0.87834
H -3.15233 0.53340 -1.34223
N 1.80368 0.37366 -0.54081
H 1.54609 2.47692 -0.56086
C -2.93839 -0.49907 -1.06255
H -3.89629 -1.02587 -0.98072
H 3.55988 0.22039 0.67751
O -0.56291 1.86245 0.05896
C 2.47787 0.33038 0.81663
H -1.96898 -2.57059 0.23629
N -2.26815 -0.46816 0.29835
H 2.10517 -1.77039 1.17584
H 2.30416 1.29583 1.29475
H -2.93486 1.51915 0.65671
C 1.92601 -0.80320 1.64907
C -2.37956 -1.84114 0.93864
H 0.18623 -2.70184 1.48501
H -3.45072 -2.05273 1.05067
C -3.01264 0.54421 1.12980
H -4.06472 0.24363 1.19547
N 0.43220 -0.63364 1.81206
H 2.40665 -0.82609 2.63466
C -0.15820 -1.96483 2.21716
H 0.61057 1.35927 2.57272
C -1.68272 -1.99489 2.28934
H -2.60385 0.60033 2.13335
H -1.95915 -2.98610 2.66890
C 0.17630 0.40679 2.86963
H 0.26568 -2.23794 3.19315
H -0.88926 0.55095 3.01700
H -2.06868 -1.28599 3.02774
H 0.62315 0.08049 3.81619
H -0.85554 2.53229 0.71094
C -1.39500 4.59434 1.57379
C -2.80170 4.42065 1.73766
C -3.33985 4.04974 2.94410
C -2.48570 3.81143 4.16183
C -1.01517 4.02787 3.91755
C -0.52757 4.39962 2.68915
H -0.99533 4.93592 0.62468
H -3.45533 4.59442 0.88712
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H -4.41369 3.92664 3.05319
H -2.82843 4.45625 4.99454
H -2.65927 2.78973 4.55255
H -0.34112 3.89021 4.75827
H 0.53951 4.55924 2.55947

66
FeO+CHD syn React (2/5)
Fe -0.20130 -0.09995 -0.03575
H 2.48971 -1.53697 -3.30485
H 0.15875 -1.50972 -3.88351
H -1.00380 0.62327 -3.97924
H 1.97646 0.12280 -3.22555
C 1.86271 -0.84510 -2.72884
H 0.22526 1.36310 -2.93249
C 0.43054 -1.37017 -2.82825
C -0.71963 0.82730 -2.93998
H -2.40240 -1.11241 -3.16789
H 1.82141 1.78032 -1.81278
H 0.36032 -2.34341 -2.33259
H 3.52505 -0.64396 -1.36675
H -1.47119 1.46245 -2.47503
N -0.60109 -0.47206 -2.18945
H 3.30020 1.72858 -0.83021
C 2.44489 -0.83081 -1.31597
C -1.94041 -1.16543 -2.17432
H -1.77090 -2.22009 -1.94907
C 2.21185 1.60435 -0.81511
H 2.29981 -1.81191 -0.85721
H -3.03625 0.53175 -1.38679
N 1.88111 0.21082 -0.35487
H 1.76339 2.31973 -0.12768
C -2.85467 -0.51746 -1.14988
H -3.82585 -1.02503 -1.12999
H 3.58702 -0.14246 0.88624
O -0.46413 1.51061 0.22617
C 2.50916 0.00764 1.01474
H -1.99414 -2.66767 0.08228
N -2.25592 -0.56326 0.24774
H 2.04679 -2.10573 1.19304
H 2.36853 0.93403 1.57321
H -2.81241 1.43814 0.69415
C 1.89446 -1.17437 1.74183
C -2.41692 -1.97208 0.81104
H 0.08249 -2.99553 1.42895
H -3.49715 -2.15810 0.86048
C -2.98570 0.44166 1.09721
H -4.05640 0.21083 1.08449
N 0.40956 -0.96782 1.90612
H 2.36779 -1.29290 2.72443
C -0.26275 -2.28950 2.19035
H 0.65243 0.95901 2.80554
C -1.79050 -2.23084 2.18104
H -2.62967 0.40747 2.12261
H -2.14248 -3.22260 2.49111
C 0.15846 0.01309 3.02013
H 0.08806 -2.64957 3.16709
H -0.90518 0.20601 3.12763
H -2.17450 -1.54210 2.93908
H 0.54295 -0.39701 3.96163
H -3.93641 20.71863 2.93902
C -4.28160 21.59448 3.51467
C -5.39294 21.18662 4.45342
C -5.34740 21.37046 5.78080
C -4.17925 22.00720 6.49675
C -3.06763 22.41446 5.55808
C -3.11319 22.23070 4.23069
H -4.67304 22.28556 2.74857
H -6.26602 20.72080 3.99988
H -6.18360 21.05330 6.40141
H -4.52452 22.88361 7.07149
H -3.78807 21.31673 7.26354
H -2.19448 22.88013 6.01165
H -2.27695 22.54777 3.61010

66
FeO+CHD syn Intermediate (2/5)
Fe -0.65421 0.76984 0.26133
H 1.90622 -0.73350 -3.16702
H -0.42842 -1.01825 -3.40927
H -1.72901 1.02361 -3.64079
H 1.24790 0.87666 -3.10544
C 1.30269 -0.06127 -2.54425
H -0.60440 2.00209 -2.66625
C -0.07201 -0.71825 -2.41374
C -1.46471 1.33865 -2.62379
H -2.91315 -0.77950 -2.60786
H 1.19500 2.61118 -1.83315
H 0.01307 -1.62381 -1.80449
H 3.10834 0.38872 -1.44006
H -2.29492 1.89075 -2.18540
N -1.15696 0.13187 -1.78147
H 2.75924 2.72635 -0.99970
C 2.06562 0.11138 -1.22883
C -2.39968 -0.72056 -1.64012
H -2.07946 -1.73156 -1.38061
C 1.68832 2.52598 -0.86755
H 2.08148 -0.84430 -0.69886
H -3.65930 0.85087 -0.84933
N 1.49234 1.15116 -0.29391
H 1.25803 3.26217 -0.19131
C -3.33993 -0.16030 -0.58729
H -4.24278 -0.78215 -0.52410
H 3.28194 1.01233 0.88391
O -1.15251 2.47317 0.45019
C 2.19798 1.09132 1.04060
H -2.22761 -2.15254 0.66555
N -2.67740 -0.08392 0.76740
H 1.91546 -1.02770 1.37671
H 2.01281 2.03926 1.55098
H -3.42565 1.85763 1.19342
C 1.71107 -0.07951 1.87749
C -2.62564 -1.45222 1.40423
H 0.04791 -2.05009 1.65419
H -3.65735 -1.75970 1.62726
C -3.47933 0.85860 1.62213
H -4.52232 0.51971 1.66851
N 0.22033 -0.00174 2.12167
H 2.23841 -0.09754 2.83936
C -0.27200 -1.39141 2.46806
H 0.38590 1.93465 3.00646
C -1.78007 -1.53552 2.67756
H -3.08083 0.88956 2.63416
H -1.93809 -2.54031 3.08926
C -0.06042 0.96791 3.23635
H 0.25405 -1.70823 3.37959
H -1.13167 1.11116 3.35518
H -2.14433 -0.85018 3.44916
H 0.36045 0.58683 4.17502
H -1.07885 3.39634 0.77723
C -0.85848 5.41911 1.43279
C -2.17969 5.61170 0.92861
C -3.27672 5.45330 1.73759
C -3.14857 5.08840 3.18895
C -1.72971 4.92812 3.65536
C -0.66346 5.09337 2.80869
H -0.00195 5.60482 0.79319
H -2.31008 5.88725 -0.11350
H -4.27732 5.60300 1.34333
H -3.66637 5.84255 3.81270
H -3.72142 4.16397 3.39761
H -1.56976 4.68385 4.70126
H 0.34924 4.98041 3.18395

66
FeO+CHD anti React (2/3)
Fe -0.13859 -0.21428 0.09552
H -2.32051 -0.28721 3.86818
H -3.67317 -0.09177 1.87223
H -3.81566 -1.72203 -0.06072
H -2.17249 -1.76460 2.96564
C -1.90082 -0.70428 2.94402
H -2.57362 -2.45890 0.96063
C -2.58555 0.03043 1.79327
C -2.73723 -1.79821 0.11429
H -3.82703 0.50624 -0.60898
H -0.81777 -2.86828 1.74501
H -2.35471 1.09561 1.84743
H -0.02152 -0.99454 3.95514
H -2.26401 -2.23461 -0.76412
N -2.17976 -0.42639 0.40438
H 0.65074 -3.05564 2.71807
C -0.38682 -0.51532 3.03826
C -2.73290 0.57271 -0.59300
H -2.45022 1.56711 -0.24764
C 0.23067 -2.60094 1.81463
H -0.14006 0.54791 3.08266
H -2.56598 -0.65019 -2.36432
N 0.40792 -1.10058 1.88389
H 0.75298 -2.99234 0.94040
C -2.16188 0.28014 -1.96241
H -2.42031 1.07628 -2.66595
H 2.06744 -0.61187 3.16452
O -0.25658 1.31120 0.63704
C 1.89513 -0.82290 2.10562
H -0.40211 2.23369 -1.74751
N -0.64118 0.14286 -1.89224
H 1.91769 1.27412 1.58723
H 2.44652 -1.73238 1.86341
H -0.67305 -1.93769 -2.40350
C 2.35648 0.33562 1.25016
C -0.00102 1.43352 -2.37325
H 1.76743 2.20932 -0.34202
H -0.34067 1.59658 -3.40375
C -0.24555 -1.01136 -2.79009
H -0.62935 -0.82984 -3.79934
N 1.90741 0.11514 -0.18005
H 3.44846 0.42692 1.28299
C 2.15961 1.39497 -0.95312
H 2.36640 -1.98025 -0.37854
C 1.52756 1.44872 -2.34301
H 0.83279 -1.11707 -2.83633
H 1.83454 2.40547 -2.78376
C 2.68999 -1.02450 -0.78919
H 3.24702 1.51846 -1.03587
H 2.54871 -1.04539 -1.86606
H 1.94568 0.68554 -3.00699
H 3.75578 -0.88404 -0.58032
H 0.02146 3.72513 1.34704
C -0.49147 4.47307 1.97387
C -1.92700 4.60518 1.52321
C -2.98051 4.40254 2.32919
C -2.85588 4.02809 3.78781
C -1.41986 3.88529 4.23620
C -0.36722 4.08630 3.42883
H 0.04998 5.41619 1.78777
H -2.08626 4.88394 0.48290
H -3.99091 4.51704 1.94085
H -3.36909 4.78003 4.41152
H -3.40544 3.09196 3.98372
H -1.26078 3.61132 5.27757
H 0.64343 3.97567 3.81821

66
FeO+CHD anti TS (2/3)
Fe -0.24462 -0.11386 0.14464
H -2.54759 -0.52138 3.82025
H -3.84642 -0.39618 1.78423
H -3.76751 -1.95557 -0.21238
H -2.21698 -1.94558 2.88014
C -2.05560 -0.86277 2.90037
H -2.51910 -2.60516 0.85931
C -2.77375 -0.16407 1.74474
C -2.69639 -1.94114 0.01748
H -3.96101 0.26774 -0.69888
H -0.73838 -2.87074 1.67172
H -2.64765 0.91468 1.83602
H -0.20045 -0.99179 3.98819
H -2.14071 -2.31642 -0.84120
N -2.27390 -0.53377 0.36277
H 0.65768 -2.96433 2.76175
C -0.56932 -0.53199 3.06172
C -2.87816 0.43270 -0.63385
H -2.69060 1.43612 -0.25641
C 0.27588 -2.52264 1.83437
H -0.42914 0.54808 3.13465
H -2.54923 -0.71271 -2.43501
N 0.32365 -1.01616 1.93300
H 0.89516 -2.85312 0.99937
C -2.23121 0.23102 -1.98876
H -2.52741 1.02870 -2.67632
H 1.88188 -0.38640 3.28089
O -0.62376 1.47276 0.69609
C 1.76779 -0.61499 2.21726
H -0.61464 2.30125 -1.70240
N -0.70775 0.20498 -1.87083
H 1.65037 1.47748 1.70576
H 2.40650 -1.47338 2.00285
H -0.57642 -1.86734 -2.38069
C 2.16454 0.57816 1.37282
C -0.14471 1.53753 -2.32515
H 1.52725 2.42266 -0.24289
H -0.46184 1.69086 -3.36516
C -0.20555 -0.91238 -2.75545
H -0.56856 -0.76131 -3.77810
N 1.76619 0.33829 -0.06699
H 3.24570 0.75317 1.43647
C 1.97508 1.62712 -0.83783
H 2.32787 -1.72929 -0.26441
C 1.37902 1.65036 -2.24629
H 0.87829 -0.94360 -2.76941
H 1.64027 2.62678 -2.67377
C 2.62321 -0.75484 -0.65136
H 3.05664 1.80886 -0.89305
H 2.52793 -0.76992 -1.73327
H 1.86437 0.91779 -2.89925
H 3.67412 -0.57156 -0.40053
H -0.27749 2.61626 1.32362
C -0.19491 3.75496 1.84592
C -1.42653 4.43587 1.39663
C -2.47413 4.64721 2.22549
C -2.44967 4.26264 3.67884
C -1.11339 3.75638 4.14631
C -0.07530 3.55018 3.30453
H 0.72075 4.11335 1.36111
H -1.48068 4.74443 0.35631
H -3.37399 5.13312 1.85756
H -2.76144 5.12045 4.29848
H -3.22823 3.50300 3.87771
H -0.99586 3.58273 5.21271
H 0.88123 3.21098 3.69367

66
FeO+CHD anti Interm (2/3)
Fe -0.22446 -0.16800 0.11764
H -2.42938 -0.44667 3.87727
H -3.77756 -0.33446 1.87800
H -3.80539 -1.93162 -0.07341
H -2.13864 -1.89270 2.95779
C -1.96536 -0.81183 2.95215
H -2.52840 -2.59216 0.95742
C -2.70245 -0.12537 1.80176
C -2.72564 -1.93871 0.11139
H -3.96184 0.29081 -0.59725
H -0.71526 -2.84422 1.71807
H -2.55159 0.95201 1.86362
H -0.07973 -0.94572 3.98828
H -2.21524 -2.34142 -0.76296
N -2.25574 -0.53587 0.41127
H 0.72323 -2.94373 2.75105
C -0.47293 -0.49342 3.06882
C -2.87393 0.43027 -0.57731
H -2.64603 1.43344 -0.22288
C 0.30930 -2.50884 1.83503
H -0.32371 0.58648 3.13417
H -2.61739 -0.76511 -2.35679
N 0.38124 -0.99717 1.91807
H 0.89131 -2.85385 0.97910
C -2.28184 0.18949 -1.94798
H -2.59775 0.96946 -2.64714
H 1.98871 -0.37859 3.21239
O -0.61430 1.51543 0.63903
C 1.84147 -0.61967 2.15590
H -0.66130 2.25742 -1.71535
N -0.75648 0.16143 -1.87808
H 1.80783 1.48275 1.63918
H 2.45609 -1.49403 1.93755
H -0.62325 -1.91414 -2.37943
C 2.24569 0.55046 1.28258
C -0.20832 1.49434 -2.35061
H 1.52314 2.40660 -0.32602
H -0.55414 1.64406 -3.38166
C -0.28983 -0.95688 -2.78349
H -0.71684 -0.81906 -3.78269
N 1.77371 0.31658 -0.13640
H 3.33442 0.68055 1.29606
C 1.95372 1.60338 -0.92410
H 2.35988 -1.74634 -0.31737
C 1.31723 1.61154 -2.31434
H 0.79149 -0.97107 -2.86614
H 1.56301 2.58564 -2.75602
C 2.60444 -0.78010 -0.75692
H 3.03247 1.78645 -1.01155
H 2.42374 -0.83169 -1.82604
H 1.78851 0.87662 -2.97469
H 3.66707 -0.56991 -0.59381
H -0.02228 2.02556 1.23178
C 0.02454 4.29470 2.38022
C -1.05195 4.84679 1.62552
C -2.34660 4.78049 2.07377
C -2.70804 4.12646 3.38180
C -1.52065 3.57616 4.12760
C -0.24225 3.67318 3.63508
H 1.04608 4.40020 2.02957
H -0.83453 5.33402 0.67889
H -3.15468 5.21024 1.48841
H -3.25667 4.84321 4.02378
H -3.45456 3.32577 3.21199
H -1.70576 3.10508 5.08886
H 0.58839 3.27888 4.21465

66
FeO+CHD anti React (2/5)
Fe -0.10021 -0.15712 0.50051
H -0.59539 -1.27808 4.66361
H -2.62155 -0.93688 3.42888
H -3.32781 -2.31145 1.40516
H -0.68500 -2.52032 3.45325
C -0.52663 -1.44479 3.58116
H -1.67203 -2.91207 1.62432
C -1.67416 -0.63328 2.96573
C -2.28264 -2.17875 1.10596
H -3.83410 -0.01786 1.32692
H 0.35165 -3.27921 1.72862
H -1.52420 0.43096 3.15466
H 1.60902 -1.58324 3.83213
H -2.19013 -2.34840 0.03435
N -1.83991 -0.78389 1.46519
H 2.08761 -3.31058 2.09320
C 0.90214 -1.04884 3.18279
C -2.83749 0.23419 0.94484
H -2.55172 1.20836 1.34300
C 1.31144 -2.83131 1.48444
H 1.04677 0.02355 3.33107
H -3.29847 -0.68314 -0.96115
N 1.28797 -1.35198 1.74646
H 1.51825 -3.01036 0.42860
C -2.85468 0.23747 -0.57966
H -3.47753 1.06523 -0.93554
H 3.24150 -0.70147 2.37207
```

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O -0.15822 1.24181 1.39584
C 2.66357 -0.77752 1.44477
H -1.38124 2.39783 -0.61220
N -1.45982 0.35713 -1.17408
H 2.20971 1.35073 1.46798
H 3.18624 -1.48679 0.80122
H -1.54417 -1.54555 -2.13623
C 2.58258 0.59191 0.77974
C -1.15443 1.80767 -1.50258
H 1.16609 2.57716 -0.05166
H -1.84685 2.11484 -2.29869
C -1.38761 -0.50089 -2.40811
H -2.15798 -0.19234 -3.12500
N 1.63089 0.55431 -0.40139
H 3.57545 0.89643 0.42794
C 1.39496 1.95972 -0.92227
H 2.14005 -1.38914 -1.16255
C 0.28086 2.09213 -1.96809
H -0.41393 -0.41001 -2.88240
H 0.29262 3.14472 -2.27794
C 2.16989 -0.34779 -1.48007
H 2.34208 2.30755 -1.35400
H 1.58052 -0.24546 -2.38643
H 0.51968 1.52960 -2.87609
H 3.20589 -0.06641 -1.69797
H -0.83579 3.57478 2.18921
C -1.46959 4.46654 2.04646
C -1.05287 5.19071 0.78796
C -1.88827 5.45515 -0.22867
C -3.34806 5.06552 -0.23307
C -3.75974 4.32074 1.01519
C -2.92390 4.05828 2.03223
H -1.26527 5.09773 2.92807
H -0.01327 5.50868 0.73151
H -1.52415 5.98627 -1.10621
H -3.97478 5.96578 -0.35352
H -3.57263 4.45741 -1.12536
H -4.79896 4.00189 1.07071
H -3.28977 3.52983 2.91097

66
FeO+CHD anti TS (2/5)
Fe -0.10538 -0.10577 0.26697
H -1.16024 -0.70446 4.43099
H -3.01163 -0.57576 2.90984
H -3.43295 -2.20105 1.00555
H -1.08846 -2.09141 3.38838
C -0.95075 -1.00561 3.39661
H -1.81243 -2.73179 1.49395
C -2.01418 -0.30522 2.53955
C -2.35993 -2.07805 0.82139
H -3.92720 0.07490 0.54658
H 0.15355 -3.05057 1.94006
H -1.90455 0.77812 2.61525
H 1.13205 -1.06772 3.94464
H -2.13529 -2.37072 -0.20353
N -1.97524 -0.64226 1.06237
H 1.81796 -3.00874 2.55194
C 0.51901 -0.63832 3.14036
C -2.88344 0.29036 0.28656
H -2.65118 1.30663 0.60660
C 1.14184 -2.62922 1.77616
H 0.64279 0.44653 3.15930
H -3.08040 -0.84961 -1.54117
N 1.09420 -1.12716 1.82190
H 1.49769 -2.95428 0.79765
C -2.68296 0.11292 -1.21590
H -3.24132 0.88742 -1.75269
H 2.95457 -0.38406 2.60778
O -0.26662 1.39827 0.95418
C 2.50474 -0.58996 1.63049
H -1.18727 2.26137 -1.31857
N -1.21742 0.16785 -1.62311
H 2.09914 1.52275 1.30079
H 3.09863 -1.37929 1.16731
H -1.17479 -1.84764 -2.31784
C 2.54196 0.67500 0.77749
C -0.85796 1.56718 -2.09531
H 1.27824 2.53297 -0.48003
H -1.44337 1.76743 -3.00335
C -0.98129 -0.84692 -2.70630
H -1.64754 -0.65221 -3.55553
N 1.75631 0.48425 -0.50511
H 3.58141 0.92177 0.52927
C 1.60511 1.80818 -1.22741
H 2.34620 -1.53546 -0.93858
C 0.62792 1.79845 -2.41090
H 0.04689 -0.80582 -3.05579
H 0.68892 2.80152 -2.85194
C 2.41644 -0.54421 -1.38414
H 2.60121 2.10241 -1.58301
H 1.93664 -0.56947 -2.35782
H 0.96996 1.12387 -3.20204
H 3.47194 -0.28170 -1.51682
H -0.58358 3.25875 1.74536
C -1.03794 4.22154 2.06695
C -1.38920 5.03447 0.84893
C -2.64458 5.39877 0.53828
C -3.84403 5.05295 1.38685
C -3.48110 4.29732 2.64170
C -2.22429 3.93563 2.94987
H -0.23892 4.71684 2.64372
H -0.56431 5.32631 0.20157
H -2.83453 5.98492 -0.35865
H -4.39173 5.97365 1.65134
H -4.56973 4.47047 0.79327
H -4.29760 4.05816 3.32014
H -2.02578 3.40490 3.87929

66
FeO+CHD anti Interm (2/5)
Fe -0.54329 -0.00236 0.18331
H -3.40267 -1.09701 3.26765
H -4.30280 -1.09902 1.05767
H -3.60685 -2.62555 -0.79694
H -2.60371 -2.37203 2.39911
C -2.67469 -1.28168 2.46698
H -2.31903 -3.01997 0.35733
C -3.29323 -0.68640 1.19246
C -2.58553 -2.37919 -0.48002
H -4.00087 -0.38006 -1.51917
H -0.69993 -2.96680 1.62245
H -3.38139 0.39628 1.29980
H -1.13888 -1.08170 3.96627
H -1.89817 -2.58544 -1.29916
N -2.50852 -0.93815 -0.07686
H 0.38274 -2.82229 3.02341
C -1.34956 -0.67897 2.96595
C -3.00681 -0.04719 -1.19184
H -3.09538 0.95975 -0.78404
C 0.15538 -2.43075 2.02468
H -1.43677 0.40690 3.04926
H -2.12023 -1.01380 -2.91872
N -0.13069 -0.95556 2.10077
H 1.00772 -2.60230 1.36665
C -2.05019 -0.06364 -2.38634
H -2.34243 0.72030 -3.09208
H 0.91221 0.03728 3.70007
O -1.24244 1.56707 0.65935
C 1.09807 -0.24201 2.65810
H -0.83918 2.22617 -1.82805
N -0.59057 0.13583 -1.98915
H 0.75936 1.80732 2.02691
H 1.92111 -0.95850 2.66247
H -0.07901 -1.88482 -2.43506
C 1.48139 1.00746 1.86201
C -0.13586 1.54846 -2.31686
H 0.89537 2.71362 0.05147
H -0.23016 1.67887 -3.40375
C 0.25229 -0.88194 -2.70625
H 0.16026 -0.75120 -3.79110
N 1.51107 0.72565 0.37702
H 2.46794 1.35807 2.19365
C 1.60428 2.01984 -0.40383
H 2.48817 -1.17700 0.47151
C 1.30576 1.89611 -1.90632
H 1.29723 -0.78021 -2.42661
H 1.50365 2.88791 -2.33315
C 2.64910 -0.18957 0.04090
H 2.61684 2.42594 -0.27141
H 2.73919 -0.29953 -1.03763
H 2.02221 1.23061 -2.39863
H 3.58849 0.22387 0.42879
H -1.62132 2.38954 1.04311
C -2.47992 4.09990 1.92304
C -1.79480 3.91887 3.16312
C -0.57554 4.50341 3.39535
C 0.09977 5.37717 2.37258
C -0.68479 5.53291 1.09778
C -1.90230 4.92747 0.91281
H -3.47183 3.68221 1.78340
H -2.25600 3.30741 3.93352
H -0.06844 4.35895 4.34496
H 0.30917 6.37328 2.80894
H 1.11178 4.98750 2.14987
H -0.25990 6.16131 0.32042
H -2.44403 5.07706 -0.01680

72
FeO+CNCH3+CHD syn React (2/3)
Fe 0.20836 -0.40767 0.00299
H 2.08759 -1.19762 -3.92989
H -0.20485 -0.45072 -3.98816
H -1.11618 1.54485 -3.21029
H 2.00901 0.41463 -3.28170
C 1.73407 -0.62169 -3.06521
H 0.43590 1.79851 -2.38162
C 0.21612 -0.79661 -3.03534
C -0.57299 1.41103 -2.26805
H -2.47809 -0.30735 -2.77795
H 2.23662 1.54794 -1.56230
H -0.02908 -1.85336 -2.94054
H 3.57631 -1.10023 -2.05929
H -1.06271 1.96896 -1.47470
N -0.52406 -0.05773 -1.93040
H 3.83960 0.99494 -1.02591
C 2.50002 -1.14899 -1.84866
C -1.93471 -0.61001 -1.87421
H -1.87009 -1.69630 -1.87708
C 2.77517 1.04201 -0.76836
H 2.25111 -2.19258 -1.65488
H -2.88387 0.95402 -0.73711
N 2.25693 -0.36442 -0.57403
H 2.63848 1.60646 0.15021
C -2.65868 -0.10865 -0.64314
H -3.61413 -0.63200 -0.53109
H 3.90396 -1.52503 0.18505
O 0.35912 1.16551 0.41679
C 3.05017 -0.96537 0.58078
H -2.18458 -2.38349 0.67357
N -1.82654 -0.29199 0.62052
H 1.94531 -2.78903 0.92968
H 3.45126 -0.13894 1.16814
H -1.83184 1.81639 0.95751
C 2.19654 -1.86585 1.44781
C -2.25935 -1.54128 1.36227
H 0.05249 -3.11532 1.85776
H -3.31997 -1.41710 1.61729
C -2.09788 0.90979 1.49515
H -3.16321 0.92651 1.75365
N 0.90144 -1.17424 1.82786
H 2.74398 -2.13517 2.35951
C -0.00722 -2.21422 2.46637
H 1.80598 0.68758 2.39060
C -1.47083 -1.81258 2.64599
H -1.50992 0.86731 2.40536
H -1.95920 -2.66333 3.13801
C 1.19069 -0.08952 2.83547
H 0.42334 -2.45628 3.44646
H 0.26141 0.36448 3.16905
H -1.57022 -0.98153 3.35019
H 1.70547 -0.52812 3.69743
H 0.68647 4.33414 -0.33321
C 0.01657 5.14025 0.00931
C -1.38814 4.88263 -0.48409
C -2.45658 4.80493 0.32447
C -2.38250 4.97236 1.82430
C -0.97257 5.19280 2.32088
C 0.09522 5.26849 1.51278
H 0.41847 6.05146 -0.46593
H -1.51279 4.76804 -1.55947
H -3.44393 4.62534 -0.09705
H -3.02551 5.81290 2.13730
H -2.82386 4.09331 2.32317
H -0.84730 5.29827 3.39693
H 1.08439 5.43580 1.93514
N 0.01789 -2.46848 -0.53623
C -0.08801 -3.59283 -0.82950
C -0.22064 -4.98971 -1.19435
H -0.61943 -5.56207 -0.35124
H -0.90130 -5.09254 -2.04493
H 0.75523 -5.40055 -1.47057

72
FeO+CNCH3+CHD syn TS (2/3)
Fe -0.04890 -0.21407 -0.22890
H 2.40716 -1.28447 -3.76287
H 0.05212 -0.98816 -4.19386
H -1.35643 0.87058 -3.86499
H 1.98339 0.36775 -3.41656
C 1.85206 -0.65623 -3.05436
H 0.07999 1.53401 -3.05583
C 0.39070 -1.09511 -3.15475
C -0.85959 1.00886 -2.89724
H -2.36420 -1.09421 -3.22715
H 1.68904 1.81475 -1.86838
H 0.31063 -2.15069 -2.89861
H 3.60122 -0.65176 -1.80157
H -1.47252 1.61016 -2.23243
N -0.59432 -0.33915 -2.27885
H 3.37940 1.57466 -1.35252
C 2.52466 -0.83925 -1.69009
C -1.88258 -1.13507 -2.24137
H -1.63094 -2.17532 -2.04227
C 2.32824 1.51262 -1.04614
H 2.40669 -1.86098 -1.33002
H -3.19529 0.39164 -1.48805
N 2.01640 0.10130 -0.61345
H 2.16019 2.18858 -0.21485
C -2.82567 -0.59008 -1.18898
H -3.69690 -1.24779 -1.09058
H 3.74068 -0.59353 0.47610
O -0.38066 1.48335 -0.14736
C 2.76273 -0.14820 0.68935
H -2.09619 -2.52353 0.50944
N -2.15250 -0.42857 0.16447
H 1.95713 -2.06960 1.25382
H 2.94939 0.81936 1.15654
H -2.63096 1.64699 0.18141
C 1.97682 -1.04560 1.62312
C -2.42178 -1.63126 1.04390
H 0.06710 -2.61393 2.02862
H -3.50992 -1.70670 1.17653
C -2.78654 0.77863 0.81253
H -3.85821 0.58580 0.94793
N 0.54336 -0.56926 1.75028
H 2.44762 -1.05919 2.61458
C -0.23797 -1.66350 2.46344
H 1.08357 1.46883 2.11056
C -1.76300 -1.55181 2.42571
H -2.33515 0.98244 1.77775
H -2.14018 -2.40658 3.00204
C 0.50203 0.68303 2.58256
H 0.09503 -1.66553 3.50979
H -0.52212 1.03271 2.67772
H -2.10520 -0.66741 2.97075
H 0.90918 0.47295 3.57872
H 0.06295 2.67189 0.24842
C 0.20673 3.93538 0.43448
C -1.17644 4.44475 0.35778
C -1.84416 4.88981 1.44664
C -1.21690 4.95699 2.81251
C 0.24752 4.61276 2.81755
C 0.89701 4.16794 1.71711
H 0.81374 4.14674 -0.45341
H -1.66389 4.43107 -0.61322
H -2.86916 5.23994 1.35555
H -1.36554 5.96137 3.24445
H -1.76164 4.29221 3.50822
H 0.78783 4.76262 3.74872
H 1.96473 3.96738 1.76597
N 0.17361 -2.35744 -0.42422
C 0.31002 -3.51224 -0.52468
C 0.47951 -4.94804 -0.64696
H 0.40260 -5.42060 0.33719
H -0.29330 -5.36479 -1.29977
H 1.46172 -5.17648 -1.07161

72
FeO+CNCH3+CHD syn Interm (2/3)
Fe -0.22589 -0.27912 -0.38707
H 2.65708 -1.30082 -3.57396
H 0.34107 -1.30411 -4.23176
H -1.25301 0.41950 -4.18800
H 2.03118 0.31258 -3.39379
C 1.97446 -0.69279 -2.96654
H -0.00354 1.29385 -3.27363
C 0.58416 -1.29839 -3.16105
C -0.89187 0.67328 -3.18428
H -2.12981 -1.60476 -3.49986
H 1.48707 1.83471 -1.99854
H 0.58961 -2.33579 -2.82814
H 3.58949 -0.42252 -1.56986
H -1.63984 1.23929 -2.63840
N -0.55826 -0.59554 -2.44451
H 3.13282 1.78026 -1.31679
C 2.53057 -0.71134 -1.53942
C -1.75534 -1.52162 -2.47162
H -1.42395 -2.51113 -2.16330
C 2.06628 1.64851 -1.10081
H 2.47759 -1.71291 -1.11298
H -3.30679 -0.11155 -1.99352
N 1.83367 0.24509 -0.58604
H 1.78093 2.37842 -0.34635
C -2.85255 -1.00588 -1.56542
H -3.64515 -1.75617 -1.47007
H 3.49010 -0.22763 0.71145
O -0.69293 1.45154 -0.48597
C 2.46930 0.15969 0.79657
H -2.15666 -2.67018 0.40578
N -2.32803 -0.63611 -0.18509
H 1.76591 -1.76580 1.47452
H 2.54766 1.17406 1.19024
H -2.95355 1.38260 -0.45277
C 1.66252 -0.71434 1.73513
C -2.59742 -1.75449 0.80131
H -0.15778 -2.41322 2.08361
H -3.68469 -1.90467 0.83985
C -3.11344 0.57718 0.25546
H -4.17585 0.30819 0.30506
N 0.18973 -0.36184 1.67207
H 2.02422 -0.59164 2.76388
C -0.57243 -1.45916 2.40530
H 0.58988 1.72683 1.97030
C -2.08911 -1.47344 2.21962
H -2.78546 0.91978 1.23122
H -2.46181 -2.28927 2.85227
C -0.04334 0.94415 2.38377
H -0.34131 -1.35023 3.47283
H -1.08119 1.24963 2.28485
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H -2.54404 -0.56575 2.62642
H 0.20053 0.82667 3.44571
H -0.15604 2.11512 -0.00899
C 0.11482 4.68627 0.60653
C -1.14227 4.63833 1.27676
C -1.22264 4.63364 2.64708
C 0.00350 4.69127 3.52154
C 1.29376 4.72791 2.74424
C 1.31736 4.73343 1.37102
H 0.15413 4.72926 -0.47688
H -2.05295 4.61075 0.68462
H -2.18959 4.60223 3.14136
H -0.05475 5.57034 4.19379
H 0.00817 3.83999 4.22943
H 2.21997 4.76799 3.31054
H 2.27063 4.78437 0.85127
N 0.20068 -2.31305 -0.35095
C 0.44003 -3.45476 -0.34049
C 0.73645 -4.87417 -0.33090
H 0.64199 -5.27123 0.68436
H 0.04136 -5.40831 -0.98572
H 1.75817 -5.04669 -0.68278

72
FeO+CNCH3+CHD syn React (2/5)
Fe 0.01524 -0.15333 0.33994
H -0.02072 -0.36025 4.79205
H 2.15577 -0.37860 3.82785
H 3.17428 1.30081 2.48192
H 0.16988 1.13113 3.92049
C 0.04447 0.05348 3.77728
H 1.53677 1.98666 2.35561
C 1.30445 -0.56793 3.15933
C 2.25674 1.32257 1.88147
H 3.65783 -0.89473 1.64620
H -0.62795 2.28608 2.39212
H 1.18525 -1.64928 3.09194
H -2.10937 0.06670 3.78856
H 2.47608 1.71524 0.89109
N 1.68576 -0.06360 1.78046
H -2.37886 2.18011 2.69411
C -1.30642 -0.25467 3.11052
C 2.68565 -1.00044 1.14640
C 2.34261 -2.02006 1.31330
C -1.57379 1.93084 1.99246
H -1.42303 -1.32762 2.95357
H 3.40508 0.21792 -0.48580
N -1.54008 0.43913 1.78250
H -1.74708 2.42546 1.03895
C 2.87448 -0.72467 -0.34515
H 3.50097 -1.51374 -0.77576
H -3.54264 -0.32007 1.94677
O 0.08777 1.40599 -0.14821
C -2.86400 0.02517 1.15885
H 1.27598 -2.73016 -1.08337
N 1.57712 -0.62899 -1.13289
H -2.49978 -2.02560 0.54729
H -3.30851 0.92126 0.72379
H 1.97256 1.39986 -1.66030
C -2.74370 -1.06597 0.09540
C 1.24578 -1.93541 -1.82987
H -1.36729 -2.84082 -1.08721
H 2.05267 -2.13228 -2.54924
C 1.73704 0.46231 -2.15942
H 2.54603 0.19464 -2.84981
N -1.68306 -0.75228 -0.93187
H -3.71624 -1.17549 -0.40308
C -1.38691 -1.98567 -1.76276
H -2.28761 1.27650 -1.23740
C -0.09284 -1.94586 -2.58784
H 0.81782 0.60164 -2.72132
H -0.09395 -2.86925 -3.18166
C -2.13023 0.37242 -1.82164
H -2.23508 -2.13506 -2.44522
H -1.36786 0.58502 -2.56833
H -0.12619 -1.13768 -3.32483
H -3.06181 0.09269 -2.32907
H -0.09412 3.54611 -1.60777
C -0.07257 4.21001 -2.48831
C 1.29137 4.15398 -3.13517
C 1.49142 3.81783 -4.41876
C 0.37505 3.46239 -5.37298
C -0.98737 3.49918 -4.72084
C -1.18664 3.83559 -3.43731
H -0.25237 5.21854 -2.07909
H 2.14067 4.40812 -2.50285
H 2.50173 3.79936 -4.82365
H 0.39300 4.14554 -6.23973
H 0.55559 2.46568 -5.80935
H -1.83576 3.24222 -5.35274
H -2.19688 3.85174 -3.03193
N -0.08580 -2.18526 0.98005
C -0.13886 -3.29595 1.33325
C -0.19873 -4.67632 1.77086
H -1.20078 -5.08162 1.60193
H 0.52553 -5.27800 1.21287
H 0.03419 -4.74210 2.83819

72
FeO+CNCH3+CHD syn TS (2/5)
Fe 0.03113 -0.12109 0.10840
H -0.07927 0.08067 4.57466
H 2.11007 -0.03889 3.65033
H 3.16278 1.47765 2.17416
H 0.13082 1.47677 3.56100
C 0.00134 0.39085 3.52459
H 1.53641 2.16247 1.93231
C 1.26872 -0.29324 2.99037
C 2.26155 1.44701 1.54895
H 3.63818 -0.79860 1.56742
H -0.64284 2.48802 1.90652
H 1.14469 -1.37457 3.03207
H -2.15347 0.40834 3.50990
H 2.51116 1.73492 0.53029
N 1.67390 0.06434 1.57387
H -2.39004 2.41105 2.24741
C -1.34378 0.02553 2.87211
C 2.67520 -0.94306 1.05851
H 2.31210 -1.93558 1.31949
C -1.59539 2.09657 1.55895
H -1.46017 -1.05721 2.81323
H 3.41563 0.10578 -0.67855
N -1.55666 0.59409 1.48524
H -1.78325 2.49917 0.56671
C 2.89776 -0.82680 -0.44923
H 3.55070 -1.64493 -0.77669
H -3.57930 -0.10682 1.67927
O 0.12072 1.40834 -0.58549
C -2.86443 0.11648 0.87825
H 1.30259 -2.90732 -0.90710
N 1.61931 -0.84175 -1.26855
H -2.47779 -1.99586 0.56890
H -3.27603 0.94905 0.30547
H 2.05299 1.07711 -2.08185
C -2.72423 -1.11347 -0.01933
C 1.28891 -2.23375 -1.76478
H -1.32200 -3.02703 -0.92019
H 2.10158 -2.54201 -2.43805
C 1.80516 0.08120 -2.44136
H 2.61151 -0.29665 -3.08302
N -1.65050 -0.94251 -1.06728
H -3.68988 -1.30181 -0.50835
C -1.34387 -2.27937 -1.71187
H -2.27492 1.01264 -1.67127
C -0.04320 -2.35334 -2.52516
H 0.88923 0.15317 -3.02225
H -0.03952 -3.35092 -2.98359
C -2.09297 0.03695 -2.11616
H -2.18616 -2.53002 -2.37201
H -1.31259 0.15229 -2.86590
H -0.07192 -1.65622 -3.36795
H -3.00790 -0.32669 -2.60068
H 0.15129 2.87854 -1.34550
C 0.14574 3.89598 -1.88397
C 1.38698 3.99709 -2.70838
C 1.37088 4.01224 -4.05637
C 0.09998 3.97030 -4.86217
C -1.14563 4.01307 -4.01775
C -1.12013 3.99829 -2.67014
H 0.15932 4.59320 -1.03190
H 2.33361 4.04846 -2.17538
H 2.30299 4.07830 -4.61254
H 0.08930 4.80373 -5.58524
H 0.09007 3.06909 -5.50150
H -2.09435 4.07973 -4.54507
H -2.05015 4.05014 -2.10867
N -0.09354 -2.22181 1.06163
C -0.15977 -3.28071 1.54989
C -0.23842 -4.59540 2.15886
H -1.21646 -5.04439 1.96156
H 0.53841 -5.24726 1.74793
H -0.09764 -4.51783 3.24128

72
FeO+CNCH3+CHD syn Interm (2/5)
Fe -0.16842 0.28524 -0.22059
H -0.28150 0.03285 4.31091
H 1.82113 -0.35691 3.29489
H 2.84938 1.52779 2.15990
H 0.07720 1.49581 3.43917
C -0.18427 0.44257 3.29755
H 1.28044 2.27715 1.78334
C 0.94728 -0.33768 2.62816
C 2.02567 1.56490 1.43646
H 3.40063 -0.61322 1.25915
H -0.75369 2.78584 1.91698
H 0.63401 -1.37168 2.45725
H -2.33250 0.69329 3.29790
H 2.40286 1.91008 0.47462
N 1.41774 0.19719 1.28988
H -2.52000 2.76702 2.10152
C -1.55475 0.28637 2.63591
C 2.44613 -0.76719 0.73974
H 2.10069 -1.77635 0.97137
C -1.68497 2.45833 1.45959
H -1.76378 -0.77763 2.49875
H 2.97970 0.42526 -0.99080
N -1.69595 0.96550 1.29287
H -1.77797 2.92653 0.48129
C 2.63222 -0.58331 -0.75668
H 3.39328 -1.28333 -1.12606
H -3.81069 0.60723 1.38952
O -0.11471 1.80801 -1.12851
C -3.00237 0.56931 0.64745
H 1.17244 -2.72867 -0.62822
N 1.33667 -0.80186 -1.50182
H -2.70585 -1.57024 0.80374
H -3.22701 1.31662 -0.11638
H 1.62476 0.89058 -2.75590
C -2.92310 -0.82069 0.04014
C 1.06001 -2.28454 -1.61971
H -1.23937 -2.77191 -0.21969
H 1.83474 -2.71407 -2.27133
C 1.45943 -0.18014 -2.86352
H 2.29737 -0.63755 -3.40548
N -1.83302 -0.90419 -1.00532
H -3.88526 -1.08691 -0.41522
C -1.48276 -2.36513 -1.20611
H -2.64245 0.73758 -2.10786
C -0.32417 -2.64443 -2.16473
H 0.54721 -0.33439 -3.43635
H -0.31785 -3.72957 -2.32864
C -2.31633 -0.28533 -2.28923
H -2.38913 -2.87131 -1.56724
H -1.51465 -0.25735 -3.02309
H -0.50075 -2.20763 -3.15254
H -3.15258 -0.87216 -2.68828
H 0.08361 2.74283 -1.36241
C 0.47188 4.75389 -1.81573
C 1.71987 4.39813 -2.41184
C 1.82018 4.14774 -3.75704
C 0.63477 4.24809 -4.67812
C -0.63956 4.64688 -3.98492
C -0.69028 4.88480 -2.63517
H 0.42543 5.00913 -0.76197
H 2.60206 4.32866 -1.78191
H 2.77662 3.88091 -4.19708
H 0.85497 4.95902 -5.49806
H 0.49014 3.29046 -5.21456
H -1.53128 4.75184 -4.59604
H -1.62780 5.18114 -2.17352
N 0.58945 -3.78691 1.63400
C 0.68231 -4.82430 2.17052
C 0.80085 -6.11300 2.83797
H 0.05783 -6.81521 2.44833
H 1.79678 -6.53605 2.67579
H 0.64232 -6.00148 3.91479

72
FeO+CNCH3+CHD anti React (2/3)
Fe -0.00281 -0.37084 0.01614
H -2.07068 0.08580 3.85290
H -3.47390 0.17148 1.90006
H -3.86433 -1.53868 0.35663
H -2.01653 -1.47962 3.09329
C -1.69899 -0.44034 2.96439
H -2.44973 -2.39199 1.00166
C -2.38475 0.21799 1.76974
C -2.78495 -1.68957 0.24267
H -3.68035 0.60016 -0.63986
H -0.80937 -2.83957 2.00754
H -2.09294 1.26754 1.72706
H 0.19833 -0.66017 3.96608
H -2.58573 -2.11527 -0.73801
N -2.07632 -0.37442 0.40320
H 0.45310 -2.81824 3.25391
C -0.17454 -0.31613 2.99250
C -2.58359 0.61777 -0.62653
H -2.26069 1.60809 -0.30613
C 0.23137 -2.60295 2.20244
H 0.12449 0.72353 2.85469
H -2.44298 -0.66387 -2.35252
N 0.52630 -1.14546 1.93031
H 0.85995 -3.23008 1.57718
C -2.04036 0.28528 -1.99615
H -2.33754 1.05333 -2.71882
H 2.30075 -0.80547 3.09425
O -0.05627 1.18288 0.54846
C 2.03394 -0.97446 2.04521
H -0.25026 2.22422 -1.55225
N -0.52307 0.16625 -1.98341
H 2.13392 1.11821 1.54217
H 2.49868 -1.91402 1.74341
H -0.72501 -1.71083 -2.99183
C 2.52707 0.16611 1.18736
C 0.10892 1.51167 -2.29534
H 1.94176 2.09468 -0.28031
H -0.25971 1.81927 -3.28262
C -0.15098 -0.79425 -3.08914
H -0.38676 -0.33115 -4.05410
N 2.06080 -0.00812 -0.24558
H 3.62259 0.21374 1.21173
C 2.30494 1.31581 -0.95100
H 2.70196 -2.04616 -0.40181
C 1.63909 1.48658 -2.31449
H 0.90674 -1.03409 -3.06295
H 1.96283 2.46592 -2.68937
C 2.85109 -1.09813 -0.91335
H 3.39197 1.42977 -1.05455
H 2.53867 -1.20970 -1.94883
H 2.01737 0.76287 -3.04320
H 3.91638 -0.84200 -0.89242
H -0.11659 3.66500 1.41093
C -0.66581 4.37983 2.04493
C -2.08999 4.49961 1.55548
C -3.16294 4.25763 2.32415
C -3.07496 3.84428 3.77487
C -1.65052 3.70441 4.25909
C -0.57829 3.94606 3.48950
H -0.13975 5.34014 1.90855
H -2.22414 4.80494 0.51906
H -4.16340 4.36553 1.90907
H -3.61407 4.57308 4.40425
H -3.61927 2.89745 3.92951
H -1.51717 3.39738 5.29486
H 0.42222 3.83527 3.90418
N 0.06716 -2.32930 -0.66216
C 0.10976 -3.43267 -1.03527
C 0.16418 -4.80620 -1.49629
H 0.53348 -5.45654 -0.69738
H -0.83370 -5.14329 -1.79283
H 0.83505 -4.88809 -2.35678

72
FeO+CNCH3+CHD anti TS (2/3)
Fe -0.18486 -0.28610 0.07732
H -2.53515 -0.26855 3.77743
H -3.81716 -0.29946 1.74630
H -3.86974 -1.99514 0.16750
H -2.19191 -1.76977 2.96720
C -2.03265 -0.68926 2.89654
H -2.37223 -2.66063 0.85004
C -2.74029 -0.09277 1.68073
C -2.77522 -1.98521 0.09856
H -3.93297 0.17820 -0.79386
H -0.70664 -2.88735 1.98559
H -2.59319 0.98618 1.67904
H -0.19733 -0.65231 4.02895
H -2.47854 -2.34438 -0.88394
N -2.26785 -0.59040 0.32537
H 0.47176 -2.70609 3.30211
C -0.54846 -0.33670 3.03702
C -2.85028 0.34340 -0.71658
H -2.67074 1.35706 -0.36508
C 0.27365 -2.49953 2.24370
H -0.40716 0.73930 2.95113
H -2.46330 -0.85747 -2.46346
N 0.34909 -1.00789 2.01249
H 1.02289 -3.00731 1.64291
C -2.19544 0.12114 -2.06188
H -2.54864 0.86994 -2.78056
H 1.95480 -0.36606 3.29466
O -0.60881 1.33646 0.56927
C 1.79824 -0.60395 2.23634
H -0.66231 2.25134 -1.54187
N -0.67825 0.18246 -1.97358
H 1.66703 1.47496 1.69189
H 2.42252 -1.46874 2.00742
H -0.61393 -1.70546 -2.98116
C 2.18723 0.57508 1.37252
C -0.18935 1.58693 -2.26405
H 1.48556 2.40581 -0.17801
H -0.53639 1.85311 -3.27202
C -0.14344 -0.72915 -3.05345
H -0.37703 -0.29787 -4.03433
N 1.81571 0.32635 -0.07476
H 3.26615 0.76062 1.45116
C 1.95143 1.65134 -0.80758
H 2.70204 -1.62197 -0.14734
C 1.33419 1.72896 -2.20398
H 0.93191 -0.85145 -2.97052
H 1.57141 2.73249 -2.58050
C 2.76419 -0.67303 -0.67455
H 3.02455 1.87727 -0.87087
H 2.51871 -0.84113 -1.72040
H 1.82629 1.04115 -2.89860
H 3.79015 -0.29202 -0.60932
H -0.24118 2.41116 1.29519
C -0.16215 3.56575 1.83221
C -1.40893 4.21005 1.37276
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C -2.46052 4.41645 2.19875
C -2.42471 4.06605 3.66126
C -1.07341 3.60666 4.13613
C -0.03436 3.40168 3.29432
H 0.74425 3.93607 1.33944
H -1.47251 4.49511 0.32625
H -3.37180 4.87324 1.82150
H -2.75849 4.92903 4.26196
H -3.18204 3.28996 3.87844
H -0.94699 3.46503 5.20631
H 0.93189 3.09949 3.69073
N 0.15203 -2.21683 -0.60653
C 0.36341 -3.29946 -0.98335
C 0.62921 -4.64688 -1.45131
H 0.77737 -5.31878 -0.60031
H -0.21193 -5.01332 -2.04726
H 1.53161 -4.65892 -2.06997

72
FeO+CNCH3+CHD anti Inter (2/3)
Fe -0.38689 -0.42655 0.20894
H -2.70587 -0.94215 3.90497
H -3.97221 -0.99545 1.86874
H -3.82624 -2.56101 0.17015
H -2.17364 -2.32922 3.00027
C -2.15343 -1.23499 3.00258
H -2.25309 -3.08939 0.80086
C -2.93023 -0.65114 1.82427
C -2.74213 -2.41289 0.10316
H -4.16715 -0.33420 -0.60512
H -0.56872 -3.17124 1.94074
H -2.91879 0.43455 1.89689
H -0.33169 -1.05395 4.14365
H -2.41254 -2.65677 -0.90418
N -2.40715 -0.98713 0.43665
H 0.58729 -2.93744 3.26807
C -0.72695 -0.70802 3.17948
C -3.10949 -0.05181 -0.52712
H -3.03849 0.94639 -0.10133
C 0.35642 -2.68199 2.22764
H -0.72513 0.38196 3.19053
H -2.60724 -1.07134 -2.35884
N 0.24175 -1.17714 2.10634
H 1.15984 -3.04369 1.59264
C -2.45395 -0.09943 -1.88680
H -2.89987 0.65245 -2.54812
H 1.75968 -0.43307 3.44064
O -1.01876 1.15699 0.84004
C 1.63361 -0.61750 2.36812
H -1.19359 2.15162 -1.19355
N -0.95505 0.13734 -1.78997
H 1.32710 1.49180 1.98367
H 2.35522 -1.38661 2.09007
H -0.66434 -1.64645 -2.93595
C 1.89317 0.65012 1.58411
C -0.64827 1.61251 -1.96722
H 0.92372 2.50281 0.17258
H -1.03512 1.90777 -2.95183
C -0.32235 -0.61517 -2.93703
H -0.62349 -0.14612 -3.88117
N 1.51555 0.46741 0.12796
H 2.95382 0.92139 1.65752
C 1.47411 1.85254 -0.50589
H 2.66018 -1.33250 -0.08408
C 0.84454 1.94414 -1.89467
H 0.76116 -0.60405 -2.86961
H 0.94760 2.99326 -2.20074
C 2.57646 -0.35534 -0.55392
H 2.50934 2.21573 -0.54925
H 2.33011 -0.49291 -1.60393
H 1.41766 1.37495 -2.63314
H 3.54054 0.16098 -0.48233
H -0.52960 1.65460 1.52456
C 0.92545 4.55954 2.59104
C 0.36457 5.24620 1.47656
C -0.97006 5.14452 1.16963
C -1.92035 4.30971 1.98909
C -1.25387 3.60407 3.14302
C 0.08864 3.74467 3.40689
H 1.97976 4.66192 2.82248
H 1.01105 5.86644 0.86154
H -1.38078 5.67958 0.31791
H -2.75202 4.93904 2.36216
H -2.42967 3.57111 1.34173
H -1.88080 2.99591 3.78947
H 0.52340 3.23486 4.26288
N 0.18996 -2.19001 -0.58468
C 0.51640 -3.21054 -1.04308
C 0.92322 -4.48094 -1.61143
H 1.43544 -5.08507 -0.85644
H 0.04825 -5.03095 -1.97069
H 1.60484 -4.31471 -2.45134

72
FeO+CNCH3+CHD anti React (2/5)
Fe -0.06035 -0.32476 0.06725
H -1.36245 -0.29617 4.25837
H -3.11186 -0.20693 2.66098
H -3.65372 -1.95025 1.16517
H -1.28091 -1.78255 3.36155
C -1.10375 -0.70598 3.27338
H -2.03048 -2.63786 1.39370
C -2.08810 -0.05722 2.29225
C -2.62421 -1.95589 0.78766
H -3.90841 0.26153 0.18152
H -0.02135 -2.98112 2.16514
H -1.90029 1.01653 2.24844
H 0.94032 -0.71180 3.96846
H -2.62504 -2.31437 -0.23950
N -2.05425 -0.57074 0.86168
H 1.48479 -2.82562 3.09411
C 0.38981 -0.40580 3.06754
C -2.83588 0.38741 -0.01561
H -2.55285 1.39871 0.27821
C 0.99832 -2.60426 2.13550
H 0.54012 0.66521 2.92192
H -2.96411 -0.81176 -1.81017
N 1.01604 -1.12193 1.88861
H 1.53763 -3.11700 1.34194
C -2.57400 0.15954 -1.50101
H -3.11551 0.91965 -2.07795
H 2.91266 -0.45707 2.64508
O -0.17976 1.20022 0.67363
C 2.45235 -0.69015 1.67681
H -0.93971 2.25181 -1.38667
N -1.10593 0.19412 -1.87026
H 2.15136 1.40442 1.21373
H 2.99316 -1.54413 1.26566
H -1.31342 -1.68440 -2.86160
C 2.59380 0.51851 0.75838
C -0.65045 1.59791 -2.21140
H 1.45554 2.37267 -0.52092
H -1.20252 1.91337 -3.10837
C -0.89675 -0.69962 -3.06047
H -1.40225 -0.27239 -3.93592
N 1.90511 0.31331 -0.57553
H 3.65949 0.71645 0.58669
C 1.79304 1.65866 -1.27318
H 2.75613 -1.61851 -0.91378
C 0.85707 1.72446 -2.48602
H 0.16171 -0.80666 -3.28543
H 1.00525 2.72376 -2.91546
C 2.66143 -0.66285 -1.42534
H 2.80686 1.94473 -1.58465
H 2.13776 -0.82272 -2.36558
H 1.17442 1.03085 -3.27116
H 3.66263 -0.26888 -1.63705
H -0.25564 3.66606 1.54415
C -0.99194 4.43948 1.81890
C -1.94095 4.66453 0.66521
C -3.27086 4.50802 0.75562
C -3.97929 4.09865 2.02588
C -3.03104 3.87994 3.18166
C -1.70132 4.03466 3.08980
H -0.39279 5.34863 1.99592
H -1.49494 4.97365 -0.27861
H -3.89909 4.68980 -0.11450
H -4.72970 4.86073 2.29697
H -4.57128 3.18502 1.84798
H -3.47937 3.58886 4.12984
H -1.07491 3.86905 3.96461
N 0.09085 -2.23886 -0.69317
C 0.17819 -3.32018 -1.11973
C 0.28933 -4.66581 -1.64645
H 1.32152 -4.86537 -1.95007
H -0.00148 -5.39302 -0.88229
H -0.36411 -4.78567 -2.51588

72
FeO+CNCH3+CHD anti TS (2/5)
Fe -0.14130 -0.23805 0.05287
H -1.65155 -0.32762 4.17125
H -3.34368 -0.35242 2.51297
H -3.74274 -2.07588 0.90454
H -1.43171 -1.79639 3.26849
C -1.32719 -0.70912 3.19404
H -2.11569 -2.67681 1.29631
C -2.32115 -0.12546 2.17872
C -2.68101 -2.02555 0.63103
H -4.03474 0.14115 -0.03638
H -0.05068 -2.89879 2.12831
H -2.20873 0.95851 2.15295
H 0.67787 -0.57177 3.98334
H -2.55780 -2.38541 -0.38876
N -2.18782 -0.61660 0.75108
H 1.37962 -2.65123 3.15526
C 0.15261 -0.30686 3.05409
C -2.95673 0.30731 -0.16808
H -2.72967 1.32807 0.13838
C 0.94397 -2.46059 2.16578
H 0.23658 0.77049 2.90782
H -2.95805 -0.88682 -1.96851
N 0.88627 -0.98048 1.91157
H 1.56181 -2.94106 1.41055
C -2.60427 0.09193 -1.63911
H -3.13063 0.84087 -2.24419
H 2.68650 -0.17732 2.76890
O -0.36865 1.34626 0.64277
C 2.30762 -0.46440 1.77981
H -1.02755 2.22995 -1.52282
N -1.11732 0.15564 -1.93586
H 1.94108 1.59825 1.22846
H 2.92259 -1.29743 1.43402
H -1.22555 -1.76201 -2.86212
C 2.45313 0.72321 0.83021
C -0.68699 1.55953 -2.31261
H 1.33986 2.48679 -0.58444
H -1.21225 1.82575 -3.24151
C -0.82477 -0.77451 -3.07952
H -1.29324 -0.39483 -3.99686
N 1.86150 0.44805 -0.53535
H 3.51998 0.96414 0.72605
C 1.72762 1.75416 -1.29201
H 2.79572 -1.46006 -0.75731
C 0.82679 1.72968 -2.53594
H 0.24685 -0.86370 -3.24195
H 0.95322 2.71276 -3.00826
C 2.70690 -0.52144 -1.30137
H 2.73775 2.06855 -1.59085
H 2.25411 -0.72802 -2.27014
H 1.19586 1.01214 -3.27591
H 3.70885 -0.10210 -1.45955
H -0.64484 2.79326 1.17622
C -0.89010 3.87332 1.56368
C -1.93976 4.43890 0.67147
C -3.21065 4.64010 1.07906
C -3.67128 4.36040 2.48363
C -2.55784 3.95805 3.41195
C -1.29008 3.75853 2.99336
H 0.08599 4.36307 1.43451
H -1.65138 4.67824 -0.34918
H -3.94828 5.04341 0.38974
H -4.19337 5.24404 2.88815
H -4.45203 3.57798 2.47372
H -2.80868 3.85212 4.46449
H -0.51689 3.48755 3.70802
N 0.15795 -2.27874 -0.70426
C 0.32567 -3.36399 -1.09681
C 0.53406 -4.71521 -1.58221
H 1.58812 -4.86638 -1.83355
H 0.24763 -5.43952 -0.81378
H -0.07023 -4.89253 -2.47689

72
FeO+CNCH3+CHD anti Inter (2/5)
Fe -0.16778 -0.19934 0.08979
H -1.61946 -0.39627 4.21684
H -3.34186 -0.42363 2.59025
H -3.77093 -2.10067 0.93968
H -1.39772 -1.84845 3.28778
C -1.30843 -0.75893 3.22817
H -2.14453 -2.70741 1.32504
C -2.33011 -0.17448 2.23944
C -2.70894 -2.04759 0.66690
H -4.06659 0.12776 0.03636
H -0.03146 -2.91495 2.09872
H -2.23471 0.91133 2.22965
H 0.70695 -0.61216 3.98648
H -2.58546 -2.39740 -0.35658
N -2.21225 -0.64245 0.80187
H 1.40191 -2.67089 3.12317
C 0.16480 -0.33738 3.07020
C -2.98904 0.29479 -0.09936
H -2.75783 1.31044 0.21870
C 0.96017 -2.47031 2.13860
H 0.23641 0.74271 2.94060
H -3.00425 -0.87142 -1.91775
N 0.89043 -0.98691 1.90586
H 1.57818 -2.93527 1.37414
C -2.64712 0.10199 -1.57661
H -3.17609 0.86062 -2.16674
H 2.69253 -0.17679 2.75681
O -0.41753 1.46636 0.72629
C 2.31072 -0.46011 1.76800
H -1.06487 2.24563 -1.48082
N -1.15966 0.16737 -1.88804
H 1.93794 1.60424 1.22926
H 2.92702 -1.28896 1.41502
H -1.28007 -1.74741 -2.81986
C 2.44733 0.73199 0.82217
C -0.73408 1.57343 -2.27300
H 1.33294 2.50485 -0.58207
H -1.27295 1.83557 -3.19496
C -0.87998 -0.75996 -3.03768
H -1.35747 -0.37582 -3.94823
N 1.84495 0.46202 -0.54079
H 3.51336 0.97524 0.71308
C 1.70291 1.76863 -1.29526
H 2.77930 -1.44393 -0.77772
C 0.77651 1.74526 -2.52157
H 0.18985 -0.84984 -3.21090
H 0.89261 2.72888 -2.99539
C 2.68535 -0.50260 -1.31658
H 2.70704 2.07995 -1.61676
H 2.22341 -0.70662 -2.28177
H 1.13269 1.02851 -3.26857
H 3.68601 -0.08312 -1.48320
H -0.54978 2.37665 1.06517
C -0.77198 4.44101 1.77836
C -1.69773 4.73191 0.73149
C -3.05053 4.58871 0.91417
C -3.63737 4.13826 2.22607
C -2.60269 3.85413 3.28304
C -1.25933 4.01153 3.04934
H 0.28938 4.61232 1.63108
H -1.31681 5.07702 -0.22574
H -3.74136 4.81756 0.10778
H -4.35513 4.89627 2.59658
H -4.27640 3.24770 2.07096
H -2.95683 3.53034 4.25755
H -0.54683 3.81068 3.84458
N 0.13315 -2.27942 -0.70254
C 0.29760 -3.36151 -1.10581
C 0.50179 -4.70897 -1.60406
H 1.55136 -4.85474 -1.87644
H 0.23271 -5.43951 -0.83525
H -0.11866 -4.88301 -2.48826

88
FeO+CNCH3+CHD+CI anti Re (0/3)
Fe -0.23299 -0.59272 -0.18397
H -1.04716 0.13081 4.05999
H -2.92840 -0.60838 2.75543
H -3.18867 -2.65653 1.66582
H -0.71871 -1.49666 3.52965
C -0.81449 -0.46748 3.16974
H -1.44574 -2.94361 1.83330
C -2.01111 -0.30293 2.23517
C -2.21320 -2.53378 1.18111
H -4.03611 -0.82806 0.42762
H 0.46685 -2.68847 2.22817
H -2.10540 0.74976 1.96837
H 1.26178 0.05476 3.43484
H -2.20808 -3.08713 0.24515
N -1.96192 -1.07515 0.92720
H 1.97188 -2.06123 2.92992
C 0.51571 0.06166 2.62922
C -3.05891 -0.51002 0.04423
H -3.00656 0.57547 0.11106
C 1.38149 -2.14708 2.01036
H 0.40003 1.08499 2.27143
H -3.02948 -2.04594 -1.46847
N 1.08506 -0.76144 1.48776
H 1.95667 -2.70403 1.27643
C -2.88410 -0.96773 -1.38335
H -3.62711 -0.47318 -2.01733
H 2.92184 0.28366 1.88111
O -0.62401 0.96079 0.16988
C 2.40768 -0.16930 1.02588
H -1.80629 1.44577 -1.81118
N -1.48594 -0.65033 -1.90006
H 1.65410 1.71980 0.29470
H 3.03159 -0.99192 0.67368
H -1.34960 -2.67633 -2.57588
C -1.16847 -1.67708 -2.96087
H -1.82322 -1.50793 -3.82346
N 1.40508 0.25675 -1.21004
H 3.17720 1.19678 -0.44618
C 0.96596 1.42061 -2.08613
H 2.58449 -1.52468 -1.38902
C -0.11285 1.12364 -3.12387
H -0.13522 -1.60362 -3.28353
H -0.26897 2.06850 -3.65884
C 2.26341 -0.68655 -2.00308
H 1.86671 1.79560 -2.59122
H 1.70838 -1.07139 -2.85510
H 0.23188 0.40982 -3.87881
H 3.14641 -0.15282 -2.37302
H 0.04648 4.32976 4.08933
C -0.99305 4.62537 4.30974
C -1.63831 5.19689 3.06893
C -2.78704 4.73693 2.55148
C -3.57507 3.59528 3.14954
C -2.90221 2.98755 4.35809
C -1.75246 3.44741 4.87537
H -0.89509 5.41028 5.07963
```

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H -1.12048 6.02075 2.58153
H -3.19201 5.18493 1.64865
H -4.58844 3.93947 3.42038
H -3.74862 2.82286 2.38185
H -3.40379 2.13946 4.82118
H -1.32459 2.96982 5.75517
N 0.26736 -2.56138 -0.62200
C 0.54414 -3.66631 -0.86857
C 0.88919 -5.04091 -1.17519
H 1.08602 -5.59447 -0.25206
H 0.06592 -5.52552 -1.70875
H 1.78407 -5.07266 -1.80395
S -5.70133 2.31338 -1.37532
O -5.88741 1.78613 0.00064
O -5.04373 1.37754 -2.32605
O -6.84365 3.08328 -1.92748
C -4.39982 3.63494 -1.13385
F -4.05110 4.23606 -2.33195
F -4.84330 4.63239 -0.27702
F -3.23428 3.10613 -0.58041
S 0.31310 5.27934 -1.43975
O 0.45396 4.45231 -0.21306
O -0.37033 4.61690 -2.58046
O 1.51023 6.08380 -1.79828
C -0.91766 6.58510 -0.91773
F -1.11537 7.52459 -1.91883
F -2.15709 6.03691 -0.61701
F -0.48296 7.26745 0.21227

88
FeO+CNCH3+CHD+CI anti TS (0/3)
Fe -0.27541 -0.61516 0.34849
H -0.92751 -1.12466 4.65758
H -2.82162 -1.61734 3.26619
H -3.00721 -3.30709 1.68877
H -0.50686 -2.49302 3.66805
C -0.70285 -1.41698 3.62332
H -1.24161 -3.48947 1.72012
C -1.96073 -1.10636 2.81280
C -2.06784 -2.98643 1.22178
H -4.03500 -1.28222 1.00543
H 0.73450 -3.17618 2.11564
H -2.14429 -0.03366 2.83924
H 1.33146 -0.79409 3.98184
H -2.07323 -3.28184 0.17533
N -1.92571 -1.49760 1.34709
H 2.21377 -2.60918 2.91952
C 0.55578 -0.64319 3.21838
C -3.09891 -0.81137 0.67656
H -3.09603 0.22650 0.99910
C 1.58719 -2.51050 2.02482
H 0.34053 0.42194 3.15515
H -3.10304 -1.91881 -1.17357
N 1.14541 -1.07214 1.88808
H 2.17078 -2.80257 1.15637
C -2.97929 -0.89086 -0.82789
H -3.76627 -0.28824 -1.29394
H 2.86232 0.06831 2.50945
O -0.91022 0.83938 1.08115
C 2.39085 -0.25774 1.57517
H -2.02679 1.60506 -0.79447
N -1.61904 -0.40423 -1.31106
H 1.48357 1.66846 1.25903
H 3.10103 -0.91602 1.07232
H -1.42251 -2.24356 -2.38939
C 2.07065 0.93944 0.70686
C -1.69289 1.06565 -1.67861
H 0.33520 2.42057 -0.33177
H -2.46080 1.16803 -2.45571
C -1.30439 -1.17867 -2.56864
H -2.00338 -0.87548 -3.35740
N 1.25902 0.53003 -0.50314
H 2.99846 1.42772 0.38148
C 0.72479 1.80505 -1.13847
H 2.56203 -1.08313 -1.04847
C -0.36905 1.63783 -2.19074
H -0.29039 -0.98862 -2.90601
H -0.57972 2.65373 -2.54603
C 2.14701 -0.17843 -1.48710
H 1.58091 2.33200 -1.58019
H 1.58152 -0.45096 -2.37536
H -0.00677 1.08814 -3.06571
H 2.96787 0.48543 -1.78378
H -0.59894 1.98604 1.72216
C -0.57654 3.07715 2.38681
C -1.02556 4.12734 1.45053
C -2.28761 4.61548 1.47233
C -3.31655 4.16362 2.47106
C -2.75166 3.28835 3.55518
C -1.48424 2.81627 3.52403
H 0.48329 3.13594 2.65970
H -0.32121 4.49345 0.70841
H -2.59378 5.36702 0.75248
H -3.82126 5.03687 2.91713
H -4.12517 3.62959 1.93841
H -3.40030 3.05800 4.39671
H -1.11237 2.20381 4.34154
N 0.30961 -2.40417 -0.54035
C 0.65358 -3.40082 -1.03742
C 1.08384 -4.64262 -1.65264
H 1.69430 -5.21875 -0.95053
H 0.21575 -5.24344 -1.93990
H 1.67916 -4.43344 -2.54658
S -5.59206 2.38172 -1.16051
O -4.88884 1.97225 0.08432
O -5.33876 1.51607 -2.34290
O -7.00091 2.81541 -0.98037
C -4.72746 3.97384 -1.62117
F -5.25659 4.52327 -2.77912
F -4.84988 4.92452 -0.61668
F -3.37157 3.77405 -1.84276
S 0.01171 6.30834 -2.57695
O 0.12665 5.01389 -1.85336
O -0.65717 6.23811 -3.90059
O 1.21616 7.17555 -2.51530
C -1.22222 7.25372 -1.54461
F -1.42712 8.53128 -2.04380
F -2.45960 6.62152 -1.51179
F -0.79455 7.38403 -0.23039

88
FeO+CNCH3+CHD+CI anti Im (0/3)
Fe -0.42062 -0.68710 0.32116
H -1.31026 -1.27336 4.58112
H -3.05635 -1.90796 3.05851
H -2.99176 -3.59066 1.47635
H -0.71120 -2.59575 3.62238
C -0.99159 -1.53936 3.56469
H -1.22116 -3.62632 1.59532
C -2.21112 -1.32345 2.67022
C -2.06071 -3.18764 1.06016
H -4.14454 -1.64071 0.74932
H 0.66608 -3.15396 2.13375
H -2.47876 -0.26898 2.68736
H 0.96110 -0.76136 4.05460
H -1.99053 -3.46930 0.01198
N -2.04876 -1.69382 1.20552
H 2.04384 -2.48446 3.03218
C 0.22146 -0.65977 3.24921
C -3.23313 -1.09307 0.47501
H -3.32937 -0.06147 0.80322
C 1.46787 -2.42333 2.10153
H -0.07714 0.38653 3.19644
H -3.03669 -2.18013 -1.37854
N 0.92359 -1.01978 1.95080
H 2.12414 -2.65709 1.26824
C -3.02108 -1.14970 -1.01886
H -3.82568 -0.60864 -1.52953
H 2.51384 0.22825 2.69199
O -1.24257 0.75005 1.06926
C 2.12334 -0.11071 1.72587
H -2.29256 1.40331 -0.86027
N -1.68152 -0.54264 -1.41002
H 1.15372 1.79429 1.38673
H 2.90599 -0.70883 1.25758
H -1.26793 -2.32808 -2.51538
C 1.78059 1.07798 0.85344
C -1.86052 0.92887 -1.73837
H -0.03395 2.45420 -0.25286
H -2.58946 0.99080 -2.55641
C -1.23312 -1.25239 -2.66480
H -1.91224 -0.98954 -3.48453
N 1.05036 0.63473 -0.39721
H 2.69806 1.61147 0.57422
C 0.44515 1.87604 -1.04258
H 2.52125 -0.84137 -0.89892
C -0.56897 1.63119 -2.15733
H -0.22312 -0.96717 -2.94272
H -0.84595 2.63013 -2.51435
C 2.03917 0.02201 -1.35124
H 1.27610 2.47743 -1.43246
H 1.53453 -0.29614 -2.25989
H -0.10389 1.13637 -3.01662
H 2.80245 0.76406 -1.61234
H -0.71634 1.47638 1.45542
C 0.00044 3.91902 2.95497
C -0.52700 4.65331 1.85267
C -1.87688 4.70383 1.60616
C -2.87853 3.99533 2.48058
C -2.24900 3.24629 3.62627
C -0.89007 3.22925 3.82875
H 1.06813 3.91174 3.14685
H 0.15369 5.19110 1.19885
H -2.26011 5.26949 0.76404
H -3.61977 4.72258 2.86843
H -3.49742 3.31293 1.86805
H -2.91183 2.71898 4.30707
H -0.48003 2.68773 4.67758
N 0.36344 -2.34288 -0.53624
C 0.81121 -3.29598 -1.03529
C 1.36979 -4.48224 -1.65515
H 2.04139 -4.99106 -0.95688
H 0.56988 -5.17151 -1.94144
H 1.93596 -4.20690 -2.55014
S -5.58812 2.42875 -1.00993
O -4.88969 1.89272 0.18899
O -5.43004 1.62032 -2.24734
O -6.95319 2.95963 -0.76476
C -4.61384 3.97770 -1.39737
F -5.11149 4.62487 -2.51792
F -4.65583 4.88016 -0.34239
F -3.27665 3.69577 -1.64490
S -0.15615 6.25551 -3.15018
O 0.05465 4.88338 -2.61807
O -1.14448 6.36433 -4.25282
O 1.07793 7.06456 -3.31649
C -1.02012 7.12040 -1.73974
F -1.25048 8.45668 -2.02891
F -2.25209 6.54267 -1.45677
F -0.26638 7.07431 -0.57309

88
FeO+CNCH3+CHD+CI anti Re (0/5)
Fe -0.01567 -0.34124 0.08059
H -1.75074 -0.26939 4.11561
H -3.31685 -0.13990 2.34298
H -3.74274 -1.87155 0.79399
H -1.61200 -1.76065 3.23250
C -1.39783 -0.68901 3.16424
H -2.17189 -2.59967 1.20005
C -2.25568 -0.01934 2.08433
C -2.67847 -1.90632 0.53145
H -3.84020 0.34401 -0.18803
H -0.25206 -2.98947 2.19563
H -2.03472 1.04796 2.06161
H 0.55565 -0.75751 4.07466
H -2.57609 -2.26983 -0.48902
N -2.08386 -0.53636 0.66519
H 1.17038 -2.86784 3.25402
C 0.11644 -0.42641 3.12209
C -2.75084 0.43909 -0.28427
H -2.46870 1.44279 0.03451
C 0.77499 -2.63659 2.25634
H 0.32356 0.63880 3.01369
H -2.74985 -0.76309 -2.07906
N 0.84688 -1.15640 2.01366
H 1.36960 -3.16358 1.51316
C -2.35575 0.19558 -1.73650
H -2.81218 0.97146 -2.36486
H 2.65957 -0.49942 2.95626
O -0.16115 1.19186 0.65937
C 2.30473 -0.75008 1.94932
H -0.65663 2.23793 -1.48231
N -0.85928 0.17648 -1.96099
H 2.09884 1.33892 1.43646
H 2.87172 -1.62148 1.61669
H -1.02965 -1.70828 -2.94786
C 2.56243 0.44050 1.03247
C -0.32237 1.55903 -2.26744
H 1.61970 2.30773 -0.39562
H -0.77356 1.88395 -3.21644
C -0.56399 -0.73953 -3.11392
H -0.96546 -0.30792 -4.04006
N 2.00846 0.22863 -0.36234
H 3.64440 0.61434 0.96496
C 2.00883 1.56484 -1.09072
H 2.84249 -1.72879 -0.58415
C 1.20692 1.63248 -2.39459
H 0.50751 -0.88267 -3.23032
H 1.42214 2.62231 -2.81422
C 2.82111 -0.78037 -1.11692
H 3.05779 1.81355 -1.29812
H 2.39260 -0.94599 -2.10390
H 1.58059 0.91671 -3.13408
H 3.84714 -0.41072 -1.23248
H -0.81284 3.43867 1.71191
C -1.47230 4.17187 2.20403
C -2.63612 4.49484 1.29672
C -3.92108 4.34973 1.65649
C -4.35732 3.84834 3.01455
C -3.19214 3.50518 3.91486
C -1.90764 3.65017 3.55296
H -0.83459 5.06209 2.33310
H -2.38232 4.86226 0.30426
H -4.71441 4.60240 0.95454
H -4.99942 4.60107 3.50410
H -5.01285 2.96841 2.89719
H -3.43863 3.12630 4.90576
H -1.11243 3.38736 4.24868
N 0.16012 -2.27293 -0.64847
C 0.25614 -3.36108 -1.05450
C 0.37693 -4.71453 -1.55966
H 0.95587 -4.71803 -2.48832
H 0.88370 -5.34681 -0.82406
H -0.61523 -5.13097 -1.75975
S 0.67918 5.66395 -1.95251
O 0.20656 4.73825 -0.88947
O 0.60686 5.12483 -3.33648
O 0.26002 7.07984 -1.79762
C 2.51987 5.75394 -1.65354
F 3.13900 6.56983 -2.59045
F 2.81360 6.26938 -0.39986
F 3.11851 4.50356 -1.74093
S 2.99879 3.38611 3.95060
O 1.80560 2.52630 3.72068
O 4.30693 2.69312 3.83100
O 2.88337 4.34272 5.07939
C 2.98831 4.50972 2.45755
F 4.06170 5.38597 2.47586
F 3.06948 3.78067 1.27643
F 1.83013 5.27127 2.39716

88
FeO+CNCH3+CHD+CI anti TS (0/5)
Fe -0.17670 -0.28058 0.10788
H -2.18601 -0.46381 4.01160
H -3.65743 -0.38791 2.16126
H -3.89042 -2.07723 0.49879
H -1.87293 -1.90598 3.09189
C -1.74646 -0.81859 3.06996
H -2.31585 -2.72059 1.02185
C -2.59593 -0.18381 1.95881
C -2.80629 -2.03723 0.33000
H -4.02887 0.17639 -0.43436
H -0.36201 -2.99638 2.10779
H -2.45073 0.89614 1.97501
H 0.14349 -0.74100 4.10832
H -2.59186 -2.36515 -0.68562
N -2.30515 -0.64400 0.54533
H 0.93630 -2.79555 3.30721
C -0.25678 -0.43578 3.13016
C -2.93949 0.32032 -0.43267
H -2.72858 1.32660 -0.07271
C 0.62391 -2.56923 2.27915
H -0.13914 0.64408 3.03660
H -2.75068 -0.82454 -2.25521
N 0.60646 -1.08238 2.06718
H 1.32594 -3.03068 1.58783
C -2.41762 0.13616 -1.85726
H -2.85267 0.91400 -2.49766
H 2.27643 -0.28625 3.16150
O -0.46133 1.28688 0.70439
C 2.03492 -0.57118 2.13032
H -0.80905 2.24157 -1.51395
N -0.90532 0.17171 -1.97438
H 1.76279 1.50043 1.57780
H 2.68820 -1.40424 1.86351
H -0.94731 -1.72589 -2.94717
C 2.30459 0.62702 1.22352
C -0.39919 1.57019 -2.26860
H 1.40515 2.43181 -0.30095
H -0.80193 1.86493 -3.24923
C -0.49896 -0.74555 -3.09292
H -0.84221 -0.33599 -4.05205
N 1.88404 0.37788 -0.20777
H 3.37799 0.85905 1.25432
C 1.86675 1.69677 -0.95787
H 2.81300 -1.54170 -0.34057
C 1.13302 1.70322 -2.30486
H 0.58208 -0.86091 -3.12629
H 1.33389 2.69025 -2.73889
C 2.80474 -0.59408 -0.87635
H 2.91142 1.99612 -1.11848
H 2.47665 -0.77884 -1.89836
H 1.57519 0.98536 -3.00375
H 3.82401 -0.18701 -0.90001
H -0.85196 2.70363 1.31831
C -1.17633 3.71532 1.80333
C -2.44776 4.14395 1.15854
C -3.62705 4.16590 1.81492
C -3.76016 3.79766 3.26874
C -2.44169 3.51582 3.93936
C -1.26703 3.50031 3.27385
H -0.32895 4.34863 1.51303
H -2.39190 4.44104 0.11480
H -4.53315 4.48115 1.30272
H -4.29060 4.60011 3.80978
H -4.43005 2.92456 3.37539
H -2.46431 3.34295 5.01295
H -0.33582 3.30729 3.80062
N 0.17211 -2.31257 -0.65136
C 0.37069 -3.39005 -1.05040
C 0.62097 -4.72997 -1.54777
H 1.08400 -4.68380 -2.53800
H 1.29248 -5.26470 -0.86938
H -0.31835 -5.28570 -1.62382
S 0.69534 5.81052 -2.03677
O 0.14631 4.94779 -0.95782
O 0.67519 5.21107 -3.39715
O 0.30795 7.24231 -1.96592
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C 2.51975 5.86611 -1.64678
F 3.20434 6.64667 -2.56813
F 2.76068 6.40356 -0.39070
F 3.09268 4.60182 -1.67605
S 3.25810 3.54754 3.99744
O 2.10038 2.61201 3.96794
O 4.57131 2.93718 3.66845
O 3.26587 4.51172 5.12683
C 2.93961 4.64994 2.52174
F 3.93640 5.60122 2.37753
F 2.89025 3.91778 1.34199
F 1.73246 5.32803 2.63749

88
FeO+CNCH3+CHD+Cl anti Im (0/5)
Fe -0.14887 -0.21879 0.11744
H -2.12801 -0.39265 4.02731
H -3.62374 -0.31013 2.19548
H -3.91050 -1.97147 0.51812
H -1.84800 -1.84139 3.10736
C -1.70620 -0.75606 3.08085
H -2.35158 -2.65116 1.04279
C -2.56346 -0.11401 1.97883
C -2.82559 -1.95708 0.34971
H -3.99851 0.28262 -0.41416
H -0.37143 -2.95374 2.10330
H -2.41067 0.96471 1.99541
H 0.19585 -0.70762 4.09637
H -2.61838 -2.29310 -0.66492
N -2.28945 -0.57728 0.56248
H 0.93819 -2.77399 3.29418
C -0.20970 -0.39557 3.12289
C -2.90590 0.40135 -0.41454
H -2.67334 1.40280 -0.05576
C 0.62372 -2.54594 2.26733
H -0.07280 0.68163 3.02732
H -2.75790 -0.74173 -2.24086
N 0.63460 -1.05930 2.05120
H 1.31225 -3.02346 1.57370
C -2.39297 0.20666 -1.84149
H -2.80404 0.99971 -2.47859
H 2.32292 -0.28494 3.13544
O -0.39487 1.45317 0.73516
C 2.07785 -0.57851 2.10790
H -0.70549 2.26984 -1.54305
N -0.87778 0.19284 -1.96707
H 1.85661 1.48898 1.52568
H 2.71002 -1.43164 1.85426
H -0.99010 -1.71390 -2.91693
C 2.37807 0.59901 1.18363
C -0.32882 1.57133 -2.28984
H 1.54241 2.40973 -0.36651
H -0.73509 1.86127 -3.27015
C -0.50767 -0.75215 -3.07542
H -0.83915 -0.34151 -4.03799
N 1.94866 0.34051 -0.24463
H 3.45730 0.80397 1.21169
C 1.96560 1.64651 -1.01671
H 2.82563 -1.60495 -0.35223
C 1.20677 1.65569 -2.35106
H 0.56843 -0.90618 -3.10918
H 1.42800 2.63061 -2.80231
C 2.84308 -0.66359 -0.89919
H 3.01684 1.90598 -1.20413
H 2.51063 -0.85320 -1.91935
H 1.61525 0.91504 -3.04667
H 3.87371 -0.28602 -0.92802
H -0.64414 2.34922 1.04650
C -1.39791 4.23969 1.88352
C -2.66624 4.37090 1.24177
C -3.83329 4.05433 1.88973
C -3.84816 3.56375 3.31413
C -2.47522 3.44041 3.92250
C -1.33708 3.77442 3.23109
H -0.50055 4.55912 1.36573
H -2.69481 4.73492 0.21837
H -4.79050 4.16365 1.38734
H -4.47725 4.23137 3.93577
H -4.38007 2.59457 3.37615
H -2.41236 3.08698 4.94816
H -0.36477 3.67771 3.70573
N 0.15307 -2.31459 -0.64996
C 0.32505 -3.39975 -1.04139
C 0.54270 -4.74920 -1.52909
H 1.04097 -4.72223 -2.50276
H 1.17008 -5.30731 -0.82768
H -0.41320 -5.27025 -1.63734
S 0.71166 5.72649 -1.99207
O 0.20841 4.82429 -0.92223
O 0.67822 5.15813 -3.36514
O 0.28735 7.14486 -1.87867
C 2.54160 5.82202 -1.63808
F 3.18729 6.63141 -2.56256
F 2.79499 6.34898 -0.38016
F 3.14423 4.57273 -1.69604
S 3.21371 3.52631 4.02337
O 2.07254 2.57294 3.95181
O 4.54852 2.93587 3.74923
O 3.16224 4.49468 5.14803
C 2.93529 4.61616 2.53035
F 3.91552 5.58948 2.42461
F 2.95457 3.87835 1.35312
F 1.70924 5.26638 2.59093
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[(TMC)FeOO]$^{2+}$ (4)

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53
FeOO syn (2/1)
Fe -0.07039 0.07349 -0.04811
H 1.70330 -1.62243 -3.68868
H -0.66761 -1.30318 -3.70566
H -1.56014 0.94548 -3.69581
H 1.44618 0.09535 -3.57459
C 1.32866 -0.83907 -3.01819
H -0.07084 1.57595 -2.96892
C -0.13787 -1.16268 -2.75468
C -1.04720 1.15315 -2.74996
H -2.89878 -0.61368 -2.61503
H 1.71730 1.78168 -2.24841
H -0.20912 -2.10043 -2.19444
H 3.26688 -0.78761 -2.06421
H -1.62172 1.88609 -2.18558
N -0.91197 -0.11883 -1.95918
H 3.37246 1.51675 -1.67463
C 2.21203 -0.87195 -1.77326
C -2.29196 -0.69291 -1.70578
H -2.17400 -1.75460 -1.47976
C 2.31948 1.55688 -1.37319
H 2.08480 -1.82999 -1.26171
H -3.10574 1.08898 -0.79818
N 1.92900 0.23111 -0.76619
H 2.18942 2.34865 -0.63833
C -2.94635 0.03622 -0.55768
H -3.92640 -0.39773 -0.32872
H 3.81317 -0.29837 0.12443
O 0.05359 2.11285 0.29767
C 2.81687 0.02539 0.44760
H -2.08543 -2.15758 0.64925
N -2.05948 -0.02789 0.67282
H 2.10778 -1.96467 0.89077
H 2.93417 0.99113 0.94229
H -2.48344 2.03200 1.06487
C 2.19475 -0.98956 1.37452
C -2.27753 -1.36202 1.37430
H 0.20114 -2.55734 1.57869
H -3.33778 -1.41234 1.65321
C -2.50675 1.08209 1.59400
H -3.53426 0.88626 1.92043
N 0.79963 -0.53918 1.76068
H 2.80450 -1.12098 2.27621
C 0.07735 -1.75805 2.31603
H 1.39210 1.41823 2.39845
C -1.40779 -1.57320 2.61235
H -1.86850 1.14972 2.46916
H -1.74835 -2.50568 3.07914
C 0.90118 0.53692 2.80917
H 0.60515 -2.06289 3.22896
H -0.08629 0.82512 3.15819
H -1.58015 -0.79708 3.36373
H 1.47845 0.16456 3.66286
O -0.76710 2.99947 -0.13989

53
FeOO syn TI (2/3)
Fe -0.07109 0.19194 -0.03188
H 1.71111 -1.66712 -3.65850
H -0.66822 -1.34530 -3.69442
H -1.58411 0.94088 -3.65127
H 1.43434 0.04884 -3.58993
C 1.32441 -0.87162 -3.00992
H -0.03440 1.50156 -2.99762
C -0.13997 -1.20492 -2.74250
C -1.01797 1.12711 -2.73216
H -2.89725 -0.62286 -2.59683
H 1.75957 1.76858 -2.29942
H -0.21002 -2.14103 -2.18017
H 3.25903 -0.77559 -2.05874
H -1.52262 1.88470 -2.13525
N -0.90292 -0.15996 -1.95364
H 3.38478 1.56591 -1.62208
C 2.20621 -0.86594 -1.76465
C -2.29384 -0.70012 -1.68549
H -2.20056 -1.75992 -1.44166
C 2.31528 1.58430 -1.38522
H 2.09027 -1.81266 -1.23230
H -3.04060 1.13115 -0.80969
N 1.93204 0.25804 -0.77549
H 2.10595 2.37830 -0.67251
C -2.92820 0.07589 -0.55686
H -3.92357 -0.31725 -0.32291
H 3.81160 -0.23395 0.13345
O 0.04052 2.12759 0.28918
C 2.80455 0.05699 0.45273
H -2.09583 -2.13059 0.62860
N -2.05667 -0.00076 0.68698
H 2.12931 -1.95921 0.85339
H 2.88834 1.01969 0.95929
H -2.40867 2.06100 1.09618
C 2.19954 -0.99159 1.35323
C -2.27085 -1.34647 1.36906
H 0.19886 -2.58340 1.54090
H -3.32963 -1.38603 1.65332
C -2.49718 1.10840 1.61175
H -3.54289 0.93669 1.88950
N 0.79792 -0.57150 1.75279
H 2.80975 -1.12895 2.25330
C 0.08089 -1.79487 2.28985
H 1.30367 1.41972 2.37517
C -1.40054 -1.59819 2.59742
H -1.89281 1.12894 2.51254
H -1.75328 -2.53818 3.03877
C 0.88270 0.51102 2.80163
H 0.60990 -2.11194 3.19796
H -0.10413 0.74156 3.19077
H -1.56179 -0.84105 3.36985
H 1.51183 0.16231 3.62762
O -0.87636 3.02140 -0.17309

53
FeOO syn TII (2/3)
Fe -0.05603 0.09066 -0.04319
H 1.69874 -1.64601 -3.67155
H -0.67629 -1.35560 -3.66657
H -1.51775 0.88178 -3.73993
H 1.42284 0.07089 -3.58979
C 1.32200 -0.85325 -3.01369
H -0.06982 1.57012 -2.98114
C -0.13780 -1.18540 -2.72585
C -1.04328 1.13189 -2.78469
H -2.90392 -0.59410 -2.60812
H 1.68110 1.78477 -2.26749
H -0.19868 -2.10797 -2.13940
H 3.26632 -0.73496 -2.07698
H -1.64475 1.86468 -2.25319
N -0.91200 -0.11951 -1.95661
H 3.32845 1.57619 -1.65389
C 2.21752 -0.85179 -1.77795
C -2.29870 -0.67701 -1.69881
H -2.19616 -1.73894 -1.46690
C 2.26879 1.58656 -1.37683
H 2.12499 -1.80982 -1.25976
H -3.06289 1.13010 -0.80163
N 1.91145 0.24816 -0.77357
H 2.09443 2.37392 -0.64763
C -2.93491 0.07452 -0.55724
H -3.92461 -0.33271 -0.32211
H 3.80301 -0.23574 0.12151
O 0.05378 1.90758 0.53238
C 2.79973 0.06233 0.44525
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N -2.04807 -0.00485 0.67271
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C 2.19757 -0.97063 1.36563
C -2.28161 -1.34184 1.36710
H 0.18883 -2.54834 1.52856
H -3.34072 -1.37497 1.65096
C -2.48386 1.10841 1.59564
H -3.51647 0.92266 1.91054
N 0.79941 -0.53508 1.76379
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C 0.07192 -1.76688 2.28599
H 1.39695 1.40162 2.45201
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H -1.85028 1.16151 2.47440
H -1.75289 -2.51262 3.05282
C 0.89632 0.51585 2.83694
H 0.60596 -2.09597 3.18629
H -0.09209 0.80531 3.17967
H -1.57011 -0.80898 3.36014
H 1.46030 0.11295 3.68469
O -0.59725 2.78030 -0.24541

53
FeOO syn sideon (2/3)
Fe -0.00471 0.02683 -0.01768
H 0.00089 -0.05812 4.42823
H 2.13847 -0.15762 3.36247
H 2.75199 1.86080 2.31123
H 0.17446 1.44531 3.56661
C 0.04340 0.36947 3.41918
H 1.13388 2.39627 1.80529
C 1.24915 -0.25925 2.72691
C 1.98693 1.78523 1.53051
H 3.69301 -0.06711 1.26330
H -0.77748 2.59069 1.93159
H 1.07173 -1.32787 2.56948
H -2.11642 0.40396 3.38962
H 2.38768 2.16365 0.59347
N 1.59001 0.33972 1.37757
H -2.52094 2.35447 2.14201
C -1.29405 0.04299 2.75969
C 2.76604 -0.42594 0.80200
H 2.65155 -1.47648 1.07354
C -1.66357 2.14092 1.49411
H -1.39588 -1.04052 2.66948
H 2.94154 0.81267 -0.96164
N -1.50846 0.64447 1.37745
H -1.83655 2.56733 0.50932
C 2.80825 -0.23666 -0.69479
H 3.63785 -0.79980 -1.13691
H -3.57761 0.11266 1.57194
O -0.77391 1.54476 -1.37092
C -2.80150 0.09509 0.79824
H 1.74637 -2.60242 -0.40004
N 1.50240 -0.70015 -1.31919
H -2.28947 -1.99171 1.07601
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C -2.59254 -1.30822 0.28111
C 1.50523 -2.21999 -1.39443
H -0.64843 -3.03197 0.09820
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C 1.43586 -0.12130 -2.71177
H 2.29929 -0.48008 -3.28251
N -1.50513 -1.30685 -0.77641
H -3.51957 -1.70078 -0.15189
C -0.95891 -2.71589 -0.90274
H -2.61856 0.09132 -1.95358
C 0.20602 -2.85940 -1.87721
H 0.52808 -0.43339 -3.21863
H 0.40854 -3.93305 -1.97113
C -2.10802 -0.85976 -2.08346
H -1.78889 -3.36212 -1.21602
H -1.34402 -0.73384 -2.84339
H -0.06346 -2.52780 -2.88409
H -2.82607 -1.61656 -2.41910
O 0.38525 2.02898 -0.80020

53
FeOO syn QI (2/5)
Fe 6.76604 3.99696 5.29152
H 3.12792 4.26992 2.79385
H 2.76716 4.05434 5.15872
H 3.42704 5.80698 6.66440
H 3.80215 5.69543 3.52869
C 3.94737 4.61547 3.43587
H 4.53907 6.42899 5.42841
C 3.78232 3.89843 4.77216
C 4.45004 5.75683 6.27703
H 3.62256 3.70959 7.57831
H 5.71688 6.73678 3.85203
H 3.92552 2.82297 4.63067
H 5.20848 4.69392 1.68570
H 5.15172 6.07889 7.04440
N 4.74963 4.33338 5.85946
H 6.42374 6.61672 2.22842
C 5.24130 4.27778 2.70017
C 4.54064 3.41953 7.05509
H 4.39756 2.40530 6.67807
C 6.53232 6.31092 3.27470
H 5.33483 3.19301 2.61061
H 5.86350 4.51140 8.37055
N 6.51494 4.80232 3.34740
H 7.47677 6.68106 3.66486
C 5.73259 3.50195 7.97802
H 5.61249 2.82783 8.83315
H 7.49906 4.38728 1.48599
O 8.25297 5.48561 5.62871
C 7.71043 4.29413 2.55715
H 6.15453 1.24463 6.74844
N 7.00116 3.13428 7.22263
H 7.17548 2.20009 2.69217
H 8.55289 4.94857 2.78404
H 8.05830 4.76654 8.10290
C 8.01359 2.86010 2.92332
C 7.09814 1.61641 7.15506
H 7.14645 0.98073 4.47865
H 7.18081 1.26074 8.18950
C 8.17101 3.68997 7.99666
H 8.19226 3.22606 8.98915
N 8.28660 2.75970 4.41133
H 8.88314 2.49577 2.36422
C 8.13041 1.31004 4.82708
H 9.82571 4.25008 4.34481
C 8.25538 1.06200 6.32785
H 9.10719 3.48104 7.48834
H 8.23960 -0.02574 6.46858
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C 9.69517 3.22443 4.67981
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H 9.22497 1.38792 6.71584
H 10.39283 2.56855 4.14666
O 7.78831 6.55841 6.28446

53
FeOO syn QII (2/5)
Fe 6.83796 4.15611 5.33092
H 3.11363 4.32758 2.81174
H 2.77725 3.94197 5.11838
H 3.28593 5.73321 6.62749
H 3.81730 5.71588 3.58770
C 3.95439 4.64000 3.44367
H 4.49069 6.42540 5.51381
C 3.81164 3.86766 4.75719
C 4.33935 5.71730 6.32637
H 3.61287 3.61104 7.58078
H 5.73371 6.81035 3.67061
H 4.02919 2.80883 4.58484
H 5.13643 4.75976 1.63648
H 4.96305 6.02600 7.16529
N 4.71765 4.32524 5.88646
H 6.48892 6.64845 2.06840
C 5.22262 4.33359 2.64487
C 4.54605 3.37494 7.05553
H 4.44712 2.36590 6.65088
C 6.56139 6.36123 3.12377
H 5.32113 3.25075 2.53758
H 5.82012 4.48023 8.41465
N 6.51502 4.85900 3.24417
H 7.49972 6.72837 3.53773
C 5.72064 3.46942 8.01403
H 5.56829 2.79368 8.86447
H 7.48480 4.32059 1.40780
O 8.31065 5.49579 5.64991
C 7.69215 4.28155 2.48419
H 6.19224 1.23907 6.81097
N 7.02368 3.12263 7.32149
H 7.12426 2.19987 2.70991
H 8.55193 4.92718 2.67286
H 8.04772 4.75445 8.23423
C 7.97906 2.85024 2.90526
C 7.13761 1.61486 7.20955
H 7.10159 1.02460 4.53385
H 7.24508 1.22420 8.23061
C 8.16123 3.67533 8.13657
H 8.15627 3.21918 9.13362
N 8.28777 2.76678 4.38540
H 8.82846 2.45598 2.33438
C 8.10671 1.33146 4.83976
H 9.85321 4.22209 4.24078
C 8.28303 1.09677 6.34002
H 9.11411 3.46357 7.65595
H 8.30615 0.00909 6.48172
C 9.70438 3.21719 4.62947
H 8.82877 0.71990 4.28241
H 9.92236 3.23178 5.69431
H 9.25521 1.45117 6.69561
H 10.39238 2.52448 4.13099
O 8.07373 6.55699 6.43552

53
FeOO syn QIII (2/5)
Fe 6.85649 4.15003 5.33282
H 3.12000 4.31573 2.81083
H 2.78748 3.89566 5.10900
H 3.24937 5.71126 6.58469
H 3.81259 5.70263 3.59971
C 3.95873 4.62930 3.44494
H 4.48980 6.41917 5.51959
C 3.82542 3.84517 4.75278
C 4.31296 5.70363 6.32045
H 3.61970 3.60110 7.58627
H 5.72706 6.81242 3.68192
H 4.06471 2.79163 4.57515
H 5.13750 4.77782 1.63802
H 4.90350 6.00893 7.18439
N 4.71658 4.31590 5.88652
H 6.48921 6.66591 2.08224
C 5.22956 4.34263 2.64253
C 4.55324 3.37033 7.05860
H 4.45975 2.35886 6.65832
C 6.55875 6.36930 3.13571
H 5.33421 3.26148 2.52354
H 5.82852 4.49108 8.40353
N 6.51681 4.86788 3.24763
H 7.49298 6.74050 3.55578
C 5.72967 3.47493 8.01547
H 5.57525 2.81032 8.87482
H 7.49181 4.33932 1.40977
O 8.24867 5.47589 5.68589
C 7.69483 4.29738 2.48729
H 6.18955 1.23791 6.84262
N 7.03262 3.12162 7.32989
H 7.12925 2.21456 2.70127
H 8.55395 4.94283 2.68066
H 8.07773 4.75147 8.22528
C 7.98257 2.86452 2.90439
C 7.14172 1.61431 7.22428
H 7.05770 1.06068 4.54418
H 7.26639 1.22316 8.24355
C 8.16801 3.66782 8.15111
H 8.14235 3.23245 9.15764
N 8.28060 2.77616 4.38673
H 8.83560 2.47205 2.33782
C 8.07441 1.34309 4.83653
H 9.87846 4.19027 4.21218
C 8.26927 1.09288 6.33271
H 9.12292 3.42573 7.68848
H 8.28449 0.00367 6.46389
C 9.70329 3.20370 4.63686
H 8.77291 0.71789 4.26433
H 9.90764 3.25029 5.70352
H 9.25014 1.43552 6.67623
H 10.38444 2.48228 4.17066
O 8.20547 6.65764 6.26191

53
FeOO syn QSI (2/5)
Fe -0.08876 0.36011 -0.01863
H 1.70512 -1.61019 -3.67230
H -0.65234 -1.51860 -3.56202
H -1.46987 0.71052 -3.83737
H 1.34317 0.08994 -3.59619
C 1.31885 -0.83004 -3.00489
H -0.14341 1.54924 -2.99602
C -0.11144 -1.23511 -2.64958
C -1.09356 1.04036 -2.86271
H -2.91940 -0.71586 -2.55353
H 1.83145 1.85905 -2.31560
H -0.10095 -2.10334 -1.98338
H 3.30704 -0.62774 -2.18063
H -1.79854 1.74322 -2.42346
N -0.93675 -0.16105 -1.96523
H 3.45387 1.68277 -1.61595
C 2.28004 -0.76768 -1.81846
C -2.30610 -0.72844 -1.64526
H -2.17288 -1.77183 -1.35356
C 2.38009 1.67376 -1.39495
H 2.24730 -1.72015 -1.28508
H -3.10231 1.11783 -0.83399
N 2.00290 0.33547 -0.81427
H 2.14819 2.45568 -0.67423
C -2.98187 0.07190 -0.54643
H -3.98150 -0.33224 -0.34682
H 3.84534 -0.19721 0.14530
O 0.19798 2.15291 0.82766
C 2.82938 0.10071 0.43129
H -2.28295 -2.07434 0.69532
N -2.16168 0.04321 0.72503
H 2.10593 -1.91464 0.77072
H 2.90302 1.05215 0.96094
H -2.41789 2.12668 1.08706
C 2.20037 -0.96797 1.30570
C -2.37181 -1.27714 1.43677
H 0.07383 -2.48787 1.31732
H -3.40487 -1.28608 1.80865
C -2.59689 1.18651 1.60549
H -3.66517 1.08627 1.82968
N 0.81155 -0.55462 1.75531
H 2.82256 -1.14902 2.18966
C 0.04278 -1.79739 2.16629
H 1.59129 1.22631 2.64714
C -1.40705 -1.55854 2.58906
H -2.04025 1.18080 2.53947
H -1.75150 -2.48866 3.05714
C 0.92807 0.40511 2.91186
H 0.59838 -2.25847 2.99346
H -0.04203 0.81982 3.17084
H -1.47960 -0.79905 3.37288
H 1.33739 -0.12827 3.77707
O -0.45811 2.28269 -0.41557

53
FeOO syn QSII (2/5)
Fe -0.00422 0.02487 -0.01548
H 0.00085 -0.05380 4.42678
H 2.13815 -0.15236 3.36218
H 2.76033 1.86130 2.30994
H 0.17063 1.44884 3.56280
C 0.04228 0.37240 3.41706
H 1.14170 2.40082 1.81046
C 1.24953 -0.25437 2.72570
C 1.99257 1.78831 1.53159
H 3.69401 -0.06685 1.26430
H -0.77467 2.59021 1.91869
H 1.07279 -1.32309 2.56807
H -2.11797 0.39970 3.38784
H 2.39196 2.16761 0.59412
N 1.59115 0.34455 1.37626
H -2.51499 2.35123 2.15404
C -1.29432 0.04175 2.75788
C 2.76637 -0.42413 0.80312
H 2.64938 -1.47406 1.07605
C -1.66628 2.13849 1.49464
H -1.39230 -1.04215 2.66744
H 2.94710 0.80952 -0.96314
N -1.50938 0.64234 1.37509
H -1.85451 2.56545 0.51270
C 2.80993 -0.23888 -0.69418
H 3.63836 -0.80536 -1.13427
H -3.57771 0.10747 1.57557
O -0.76305 1.52875 -1.37139
C -2.80372 0.09304 0.79966
H 1.74333 -2.60245 -0.39833
N 1.50255 -0.69986 -1.31721
H -2.28795 -1.99255 1.07222
H -3.12051 0.76959 0.00454
H 1.48006 0.96201 -2.65766
C -2.59314 -1.30836 0.27873
C 1.50526 -2.21960 -1.39333
H -0.64879 -3.02735 0.09573
H 2.32729 -2.49911 -2.06394
C 1.43829 -0.12310 -2.71088
H 2.29474 -0.49307 -3.28494
N -1.50608 -1.30253 -0.77900
H -3.51979 -1.70204 -0.15406
C -0.95942 -2.71186 -0.90535
H -2.62527 0.09097 -1.95611
C 0.20598 -2.85643 -1.87882
H 0.52431 -0.42363 -3.21363
H 0.40656 -3.93035 -1.97411
C -2.11240 -0.85910 -2.08558
H -1.78941 -3.35832 -1.21811
H -1.34977 -0.73302 -2.84703
H -0.06160 -2.52262 -2.88552
H -2.82979 -1.61729 -2.41955
O 0.37639 2.01765 -0.78238

53
FeOO syn QSIII (2/5)
Fe -0.00350 0.06293 -0.03978
H 0.00741 0.05664 4.44765
H 2.12711 -0.12337 3.40653
H 2.83526 1.86128 2.30436
H 0.17103 1.51977 3.52061
C 0.03909 0.43837 3.41963
H 1.21551 2.41765 1.82144
C 1.24930 -0.21932 2.75371
C 2.05568 1.78917 1.53718
H 3.70750 -0.15022 1.29009
H -0.87679 2.64129 1.89701
H 1.05685 -1.28723 2.60891
H -2.12264 0.43343 3.45353
H 2.44927 2.15404 0.59049
N 1.62623 0.35273 1.40132
H -2.60852 2.37866 2.19250
C -1.31359 0.08772 2.79671
C 2.76573 -0.46219 0.82340
H 2.59881 -1.50646 1.09409
C -1.77508 2.16154 1.51439
H -1.39710 -0.99865 2.71556
H 3.03604 0.75126 -0.95298
N -1.57836 0.67249 1.41847
H -2.00004 2.56444 0.52806
C 2.85375 -0.29088 -0.68378
H 3.68780 -0.88249 -1.07974
H -3.60968 0.01240 1.62376
O -0.74144 1.54603 -1.41546
C -2.83745 0.05114 0.84585
H 1.74156 -2.62831 -0.45218
N 1.56709 -0.71793 -1.36476
H -2.22002 -2.01541 1.09149
H -3.20077 0.71492 0.05910
H 1.62076 0.96220 -2.67877
C -2.57833 -1.34700 0.30625
C 1.52105 -2.23439 -1.44743
H -0.64170 -3.05697 0.03479
H 2.33707 -2.54354 -2.11384
C 1.53621 -0.12118 -2.74800
H 2.37532 -0.51208 -3.33459
N -1.53652 -1.32796 -0.79300
H -3.51056 -1.77194 -0.08483
C -0.96441 -2.72414 -0.95687
H -2.67065 0.08838 -1.92845
C 0.20142 -2.83065 -1.94122
H 0.60657 -0.37304 -3.25369
H 0.38682 -3.90208 -2.08584
C -2.17176 -0.86707 -2.07784
H -1.78333 -3.37977 -1.28068
H -1.42259 -0.74260 -2.85579
H -0.06863 -2.45130 -2.93134
H -2.90668 -1.61193 -2.40458
O 0.34869 2.06083 -0.77220

53
FeOO syn sideon (2/7)
Fe -0.00311 0.04526 -0.02935
H 0.00745 0.06097 4.45081
H 2.13021 -0.10491 3.41454
H 2.84747 1.86956 2.30307
H 0.16237 1.52448 3.52270
C 0.03815 0.44204 3.42248
H 1.22544 2.42746 1.83123
C 1.25489 -0.20741 2.75917
C 2.06280 1.79767 1.54072
H 3.71037 -0.14538 1.29018
H -0.87039 2.63698 1.88980
H 1.06908 -1.27690 2.61689
H -2.12421 0.42210 3.45329
H 2.45170 2.16274 0.59195
N 1.62966 0.36320 1.40589
H -2.59731 2.37256 2.20912
C -1.31174 0.08238 2.79746
C 2.76595 -0.45548 0.82725
H 2.59727 -1.49884 1.10098
C -1.77328 2.15603 1.51936
H -1.38782 -1.00457 2.71474
H 3.03593 0.75010 -0.95407
N -1.57598 0.66722 1.41883
H -2.01315 2.56053 0.53710
C 2.85233 -0.29091 -0.68129
H 3.68633 -0.88454 -1.07466
H -3.60790 0.00722 1.62363
O -0.75635 1.57299 -1.39209
C -2.83584 0.04773 0.84553
H 1.72998 -2.62832 -0.44338
N 1.56548 -0.71917 -1.36134
H -2.21926 -2.01942 1.08361
H -3.19952 0.71389 0.06087
H 1.64080 0.95383 -2.68408
C -2.57958 -1.34947 0.30045
C 1.51845 -2.23597 -1.44136
H -0.65726 -3.06721 0.02173
H 2.33934 -2.54838 -2.10033
C 1.53699 -0.12836 -2.74719
H 2.36584 -0.53526 -3.33761
N -1.54141 -1.33031 -0.80190
H -3.51446 -1.77233 -0.08696
C -0.97240 -2.72766 -0.97012
H -2.67332 0.09020 -1.93408
C 0.20151 -2.83086 -1.94579
H 0.60027 -0.36609 -3.24692
H 0.38773 -3.90181 -2.09305
C -2.17905 -0.86777 -2.08419
H -1.78973 -3.38025 -1.30422
H -1.43153 -0.74748 -2.86481
H -0.06118 -2.44760 -2.93642
H -2.91916 -1.60817 -2.41000
O 0.36595 2.05286 -0.80894

53
FeOO syn unbound (2/7)
Fe -0.07242 0.14598 -0.05920
H 1.74847 -1.50180 -3.78684
H -0.61256 -1.39172 -3.77509
H -1.69291 0.80011 -3.74937
H 1.38413 0.18559 -3.57196
C 1.33808 -0.78368 -3.06533
H -0.21887 1.50152 -3.03935
C -0.11181 -1.21424 -2.81228
C -1.17172 1.02744 -2.81066
H -2.91228 -0.90485 -2.58311
H 1.80941 1.84530 -2.19430
H -0.11963 -2.15895 -2.25801
H 3.31259 -0.72047 -2.18886
H -1.76701 1.73183 -2.22934
N -0.95012 -0.23311 -2.02423
H 3.46853 1.61418 -1.59755
C 2.27088 -0.82055 -1.84878
C -2.27862 -0.86841 -1.68663
H -2.08133 -1.89993 -1.38354
C 2.40628 1.59261 -1.31867
H 2.17970 -1.79504 -1.35999
H -3.20715 0.91894 -0.88753
N 2.02374 0.23856 -0.79845
H 2.22218 2.33856 -0.54469
C -2.99843 -0.10726 -0.57804
H -3.96612 -0.58474 -0.37292
H 3.84639 -0.43294 0.12177
O 0.33938 3.62334 0.83356
C 2.85538 -0.06951 0.42520
H -2.22330 -2.16008 0.76309
N -2.17669 -0.04555 0.68832
H 2.03741 -2.04417 0.78703
H 3.00740 0.86738 0.96477
H -2.48633 2.04435 0.92753
C 2.18287 -1.10251 1.32290
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C -2.36144 -1.33137 1.46381
H 0.09248 -2.59897 1.55570
H -3.40475 -1.36635 1.81193
C -2.62560 1.13092 1.50731
H -3.68466 1.03184 1.78108
N 0.82416 -0.63243 1.78566
H 2.82142 -1.31195 2.19170
C 0.04276 -1.81407 2.31767
H 1.54736 1.26405 2.45990
C -1.42359 -1.52851 2.65979
H -2.03334 1.20455 2.41856
H -1.79166 -2.41309 3.19532
C 0.98177 0.41740 2.84967
H 0.56027 -2.18847 3.21289
H 0.00636 0.78139 3.16756
H -1.51292 -0.70498 3.37559
H 1.50851 -0.00124 3.71669
O -0.56625 3.71665 -0.02925

53
FeOO anti (2/1)
Fe -0.04074 -0.34339 -0.09796
H 1.83125 -1.19482 -3.96813
H -0.56695 -0.89032 -4.01216
H -1.88356 1.09622 -3.30453
H 1.47789 0.44608 -3.51560
C 1.39644 -0.58729 -3.16446
H -0.24142 1.58470 -2.85655
C -0.06526 -1.02279 -3.04499
C -1.15640 1.12976 -2.48623
H -2.79802 -0.92097 -2.72355
H 1.46369 1.79186 -1.86906
H -0.11451 -2.08432 -2.79626
H 3.31573 -0.59482 -2.18635
H -1.54751 1.74946 -1.68070
N -0.88085 -0.27597 -2.00119
H 3.14081 1.68697 -1.29984
C 2.27244 -0.81784 -1.92963
C -2.19422 -1.00291 -1.81146
H -1.97724 -2.05951 -1.65596
C 2.09465 1.49471 -1.03765
H 2.22387 -1.86396 -1.61630
H -3.33468 0.57057 -0.87191
N 1.91308 0.02754 -0.71844
H 1.82614 2.09280 -0.16625
C -2.94027 -0.41722 -0.62984
H -3.79408 -1.04873 -0.36693
H 3.75202 -0.80536 0.03841
O -0.62750 -3.36727 -0.43654
C 2.85846 -0.31261 0.43250
H -2.19978 -2.33225 1.04639
N -2.01772 -0.27344 0.58028
H 2.02470 -2.20786 1.05590
H 3.18412 0.62274 0.88944
H -2.06205 1.86651 0.50657
C 2.17016 -1.20140 1.44837
C -2.30662 -1.38261 1.57718
H 0.17920 -2.62590 2.13275
H -3.35857 -1.28955 1.87583
C -2.31373 1.07203 1.20988
H -3.37909 1.13079 1.45711
N 0.80593 -0.63373 1.78404
H 2.77329 -1.28018 2.36118
C 0.05645 -1.65749 2.62076
H 1.38737 1.43006 1.95641
C -1.43043 -1.36642 2.83292
H -1.73534 1.21538 2.11657
H -1.80884 -2.16556 3.48263
C 0.97873 0.63639 2.57943
H 0.55885 -1.71721 3.59467
H 0.02218 0.96829 2.97312
H -1.57840 -0.44478 3.40392
H 1.65637 0.45258 3.42054
O 0.26856 -2.44695 -0.33739

53
FeOO anti (2/3)
Fe -0.02788 -0.43517 -0.10823
H 1.83923 -1.17188 -3.97972
H -0.56366 -0.87501 -4.02306
H -1.91566 1.11130 -3.26386
H 1.48039 0.46579 -3.52008
C 1.39976 -0.56963 -3.17487
H -0.25056 1.57777 -2.88514
C -0.05873 -1.01512 -3.05877
C -1.15426 1.13287 -2.47720
H -2.77679 -0.97328 -2.71766
H 1.47368 1.80797 -1.87062
H -0.10200 -2.07305 -2.79951
H 3.31487 -0.59162 -2.18953
H -1.50310 1.75488 -1.65433
N -0.87437 -0.27571 -2.01416
H 3.14966 1.69952 -1.29482
C 2.26935 -0.80887 -1.93850
C -2.17681 -1.02288 -1.80135
H -1.93261 -2.06812 -1.61027
C 2.10200 1.50976 -1.03788
H 2.20537 -1.85262 -1.62200
H -3.31260 0.58119 -0.90437
N 1.92183 0.04288 -0.72560
H 1.83045 2.10456 -0.16552
C -2.93282 -0.40714 -0.64280
H -3.79496 -1.02539 -0.37681
H 3.75445 -0.80205 0.02865
O -0.50556 -3.43772 0.01039
C 2.86087 -0.31548 0.42940
H -2.20548 -2.31661 1.03293
N -2.02545 -0.25234 0.58026
H 2.01545 -2.21971 1.01923
H 3.18334 0.61447 0.89848
H -2.06797 1.88869 0.51969
C 2.17218 -1.22285 1.42935
C -2.30993 -1.37087 1.57065
H 0.14707 -2.64034 2.08406
H -3.36083 -1.27117 1.86956
C -2.33488 1.08916 1.21112
H -3.40572 1.14122 1.43303
N 0.80793 -0.65570 1.77912
H 2.77211 -1.31280 2.34252
C 0.04968 -1.68368 2.59948
H 1.37366 1.41614 1.93418
C -1.43108 -1.36941 2.82394
H -1.77799 1.22475 2.13245
H -1.81707 -2.16959 3.46768
C 0.97150 0.62331 2.56195
H 0.55856 -1.76299 3.56828
H 0.01376 0.94793 2.95705
H -1.56610 -0.45119 3.40321
H 1.65381 0.44612 3.40013
O 0.14252 -2.33030 -0.43921

53
FeOO anti QI (2/5)
Fe -0.03244 -0.35893 -0.10125
H 1.84022 -1.23307 -3.94312
H -0.56600 -0.92984 -3.99620
H -1.90400 1.08027 -3.26811
H 1.47589 0.41565 -3.53044
C 1.39854 -0.60969 -3.15573
H -0.23486 1.54279 -2.90021
C -0.06015 -1.05378 -3.03026
C -1.14166 1.11383 -2.48320
H -2.78054 -0.98034 -2.69398
H 1.49620 1.81632 -1.90930
H -0.10612 -2.10946 -2.76149
H 3.31411 -0.59449 -2.17186
H -1.48591 1.75332 -1.67114
N -0.87162 -0.29433 -1.99602
H 3.16798 1.70312 -1.32384
C 2.27021 -0.81040 -1.91360
C -2.18621 -1.01768 -1.77364
H -1.96325 -2.06272 -1.55526
C 2.11736 1.53041 -1.06662
H 2.21176 -1.84575 -1.57016
H -3.28429 0.62884 -0.90373
N 1.92034 0.07256 -0.72135
H 1.84949 2.14758 -0.20877
C -2.93286 -0.36623 -0.62901
H -3.81303 -0.95741 -0.35969
H 3.76959 -0.72242 0.04769
O -0.68266 -3.43930 -0.38145
C 2.85628 -0.26704 0.44104
H -2.17434 -2.29828 0.99133
N -2.02439 -0.22416 0.59308
H 2.02770 -2.19213 0.98461
H 3.14378 0.66734 0.92376
H -2.09550 1.91497 0.56343
C 2.17496 -1.20300 1.41832
C -2.29802 -1.37069 1.55582
H 0.17178 -2.64405 2.07827
H -3.35122 -1.29244 1.85314
C -2.34538 1.10228 1.24624
H -3.41496 1.13829 1.47893
N 0.80547 -0.65198 1.77326
H 2.77226 -1.31137 2.33114
C 0.05691 -1.68890 2.59151
H 1.33325 1.43150 1.95255
C -1.42633 -1.38804 2.81331
H -1.78160 1.23256 2.16427
H -1.81130 -2.20068 3.44191
C 0.96134 0.61850 2.57367
H 0.56528 -1.76503 3.56085
H 0.00549 0.91612 2.99380
H -1.56799 -0.48041 3.40771
H 1.66416 0.44138 3.39463
O 0.24488 -2.47357 -0.36390

53
FeOO anti QII (2/5)
Fe -0.03796 -0.38157 -0.10614
H 1.84157 -1.19092 -3.96581
H -0.54123 -0.95361 -4.06659
H -1.90092 1.06765 -3.41899
H 1.45391 0.44240 -3.51980
C 1.38867 -0.59127 -3.16599
H -0.27227 1.56688 -2.92177
C -0.07412 -1.05407 -3.07802
C -1.19623 1.10618 -2.58050
H -2.86204 -0.97444 -2.70845
H 1.56302 1.84077 -1.90020
H -0.11608 -2.10807 -2.79901
H 3.32442 -0.61013 -2.21945
H -1.61341 1.72425 -1.78538
N -0.92546 -0.28878 -2.08362
H 3.24720 1.70324 -1.35015
C 2.28256 -0.80276 -1.93249
C -2.22548 -1.01438 -1.81559
H -1.99363 -2.06204 -1.61922
C 2.19962 1.54024 -1.07209
H 2.21515 -1.83719 -1.58677
H -3.35041 0.59802 -0.90507
N 1.98014 0.08864 -0.73220
H 1.95466 2.15541 -0.20567
C -2.96988 -0.38850 -0.63738
H -3.83488 -1.00870 -0.38108
H 3.78858 -0.76885 0.05886
O -0.64867 -3.39785 -0.43855
C 2.88465 -0.28380 0.44113
H -2.16039 -2.30126 1.00531
N -2.08914 -0.22020 0.59884
H 2.03628 -2.19731 1.03058
H 3.19754 0.64497 0.91958
H -2.21861 1.90924 0.54373
C 2.20208 -1.20544 1.45237
C -2.30446 -1.37520 1.56843
H 0.18833 -2.64290 2.13928
H -3.35695 -1.33715 1.87902
C -2.42164 1.09975 1.24565
H -3.48106 1.11751 1.52546
N 0.85303 -0.65360 1.86845
H 2.84490 -1.31429 2.33490
C 0.06979 -1.68703 2.65225
H 1.46151 1.39420 2.07920
C -1.42248 -1.36573 2.82781
H -1.81792 1.25608 2.13603
H -1.82344 -2.15573 3.47543
C 1.03437 0.59684 2.68622
H 0.53476 -1.78255 3.64236
H 0.07407 0.93673 3.06704
H -1.56258 -0.44057 3.39539
H 1.69815 0.39047 3.53373
O 0.18099 -2.35352 -0.32010

53
FeOO anti sideon (2/5)
Fe -0.02586 -0.57337 -0.12092
H 1.83798 -0.96763 -4.06145
H -0.54365 -0.88987 -4.08420
H -1.81985 1.08035 -3.42276
H 1.37345 0.60440 -3.48960
C 1.38077 -0.45287 -3.20675
H -0.29755 1.63917 -2.70108
C -0.05307 -1.00185 -3.10838
C -1.22001 1.09859 -2.50563
H -2.85856 -0.96339 -2.74181
H 1.50718 1.85959 -1.72885
H -0.03585 -2.06663 -2.86683
H 3.33872 -0.35592 -2.31755
H -1.76840 1.63027 -1.73117
N -0.92415 -0.31178 -2.07290
H 3.18025 1.75415 -1.14538
C 2.33571 -0.69413 -2.02480
C -2.22217 -1.05980 -1.85307
H -1.98347 -2.11650 -1.72858
C 2.13679 1.51364 -0.91327
H 2.39904 -1.75883 -1.79945
H -3.46971 0.42854 -0.88609
N 1.98565 0.02528 -0.72754
H 1.83899 2.03580 -0.00456
C -2.97992 -0.51343 -0.63480
H -3.76898 -1.21998 -0.36225
H 3.73219 -1.00996 -0.00899
O -0.56334 -2.67129 -0.05894
C 2.90463 -0.43047 0.40973
H -2.35564 -2.26908 1.21398
N -2.09262 -0.25781 0.58737
H 2.03253 -2.29665 1.12475
H 3.33818 0.46392 0.85977
H -2.09563 1.87138 0.35367
C 2.19678 -1.27767 1.47757
C -2.37448 -1.28302 1.67921
H 0.09130 -2.63734 2.21264
H -3.39891 -1.10202 2.03158
C -2.36974 1.13236 1.10654
H -3.43448 1.23179 1.34461
N 0.84773 -0.69130 1.84259
H 2.82977 -1.33193 2.37202
C 0.03570 -1.65641 2.68899
H 1.57103 1.32454 1.95444
C -1.43306 -1.24828 2.89536
H -1.79082 1.32654 2.00619
H -1.84575 -1.97636 3.60538
C 1.03462 0.60960 2.57375
H 0.52516 -1.73297 3.66855
H 0.07242 1.03975 2.83660
H -1.50032 -0.28604 3.41191
H 1.60759 0.43165 3.49101
O 0.65814 -2.59675 -0.66088

53
FeOO anti sideon (2/7)
Fe -0.03059 -0.49334 -0.12362
H 1.83690 -0.95656 -4.05791
H -0.53986 -0.89858 -4.08718
H -1.83066 1.05201 -3.45812
H 1.36416 0.61062 -3.47910
C 1.37740 -0.44787 -3.20064
H -0.32425 1.63634 -2.71998
C -0.05512 -1.00445 -3.10762
C -1.24379 1.08671 -2.53306
H -2.86766 -0.98255 -2.73956
H 1.55760 1.88160 -1.72432
H -0.03390 -2.06886 -2.86540
H 3.34109 -0.35722 -2.32388
H -1.80894 1.61989 -1.77120
N -0.93581 -0.31511 -2.08031
H 3.22901 1.74717 -1.13896
C 2.33803 -0.68742 -2.02156
C -2.22735 -1.06993 -1.85242
H -1.98357 -2.12492 -1.72458
C 2.18128 1.52389 -0.90817
H 2.39879 -1.75185 -1.79360
H -3.48063 0.41676 -0.89145
N 2.00136 0.03769 -0.72422
H 1.89039 2.04814 0.00186
C -2.98729 -0.52208 -0.63486
H -3.77506 -1.23008 -0.36160
H 3.73647 -1.01872 -0.00832
O -0.55363 -2.65466 -0.05072
C 2.91152 -0.43559 0.41118
H -2.35664 -2.26914 1.21822
N -2.10330 -0.25734 0.58715
H 2.02256 -2.29990 1.11261
H 3.35184 0.45079 0.87062
H -2.15079 1.86937 0.35046
C 2.19367 -1.28442 1.47145
C -2.37791 -1.28154 1.67978
H 0.08474 -2.63315 2.20809
H -3.40251 -1.10570 2.03513
C -2.40109 1.12681 1.10886
H -3.46382 1.20963 1.36234
N 0.85079 -0.68832 1.84140
H 2.82651 -1.35172 2.36551
C 0.03392 -1.65196 2.68440
H 1.60741 1.31414 1.98711
C -1.43299 -1.23873 2.89282
H -1.81074 1.33420 1.99887
H -1.84525 -1.95835 3.61171
C 1.05956 0.59800 2.59573
H 0.52306 -1.73416 3.66394
H 0.10312 1.03979 2.86290
H -1.49559 -0.27101 3.39995
H 1.62864 0.39627 3.51043
O 0.63524 -2.55464 -0.67044

67
FeOO+CHD syn React (2/1)
Fe 6.21567 4.01914 4.90597
H 2.35603 4.01799 2.81916
H 2.55630 5.49051 4.69290
H 4.03195 7.39090 4.50002
H 3.57129 5.18710 2.38527
C 3.37687 4.34361 3.05438
H 5.02513 6.58958 3.26875
C 3.36785 4.77219 4.51836
C 4.89150 6.73095 4.33706
H 3.85586 6.55767 6.66074
H 5.68592 5.38194 1.94536
H 3.18023 3.89943 5.15230
H 4.12990 2.81580 1.72337
H 5.78649 7.20418 4.73828
N 4.65307 5.41447 5.02402
H 5.95052 4.01374 4.84947
C 4.29259 3.15888 2.75300
C 4.47023 5.66302 6.50934
H 3.92297 4.81492 6.92508
C 6.19701 4.43086 1.83264
H 4.04754 2.33022 3.42247
H 6.35039 6.68821 6.77205
N 5.77677 3.45421 2.90376
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H 7.27101 4.59595 1.89108
C 5.81932 5.81984 7.16586
H 5.71439 5.96247 8.24773
H 6.12184 1.63022 1.82006
O 7.82041 5.03332 4.13648
C 6.55996 2.17773 2.66258
H 5.19906 3.30137 7.71283
N 6.67569 4.59798 6.89172
H 5.55055 1.03185 4.18694
H 7.57403 2.46229 2.37628
H 8.36257 5.89199 6.63419
C 6.56297 1.33481 3.91323
C 6.26951 3.48145 7.84316
H 5.60961 1.31914 6.27793
H 6.42530 3.85176 8.86412
C 8.10418 4.99062 7.18551
H 8.20500 5.19587 8.25730
N 7.13306 2.13849 5.06421
H 7.15368 0.42267 3.76966
C 6.69458 1.44634 6.34662
H 8.94065 2.65459 4.04029
C 7.03317 2.17424 7.64311
H 8.79596 4.19957 6.91580
H 6.73271 1.50676 8.46012
C 8.63440 2.15103 4.95619
H 7.14816 0.44676 6.34875
H 9.07463 2.67398 5.79983
H 8.11132 2.31150 7.76552
H 9.00978 1.12151 4.94764
O 8.07145 6.27826 4.35453
H 10.70942 6.90951 4.88631
C 11.16334 7.55436 5.65700
C 10.13893 8.54198 6.16484
C 9.83163 8.69096 7.46247
C 10.47431 7.88922 8.57004
C 11.44634 6.85325 8.05531
C 11.75354 6.70453 6.75788
H 11.96837 8.09006 5.12489
H 9.64415 9.15797 5.41620
H 9.08810 9.42693 7.76295
H 10.98827 8.56771 9.27275
H 9.69622 7.40403 9.18257
H 11.91254 6.21114 8.80034
H 12.46824 5.94199 6.45367

67
FeOO+CHD syn TS (2/1)
Fe 6.24553 4.23935 5.03805
H 2.24572 4.12476 3.16180
H 2.26574 4.29843 5.55465
H 3.14623 6.26352 6.65615
H 2.99400 5.64919 3.54603
C 3.14899 4.56745 3.60027
H 4.05326 6.66693 5.18409
C 3.21386 4.07816 5.04452
C 4.09708 6.12732 6.12598
H 3.52443 4.30282 7.84019
H 4.84189 6.72545 3.40122
H 3.34880 2.99179 5.05033
H 4.10155 4.35508 1.67355
H 4.90985 6.54605 6.71726
N 4.33565 4.66244 5.88076
H 5.32520 6.39542 1.72548
C 4.32094 4.12284 2.72479
C 4.34218 3.93596 7.20711
H 4.15403 2.87837 7.01033
C 5.58743 6.23920 2.77924
H 4.44138 3.03922 2.80677
H 5.84877 5.19046 8.10395
N 5.65367 4.76191 3.06639
H 6.55773 6.68757 2.98419
C 5.67529 4.13448 7.88988
H 5.70993 3.59369 8.84385
H 6.32911 4.09942 1.13441
O 7.29859 6.05982 5.07425
C 6.71947 4.18656 2.15614
H 5.92431 1.73353 6.81301
N 6.80073 3.66269 6.99153
H 6.35443 2.12297 2.67271
H 7.54831 4.89643 2.12894
H 7.96343 5.34692 7.58264
C 7.17550 2.84289 2.67255
C 6.89926 2.14987 7.08163
H 6.69002 1.15896 4.51673
H 7.09184 1.89560 8.13273
C 8.07297 4.26694 7.52449
H 8.27432 3.87053 8.52699
N 7.66894 2.98019 4.09624
H 7.97230 2.43261 2.03965
C 7.67938 1.58867 4.70250
H 9.03758 4.57529 3.69616
C 7.97794 1.52518 6.19741
H 8.91286 4.03387 6.87759
H 8.02369 0.46109 6.46136
C 9.05963 3.55617 4.07835
H 8.41335 0.98774 4.14795
H 9.47568 3.57890 5.08175
H 8.97032 1.92271 6.43131
H 9.70752 2.93803 3.44487
O 7.26282 6.97494 6.09178
H 8.41409 7.49341 6.20916
C 9.61480 8.13429 6.31700
C 9.82857 8.23391 7.75635
C 10.71784 7.43068 8.40107
C 11.57167 6.43534 7.67287
C 11.41610 6.46509 6.18154
C 10.51765 7.27934 5.55912
H 9.25254 9.03480 5.81220
H 9.24146 8.95777 8.31335
H 10.85032 7.50955 9.47607
H 12.63304 6.58577 7.94081
H 11.36485 5.41580 8.05118
H 12.07294 5.82601 5.59874
H 10.45237 7.29319 4.47560

67
FeOO+CHD syn Interm (2/1)
Fe 6.27843 4.21063 5.01961
H 2.23534 4.09881 3.29423
H 2.37508 4.35114 5.67724
H 3.25547 6.36489 6.62650
H 2.98059 5.64419 3.58969
C 3.15265 4.56748 3.67147
H 4.15528 6.73432 5.14287
C 3.29558 4.12512 5.12387
C 4.20620 6.22490 6.09973
H 3.70570 4.53302 7.91032
H 4.78762 6.69719 3.37039
H 3.44316 3.04074 5.15893
H 4.04501 4.33143 1.71475
H 5.02376 6.65620 6.67079
N 4.44753 4.75054 5.90466
H 5.35268 6.36921 1.72434
C 4.28803 4.10283 2.76041
C 4.46810 4.08004 7.26750
H 4.20023 3.03055 7.13152
C 5.56781 6.21882 2.78857
H 4.39985 3.01861 2.84664
H 6.10007 5.27179 8.01514
N 5.63073 4.73806 3.06778
H 6.52417 6.66590 3.04647
C 5.84046 4.22232 7.87432
H 5.89442 3.72093 8.84758
H 6.29046 4.12853 1.11748
O 7.31497 5.66092 4.94192
C 6.68762 4.17875 2.13815
H 5.84685 1.76940 6.81375
N 6.88049 3.63166 6.94200
H 6.30551 2.10275 2.58802
H 7.52080 4.88367 2.13570
H 8.21369 5.21539 7.41312
C 7.12924 2.81835 2.61223
C 6.85888 2.11506 7.04238
H 6.49726 1.18470 4.47481
H 7.06718 1.85671 8.08828
C 8.21872 4.13092 7.42842
H 8.37276 3.77397 8.45333
N 7.62756 2.91737 4.04212
H 7.92605 2.42168 1.97331
C 7.52657 1.51966 4.64111
H 9.09543 4.39230 3.57754
C 7.85684 1.40889 6.12541
H 9.02745 3.76430 6.80684
H 7.81115 0.34157 6.37469
C 9.05218 3.39978 4.02200
H 8.18836 0.86693 4.05773
H 9.45196 3.46215 5.02823
H 8.88636 1.71020 6.33591
H 9.66379 2.70273 3.43814
O 7.19971 6.63094 6.08655
H 8.10012 7.06172 6.07063
C 9.76833 8.39484 6.32082
C 9.68689 8.34291 7.74577
C 10.48280 7.49633 8.47566
C 11.49221 6.58788 7.82470
C 11.52761 6.70268 6.32349
C 10.70853 7.56508 5.63867
H 9.17951 9.12005 5.76794
H 8.98048 8.99234 8.25535
H 10.40936 7.47022 9.55911
H 12.49949 6.78488 8.24118
H 11.30401 5.53767 8.12107
H 12.24104 6.08130 5.78977
H 10.77670 7.62830 4.55620

67
FeOO+CHD syn React (2/3)
Fe 6.14095 4.21031 5.34269
H 2.71747 4.15922 2.51265
H 2.16042 3.95433 4.83719
H 2.60415 5.83108 6.34717
H 3.20898 5.64309 3.27664
C 3.44633 4.57720 3.21761
H 3.78099 6.46033 5.18057
C 3.21633 3.86917 4.54929
C 3.65645 5.81242 6.04264
H 2.82057 3.76896 7.35364
H 4.99041 6.83017 3.70106
H 3.45299 2.80553 4.44862
H 4.84600 4.74240 1.58396
H 4.28027 6.19277 6.84952
N 4.04501 4.39558 5.70481
H 5.94525 6.76028 2.20746
C 4.82282 4.33591 2.60268
C 3.79033 3.51254 6.91239
H 3.73007 2.47917 6.56624
C 5.91366 6.46556 3.26226
H 5.00775 3.26108 2.53593
H 4.95027 4.73436 8.26565
N 5.99330 4.96178 3.34677
H 6.75678 6.89840 3.79505
C 4.89918 3.70159 7.91821
H 4.74734 3.06217 8.79496
H 7.16776 4.58829 1.59006
O 6.96526 5.91621 5.86329
C 7.29070 4.53698 2.67777
H 5.54570 1.44973 6.69104
N 6.24309 3.37183 7.28938
H 6.91000 2.41147 2.80826
H 8.05759 5.26185 2.95546
H 7.15563 5.02863 8.27268
C 7.66425 3.14041 3.10987
C 6.41000 1.86017 7.21881
H 6.85373 1.19424 4.56661
H 6.37696 1.49320 8.25178
C 7.30921 3.95644 8.18408
H 7.22715 3.49089 9.17241
N 7.77956 3.08747 4.62086
H 8.61669 2.83649 2.66078
C 7.73940 1.63075 5.03759
H 9.05383 4.80637 4.84633
C 7.69261 1.38227 6.54248
H 8.30100 3.76496 7.78828
H 7.72766 0.29435 6.67729
C 9.07762 3.73534 5.04144
H 8.62348 1.14214 4.60834
H 9.24967 3.58433 6.10242
H 8.58475 1.76225 7.04819
H 9.90271 3.27704 4.48555
O 6.59087 6.67645 6.92724
H 8.80251 8.19639 6.82476
C 9.83687 8.45030 6.54096
C 10.80770 7.80601 7.50298
C 11.80192 6.99126 7.12033
C 12.07357 6.62357 5.68007
C 11.07965 7.23688 4.72081
C 10.08495 8.05194 5.10494
H 9.88828 9.54866 6.63739
H 10.66999 8.03467 8.55836
H 12.46850 6.56102 7.86563
H 13.09726 6.92898 5.40257
H 12.07841 5.52640 5.56658
H 11.20869 6.99680 3.66686
H 9.40910 8.46983 4.36068

67
FeOO+CHD syn TS (2/3)
Fe 6.31089 4.25740 5.24056
H 2.59652 4.27458 2.76989
H 2.27423 4.28259 5.15557
H 3.06377 6.16031 6.57984
H 3.26232 5.76527 3.37154
C 3.42045 4.68307 3.36795
H 4.02939 6.62611 5.16913
C 3.28055 4.08322 4.76423
C 4.03671 6.04841 6.08794
H 3.17926 4.14737 7.58037
H 5.14302 6.82863 3.58963
H 3.40822 2.99783 4.70908
H 4.66206 4.64478 1.60231
H 4.82706 6.43788 6.72823
N 4.27539 4.58902 5.78862
H 5.93939 6.62714 2.01754
C 4.71014 4.30317 2.64421
C 4.07791 3.79322 7.06232
H 3.90689 2.75165 6.78482
C 5.99185 6.37937 3.08398
H 4.81118 3.21510 2.63246
H 5.46074 4.98187 8.22224
N 5.98150 4.88007 3.24133
H 6.90826 6.77045 3.51887
C 5.29677 3.94040 7.94074
H 5.18889 3.35891 8.86346
H 6.96142 4.37234 1.40078
O 7.42840 5.73081 5.55410
C 7.17534 4.33991 2.47527
H 5.61944 1.59804 6.79079
N 6.53354 3.47325 7.19577
H 6.65479 2.25526 2.72785
H 8.01338 5.01172 2.66591
H 7.68026 5.11070 7.91774
C 7.48961 2.93144 2.92084
C 6.56801 1.95497 7.19866
H 6.64347 1.13762 4.55971
H 6.62021 1.64069 8.24893
C 7.72896 4.02392 7.93219
H 7.70683 3.65527 8.96466
N 7.76098 2.91992 4.41031
H 8.36142 2.54003 2.38327
C 7.61850 1.49573 4.90462
H 9.24281 4.46659 4.34257
C 7.71931 1.32536 6.41769
H 8.65331 3.70224 7.46367
H 7.67535 0.24709 6.61489
C 9.15884 3.42836 4.65612
H 8.39160 0.89288 4.40965
H 9.39931 3.37584 5.71303
H 8.69217 1.64809 6.79985
H 9.87057 2.80941 4.09771
O 7.08213 6.75324 6.49670
H 8.23860 7.56336 6.59833
C 9.25694 8.25206 6.60506
C 10.06575 7.79293 7.75369
C 11.18442 7.04929 7.59521
C 11.72624 6.67678 6.24336
C 10.97890 7.29983 5.09835
C 9.86068 8.04410 5.27466
H 8.79120 9.23576 6.74233
H 9.72003 8.05435 8.75010
H 11.74694 6.71382 8.46248
H 12.79509 6.94467 6.18112
H 11.73029 5.57656 6.13145
H 11.38871 7.15510 4.10213
H 9.36456 8.49418 4.41914

67
FeOO+CHD syn Interm (2/3)
Fe 6.32820 4.22798 5.23781
H 2.59883 4.28080 2.78421
H 2.29024 4.29853 5.17197
H 3.11226 6.18611 6.56043
H 3.28431 5.76490 3.37961
C 3.43040 4.68101 3.37717
H 4.09635 6.62283 5.15364
C 3.29167 4.08552 4.77542
C 4.08667 6.05264 6.07683
H 3.20460 4.19113 7.59518
H 5.18119 6.80274 3.55972
H 3.40645 2.99857 4.72397
H 4.66349 4.62983 1.60640
H 4.88021 6.43128 6.71795
N 4.29772 4.58468 5.79159
H 6.00925 6.58325 2.00731
C 4.71105 4.28414 2.64687
C 4.09098 3.80886 7.07624
H 3.89278 2.76841 6.81336
C 6.03464 6.33908 3.07544
H 4.79517 3.19491 2.63112
H 5.50534 4.98122 8.21513
N 5.99569 4.84018 3.23668
H 6.94789 6.71440 3.53026
C 5.31868 3.94079 7.94468
H 5.20630 3.36932 8.87310
H 6.96005 4.31269 1.39473
O 7.53976 5.64717 5.51413
C 7.17662 4.27412 2.46845
H 5.57799 1.58852 6.80398
N 6.54106 3.44228 7.19593
H 6.61346 2.19950 2.71983
H 8.02885 4.92848 2.65693
H 7.72757 5.05152 7.91607
C 7.46218 2.85845 2.91112
C 6.53876 1.92277 7.20191
H 6.56515 1.09603 4.56764
H 6.59151 1.61208 8.25319
C 7.75417 3.96474 7.92372
H 7.73275 3.59091 8.95424
N 7.73881 2.83990 4.39945
H 8.32385 2.45050 2.36981
C 7.55480 1.42405 4.90094
H 9.27296 4.33105 4.29256
C 7.66638 1.25985 6.41415
H 8.66734 3.62632 7.44552
H 7.59610 0.18443 6.61880
C 9.15321 3.30620 4.63669
H 8.30307 0.79395 4.40172
H 9.39013 3.27710 5.69504
H 8.65090 1.55975 6.78502
H 9.84367 2.64706 4.09771
O 7.12173 6.71421 6.48191

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H 7.94235 7.27979 6.51111
C 9.52194 8.68754 6.70399
C 10.11828 7.97223 7.78657
C 11.11624 7.05555 7.57218
C 11.64406 6.75574 6.19403
C 10.98249 7.55965 5.10601
C 9.98708 8.46578 5.37244
H 8.77952 9.45447 6.90104
H 9.77232 8.16660 8.79791
H 11.56140 6.52177 8.40695
H 12.73965 6.91443 6.16683
H 11.54516 5.67385 5.97846
H 11.32823 7.40604 4.08771
H 9.54309 9.03385 4.55969

67
FeOO+CHD syn QI React (2/5)
Fe 6.09894 4.12663 5.26110
H 2.55347 4.25800 2.62787
H 2.11409 4.08791 4.98799
H 2.75536 5.86767 6.56523
H 3.15014 5.71669 3.36329
C 3.33638 4.64134 3.29363
H 3.79664 6.47147 5.26531
C 3.14247 3.94020 4.63459
C 3.76232 5.82397 6.13642
H 2.88501 3.75148 7.41466
H 4.99836 6.82343 3.75011
H 3.30416 2.86507 4.51217
H 4.65573 4.74915 1.58993
H 4.49004 6.18583 6.86056
N 4.06998 4.39904 5.74497
H 5.80907 6.72796 2.17481
C 4.66781 4.34230 2.60866
C 3.84002 3.49489 6.94273
H 3.76277 2.46941 6.57640
C 5.86242 6.42617 3.22674
H 4.80586 3.26074 2.53317
H 5.03969 4.67123 8.30043
N 5.89582 4.91879 3.29809
H 6.76651 6.82778 3.67781
C 4.98164 3.65155 7.91706
H 4.86006 2.98241 8.77591
H 6.94792 4.49705 1.47341
O 7.15236 5.86976 5.75900
C 7.13833 4.45756 2.55148
H 5.59603 1.40573 6.68968
N 6.29890 3.34377 7.22272
H 6.71842 2.34489 2.74597
H 7.93760 5.16741 2.76850
H 7.21308 5.01449 8.18610
C 7.50823 3.06003 2.98402
C 6.48189 1.83232 7.16683
H 6.79218 1.13704 4.51044
H 6.50533 1.48016 8.20518
C 7.40312 3.95269 8.05281
H 7.42198 3.45992 9.03111
N 7.71753 3.03311 4.48599
H 8.42289 2.72424 2.48216
C 7.70138 1.58153 4.92611
H 9.02195 4.74018 4.60485
C 7.73442 1.35845 6.43474
H 8.36778 3.82371 7.57261
H 7.79122 0.27360 6.58649
C 9.04452 3.67295 4.81587
H 8.56180 1.08767 4.45677
H 9.27535 3.53852 5.86820
H 8.64500 1.75935 6.88893
H 9.82976 3.19413 4.22101
O 6.75197 6.72831 6.70665
H 8.80725 8.44252 6.49422
C 9.88599 8.62418 6.35871
C 10.64061 8.14855 7.57810
C 11.62967 7.24397 7.53351
C 12.11065 6.59422 6.25683
C 11.34904 7.06109 5.03786
C 10.35890 7.96568 5.08378
H 9.97379 9.72046 6.26778
H 10.34424 8.58115 8.53210
H 12.13345 6.94465 8.45085
H 13.18853 6.78787 6.12102
H 12.04080 5.49678 6.34504
H 11.64642 6.62966 4.08367
H 9.85550 8.26516 4.16605

67
FeOO+CHD syn QI TS (2/5)
Fe 6.28681 4.26460 5.23961
H 2.58437 4.24267 2.74914
H 2.24315 4.24777 5.13291
H 2.98907 6.11694 6.55380
H 3.23810 5.73705 3.35609
C 3.40141 4.65548 3.35379
H 3.98682 6.60766 5.17324
C 3.25438 4.05603 4.74952
C 3.97590 6.02003 6.08605
H 3.14345 4.08501 7.55975
H 5.10821 6.82037 3.59653
H 3.38998 2.97145 4.69418
H 4.65171 4.61273 1.59453
H 4.74269 6.41292 6.75190
N 4.24008 4.56782 5.77738
H 5.86593 6.61939 2.00388
C 4.69947 4.28325 2.64057
C 4.05400 3.75863 7.04318
H 3.91188 2.71514 6.75603
C 5.94796 6.37766 3.07003
H 4.81350 3.19619 2.64141
H 5.39800 4.96830 8.22625
N 5.96104 4.87997 3.23905
H 6.86993 6.78571 3.47752
C 5.26324 3.92583 7.93304
H 5.15995 3.33422 8.85005
H 6.94219 4.36908 1.39823
O 7.32218 5.83376 5.58544
C 7.16041 4.35396 2.47239
H 5.66092 1.59761 6.77444
N 6.51778 3.49576 7.19535
H 6.67971 2.26420 2.75027
H 7.98801 5.04226 2.65020
H 7.60616 5.15521 7.96097
C 7.50327 2.95709 2.93333
C 6.59247 1.97942 7.19949
H 6.73292 1.14072 4.56875
H 6.63462 1.66397 8.25001
C 7.69228 4.07110 7.94541
H 7.68803 3.67884 8.96949
N 7.77778 2.96651 4.42151
H 8.38069 2.57597 2.39669
C 7.68803 1.54066 4.92298
H 9.20762 4.56394 4.35649
C 7.77382 1.38236 6.43804
H 8.62744 3.79792 7.46710
H 7.76276 0.30424 6.64122
C 9.15914 3.52047 4.66132
H 8.49078 0.96568 4.44194
H 9.40942 3.46497 5.71638
H 8.73037 1.73878 6.83117
H 9.88887 2.93196 4.09294
O 7.04214 6.84382 6.53423
H 8.27726 7.58525 6.61002
C 9.32264 8.22239 6.59214
C 10.12087 7.76281 7.74597
C 11.22666 6.99599 7.59648
C 11.75947 6.59788 6.25014
C 11.01444 7.20333 5.09610
C 9.90834 7.97012 5.26304
H 8.88867 9.22361 6.71200
H 9.78122 8.04461 8.73866
H 11.78423 6.66259 8.46748
H 12.83029 6.85742 6.17984
H 11.75951 5.49567 6.15831
H 11.41429 7.02835 4.10091
H 9.41295 8.40827 4.40121

67
FeOO+CHD syn QI Interm (2/5)
Fe 6.44578 4.08534 5.48827
H 3.21198 5.14545 2.38865
H 2.43122 4.56219 4.52850
H 3.00424 6.09040 6.35009
H 3.98888 6.28428 3.45282
C 3.97571 5.22576 3.17349
H 4.48806 6.61212 5.50920
C 3.49419 4.34904 4.33294
C 4.07092 5.87539 6.19353
H 2.71959 3.81908 6.98201
H 5.95908 7.02313 3.88667
H 3.56820 3.29603 4.04012
H 5.43554 5.33474 1.58074
H 4.60831 5.96361 7.13665
N 4.24708 4.49451 5.63375
H 7.06881 6.91108 2.50243
C 5.30144 4.80000 2.53555
C 3.69630 3.48279 6.60455
H 3.52567 2.55587 6.05161
C 6.82172 6.48910 3.48819
H 5.24965 3.73248 2.30211
H 4.79887 4.16334 8.33634
N 6.52313 5.02763 3.38123
H 7.65712 6.62343 4.17419
C 4.64097 3.23975 7.77417
H 4.19038 2.51118 8.46542
H 7.72407 4.49918 1.67954
O 7.91793 5.17725 6.24620
C 7.70589 4.33191 2.76754
H 5.03483 1.15352 6.31379
N 5.98583 2.76037 7.30735
H 6.79239 2.37258 2.65685
H 8.60598 4.79574 3.17855
H 7.00061 4.03445 8.65696
C 7.70196 2.83324 3.05082
C 5.91092 1.29870 6.95228
H 6.33945 1.00718 4.25307
H 5.73341 0.73018 7.87999
C 6.98835 2.97729 8.39490
H 6.73058 2.38652 9.28650
N 7.75779 2.53965 4.52426
H 8.55274 2.36046 2.53749
C 7.30049 1.12543 4.76556
H 9.47555 3.75923 4.84711
C 7.13769 0.72176 6.23590
H 7.98378 2.69370 8.05687
H 7.01380 -0.36922 6.24317
C 9.15554 2.73339 5.02691
H 8.01708 0.44202 4.28163
H 9.19662 2.55911 6.10020
H 8.05411 0.90951 6.80487
H 9.84317 2.04029 4.52058
O 7.20894 6.19298 7.15873
H 7.66246 6.02219 8.01470
C 10.04106 9.84519 6.78525
C 11.36006 10.02755 6.30206
C 12.00986 8.97287 5.70556
C 11.35298 7.66050 5.56421
C 9.98253 7.53592 6.09081
C 9.35771 8.61487 6.68236
H 9.53831 10.68567 7.25323
H 11.84040 10.99195 6.40638
H 13.01958 9.08208 5.32460
H 11.36829 7.35118 4.49902
H 11.99433 6.87291 6.00927
H 9.46217 6.57963 6.00580
H 8.35073 8.51037 7.06414

67
FeOO+CHD syn QII React (2/5)
Fe 6.72910 4.04544 5.25633
H 2.96410 4.38667 2.77294
H 2.66796 4.28087 5.11008
H 3.42329 6.24421 6.28893
H 3.84089 5.76331 3.37344
C 3.85593 4.66975 3.34599
H 4.73325 6.60870 5.13685
C 3.67996 4.06648 4.74137
C 4.46866 6.04459 6.02845
H 3.52723 4.25624 7.58960
H 5.90619 6.62333 3.28376
H 3.79283 2.97890 4.69177
H 4.98768 4.48099 1.51394
H 5.11597 6.37279 6.84178
N 4.65646 4.56408 5.79143
H 6.60615 6.18673 1.70909
C 5.05363 4.14022 2.55613
C 4.39634 3.81784 7.08524
H 4.13944 2.78854 6.82735
C 6.65900 6.01056 2.78988
H 5.01712 3.04845 2.54744
H 5.86045 4.89881 8.26145
N 6.41771 4.55109 3.07785
H 7.64427 6.29550 3.15607
C 5.60959 3.86905 7.99889
H 5.40148 3.33265 8.93258
H 7.26486 3.68655 1.30760
O 8.35713 5.18384 5.34887
C 7.48663 3.73800 2.38084
H 5.71523 1.47019 7.08716
N 6.82668 3.26045 7.32870
H 6.63450 1.79895 2.84736
H 8.43143 4.27325 2.49318
H 8.11123 4.82149 8.00970
C 7.57847 2.33560 2.95807
C 6.72281 1.74690 7.40573
H 6.47343 0.87957 4.82049
H 6.82327 1.47193 8.46406
C 8.05950 3.73422 8.05180
H 8.01731 3.41379 9.09944
N 7.91606 2.37381 4.43313
H 8.34687 1.76112 2.42695
C 7.52803 1.04970 5.05947
H 9.67934 3.52925 4.06381
C 7.73730 0.96426 6.57186
H 8.95439 3.31930 7.59241
H 7.60624 -0.09036 6.84392
C 9.39191 2.62735 4.59967
H 8.11566 0.26738 4.56045
H 9.64339 2.76544 5.64773
H 8.76660 1.20598 6.85301
H 9.95020 1.77163 4.20305
O 8.29182 6.39257 5.94213
H 10.71539 6.94814 6.81229
C 11.80625 6.86419 6.95183
C 12.19630 5.40883 7.06368
C 13.08152 4.81261 6.25091
C 13.79880 5.52760 5.12942
C 13.40664 6.98236 5.01572
C 12.52122 7.57742 5.82823
H 12.00263 7.37892 7.90803
H 11.72151 4.83782 7.85994
H 13.32143 3.75972 6.38827
H 14.89004 5.44399 5.27100
H 13.60919 5.01176 4.17281
H 13.88655 7.55460 4.22382
H 12.28470 8.63145 5.69357

67
FeOO+CHD syn QIII React (2/5)
Fe 6.87471 4.05912 5.27597
H 3.13025 4.54345 2.81067
H 2.79857 4.32107 5.13292
H 3.53215 6.17705 6.47422
H 4.01231 5.87901 3.49272
C 4.01743 4.78788 3.40867
H 4.81918 6.63087 5.32831
C 3.81661 4.11791 4.77137
C 4.57667 6.00635 6.18595
H 3.65064 4.09248 7.61697
H 6.06540 6.73491 3.48310
H 3.92015 3.03300 4.66519
H 5.15251 4.66724 1.57337
H 5.23070 6.29501 7.00901
N 4.78416 4.55080 5.85302
H 6.73381 6.40538 1.86919
C 5.22229 4.29238 2.60491
C 4.54049 3.72156 7.09243
H 4.32523 2.70053 6.76995
C 6.80905 6.15637 2.93564
H 5.18791 3.20094 2.55772
H 5.96543 4.78125 8.33317
N 6.58053 4.68681 3.14393
H 7.79946 6.42776 3.29942
C 5.74392 3.75743 8.02371
H 5.52886 3.18198 8.93407
H 7.43111 3.90256 1.33433
O 8.47131 5.24663 5.51091
C 7.65095 3.91375 2.41022
H 5.90491 1.40999 7.02875
N 6.98025 3.20740 7.35184
H 6.82338 1.94560 2.79425
H 8.59251 4.45079 2.54387
H 8.22404 4.75859 8.11223
C 7.76294 2.48578 2.92806
C 6.90713 1.69440 7.35878
H 6.66992 0.94251 4.73087
H 7.01501 1.36319 8.40166
C 8.18858 3.66915 8.11421
H 8.14225 3.30939 9.15037
N 8.09970 2.46329 4.40186
H 8.53466 1.94416 2.36672
C 7.72376 1.11234 4.97532
H 9.85686 3.63286 4.06488
C 7.93419 0.97003 6.48530
H 9.09806 3.29038 7.65063
H 7.83016 -0.09834 6.71346
C 9.57231 2.71661 4.57902
H 8.31537 0.35070 4.44817
H 9.81813 2.83358 5.63160
H 8.95856 1.22563 6.77356
H 10.14140 1.87568 4.16430
O 8.41294 6.48293 5.99119
H 10.16983 7.02381 6.32568
C 11.28417 7.04669 6.50160
C 11.66556 5.79516 7.22454
C 12.48417 4.86204 6.69426
C 13.11959 5.00550 5.33965
C 12.79067 6.30140 4.65188
C 11.97131 7.23001 5.18619
H 11.39730 7.93460 7.14479
H 11.24745 5.65052 8.21761
H 12.72985 3.96715 7.26075
H 14.21497 4.89904 5.42999
H 12.83053 4.15460 4.69683
H 13.26424 6.48094 3.68989
H 11.77866 8.15772 4.65318

67
FeOO+CHD syn QIII React (2/5)
Fe 6.95435 4.06007 5.27649
H 3.19833 4.65502 2.83094
H 2.88154 4.42054 5.15035
H 3.66981 6.26878 6.47646
H 4.12539 5.96046 3.51201
C 4.09847 4.87008 3.42089
H 4.97653 6.68228 5.33694
C 3.89332 4.19790 4.78198
C 4.70991 6.06524 6.19283
H 3.73531 4.18629 7.63047
H 6.20680 6.74960 3.48439
H 3.97340 3.11151 4.67040
H 5.21438 4.73644 1.57512
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H 5.36889 6.33320 7.01903
N 4.87542 4.60504 5.86087
H 6.88518 6.40928 1.87673
C 5.28079 4.34630 2.60163
C 4.60841 3.78374 7.10076
H 4.35344 2.77184 6.77815
C 6.93652 6.14850 2.94225
H 5.20913 3.25730 2.54041
H 6.07904 4.78557 8.33577
N 6.65196 4.68767 3.13661
H 7.92992 6.37779 3.32623
C 5.81649 3.77098 8.02717
H 5.58129 3.20411 8.93838
H 7.47166 3.87872 1.32299
O 8.55427 5.17673 5.49688
C 7.69258 3.88073 2.39901
H 5.88512 1.42051 7.02140
N 7.02747 3.17450 7.35077
H 6.79631 1.94460 2.78744
H 8.65233 4.38477 2.53289
H 8.34689 4.67281 8.08400
C 7.75673 2.44881 2.91439
C 6.89828 1.66690 7.34897
H 6.62461 0.93998 4.71614
H 6.99863 1.32275 8.38882
C 8.25498 3.58719 8.10865
H 8.18940 3.24788 9.15104
N 8.10349 2.41029 4.38498
H 8.50278 1.87946 2.34542
C 7.68496 1.07262 4.95615
H 9.89425 3.52271 4.04462
C 7.89523 0.91321 6.46471
H 9.14366 3.15250 7.65344
H 7.75498 -0.15274 6.68532
C 9.58487 2.61064 4.55136
H 8.24673 0.29188 4.42373
H 9.84166 2.70965 5.60318
H 8.92918 1.13070 6.75044
H 10.12125 1.75427 4.12381
O 8.51547 6.41196 6.10603
H 9.91135 6.79116 6.30738
C 11.09583 7.04076 6.49875
C 11.60748 5.91376 7.29540
C 12.43892 4.97928 6.76723
C 12.94477 5.05714 5.35881
C 12.51529 6.28656 4.61706
C 11.68287 7.21157 5.15981
H 10.95669 7.97313 7.06122
H 11.28017 5.83290 8.32777
H 12.78867 4.15017 7.37579
H 14.04707 4.98441 5.35415
H 12.63528 4.15438 4.79899
H 12.92163 6.43285 3.62038
H 11.41114 8.09980 4.59716

67
FeOO+CHD syn QIII Interm (2/5)
Fe 7.21643 3.60967 5.27744
H 3.81986 5.80142 3.10015
H 3.59722 5.64351 5.43894
H 5.26202 6.75563 6.89229
H 5.26793 6.53773 3.72627
C 4.75993 5.57396 3.62001
H 6.39687 6.69718 5.52090
C 4.36512 4.99819 4.98367
C 6.03759 6.15562 6.39488
H 4.29785 4.77875 7.76920
H 7.38450 6.44047 3.46115
H 3.91659 4.00979 4.83650
H 5.54427 5.03225 1.67858
H 6.88363 6.01626 7.06746
N 5.48385 4.82483 5.98116
H 7.84667 5.87108 1.84033
C 5.54546 4.62886 2.70444
C 4.93705 4.10184 7.18310
H 4.30035 3.29256 6.81639
C 7.80363 5.60133 2.90626
H 5.03072 3.66384 2.67258
H 6.67416 4.35786 8.44580
N 6.97111 4.37608 3.11195
H 8.80425 5.40168 3.28839
C 6.04454 3.54780 8.07024
H 5.59908 3.05184 8.94605
H 7.25453 3.36424 1.23754
O 9.08869 4.19782 5.43461
C 7.54705 3.25538 2.29312
H 5.23461 1.40600 6.89264
N 6.93091 2.59367 7.32024
H 6.01853 1.79965 2.77122
H 8.63532 3.34536 2.33410
H 8.69332 3.46896 8.09526
C 7.10774 1.88860 2.80323
C 6.26433 1.24768 7.22719
H 5.68984 0.72195 4.59687
H 6.21335 0.82000 8.24194
C 8.24089 2.47993 8.03300
H 8.09870 2.07619 9.04643
N 7.54027 1.65322 4.22500
H 7.51660 1.10343 2.14951
C 6.74590 0.50491 4.79023
H 9.57574 2.19407 3.88074
C 6.93344 0.23834 6.28747
H 8.91601 1.82543 7.48337
H 6.46117 -0.73219 6.48924
C 9.00746 1.34785 4.26593
H 7.00319 -0.40569 4.22572
H 9.32753 1.17634 5.29233
H 7.98980 0.10057 6.53959
H 9.22834 0.45314 3.66565
O 9.25849 5.28619 6.48857
H 10.06611 4.96776 6.95191
C 10.36444 7.56446 5.75537
C 10.93849 7.90175 7.01006
C 12.29968 7.84614 7.16919
C 13.18651 7.44523 6.05695
C 12.52477 7.12351 4.77559
C 11.16175 7.18818 4.64265
H 9.29507 7.65790 5.62645
H 10.29414 8.20314 7.82610
H 12.76052 8.10248 8.11715
H 13.95471 8.22589 5.89319
H 13.81537 6.58983 6.37435
H 13.15299 6.84034 3.93775
H 10.68377 6.95995 3.69916

67
FeOO+CHD syn QSIII React (2/5)
Fe 6.45951 3.76861 5.14711
H 2.47906 4.74524 3.28990
H 2.48654 4.56610 5.65274
H 3.65874 6.28945 6.79371
H 3.59177 5.97030 3.82609
C 3.46475 4.88618 3.75054
H 4.84752 6.57408 5.50211
C 3.39183 4.22903 5.13088
C 4.62700 5.97841 6.38436
H 3.70410 4.18765 7.97332
H 5.72350 6.58680 3.58366
H 3.32924 3.14188 5.02006
H 4.31041 4.65805 1.77310
H 5.40509 6.16310 7.12261
N 4.57250 4.51418 6.03901
H 6.05293 6.23693 1.87313
C 4.47600 4.26409 2.78435
C 4.42924 3.70166 7.30977
H 4.01922 2.72756 7.03622
C 6.28894 5.95184 2.90485
H 4.31687 3.18354 2.74833
H 6.16742 4.53594 8.29900
N 5.93982 4.50216 3.11986
H 7.35245 6.10138 3.08350
C 5.76633 3.55960 8.02036
H 5.64039 2.98247 8.94425
H 6.41909 3.70580 1.18469
O 8.32013 4.84801 5.05957
C 6.80817 3.65469 2.20888
H 5.48860 1.22210 6.92934
N 6.79993 2.87856 7.14188
H 5.86326 1.75876 2.67732
H 7.80518 4.09950 2.20106
H 8.31647 4.25196 7.74860
C 6.85844 2.20761 2.67267
C 6.54887 1.38017 7.14124
H 5.91726 0.68947 4.55867
H 6.74227 1.02093 8.16039
C 8.16840 3.17440 7.69868
H 8.25182 2.75217 8.70671
N 7.41514 2.10325 4.07896
H 7.48163 1.61834 1.98970
C 7.00270 0.76960 4.67431
H 9.21285 3.11536 3.50310
C 7.38102 0.57167 6.14373
H 8.94134 2.73874 7.06906
H 7.18830 -0.48399 6.37202
C 8.91629 2.21250 4.03342
H 7.46373 -0.01818 4.06418
H 9.32939 2.25656 5.03827
H 8.45425 0.70753 6.30718
H 9.32609 1.33751 3.51576
O 7.42043 5.58237 5.78217
H 8.10323 8.20323 5.29504
C 8.92247 8.91641 5.48778
C 8.89261 9.34771 6.93526
C 9.92639 9.19627 7.77609
C 11.24626 8.58019 7.37483
C 11.27532 8.14593 5.92807
C 10.24125 8.29781 5.08728
H 8.69800 9.77710 4.83472
H 7.96931 9.80437 7.28750
H 9.83952 9.52975 8.80861
H 12.06598 9.29341 7.56758
H 11.47427 7.72179 8.02928
H 12.20012 7.69331 5.57483
H 10.33033 7.96890 4.05333

67
FeOO+CHD syn QSIII TS (2/5)
Fe 6.55645 3.98565 5.22666
H 2.63189 4.74769 3.09312
H 2.49040 4.53183 5.44781
H 3.46744 6.29333 6.69954
H 3.64258 6.02147 3.71460
C 3.57605 4.93326 3.62055
H 4.71608 6.67886 5.48977
C 3.44966 4.25736 4.98766
C 4.47816 6.05359 6.34671
H 3.56312 4.17918 7.83470
H 5.72127 6.73608 3.60455
H 3.45944 3.16991 4.86045
H 4.56755 4.77593 1.70532
H 5.19747 6.27198 7.13352
N 4.54706 4.59872 5.97513
H 6.29544 6.42557 1.95110
C 4.68275 4.37565 2.72204
C 4.36383 3.75350 7.21689
H 4.03387 2.76273 6.89749
C 6.40313 6.13768 3.00407
H 4.57624 3.28975 2.66193
H 5.99055 4.66383 8.31714
N 6.10037 4.67408 3.16581
H 7.42434 6.32367 3.33179
C 5.64822 3.66922 8.02552
H 5.47375 3.09666 8.94551
H 6.76663 3.93549 1.26417
O 8.31153 5.02901 5.31476
C 7.07156 3.88216 2.31699
H 5.52769 1.32551 6.94468
N 6.76440 3.02570 7.23243
H 6.16773 1.94731 2.69140
H 8.04662 4.36603 2.40124
H 8.19654 4.44645 7.90242
C 7.14388 2.43105 2.76516
C 6.56978 1.52365 7.20657
H 6.10338 0.88613 4.57785
H 6.72855 1.15491 8.22933
C 8.07485 3.36517 7.88992
H 8.08134 2.97769 8.91597
N 7.60296 2.32687 4.20308
H 7.83380 1.87417 2.11908
C 7.17971 0.98088 4.75500
H 9.39587 3.40643 3.78130
C 7.47769 0.76006 6.23992
H 8.90248 2.92211 7.34024
H 7.30478 -0.30588 6.43482
C 9.09833 2.47609 4.26122
H 7.68469 0.20665 4.16080
H 9.44115 2.50460 5.29242
H 8.53545 0.92448 6.46674
H 9.57068 1.63116 3.74534
O 7.33241 5.76167 6.05824
H 7.72977 7.47739 5.83948
C 8.43237 8.37519 5.79710
C 8.87925 8.64985 7.19413
C 10.14334 8.42267 7.60978
C 11.22098 7.91829 6.69365
C 10.79463 7.78386 5.26267
C 9.52401 8.01733 4.85247
H 7.78015 9.16794 5.40108
H 8.13346 9.02549 7.88947
H 10.42572 8.62080 8.64030
H 12.10617 8.57536 6.75655
H 11.60223 6.94667 7.06009
H 11.56040 7.51204 4.54118
H 9.27190 7.93909 3.79860

67
FeOO+CHD syn QSIII Inter (2/5)
Fe 6.48637 4.15185 4.76918
H 3.91133 3.37338 1.06136
H 2.73549 3.56967 3.08697
H 2.74983 5.74892 4.18713
H 4.35766 4.94775 1.65613
C 4.48170 3.87801 1.85234
H 4.30427 6.14983 3.41537
C 3.82903 3.47332 3.17826
C 3.84308 5.68444 4.28503
H 2.57509 3.91624 5.67024
H 6.13306 6.10585 2.06124
H 4.04974 2.41885 3.37737
H 6.22962 3.55647 0.61964
H 4.16934 6.23432 5.16622
N 4.26975 4.25013 4.39467
H 7.48885 5.61951 1.01838
C 5.94049 3.44447 1.67754
C 3.63550 3.62995 5.61226
H 3.66981 2.54497 5.48476
C 7.09518 5.59431 2.04531
H 6.01918 2.38121 1.92305
H 4.32179 5.12509 7.01627
N 6.94082 4.18457 2.52157
H 7.77672 6.11481 2.71866
C 4.34805 4.03971 6.89492
H 3.82800 3.60144 7.76060
H 8.50010 3.21306 1.40717
O 7.64270 5.71278 5.20228
C 8.27722 3.49804 2.44680
H 5.19538 1.62569 6.56418
N 5.79260 3.62771 6.88666
H 7.57397 1.54034 3.04294
H 9.03464 4.22537 2.74869
H 6.46100 5.49373 7.62489
C 8.34032 2.26203 3.33731
C 5.91092 2.16006 7.19622
H 6.91153 0.88311 4.97458
H 5.59935 2.00354 8.24220
C 6.53617 4.44171 7.89716
H 6.11967 4.28274 8.90337
N 8.11228 2.59984 4.78424
H 9.31560 1.76800 3.21128
C 7.73280 1.34896 5.53018
H 9.61097 4.11368 4.81263
C 7.30069 1.54435 6.98844
H 7.58906 4.16278 7.90613
H 7.26207 0.54146 7.43398
C 9.34642 3.21362 5.36736
H 8.58724 0.65333 5.49876
H 9.16833 3.50526 6.40057
H 8.06351 2.08235 7.56056
H 10.18359 2.50116 5.32974
O 6.59750 6.77119 5.60144
H 6.65579 7.39669 4.84405
C 9.35615 7.15273 7.33593
C 10.60888 6.86783 7.93362
C 11.13427 7.73859 8.85935
C 10.41607 8.96928 9.23848
C 9.11998 9.20946 8.57830
C 8.61849 8.31891 7.65901
H 8.92796 6.46572 6.60053
H 11.14061 5.96562 7.65813
H 12.08980 7.54211 9.33404
H 10.28364 8.99819 10.33882
H 11.07818 9.84590 9.09014
H 8.57430 10.10917 8.84250
H 7.66522 8.47655 7.17233

67
FeOO+CHD syn React sideon(2/7)
Fe 6.20237 4.08083 5.35397
H 2.67842 4.12954 2.58324
H 2.16846 3.80661 4.87610
H 2.52426 5.68863 6.29155
H 3.25430 5.56713 3.37538
C 3.44845 4.49509 3.27388
H 3.83940 6.37004 5.30862
C 3.22873 3.75424 4.59493
C 3.60640 5.67870 6.11508
H 2.86933 3.61092 7.43330
H 5.14163 6.72977 3.68956
H 3.49128 2.69822 4.47411
H 4.77035 4.63066 1.56925
H 4.11853 6.01657 7.01401
N 4.04049 4.28127 5.76417
H 5.93410 6.59989 2.10453
C 4.79119 4.22588 2.58970
C 3.83065 3.37524 6.96120
H 3.77048 2.34876 6.59369
C 5.99700 6.31379 3.16081
H 4.94018 3.14598 2.51267
H 5.01081 4.55871 8.34108
N 6.01248 4.81177 3.27699
H 6.91135 6.72322 3.58804
C 4.95408 3.53201 7.97423
H 4.76911 2.88562 8.84092
H 7.13311 4.31450 1.51493
O 7.68200 5.63078 5.72086
C 7.26625 4.28615 2.60324
H 5.55092 1.27706 6.83453
N 6.30407 3.19031 7.37223
H 6.77658 2.18208 2.80284
H 8.08056 4.97023 2.84893
H 7.23624 4.84554 8.34618
C 7.58922 2.86805 3.04942
C 6.45553 1.67919 7.29728
H 6.65881 1.02815 4.62803
H 6.49264 1.30737 8.32967
C 7.37988 3.77010 8.25266
H 7.32498 3.31200 9.24692
N 7.80805 2.80074 4.54657
H 8.48756 2.51097 2.53159
C 7.62658 1.36795 5.01133
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H 9.35405 4.27972 4.45665
C 7.67801 1.17020 6.52816
H 8.36481 3.57845 7.83185
H 7.71066 0.08639 6.69606
C 9.19262 3.28829 4.87596
H 8.40816 0.76306 4.53276
H 9.33159 3.34768 5.95282
H 8.61094 1.55207 6.95374
H 9.93236 2.59462 4.45880
O 6.50961 6.04921 6.25287
H 8.36491 8.54005 6.13357
C 9.44120 8.76163 6.04105
C 10.17730 8.24389 7.25461
C 11.20278 7.38200 7.18864
C 11.74611 6.82750 5.89227
C 10.99881 7.33126 4.67954
C 9.97194 8.19259 4.74627
H 9.49300 9.86358 6.01402
H 9.83734 8.60941 8.22198
H 11.69264 7.05030 8.10238
H 12.81787 7.07380 5.79992
H 11.72226 5.72487 5.91635
H 11.33858 6.96564 3.71213
H 9.48118 8.52304 3.83241

67
FeOO+CHD syn TS sideon (2/7)
Fe 6.66713 3.95702 5.25958
H 2.82222 5.06411 3.09766
H 2.65837 4.83115 5.43922
H 3.75605 6.50500 6.70751
H 3.96525 6.22168 3.71599
C 3.78367 5.14673 3.61989
H 5.03644 6.79410 5.50572
C 3.59613 4.48241 4.98503
C 4.74749 6.18749 6.36089
H 3.66732 4.41251 7.83271
H 6.10302 6.72483 3.51331
H 3.51918 3.39782 4.85542
H 4.74633 4.88992 1.70039
H 5.47676 6.34483 7.15325
N 4.70831 4.73154 5.98379
H 6.67773 6.29486 1.88972
C 4.82019 4.47688 2.71613
C 4.42880 3.90932 7.22372
H 4.00724 2.95558 6.90072
C 6.72996 6.03254 2.95361
H 4.59487 3.40970 2.65184
H 6.13644 4.65473 8.32614
N 6.26066 4.61869 3.15865
H 7.75908 6.11252 3.30088
C 5.69125 3.69891 8.04290
H 5.45278 3.15724 8.96767
H 6.83836 3.76897 1.27608
O 8.45113 4.77104 5.32580
C 7.13422 3.70212 2.33092
H 5.31111 1.38390 6.96558
N 6.73316 2.93239 7.26087
H 6.01218 1.89533 2.74144
H 8.15863 4.07218 2.40716
H 8.31836 4.17556 7.93444
C 7.03877 2.26173 2.80653
C 6.36611 1.46478 7.23857
H 5.84014 0.86025 4.62594
H 6.46872 1.08561 8.26509
C 8.06517 3.11714 7.93626
H 8.00965 2.74571 8.96729
N 7.48315 2.12892 4.24311
H 7.65611 1.61613 2.16887
C 6.92043 0.84073 4.80253
H 9.37923 3.01230 3.81307
C 7.19043 0.59689 6.28734
H 8.83964 2.56757 7.40509
H 6.90269 -0.44254 6.48939
C 8.98426 2.12835 4.31142
H 7.34060 0.01364 4.21253
H 9.31835 2.15098 5.34546
H 8.25932 0.64858 6.51632
H 9.37500 1.22792 3.82116
O 7.74732 5.67955 6.23995
H 8.00833 7.00652 5.83899
C 8.36487 8.20003 5.65121
C 8.53951 8.71287 7.01703
C 9.77117 8.87371 7.56744
C 11.03123 8.60290 6.80352
C 10.81715 8.25727 5.36181
C 9.57632 8.10065 4.82856
H 7.47340 8.56315 5.12887
H 7.64749 8.93224 7.59597
H 9.87415 9.23196 8.58748
H 11.71231 9.46859 6.88355
H 11.60194 7.79411 7.29997
H 11.69945 8.15970 4.73615
H 9.46332 7.87802 3.77193

67
FeOO+CHD syn Inter sideon(2/7)
Fe 6.44290 3.94181 5.22009
H 2.57972 4.57319 2.96535
H 2.39300 4.40844 5.31543
H 3.33523 6.20754 6.62079
H 3.55421 5.87989 3.57330
C 3.51094 4.78881 3.50424
H 4.52651 6.58945 5.35411
C 3.36658 4.14107 4.88295
C 4.33822 5.98517 6.23882
H 3.36557 4.14067 7.72341
H 5.60825 6.64299 3.46827
H 3.39817 3.05159 4.78088
H 4.53697 4.60203 1.61020
H 5.08706 6.24241 6.98524
N 4.42962 4.51786 5.90012
H 6.21092 6.29411 1.83286
C 4.64437 4.23215 2.63934
C 4.19671 3.70403 7.15680
H 3.89090 2.70183 6.85028
C 6.31382 6.04317 2.89579
H 4.56345 3.14280 2.60730
H 5.75803 4.66238 8.31122
N 6.04320 4.57737 3.10294
H 7.32277 6.27210 3.23520
C 5.44790 3.65801 8.01569
H 5.25234 3.09052 8.93458
H 6.77096 3.78504 1.24541
O 7.85462 5.16670 5.44975
C 7.05297 3.78252 2.30594
H 5.41579 1.30083 6.94106
N 6.60129 3.03122 7.26584
H 6.19933 1.83126 2.70929
H 8.01303 4.29605 2.38743
H 7.99059 4.49006 7.95420
C 7.15298 2.35278 2.81145
C 6.43927 1.52619 7.24989
H 6.11287 0.80026 4.61218
H 6.55761 1.17214 8.28341
C 7.88171 3.40701 7.96214
H 7.85843 3.04121 8.99625
N 7.54137 2.31658 4.27465
H 7.89616 1.79788 2.22623
C 7.17218 0.95780 4.83807
H 9.27300 3.53724 3.96809
C 7.41097 0.77433 6.33774
H 8.73479 2.96252 7.45391
H 7.26103 -0.29333 6.54202
C 9.02007 2.57429 4.40957
H 7.74792 0.20633 4.28077
H 9.30832 2.59600 5.45721
H 8.45266 0.97204 6.60826
H 9.57690 1.78079 3.89761
O 7.51973 6.21635 6.44245
H 8.09119 6.98255 6.14912
C 8.97001 8.83822 5.69567
C 9.24657 9.08099 7.07622
C 10.44686 8.72392 7.63652
C 11.53971 8.06697 6.83545
C 11.18803 7.86622 5.38498
C 9.97147 8.24040 4.87147
H 8.03955 9.18525 5.25757
H 8.48685 9.56018 7.68740
H 10.64105 8.91497 8.68800
H 12.47411 8.65514 6.91910
H 11.81542 7.09795 7.29585
H 11.94026 7.41592 4.74375
H 9.76146 8.08883 3.81631

67
FeOO+CHD syn React unboun(2/7)
Fe 6.07574 3.95675 5.31616
H 2.60705 4.20187 2.49336
H 2.04023 3.97852 4.78128
H 2.56827 5.79985 6.33456
H 3.28858 5.60363 3.26608
C 3.39757 4.51735 3.18638
H 3.81275 6.36019 5.19304
C 3.09748 3.82580 4.52027
C 3.62295 5.70892 6.04411
H 2.68545 3.61556 7.30113
H 5.20939 6.62617 3.51957
H 3.25935 2.74797 4.41413
H 4.72984 4.50950 1.48464
H 4.25292 6.04130 6.86964
N 3.93965 4.28367 5.69079
H 6.11238 6.43214 2.00051
C 4.72601 4.13816 2.52060
C 3.67122 3.38589 6.87446
H 3.63684 2.35817 6.50373
C 6.07140 6.14475 3.05998
H 4.80396 3.04760 2.47668
H 4.76822 4.55953 8.32737
N 5.97346 4.65502 3.20096
H 6.97285 6.49367 3.56527
C 4.74427 3.53636 7.94713
H 4.50869 2.88209 8.79740
H 7.04575 3.95474 1.47424
O 8.12339 6.82120 5.88590
C 7.18856 4.02282 2.56107
H 5.44563 1.25882 6.96669
N 6.12122 3.21347 7.41539
H 6.63617 1.96063 2.94287
H 8.03533 4.69067 2.73158
H 6.98021 4.97389 8.24078
C 7.47635 2.63544 3.12627
C 6.32498 1.71458 7.43150
H 6.63517 0.86997 4.81085
H 6.34667 1.38984 8.48269
C 7.14668 3.89626 8.27264
H 7.07657 3.54814 9.31202
N 7.70038 2.68120 4.61960
H 8.35766 2.20786 2.62978
C 7.57392 1.28642 5.19121
H 9.14326 4.25755 4.50671
C 7.58504 1.20368 6.72225
H 8.14954 3.68875 7.90151
H 7.66368 0.13736 6.97029
C 9.05806 3.25196 4.91862
H 8.39496 0.67698 4.78685
H 9.21293 3.31472 5.99410
H 8.48809 1.65979 7.14016
H 9.83779 2.61531 4.48109
O 7.41977 7.31170 6.80402
H 9.33466 9.23748 7.32418
C 10.37722 9.28482 6.96462
C 11.17001 8.13594 7.54175
C 11.82772 7.23855 6.79272
C 11.85558 7.27123 5.28272
C 11.05334 8.41311 4.70548
C 10.39578 9.31099 5.45517
H 10.75790 10.24119 7.36168
H 11.19338 8.05805 8.62718
H 12.38432 6.43526 7.27212
H 12.89913 7.33067 4.92879
H 11.48673 6.31273 4.87955
H 11.02908 8.49098 3.62003
H 9.83915 10.11405 4.97553

67
FeOO+CHD syn TS unbound(2/7)
Fe 6.23298 4.16763 5.26191
H 2.55068 4.53855 2.75746
H 2.14414 4.35747 5.07987
H 2.83690 6.11838 6.62151
H 3.34600 5.91613 3.46290
C 3.40338 4.82581 3.38606
H 4.00568 6.66528 5.39516
C 3.17375 4.15762 4.74732
C 3.86419 6.00400 6.24892
H 3.01372 3.93992 7.57803
H 5.26183 6.87692 3.57966
H 3.27846 3.07328 4.63504
H 4.59140 4.73271 1.58098
H 4.56823 6.30398 7.02510
N 4.11815 4.58074 5.84906
H 5.96561 6.65436 1.96057
C 4.66157 4.38770 2.62301
C 3.93146 3.67006 7.03708
H 3.79725 2.65405 6.65728
C 6.05742 6.38637 3.02126
H 4.70815 3.29454 2.60392
H 5.25160 4.74985 8.36846
N 5.97248 4.89439 3.18738
H 7.01567 6.73613 3.40363
C 5.12047 3.73490 7.98801
H 4.93843 3.08333 8.85337
H 6.91833 4.24534 1.37096
O 7.70449 5.82264 5.52194
C 7.13516 4.26759 2.44749
H 5.58599 1.45353 6.79681
N 6.41334 3.33666 7.31303
H 6.58124 2.20400 2.79668
H 7.99885 4.92064 2.59027
H 7.45048 4.97119 8.19221
C 7.44620 2.85751 2.93652
C 6.51231 1.82709 7.24353
H 6.64881 1.07641 4.58725
H 6.55690 1.44891 8.27543
C 7.55926 3.89090 8.10976
H 7.57070 3.44618 9.11357
N 7.80063 2.83429 4.40453
H 8.27078 2.43903 2.34303
C 7.62843 1.42630 4.92994
H 9.32796 4.31642 4.22749
C 7.70749 1.27740 6.45350
H 8.50599 3.67461 7.61778
H 7.73446 0.19865 6.65481
C 9.21234 3.29881 4.59856
H 8.39101 0.78634 4.46157
H 9.46568 3.29847 5.65775
H 8.65417 1.66372 6.84412
H 9.90821 2.63495 4.06717
O 7.45625 6.71446 6.52310
H 8.41630 7.55741 6.48692
C 9.44564 8.43950 6.40477
C 10.22024 8.16392 7.60862
C 11.37467 7.44402 7.56082
C 11.94740 6.93651 6.27139
C 11.19829 7.37328 5.04904
C 10.04337 8.09541 5.12370
H 8.79851 9.32099 6.42640
H 9.84144 8.52924 8.55816
H 11.92940 7.23373 8.47035
H 13.00772 7.23520 6.18760
H 12.00479 5.83090 6.29769
H 11.62153 7.11327 4.08336
H 9.53729 8.41181 4.21698

67
FeOO+CHD syn Intm unbound(2/7)
Fe 6.33996 4.28860 5.29384
H 2.52227 4.53940 2.87396
H 2.26061 4.22957 5.20040
H 2.93689 6.02185 6.68318
H 3.31247 5.91493 3.58806
C 3.39970 4.83109 3.46479
H 4.09832 6.62458 5.47624
C 3.27572 4.09709 4.80165
C 3.96659 5.94393 6.31504
H 3.14076 3.85799 7.60228
H 5.23307 6.93765 3.57675
H 3.43285 3.02541 4.64354
H 4.51518 4.85221 1.61159
H 4.65977 6.24037 7.10123
N 4.24324 4.52579 5.88820
H 5.94405 6.72103 1.96186
C 4.62629 4.45571 2.63046
C 4.06589 3.59836 7.07277
H 3.94746 2.58598 6.68110
C 6.03309 6.45101 3.02137
H 4.68537 3.36673 2.55457
H 5.36866 4.69019 8.41573
N 5.94594 4.95583 3.17552
H 6.98883 6.79556 3.41281
C 5.25071 3.67963 8.01983
H 5.09349 3.01114 8.87558
H 6.84941 4.32905 1.33149
O 7.57826 5.67729 5.58941
C 7.08664 4.33253 2.40308
H 5.69584 1.41343 6.88613
N 6.53753 3.31073 7.31456
H 6.49670 2.27379 2.73420
H 7.96171 4.97077 2.53939
H 7.59743 4.97620 8.11150
C 7.36831 2.91662 2.87534
C 6.65186 1.80340 7.24562
H 6.54230 1.15360 4.58242
H 6.79334 1.43627 8.27177
C 7.69174 3.89126 8.08479
H 7.69368 3.49378 9.10749
N 7.71924 2.88921 4.34808
H 8.19389 2.48409 2.29684
C 7.55544 1.46918 4.85148
H 9.25651 4.36806 4.14822
C 7.77289 1.26984 6.35222
H 8.63489 3.63489 7.60598
H 7.80702 0.18539 6.51586
C 9.13705 3.36087 4.54294
H 8.26109 0.84098 4.29108
H 9.38580 3.38266 5.60114
H 8.75291 1.63727 6.67092
H 9.82181 2.67817 4.02607
O 7.18842 6.86237 6.36259
H 8.01671 7.42230 6.30078
C 9.65035 8.71821 6.07278
C 10.05837 8.46454 7.41777
C 11.02883 7.53794 7.70634
C 11.72275 6.74529 6.63037
C 11.26195 7.08527 5.23752
C 10.28451 8.01832 5.00095
H 8.93512 9.50671 5.85948
H 9.58975 9.02331 8.22307
H 11.32835 7.35762 8.73475
H 12.81877 6.88112 6.70920
H 11.59385 5.66098 6.81693
H 11.73973 6.56734 4.41071
H 9.98711 8.24115 3.98002

83
FeOO+CHD+CI syn Re unboun(0/7)
Fe 6.33887 3.49426 5.24894
H 3.22898 4.69001 2.27540
H 2.47547 4.51537 4.51003
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H 3.30776 6.11207 6.11477
H 4.19737 5.83636 3.15846
C 4.02879 4.76320 3.02367
H 4.78382 6.37588 5.15741
C 3.48046 4.11912 4.30241
C 4.33683 5.76839 5.94267
H 2.86110 3.94001 7.06162
H 6.31379 6.33102 3.57267
H 3.38539 3.03842 4.15165
H 5.41272 4.47017 1.39075
H 4.91763 5.90489 6.85482
N 4.32623 4.32045 5.53873
H 7.15217 5.97420 2.04619
C 5.25620 4.08094 2.40849
C 3.77701 3.47980 6.66602
H 3.50044 2.50908 6.24583
C 7.03020 5.66443 3.09379
H 5.05897 3.00825 2.32016
H 5.06603 4.28533 8.21489
N 6.55171 4.24457 3.16718
H 7.98972 5.75131 3.60221
C 4.79690 3.31742 7.78779
H 4.35958 2.71307 8.59504
H 7.50496 3.35704 1.45903
O 8.37460 6.10329 6.67226
C 7.60212 3.34565 2.55374
H 4.93835 0.97454 6.71437
N 6.06900 2.66492 7.29651
H 6.50882 1.48568 2.80001
H 8.57965 3.76484 2.79901
H 7.27925 4.10581 8.28555
C 7.48124 1.91245 3.06013
C 5.87535 1.16774 7.24558
H 6.10909 0.37312 4.60995
H 5.74656 0.81053 8.27869
C 7.18651 3.02110 8.23296
H 6.98338 2.62985 9.23988
N 7.61734 1.84650 4.56187
H 8.25170 1.28709 2.58841
C 7.10120 0.51442 5.05219
H 9.43577 2.98118 4.56798
C 7.00117 0.37125 6.57505
H 8.12728 2.60183 7.87794
H 6.78778 -0.68751 6.77089
C 9.05681 2.03472 4.95370
H 7.75734 -0.27367 4.65373
H 9.15201 2.04352 6.03860
H 7.96519 0.56279 7.05701
H 9.66308 1.21231 4.55039
O 7.63943 7.03754 6.27148
H 8.45207 9.68693 6.69796
C 9.32645 10.18674 7.14798
C 10.15425 9.17692 7.90796
C 11.45742 8.96138 7.67277
C 12.25132 9.69870 6.61922
C 11.41646 10.69268 5.84577
C 10.11374 10.90925 6.08057
H 8.88865 10.91647 7.85081
H 9.63506 8.61305 8.68008
H 11.99869 8.22002 8.25822
H 13.10804 10.21368 7.08727
H 12.71115 8.97770 5.92350
H 11.92644 11.25038 5.06209
H 9.57012 11.64165 5.48621
C 5.88791 7.06319 11.58973
F 5.63670 5.78647 12.07130
F 6.66377 7.71816 12.53561
F 4.67202 7.72625 11.51742
S 6.74456 7.01221 9.93289
O 6.93177 8.44993 9.61249
O 5.75638 6.29844 9.07765
O 7.98611 6.25510 10.22913
C 12.55970 6.47034 3.13112
F 13.17976 7.59220 3.66599
F 13.51200 5.46452 3.06068
F 12.18770 6.78333 1.83212
S 11.08972 5.95224 4.15808
O 10.21282 7.14830 4.10667
O 10.58086 4.76488 3.41669
O 11.69751 5.65519 5.47928

83
FeOO+CHD+CI syn Re sideon(0/7)
Fe 6.23520 3.36090 5.27415
H 3.13735 4.55778 2.24573
H 2.36870 4.39459 4.48243
H 3.19536 6.03747 5.96755
H 4.09101 5.71558 3.12947
C 3.92699 4.64121 3.00295
H 4.76638 6.25589 5.16408
C 3.37314 4.00027 4.27663
C 4.22732 5.67018 5.90558
H 2.74649 3.93557 7.06217
H 6.20100 6.19753 3.63820
H 3.28400 2.91881 4.13167
H 5.35052 4.33328 1.40552
H 4.71522 5.80119 6.87058
N 4.20981 4.21359 5.52119
H 6.99602 5.84653 2.08990
C 5.15753 3.94695 2.41553
C 3.61454 3.40405 6.65308
H 3.25178 2.46348 6.23337
C 6.91061 5.53992 3.13955
H 4.95373 2.87723 2.32473
H 4.99168 4.10574 8.17681
N 6.44142 4.10910 3.20525
H 7.88460 5.63484 3.61676
C 4.63629 3.16446 7.75261
H 4.17799 2.58568 8.56497
H 7.49244 3.31559 1.51360
O 8.09478 4.32269 5.81742
C 7.51702 3.22234 2.60688
H 4.54911 0.87285 6.54520
N 5.84460 2.40978 7.22856
H 6.35382 1.38801 2.65741
H 8.48340 3.59788 2.95083
H 7.17148 3.63658 8.37735
C 7.31608 1.76965 3.00522
C 5.49370 0.93902 7.09095
H 5.67898 0.32931 4.42080
H 5.31750 0.55564 8.10494
C 6.97519 2.57868 8.21070
H 6.69775 2.11414 9.16486
N 7.35803 1.60798 4.50940
H 8.09782 1.14788 2.55159
C 6.67142 0.31060 4.88320
H 9.31949 2.47010 4.57718
C 6.53475 0.06598 6.38692
H 7.87906 2.09846 7.83956
H 6.19307 -0.97008 6.50357
C 8.79212 1.60179 4.97014
H 7.24077 -0.50926 4.42463
H 8.84323 1.63023 6.05627
H 7.50492 0.10651 6.89139
H 9.28122 0.68665 4.61355
O 7.07416 5.10116 6.26019
H 8.48396 9.25494 6.08659
C 9.23592 9.96114 6.47717
C 10.19208 9.23228 7.39238
C 11.52063 9.20856 7.20737
C 12.21883 9.90468 6.06175
C 11.26093 10.63158 5.14680
C 9.93269 10.65635 5.33124
H 8.64671 10.69201 7.05726
H 9.74434 8.70973 8.23494
H 12.15585 8.66586 7.90552
H 12.97127 10.61049 6.45361
H 12.80368 9.17214 5.48172
H 11.70085 11.15599 4.30020
H 9.29825 11.20059 4.63375
C 6.55125 6.93810 11.35491
F 6.21286 5.77815 12.03647
F 7.66358 7.47945 11.98255
F 5.50504 7.83414 11.51405
S 6.89139 6.59304 9.55267
O 7.23017 7.93406 9.01300
O 5.59348 6.03181 9.08466
O 8.01397 5.62246 9.60969
C 12.49427 5.99320 3.35428
F 13.11099 7.13347 3.85238
F 13.43548 4.97464 3.36782
F 12.17039 6.24338 2.02917
S 10.98371 5.54021 4.35389
O 10.10716 6.72717 4.18667
O 10.50999 4.30558 3.66723
O 11.53628 5.33505 5.71565

83
FeOO+CHD+CI syn Re QSIII(0/5)
Fe 6.34793 3.50245 5.28102
H 3.23717 4.66890 2.23934
H 2.48760 4.55391 4.48367
H 3.36614 6.24616 5.89739
H 4.20843 5.83475 3.09279
C 4.03434 4.75974 2.98769
H 4.94334 6.40037 5.08989
C 3.48750 4.14812 4.27828
C 4.38906 5.85280 5.84854
H 2.87414 4.19792 7.06665
H 6.33432 6.30296 3.54307
H 3.39004 3.06432 4.15911
H 5.44750 4.41614 1.38815
H 4.87941 6.00204 6.80937
N 4.33445 4.38472 5.51121
H 7.15172 5.88230 2.02472
C 5.25291 4.04374 2.40294
C 3.72551 3.62972 6.67284
H 3.33639 2.68480 6.28847
C 7.04156 5.61550 3.08300
H 5.03403 2.97605 2.32487
H 5.12944 4.35433 8.15883
N 6.54235 4.19698 3.18628
H 8.00896 5.71002 3.57414
C 4.74988 3.40633 7.77185
H 4.28754 2.86656 8.60833
H 7.57530 3.34172 1.51357
O 8.20986 4.38647 5.80616
C 7.59792 3.27314 2.60864
H 4.58727 1.09033 6.63676
N 5.93407 2.60703 7.26105
H 6.39567 1.46560 2.70042
H 8.57423 3.63259 2.94231
H 7.30355 3.82832 8.36586
C 7.36504 1.83514 3.04092
C 5.54228 1.14414 7.16475
H 5.67155 0.49656 4.50524
H 5.37344 0.78969 8.19043
C 7.07577 2.77219 8.23089
H 6.79003 2.34541 9.19998
N 7.40229 1.70964 4.54948
H 8.13402 1.18540 2.60601
C 6.66883 0.44637 4.95479
H 9.39957 2.48822 4.56927
C 6.54719 0.22909 6.46350
H 7.96233 2.25385 7.87000
H 6.17668 -0.79429 6.60172
C 8.83651 1.66617 5.00960
H 7.19978 -0.40074 4.50001
H 8.89374 1.74926 6.09234
H 7.52498 0.24924 6.95411
H 9.28265 0.71352 4.69877
O 7.22279 5.26059 6.17956
H 8.31259 8.45910 6.29938
C 8.95865 9.29031 6.63105
C 10.14763 8.74015 7.38333
C 11.42006 8.94798 7.01257
C 11.81566 9.75442 5.79668
C 10.62727 10.34566 5.07432
C 9.35519 10.13812 5.44538
H 8.32078 9.87081 7.31732
H 9.92408 8.15209 8.27089
H 12.23287 8.52491 7.60052
H 12.51362 10.55694 6.08967
H 12.39663 9.12234 5.10410
H 10.84532 10.96872 4.20856
H 8.54439 10.59368 4.87933
C 6.22654 6.69109 11.52894
F 5.77213 5.42059 11.85249
F 7.22127 7.01997 12.43811
F 5.17356 7.57155 11.72637
S 6.86062 6.76231 9.77520
O 7.28145 8.17790 9.63133
O 5.66040 6.37509 8.98236
O 7.95984 5.76341 9.78218
C 12.68520 5.84653 3.16310
F 13.25769 7.01616 3.64663
F 13.66532 4.86557 3.18725
F 12.34974 6.06744 1.83585
S 11.19635 5.34952 4.17330
O 10.27339 6.49700 3.98154
O 10.76963 4.08275 3.51478
O 11.75980 5.19385 5.53699

83
FeOO+CHD+CI syn TS QSIII(0/5)
Fe 6.62702 3.83148 5.40200
H 3.43541 4.99169 2.40846
H 2.70859 4.74653 4.64629
H 3.50798 6.43038 6.07852
H 4.36953 6.15772 3.30368
C 4.23565 5.08212 3.15374
H 5.10874 6.67720 5.33893
C 3.72667 4.39747 4.42343
C 4.54768 6.07897 6.05284
H 3.13328 4.33255 7.22705
H 6.46068 6.66777 3.77411
H 3.67898 3.31544 4.26176
H 5.65430 4.86496 1.53582
H 4.99193 6.20878 7.03844
N 4.56796 4.62527 5.66154
H 7.35056 6.35594 2.26749
C 5.47614 4.43844 2.53295
C 3.99194 3.80390 6.79440
H 3.61698 2.86983 6.37137
C 7.20626 6.02978 3.30473
H 5.29177 3.36928 2.40466
H 5.41040 4.47762 8.28730
N 6.75456 4.59589 3.32500
H 8.14974 6.11826 3.83878
C 5.03087 3.54271 7.87272
H 4.57659 2.97831 8.69819
H 7.83031 3.86769 1.62024
O 8.39924 4.64798 5.93108
C 7.84070 3.73997 2.71078
H 4.86572 1.27944 6.63706
N 6.21140 2.76803 7.32801
H 6.69288 1.89839 2.69025
H 8.80114 4.10831 3.07349
H 7.62974 3.93483 8.40107
C 7.64799 2.27478 3.06225
C 5.82908 1.31345 7.15159
H 5.93728 0.86837 4.44932
H 5.68130 0.88944 8.15462
C 7.35040 2.88840 8.30307
H 7.03710 2.50471 9.28120
N 7.67339 2.06773 4.55981
H 8.43887 1.67288 2.59769
C 6.93916 0.78487 4.88380
H 9.67689 2.81703 4.59494
C 6.83089 0.45721 6.37412
H 8.20894 2.31664 7.95663
H 6.46825 -0.57620 6.44121
C 9.10254 1.99922 5.02740
H 7.46083 -0.03292 4.36692
H 9.15506 2.07540 6.11050
H 7.81480 0.44873 6.85308
H 9.54167 1.04591 4.70676
O 7.39219 5.48558 6.51606
H 7.82479 7.19688 6.42345
C 8.26903 8.23149 6.62684
C 9.38780 8.03727 7.59103
C 10.68084 8.24576 7.25033
C 11.09871 8.72096 5.89040
C 9.95066 9.06629 4.98853
C 8.65986 8.85308 5.33096
H 7.40822 8.73867 7.09093
H 9.12030 7.70376 8.58976
H 11.47018 8.08119 7.97965
H 11.77908 9.58522 5.98358
H 11.72085 7.94532 5.40348
H 10.19391 9.51453 4.02856
H 7.86159 9.13012 4.64720
C 5.37334 7.33166 11.88931
F 4.16556 6.69822 12.14268
F 6.13473 7.25218 13.04619
F 5.10032 8.67174 11.66063
S 6.25619 6.55536 10.44015
O 7.49935 7.36289 10.33611
O 5.28460 6.74467 9.32899
O 6.44515 5.15047 10.88145
C 13.01706 5.24231 1.85433
F 13.49823 6.50534 1.54200
F 14.08736 4.48905 2.31251
F 12.57455 4.66269 0.67445
S 11.65148 5.33148 3.12328
O 10.61848 6.15284 2.44288
O 11.29396 3.90043 3.31800
O 12.31869 5.97825 4.28371

83
FeOO+CHD+CI syn Im QSIII(0/5)
Fe 6.34081 3.56497 5.17662
H 2.78837 3.96061 2.32069
H 2.24351 3.88342 4.60096
H 2.98143 5.75663 5.88261
H 3.71399 5.26502 3.01490
C 3.64072 4.17334 2.97947
H 4.46200 6.05116 4.92416
C 3.27884 3.59777 4.35262
C 4.04022 5.48587 5.75293
H 2.82410 3.67867 7.13836
H 5.72086 6.04344 2.98963
H 3.31250 2.50368 4.30217
H 4.87660 3.81087 1.23948
H 4.59271 5.75685 6.65195
N 4.16644 4.01293 5.49682
H 6.50551 5.53420 1.47252
C 4.87407 3.55367 2.31220
C 3.75025 3.25040 6.72554
H 3.52018 2.22778 6.41475
C 6.48350 5.39247 2.56459
H 4.79605 2.46468 2.38165
H 5.07153 4.27364 8.10581
N 6.19494 3.96423 2.89856
H 7.44580 5.67288 2.98679
C 4.83638 3.25332 7.79419
H 4.47001 2.71726 8.68488
H 7.19025 3.00629 1.25380
O 7.72072 4.84256 5.67051
C 7.29807 3.10778 2.34590
H 5.02790 0.87073 6.83905
N 6.10846 2.62776 7.29862
H 6.38313 1.19449 2.78694
H 8.23845 3.63159 2.53210
H 7.34062 4.14073 8.12926
C 7.32189 1.72145 2.97745
C 5.98216 1.13135 7.30674
H 6.05929 0.27603 4.70087
H 5.93099 0.79303 8.35565
C 7.23534 3.05897 8.18196
```

H 7.04882 2.75010 9.22269	H 8.08439 0.63705 6.98467	H 8.82910 9.54400 8.01714	O 6.78106 8.60686 8.73087
N 7.51451 1.77899 4.46829	H 9.58008 1.20044 4.46059	H 9.82371 7.30148 8.28291	O 5.52884 6.44890 9.01845
H 8.12388 1.12406 2.51721	O 7.21932 6.28637 5.55717	H 12.33365 7.18368 7.97553	O 8.01436 6.52226 9.38883
C 7.07878 0.46295 5.05634	H 7.95719 6.67042 5.01605	H 11.58351 7.05779 6.44655	C 11.75680 7.19786 2.82320
H 9.28423 2.95143 4.26893	C 10.59513 10.37930 7.06421	H 13.49712 8.73977 6.37565	F 12.11725 8.34525 3.51382
C 7.10027 0.37087 6.58546	C 9.83689 9.35384 7.66665	H 12.46057 10.99425 6.15223	F 12.91504 6.48977 2.54986
H 8.17025 2.60813 7.84888	C 10.39471 8.09745 7.81178	C 6.44494 7.66332 11.16297	F 11.20398 7.58751 1.61587
H 6.96555 -0.69051 6.83338	C 11.73254 7.80746 7.29477	F 6.36816 6.51354 11.93440	S 10.55814 6.16617 3.81350
C 8.95527 2.04797 4.78102	C 12.48705 8.92571 6.72459	F 7.47812 8.43759 11.67163	O 9.41747 7.10536 4.00943
H 7.72268 -0.32961 4.64010	C 11.91340 10.17259 6.59685	F 5.26570 8.36905 11.34888	O 10.30072 5.00351 2.93430
H 9.08552 2.20284 5.85102	H 10.15340 11.36514 6.95937	S 6.72398 7.26197 9.36189	O 11.33282 5.86304 5.05427