

Support Information

Theoretical Study on Catalytic Mechanism of Human Deoxyhypusine Hydroxylase

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Section 1. Geometric structures of intermediates and transition states along the catalytic reaction process of hDOHH.

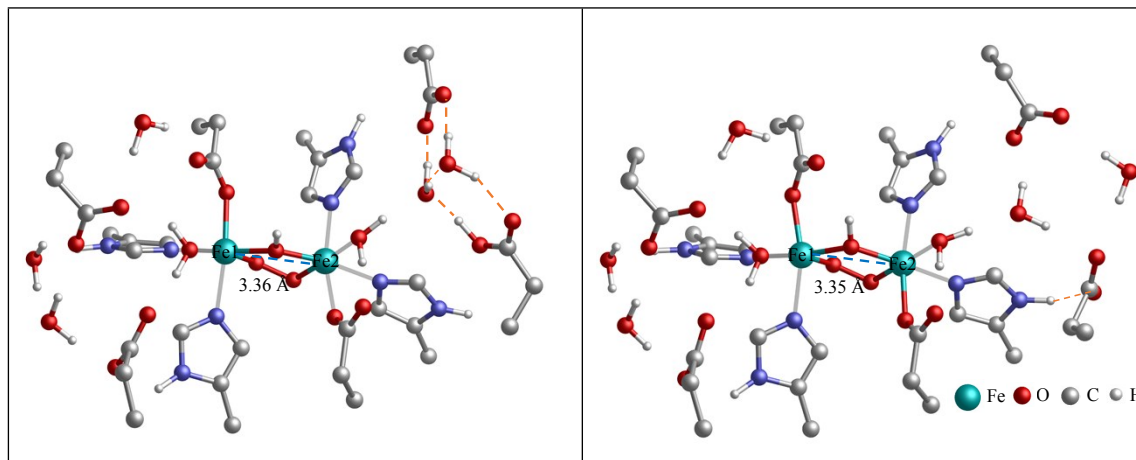


Fig. S1 The geometric structures of Int A in protonated (left) and unprotonated (right) states.

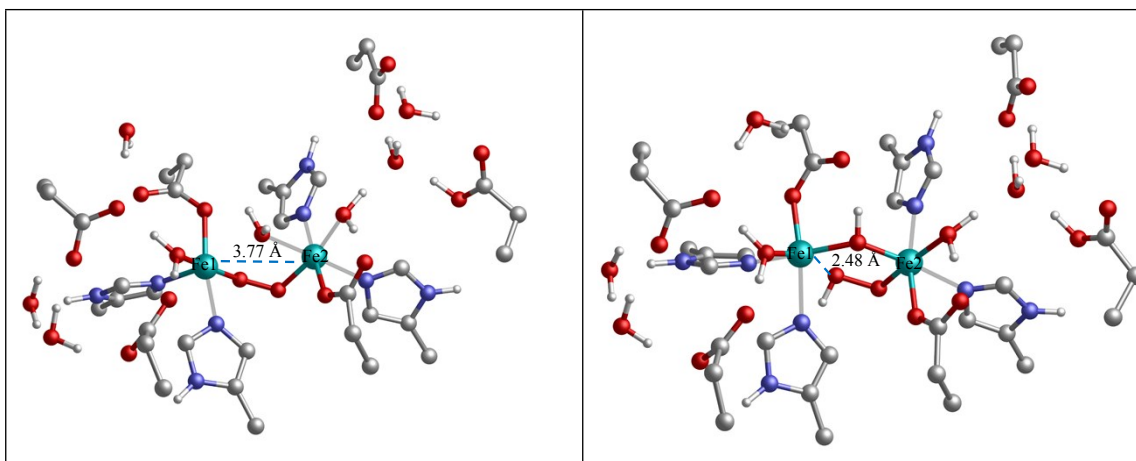


Fig. S2 Geometric structures of Int A with one protonate added to the bridge hydroxo group (left) or peroxy group (right) respectively.

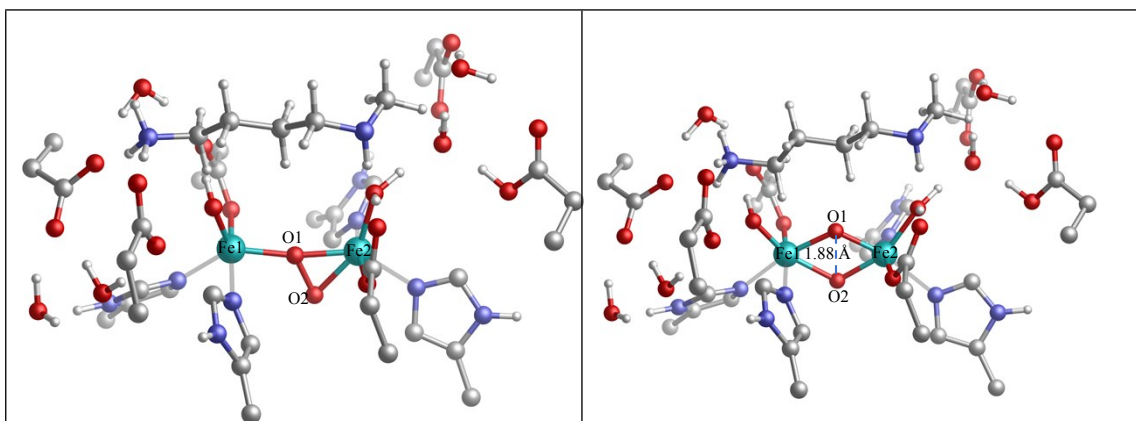
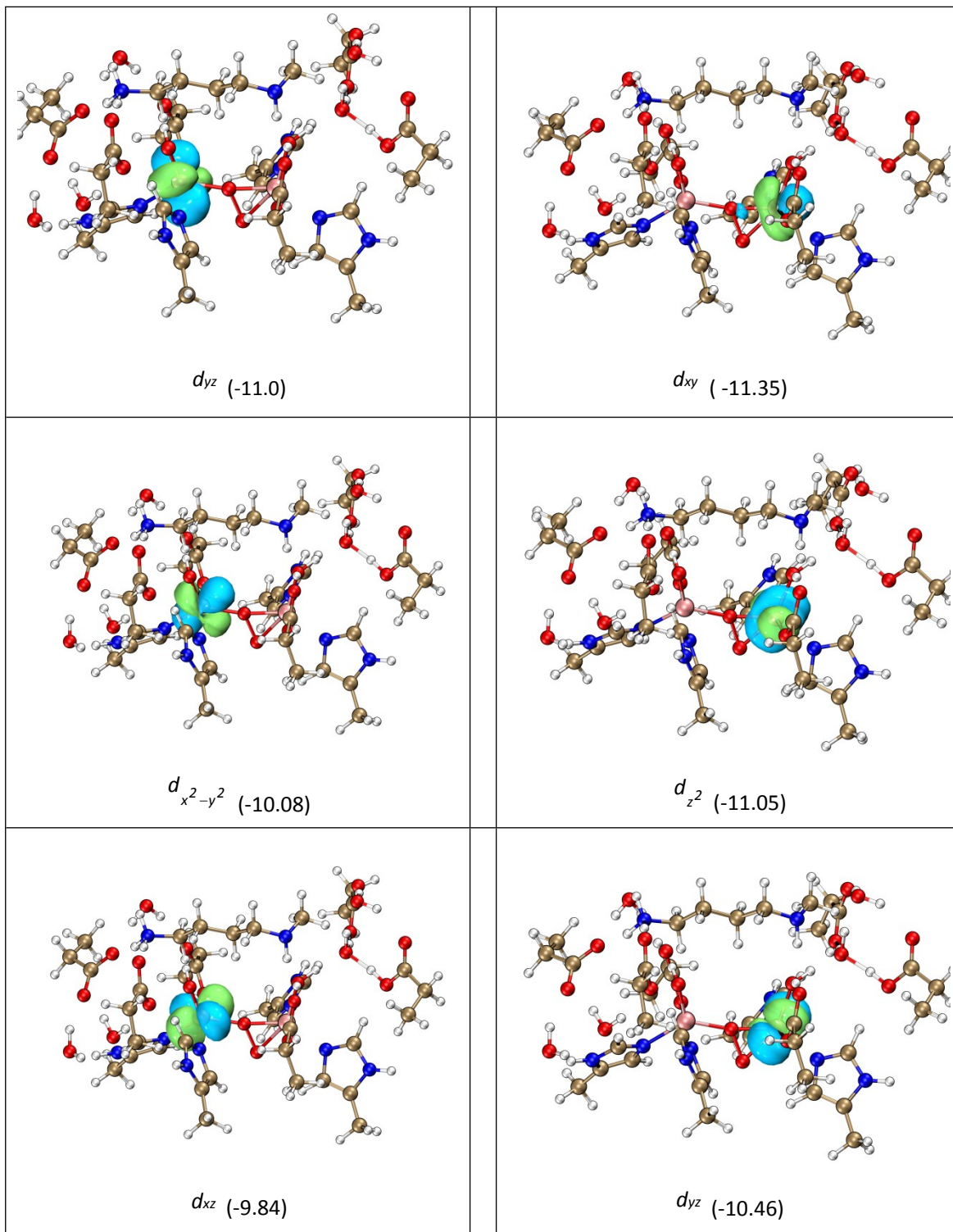


Fig. S3 The geometric structures of Int C (left) and TS_{CD} (right).



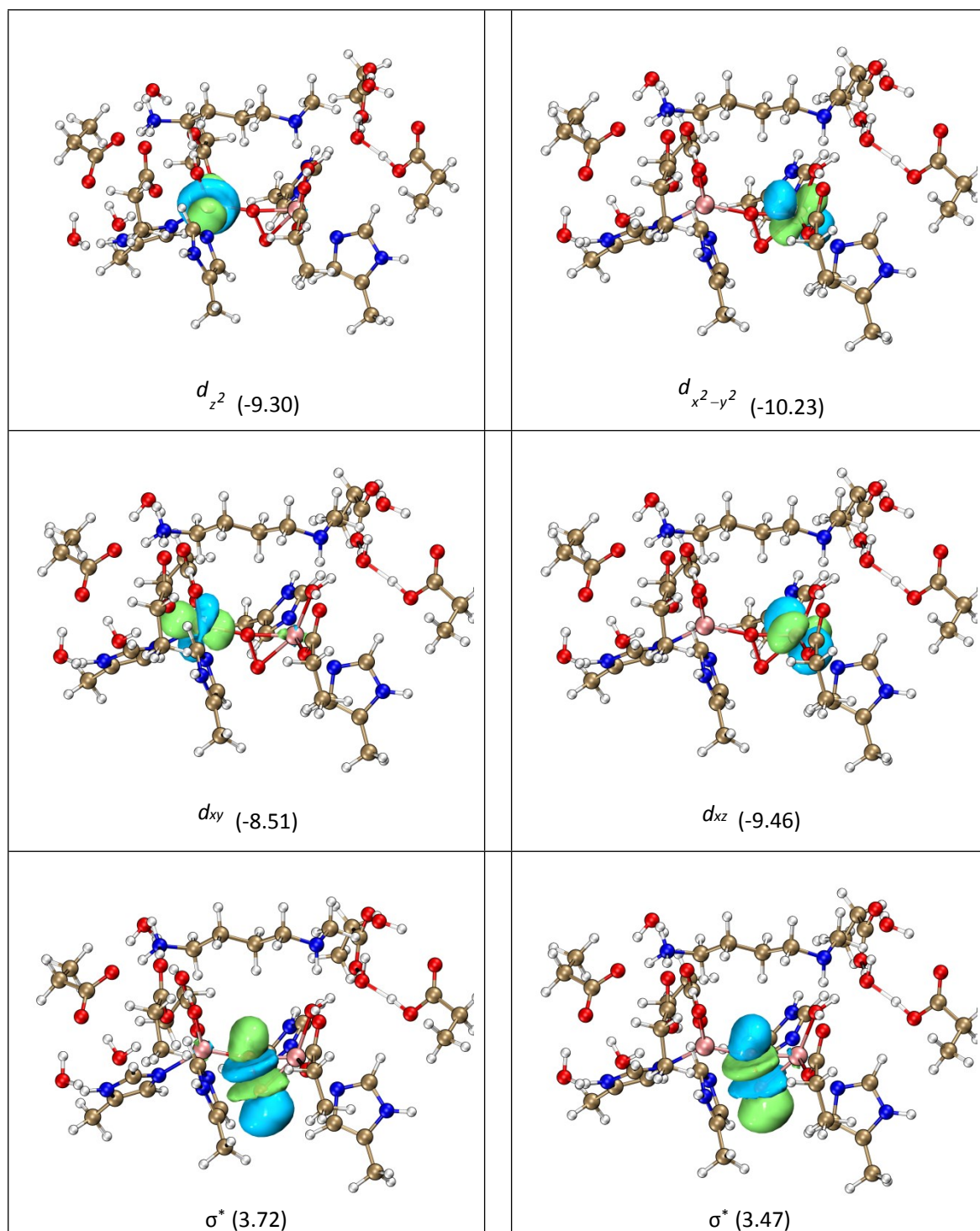


Fig. S4 The frontier molecular orbitals (FMOs) of Int C. Left panel lists α orbitals and right panel lists β orbitals. The energy level (in eV) of these orbitals are labeled.

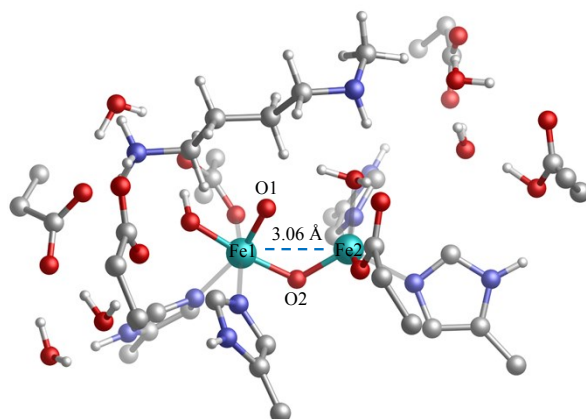


Fig. S5 The geometric structure of Int D_{open1}.

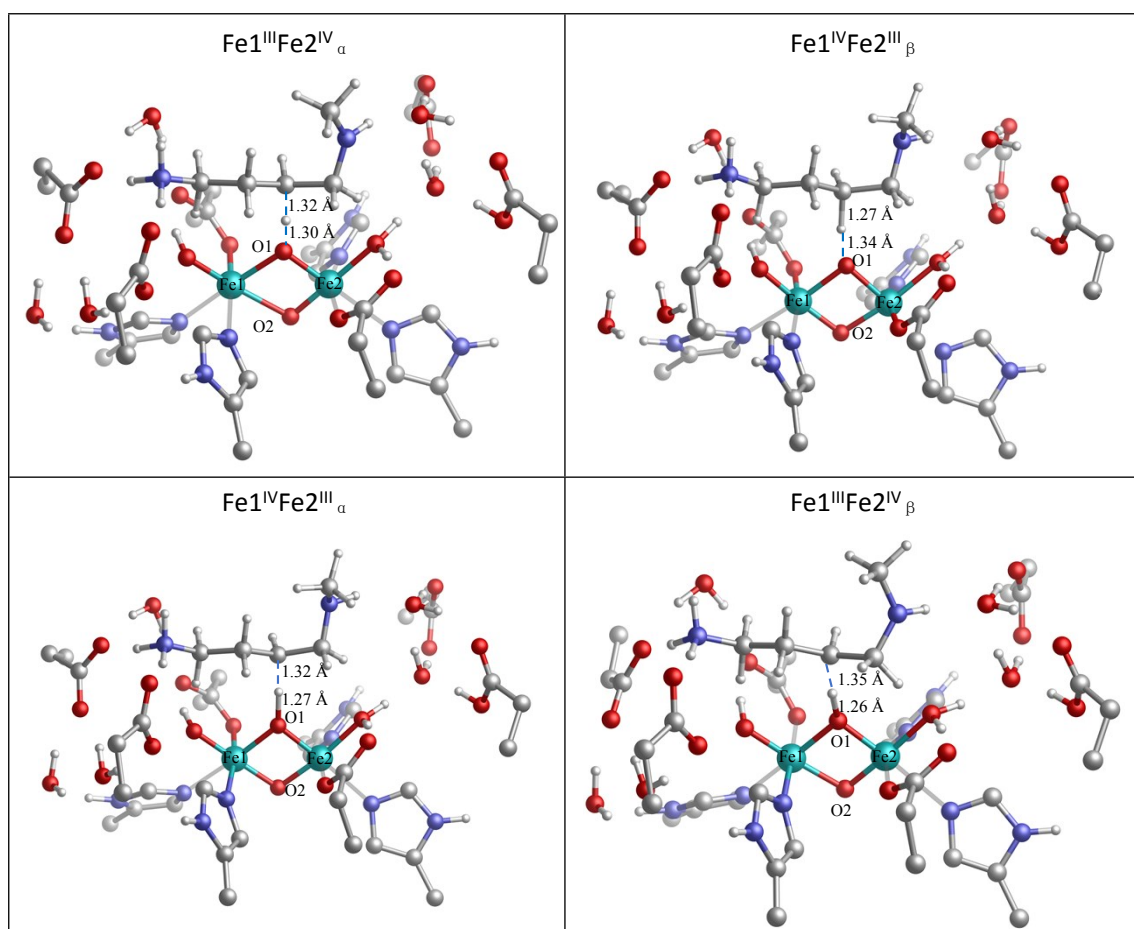


Fig. S6 The geometric structures of TS_{D_E} in different electronic states. Distances (in Å) of Cy-H and O1-H are labeled in the structures.

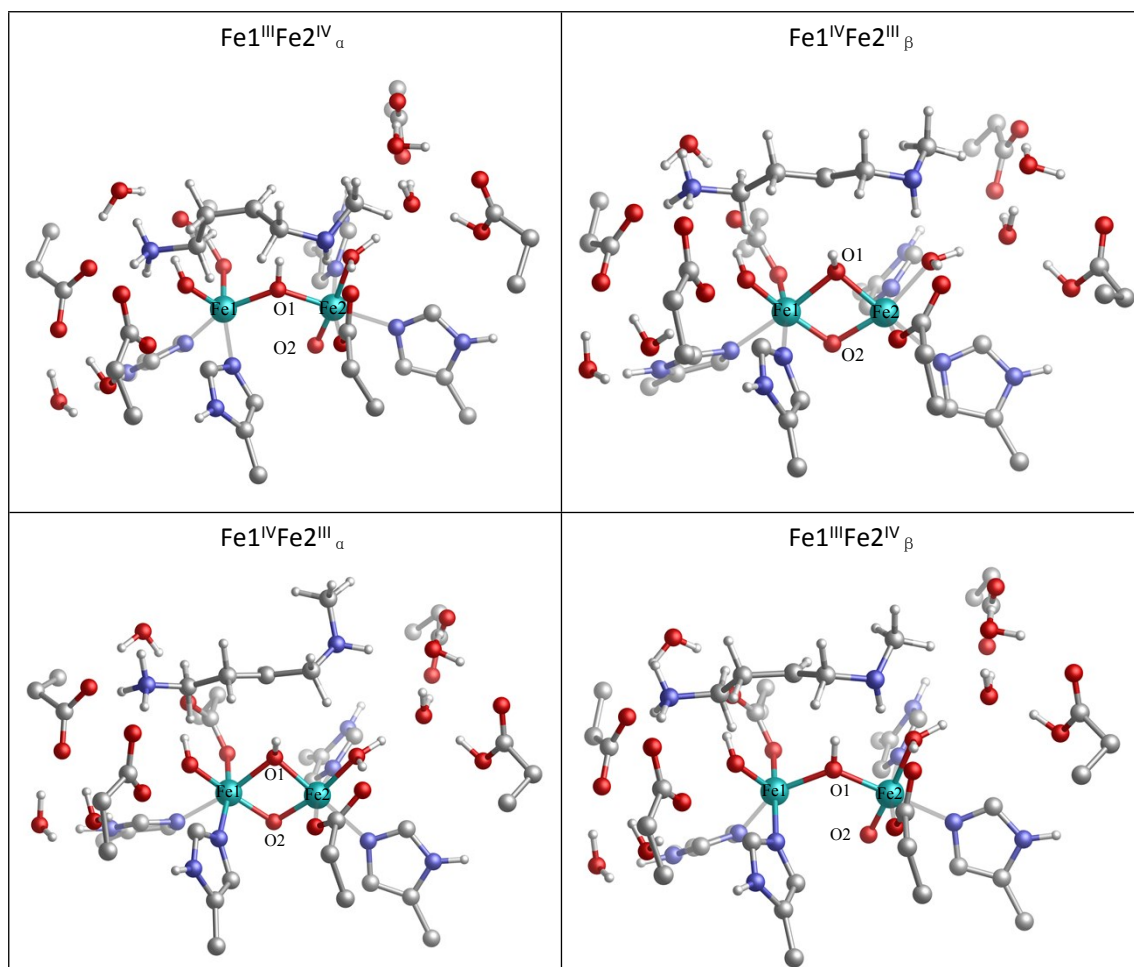


Fig. S7 The geometric structures of Int E in different electronic states.

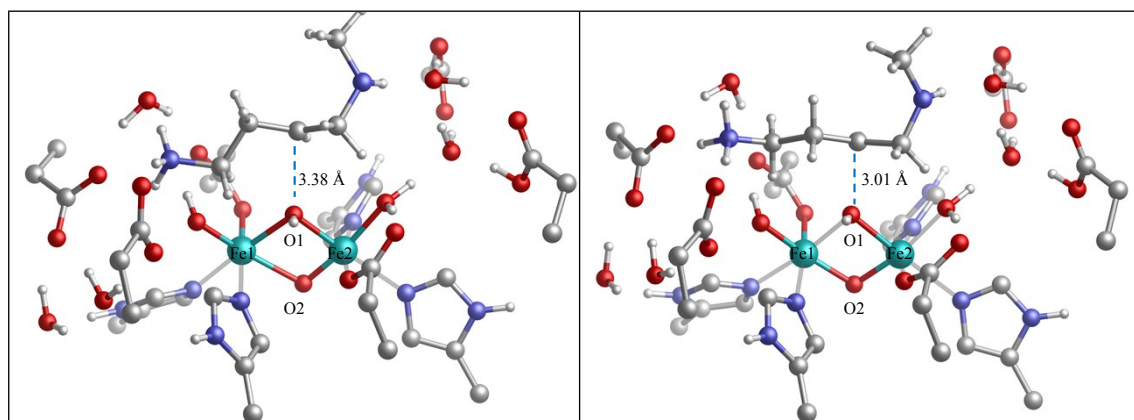


Fig. S8 The geometric structures of TS_{EF} ($\text{Fe1}^{\text{III}}\text{Fe2}^{\text{IV}}_{\alpha}$) (left) and TS_{EF} ($\text{Fe1}^{\text{IV}}\text{Fe2}^{\text{III}}_{\beta}$) (right) with Cy-O1 distances marked.

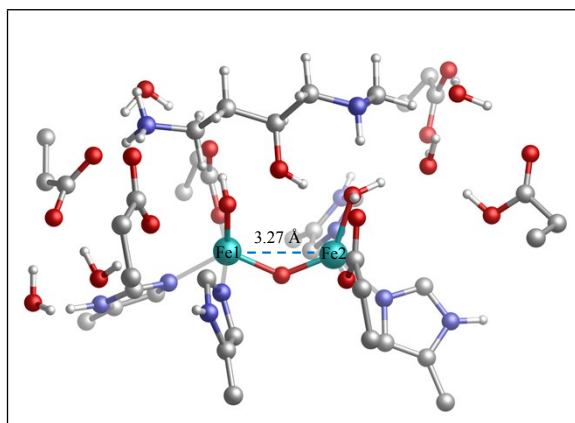


Fig. S9 The geometric structure of product F (pro F). The Fe-Fe distance is 3.27 Å in this structure.

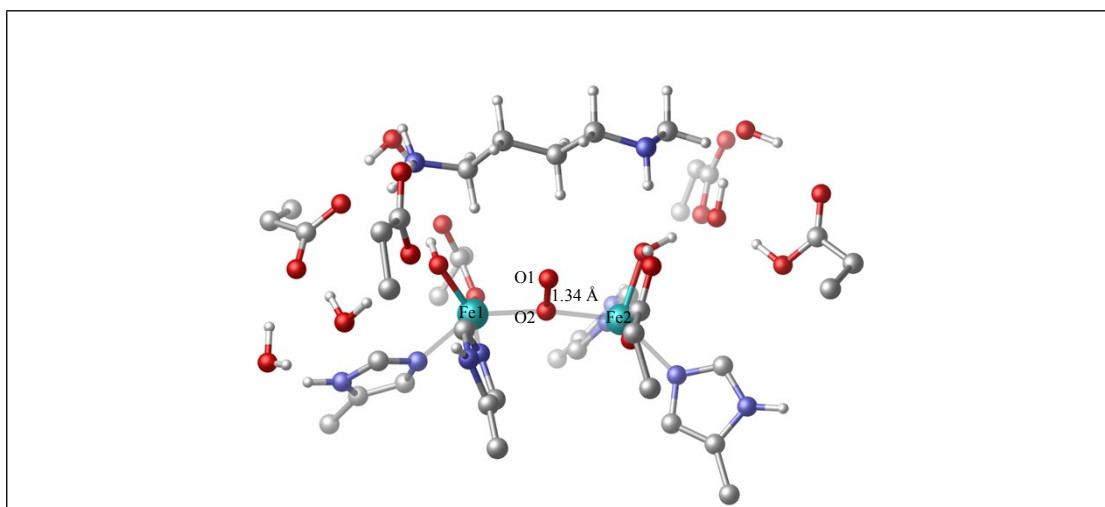


Fig. S10 The geometric structure of Int D1 with O-O distance labelled.

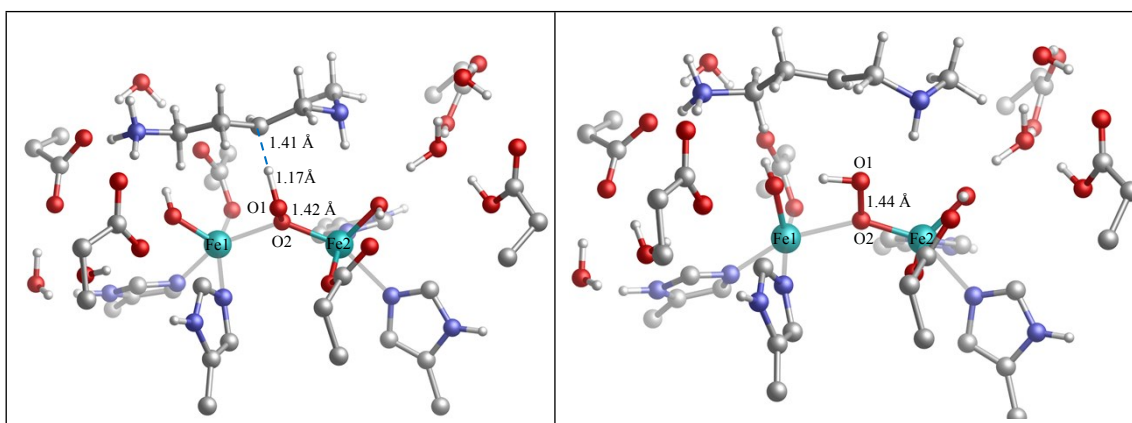


Fig. S11 The left panel shows the geometric structure of $TS_{CE1-\beta}$, in which a β electron is transferred to the Fe1. The right panel presents the corresponding structure of Int $E1_{\beta}$.

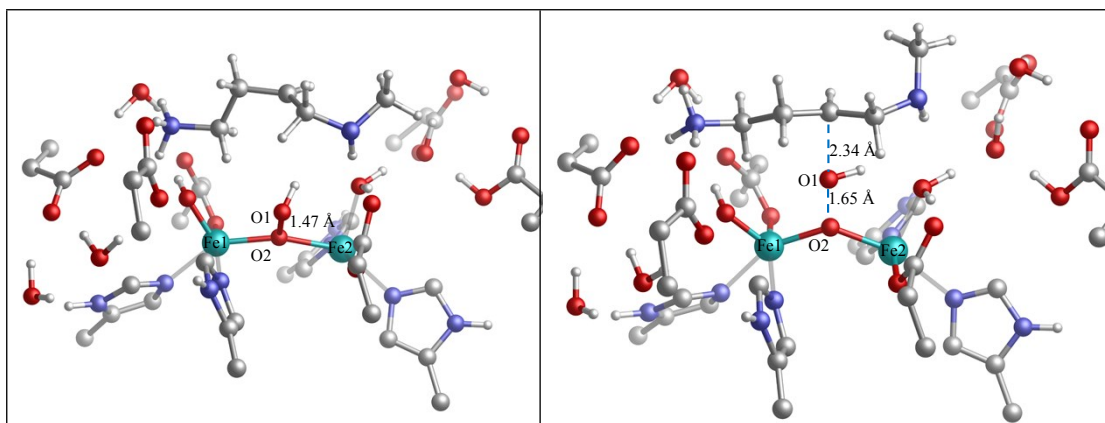


Fig. S12 The structures of Int E1 $_{\alpha}$ and TS $_{EF1-\alpha}$. The distance of O1-O2 in the Int E1 $_{\alpha}$ is 1.47 Å. The distances of Cy-O1 and O1-O2 are 2.34 Å and 1.65 Å, respectively.

Section 2. Atomic spin populations of the intermediates and transition states along the catalytic reaction pathways of hDOHH.

Table S1 The atomic spin populations on the ligation atoms of two Fe ions.

species	Fe1	O _{Glu90}	N _{His89}	N _{His207}	O _{OH/WAT2001}	Fe2	O _{Glu241}	N _{His240}	N _{His56}	O _{WAT2002}
Int A	4.19	0.11	0.07	0.07	0.05	-4.10	-0.08	-0.04	-0.06	-0.05
Int B	4.10	0.10	0.07	0.07	0.02	-4.16	-0.10	-0.06	-0.07	-0.07
Int B'	4.10	0.11	0.09	0.07	0.35	-4.03	-0.09	-0.07	-0.06	-0.08
Int C	4.10	0.11	0.08	0.07	0.41	-4.11	-0.10	-0.06	-0.07	-0.08
TS _{CD}	3.87	0.11	0.06	0.08	0.33	-4.11	-0.12	-0.04	-0.08	-0.10
Int D _{diamond}	3.41	0.10	0.04	0.08	0.14	-3.49	-0.12	-0.01	-0.10	-0.04
Int D _{open2}	4.11	0.11	0.07	0.07	0.41	-3.08	-0.11	0.00	-0.09	-0.08
TS _{DE} (Fe ^{III} Fe ^{IV} $_{\alpha}$)	4.12	0.1	0.06	0.06	0.35	-3.44	-0.1	-0.02	-0.07	-0.03
TS _{DE} (Fe ^{IV} Fe ^{III} $_{\beta}$)	3.36	0.07	0.05	0.05	0.10	-4.1	-0.11	-0.03	-0.07	-0.06
TS _{DE} (Fe ^{IV} Fe ^{III} $_{\alpha}$)	3.42	0.06	0.06	0.03	0.13	-2.98	-0.09	0.00	-0.06	-0.01
TS _{DE} (Fe ^{III} Fe ^{IV} $_{\beta}$)	2.55	-0.01	0.01	-0.02	0.08	-3.05	-0.07	-0.01	-0.05	0.00
Int E(Fe ^{III} Fe ^{IV} $_{\alpha}$)	4.14	0.12	0.07	0.07	0.41	-3.13	-0.08	-0.04	-0.06	0.00
Int E(Fe ^{IV} Fe ^{III} $_{\beta}$)	3.37	0.07	0.06	0.05	0.08	-4.19	-0.1	-0.05	-0.08	-0.07
Int E(Fe ^{IV} Fe ^{III} $_{\alpha}$)	3.44	0.06	0.07	0.03	0.12	-2.83	-0.08	0.00	-0.06	0.01
Int E(Fe ^{III} Fe ^{IV} $_{\beta}$)	2.80	-0.04	0.04	-0.03	0.07	-3.13	-0.08	-0.03	-0.07	0.01
TS _{EF} (Fe ^{III} Fe ^{IV} $_{\alpha}$)	4.16	0.11	0.07	0.06	0.35	-3.76	-0.08	-0.04	-0.06	-0.03
TS _{EF} (Fe ^{IV} Fe ^{III} $_{\beta}$)	3.92	0.09	0.06	0.06	0.14	-4.13	-0.08	-0.04	-0.07	-0.05
Pro F	4.09	0.09	0.06	0.07	0.37	-4.09	-0.09	-0.07	-0.07	-0.08
Int D1	4.13	0.12	0.09	0.06	0.42	-3.76	-0.05	-0.03	-0.02	-0.07
TS _{CE1-alpha}	4.11	0.13	0.07	0.06	0.40	-3.76	-0.04	-0.02	-0.02	-0.05
TS _{CE1-beta}	3.73	0.03	0.03	0.02	0.20	-4.10	-0.14	-0.05	-0.05	-0.25
Int E1 $_{\alpha}$	4.13	0.12	0.08	0.06	0.40	-3.76	-0.04	-0.02	-0.03	-0.05
Int E1 $_{\beta}$	3.74	0.04	0.03	0.02	0.11	-4.07	-0.11	-0.05	-0.05	-0.25
TS _{EF1-alpha}	4.09	0.11	0.06	0.06	0.40	-3.78	-0.06	-0.02	-0.02	-0.04

Table S2 The atomic spin populations on two iron centers and the substrate of the reaction intermediates and transition states along the reaction pathway I and pathway II of hDOHH.

Species	Fe1	Fe2	O1	O2	Substrate
Int A	+4.5	-4.3	+0.2	-0.3	–
Int B	+4.4	-4.5	+0.3	-0.2	–
Int B'	+4.7	-4.3	0.0	-0.4	–
Int C	+4.8	-4.4	-0.1	-0.3	–
TS _{CD}	+4.5	-4.5	0.0	0.0	–
Int D _{diamond}	+3.8	-3.8	0.0	0.0	–
Int D _{open2}	+4.8	-3.4	-1.1	-0.4	
TS _{DE} (Fe ^{III} Fe ^{IV} _α)	+4.7	-3.7	-0.2	-0.2	-0.6
TS _{DE} (Fe ^{IV} Fe ^{III} _β)	+3.6	-4.4	+0.2	0.0	+0.4
TS _{DE} (Fe ^{IV} Fe ^{III} _α)	+3.7	-3.1	-0.2	0.0	-0.4
TS _{DE} (Fe ^{III} Fe ^{IV} _β)	+2.6	-3.2	0.0	-0.1	+0.7
Int E (Fe ^{III} Fe ^{IV} _α)	+4.8	-3.3	0.0	-0.5	-1.0
Int E (Fe ^{IV} Fe ^{III} _β)	+3.6	-4.5	0.0	0.0	+1.0
Int E (Fe ^{IV} Fe ^{III} _α)	+3.7	-3.0	0.0	+0.1	-1.0
Int E (Fe ^{III} Fe ^{IV} _β)	+2.8	-3.3	0.0	-0.5	+1.0
TS _{EF} (Fe ^{III} Fe ^{IV} _α)	+4.8	-4.0	0.0	-0.2	-0.7
TS _{EF} (Fe ^{IV} Fe ^{III} _β)	+4.3	-4.4	-0.2	-0.3	+0.6
Pro F	+4.7	-4.4	–	-0.3	–
Int D1	4.8	-3.9	-0.64	-0.29	–
TS _{CE1-α}	+4.8	-3.9	-0.4	0.0	-0.6
TS _{CE1-β}	+4.0	-4.6	+0.2	-0.2	+0.6
Int E1 _α	+4.8	-3.9	0.0	0.0	-1.0
Int E1 _β	+3.9	-4.5	0.0	-0.3	+1.0
TS _{EF1-α}	+4.7	-3.9	0.0	-0.1	-0.8

Section 3. The relative energies of different electronic states of Int A and C.

Scheme S1 The electronic states and corresponding energies of Int A and Int C.

	HH	HM	HL	MM	ML	LL
Energy for Int A	0.0	7.4	13.1	19.5	24.9	26.7
Energy for Int C	0.0	11.0	15.0	27.8	27.8	38.0

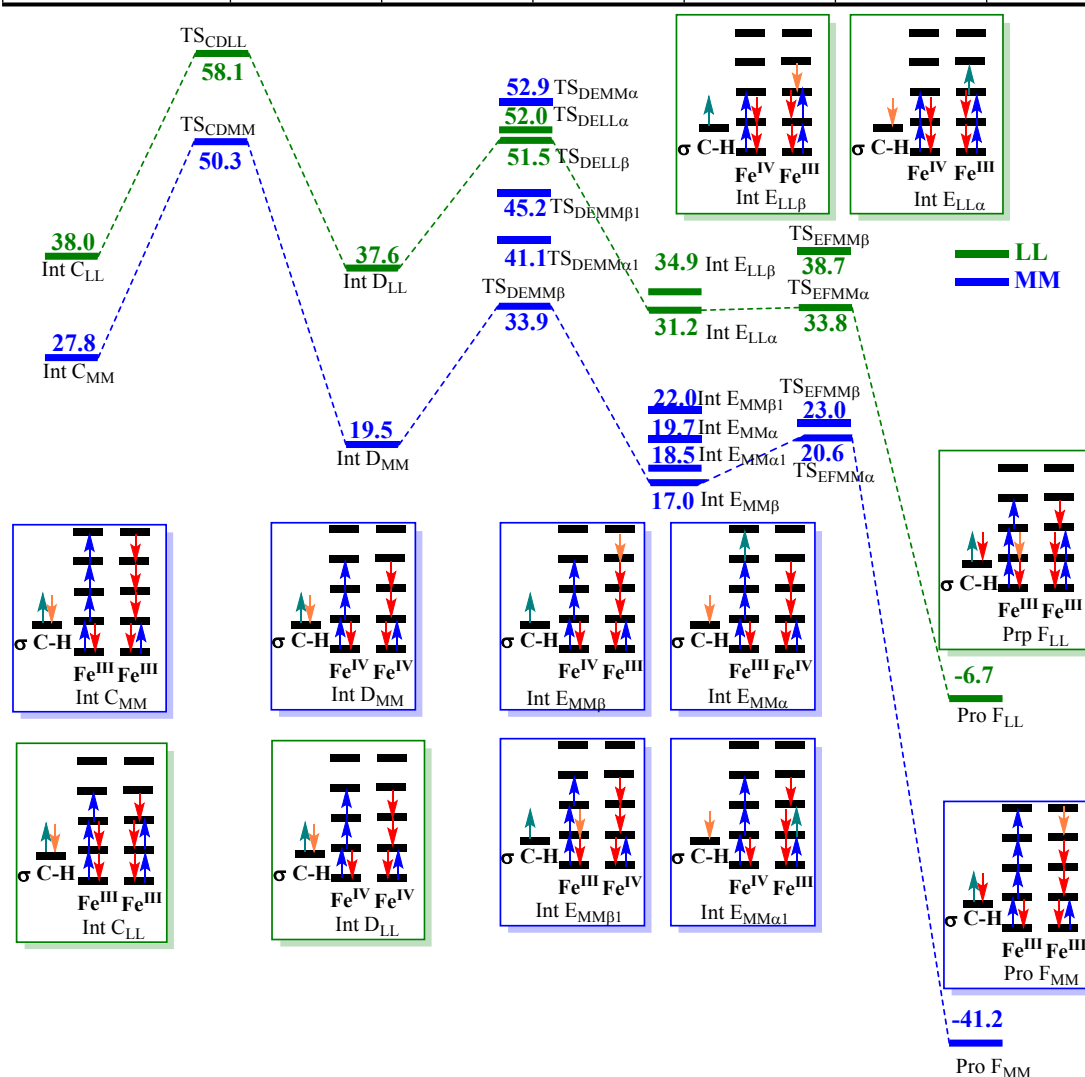


Fig. S13 The energy profiles of the structures with antiferromagnetically (A) coupled middle spin (M) and low spin (L) diiron core (S=0) along the pathway I. The relative energies (in kcal·mol⁻¹) and the electronic states of intermediates are labeled on the figure.

Section 4. Cartesian coordinates of the important stationary point structures.

Int A

C	0.58983300	0.61687100	0.00001800	C	8.72285000	10.21088800	5.01099600
C	0.46547700	1.62393800	1.10274900	C	8.92923100	8.73377900	5.33608100
N	-0.32275900	1.44976900	2.23606100	C	8.42800000	7.83994200	4.18843200
C	1.03077000	2.86016500	1.25904500	O	8.76529300	8.22211100	3.01316800
C	-0.20093200	2.55325000	3.01822400	O	7.74890000	6.83628900	4.49598900
N	0.60658400	3.42934100	2.44499300	C	-3.65216200	8.85487600	6.55002400
C	-2.37116600	-0.87608700	4.64499800	C	-4.56632400	7.66914800	6.92039200
C	-2.38450500	-0.55129900	6.13954800	C	-3.85737800	6.32798600	6.99240900
C	-2.26728000	0.94556600	6.48544300	O	-3.83386100	5.67112400	8.02815800
O	-2.18482700	1.75189200	5.49807300	O	-3.29678800	5.97733000	5.85192100
O	-2.29303100	1.23189200	7.70233400	Fe	4.44679600	4.68493400	2.37148500
C	7.41282800	2.90290500	-2.17101400	Fe	1.24727900	5.48200800	3.00302300
C	7.05485200	3.44565800	-0.83553100	O	0.49204400	5.14538500	4.94012700
N	7.97436100	3.68358800	0.16765700	O	-1.66871600	4.13013000	6.10981000
C	5.83342800	3.77040300	-0.30403500	O	-1.78016800	3.71105600	8.69226900
C	7.30242400	4.12872900	1.24915800	O	7.29065900	0.78616600	5.86619100
N	6.00215100	4.19443400	0.99430200	O	10.62068400	3.96739100	0.73866700
C	4.44181600	0.09288900	1.14499800	O	10.60794200	6.34901700	2.11768500
C	4.13925100	0.33709200	2.63173200	H	1.59854800	0.64360500	-0.41922700
C	4.58958300	1.72590200	3.11416300	H	-0.11922200	0.80529900	-0.81744100
O	4.11723600	2.69870800	2.40559900	H	1.75940300	3.36565200	0.64379000
O	5.32067800	1.84184600	4.10329900	H	-0.70238400	2.63813300	3.97062700
C	-2.63617500	8.68886600	0.02597800	H	-2.96873000	-1.77287600	4.43207400
C	-2.03974900	7.70804700	0.99107600	H	-2.80554500	-0.04112600	4.08868500
N	-2.63616600	7.39511700	2.20709800	H	-1.59077900	-1.07808700	6.68097300
C	-0.87434200	6.98148400	0.98559900	H	-3.32262900	-0.89221000	6.59504800
C	-1.82841000	6.52492300	2.87182300	H	8.26938000	3.43159600	-2.60837800
N	-0.75757500	6.25506300	2.15421900	H	6.56892000	3.02766200	-2.85718100
C	1.06183100	10.26886400	3.42699800	H	4.85290900	3.72989800	-0.75485500
C	1.68273100	9.53555200	4.61776400	H	7.80648400	4.36496100	2.17934000
C	1.27022300	8.06653100	4.65564300	H	4.02799200	-0.86555300	0.80664900
O	1.33627900	7.46995800	3.52382200	H	4.01278200	0.89741700	0.54208200
O	0.90700300	7.55700900	5.73952100	H	4.62289900	-0.41722500	3.25935100
C	9.54281100	0.93491200	3.35500400	H	3.05629400	0.26993400	2.79833100
C	10.12999800	2.00114500	4.29311600	H	-3.58648200	8.33606700	-0.39657400
C	9.23228700	3.23880300	4.17594200	H	-1.94453300	8.85308400	-0.80370500
O	9.55069600	4.05160300	3.24564800	H	-0.09106400	6.94366200	0.24266600
O	8.20955900	3.30406700	4.90000300	H	-2.04695700	6.16210500	3.86459100
C	4.76484700	10.35186100	1.08097200	H	1.46701700	11.28425500	3.33259600
C	5.06557000	8.97614000	1.56704300	H	1.27479400	9.72367000	2.50542400
N	6.34959400	8.49039400	1.76583000	H	1.41833800	10.00301900	5.57078100
C	4.23979300	7.89273100	1.74354400	H	2.77613100	9.55329600	4.52688800
C	6.25460400	7.18091600	2.06270600	H	8.63202400	0.52995200	3.80488200
N	4.99713000	6.78092000	2.06197200	H	9.28848700	1.38193800	2.38704700

H	10.14393700	1.62476400	5.32118000	H	-0.86607700	0.63787300	2.48925000
H	11.15010800	2.26764900	3.99478700	O	3.02808400	5.06489800	3.68180400
H	3.70644500	10.40158300	0.80473700	H	3.11835800	4.67259400	4.55933500
H	5.34024100	10.58194800	0.17324000	H	6.54849500	5.54307100	4.13331500
H	3.16640500	7.82264200	1.65826500	Int B			
H	7.12146500	6.60393800	2.32024500	C	-0.11697300	0.99112900	-0.00017100
H	9.23571300	10.86369400	5.73153100	C	-0.30013800	2.00870200	1.08561000
H	9.12176500	10.41534200	4.01431100	N	-0.89824500	1.75219600	2.31333100
H	8.43019200	8.44240300	6.26473700	C	0.08354300	3.31990200	1.15643200
H	10.00247100	8.53425500	5.45969100	C	-0.84611200	2.87723400	3.06806400
H	-2.76474300	8.89009700	7.18808900	N	-0.25120000	3.84813200	2.39025800
H	-3.31925700	8.80703400	5.51082500	C	-3.07781700	-0.50153100	4.64512800
H	-5.02512000	7.83775700	7.89820400	C	-3.07956000	-0.16940000	6.13672600
H	-5.37594500	7.59160200	6.18232900	C	-2.84428600	1.31214000	6.47609400
H	-0.29225100	4.69294700	5.33715800	O	-2.72448600	2.10845300	5.48074700
H	0.61854100	6.03499200	5.40200000	O	-2.82578300	1.60752400	7.68953700
H	-1.94493200	3.16008500	5.85689800	C	6.70672300	3.27727100	-2.17085000
H	-1.50228400	4.06285000	7.09981600	C	6.28684500	3.91595200	-0.89647400
H	-2.61154500	4.21590500	8.67256300	N	7.06917600	4.79868700	-0.17054300
H	-2.01910500	2.78327700	8.43701800	C	5.06601500	3.92362300	-0.28272900
H	6.49588000	0.88400500	5.31419700	C	6.32135800	5.30780200	0.82529000
H	7.69098500	1.66889200	5.72855000	N	5.09463400	4.79725700	0.78548700
H	10.66262800	4.94046600	0.88836400	C	3.73559900	0.46713400	1.14590500
H	10.40787000	3.69972500	1.66509000	C	3.40105400	0.86652100	2.58999500
H	9.94704300	7.06277800	2.24476200	C	3.44999900	2.36917900	2.87659200
H	10.30447300	5.67736100	2.76049400	O	3.23899100	3.12635100	1.85836000
O	5.96013000	4.77248000	3.94625800	O	3.61859900	2.77968500	4.04391900
H	6.47923500	3.99342100	4.24876900	C	-3.34290100	9.06304400	0.02592100
H	-2.66924100	5.12687300	5.97773700	C	-2.80683100	8.09045900	1.02502900
H	-1.39682300	-1.07763300	4.25137400	N	-3.42787200	7.81809900	2.23813100
H	0.40620800	-0.37350500	0.36094800	C	-1.64440400	7.37093800	1.06168500
H	5.49809900	0.07607900	0.97490700	C	-2.63552100	6.97516700	2.95024100
H	7.65797900	1.86146400	-2.15410700	N	-1.54807900	6.68815300	2.25936800
H	10.23077600	0.13870200	3.16060900	C	0.35513700	10.64327000	3.42699400
H	7.68858400	10.48493500	5.02438900	C	0.98039100	9.91056800	4.62017600
H	4.93700700	11.15594000	1.76569400	C	0.62272300	8.42693800	4.66490100
H	-0.00002900	10.35531200	3.52655200	O	0.71448200	7.81027600	3.54432300
H	-2.81455800	9.63060200	0.50170800	O	0.28652200	7.90533800	5.75391400
H	-4.23014000	9.74019500	6.71460600	C	8.83508500	1.30886500	3.35419900
O	3.12911300	4.95162300	0.96475600	C	9.53954600	2.62250300	3.01916300
O	2.01086900	5.72700200	1.28887800	C	8.74247100	3.92014600	3.19553900
H	-3.51290100	7.74927200	2.55695600	O	9.31934200	4.96200700	2.76433700
H	7.24091600	8.95363200	1.94176200	O	7.61280400	3.88390600	3.76031700
H	9.02012200	3.67580400	0.16335900	C	4.05789600	10.72613200	1.08082400

C	4.15413700	9.36514700	1.68204600	H	0.57318900	10.10342700	2.50288500
N	5.09987800	8.97050700	2.61681500	H	0.69347300	10.36472000	5.57255700
C	3.45440000	8.22515900	1.38400100	H	2.07429200	9.96621200	4.54690300
C	4.95325500	7.64819200	2.84130000	H	8.51070800	1.26636800	4.39703500
N	3.96714500	7.16507200	2.10600000	H	7.94862000	1.16166900	2.72916900
C	8.01604600	10.58505100	5.01127100	H	10.44311600	2.73533200	3.63346300
C	8.32759000	9.53525100	6.07588700	H	9.90140800	2.60835500	1.98352400
C	7.60108500	8.19917500	5.86216900	H	3.06141500	10.86351300	0.65235100
O	6.99681600	8.02830900	4.76041200	H	4.78144700	10.84961100	0.26360300
O	7.67147500	7.36162400	6.80469900	H	2.60889500	8.09017400	0.72840000
C	-4.35864000	9.22911700	6.55005900	H	5.59727300	7.12308400	3.52536800
C	-5.19731600	8.04356500	7.06650700	H	8.60121900	11.49864100	5.17457900
C	-4.45846600	6.71866300	7.09821300	H	8.25974400	10.20622000	4.01454000
O	-4.31184200	6.08129600	8.13286700	H	8.07936600	9.89515500	7.08088700
O	-4.00983900	6.34560900	5.90822900	H	9.40329800	9.31727700	6.09711000
Fe	3.34134000	5.14300000	1.85347300	H	-3.41684300	9.32026800	7.09871800
Fe	0.38973400	5.88014000	2.97367100	H	-4.12469100	9.13026300	5.48713400
O	-0.23340600	5.51493600	4.89747000	H	-5.54176100	8.23823600	8.08499600
O	-2.31425000	4.50882700	6.06193500	H	-6.08548300	7.92404000	6.43225400
O	-2.26432300	4.07501800	8.62528300	H	-1.03742000	5.07495100	5.30899000
O	6.12350800	2.34676900	5.55447300	H	-0.04510300	6.37050400	5.39376400
O	9.55380200	5.90888800	0.23042500	H	-2.55073800	3.52277100	5.81479700
O	8.20173900	7.34589300	2.33341700	H	-2.12156500	4.43760900	7.05178700
H	0.90533100	1.02430300	-0.38635400	H	-3.09470200	4.57389800	8.70791800
H	-0.79737900	1.16436200	-0.84262900	H	-2.51423600	3.14052200	8.40042600
H	0.63052600	3.90462900	0.43493300	H	5.22581000	2.34255200	5.17655200
H	-1.25012000	2.91244100	4.06904800	H	6.67995600	2.67428400	4.81832800
H	-3.67247300	-1.40193200	4.44334600	H	9.20678800	6.73814500	0.60714800
H	-3.51587500	0.32677900	4.08261800	H	9.72055200	5.40215600	1.05851300
H	-2.34269600	-0.76154800	6.69072000	H	7.86837100	7.77601000	3.14426200
H	-4.04995600	-0.42672300	6.57903000	H	8.57500200	6.49222700	2.66831900
H	7.58272800	3.79351400	-2.57947800	O	2.22258700	5.24741800	3.42469200
H	5.91020700	3.38944700	-2.91538600	H	2.34192300	4.46308000	3.99110900
H	4.17324400	3.37355000	-0.53254500	H	-3.38499800	5.51066300	5.99272300
H	6.71652300	6.03419300	1.52548600	H	-2.10361100	-0.70374400	4.25125700
H	3.36132600	-0.54080900	0.93008500	H	-0.30051500	0.00066400	0.36107100
H	3.27616600	1.16519800	0.44421000	H	4.79107400	0.45033800	0.97422400
H	4.04724000	0.36182000	3.31442600	H	6.95071500	2.23554400	-2.15423000
H	2.37418000	0.56058600	2.83321800	H	9.52454300	0.51312000	3.16120700
H	-4.28152300	8.72742900	-0.43304100	H	6.98173700	10.85912500	5.02418700
H	-2.61289800	9.21195700	-0.77234600	H	4.23041300	11.53005800	1.76577100
H	-0.84800200	7.30942600	0.33681600	H	-0.70680700	10.72934400	3.52654700
H	-2.88244300	6.63638800	3.94538200	H	-3.52135100	10.00484200	0.50173000
H	0.75901600	11.65872800	3.34100000	H	-4.93702300	10.11432200	6.71461500

O	2.04601800	5.54070000	0.58366500	C	5.10084900	3.91607000	-0.24354400
O	0.97931100	6.24280100	1.16940300	C	6.42306100	5.12470300	0.98917900
C	0.24761900	6.16258900	8.92291800	N	5.17270700	4.68452900	0.89911200
N	1.18738400	7.27503100	8.79576500	C	3.76301000	0.46877300	1.16385200
C	2.58780100	6.86833600	8.70922300	C	3.40427700	0.71595900	2.63178300
C	3.02452300	6.20784800	7.38655200	C	3.65225700	2.15794300	3.06991300
C	4.50875800	5.81537200	7.37113500	O	3.23659000	3.05049800	2.23002700
C	4.99486400	5.51004300	5.95551300	O	4.18796000	2.38967800	4.16750800
N	6.44635400	5.16146400	5.93991200	C	-3.32028300	9.05922200	0.03169400
H	0.43247800	5.62704700	9.86164400	C	-2.92068900	8.01890200	1.01394100
H	0.27876500	5.41909400	8.11101700	N	-3.65228100	7.71397300	2.15395800
H	0.94731100	7.80190900	7.95693800	C	-1.80368400	7.23959100	1.09535800
H	3.21624600	7.75666400	8.87181900	C	-2.96582100	6.79772200	2.87908000
H	2.79552900	6.19027700	9.54957800	N	-1.84152300	6.49142500	2.25569400
H	2.40707600	5.32532300	7.18137800	C	0.37318900	10.64398000	3.43564800
H	4.67386000	4.94393700	8.02004300	C	1.00377400	9.85022000	4.58876300
H	5.12152400	6.63189100	7.77516800	C	0.62703300	8.36918700	4.67370800
H	4.87587300	6.39790500	5.33504800	O	0.16856100	7.82940700	3.59970800
H	4.44800000	4.68223200	5.49932900	O	0.81798200	7.75622100	5.74808100
H	6.56710700	4.24399500	6.38686700	C	8.85937200	1.31541300	3.37681500
H	6.80855000	4.99784700	4.97822100	C	9.69232300	2.58417000	3.60227200
H	-0.77450200	6.54842100	8.96715000	C	8.88620800	3.87050800	3.80532800
H	2.82117200	6.91344900	6.57054200	O	9.26064200	4.88524500	3.14824700
H	7.01135400	5.97425600	6.36709600	O	7.93705500	3.83935900	4.63720200
H	-4.31880100	8.17251400	2.55140600	C	4.07833100	10.72800200	1.09325800
H	5.80976000	9.51220400	3.09251400	C	4.15729100	9.37119600	1.71746400
H	8.06449500	5.08434200	-0.26980600	N	4.95327400	9.05266900	2.81216900
H	-1.33110600	0.89279600	2.62031900	C	3.55375600	8.18902200	1.37182200
				C	4.81299500	7.73559500	3.08082800
				N	3.97188700	7.18505800	2.22094600
				C	8.03257400	10.59194600	5.02782700
				C	8.38662000	9.62702100	6.15298500
				C	7.59191300	8.31495500	6.09240600
				O	6.92382900	8.07116700	5.05012900
				O	7.68782200	7.56808700	7.11167300
				C	-4.34281700	9.22839000	6.55468900
				C	-5.03852600	7.99544900	7.15891800
				C	-4.17630300	6.74142600	7.20800600
				O	-4.02162300	6.10257300	8.23870400
				O	-3.63363400	6.42466600	6.03731700
				Fe	3.63582400	5.03287600	2.22303900
				Fe	0.01547200	5.87671800	3.04137400
				O	0.25880400	5.32986700	4.96273200
				O	-1.93502900	4.53555100	6.14815400

Int B'

O	-1.98513200	4.02284600	8.67616100	H	-0.54596800	4.95148000	5.43852000
O	6.42565900	1.98470000	6.06188400	H	0.51892300	6.18551800	5.43410900
O	9.58329900	5.74553400	0.60021100	H	-2.28894800	3.59999600	5.89212400
O	8.10866400	7.23931200	2.63337200	H	-1.77450300	4.42089300	7.14499300
H	0.93753200	1.03467800	-0.36035900	H	-2.79261400	4.55414800	8.77941300
H	-0.76432000	1.15891400	-0.83340200	H	-2.28073900	3.10413100	8.43304200
H	0.63248100	3.91375100	0.54077400	H	5.63499700	1.95224400	5.49892600
H	-1.34116400	2.79207700	4.09135100	H	7.04495000	2.52967400	5.53579200
H	-3.65539600	-1.40246500	4.47982300	H	9.22066600	6.58191100	0.94385000
H	-3.49091400	0.31576600	4.07724800	H	9.68386000	5.24428200	1.44383700
H	-2.33875000	-0.75083500	6.70975100	H	7.70317000	7.68179100	3.40446500
H	-4.02927800	-0.35092200	6.58053900	H	8.48984100	6.41459800	3.02227100
H	7.59834200	3.80631400	-2.57286700	O	4.15106400	5.09535900	3.96542500
H	5.92019100	3.37744200	-2.87603400	H	4.22467800	4.16070300	4.27112400
H	4.18048100	3.43916800	-0.54371100	H	-2.98434800	5.61642900	6.12478800
H	6.82687600	5.78613900	1.74958200	H	-2.07913400	-0.71727800	4.26022700
H	3.36785800	-0.49651300	0.82343300	H	-0.26620000	-0.00681400	0.37574100
H	3.33445600	1.25599200	0.53989000	H	4.82332400	0.44603500	1.00300900
H	3.95013200	0.04909800	3.30426100	H	6.99000000	2.23665300	-2.11746100
H	2.33300400	0.52665400	2.78218600	H	9.55110500	0.50982400	3.20287000
H	-4.23017600	8.79168600	-0.52096700	H	6.99521100	10.85164700	5.07142400
H	-2.51996100	9.20167000	-0.69763400	H	4.25203000	11.52439800	1.80645800
H	-0.94993000	7.19160500	0.43698400	H	-0.68921400	10.71776100	3.55305800
H	-3.29291300	6.43932200	3.84470900	H	-3.49510800	9.99478200	0.51987300
H	0.78160500	11.66017800	3.40486500	H	-4.92745800	10.09566000	6.72903400
H	0.57820900	10.15512600	2.48051300	O	1.06988200	6.17489700	1.56489700
H	0.78102200	10.30253700	5.56063300	O	2.10226500	5.37725100	1.10613000
H	2.09790500	9.86422400	4.49546300	C	0.39082500	6.48502200	9.34770500
H	8.22258500	1.08940000	4.23558300	N	1.32065700	7.55005100	8.97944100
H	8.21779700	1.41449600	2.49386300	C	2.73266500	7.18031600	9.06804400
H	10.30553600	2.44940300	4.50449400	C	3.23295300	6.14017600	8.04626500
H	10.38595800	2.74049500	2.77000200	C	4.75597000	5.94215100	8.08006600
H	3.09034900	10.88300600	0.65098700	C	5.23231700	5.12204000	6.88024200
H	4.82034400	10.85163900	0.29341100	N	6.72003800	5.16878500	6.72173300
H	2.83288200	7.99276700	0.59306500	H	0.53774300	6.22045000	10.40277600
H	5.32937800	7.23723100	3.88525300	H	0.46805500	5.55387200	8.76505200
H	8.61547000	11.51925600	5.09297500	H	1.12462200	7.84762700	8.02445400
H	8.23074300	10.13481200	4.05415000	H	3.32637300	8.09714700	8.94236800
H	8.22164400	10.07655400	7.13891200	H	2.92826000	6.82658500	10.09125500
H	9.45207400	9.36469800	6.11925600	H	2.72760800	5.17869200	8.20073000
H	-3.36431700	9.38799200	7.01859500	H	5.06083100	5.46706100	9.02408100
H	-4.17911200	9.11050900	5.48008400	H	5.25316300	6.91978800	8.04800100
H	-5.35223700	8.19342200	8.18649300	H	4.80024800	5.51942800	5.96050100
H	-5.94310400	7.75998100	6.58207800	H	4.95237000	4.06708700	6.94530200

H	7.16512800	4.54671100	7.39628200	C	9.69467200	2.57916800	3.41871900
H	7.03895000	4.82832500	5.78696600	C	8.97228400	3.88162600	3.76744800
H	-0.63779700	6.84519900	9.24347400	O	9.29369000	4.90302200	3.09312700
H	2.94288800	6.48436200	7.04539100	O	8.15825000	3.85750600	4.73184900
H	7.10628200	6.18313300	6.86130800	C	4.05793500	10.72610400	1.08084500
H	-4.54091100	8.11195500	2.41777600	C	4.21416500	9.38147900	1.72111700
H	5.59778900	9.63851000	3.32594000	N	5.07587600	9.11892900	2.77954400
H	8.15293300	4.92715800	-0.10784600	C	3.64762500	8.16734700	1.42651500
H	-1.32079800	0.81191400	2.59902000	C	5.01255700	7.80153200	3.07870600
Int C				N	4.15872800	7.19852300	2.26727300
C	-0.11698500	0.99112600	-0.00014900	C	8.01612800	10.58506700	5.01126400
C	-0.33698800	1.98967800	1.09684700	C	8.38921100	9.73114900	6.21591200
N	-1.02660200	1.69779100	2.26700200	C	7.72546500	8.34714900	6.21902600
C	0.03980000	3.29792400	1.23780700	O	7.08365800	7.98678600	5.19612600
C	-1.03896100	2.79915800	3.05695700	O	7.90019300	7.66381500	7.27348600
N	-0.40167100	3.79049000	2.45374800	C	-4.35862400	9.22912300	6.55006300
C	-3.07782800	-0.50157500	4.64513600	C	-5.18297700	8.01847000	7.02916100
C	-3.08367800	-0.16705500	6.13894100	C	-4.40073800	6.71764600	7.10480800
C	-2.86517000	1.31415800	6.50270100	O	-4.31999200	6.06758400	8.13794700
O	-2.78945800	2.14276400	5.52902500	O	-3.83316800	6.37908700	5.95430500
O	-2.81745300	1.58027400	7.72188100	Fe	3.82749800	5.06788000	2.43066000
C	6.70671100	3.27727000	-2.17077900	Fe	0.13313100	5.83701400	3.04331100
C	6.31190300	3.91283400	-0.87486400	O	-0.07143500	5.43252100	5.00113800
N	7.14285500	4.72728200	-0.11892800	O	-2.17214900	4.50045600	6.17842700
C	5.09658100	3.95808900	-0.24004800	O	-2.27675800	4.04118500	8.72291100
C	6.43420300	5.22535100	0.91096800	O	6.61422000	1.96990100	6.09146600
N	5.18185400	4.78031700	0.86506900	O	9.58330500	5.77349300	0.55297200
C	3.73563500	0.46702900	1.14584500	O	8.17369300	7.28453200	2.68304000
C	3.41074300	0.74568600	2.61668900	H	0.91279100	1.03428000	-0.36385700
C	3.81596200	2.15237500	3.05202200	H	-0.78374100	1.16249200	-0.85392200
O	3.42665100	3.09383800	2.25491400	H	0.62124000	3.92746800	0.58370400
O	4.45266000	2.31271000	4.10857400	H	-1.51000300	2.79618600	4.03077200
C	-3.34290400	9.06301800	0.02592100	H	-3.67388400	-1.40077300	4.44416100
C	-2.87457400	8.04556400	1.00367900	H	-3.51751000	0.32672500	4.08229800
N	-3.58698300	7.69310200	2.14101400	H	-2.34268900	-0.75453900	6.69178900
C	-1.72033500	7.31660300	1.07355900	H	-4.05231800	-0.43807900	6.57718400
C	-2.85663300	6.79516700	2.84839400	H	7.57240300	3.79715800	-2.59570300
N	-1.72214000	6.54878800	2.21884600	H	5.89128700	3.38969500	-2.89395200
C	0.35514700	10.64327300	3.42699000	H	4.17580500	3.45839800	-0.49778800
C	0.97403400	9.86132300	4.59392800	H	6.85660300	5.90099500	1.64902800
C	0.59509300	8.38087200	4.66165300	H	3.33463800	-0.50463800	0.83345000
O	0.38274400	7.80074600	3.53499100	H	3.29745800	1.24230600	0.51279600
O	0.54225200	7.81702500	5.77887100	H	3.89879200	0.02650100	3.27961500
C	8.83486700	1.30890600	3.35409500	H	2.32780700	0.66238500	2.77595700

H	-4.26802400	8.76116200	-0.48176900	H	6.98174900	10.85914600	5.02421600
H	-2.57987700	9.21281500	-0.74127300	H	4.23036700	11.53006700	1.76576900
H	-0.87337600	7.31477400	0.40454000	H	-0.70681500	10.72934400	3.52654900
H	-3.16988800	6.40302600	3.80508700	H	-3.52136300	10.00486100	0.50174000
H	0.76896500	11.65709300	3.38376800	H	-4.93703400	10.11434100	6.71459700
H	0.56926800	10.13875700	2.48195000	O	1.93684500	5.47895400	2.54558500
H	0.73038600	10.31250700	5.56029100	O	1.20918400	5.98385900	1.38669700
H	2.06876400	9.88316800	4.50705400	C	0.57783000	6.04394200	9.12800000
H	8.29738500	1.12780000	4.28759700	N	1.43515400	7.20574700	8.90997900
H	8.10548700	1.35612000	2.53833200	C	2.86637600	6.94091300	9.03553100
H	10.46171900	2.44081000	4.19456300	C	3.49602900	6.00947100	7.98101000
H	10.23147800	2.72258300	2.47538400	C	5.02168800	5.88511300	8.11815600
H	3.04673500	10.83629600	0.67960700	C	5.61921700	5.13067600	6.93154200
H	4.75899900	10.86014800	0.24656300	N	7.11340600	5.20048600	6.89810200
H	2.88311800	7.92545100	0.70415200	H	0.72681100	5.66495600	10.14698300
H	5.58370600	7.34345600	3.87186100	H	0.73509500	5.19792400	8.43868200
H	8.59564700	11.51709800	4.99120600	H	1.24311600	7.59244600	7.98684500
H	8.22141300	10.04503800	4.08255100	H	3.39005500	7.90699700	8.99868800
H	8.13819900	10.22914700	7.15962800	H	3.04715700	6.53346600	10.04160600
H	9.47403000	9.56688600	6.24744100	H	3.03763100	5.01403100	8.03223400
H	-3.42788400	9.32086100	7.11788500	H	5.27675000	5.38625500	9.06515700
H	-4.09833500	9.14933000	5.49154700	H	5.47280000	6.88461500	8.15874500
H	-5.58358400	8.20023600	8.02922900	H	5.27954100	5.57093200	5.99457400
H	-6.03632100	7.86569600	6.35508400	H	5.34942100	4.07112500	6.92003200
H	-0.85768400	5.00230400	5.46641500	H	7.51735800	4.59914500	7.61561100
H	0.17246400	6.29125900	5.47865300	H	7.47878300	4.85531300	5.97931100
H	-2.48166400	3.54264900	5.91377500	H	-0.47215900	6.33788500	9.04329500
H	-2.02910700	4.40977700	7.17736800	H	3.25686600	6.40526600	6.98489700
H	-3.10664000	4.54558800	8.77092700	H	7.45125700	6.23084600	7.04662000
H	-2.52565300	3.11147900	8.47844000	H	-4.49144600	8.04614900	2.41461000
H	5.85074200	1.88362200	5.49857300	H	5.69731100	9.75862700	3.25414000
H	7.22230400	2.54169600	5.58115200	H	8.14963000	4.96875500	-0.18754700
H	9.24763500	6.61827000	0.90038900	H	-1.45124100	0.81823300	2.52355900
H	9.67588800	5.26585900	1.39537400	TS _{CD}			
H	7.81920700	7.69440900	3.49575700	C	-0.11696900	0.99111600	-0.00014100
H	8.55432600	6.43726200	3.02172000	C	-0.28915200	2.00419500	1.09044500
O	4.63789800	4.99725200	4.03075400	N	-1.04712900	1.79726700	2.23584700
H	4.72692100	4.04619500	4.28725000	C	0.21060400	3.27002600	1.23443600
H	-3.20620600	5.55222100	6.07710300	C	-0.97780600	2.90529800	3.01326200
H	-2.10360000	-0.70371700	4.25124200	N	-0.22402300	3.82191100	2.42539600
H	-0.30051100	0.00065800	0.36106300	C	-3.07782500	-0.50157200	4.64513200
H	4.79102200	0.45036600	0.97418500	C	-3.07868200	-0.15595800	6.13409600
H	6.95072300	2.23552300	-2.15423700	C	-2.85855200	1.32923900	6.46287300
H	9.52470900	0.51316300	3.16129900	O	-2.80724000	2.12980400	5.46221000

O	-2.78752600	1.63019800	7.67170000	Fe	3.67294900	5.08958100	2.41597600
C	6.70670600	3.27725700	-2.17076800	Fe	0.49361000	5.80371600	3.06684000
C	6.18684600	3.92074100	-0.92445900	O	-0.36635000	5.59174700	4.84881800
N	6.95661000	4.78484500	-0.16427800	O	-2.30356100	4.49389200	6.04331600
C	4.93457100	3.96652100	-0.35849700	O	-2.25141800	4.11622000	8.60388600
C	6.18600500	5.30348000	0.80560700	O	6.64265700	2.49622500	6.19652800
N	4.94238400	4.83558800	0.71554300	O	9.45958100	5.80721600	0.27550400
C	3.73565000	0.46704600	1.14584100	O	8.14749300	7.25252700	2.41527000
C	3.41888900	0.74358700	2.61995700	H	0.90290200	1.02470800	-0.39094600
C	3.83959000	2.15585800	3.01585200	H	-0.80376200	1.16776700	-0.83742000
O	3.36198500	3.07817400	2.25165900	H	0.89348500	3.80709700	0.59797500
O	4.59381700	2.33239800	3.99308800	H	-1.46693300	2.95757000	3.97476400
C	-3.34292600	9.06303100	0.02594300	H	-3.66999100	-1.40553000	4.45315000
C	-2.69035100	8.08659100	0.95456200	H	-3.52418500	0.31970300	4.07803900
N	-3.27940700	7.65861000	2.13578200	H	-2.33470400	-0.73520800	6.69137200
C	-1.47710000	7.44471600	0.92631000	H	-4.04582900	-0.41933500	6.58036800
C	-2.42981900	6.80769000	2.76232800	H	7.61266300	3.79972600	-2.49701300
N	-1.32695800	6.65532700	2.05013600	H	5.97658200	3.39947100	-2.98020200
C	0.35514200	10.64327800	3.42699000	H	4.03982000	3.43623200	-0.64665300
C	0.99697200	9.88754600	4.59538000	H	6.57373600	5.99124200	1.54713400
C	0.62446300	8.41039000	4.63332200	H	3.33410200	-0.50411400	0.83201600
O	0.71886600	7.78314500	3.51502600	H	3.29675500	1.24533200	0.51774700
O	0.26210700	7.89809000	5.71920600	H	3.91857600	0.02913600	3.27930400
C	8.83487100	1.30892000	3.35408400	H	2.33762500	0.66192700	2.78725500
C	9.66675500	2.59992400	3.38109100	H	-4.30102600	8.68829200	-0.35484500
C	8.88279000	3.90924300	3.52660400	H	-2.69315700	9.23978200	-0.83444500
O	9.24504800	4.86062100	2.76996600	H	-0.70036800	7.51138300	0.17896500
O	7.97942600	3.97609600	4.39948600	H	-2.63254900	6.37124000	3.72784600
C	4.05792800	10.72608900	1.08083500	H	0.75896200	11.65997800	3.36038300
C	4.20177500	9.38661200	1.71966600	H	0.57096800	10.12803000	2.48778200
N	5.14138100	9.08997000	2.69716400	H	0.73359800	10.33080200	5.55920200
C	3.55540200	8.20086600	1.48586700	H	2.08886500	9.93407500	4.49714600
C	5.04531500	7.77743500	3.00399500	H	8.31438000	1.13630200	4.29916700
N	4.09348600	7.21416800	2.28300200	H	8.08902800	1.32938900	2.55226800
C	8.01612000	10.58507100	5.01127000	H	10.36568700	2.55243500	4.22839800
C	8.35090000	9.63220400	6.15892200	H	10.27938700	2.67146400	2.47668900
C	7.62442400	8.28038700	6.06068700	H	3.04968800	10.84156800	0.67362100
O	7.11478600	7.97950200	4.94258900	H	4.76393300	10.85750400	0.24976400
O	7.60042700	7.56743600	7.10348200	H	2.73499500	7.99408600	0.81682100
C	-4.35863400	9.22913200	6.55004600	H	5.68121700	7.29838700	3.72924300
C	-5.23019200	8.02719200	6.96370500	H	8.60064900	11.51150600	5.07985900
C	-4.47644400	6.71203200	7.00487700	H	8.24037000	10.11679000	4.04908200
O	-4.33957800	6.07152200	8.03852200	H	8.11795300	10.07532800	7.13347800
O	-3.99059200	6.35380500	5.82267100	H	9.42861500	9.42181800	6.17467400

H	-3.45250800	9.29011200	7.15975200	H	4.70758500	5.40161100	8.58173300
H	-4.05879300	9.17114200	5.50070500	H	5.02238900	7.06323100	8.08467500
H	-5.64583200	8.18628400	7.96148000	H	4.66038400	6.49025200	5.71244600
H	-6.06865300	7.92523400	6.26281800	H	4.28121100	4.82606200	6.11830700
H	-1.09910300	5.06027100	5.31553900	H	6.49540700	4.41834900	6.69590900
H	-0.15078600	6.43826700	5.36723600	H	6.57753300	5.27032600	5.31841100
H	-2.57233600	3.50435500	5.80664600	H	-0.88442400	6.84408000	9.31176500
H	-2.11623900	4.44045400	7.03751600	H	2.65732500	6.96981600	6.92983400
H	-3.08888400	4.60469400	8.67880000	H	6.90243900	6.15366500	6.71131500
H	-2.49122300	3.17588400	8.39706300	H	-4.18280500	7.93184300	2.49272500
H	5.87582800	2.25594500	5.65161500	H	5.83111600	9.69695000	3.11751500
H	7.26875700	2.86277200	5.52645500	H	7.96435200	5.04727100	-0.22419500
H	9.14076900	6.63273400	0.68540600	H	-1.55157300	0.96179000	2.49673300
H	9.61300100	5.26762000	1.08773000	Int D _{diamond}			
H	7.89728300	7.69092900	3.25052800	C	-0.11696700	0.99112600	-0.00014400
H	8.49418800	6.37567300	2.72435500	C	-0.24885000	2.01872700	1.07230400
O	4.99303900	4.93517100	3.62182700	N	-0.87841400	1.81987200	2.29310300
H	5.06572200	3.97426600	3.86565500	C	0.21971100	3.30140900	1.12630900
H	-3.37286400	5.52511200	5.93158700	C	-0.76254000	2.95290900	3.02729600
H	-2.10360500	-0.70372000	4.25124700	N	-0.10194300	3.86973300	2.33939400
H	-0.30052600	0.00066400	0.36105600	C	-3.07782800	-0.50157100	4.64513500
H	4.79101200	0.45035100	0.97418900	C	-3.63684600	0.02603800	5.96113700
H	6.95072600	2.23553400	-2.15424400	C	-3.35121000	1.51551900	6.19282600
H	9.52470800	0.51315600	3.16130800	O	-3.02586100	2.18266300	5.14677200
H	6.98175700	10.85914300	5.02421000	O	-3.47927200	1.94585100	7.35736400
H	4.23037500	11.53007700	1.76577900	C	6.70669400	3.27727000	-2.17078000
H	-0.70681000	10.72934100	3.52654700	C	6.11513000	3.91074700	-0.93897400
H	-3.52134200	10.00485200	0.50171900	N	6.85735200	4.74466900	-0.11810000
H	-4.93702400	10.11433000	6.71461000	C	4.83246200	3.97732900	-0.43546100
O	1.86758400	5.60910100	1.75847600	C	6.04421000	5.26248000	0.81935000
O	2.19895500	5.29674200	3.58619900	N	4.79771900	4.82585900	0.65859600
C	0.15872700	6.51796000	9.36636500	C	3.73564200	0.46705300	1.14584500
N	1.03835100	7.64017400	9.04096500	C	3.37884300	0.81069400	2.59671400
C	2.46412600	7.30642900	9.03652000	C	3.72321000	2.25409400	2.93854700
C	2.93945000	6.44531900	7.85289000	O	3.16408300	3.14277200	2.19648400
C	4.45110800	6.16135700	7.83072200	O	4.51427400	2.49146700	3.88059300
C	4.85680600	5.69818700	6.43356300	C	-3.34291500	9.06301900	0.02593000
N	6.30333200	5.35759700	6.31023800	C	-2.57846800	8.09514200	0.89362300
H	0.34661700	6.19440000	10.39782000	N	-3.14429500	7.47876100	2.00173700
H	0.25262600	5.63045900	8.72145600	C	-1.29401700	7.59630700	0.85261700
H	0.78653100	7.99165600	8.11776900	C	-2.22136200	6.66713000	2.56820600
H	3.03615000	8.24571100	9.03405700	N	-1.08379900	6.71057200	1.89786200
H	2.69871400	6.80822200	9.98792400	C	0.35514800	10.64327600	3.42698800
H	2.39161700	5.49509900	7.83519000	C	1.01135400	9.88761900	4.58761300

C	0.72226400	8.39039000	4.55318900	H	3.34675400	-0.52273100	0.87891600
O	0.93005700	7.81563800	3.42796400	H	3.29259500	1.20197500	0.46890000
O	0.30602600	7.82769100	5.59739300	H	3.89494300	0.15456600	3.30205900
C	8.83487000	1.30891700	3.35409300	H	2.29904500	0.68891100	2.74375500
C	9.65269900	2.60580900	3.37714800	H	-4.31122400	8.64545100	-0.27400600
C	8.86496700	3.88678800	3.66205900	H	-2.77464100	9.25823700	-0.88728900
O	9.18162600	4.91043700	2.99347200	H	-0.50975800	7.81934400	0.14461400
O	7.99330500	3.84364800	4.57597900	H	-2.40861900	6.10322900	3.46349700
C	4.05792600	10.72608900	1.08082700	H	0.75138200	11.66365300	3.36136000
C	4.14664300	9.38402000	1.72382400	H	0.57242100	10.13353300	2.48515400
N	4.98514200	9.07410000	2.78736200	H	0.69744000	10.27887800	5.55870700
C	3.51716400	8.20743400	1.41819500	H	2.10042600	10.00130700	4.51933800
C	4.85271700	7.76298300	3.07652100	H	8.31679300	1.13455300	4.29981400
N	3.97137000	7.21515600	2.25792200	H	8.08512300	1.32485800	2.55555000
C	8.01612700	10.58506300	5.01127500	H	10.41703400	2.53021700	4.16408600
C	8.34655500	9.64487200	6.16470500	H	10.19252700	2.73648000	2.43380700
C	7.58312400	8.31454500	6.10590700	H	3.06614200	10.86620500	0.64224200
O	6.91942200	8.05522200	5.06326700	H	4.79193100	10.83610300	0.27137400
O	7.69476000	7.56961800	7.12401900	H	2.76023700	8.00627000	0.67729000
C	-4.35863200	9.22912300	6.55006400	H	5.41673700	7.27271000	3.85184300
C	-5.37005500	8.15894900	6.07771200	H	8.60475200	11.50940700	5.06795100
C	-4.77584600	6.77431500	6.17663800	H	8.23308600	10.10779200	4.05122100
O	-4.75724700	6.16976200	7.24092400	H	8.13939100	10.10925000	7.13584300
O	-4.24328500	6.33934600	5.04353600	H	9.41754200	9.40467400	6.17357400
Fe	3.41899400	5.18055400	2.36090800	H	-3.89596600	8.93132200	7.49419000
Fe	0.76595000	5.80347200	2.90528500	H	-3.57386400	9.41416800	5.81294800
O	-0.29973200	5.60209200	4.59322100	H	-6.24610500	8.18402300	6.73221500
O	-2.50595600	4.58507400	5.49259200	H	-5.69583600	8.36793600	5.05363200
O	-2.69401900	4.41328100	8.07467000	H	-1.13260500	5.13438600	4.90397100
O	6.49728800	2.05960900	6.05349100	H	-0.09126500	6.42257200	5.16172400
O	9.32025800	5.82118000	0.45358400	H	-2.77268100	3.57429400	5.33536400
O	7.94698200	7.24031200	2.55540800	H	-2.41783200	4.61363300	6.50330100
H	0.89235600	1.00894600	-0.42034900	H	-3.51333500	4.93814000	8.05008400
H	-0.81953500	1.16642900	-0.82494500	H	-2.98988500	3.47504300	7.93255100
H	0.80879200	3.84375200	0.40545300	H	5.75125400	1.96014100	5.44148000
H	-1.16675700	3.03751500	4.02246700	H	7.13838000	2.56457500	5.51198400
H	-3.32441900	-1.55969100	4.49468800	H	8.95765500	6.63690200	0.84617000
H	-3.48163700	0.07151800	3.80575100	H	9.49823400	5.30522300	1.27434800
H	-3.24270500	-0.52755600	6.81954600	H	7.66371100	7.69955500	3.36857300
H	-4.72703100	-0.10494700	5.99240500	H	8.32736600	6.39572900	2.90064300
H	7.62745400	3.80715800	-2.43769600	O	4.77372500	4.98762000	3.44289500
H	6.02042100	3.41125300	-3.01556300	H	4.79865900	4.01347100	3.74192200
H	3.94185800	3.47802200	-0.78633500	H	-3.62127000	5.52222700	5.23582600
H	6.40425300	5.93216400	1.59006400	H	-1.98559900	-0.40967500	4.62383600

H	-0.30052800	0.00065500	0.36106000	C	-3.07782900	-0.50157200	4.64513500
H	4.79102100	0.45034600	0.97418600	C	-3.72339800	-0.11454700	5.97471600
H	6.95073800	2.23551900	-2.15423700	C	-3.43514400	1.33112400	6.41322500
H	9.52470900	0.51315400	3.16130100	O	-3.12324000	2.14475100	5.47323800
H	6.98175000	10.85914800	5.02420800	O	-3.55203300	1.59366600	7.62769700
H	4.23037600	11.53007700	1.76578500	C	6.70670000	3.27726300	-2.17077900
H	-0.70681700	10.72934300	3.52654800	C	6.15510000	3.88516700	-0.90865500
H	-3.52135100	10.00486200	0.50172900	N	6.89818900	4.71408300	-0.08130300
H	-4.93702800	10.11434000	6.71459700	C	4.88591500	3.90703300	-0.37718600
O	1.83826200	5.70313200	1.48481600	C	6.09300600	5.19890300	0.88112000
O	2.17881900	5.29631200	3.75908700	N	4.85398600	4.73341200	0.73382100
C	0.29229600	5.91226700	9.00974700	C	3.73563500	0.46705900	1.14584800
N	1.07605600	7.11365200	8.73485100	C	3.36090100	0.74832300	2.60228500
C	2.52177300	6.91376600	8.77924500	C	3.57601300	2.20152300	3.01231100
C	3.13090300	6.02380100	7.67786800	O	3.10072600	3.07988100	2.18645900
C	4.65768800	5.90515900	7.78313400	O	4.14978400	2.45499700	4.08673900
C	5.25004000	5.19142600	6.57029200	C	-3.34292000	9.06301600	0.02593200
N	6.74380900	5.17663600	6.60261200	C	-2.71463000	8.06840200	0.95259400
H	0.48906900	5.57798800	10.03708100	N	-3.40827000	7.51975300	2.02099600
H	0.48541500	5.05529100	8.34303500	C	-1.45982800	7.51456600	1.03922900
H	0.81802000	7.48290300	7.82072300	C	-2.58145200	6.68942600	2.69901900
H	3.00252200	7.90155900	8.73079000	N	-1.39040400	6.66368600	2.12634600
H	2.77449700	6.49934000	9.76685200	C	0.35516500	10.64329400	3.42698400
H	2.68256000	5.02334600	7.70987900	C	0.96241100	9.88409100	4.61635200
H	4.92890100	5.37163600	8.70627200	C	0.50633300	8.42995500	4.63367700
H	5.10959000	6.90254400	7.85598900	O	0.70670600	7.77522300	3.56273700
H	4.96339800	5.69883200	5.64999200	O	-0.05387600	7.97312300	5.67305500
H	4.92294200	4.15160800	6.49547000	C	8.83486700	1.30891500	3.35408700
H	7.06557700	4.49449600	7.28947800	C	9.66119500	2.59315300	3.49008200
H	7.15017300	4.85953800	5.69045800	C	8.85269900	3.84291900	3.83947400
H	-0.77500300	6.13349600	8.93462300	O	9.07896700	4.88616600	3.16453300
H	2.86118900	6.44591000	6.70084400	O	8.04661700	3.74610300	4.80856800
H	7.13958900	6.16705100	6.82959000	C	4.05792700	10.72609200	1.08083000
H	-4.07334200	7.60822300	2.37508000	C	4.09356700	9.37069300	1.70350600
H	5.64770900	9.66557800	3.27021500	N	4.82842800	9.02706400	2.82941100
H	7.86521000	5.00537700	-0.12797600	C	3.50227200	8.19995300	1.30405000
H	-1.37439200	0.99820300	2.60868900	C	4.66781400	7.70733600	3.06400400
Int D _{open2}				N	3.87199400	7.17622800	2.14857800
C	-0.11697900	0.99112100	-0.00015300	C	8.01612000	10.58505800	5.01126800
C	-0.44255000	1.98277200	1.07466400	C	8.31996500	9.62796900	6.15466500
N	-1.13766200	1.65897600	2.23184400	C	7.48558700	8.34019600	6.10601200
C	-0.12868400	3.30591500	1.22515100	O	6.76346000	8.12671000	5.09296600
C	-1.20670800	2.75995800	3.02393300	O	7.61275700	7.58328400	7.11431400
N	-0.60181700	3.77774300	2.43357500	C	-4.35863200	9.22912100	6.55004600

C	-5.03725200	8.08092000	7.31850800	H	8.61287600	11.50298800	5.08153600
C	-4.27112700	6.76963400	7.34443600	H	8.22937800	10.11508300	4.04667100
O	-4.04464100	6.17531900	8.39064300	H	8.15053000	10.09870400	7.13026300
O	-3.90917800	6.34579000	6.14119300	H	9.37650100	9.33117900	6.14836700
Fe	3.38358800	5.07209100	2.26302800	H	-3.34054600	9.40274300	6.91039800
Fe	0.28010700	5.72363800	3.20460300	H	-4.30564300	9.01908400	5.47877300
O	-0.88953700	5.83545400	4.75674700	H	-5.20440400	8.36240200	8.36100400
O	-2.28295000	4.37224800	6.24064000	H	-6.02160100	7.87868400	6.87452800
O	-2.41343500	3.79755200	8.77633800	H	-1.27695500	5.11368300	5.36724400
O	6.36812200	1.78510200	5.93616600	H	-0.56699800	6.69129800	5.28617000
O	9.30498400	5.79839500	0.62560400	H	-2.67930000	3.45874200	5.92155500
O	7.82732600	7.19320200	2.65779000	H	-2.10324500	4.21336800	7.21902400
H	0.93524800	1.05901000	-0.28800900	H	-3.09354200	4.48780600	8.86616900
H	-0.72548200	1.13608700	-0.90097300	H	-2.89044300	2.98224700	8.47978500
H	0.45143100	3.93764500	0.57302000	H	5.60379600	1.83273000	5.33885300
H	-1.69955300	2.74216200	3.98698800	H	7.01489500	2.38489500	5.51671400
H	-3.34482000	-1.52369200	4.35013200	H	8.92359900	6.61378400	1.00119600
H	-3.40668600	0.18464300	3.85877400	H	9.44257900	5.28258400	1.45559000
H	-3.40286800	-0.77713600	6.78466700	H	7.49226700	7.67751000	3.43754000
H	-4.81468200	-0.22297700	5.90639300	H	8.21547600	6.37404600	3.04945900
H	7.61598100	3.81095000	-2.46637200	O	4.09742300	5.10785000	3.91978400
H	5.98681700	3.41161000	-2.98603000	H	4.17205800	4.16440500	4.21733700
H	4.00192100	3.38909400	-0.71709900	H	-3.32088100	5.50317500	6.22221800
H	6.44785700	5.88391800	1.64534500	H	-1.98518600	-0.44865400	4.70994300
H	3.34897300	-0.51025700	0.83136200	H	-0.30051700	0.00065700	0.36106400
H	3.29757500	1.22876300	0.49615000	H	4.79102800	0.45034200	0.97418400
H	3.91403000	0.11039400	3.29601900	H	6.95073300	2.23552500	-2.15423800
H	2.29217600	0.54204300	2.74675200	H	9.52470900	0.51315800	3.16130600
H	-4.29643100	8.69647200	-0.37298000	H	6.98175400	10.85915300	5.02421400
H	-2.68086900	9.24311300	-0.82483800	H	4.23037400	11.53007400	1.76578200
H	-0.60144300	7.68278000	0.40693800	H	-0.70682600	10.72932700	3.52655100
H	-2.85531900	6.17966700	3.60783100	H	-3.52134700	10.00486400	0.50172600
H	0.76569800	11.65729800	3.36063400	H	-4.93702600	10.11434000	6.71461100
H	0.57802400	10.11636200	2.49635800	O	1.50508900	5.56563000	2.02729100
H	0.69536000	10.34917600	5.56879900	O	1.34744500	4.97437500	4.33344600
H	2.05551200	9.88433200	4.53194800	C	0.27654300	5.88290700	8.89898400
H	8.25858900	1.09477800	4.25686100	N	1.13137200	7.03583900	8.63705800
H	8.13503800	1.37449500	2.51315900	C	2.56306800	6.78544900	8.75665100
H	10.39399700	2.45859200	4.29821400	C	3.20500200	5.78793100	7.76844500
H	10.23021500	2.78444800	2.57472700	C	4.73176200	5.73368100	7.93016400
H	3.08433300	10.89617300	0.61165800	C	5.41315000	4.90125700	6.84463500
H	4.81631500	10.82320200	0.29208400	N	6.89772000	5.09158200	6.85957900
H	2.82601700	8.03709900	0.47823200	H	0.43759500	5.53163700	9.92597700
H	5.13841300	7.19245500	3.88473200	H	0.42498000	5.01708000	8.23269400

H	0.91906400	7.41269000	7.71494400	C	-2.38614100	6.70274600	2.65620900
H	3.07826300	7.75094000	8.65027100	N	-1.22950100	6.68663900	2.02121100
H	2.75973600	6.44767600	9.78584500	C	0.35514400	10.64327200	3.42699300
H	2.77755500	4.78689000	7.90567100	C	0.94296200	9.88128800	4.61672700
H	4.98925900	5.34231400	8.92626100	C	0.45220800	8.44632700	4.54769200
H	5.13782900	6.75216400	7.88374000	O	0.90803300	7.77112900	3.57079900
H	5.08218900	5.21843200	5.85576000	O	-0.39086900	8.04336700	5.39834400
H	5.22162100	3.82796800	6.92943900	C	8.83484700	1.30892200	3.35407700
H	7.31587200	4.61016500	7.65504100	C	9.18329500	1.97730300	4.68844900
H	7.33405800	4.69093500	5.99093400	C	8.59272300	3.38470500	4.84239200
H	-0.77333700	6.17969900	8.82102000	O	8.75993700	4.18426200	3.88717900
H	2.95930400	6.08753000	6.74137000	O	8.01352500	3.63258500	5.94721200
H	7.15793800	6.15161600	6.92537100	C	4.05792700	10.72608900	1.08084200
H	-4.36378700	7.71590000	2.27802500	C	4.18222500	9.38510400	1.73100300
H	5.45661300	9.59139200	3.38691700	N	5.15104600	9.07010700	2.67763100
H	7.90455300	4.98456800	-0.07808900	C	3.48673000	8.21779300	1.54697900
H	-1.51899700	0.75834700	2.48294700	C	5.01880000	7.76771600	3.01759500
$TS_{DE} (Fe1^{III}Fe2^{IV}_{\alpha})$				N	4.01917400	7.22620100	2.34343800
C	-0.11697200	0.99111100	-0.00015000	C	8.01611900	10.58506000	5.01126800
C	-0.25138800	1.99957400	1.09832700	C	8.30333100	9.67472800	6.20707200
N	-1.00488600	1.80026100	2.24851900	C	7.42722700	8.41057500	6.18532500
C	0.28600600	3.24899000	1.25087900	O	7.06693300	7.98443600	5.05466800
C	-0.89372200	2.89966700	3.03545900	O	7.13902000	7.88906900	7.30137600
N	-0.11912500	3.79821500	2.45013100	C	-4.35857500	9.22916200	6.55008300
C	-3.07782700	-0.50157400	4.64512800	C	-4.71337200	8.18774200	7.62322700
C	-3.06021500	-0.14298500	6.13178700	C	-4.02594000	6.84478800	7.44417100
C	-2.79119000	1.34001300	6.41863200	O	-3.51485400	6.23760800	8.37872400
O	-2.94967200	2.12913100	5.42270100	O	-4.07131300	6.40977600	6.19378700
O	-2.48844700	1.65450600	7.59098200	Fe	3.59243600	5.11663100	2.56147500
C	6.70670100	3.27727600	-2.17077700	Fe	0.71592700	5.74032800	3.09282400
C	6.18168500	3.87569300	-0.90096500	O	-0.50630600	5.67986400	4.65807900
N	6.99369000	4.44821700	0.06374500	O	-2.43813700	4.49888400	5.85318800
C	4.89707100	4.10440800	-0.45889300	O	-1.60580600	4.04662900	8.35124700
C	6.20615500	4.97621300	1.02072700	O	5.97054800	1.71001300	6.43133700
N	4.91949200	4.78860300	0.74183500	O	9.47514300	4.85854500	1.23794000
C	3.73564500	0.46704300	1.14584700	O	8.27333700	6.66717400	2.95139300
C	3.40784100	0.77490000	2.61280200	H	0.89321400	1.01725900	-0.41588300
C	3.89188200	2.17433200	2.98231700	H	-0.82189600	1.17691700	-0.82069400
O	3.24896600	3.12915400	2.39911900	H	0.96621100	3.78549300	0.61072700
O	4.86111600	2.30478800	3.75596200	H	-1.38093400	2.96843500	3.99573300
C	-3.34292700	9.06300400	0.02591800	H	-3.66660900	-1.41058600	4.46806900
C	-2.64385100	8.08506500	0.92704200	H	-3.53334700	0.31352600	4.07830100
N	-3.26768700	7.52661900	2.03268300	H	-2.33658100	-0.73893200	6.69640800
C	-1.37892000	7.54087200	0.94330400	H	-4.03933300	-0.36169400	6.57876300

H	7.60751500	3.81070400	-2.49567800	O	5.08744500	4.99142400	3.60963800
H	5.96245300	3.40594500	-2.96454100	H	5.27236300	4.03245500	3.74849900
H	3.96693200	3.82410200	-0.93268600	H	-3.49269700	5.56738200	6.08705600
H	6.60354100	5.47501200	1.89314400	H	-2.10360300	-0.70372100	4.25124900
H	3.33246500	-0.50840400	0.84803300	H	-0.30052200	0.00066700	0.36106000
H	3.30170100	1.23336100	0.49727900	H	4.79101600	0.45035400	0.97418700
H	3.88217100	0.05036600	3.28017600	H	6.95073200	2.23551600	-2.15423600
H	2.32315400	0.73396100	2.76299500	H	9.52472300	0.51315300	3.16131500
H	-4.30586700	8.67076300	-0.32334100	H	6.98175700	10.85915100	5.02421400
H	-2.72743300	9.25114400	-0.85764400	H	4.23037700	11.53007800	1.76577500
H	-0.56457800	7.71260800	0.25487100	H	-0.70681500	10.72934400	3.52654600
H	-2.61943200	6.17138100	3.56388400	H	-3.52134300	10.00487400	0.50173900
H	0.76522000	11.65791000	3.35962200	H	-4.93707000	10.11430900	6.71457800
H	0.58345800	10.11678600	2.49732900	O	1.70984300	5.70880400	1.73568800
H	0.63835500	10.32913500	5.56662700	O	2.20275900	5.29355300	4.06563900
H	2.03593200	9.87727900	4.55709300	C	1.71932200	5.53308700	9.76054600
H	7.81171000	0.92099900	3.35979200	N	0.97819300	5.31458200	8.54990800
H	8.91742200	2.03055000	2.53710600	C	1.30120400	5.90700300	7.28516500
H	8.86323300	1.35875000	5.53115500	C	2.52114200	5.19221200	6.65851500
H	10.27386000	2.09344700	4.76084200	C	3.87101000	5.68722500	7.15759400
H	3.05345800	10.84630500	0.66614900	C	5.05166100	4.92717400	6.56799900
H	4.77133800	10.84808200	0.25441500	N	6.37244500	5.35633500	7.12039900
H	2.63168700	8.02299200	0.91935300	H	2.04432000	6.57874000	9.83028800
H	5.65045200	7.27327700	3.73802700	H	2.61852100	4.90066900	9.85556800
H	8.61550700	11.50313300	5.03901400	H	0.18637000	4.66924900	8.56918800
H	8.22661900	10.06215900	4.07517200	H	0.43767000	5.80556100	6.63731800
H	8.14449000	10.19495300	7.15737200	H	1.52239000	6.97661100	7.39665800
H	9.35342600	9.35237600	6.19863000	H	2.42311400	4.10151400	6.72720200
H	-3.29449500	9.48158000	6.57590400	H	3.88842500	5.59049300	8.25744800
H	-4.58535500	8.84235200	5.55372200	H	3.97403900	6.76143700	6.95175100
H	-4.46823500	8.54565100	8.62626500	H	5.10004800	5.10734500	5.49351500
H	-5.79567300	7.99866300	7.60312600	H	4.97368300	3.84687000	6.72798900
H	-1.24178500	5.09999900	5.01012600	H	6.47506000	5.06889100	8.09414900
H	-0.58109900	6.64321500	5.03984800	H	7.12229900	4.83787000	6.56711900
H	-2.73127800	3.49998200	5.67213900	H	1.07520200	5.31198600	10.61782700
H	-1.99548000	4.42715400	6.74129500	H	2.34392500	5.34298800	5.35811600
H	-2.33455400	4.63195900	8.62646400	H	6.57389300	6.41945100	7.08786500
H	-1.97801100	3.13430900	8.17864800	H	-4.20649700	7.71536700	2.34965500
H	5.56935700	1.75427600	5.54725300	H	5.85661900	9.66985200	3.08057600
H	6.74914400	2.29458700	6.34639000	H	8.02055600	4.46299700	0.19396400
H	9.24104200	5.74746500	1.57321000	H	-1.54058600	0.98089900	2.49625900
H	9.38102400	4.34415200	2.06709100	TS _{DE} (Fe ^{IV} Fe ^{III} _β)			
H	7.97490400	7.32626200	3.60637000	C	-0.11696100	0.99113500	-0.00014200
H	8.33341400	5.84109800	3.48300700	C	-0.26283600	2.00435200	1.09112400

N	-1.05914900	1.83831000	2.21824700	C	7.43284500	8.39132800	6.17787700
C	0.30665700	3.23776400	1.24877500	O	6.89333400	8.06746400	5.08327700
C	-0.94043200	2.94190900	2.99818300	O	7.33210600	7.76148600	7.26964500
N	-0.11875400	3.81069400	2.43047600	C	-4.35862200	9.22912000	6.55006800
C	-3.07782700	-0.50155300	4.64513100	C	-4.70583900	8.19077600	7.62736600
C	-3.61678900	-0.07271000	6.01021400	C	-4.01531500	6.84864400	7.44990000
C	-3.29626500	1.39326400	6.32936300	O	-3.51721800	6.24054300	8.39086900
O	-3.27762100	2.17190300	5.30883100	O	-4.04520300	6.42026600	6.19834800
O	-3.09919800	1.70906600	7.52134200	Fe	3.43400600	5.19518800	2.43801400
C	6.70670900	3.27726800	-2.17077000	Fe	0.68859500	5.76727700	3.05538800
C	6.13691700	3.89880000	-0.92666000	O	-0.57712400	5.62965100	4.65708900
N	6.91580300	4.59359600	-0.01617700	O	-2.50690900	4.44502000	5.84422400
C	4.84288900	4.06657800	-0.47841700	O	-1.76226100	3.92778100	8.34183100
C	6.10610200	5.12747000	0.91794600	O	6.40494200	1.54548100	5.95296300
N	4.83402900	4.83221000	0.67363700	O	9.39574200	5.27472400	0.97717300
C	3.73563800	0.46704600	1.14584500	O	8.05477300	6.98066000	2.79845800
C	3.40286700	0.83809200	2.59659500	H	0.89617500	1.02125300	-0.40788300
C	3.85378500	2.26039700	2.90037300	H	-0.81546700	1.17133200	-0.82761900
O	3.19354000	3.17783700	2.28772200	H	1.02709300	3.74577100	0.62999800
O	4.82398100	2.45135400	3.66730300	H	-1.45756000	3.04140400	3.94046700
C	-3.34293700	9.06299700	0.02593900	H	-3.32982900	-1.54384600	4.41670200
C	-2.64409500	8.07754000	0.90818700	H	-3.49425200	0.14000000	3.86369700
N	-3.26006300	7.49286600	2.00344600	H	-3.21759400	-0.69425500	6.81690600
C	-1.37977600	7.53729300	0.89980500	H	-4.70934400	-0.18722500	6.03316100
C	-2.37365500	6.65614000	2.59992500	H	7.62017300	3.80874700	-2.46063200
N	-1.22173200	6.65852800	1.95448200	H	5.99804600	3.40806000	-2.99683200
C	0.35516400	10.64330400	3.42697800	H	3.92707000	3.69216500	-0.91255200
C	0.97523600	9.85894100	4.58725100	H	6.48281800	5.71073300	1.74635900
C	0.51492900	8.40838800	4.56290000	H	3.34092600	-0.52487800	0.89681900
O	0.85985700	7.74648000	3.51817600	H	3.29383900	1.19558200	0.46034700
O	-0.17338600	7.97068300	5.51495200	H	3.89297600	0.15786100	3.29802700
C	8.83485400	1.30891900	3.35409200	H	2.31981000	0.78336800	2.75125500
C	9.63638200	2.36771800	4.13801700	H	-4.30803700	8.67593400	-0.32407800
C	8.83657500	3.63037600	4.44986500	H	-2.73215500	9.25587500	-0.86014100
O	8.77528600	4.50537800	3.54640500	H	-0.57306900	7.72953000	0.20775100
O	8.28556500	3.68566000	5.59385200	H	-2.59070100	6.10708600	3.50072400
C	4.05792600	10.72608500	1.08082900	H	0.76395100	11.65948100	3.37889500
C	4.13814300	9.38374800	1.73502200	H	0.57438400	10.14201400	2.48060200
N	5.01244000	9.07617300	2.77188700	H	0.70694000	10.29621900	5.55252500
C	3.48380200	8.20812000	1.47166500	H	2.06678300	9.86794100	4.49245800
C	4.87540700	7.77090800	3.08600000	H	7.99181700	0.94037600	3.94459800
N	3.95909400	7.22202100	2.30908200	H	8.46539300	1.71029800	2.40582500
C	8.01612500	10.58506100	5.01128000	H	9.98185600	1.93038000	5.08036200
C	8.30703500	9.65587400	6.18954700	H	10.51551600	2.65888600	3.55149200

H	3.06852400	10.86769800	0.63756700	C	5.34985500	4.79697200	6.39841000
H	4.79624900	10.82831200	0.27431200	N	6.63822900	5.23085800	7.01495600
H	2.70235500	7.99890600	0.75882400	H	1.14796600	6.35175700	9.65910000
H	5.45018300	7.28692700	3.85696600	H	2.71052900	5.51930900	9.69313500
H	8.61481600	11.50275600	5.05951400	H	0.36013100	4.21363500	8.47277800
H	8.23040700	10.08676500	4.06224900	H	0.68130300	5.01655500	6.47088900
H	8.16054200	10.16425200	7.14883200	H	1.50318400	6.37010100	7.23107200
H	9.35585600	9.33049200	6.17591100	H	2.84778600	3.70688100	6.42777300
H	-3.29533900	9.48578200	6.57349500	H	4.11568300	5.14421300	8.13630100
H	-4.58749300	8.83909000	5.55452000	H	4.10409800	6.47238200	6.97926400
H	-4.45797300	8.55299900	8.62820200	H	5.39428600	5.11755300	5.36012800
H	-5.78762800	7.99825000	7.61275300	H	5.34174000	3.70295600	6.41720300
H	-1.31299800	5.07423800	5.05123000	H	6.73230500	4.87200500	7.96535500
H	-0.51252000	6.52574700	5.13505800	H	7.40122700	4.78174000	6.42469900
H	-2.90552700	3.48467000	5.61229700	H	1.31799400	4.78673300	10.49369300
H	-2.08860800	4.30262800	6.73903300	H	2.64336000	5.10837700	5.26789100
H	-2.40117000	4.61252700	8.61370600	H	6.80268100	6.30466100	7.05192000
H	-2.28015200	3.09467200	8.19154700	H	-4.19723000	7.67153400	2.33112500
H	5.86167300	1.72172900	5.16677000	H	5.68455600	9.67191900	3.23518500
H	7.12921500	2.19625500	5.87996200	H	7.94246900	4.71193600	0.07561000
H	9.11993000	6.14968100	1.31036600	H	-1.62430200	1.03666100	2.45908300
H	9.34726300	4.75764600	1.81307700	Int E (Fe ^{III} Fe ^{IV} _α)			
H	7.74869400	7.56463300	3.51814400	C	-0.11697400	0.99111600	-0.00015000
H	8.21386800	6.12918000	3.26564100	C	-0.21969300	2.03176800	1.06307400
O	4.88084700	5.02882500	3.44228200	N	-0.83059900	1.84581300	2.29431600
H	5.03099500	4.04776300	3.59459300	C	0.21694400	3.32878400	1.08240000
H	-3.48541600	5.55894600	6.09234400	C	-0.74071000	2.99617800	3.00195600
H	-1.98559900	-0.40969200	4.62383900	N	-0.11358700	3.91429300	2.28426100
H	-0.30053300	0.00064700	0.36105800	C	-3.07782600	-0.50156500	4.64512800
H	4.79102400	0.45035000	0.97418400	C	-3.04712500	-0.04986200	6.10411800
H	6.95072500	2.23552100	-2.15424300	C	-2.68723100	1.42902900	6.32390600
H	9.52472000	0.51315400	3.16130100	O	-2.67625200	2.16868100	5.27718700
H	6.98175000	10.85914800	5.02420500	O	-2.48108500	1.78400700	7.50357600
H	4.23037500	11.53008100	1.76578600	C	6.70668800	3.27728500	-2.17078000
H	-0.70682700	10.72932100	3.52655400	C	6.26738600	3.92325100	-0.89455200
H	-3.52133200	10.00488000	0.50172300	N	7.06537800	4.80533000	-0.18380100
H	-4.93703700	10.11434000	6.71459300	C	5.05572900	3.93814500	-0.24751200
O	1.91706100	5.61079800	1.62705100	C	6.34757900	5.30706600	0.83550800
O	2.21801700	5.28492200	4.01407700	N	5.11386300	4.80590200	0.82552200
C	1.62853700	5.35708000	9.61268600	C	3.73564900	0.46704600	1.14584600
N	1.29650700	4.61008100	8.41540600	C	3.43324100	0.74767600	2.62418900
C	1.50209900	5.27278400	7.13878600	C	3.93476600	2.12520800	3.05390800
C	2.81520600	4.80099000	6.48598300	O	3.46858200	3.10286600	2.34305700
C	4.10399800	5.37748800	7.05862400	O	4.72423800	2.23187900	4.00861000

C	-3.34292100	9.06301100	0.02591900	H	-3.65094900	-1.43060600	4.53234200
C	-2.76715600	8.07941500	0.99295400	H	-3.55091300	0.26799600	4.02981900
N	-3.38101900	7.72473200	2.18837200	H	-2.36465300	-0.65698400	6.70819500
C	-1.58058600	7.39706200	0.99906300	H	-4.03840300	-0.18622700	6.55640800
C	-2.56314100	6.87254500	2.85875500	H	7.58947400	3.79633100	-2.55974800
N	-1.46636200	6.65674700	2.15746200	H	5.92400600	3.39222900	-2.93007700
C	0.35514600	10.64327100	3.42699300	H	4.15533200	3.38990300	-0.47712700
C	0.99921100	9.87325000	4.58173300	H	6.76018300	6.01064000	1.55212900
C	0.71316100	8.37829600	4.52165400	H	3.32821700	-0.50311900	0.83893400
O	0.71762100	7.86933900	3.35024800	H	3.29540100	1.24463500	0.51725900
O	0.50684500	7.75119800	5.59385000	H	3.89299500	-0.00371900	3.27141500
C	8.83485600	1.30891300	3.35408500	H	2.34919500	0.72277500	2.79037200
C	9.62663000	2.60516800	3.13582400	H	-4.28883100	8.71754700	-0.41008200
C	8.92072300	3.93176200	3.44542400	H	-2.63842200	9.22386900	-0.79305200
O	9.29226100	4.92258100	2.74114200	H	-0.77989100	7.40170500	0.27621600
O	8.09014600	3.98323600	4.38504500	H	-2.79614000	6.47092100	3.83273200
C	4.05792400	10.72609100	1.08083600	H	0.75261400	11.66425100	3.37716100
C	4.19352100	9.37500200	1.71778600	H	0.57353300	10.14330700	2.48142700
N	5.08959300	9.09712100	2.74186500	H	0.68773000	10.24895000	5.56014100
C	3.58628200	8.17160700	1.45228000	H	2.09034900	9.98106300	4.52712000
C	5.00921800	7.78540500	3.04746200	H	8.45669000	1.22916500	4.37610700
N	4.10782000	7.19275100	2.27966000	H	7.98491600	1.22821500	2.66894800
C	8.01612300	10.58505300	5.01126800	H	10.52124800	2.58452800	3.77568300
C	8.36440600	9.66126400	6.17756800	H	9.99928200	2.65249800	2.10692400
C	7.64430400	8.30409400	6.12524700	H	3.05232600	10.84546500	0.66837000
O	7.02295000	8.01768600	5.05975100	H	4.76878400	10.85224800	0.25357700
O	7.73632500	7.57258200	7.15147100	H	2.78950900	7.94579400	0.76097700
C	-4.35859600	9.22914500	6.55008700	H	5.61694100	7.32567600	3.80952500
C	-5.08953200	8.05315700	7.22243900	H	8.60094400	11.51292300	5.05291800
C	-4.32504300	6.74728800	7.13299600	H	8.23356100	10.09445100	4.05826200
O	-3.94637300	6.13801900	8.12374700	H	8.13806700	10.12770900	7.14342000
O	-4.11684200	6.36383400	5.87869600	H	9.44264700	9.45573600	6.19274200
Fe	3.91631000	5.05495500	2.55845700	H	-3.36361300	9.37672400	6.98029000
Fe	0.48775300	5.90197400	2.77676700	H	-4.24399000	9.06410500	5.47577400
O	-0.11996700	5.50996700	4.64757900	H	-5.25792900	8.25970600	8.28191600
O	-2.30380000	4.61970200	5.70701800	H	-6.06797200	7.91206300	6.74574400
O	-1.72644800	4.27649400	8.20439400	H	-1.00786700	5.16000700	4.96295500
O	6.78288200	2.55703200	6.21536700	H	0.11367200	6.36101200	5.17347800
O	9.53508700	5.87800300	0.27480500	H	-2.52625500	3.61865300	5.52269400
O	8.17098200	7.33051400	2.52459000	H	-1.95528800	4.57743800	6.66140900
H	0.88317000	0.99781000	-0.44277200	H	-2.52696000	4.75610200	8.47848100
H	-0.83347600	1.17133400	-0.81172700	H	-1.99948900	3.32878000	8.07981800
H	0.76126500	3.88383900	0.33527300	H	6.02423700	2.25840500	5.68927200
H	-1.13537400	3.08394200	4.00083100	H	7.39426700	2.91336300	5.52316700

H	9.21429400	6.71306100	0.65735400	H	-1.29507900	1.01666200	2.63745000
H	9.65452200	5.34601600	1.10213900	Int E (Fe1 ^{IV} Fe2 ^{III} _β)			
H	7.84528100	7.69992300	3.36722600	C	-0.11697500	0.99110600	-0.00015200
H	8.56268000	6.46117800	2.79546200	C	-0.18905800	2.00360400	1.09272200
O	5.13503600	4.91169800	3.88143300	N	-0.91540900	1.85730100	2.26722500
H	5.27459200	3.94971100	4.05501700	C	0.38193100	3.24307900	1.18741100
H	-3.45984700	5.56388300	5.84569000	C	-0.75838500	2.97462400	3.01414300
H	-2.10360200	-0.70372800	4.25124900	N	0.01864800	3.83791500	2.37813500
H	-0.30052200	0.00066300	0.36106200	C	-3.07782000	-0.50155900	4.64512800
H	4.79101400	0.45035100	0.97418700	C	-3.43713400	0.07623400	6.00781600
H	6.95074400	2.23550700	-2.15423200	C	-3.28626800	1.59980000	6.09949800
H	9.52471800	0.51316000	3.16130900	O	-3.09251900	2.20763200	4.98825500
H	6.98175200	10.85915500	5.02421300	O	-3.39128300	2.10816800	7.23608300
H	4.23038000	11.53007900	1.76577800	C	6.70669700	3.27727900	-2.17077800
H	-0.70681700	10.72934400	3.52654500	C	6.18248700	4.04204900	-0.98888400
H	-3.52134800	10.00486800	0.50173700	N	6.96650000	4.86316400	-0.19188900
H	-4.93705400	10.11432500	6.71457800	C	4.92408700	4.11273200	-0.43500500
O	1.07655900	6.13814600	1.27959600	C	6.19006800	5.37249200	0.78606400
O	2.20420900	5.35497100	3.46720200	N	4.93847800	4.94610600	0.66789500
C	0.42510400	7.24807700	9.26752500	C	3.73565300	0.46705200	1.14584900
N	1.50436800	8.00049600	8.63491500	C	3.65172300	0.83201900	2.62994000
C	2.85080000	7.58044500	9.02937600	C	4.03885800	2.28073400	2.91147700
C	3.31061100	6.23301100	8.55315100	O	3.40687400	3.16983400	2.22818400
C	4.74418900	5.91917300	8.24786600	O	4.92068200	2.51481500	3.76679800
C	4.97739600	5.77574900	6.73366800	C	-3.34293000	9.06301400	0.02594200
N	6.38095900	5.40017400	6.40576600	C	-2.58937100	8.06230900	0.85660200
H	0.46948600	7.39273400	10.35534700	N	-3.18386200	7.31635500	1.86531600
H	0.41568300	6.16231900	9.07549300	C	-1.28007900	7.63603800	0.84687100
H	1.39969800	7.93987200	7.62269000	C	-2.24792600	6.50270000	2.40695600
H	3.56644200	8.34168400	8.68173800	N	-1.07822600	6.66556500	1.81430600
H	2.89087200	7.63631400	10.13425500	C	0.35514000	10.64326500	3.42699400
H	2.57184300	5.44353300	8.43058500	C	0.79800800	9.85947900	4.66386100
H	5.04596700	4.97946100	8.73707900	C	0.54567000	8.35522000	4.59582000
H	5.40897400	6.70566300	8.62666500	O	0.90678800	7.75470100	3.51715600
H	4.78201800	6.72197900	6.22719500	O	0.03133000	7.80272800	5.59673800
H	4.31949700	5.02028900	6.30225400	C	8.83485000	1.30891600	3.35408600
H	6.59078300	4.42579600	6.68856300	C	9.25580400	2.66757700	2.79738500
H	6.50484000	5.39975300	5.38262500	C	8.93364600	3.90498000	3.63893600
H	-0.53595300	7.64091000	8.92004500	O	9.28637600	5.01006700	3.13665900
H	2.07627800	4.93105400	4.32757100	O	8.36708500	3.74442000	4.75700500
H	7.04164400	6.15575700	6.78576900	C	4.05792600	10.72609500	1.08083700
H	-4.28169000	8.03629100	2.51950400	C	4.18355200	9.38409900	1.71843000
H	5.75037700	9.71671100	3.18968400	N	5.06302000	9.11589600	2.76118700
H	8.06397500	5.08250900	-0.28612600	C	3.54960600	8.19529000	1.47918700

C	4.95394200	7.81506800	3.10183100	H	9.29350700	1.10746100	4.32576300
N	4.04341400	7.23684700	2.33736900	H	7.75206700	1.23235200	3.47392400
C	8.01612200	10.58506300	5.01127000	H	10.33839300	2.68702200	2.61399100
C	8.39706700	9.71818100	6.20561600	H	8.79502300	2.83197700	1.81447600
C	7.71582800	8.34162400	6.20145300	H	3.10062500	10.81515400	0.56220800
O	7.01600700	8.02350500	5.20110000	H	4.85685400	10.91877100	0.35370500
O	7.92342800	7.62306000	7.22483300	H	2.77218300	7.95488800	0.77218600
C	-4.35860200	9.22914800	6.55006600	H	5.54850300	7.34808000	3.86995100
C	-5.40729900	8.38381600	5.79027900	H	8.49353300	11.57136100	5.05658200
C	-5.01448400	6.92528900	5.78746700	H	8.31308100	10.10544900	4.07374300
O	-5.09383100	6.24568800	6.80118500	H	8.14869000	10.21022100	7.15365300
O	-4.53119500	6.49140500	4.62700800	H	9.48056800	9.54761700	6.23545400
Fe	3.57669300	5.19977500	2.39714700	H	-4.09618800	8.75120000	7.49655200
Fe	0.76631200	5.78788700	2.94746100	H	-3.44886500	9.39043300	5.96745700
O	-0.37161800	5.46935900	4.67485300	H	-6.36691800	8.46043700	6.31123200
O	-2.85803700	4.68898100	5.13816800	H	-5.53684100	8.75506900	4.76929700
O	-2.90674300	4.67949500	7.73997300	H	-1.29608300	5.13088200	4.81287600
O	6.63059700	1.92947100	6.03423000	H	-0.27110400	6.33132600	5.19129000
O	9.41127200	5.87001200	0.56002300	H	-3.02526200	3.65962400	5.05163700
O	8.12250100	7.39925400	2.69051900	H	-2.78857400	4.79364800	6.14420200
H	0.86387600	1.02591900	-0.48052700	H	-3.77636800	5.11121700	7.76842600
H	-0.87076300	1.17429700	-0.77720500	H	-3.09505800	3.70293700	7.66946700
H	1.05877100	3.74328300	0.51454400	H	5.93634000	1.90121300	5.35672400
H	-1.21815800	3.08514000	3.98185900	H	7.34076700	2.41429900	5.57033000
H	-3.33092300	-1.56743300	4.58309700	H	9.07319600	6.71625900	0.90127600
H	-3.61795900	0.02675200	3.85499300	H	9.53394800	5.37881700	1.41029100
H	-2.83857300	-0.36980300	6.80937100	H	7.75451800	7.79534200	3.50370400
H	-4.48204000	-0.15379700	6.25505200	H	8.51604800	6.56336600	3.03105900
H	7.06323400	3.94399100	-2.96575400	O	4.98156900	5.08702600	3.47510800
H	5.91241400	2.65292000	-2.58805000	H	5.11181200	4.11644900	3.69832500
H	4.02184700	3.60713700	-0.74465600	H	-3.97592000	5.63090700	4.80601000
H	6.58160200	6.01893700	1.56152700	H	-2.00375900	-0.41775200	4.43837000
H	3.39810100	-0.56220900	0.97962700	H	-0.27525400	-0.03286200	0.35317000
H	3.09881200	1.13704500	0.56210300	H	4.75170600	0.54870600	0.74668600
H	4.29392200	0.18860800	3.23671000	H	7.54140100	2.62228400	-1.89559600
H	2.61900100	0.69888900	2.97599100	H	9.17989000	0.56110900	2.63494500
H	-4.18614000	8.60001000	-0.50035200	H	6.93171600	10.73595200	4.98777200
H	-2.67597700	9.49165300	-0.72593500	H	4.11024400	11.51327300	1.84214100
H	-0.47453200	7.96614300	0.20775500	H	-0.72916600	10.66884800	3.27593000
H	-2.45484900	5.83676700	3.22723000	H	-3.73802600	9.88936600	0.62798000
H	0.68982400	11.68460900	3.49841400	H	-4.84896700	10.18356500	6.76588000
H	0.80260600	10.20584800	2.53020900	O	2.06748100	5.59843100	1.56761900
H	0.31987800	10.23294300	5.57284100	O	2.33919100	5.19858900	3.96716100
H	1.88128900	9.98730300	4.79027300	C	0.56102700	5.26305500	8.64463500

N	1.23027900	6.53452400	8.39413400	C	3.39048000	0.76205700	2.61222100
C	2.67334500	6.51457100	8.59191100	C	3.81535700	2.17138600	3.02458400
C	3.50767700	5.65275600	7.68413200	O	3.24136900	3.11669200	2.34942200
C	5.00016200	5.68471500	7.80376200	O	4.65896300	2.32128400	3.92444600
C	5.71772300	5.05578000	6.60867900	C	-3.34292900	9.06301300	0.02590900
N	7.20024000	5.14884300	6.75298400	C	-2.63642600	8.11344300	0.95010700
H	0.67826800	4.99674200	9.70387300	N	-3.20579700	7.68478000	2.14060900
H	0.93685000	4.40937800	8.05263800	C	-1.39946400	7.51166600	0.93048900
H	0.99762100	6.88595700	7.46828600	C	-2.32354100	6.87488500	2.77811900
H	3.04595200	7.55045400	8.53489000	N	-1.21627700	6.74796300	2.06935600
H	2.85459700	6.21243500	9.64296400	C	0.35519400	10.64326200	3.42699100
H	3.04323500	4.79566300	7.19752500	C	0.97439400	9.91254700	4.62422900
H	5.30998600	5.15503100	8.72771800	C	0.59233300	8.43668600	4.61718000
H	5.35167400	6.71798700	7.93188700	O	0.98890800	7.78001200	3.59306500
H	5.46527800	5.57637100	5.68548200	O	-0.07465100	7.96998100	5.57704000
H	5.47638600	3.99653500	6.49152600	C	8.83484300	1.30892200	3.35408600
H	7.51121800	4.55965500	7.52563700	C	9.67764200	2.59190000	3.43777900
H	7.68279900	4.77675200	5.89017200	C	8.90586300	3.90526400	3.61837000
H	-0.50924200	5.35779300	8.44161700	O	9.23541900	4.85653700	2.84915500
H	2.68312400	5.52188900	4.81141000	O	8.04430400	3.97466100	4.53381100
H	7.50391500	6.18164500	6.93842800	C	4.05790800	10.72609100	1.08082200
H	-4.12054000	7.39411300	2.23753100	C	4.16042000	9.38682800	1.72818200
H	5.73056000	9.73929900	3.19341400	N	5.10851200	9.07007100	2.69200700
H	7.97903500	5.09048100	-0.19706400	C	3.46844600	8.22186400	1.52127400
H	-1.49000800	1.07666600	2.55256300	C	4.97540000	7.76562900	3.01356400
TS_{EF} (Fe^{III}Fe^{IV}α)				N	3.98805200	7.22553600	2.32079000
C	-0.11698200	0.99112500	-0.00014800	C	8.01611200	10.58504800	5.01126900
C	-0.23464200	2.00644800	1.09151900	C	8.33735100	9.63326400	6.16744200
N	-0.94559300	1.81546900	2.27062700	C	7.55625900	8.30774600	6.10756800
C	0.29088200	3.26364000	1.20418300	O	7.00973500	8.01192500	5.00489000
C	-0.82381300	2.92646000	3.03627100	O	7.52540000	7.61004000	7.16108500
N	-0.08068400	3.82485700	2.40889100	C	-4.35859000	9.22913700	6.55006200
C	-3.07782100	-0.50155400	4.64513000	C	-4.88302700	8.13274200	7.49219400
C	-3.04723800	-0.10161300	6.12058300	C	-4.19328900	6.79403000	7.31397600
C	-2.73812200	1.38238700	6.36368400	O	-3.72512300	6.16358000	8.25386600
O	-2.87481400	2.14404000	5.34278400	O	-4.17574000	6.39914800	6.04808800
O	-2.42854100	1.72322900	7.52576300	Fe	3.61374500	5.08658900	2.43091100
C	6.70668000	3.27729000	-2.17078200	Fe	0.67810900	5.77386300	2.97244300
C	6.15711300	3.92289000	-0.94137400	O	-0.40269800	5.61183200	4.69084500
N	6.91457600	4.77590400	-0.15806200	O	-2.49159600	4.55338200	5.74959400
C	4.88808200	3.98730800	-0.41417800	O	-1.61708100	4.18543200	8.21718700
C	6.11962100	5.30055200	0.78965500	O	6.52599400	2.56618100	6.21450800
N	4.87339400	4.84956300	0.66384300	O	9.41950500	5.79686700	0.34271100
C	3.73563500	0.46704000	1.14584700	O	8.11906000	7.25548900	2.49092100

H	0.88841200	1.01168800	-0.42807000	H	-2.37984400	4.70106300	8.53365200
H	-0.82931300	1.17755900	-0.81410100	H	-1.92447900	3.24610700	8.08162800
H	0.94114600	3.80231400	0.53517700	H	5.80672500	2.33863200	5.60076700
H	-1.28082100	3.00597400	4.01004000	H	7.23171600	2.88142600	5.59702800
H	-3.65929800	-1.42052500	4.49790100	H	9.08929000	6.61982700	0.74786700
H	-3.54308700	0.29464300	4.05985000	H	9.57286200	5.26010600	1.15612000
H	-2.33793400	-0.70095900	6.69993200	H	7.83156400	7.68292900	3.31924000
H	-4.03065400	-0.28200800	6.57530200	H	8.46237700	6.37935300	2.80063600
H	7.62059500	3.79931900	-2.47608300	O	5.10411600	4.99392300	3.52139200
H	5.99758000	3.40053900	-2.99893300	H	5.25856500	4.05018500	3.73899300
H	3.99461500	3.47504000	-0.73914800	H	-3.57781100	5.56337600	5.94609900
H	6.49308900	5.97098200	1.55224500	H	-2.10360400	-0.70373700	4.25124700
H	3.33588300	-0.50760300	0.84058300	H	-0.30051600	0.00066200	0.36106500
H	3.30021300	1.23445900	0.50020100	H	4.79102700	0.45035500	0.97418700
H	3.87214800	0.04535500	3.28264100	H	6.95075200	2.23550100	-2.15423200
H	2.30502200	0.68655400	2.74944200	H	9.52472900	0.51315500	3.16130900
H	-4.30579500	8.66233300	-0.31381200	H	6.98176100	10.85916000	5.02421200
H	-2.72834300	9.24337300	-0.85926200	H	4.23039100	11.53007900	1.76578900
H	-0.62478000	7.58283100	0.18147100	H	-0.70685400	10.72934500	3.52655300
H	-2.51777200	6.43332300	3.74161500	H	-3.52134100	10.00486600	0.50174300
H	0.75825500	11.65875700	3.33743900	H	-4.93705800	10.11433000	6.71459600
H	0.58132100	10.10199400	2.50503100	O	1.70924200	5.71514500	1.60784300
H	0.65989600	10.35848500	5.57165800	O	2.26708400	5.35118300	4.05020100
H	2.06681900	9.97211500	4.55905400	C	1.68701000	4.64243900	10.11430600
H	8.28927200	1.11603000	4.28112200	N	0.95490000	5.48724600	9.18520400
H	8.11017200	1.35622700	2.53452400	C	1.73631500	6.32946800	8.26651200
H	10.36296100	2.50607000	4.29308200	C	2.63149900	5.50267900	7.40571900
H	10.30181600	2.68637900	2.54356600	C	4.09858000	5.35195500	7.60457900
H	3.06136000	10.85858300	0.65061800	C	4.82992900	5.76054300	6.30647200
H	4.78419300	10.83987700	0.26454200	N	6.27232000	5.40271800	6.29150600
H	2.62693400	8.02828300	0.87556300	H	2.37172800	5.25822200	10.71169000
H	5.61232800	7.26435700	3.72021100	H	2.28127700	3.83126400	9.66159300
H	8.60734900	11.50692800	5.07815200	H	0.18572600	4.99192100	8.72979600
H	8.23789300	10.10967100	4.05190100	H	1.02730500	6.89675900	7.65184500
H	8.14130200	10.10072100	7.13911000	H	2.32108200	7.04495800	8.86017100
H	9.40616800	9.38116500	6.16678700	H	2.16115500	4.88201100	6.64422600
H	-3.30291100	9.44692500	6.73564100	H	4.33985700	4.29286100	7.80074100
H	-4.46432600	8.92421900	5.50622600	H	4.45003300	5.94141100	8.45937100
H	-4.77064700	8.42323200	8.53946300	H	4.77409400	6.83977000	6.14925100
H	-5.95428700	7.97800300	7.30547600	H	4.37610300	5.26303500	5.45340700
H	-1.22359600	5.12549100	4.98405700	H	6.41248800	4.41904000	6.59533500
H	-0.34187000	6.50337600	5.17272000	H	6.61191600	5.39631600	5.31494500
H	-2.72688300	3.54368300	5.57611500	H	0.96851300	4.17937100	10.79785800
H	-2.05556800	4.51281200	6.64933200	H	2.48577900	6.19282400	4.47884800

H	6.84939600	6.15933800	6.78474300	C	4.05796900	10.72608600	1.08084900
H	-4.11698800	7.93430300	2.49479500	C	4.20968000	9.38662100	1.72204300
H	5.82656400	9.65719800	3.09212600	N	5.19753000	9.07657700	2.65068500
H	7.92397800	5.02806500	-0.19217600	C	3.51867500	8.21676300	1.54578800
H	-1.47103200	0.99857400	2.54791800	C	5.07930300	7.77152000	2.98950200
TS _{EF} (Fe ^I Fe ^{II} _β)				N	4.07021300	7.22985600	2.33199000
C	-0.11700900	0.99114800	-0.00016100	C	8.01607400	10.58505500	5.01120300
C	-0.23590300	2.00265400	1.09668500	C	8.30672900	9.68509100	6.21492300
N	-1.00927200	1.83145200	2.23960200	C	7.45159800	8.40694300	6.19990200
C	0.33565400	3.23605800	1.24800800	O	7.11026200	7.95535200	5.07512500
C	-0.87699700	2.93176400	3.02099200	O	7.16234200	7.89344500	7.32249300
N	-0.06941600	3.80482000	2.44008300	C	-4.35863100	9.22912000	6.55004000
C	-3.07777200	-0.50147000	4.64513000	C	-4.74501600	8.18893600	7.61338700
C	-3.05504200	-0.13955500	6.13044300	C	-4.08381900	6.83433200	7.42998900
C	-2.78164700	1.34515000	6.40639800	O	-3.58426700	6.21560000	8.36292100
O	-2.95052200	2.12571500	5.40578200	O	-4.13726500	6.40807200	6.17753600
O	-2.46755100	1.66660900	7.57365400	Fe	3.54750600	5.12378000	2.46196600
C	6.70677600	3.27729100	-2.17073600	Fe	0.73100000	5.76694300	3.01597600
C	6.19540400	3.86665500	-0.89228500	O	-0.46789500	5.60607700	4.72706500
N	7.01793300	4.38921400	0.09216000	O	-2.52020300	4.51183400	5.84998900
C	4.91488600	4.10597900	-0.44577300	O	-1.59947300	4.08664200	8.31170600
C	6.24032100	4.89969000	1.06638000	O	5.87492000	1.86283300	6.49007600
N	4.95305400	4.74855700	0.77597700	O	9.51295600	4.86725300	1.19953600
C	3.73564800	0.46692500	1.14587500	O	8.32938300	6.70953900	2.92438200
C	3.41916600	0.76636300	2.61923400	H	0.88911500	1.01503000	-0.42557300
C	3.87117100	2.17567900	3.00264000	H	-0.82892000	1.17866300	-0.81457000
O	3.23854800	3.11511000	2.38986000	H	1.04388300	3.75289900	0.62190300
O	4.79930000	2.32995100	3.82200000	H	-1.37201800	3.02026300	3.97580300
C	-3.34287700	9.06299700	0.02592800	H	-3.66649200	-1.41124400	4.47052100
C	-2.62367700	8.10523800	0.92886900	H	-3.53416000	0.31320500	4.07867600
N	-3.20827700	7.58663800	2.07480700	H	-2.33077800	-0.73514900	6.69470100
C	-1.36188400	7.55771200	0.91498100	H	-4.03353000	-0.35367700	6.58118100
C	-2.30862400	6.77980300	2.69241800	H	7.60387100	3.81128100	-2.50528300
N	-1.17607900	6.73866500	2.01424900	H	5.95228600	3.40647800	-2.95430500
C	0.35516500	10.64329300	3.42696200	H	3.97835600	3.86062500	-0.92548500
C	0.97340900	9.88834500	4.60733800	H	6.63800200	5.36755000	1.95438600
C	0.50829400	8.44014200	4.57920300	H	3.33118000	-0.50732200	0.84671100
O	1.01359500	7.72691700	3.64305300	H	3.29849400	1.23757000	0.50532000
O	-0.34223800	8.05825600	5.42162200	H	3.91136800	0.04719400	3.27970700
C	8.83480800	1.30886100	3.35405700	H	2.33696000	0.70392400	2.78113200
C	9.25002900	2.02870600	4.64274700	H	-4.30771600	8.66077400	-0.30636800
C	8.62180200	3.41788800	4.78250500	H	-2.74029000	9.24975900	-0.86652100
O	8.80151900	4.22154200	3.83281800	H	-0.57474800	7.70218800	0.18956000
O	7.99286300	3.65078300	5.86197000	H	-2.50601500	6.27471900	3.62354900

H	0.76211900	11.65862100	3.35212600	H	-4.93703100	10.11434000	6.71461200
H	0.57668500	10.11906300	2.49321300	O	1.94189500	5.60480300	1.65772700
H	0.68455100	10.34102900	5.55982100	O	2.33752700	5.29641600	4.17349900
H	2.06470200	9.90432700	4.52087500	C	1.64106700	5.27966400	10.03425100
H	7.81791200	0.91184800	3.42771400	N	0.88418700	5.58477200	8.84201100
H	8.86892200	1.99965300	2.50728100	C	1.48484900	6.33705100	7.74475300
H	9.00566500	1.42785100	5.52311900	C	2.59002100	5.51656400	7.16515700
H	10.33817500	2.17911600	4.63449700	C	4.00308300	5.74855800	7.56090100
H	3.04548300	10.83430500	0.68285500	C	5.03198600	5.03135800	6.68677800
H	4.75589100	10.86181600	0.24328400	N	6.42663400	5.36429600	7.09626700
H	2.65924400	8.00978900	0.92824500	H	2.12575500	6.18954400	10.41146700
H	5.72460300	7.27621500	3.69656000	H	2.42230300	4.50662900	9.92770600
H	8.61453000	11.50362700	5.03169100	H	0.17363300	4.90058000	8.57866100
H	8.22745900	10.05521800	4.07911400	H	0.70859500	6.54864400	7.00748800
H	8.13598000	10.21003800	7.16045200	H	1.86373000	7.29573700	8.12390100
H	9.36110300	9.37686800	6.21476400	H	2.32079400	4.60681300	6.63549900
H	-3.29362500	9.47398100	6.59658700	H	4.10633100	5.41355700	8.61537800
H	-4.57348000	8.84897100	5.54858600	H	4.20942100	6.82938800	7.59676800
H	-4.50229000	8.53688200	8.62052400	H	4.93447600	5.32479300	5.63927900
H	-5.83089200	8.02376900	7.58042500	H	4.93141900	3.94220000	6.73909500
H	-1.24748400	5.08344300	5.05468900	H	6.61971000	5.00454800	8.03188900
H	-0.53075400	6.53919800	5.10308400	H	7.10583500	4.84974900	6.45037700
H	-2.77992800	3.50992100	5.66293800	H	0.94461800	4.92840300	10.80260300
H	-2.06254400	4.45074800	6.73271100	H	2.66610600	6.09906300	4.60607000
H	-2.33774400	4.64275800	8.61828400	H	6.65459400	6.42804800	7.10772300
H	-1.94851500	3.16460300	8.15423300	H	-4.13503200	7.78687100	2.41943400
H	5.45896400	1.84600500	5.61116200	H	5.90305200	9.68439000	3.04117100
H	6.69767500	2.36489300	6.32919000	H	8.04666000	4.41700400	0.20262200
H	9.27525000	5.76149400	1.51562500	H	-1.56562100	1.02686500	2.49052300
H	9.43198100	4.36989300	2.04087400	Pro F			
H	8.02840000	7.35823400	3.58729700	C	-0.11700700	0.99114400	-0.00015800
H	8.39510700	5.87869900	3.44740900	C	-0.31198900	2.01186200	1.07226100
O	5.00536400	5.02827100	3.58649400	N	-0.98631400	1.78195400	2.26364500
H	5.12638600	4.07184300	3.80082700	C	0.11966100	3.30510300	1.16304700
H	-3.56160400	5.55703200	6.06610700	C	-0.93386300	2.90610100	3.01707700
H	-2.10362100	-0.70380200	4.25124900	N	-0.26814100	3.85213000	2.37144100
H	-0.30049800	0.00064400	0.36107200	C	-3.07777300	-0.50146700	4.64513100
H	4.79100800	0.45040900	0.97415800	C	-3.05108100	-0.08857800	6.11843000
H	6.95066800	2.23551100	-2.15423600	C	-2.72490100	1.39377800	6.37373500
H	9.52475200	0.51318300	3.16130900	O	-2.84417800	2.17248900	5.36274300
H	6.98178600	10.85915800	5.02427500	O	-2.42075400	1.71437700	7.54184400
H	4.23033800	11.53011400	1.76577800	C	6.70678800	3.27730000	-2.17074200
H	-0.70683700	10.72934000	3.52656700	C	6.19940600	3.89128000	-0.89910900
H	-3.52139200	10.00487200	0.50174100	N	6.96902100	4.70204600	-0.07901900

C	4.9385200	3.93389400	-0.35446800	O	-1.59712100	4.19305600	8.27637600
C	6.18163100	5.20010200	0.89325900	O	6.21065800	1.88748500	5.85027900
N	4.93516800	4.75600000	0.75700900	O	9.41605600	5.73714800	0.61316200
C	3.73564700	0.46694400	1.14588200	O	7.96224400	7.14961400	2.62702800
C	3.37889500	0.77130200	2.60063100	H	0.90932500	1.02457600	-0.37525500
C	3.51546000	2.24318100	2.98708800	H	-0.78857500	1.15543100	-0.85229600
O	3.16872100	3.09126500	2.07953700	H	0.72809700	3.87294700	0.47954200
O	3.89146100	2.52947200	4.14181800	H	-1.38362200	2.95422200	3.99669500
C	-3.34288400	9.06298900	0.02592700	H	-3.65933400	-1.42116500	4.50339900
C	-2.70168900	8.10883000	0.98168700	H	-3.54265400	0.29115400	4.05317700
N	-3.27180900	7.75650400	2.19832600	H	-2.35377500	-0.69512800	6.70479600
C	-1.50058400	7.45018600	0.96007200	H	-4.03997600	-0.25794800	6.56556000
C	-2.42436500	6.92927500	2.85618200	H	7.60550800	3.80680800	-2.50492600
N	-1.34223300	6.72455700	2.12431400	H	5.95837000	3.40469800	-2.96099000
C	0.35517100	10.64329100	3.42696100	H	4.04105900	3.43318000	-0.68365400
C	0.97168900	9.83787500	4.58046200	H	6.55659900	5.88282300	1.64992900
C	0.54615500	8.37805600	4.54548300	H	3.35184100	-0.51758700	0.85042500
O	0.93210800	7.72028300	3.49988400	H	3.29284300	1.21868900	0.48865800
O	-0.14686200	7.90565900	5.46964200	H	3.97234100	0.17851700	3.30174500
C	8.83479600	1.30884900	3.35407200	H	2.32612600	0.51366000	2.78152500
C	9.67048400	2.56234100	3.64961400	H	-4.29828800	8.68645600	-0.35939200
C	8.86094500	3.84286400	3.86436000	H	-2.68166000	9.23111200	-0.82686600
O	9.19738900	4.85406400	3.18560400	H	-0.73357100	7.45966800	0.20062200
O	7.93744800	3.80517700	4.72797100	H	-2.61769800	6.53862100	3.84427500
C	4.05797400	10.72609300	1.08084600	H	0.76583500	11.65907800	3.40033200
C	4.17258800	9.37312500	1.70100700	H	0.57841500	10.16078800	2.47118700
N	4.91881300	9.06854900	2.83115800	H	0.68979700	10.25592200	5.55000600
C	3.63183900	8.17761000	1.30955200	H	2.06387400	9.85664100	4.50315800
C	4.80561200	7.74440000	3.08016700	H	8.17387400	1.05224000	4.18548700
N	4.03776700	7.17798800	2.16632200	H	8.21686400	1.44928300	2.45968800
C	8.01606900	10.58506100	5.01120700	H	10.25087000	2.39219900	4.56698500
C	8.33382800	9.64539200	6.16909700	H	10.38941400	2.73957400	2.84354700
C	7.54444700	8.32864400	6.12191100	H	3.05809700	10.86044700	0.65780700
O	6.92120400	8.04339500	5.06216600	H	4.77659400	10.85545900	0.26039100
O	7.60274600	7.61812600	7.16913400	H	2.95440300	7.97370900	0.49466300
C	-4.35862600	9.22911700	6.55004000	H	5.30058700	7.27345400	3.91359800
C	-4.98297500	8.05140300	7.31488700	H	8.60799500	11.50713200	5.06723600
C	-4.18761100	6.76184400	7.19712100	H	8.22937800	10.10298800	4.05304900
O	-3.82016300	6.12630500	8.17492900	H	8.14003900	10.11934900	7.13806200
O	-3.95575600	6.41191500	5.93592800	H	9.40020500	9.38399800	6.17341100
Fe	3.36056800	5.13337600	2.15679900	H	-3.33336300	9.41610000	6.88307900
Fe	0.46606600	5.86961400	2.88727000	H	-4.32486800	9.02250200	5.47692200
O	0.01482300	5.44300700	4.80394600	H	-5.07011000	8.27779600	8.38013600
O	-2.22646500	4.56610700	5.77695600	H	-5.99429500	7.85933800	6.93233100

H	-0.82928000	4.98357100	5.09053900	H	7.01105700	4.61271700	7.56558100
H	-0.01711600	6.35544500	5.24908800	H	7.24145900	4.79934600	5.92903900
H	-2.55409100	3.58958700	5.61488300	H	1.44009000	4.23983400	10.69127500
H	-1.87425400	4.51282200	6.72252200	H	3.01783800	6.27322600	5.28753700
H	-2.37140500	4.70114900	8.57263600	H	7.06573100	6.21643500	6.92925700
H	-1.90365800	3.25661100	8.14553000	H	-4.16370100	8.06377700	2.55683700
H	5.42718400	1.95461500	5.27886700	H	5.51130200	9.67109500	3.38563300
H	6.86548200	2.46717600	5.41456000	H	7.97934400	4.94839900	-0.08767600
H	9.04384700	6.55164500	1.00146000	H	-1.44490300	0.93146000	2.55816400
H	9.56390800	5.21523300	1.43453500	$T_{S_{CE1-\alpha}}$			
H	7.65490300	7.65387500	3.40564800	C	-0.11698600	0.99112500	-0.00015000
H	8.34278200	6.32846900	3.02635500	C	-0.20666300	1.99910400	1.11592000
O	3.37706500	5.15562300	4.00402500	N	-0.88278600	1.76502000	2.30615300
H	3.53968300	4.22965600	4.30789700	C	0.28129400	3.27542200	1.25618300
H	-3.31682700	5.59862600	5.90337100	C	-0.77861200	2.86301900	3.09635700
H	-2.10362000	-0.70380500	4.25124900	N	-0.07838900	3.80514000	2.48307000
H	-0.30050000	0.00064800	0.36106900	C	-3.07783000	-0.50157100	4.64513600
H	4.79101400	0.45039300	0.97415300	C	-3.09534100	-0.22826000	6.14936800
H	6.95065800	2.23550400	-2.15423400	C	-2.99270400	1.25669200	6.52667500
H	9.52475900	0.51319200	3.16129700	O	-2.69289400	2.06023600	5.57580900
H	6.98179000	10.85915300	5.02427000	O	-3.22801300	1.54828900	7.71795600
H	4.23033200	11.53010800	1.76578000	C	6.70671500	3.27727400	-2.17077500
H	-0.70684300	10.72934200	3.52656800	C	6.21062000	3.93940600	-0.92297400
H	-3.52138600	10.00488000	0.50174200	N	6.97714400	4.83021800	-0.18533500
H	-4.93703600	10.11434200	6.71461200	C	4.95999700	3.99734000	-0.35549700
O	1.69313100	5.67021300	1.61919700	C	6.20247000	5.37173900	0.77006900
O	2.88825800	6.82700700	6.09040000	N	4.96169200	4.89383400	0.69597000
C	2.11880400	4.78008600	10.02171200	C	3.73563300	0.46702600	1.14584100
N	1.35612800	5.74244600	9.24620400	C	3.44148000	0.80184900	2.61412400
C	2.11057900	6.61496800	8.35316900	C	4.03461400	2.16415700	2.93735200
C	2.96992000	5.97406500	7.22657200	O	3.44461600	3.14659000	2.32050200
C	4.45110500	5.79108800	7.63102400	O	5.03159000	2.26390000	3.66701400
C	5.26347200	5.09773800	6.53861500	C	-3.34290500	9.06301900	0.02592200
N	6.73857900	5.18384300	6.76594900	C	-2.73377800	8.09480500	0.99760900
H	2.85026600	5.30976900	10.64749400	N	-3.35199800	7.74159100	2.18831600
H	2.67510300	4.02259500	9.43952400	C	-1.53594900	7.42298700	1.02855500
H	0.59828100	5.27526100	8.75307500	C	-2.53140200	6.90379300	2.87399600
H	1.39250100	7.26415800	7.84306800	N	-1.41918500	6.68787500	2.19452800
H	2.75119100	7.26446100	8.96965600	C	0.35514700	10.64327400	3.42698800
H	2.53342400	4.98951300	6.98828400	C	0.98475800	9.94276600	4.63240500
H	4.51908700	5.22782100	8.57143200	C	0.53927900	8.48594900	4.70030600
H	4.87138700	6.78811200	7.81196000	O	0.77053300	7.79534500	3.64816700
H	5.08097300	5.57829400	5.57963200	O	-0.02806600	8.08081100	5.74499400
H	5.02065700	4.03651400	6.44115400	C	8.83487100	1.30890600	3.35410600

C	9.66565400	2.58896300	3.53745300	H	-4.29320600	8.69827400	-0.38292400
C	8.86475900	3.82612800	3.95159400	H	-2.66026500	9.22768600	-0.81086900
O	8.96456200	4.85707900	3.23396800	H	-0.74663500	7.43898400	0.29109400
O	8.18673400	3.72446200	5.01945500	H	-2.76922400	6.52297700	3.85584000
C	4.05793300	10.72610100	1.08084800	H	0.75387600	11.65798000	3.30467700
C	4.06682100	9.37398300	1.73735200	H	0.57110500	10.07722400	2.51746000
N	4.71890400	9.09357600	2.92977900	H	0.72164400	10.43894200	5.57023000
C	3.53569400	8.16726000	1.34657500	H	2.07679800	9.95529000	4.53300100
C	4.57312400	7.78348200	3.20975000	H	8.25197400	1.07448100	4.24752500
N	3.85999200	7.18500300	2.26621500	H	8.14394500	1.39606800	2.50888100
C	8.01612900	10.58506600	5.01125600	H	10.40457600	2.41452200	4.33153400
C	8.27429000	9.60578100	6.15230600	H	10.22200000	2.81777400	2.62287000
C	7.32642900	8.39684500	6.11411500	H	3.09452400	10.90440300	0.59434500
O	6.57845300	8.26870300	5.10345400	H	4.83279500	10.79603500	0.30678400
O	7.37931400	7.61518700	7.10601600	H	2.94442700	7.95075300	0.46916600
C	-4.35862100	9.22912000	6.55005700	H	5.04648600	7.32213100	4.06202400
C	-5.35675600	8.07059100	6.78251600	H	8.62541900	11.49227800	5.10266500
C	-4.72782000	6.69827300	6.90356700	H	8.23181000	10.11998800	4.04519600
O	-4.75313200	6.06330900	7.95020500	H	8.16228800	10.08887800	7.13045400
O	-4.16343900	6.28048300	5.77929600	H	9.30168100	9.22149500	6.12515000
Fe	3.90644200	5.03132000	2.58401600	H	-3.53445900	9.20171700	7.26742900
Fe	0.35968100	5.79012200	3.35532600	H	-3.93974500	9.22358000	5.54144800
O	-0.60628400	5.67707500	5.12878500	H	-5.91019500	8.24352700	7.70885400
O	-2.54942900	4.44221700	6.27124500	H	-6.08204000	8.04980400	5.95886000
O	-2.88985000	3.98648200	8.83255100	H	-1.34776200	5.16920400	5.56819900
O	6.62374300	1.63180800	6.05999700	H	-0.46639500	6.58831800	5.54553800
O	9.38372800	5.79623200	0.71268900	H	-2.66231900	3.44427400	5.97601600
O	7.88420000	7.29064200	2.72753300	H	-2.49918600	4.38962100	7.27197900
H	0.87836100	1.00691900	-0.45145100	H	-3.70249600	4.51563300	8.76683600
H	-0.84810200	1.19370800	-0.79248100	H	-3.11027400	3.07132900	8.52129400
H	0.88990500	3.83222600	0.55951600	H	5.98883300	1.64000900	5.32506200
H	-1.21818900	2.90157300	4.08353600	H	7.28991500	2.27890200	5.75383300
H	-3.68198300	-1.38552800	4.40217700	H	9.03889300	6.63446000	1.06832000
H	-3.49942300	0.35122700	4.10720900	H	9.41738900	5.26151700	1.54175600
H	-2.28913500	-0.76105400	6.66780900	H	7.43318800	7.74144700	3.46651100
H	-4.02407300	-0.59537000	6.59963400	H	8.17291500	6.43646400	3.12330400
H	7.60557300	3.79548900	-2.52319300	O	5.38671300	4.98367200	3.61298300
H	5.95973200	3.39431600	-2.96524300	H	5.64498700	4.04166100	3.72720100
H	4.06797000	3.45662600	-0.63402600	H	-3.58909200	5.42979600	5.97658600
H	6.57997900	6.06895900	1.51153400	H	-2.10359800	-0.70372000	4.25124300
H	3.33007600	-0.51365800	0.87180400	H	-0.30051100	0.00065800	0.36106300
H	3.29280800	1.22127700	0.49020000	H	4.79102300	0.45036800	0.97418700
H	3.88313500	0.05703900	3.28099500	H	6.95071900	2.23552100	-2.15423900
H	2.36069000	0.83699500	2.78580600	H	9.52470600	0.51316300	3.16129100

H	6.98174900	10.85914900	5.02422200	O	-3.91654600	1.49583000	7.63605600
H	4.23036900	11.53006800	1.76576700	C	6.70670700	3.27726900	-2.17078700
H	-0.70681500	10.72934400	3.52655000	C	6.18979000	3.92829700	-0.92994300
H	-3.52136200	10.00486100	0.50173900	N	6.95678800	4.74444900	-0.11375600
H	-4.93703700	10.11434200	6.71460200	C	4.91143300	4.03974400	-0.43602100
O	2.32357000	4.32532100	4.76683500	C	6.14536700	5.29545500	0.81215600
O	2.32286500	5.34450000	3.76829700	N	4.88999600	4.89084500	0.64742400
C	0.52645400	4.34120400	9.14592400	C	3.73563000	0.46705000	1.14584600
N	0.51693700	5.32820300	8.07634800	C	3.39294200	0.71486100	2.61582300
C	1.79404000	5.92627800	7.73805000	C	3.74161600	2.14468100	3.03753100
C	2.88112000	5.01363200	7.17403900	O	3.27312900	3.05460500	2.25730700
C	4.30318100	5.51341300	7.34597200	O	4.43321200	2.33820600	4.05535100
C	5.32084000	4.62789400	6.63922100	C	-3.34291100	9.06300600	0.02592800
N	6.72990100	5.10117200	6.81201700	C	-2.81730400	8.07484100	1.02317800
H	0.89808700	4.81183600	10.06613200	N	-3.46297400	7.81681700	2.22420100
H	1.14917100	3.44508500	8.96491300	C	-1.68575300	7.29859200	1.07259900
H	0.07197200	4.96471700	7.24062800	C	-2.71875800	6.93361000	2.93909100
H	1.60966300	6.76077200	7.05054800	N	-1.63450400	6.59663500	2.26261600
H	2.19993400	6.38719800	8.65647500	C	0.35515300	10.64328300	3.42698000
H	2.76868300	3.96045300	7.45782500	C	0.93204000	9.79588500	4.57125900
H	4.51332600	5.56020200	8.42935600	C	0.29012500	8.41607200	4.62738200
H	4.39870300	6.54359900	6.97896700	O	0.51963300	7.66697400	3.59032100
H	5.12775900	4.65906000	5.57081200	O	-0.41454200	8.09151700	5.60039100
H	5.28212000	3.58347600	6.95964700	C	8.83485400	1.30892600	3.35409300
H	7.12379100	4.75539200	7.68658900	C	9.67934500	2.51412200	3.81026400
H	7.32761900	4.71083000	6.02917200	C	8.87620100	3.74867400	4.23598700
H	-0.50086400	4.01525900	9.32785800	O	8.95267100	4.77495500	3.51312800
H	2.60121100	4.81580500	5.82609800	O	8.21603900	3.63787100	5.31798500
H	6.85376100	6.18143900	6.84106800	C	4.05792500	10.72609100	1.08083300
H	-4.25512900	8.05225900	2.51316400	C	3.98466200	9.39315800	1.76531100
H	5.32124400	9.68138700	3.49231800	N	4.62584500	9.09108200	2.95816000
H	7.99109200	5.04772500	-0.17790100	C	3.37544800	8.21570000	1.39848500
H	-1.37734300	0.92619800	2.57520600	C	4.39578400	7.79063300	3.25303600
TS_{CE1-β}				N	3.64044200	7.22552600	2.32432200
C	-0.11696900	0.99113600	-0.00014100	C	8.01612500	10.58504500	5.01126300
C	-0.40344900	2.06536400	1.01117400	C	8.24813100	9.60437000	6.15759000
N	-1.63641500	2.23269400	1.63309100	C	7.23080300	8.44780800	6.15228300
C	0.36909100	3.09335200	1.49386100	O	6.45337800	8.35182400	5.16344900
C	-1.56860200	3.31774000	2.44351700	O	7.27150400	7.67942800	7.15775600
N	-0.36848400	3.87064600	2.37555600	C	-4.35862400	9.22912300	6.55005700
C	-3.07782200	-0.50156000	4.64513000	C	-5.30062400	8.10349800	7.03438200
C	-3.79666400	-0.22849200	5.96404700	C	-4.67766100	6.73479000	7.16246900
C	-3.63390000	1.18957300	6.48374000	O	-4.64415800	6.12839100	8.22522300
O	-3.18183800	2.02318900	5.56155600	O	-4.19412900	6.26988900	6.01660600

Fe	3.79814900	5.04255500	2.54589700	H	-3.43881000	9.27775900	7.13733300
Fe	0.12134100	5.74542900	3.51075400	H	-4.09281200	9.13001900	5.49581000
O	-0.91930900	5.53992500	5.03466000	H	-5.70309600	8.35523200	8.01844900
O	-2.62754100	4.31381700	6.44321400	H	-6.14906900	8.02527400	6.34173300
O	-3.03027200	3.88895200	8.96684700	H	-1.82657200	4.71461300	5.96811600
O	6.48718800	1.43689700	5.89828700	H	-0.83144000	6.44632900	5.45007900
O	9.34737700	5.66228200	0.93981400	H	-2.99402400	2.95482500	5.95247100
O	7.92540100	7.23826100	2.90054800	H	-2.48004300	4.21461100	7.43395900
H	0.93666400	1.04660800	-0.28206500	H	-3.72769800	4.56698000	8.90071300
H	-0.71257600	1.13050900	-0.91156200	H	-3.44777200	3.04810900	8.69954300
H	1.42746800	3.25739600	1.34370200	H	5.79140000	1.60711300	5.23797600
H	-2.38580100	3.65164900	3.06354800	H	7.15359500	2.12782800	5.71017100
H	-3.28930400	-1.51996700	4.29959100	H	8.96808000	6.49254200	1.28133700
H	-3.40865600	0.19562500	3.87154300	H	9.37117200	5.13685300	1.77306700
H	-3.45951200	-0.90118600	6.75895600	H	7.34929500	7.67835800	3.55176000
H	-4.87520900	-0.40742300	5.85996400	H	8.14643500	6.38317700	3.33032500
H	7.60977000	3.79700800	-2.51227200	O	5.30467900	5.08311600	3.62599600
H	5.96921500	3.39429100	-2.97450700	H	5.52056100	4.15476000	3.80834500
H	4.01212700	3.56169300	-0.79819500	H	-3.64832500	5.42334300	6.20428600
H	6.50782400	5.93654700	1.60622400	H	-1.99060200	-0.40388800	4.73520100
H	3.33757700	-0.49647400	0.80076700	H	-0.30052700	0.00064800	0.36106100
H	3.31177000	1.26035400	0.52527400	H	4.79103100	0.45034900	0.97418600
H	3.91226500	0.01302600	3.27378200	H	6.95072900	2.23552200	-2.15423200
H	2.31322900	0.57950900	2.76724800	H	9.52472200	0.51315000	3.16130200
H	-4.27967800	8.72933000	-0.43748300	H	6.98174900	10.85916300	5.02421800
H	-2.61086200	9.21504800	-0.77012500	H	4.23037700	11.53007500	1.76578100
H	-0.89804400	7.22035900	0.33768900	H	-0.70682000	10.72934000	3.52655400
H	-2.97086000	6.60691500	3.93758000	H	-3.52135400	10.00487200	0.50173100
H	0.78456400	11.65070600	3.43039800	H	-4.93703300	10.11433900	6.71460200
H	0.57745600	10.17698000	2.46351300	O	1.91325500	5.10208500	3.71838300
H	0.76822700	10.28240500	5.53645900	O	2.19375300	5.83109700	4.90995600
H	2.00889200	9.66019100	4.42645000	C	0.57193300	2.34413200	6.80195600
H	8.12564800	0.99860200	4.12550500	N	0.50285100	3.75823600	7.15154900
H	8.28074600	1.53297400	2.43612100	C	1.72046800	4.31171600	7.73462500
H	10.27803700	2.20698500	4.67751200	C	2.95519000	4.32423000	6.85278200
H	10.37271000	2.80511600	3.01421800	C	4.20851300	4.96322800	7.42604300
H	3.12598800	10.93298800	0.54602000	C	5.40531600	4.56042300	6.57602000
H	4.87102400	10.75680800	0.34346500	N	6.72214900	5.13384200	6.97777400
H	2.76942200	8.02705000	0.52338400	H	0.73039700	1.75079300	7.71148700
H	4.84788400	7.30250300	4.10141600	H	1.36208000	2.06770800	6.08370200
H	8.63542600	11.48578400	5.10055200	H	0.25168100	4.31033000	6.33458200
H	8.22680600	10.10877600	4.04954500	H	1.50089700	5.33344700	8.07398500
H	8.18284000	10.10238200	7.13293900	H	1.95151000	3.73808800	8.65063600
H	9.25104300	9.16187900	6.11317300	H	3.14932000	3.38896000	6.31782900

H	4.33171400	4.62871600	8.47285100	C	0.41989000	8.41967700	4.69063100
H	4.10574300	6.05667300	7.47018200	O	0.16113300	7.84026000	3.58307400
H	5.24860000	4.89297300	5.54744000	O	0.29616600	7.90000200	5.83221800
H	5.52185500	3.47358400	6.57019700	C	8.83486500	1.30892100	3.35409500
H	7.00804600	4.81276500	7.90300200	C	9.61781600	2.61146400	3.14474800
H	7.41920900	4.74226600	6.27797200	C	8.88581400	3.92677900	3.44132000
H	-0.38899100	2.03959200	6.37382800	O	9.24274100	4.92252800	2.73665800
H	2.56622800	5.07268800	5.72384800	O	8.04483500	3.96449600	4.37246400
H	6.78693500	6.21862500	6.97853400	C	4.05792700	10.72608700	1.08082600
H	-4.32837000	8.22991600	2.53731400	C	4.17866900	9.37112400	1.71171900
H	5.28059000	9.63536900	3.50709700	N	5.00970700	9.08658000	2.78518600
H	7.97348000	4.91702800	-0.04861000	C	3.61404900	8.16131600	1.38574800
H	-2.43315300	1.61922100	1.55334700	C	4.93157800	7.76805300	3.06056800
Int E1 _α				N	4.09423400	7.17328300	2.22622300
C	-0.11697600	0.99113600	-0.00014200	C	8.01613100	10.58505400	5.01126600
C	-0.32481500	1.98662800	1.10279700	C	8.36351700	9.64365100	6.16142600
N	-1.12746800	1.73496400	2.20611900	C	7.64011400	8.29047600	6.08786800
C	0.14068100	3.26029400	1.30856600	O	6.95426100	8.05259400	5.04926100
C	-1.11763000	2.82343700	3.01607000	O	7.79151100	7.51529400	7.07378600
N	-0.35793800	3.77302000	2.49201300	C	-4.35862700	9.22912200	6.55006200
C	-3.07782800	-0.50156900	4.64513400	C	-5.26697000	8.01903800	6.85203000
C	-3.77122500	-0.07813400	5.93762300	C	-4.51643800	6.71234900	7.04033900
C	-3.49987400	1.37392100	6.37053500	O	-4.53707800	6.10920900	8.10603500
O	-3.01884000	2.15509200	5.47773900	O	-3.85306100	6.32365600	5.96267200
O	-3.79070300	1.66578400	7.54988100	Fe	3.85885000	5.02834200	2.55175600
C	6.70669600	3.27727400	-2.17078300	Fe	0.01286100	5.78481300	3.29172800
C	6.23507700	3.91103300	-0.90022000	O	-0.10183200	5.39969200	5.32949000
N	7.00744100	4.80814100	-0.18146200	O	-2.29270000	4.40630200	6.37361600
C	5.01682900	3.89981200	-0.26474300	O	-2.86679400	3.86799000	8.85174400
C	6.27036000	5.29493900	0.83023800	O	6.74544900	2.52520400	6.20621000
N	5.04583000	4.77017200	0.80835000	O	9.45910700	5.90328300	0.27809500
C	3.73563500	0.46704800	1.14584400	O	8.07575100	7.30766300	2.51068300
C	3.40256100	0.73657000	2.61818000	H	0.90951100	1.03395800	-0.37223800
C	3.87743800	2.11768900	3.05767600	H	-0.79152600	1.16694700	-0.84724900
O	3.39278400	3.09444100	2.35211800	H	0.82572300	3.82468200	0.69420800
O	4.67063800	2.22922500	4.00658900	H	-1.66579300	2.84362500	3.94923200
C	-3.34290700	9.06301400	0.02592600	H	-3.30436000	-1.54353300	4.38878400
C	-2.90089500	8.03446200	1.01326500	H	-3.40624400	0.13517200	3.81632100
N	-3.62215300	7.71818100	2.15463500	H	-3.48001000	-0.72421700	6.77245200
C	-1.78128400	7.24956300	1.08863500	H	-4.85944600	-0.19039500	5.83963600
C	-2.92979200	6.78989600	2.86389800	H	7.59970800	3.79952500	-2.53040700
N	-1.80770400	6.48335600	2.23754800	H	5.94529000	3.39764800	-2.95076300
C	0.35515100	10.64328000	3.42699300	H	4.13244800	3.32926800	-0.50320400
C	0.94200900	9.85256400	4.60000400	H	6.66461400	6.00407200	1.55172100

H	3.33228900	-0.50104400	0.82611100	H	-0.30052100	0.00064800	0.36106200
H	3.29968900	1.24576600	0.51501700	H	4.79102600	0.45035000	0.97418700
H	3.86059100	-0.00987000	3.27195500	H	6.95073700	2.23551500	-2.15423400
H	2.31583500	0.69643100	2.76067400	H	9.52471200	0.51315300	3.16130100
H	-4.26191500	8.76957000	-0.49749000	H	6.98174500	10.85915600	5.02421600
H	-2.56550800	9.20831200	-0.72770900	H	4.23037700	11.53008000	1.76578600
H	-0.94962800	7.20948200	0.40075100	H	-0.70681900	10.72934000	3.52654300
H	-3.25996500	6.42277700	3.82631400	H	-3.52135900	10.00486700	0.50173200
H	0.77683600	11.65406900	3.38283100	H	-4.93703100	10.11434100	6.71459900
H	0.56476600	10.13276700	2.48432300	O	2.01478300	5.41133900	3.21264000
H	0.75888400	10.34611600	5.55887300	O	2.41172500	6.18470000	4.40128500
H	2.03202100	9.77544100	4.49028100	C	0.99844800	8.35793500	9.47025200
H	8.45095400	1.22367500	4.37351200	N	1.91502300	8.70069300	8.39257300
H	7.98824200	1.22758500	2.66460200	C	3.27168400	8.19245300	8.57553500
H	10.50231500	2.60292200	3.79863900	C	3.46999800	6.70407900	8.49798100
H	10.00506200	2.66200500	2.12139100	C	4.81736200	6.11508600	8.20552300
H	3.05697500	10.85628800	0.65987400	C	4.99022800	5.83194800	6.70147100
H	4.77662800	10.84826800	0.25985900	N	6.36805100	5.37765300	6.36317200
H	2.89455300	7.94768800	0.60923400	H	1.31963900	8.84766300	10.39990900
H	5.50195500	7.30319900	3.84723200	H	0.90271400	7.27871300	9.68801000
H	8.60098600	11.51221700	5.06797300	H	1.52647600	8.38440600	7.50354600
H	8.23374900	10.11047400	4.05006500	H	3.92452800	8.67510000	7.82964200
H	8.13580000	10.09476700	7.13448300	H	3.63853300	8.57285400	9.54828100
H	9.44104000	9.43606600	6.17676500	H	2.60963400	6.04607600	8.59450000
H	-3.49969700	9.25609000	7.22707500	H	4.96609500	5.18169500	8.76734000
H	-3.97717400	9.21319900	5.52618600	H	5.61303800	6.80843500	8.50815600
H	-5.82720200	8.18992900	7.77428600	H	4.81774200	6.74195400	6.12695300
H	-5.99475400	7.89142900	6.04009300	H	4.28771100	5.07563900	6.34955100
H	-0.87590400	4.94187900	5.76486300	H	6.54874100	4.40669200	6.67381700
H	-0.03242800	6.34454900	5.68562200	H	6.47571300	5.33829200	5.33874000
H	-2.63065300	3.49807600	6.00161300	H	-0.00054500	8.73121100	9.22368200
H	-2.30778800	4.25555400	7.37210400	H	2.04758000	5.61116400	5.10271900
H	-3.57101300	4.53898100	8.80629700	H	7.06411100	6.11524000	6.71197400
H	-3.27274200	3.04083500	8.48711100	H	-4.50634700	8.11637200	2.43243300
H	5.98418000	2.23297300	5.68055500	H	5.63760900	9.70238600	3.28383100
H	7.35550800	2.88448600	5.51557900	H	8.00417500	5.10292400	-0.27203300
H	9.12796800	6.72843300	0.67447800	H	-1.62091600	0.87970500	2.41879800
H	9.59571100	5.36439200	1.09820000	TS _{EF1-α}			
H	7.75780400	7.69277100	3.34921100	C	-0.11698000	0.99112900	-0.00014300
H	8.47670600	6.44510400	2.79054100	C	-0.26437700	2.01464600	1.08615300
O	5.09939000	4.88778700	3.85100300	N	-1.08786300	1.85422700	2.19081300
H	5.23579500	3.92673500	4.02731400	C	0.28725900	3.25968900	1.25171200
H	-3.24902600	5.48416300	6.16418800	C	-1.00745200	2.96496100	2.96317000
H	-1.99059800	-0.40388000	4.73519800	N	-0.18219700	3.84375800	2.41299100

C	-3.07782800	-0.50157100	4.64513400	C	-5.25794800	8.05556000	6.98795800
C	-3.77669600	-0.06198600	5.92655700	C	-4.54748700	6.72042300	7.06320700
C	-3.51340800	1.40189200	6.30630800	O	-4.46103300	6.09210400	8.11080000
O	-3.09999000	2.16111300	5.35976000	O	-4.04776500	6.33191600	5.90031400
O	-3.74107800	1.72731800	7.49033400	Fe	3.80819500	5.01773000	2.62234800
C	6.70669500	3.27726700	-2.17078200	Fe	0.32550000	5.79467300	3.26045400
C	6.17502500	3.91779600	-0.92233300	O	-0.20698600	5.44017300	5.27842900
N	6.92140600	4.80433500	-0.16102600	O	-2.43965100	4.43588100	6.13763500
C	4.91808400	3.94828400	-0.36208900	O	-2.68795500	3.90646400	8.67871400
C	6.12929400	5.31718700	0.79713400	O	6.62685200	1.70703100	6.11170200
N	4.89554500	4.82577900	0.70620200	O	9.33554300	5.81639400	0.66880600
C	3.73564000	0.46704900	1.14585000	O	7.88155500	7.28830600	2.70745700
C	3.43673400	0.74275700	2.62408300	H	0.89634100	1.01791000	-0.40803200
C	3.96799200	2.12041300	2.99968400	H	-0.81548600	1.17247200	-0.82690500
O	3.39768300	3.08656700	2.35168700	H	1.01754800	3.74951400	0.62659600
O	4.89596200	2.23790600	3.81590300	H	-1.54975100	3.05553000	3.89330800
C	-3.34291700	9.06302000	0.02593000	H	-3.30101000	-1.54740400	4.40125800
C	-2.80646400	8.07753900	1.02012500	H	-3.40498100	0.12336600	3.80757600
N	-3.45603200	7.78137200	2.20950000	H	-3.47929200	-0.68182400	6.77845200
C	-1.65216600	7.33725800	1.07362600	H	-4.86388900	-0.18526300	5.82851600
C	-2.69101600	6.90680900	2.91656100	H	7.61488300	3.80143400	-2.48792500
N	-1.58803000	6.61620700	2.25231300	H	5.98247300	3.40274600	-2.98488300
C	0.35515000	10.64328300	3.42698700	H	4.03695800	3.39995600	-0.66067000
C	0.97011800	9.86655600	4.59388800	H	6.49296000	6.00810300	1.54884700
C	0.51091200	8.41433000	4.62387300	H	3.32808500	-0.50079200	0.83013600
O	0.62912000	7.77134400	3.51933700	H	3.29827700	1.24997200	0.52175100
O	0.05251300	7.94730300	5.69394100	H	3.90373400	-0.00674900	3.26815100
C	8.83486200	1.30892800	3.35408800	H	2.35455900	0.72886500	2.79675700
C	9.66045200	2.59624600	3.50122500	H	-4.28141900	8.72584700	-0.43133900
C	8.86309300	3.83888000	3.90938300	H	-2.61619400	9.21634000	-0.77489500
O	8.97942900	4.86734000	3.18985600	H	-0.85616200	7.29787700	0.34426300
O	8.17968400	3.74769800	4.97306600	H	-2.97181600	6.55389800	3.89829500
C	4.05793300	10.72608300	1.08083100	H	0.76520900	11.65854100	3.37264000
C	4.10314100	9.37380700	1.73260300	H	0.57173300	10.13358900	2.48493100
N	4.78109400	9.09734000	2.91146300	H	0.72814400	10.32529800	5.55604800
C	3.58526800	8.16077400	1.34459600	H	2.06230000	9.85642600	4.49149600
C	4.66312800	7.77963500	3.18374500	H	8.26871500	1.08784700	4.26196600
N	3.94398400	7.17937900	2.24909400	H	8.12806800	1.37897100	2.52030800
C	8.01612500	10.58504600	5.01125900	H	10.41573000	2.43930400	4.28385800
C	8.29582300	9.63626100	6.17232100	H	10.19922600	2.81284200	2.57326300
C	7.38699200	8.39759300	6.15156300	H	3.08231300	10.89011200	0.61376400
O	6.66119400	8.22009400	5.13378700	H	4.81604300	10.81382900	0.29185000
O	7.44908600	7.64241900	7.16449500	H	2.98285300	7.94074900	0.47542300
C	-4.35862800	9.22912300	6.55005800	H	5.14442200	7.31599600	4.03023800

H	8.62080100	11.49814300	5.07459500	H	-3.52135000	10.00486200	0.50172800
H	8.22708400	10.09883500	4.05472100	H	-4.93703000	10.11433900	6.71460200
H	8.16577600	10.13433400	7.14062500	O	2.20966400	5.31365200	3.63157900
H	9.33496000	9.28377800	6.15540900	O	2.55811000	5.21443900	5.24430400
H	-3.44792800	9.28377300	7.15268900	C	0.64145400	4.57902300	9.49734300
H	-4.06961400	9.15637500	5.49898400	N	0.64898400	5.58153000	8.44049200
H	-5.67322400	8.24967100	7.97978400	C	1.95137600	6.13641700	8.10365500
H	-6.09788400	7.96061500	6.28742700	C	2.99059300	5.20223800	7.54147100
H	-1.07325900	5.03038300	5.57663900	C	4.43225600	5.59432500	7.61826400
H	-0.18769600	6.41853000	5.57293100	C	5.31751300	4.76637900	6.69415100
H	-2.76473900	3.49555400	5.80022000	N	6.76197400	5.13739200	6.80287600
H	-2.35953800	4.29573200	7.13364600	H	0.94462800	5.04643600	10.44403400
H	-3.38804000	4.58185200	8.73180700	H	1.31310900	3.71543300	9.33290000
H	-3.13733100	3.07918500	8.36570500	H	0.20186600	5.21990900	7.60463800
H	5.96340400	1.68358400	5.40269900	H	1.79739500	6.96490200	7.39696400
H	7.28427200	2.33604300	5.75277600	H	2.36466400	6.60553800	9.01530500
H	8.97995300	6.64489800	1.03791600	H	2.76567500	4.13829300	7.50121900
H	9.39978300	5.27933800	1.49406700	H	4.76114000	5.48725400	8.67114700
H	7.47416300	7.74138000	3.46980200	H	4.55167300	6.65964100	7.38153300
H	8.18144500	6.43123800	3.09055400	H	5.02880300	4.95200400	5.66280300
O	5.28505500	4.94725400	3.65567000	H	5.24538100	3.69118100	6.88124500
H	5.47929800	4.00069400	3.84095500	H	7.18014100	4.71692500	7.63280200
H	-3.44418800	5.48322300	6.02094700	H	7.29864100	4.75480400	5.97615500
H	-1.99059800	-0.40387700	4.73519700	H	-0.37834500	4.20174700	9.61099500
H	-0.30051700	0.00065300	0.36106200	H	1.63186600	5.01874900	5.49279100
H	4.79102200	0.45035200	0.97418300	H	6.93751900	6.20798900	6.87847300
H	6.95073900	2.23552200	-2.15423600	H	-4.34384100	8.14958000	2.51608500
H	9.52471500	0.51314900	3.16130500	H	5.37708000	9.69765600	3.46619400
H	6.98175000	10.85916300	5.02422300	H	7.93063700	5.04750900	-0.15537300
H	4.23037200	11.53008100	1.76578400	H	-1.63716500	1.04169100	2.43345400
H	-0.70681700	10.72933900	3.52654800				