

## A Density Functional Theory Analysis of the C-H Activation Reactivity of Iron(IV)-Oxo complexes with 'O' Substituted Tetramethyl-cyclam Macrocycle

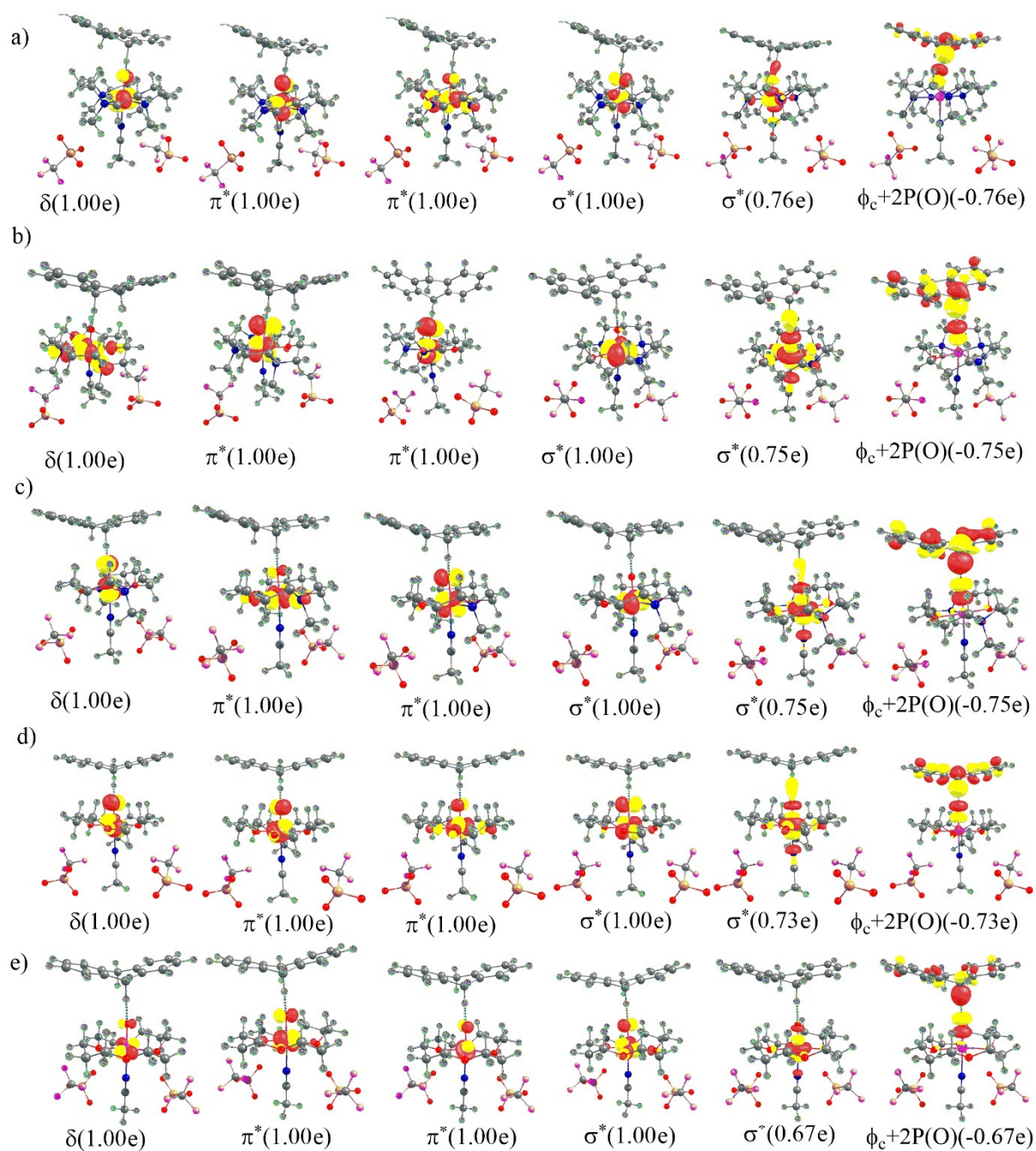
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**Full citation of Gaussian 16:** *Gaussian 16*, Revision B.01, Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.V.; Bloino, J., Janesko, B.G., Gomperts, R., Mennucci, B., Hratchian, H.P., Ortiz, J.V., Izmaylov, A.F., Sonnenberg, J.L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V.G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery Jr., J.A., Peralta, J.E., Ogliaro, F., Bearpark, M.J., Heyd, J.J., Brothers, E.N., Kudin, K.N., Staroverov, V.N., Keith, T.A., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A.P., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Millam, J.M., Klene, M., Adamo, C., Cammi, R., Ochterski, J.W., Martin, R.L., Morokuma, K., Farkas, O., Foresman, J.B., Fox, D.J. Gaussian, Inc., Wallingford CT (2016) Wallingford, E.U.A.



**Figure S1.** Spin Natural orbitals and their occupations in transition states for  $^5TS$  of a)  $N_4$  b)  $N_3O_1$  c)  $N_2O_2$  (d)  $NO_3$  and e)  $O_4$  framework

**Table S1.** Relative energies (in kcal mol<sup>-1</sup>) of oxidants, TS and intermediates computed at different levels of theory where B1 is 6-31G\*/LANL2DZ(Fe) and B2 is Def2tzvpp and B3 is 6-311++G(2d,2p)/SDD(Fe).

Reactions	Spin State	Species	B1 + ZPE	B2 +ZPE	G <sub>298K</sub> (B2)	B3 + ZPE	G <sub>298K</sub> (B3)
N4	S=1	<sup>3</sup> R+S	0.0	0.0	0.0	0.0	0.3
		<sup>3</sup> TS	25.9	21.7	34.5	20.2	33.2
		<sup>3</sup> IH	1.2	-8.6	1.1	-6.2	3.0
	S=2	<sup>5</sup> R+S	5.5	2.1	1.1	0.7	0.0
		<sup>5</sup> TS	19.0	12.8	23.1	9.0	20.9
		<sup>5</sup> IH	1.8	-14.6	-5.0	-9.0	0.1
N3O	S=1	<sup>3</sup> R+S	0.0	0.0	0.0	0.0	0.0
		<sup>3</sup> TS	23.7	20.1	31.0	18.6	29.5
		<sup>3</sup> IH	-1.0	-7.8	0.6	-20.8	-15.2
	S=2	<sup>5</sup> R+S	5.0	2.8	1.7	1.2	0.2
		<sup>5</sup> TS	16.6	10.5	20.1	6.2	15.8
		<sup>5</sup> IH	-11.3	-14.1	-10.1	-10.4	-2.0
N2O2	S=1	<sup>3</sup> R+S	0.0	0.0	0.0	0.4	0.6
		<sup>3</sup> TS	21.1	17.8	29.5	16.3	28.5
		<sup>3</sup> IH	-3.0	-10.0	-1.5	-12.2	-3.4
	S=2	<sup>5</sup> R+S	3.6	1.4	1.1	0.0	0.0
		<sup>5</sup> TS	14.4	8.6	18.4	4.6	14.8
		<sup>5</sup> IH	-16.4	-18.9	-11.6	-25.5	-17.8
NO3	S=1	<sup>3</sup> R+S	0.0	0.0	0.0	2.8	4.3
		<sup>3</sup> TS	17.1	14.3	27.1	12.4	25.3
		<sup>3</sup> IH	-6.6	-12.7	-3.1	-15.5	-5.8
	S=2	<sup>5</sup> R+S	6.4	3.6	3.6	0.0	0.0
		<sup>5</sup> TS	13.0	7.2	17.5	2.8	13.2
		<sup>5</sup> IH	-21.3	-23.6	-12.3	-30.9	-19.7
O4	S=1	<sup>3</sup> R+S	0.0	0.0	0.5	0.0	0.7
		<sup>3</sup> TS	14.7	12.1	20.8	10.0	22.3
		<sup>3</sup> IH	-8.2	-14.3	-7.8	-17.3	-9.3
	S=2	<sup>5</sup> R+S	5.3	2.5	0.0	0.8	0.0
		<sup>5</sup> TS	11.3	5.8	13.7	1.4	12.2
		<sup>5</sup> IH	-24.3	-24.1	-23.0	-39.5	-34.4

**Table S2.** Calculated LUMO energies for quintet states.

Reactions	Spin State	LUMO (eV)
N4	S=2	-3.56
N3O	S=2	-3.58
N2O2	S=2	-3.96
NO3	S=2	-4.24
O4	S=2	-4.60

**Table S3.** Calculated distortion energies for quintet states.

Reactions	Spin State	Distortion Energy (kcal mol <sup>-1</sup> )
N4	S=2	13.10
N3O	S=2	12.37
N2O2	S=2	11.65
NO3	S=2	8.72
O4	S=2	4.88

**Table S4.** Spin densities and spin charges for oxidants.

Species	Spin State	Mulliken Spin Density				Mulliken Charges			
		Fe	O	N <sub>ax</sub>	Rest	Fe	O	N <sub>ax</sub>	Rest
N4	S=1	1.321	0.814	-0.024	-0.111	0.405	-0.454	-0.196	0.245
	S=2	2.998	0.660	-0.020	0.362	0.552	-0.444	-0.216	0.108
N3O	S=1	1.330	0.823	-0.024	-0.129	0.469	-0.440	-0.209	0.180
	S=2	3.012	0.688	-0.019	0.319	0.606	-0.430	-0.237	0.061
N2O2	S=1	1.227	0.842	-0.019	-0.050	0.517	-0.431	-0.229	0.143
	S=2	3.040	0.723	-0.019	0.256	0.640	-0.425	-0.269	0.050
NO3	S=1	1.204	0.860	-0.017	-0.047	0.621	-0.410	-0.231	0.020
	S=2	3.060	0.687	-0.014	0.267	0.730	-0.402	-0.267	-0.061
O4	S=1	1.149	0.886	-0.014	-0.021	0.704	-0.390	-0.226	-0.088
	S=2	3.079	0.656	-0.008	0.273	0.811	-0.519	-0.264	-0.028

Species		Mulliken Charges					Mulliken Spin Density				
		Fe	O	H	DHA	Rest	Fe	O	H	DHA	Rest
N4	<sup>3</sup> TS	0.457	-0.637	0.321	0.004	-0.145	1.066	0.586	-0.046	0.507	-0.113
	<sup>3</sup> IH	0.411	-0.723	0.408	0.340	-0.436	1.016	0.113	-0.005	1.000	-0.124
	<sup>5</sup> TS	0.648	-0.666	0.328	0.049	-0.359	3.758	0.284	0.015	-0.378	0.321
	<sup>5</sup> IH	0.623	-0.772	0.431	0.050	-0.332	4.032	0.381	0.005	-0.046	-0.372
N3O	<sup>3</sup> TS	0.513	-0.620	0.319	0.021	-0.233	1.002	0.617	-0.046	0.515	-0.088
	<sup>3</sup> IH	0.464	-0.715	0.417	0.314	-0.480	0.977	0.126	-0.005	1.000	-0.098
	<sup>5</sup> TS	0.698	-0.651	0.322	0.061	-0.430	3.762	0.301	0.010	0.466	-0.539
	<sup>5</sup> IH	0.475	-0.832	0.388	0.932	-0.963	3.706	0.099	0.003	0.308	-0.116
N2O2	<sup>3</sup> TS	0.559	-0.613	0.313	0.040	-0.299	0.962	0.623	-0.040	0.051	0.404
	<sup>3</sup> IH	0.516	-0.715	0.417	0.034	-0.252	0.939	0.130	-0.005	0.980	-0.044
	<sup>5</sup> TS	0.727	-0.641	0.318	0.074	-0.478	3.757	0.328	0.006	0.464	-0.555
	<sup>5</sup> IH	0.490	-0.838	0.387	0.943	-0.982	3.692	0.109	0.003	0.028	0.168
NO3	<sup>3</sup> TS	0.654	-0.586	0.314	0.034	-0.416	0.930	0.655	-0.042	0.499	-0.042
	<sup>3</sup> IH	0.612	-0.709	0.424	0.038	-0.365	0.920	0.130	-0.005	1.000	-0.045
	<sup>5</sup> TS	0.801	-0.609	0.306	0.068	-0.566	3.737	0.355	0.002	-0.425	0.331
	<sup>5</sup> IH	0.557	-0.836	0.391	0.903	-1.015	3.689	0.102	0.003	0.041	0.165
O4	<sup>3</sup> TS	0.723	-0.573	0.312	0.048	-0.510	0.889	0.675	-0.037	0.492	-0.019
	<sup>3</sup> IH	0.692	-0.704	0.428	0.039	-0.455	0.884	0.141	-0.005	0.998	-0.018
	<sup>5</sup> TS	0.849	-0.558	0.283	0.037	-0.611	3.653	0.396	0.001	-0.347	0.291
	<sup>5</sup> IH	0.544	-0.864	0.377	1.014	-1.071	3.688	0.152	0.005	0.000	0.155

**Table S5.** Spin densities and spin charges for TS and intermediates

**Table S6.** Stability constants for all the complexes.

Complex	log $\beta$
N4	28.19
N3O	28.19
N2O2	28.17
NO3	28.17
O4	28.16

**Table S7.** Spin state gap using different functionals where optimisation is done using 6-31G\*/LANL2DZ(Fe) and Def2tzvpp for refinement.

Complex	B3LYP	TPSSH	M06L
N4	2.1	3.2	2.9
N3O	2.8	3.3	3.1
N2O2	1.4	1.6	1.2

NO3	3.6	3.2	1.6
O4	2.5	1.6	1.2

**Cartesian coordinates of optimized geometries of stationary points of quintet state**

**Oxidants**

**N<sub>4</sub>**

Fe	0.657740000	-2.094012000	0.061875000
O	1.067535000	-3.639410000	0.305422000
N	2.147133000	-1.578686000	1.464894000
N	-0.646939000	-2.141232000	1.776348000
N	-0.892857000	-2.696171000	-1.310346000
N	1.896487000	-2.133263000	-1.646887000
C	1.681465000	-2.291213000	2.695484000
H	2.306714000	-1.995316000	3.547638000
H	1.813337000	-3.359108000	2.523592000
C	0.234554000	-1.966764000	2.986258000
H	0.138772000	-0.932993000	3.319323000
H	-0.133798000	-2.601815000	3.799405000
C	-1.278279000	-3.503575000	1.807680000
H	-1.898351000	-3.550980000	2.712819000
H	-0.472888000	-4.231759000	1.909249000
C	-2.157380000	-3.851022000	0.603670000
H	-2.568804000	-4.846360000	0.814682000
H	-3.024810000	-3.185852000	0.554316000
C	-1.486775000	-3.964749000	-0.767718000
H	-0.687678000	-4.706262000	-0.735121000
H	-2.238909000	-4.304547000	-1.492105000
C	-0.212724000	-2.984162000	-2.624399000
H	-0.680395000	-3.856244000	-3.094149000
H	-0.389233000	-2.133154000	-3.282460000
C	1.270398000	-3.221477000	-2.462597000
H	1.749976000	-3.259970000	-3.448993000
H	1.458769000	-4.163633000	-1.948761000
C	3.307787000	-2.547206000	-1.363549000
H	3.862996000	-2.462940000	-2.306396000
H	3.286429000	-3.602004000	-1.081118000
C	4.009318000	-1.757881000	-0.266815000
H	3.986831000	-0.679893000	-0.452643000
H	5.066403000	-2.049189000	-0.299933000
C	3.502921000	-2.114766000	1.124221000
H	3.453909000	-3.201797000	1.217034000
H	4.198041000	-1.742767000	1.887667000
C	2.269556000	-0.117695000	1.731618000
H	2.985861000	0.036620000	2.548506000
H	1.308264000	0.301993000	2.018246000
H	2.625448000	0.393013000	0.839418000
C	-1.712484000	-1.105262000	1.898621000
H	-2.237352000	-1.250864000	2.851938000
H	-2.438877000	-1.168275000	1.096182000
H	-1.265303000	-0.114412000	1.889513000
C	-1.987958000	-1.734065000	-1.623362000
H	-2.651354000	-2.186567000	-2.371968000
H	-1.564812000	-0.819422000	-2.034116000
H	-2.579379000	-1.486529000	-0.749020000
C	1.923048000	-0.861792000	-2.424825000

H	2.481379000	-1.027581000	-3.355038000
H	2.411650000	-0.076868000	-1.848508000
H	0.912711000	-0.541633000	-2.670117000
N	0.143926000	-0.089341000	-0.248612000
C	-0.140610000	1.019381000	-0.415042000
C	-0.496917000	2.407095000	-0.635240000
H	-1.421615000	2.441030000	-1.221577000
H	0.325679000	2.914648000	-1.152689000
H	-0.675626000	2.890582000	0.329803000
O	-3.643560000	1.655974000	-1.452141000
O	-4.696944000	-0.118330000	-0.037675000
C	-5.761742000	2.280041000	-0.028829000
F	-6.407094000	2.051513000	1.129370000
F	-6.598846000	1.973523000	-1.036244000
F	-5.493476000	3.596412000	-0.099602000
S	3.609586000	3.242174000	-0.877733000
O	3.713019000	1.761304000	-0.948458000
O	2.445060000	3.818732000	-1.593006000
O	4.885004000	3.967954000	-1.052764000
C	3.191909000	3.542492000	0.907464000
F	3.112252000	4.857195000	1.171302000
F	4.122557000	3.009878000	1.719161000
F	2.004003000	2.986698000	1.228992000
S	-4.201665000	1.276320000	-0.129797000
O	-3.419773000	1.746133000	1.038208000

**N<sub>3</sub>O**

Fe	0.590956000	1.897017000	0.163899000
O	1.194358000	3.272264000	0.768486000
N	0.715535000	2.787756000	-1.791812000
N	-1.428697000	2.818814000	0.195806000
N	0.500344000	1.022650000	2.155279000
C	-0.069063000	4.043296000	-1.577299000
H	-0.201742000	4.558997000	-2.537075000
H	0.513336000	4.686280000	-0.918325000
C	-1.448429000	3.755227000	-0.981866000
H	-2.090393000	3.310170000	-1.742916000
H	-1.908589000	4.704793000	-0.687066000
C	-1.501858000	3.577495000	1.488416000
H	-2.496598000	4.041988000	1.539133000
H	-0.761382000	4.377181000	1.434782000
C	-1.293767000	2.756828000	2.772539000
H	-1.473981000	3.462529000	3.593444000
H	-2.075282000	1.997464000	2.870438000
C	0.085812000	2.142598000	3.065953000
H	0.861236000	2.908987000	3.020522000
H	0.068483000	1.737738000	4.086859000
C	1.892236000	0.536240000	2.462512000
H	2.089414000	0.651205000	3.534993000
H	1.922457000	-0.526402000	2.216072000
C	2.983194000	1.227763000	1.669832000
H	3.931361000	0.708780000	1.845103000
H	3.099210000	2.285473000	1.928592000
C	3.656381000	1.690122000	-0.588914000
H	4.487061000	0.977572000	-0.616661000

H	4.010342000	2.627128000	-0.140972000	H	-1.024573000	-0.241902000	3.683474000
C	3.123694000	1.940663000	-1.991349000	H	-1.241001000	0.652700000	2.150421000
H	2.713587000	1.014266000	-2.406838000	C	-2.159551000	-1.296834000	2.184124000
H	3.998229000	2.188522000	-2.605075000	H	-3.138632000	-0.860480000	2.401018000
C	2.141579000	3.113627000	-2.123275000	H	-2.060171000	-2.265516000	2.685779000
H	2.454551000	3.926958000	-1.464074000	C	-2.881371000	-2.586166000	0.252737000
H	2.153757000	3.493620000	-3.152717000	H	-3.919708000	-2.283679000	0.414329000
C	0.113676000	1.993259000	-2.895898000	H	-2.670086000	-3.482831000	0.847093000
H	0.089560000	2.607343000	-3.805022000	C	-2.636388000	-2.828731000	-1.232955000
H	-0.900120000	1.689444000	-2.638304000	H	-2.803096000	-1.898504000	-1.784746000
H	0.709859000	1.101349000	-3.082425000	H	-3.430076000	-3.515779000	-1.550962000
C	-2.578252000	1.888314000	0.065248000	C	-1.312004000	-3.503341000	-1.632464000
H	-3.515445000	2.461237000	0.051448000	H	-1.102930000	-4.339646000	-0.962506000
H	-2.612917000	1.182143000	0.890836000	H	-1.400843000	-3.897277000	-2.651783000
H	-2.487904000	1.331390000	-0.865971000	C	-0.176230000	-1.645121000	-2.761489000
C	-0.418752000	-0.137100000	2.337351000	H	-0.208223000	-2.226923000	-3.689952000
H	-0.431373000	-0.414630000	3.400001000	H	0.699915000	-0.999204000	-2.772840000
H	-0.055812000	-0.983918000	1.758443000	H	-1.069042000	-1.026447000	-2.690819000
H	-1.430673000	0.098392000	2.022354000	N	-0.004727000	0.173705000	-0.470642000
N	0.001653000	0.097754000	-0.634312000	C	0.015857000	1.274184000	-0.825144000
C	-0.238785000	-0.957425000	-1.044019000	C	0.033071000	2.647691000	-1.281973000
C	-0.554209000	-2.273765000	-1.557507000	H	0.956621000	3.131195000	-0.938618000
H	-1.419407000	-2.676369000	-1.014168000	H	-0.852312000	3.163597000	-0.888961000
H	0.310924000	-2.934539000	-1.419973000	H	0.002743000	2.658833000	-2.377217000
H	-0.797421000	-2.194494000	-2.622610000	O	3.199871000	3.595185000	-0.467205000
O	2.639957000	1.119746000	0.271163000	O	5.314387000	2.893539000	0.674638000
O	-3.372424000	-3.293224000	-0.001006000	C	4.117224000	1.179738000	-0.909408000
O	-5.569613000	-2.582939000	0.963689000	F	4.628143000	0.076664000	-0.329530000
C	-4.548785000	-1.179039000	-1.002734000	F	4.942240000	1.537874000	-1.909042000
F	-5.169910000	-0.024700000	-0.696490000	F	2.933353000	0.841421000	-1.461680000
F	-5.324449000	-1.849599000	-1.870683000	S	3.917874000	2.561113000	0.319714000
F	-3.400161000	-0.865559000	-1.643140000	O	3.118213000	1.938543000	1.401661000
S	-4.214954000	-2.188251000	0.521803000	O	-5.253035000	3.016326000	0.785481000
O	-3.512175000	-1.232097000	1.410379000	O	-3.072894000	3.570920000	-0.311856000
O	3.649591000	-4.297532000	1.176560000	C	-4.141358000	1.220323000	-0.767917000
O	2.006324000	-4.294899000	-0.714546000	F	-2.973800000	0.795932000	-1.292429000
C	3.692229000	-2.300976000	-0.527306000	F	-4.917583000	1.631002000	-1.786356000
F	2.933087000	-1.538777000	-1.338483000	F	-4.743039000	0.160970000	-0.193280000
F	4.617338000	-2.911676000	-1.288069000	S	-3.875085000	2.589971000	0.460774000
F	4.339069000	-1.483234000	0.326572000	O	-3.145995000	1.918447000	1.564022000
S	2.655208000	-3.541431000	0.387179000	O	-2.047824000	-1.498616000	0.749893000
O	1.731322000	-2.688542000	1.176514000	O	0.230470000	-0.772581000	2.099435000
		<b>N<sub>2</sub>O<sub>2</sub></b>		O	2.077081000	-1.838315000	0.061603000
Fe	-0.011786000	-1.740710000	0.300450000			<b>NO<sub>3</sub></b>	
O	-0.027154000	-3.216961000	0.966396000	Fe	-0.024838000	-1.773042000	0.335068000
N	-0.109606000	-2.595820000	-1.613966000	O	-0.077914000	-3.219082000	1.056545000
C	1.180222000	-3.362328000	-1.657651000	N	-0.170298000	-2.616644000	-1.509719000
H	1.365733000	-3.708385000	-2.681406000	C	1.120973000	-3.377087000	-1.615450000
H	1.072456000	-4.231266000	-1.007725000	H	1.270393000	-3.707828000	-3.649555000
C	2.363192000	-2.501894000	-1.201967000	H	1.044361000	-4.253956000	-0.971369000
H	2.596450000	-1.705716000	-1.909935000	C	2.275234000	-2.497765000	-1.173921000
H	3.243496000	-3.138468000	-1.084835000	H	2.492455000	-1.683873000	-1.865747000
C	2.798329000	-2.329992000	1.230591000	H	3.176486000	-3.097407000	-1.035248000
H	3.860494000	-2.319573000	0.972144000	C	2.701629000	-2.308479000	1.256027000
H	2.484082000	-3.359982000	1.433278000	H	3.746856000	-2.290946000	0.940685000
C	2.553146000	-1.408011000	2.420411000	H	2.403620000	-3.335405000	1.490619000
H	3.236012000	-1.743846000	3.211576000	C	2.504307000	-1.360956000	2.427639000
H	2.839690000	-0.384069000	2.154536000	H	3.181654000	-1.705990000	3.219401000
C	1.156620000	-1.402785000	3.034211000	H	2.816875000	-0.350851000	2.140832000
H	0.797714000	-2.410400000	3.270782000	C	1.107430000	-1.312238000	3.025871000
H	1.152327000	-0.792271000	3.941239000	H	0.740763000	-2.299004000	3.328104000
C	-1.066378000	-0.327547000	2.595179000	H	1.088558000	-0.634118000	3.882843000

C	-1.073527000	-0.221348000	2.465730000	C	-1.157951000	-0.537086000	2.387463000
H	-1.065377000	-0.096405000	3.550782000	H	-1.171831000	-0.514770000	3.478684000
H	-1.189287000	0.747861000	1.980917000	H	-1.318183000	0.463361000	1.984741000
C	-2.171126000	-1.169527000	2.050653000	C	-2.184644000	-1.508307000	1.854850000
H	-3.147654000	-0.687615000	2.139480000	H	-3.190284000	-1.089046000	1.938386000
H	-2.151353000	-2.101430000	2.624360000	H	-2.136889000	-2.486805000	2.342479000
C	-2.888398000	-2.537471000	0.207098000	C	-2.788300000	-2.592542000	-0.245656000
H	-3.889612000	-2.126394000	0.357482000	H	-3.783269000	-2.153007000	-0.145936000
H	-2.746574000	-3.404666000	0.861089000	H	-2.757327000	-3.558141000	0.270879000
C	-2.678933000	-2.900656000	-1.249158000	C	-2.406294000	-2.716903000	-1.709783000
H	-2.869657000	-2.031284000	-1.884955000	H	-2.393547000	-1.730263000	-2.184308000
H	-3.456574000	-3.635817000	-1.489117000	H	-3.205669000	-3.293633000	-2.190895000
C	-1.336334000	-3.560536000	-1.565365000	C	-1.112265000	-3.460909000	-1.985521000
H	-1.139202000	-4.366560000	-0.856032000	H	-1.065491000	-4.417920000	-1.454366000
H	-1.360066000	-3.986765000	-2.574845000	H	-0.984868000	-3.630990000	-3.058165000
C	-0.269235000	-1.653584000	-2.650559000	N	0.032503000	-0.008525000	-0.666682000
H	-0.363819000	-2.231338000	-3.576443000	C	0.017143000	1.066458000	-1.091554000
H	0.623144000	-1.034712000	-2.704001000	C	-0.007316000	2.419816000	-1.611931000
H	-1.138008000	-1.010491000	-2.531538000	H	0.872345000	2.963100000	-1.245436000
N	0.029311000	0.174697000	-0.483737000	H	-0.928702000	2.911894000	-1.274684000
C	0.085166000	1.269147000	-0.851764000	H	0.012763000	2.388335000	-2.706489000
C	0.144974000	2.635084000	-1.334010000	O	3.062013000	3.655133000	-0.443578000
H	1.058656000	3.114667000	-0.962154000	O	5.103941000	2.965652000	0.831932000
H	-0.748408000	3.171610000	-0.991453000	C	4.082178000	1.286746000	-0.904083000
H	0.162707000	2.625673000	-2.429518000	F	4.534298000	0.156942000	-0.324373000
O	3.340840000	3.562342000	-0.502478000	F	5.003247000	1.687070000	-1.796833000
O	5.408726000	2.789160000	0.678782000	F	2.961908000	0.972656000	-1.589653000
C	4.177299000	1.113068000	-0.918894000	S	3.748649000	2.611912000	0.357761000
F	4.625156000	-0.008951000	-0.321683000	O	2.888777000	1.923034000	1.350085000
F	5.040661000	1.429209000	-1.899392000	O	-5.120499000	3.123299000	0.861333000
F	2.993433000	0.821850000	-1.497907000	O	-3.010463000	3.466114000	-0.438988000
S	4.007287000	2.507063000	0.300533000	C	-4.234836000	1.156346000	-0.632386000
O	3.166800000	1.917349000	1.370138000	F	-3.130239000	0.606602000	-1.174620000
O	-5.164271000	3.219428000	0.721076000	F	-5.039701000	1.536207000	-1.638813000
O	-3.001217000	3.530985000	-0.498308000	F	-4.872947000	0.191530000	0.063075000
C	-4.216436000	1.212591000	-0.676608000	S	-3.799695000	2.591906000	0.463539000
F	-3.095404000	0.661683000	-1.181597000	O	-3.022217000	1.951115000	1.552414000
F	-5.002359000	1.560143000	-1.710253000	O	-1.879523000	-1.677992000	0.438578000
F	-4.860726000	0.259439000	0.028005000	O	0.169773000	-0.957294000	1.930989000
S	-3.826753000	2.680764000	0.394415000	O	1.982236000	-1.880392000	0.031141000
O	-3.094188000	2.075466000	1.533756000	O	0.030194000	-2.650838000	-1.569540000
O	-1.959559000	-1.495830000	0.640145000				
O	0.206882000	-0.755992000	2.027351000				
O	1.923680000	-1.860235000	0.096788000				

**O<sub>4</sub>**

Fe	0.048883000	-1.920109000	0.249908000
O	0.025821000	-3.385707000	0.933522000
C	1.315073000	-3.300946000	-1.804452000
H	1.422414000	-3.472832000	-2.879223000
H	1.328933000	-4.253570000	-1.266136000
C	2.364611000	-2.337218000	-1.304172000
H	2.418058000	-1.439663000	-1.920343000
H	3.343398000	-2.817138000	-1.256480000
C	2.786876000	-2.337546000	1.166087000
H	3.830169000	-2.245244000	0.857992000
H	2.547484000	-3.387925000	1.360260000
C	2.513197000	-1.435316000	2.358680000
H	3.187807000	-1.760368000	3.160905000
H	2.773884000	-0.402618000	2.101983000
C	1.104242000	-1.479619000	2.929288000
H	0.786864000	-2.489614000	3.208027000
H	1.030360000	-0.815592000	3.793343000

**TS**

**N<sub>4</sub>**

Fe	-0.601789000	-0.235085000	-0.099054000
O	-2.244110000	-0.686990000	-0.269082000
N	-1.056033000	1.585552000	-1.276836000
N	-0.064948000	-1.058469000	-2.142418000
N	-0.096544000	-2.154651000	0.996042000
N	-1.076626000	0.469913000	1.946448000
C	-1.556201000	0.974659000	-2.541744000
H	-1.730760000	1.759650000	-3.291716000
H	-2.508787000	0.496943000	-2.318543000
C	-0.572680000	-0.039747000	-3.125937000
H	0.295301000	0.484932000	-3.528213000
H	-1.054068000	-0.549668000	-3.969448000
C	-0.842074000	-2.335389000	-2.245639000
H	-0.658113000	-2.757007000	-3.245199000
H	-1.898877000	-2.076145000	-2.180229000
C	-0.503973000	-3.422836000	-1.210388000
H	-1.080883000	-4.302860000	-1.523709000



H	0.544289000	-3.722459000	-1.304100000	C	-5.438401000	-3.538411000	2.546990000
C	-0.868766000	-3.213150000	0.270315000	C	-6.264074000	0.342914000	0.822171000
H	-1.925610000	-2.962922000	0.362764000	C	-4.669463000	-1.598246000	-0.619424000
H	-0.699628000	-4.166015000	0.794036000	C	-5.421568000	-0.574366000	-1.380691000
C	-0.626344000	-1.959722000	2.390422000	C	-6.210648000	0.371598000	-0.689291000
H	-1.123973000	-2.877177000	2.727821000	C	-6.918137000	1.333477000	-1.417717000
H	0.232865000	-1.806294000	3.044935000	H	-7.536950000	2.053594000	-0.887299000
C	-1.600418000	-0.791736000	2.547110000	C	-6.842762000	1.375392000	-2.811644000
H	-1.791834000	-0.642103000	3.619467000	C	-6.057799000	0.440944000	-3.499173000
H	-2.546155000	-1.017848000	2.057962000	C	-5.354183000	-0.525550000	-2.786449000
C	-2.163022000	1.495185000	1.866754000	H	-7.226838000	0.729952000	1.174904000
H	-2.314064000	1.901641000	2.876891000	H	-6.627277000	-2.864746000	4.221541000
H	-3.079549000	0.977056000	1.577349000	H	-7.121539000	-0.652479000	3.217574000
C	-1.913734000	2.653336000	0.889353000	H	-4.336638000	-3.927620000	0.737323000
H	-0.931894000	3.110001000	1.050101000	H	-5.228417000	-4.512932000	2.979214000
H	-2.645206000	3.428017000	1.152634000	H	-3.530011000	-1.119821000	-0.422580000
C	-2.151082000	2.342278000	-0.596101000	H	-7.400657000	2.128891000	-3.361081000
H	-3.065719000	1.755225000	-0.697427000	H	-6.004443000	0.463923000	-4.584167000
H	-2.296582000	3.284716000	-1.143177000	H	-4.753644000	-1.263721000	-3.312863000
C	0.085094000	2.492817000	-1.540796000	H	-5.507329000	1.046168000	1.210555000
H	-0.230602000	3.297482000	-2.220099000	H	-4.394772000	-2.470199000	-1.221815000
H	0.909895000	1.945763000	-1.995699000			<b>N<sub>3</sub>O</b>	
H	0.433976000	2.929792000	-0.606350000	Fe	0.350988000	-0.373542000	0.298181000
C	1.364355000	-1.310126000	-2.453818000	O	2.031258000	-0.636767000	0.467603000
H	1.457961000	-1.722850000	-3.468898000	N	0.065963000	-0.934775000	2.413789000
H	1.810188000	-2.007567000	-1.749706000	N	-0.003148000	-2.511992000	-0.065100000
H	1.917942000	-0.372795000	-2.401927000	N	0.500339000	0.225802000	-1.845957000
C	1.326077000	-2.563690000	1.110981000	C	0.705353000	-2.284624000	2.387028000
H	1.397524000	-3.514958000	1.656348000	H	0.555462000	-2.789110000	3.351739000
H	1.881392000	-1.801349000	1.656716000	H	1.772932000	-2.138293000	2.235776000
H	1.785422000	-2.688230000	0.134527000	C	0.123012000	-3.176100000	1.282464000
C	0.054517000	0.998197000	2.745829000	H	-0.873816000	-3.511912000	1.572150000
H	-0.283817000	1.206201000	3.771015000	H	0.748141000	-4.071124000	1.191209000
H	0.435462000	1.918490000	2.301810000	C	1.093376000	-2.940967000	-0.994733000
H	0.865375000	0.270818000	2.782011000	H	0.949908000	-4.010911000	-1.203790000
N	1.509571000	0.382105000	0.141404000	H	2.032355000	-2.825755000	-0.454005000
C	2.624603000	0.680351000	0.229180000	C	1.173064000	-2.207093000	-2.347932000
C	4.022344000	1.049735000	0.345128000	H	1.980822000	-2.712942000	-2.892488000
H	4.585469000	0.204715000	0.760393000	H	0.270026000	-2.400922000	-2.934752000
H	4.110358000	1.934889000	0.986200000	C	1.531271000	-0.707949000	-2.403999000
H	4.415686000	1.285819000	-0.649055000	H	2.462013000	-0.523768000	-1.867376000
O	5.649267000	-1.768559000	1.128331000	H	1.686737000	-0.440669000	-3.459648000
O	4.486414000	-3.973208000	0.907550000	C	0.973033000	1.652531000	-1.823901000
C	6.613634000	-3.526906000	-0.566196000	H	1.658018000	1.831041000	-2.662901000
F	6.288950000	-4.501666000	-1.435169000	H	0.092842000	2.283122000	-1.962279000
F	7.436857000	-4.054802000	0.357879000	C	1.646707000	2.076553000	-0.530702000
F	7.298504000	-2.585123000	-1.240146000	H	1.790595000	3.162072000	-0.545073000
S	5.094474000	-2.808881000	0.225365000	H	2.610817000	1.586416000	-0.370287000
O	4.332541000	-2.283419000	-0.933252000	C	1.277341000	2.164527000	1.847326000
S	2.613473000	4.859840000	1.352687000	H	1.153948000	3.252085000	1.891173000
O	1.338671000	4.107964000	1.479141000	H	2.347686000	1.930073000	1.892762000
O	3.817474000	4.126251000	1.813928000	C	0.534524000	1.507519000	3.005641000
O	2.545595000	6.281511000	1.751859000	H	-0.541344000	1.686371000	2.903992000
C	2.861509000	4.948414000	-0.486567000	H	0.847935000	2.055090000	3.903159000
F	3.963364000	5.653165000	-0.793727000	C	0.843058000	0.021093000	3.263003000
F	1.811282000	5.534309000	-1.089694000	H	1.904272000	-0.164138000	3.084153000
F	3.001514000	3.715551000	-1.019037000	H	0.634601000	-0.216624000	4.315013000
C	-6.224866000	-2.612375000	3.244161000	C	-1.322035000	-1.040054000	2.924736000
C	-6.502242000	-1.365883000	2.678710000	H	-1.310445000	-1.486808000	3.928532000
C	-5.996859000	-1.019870000	1.421411000	H	-1.929549000	-1.657839000	2.264868000
C	-5.207712000	-1.953882000	0.713985000	H	-1.775436000	-0.050989000	2.983239000
C	-4.935814000	-3.209166000	1.291499000	C	-1.333706000	-2.855469000	-0.629339000

H	-1.421448000	-3.944507000	-0.743410000	H	0.468488000	-2.306165000	3.701097000
H	-1.474232000	-2.392309000	-1.602425000	H	1.693983000	-1.797913000	2.517613000
H	-2.118740000	-2.502998000	0.037067000	C	-0.020772000	-2.798332000	1.665538000
C	-0.722381000	0.190712000	-2.690471000	H	-1.080426000	-2.966684000	1.859678000
H	-0.468652000	0.498296000	-3.714902000	H	0.490979000	-3.764356000	1.673905000
H	-1.464915000	0.878742000	-2.289255000	C	1.072630000	-2.820076000	-0.537937000
H	-1.145877000	-0.809993000	-2.725484000	H	0.903595000	-3.901580000	-0.541509000
N	-1.766901000	0.271343000	0.267091000	H	2.051980000	-2.608753000	-0.100749000
C	-2.840435000	0.703684000	0.277275000	C	0.970774000	-2.297711000	-1.968756000
C	-4.192668000	1.227530000	0.302386000	H	1.756316000	-2.828836000	-2.521738000
H	-4.850065000	0.556089000	-0.263915000	H	0.022947000	-2.625088000	-2.406627000
H	-4.206913000	2.234993000	-0.131062000	C	1.200677000	-0.800020000	-2.239323000
H	-4.537950000	1.275183000	1.340948000	H	2.154040000	-0.478231000	-1.818955000
O	0.763601000	1.735956000	0.562848000	H	1.237172000	-0.652651000	-3.327819000
O	-6.092784000	-1.172956000	-1.087074000	C	0.430353000	1.555008000	-1.928494000
O	-6.884290000	-3.544072000	-1.033726000	H	0.984690000	1.678736000	-2.867492000
C	-5.309872000	-2.707105000	0.887384000	H	-0.527813000	2.068596000	-2.024017000
F	-4.906790000	-3.944224000	1.225150000	C	1.207310000	2.222867000	-0.803325000
F	-6.358014000	-2.385021000	1.663745000	H	1.233077000	3.303282000	-0.976661000
F	-4.302259000	-1.854578000	1.192485000	H	2.228764000	1.844760000	-0.707037000
S	-5.746342000	-2.606353000	-0.915593000	C	1.171621000	2.524244000	1.603519000
O	-4.496511000	-3.035790000	-1.584600000	H	1.035051000	3.609451000	1.554265000
O	-2.262749000	5.907630000	-1.900245000	H	2.240539000	2.295647000	1.530285000
O	-3.969705000	4.432181000	-0.812584000	C	0.583916000	1.989349000	2.907785000
C	-1.607753000	4.643013000	0.303180000	H	-0.495563000	2.174525000	2.920794000
F	-1.834471000	3.540475000	1.043639000	H	1.007580000	2.624720000	3.695399000
F	-1.949399000	5.710500000	1.045946000	C	0.913566000	0.533084000	3.299079000
F	-0.282810000	4.715909000	0.065954000	H	1.949792000	0.307882000	3.041294000
S	-2.572972000	4.599966000	-1.284807000	H	0.802448000	0.421882000	4.385786000
O	-2.013947000	3.418596000	-1.987605000	C	-1.295044000	-0.490065000	3.283564000
C	6.006817000	2.421969000	1.755529000	H	-1.185132000	-0.764561000	4.341199000
C	5.361233000	1.196012000	1.888587000	H	-1.961690000	-1.201016000	2.797949000
C	5.284188000	0.302743000	0.802659000	H	-1.742248000	0.500800000	3.217990000
C	5.865782000	0.658926000	-0.434416000	C	-1.168222000	-0.229474000	-2.342506000
C	6.516897000	1.890898000	-0.553119000	H	-1.038006000	-0.246624000	-3.433530000
C	6.586145000	2.771343000	0.528979000	H	-1.903476000	0.531434000	-2.088366000
C	4.594431000	-1.002250000	0.937286000	H	-1.539243000	-1.198240000	-2.009615000
C	5.759261000	-0.286169000	-1.610587000	N	-1.913658000	0.215674000	0.493995000
C	5.626789000	-1.741001000	-1.218373000	C	-3.048858000	0.437704000	0.505325000
C	5.046793000	-2.079011000	0.024167000	C	-4.476193000	0.690502000	0.523960000
C	4.895285000	-3.434260000	0.373832000	H	-4.983235000	-0.091756000	-0.054877000
H	4.454989000	-3.686589000	1.335664000	H	-4.678329000	1.680035000	0.096069000
C	5.316549000	-4.441804000	-0.489128000	H	-4.832622000	0.661455000	1.559465000
C	5.896595000	-4.104310000	-1.718724000	O	0.501528000	1.968710000	0.439742000
C	6.051430000	-2.762415000	-2.074025000	O	-5.640697000	-2.141372000	-0.928323000
H	4.496729000	-1.332481000	1.976795000	O	-5.311419000	-4.559318000	-1.477463000
H	6.067640000	3.100194000	2.602178000	C	-4.074808000	-3.570202000	0.612417000
H	4.921551000	0.910112000	2.841164000	F	-3.098939000	-4.497685000	0.628101000
H	6.977782000	2.160253000	-1.500644000	F	-5.062504000	-3.996050000	1.417810000
H	7.097827000	3.723665000	0.419089000	F	-3.567575000	-2.439511000	1.152673000
H	4.870278000	-0.004891000	-2.201096000	S	-4.691102000	-3.266759000	-1.114669000
H	5.202937000	-5.484534000	-0.205726000	O	-3.452867000	-2.927774000	-1.854597000
H	6.234664000	-4.885148000	-2.394621000	O	-3.209114000	5.427756000	-1.975537000
H	6.511547000	-2.503634000	-3.024853000	O	-4.660045000	3.901773000	-0.618312000
H	6.611466000	-0.150757000	-2.285942000	C	-2.253467000	4.453773000	0.264280000
H	3.406640000	-0.799129000	0.668878000	F	-2.309887000	3.416920000	1.122809000
		<b>N<sub>2</sub>O<sub>2</sub></b>		F	-2.644986000	5.554943000	0.929957000
Fe	0.245969000	-0.122136000	0.486663000	F	-0.965674000	4.627038000	-0.092315000
O	1.944923000	-0.274712000	0.575694000	S	-3.330173000	4.161023000	-1.223254000
N	0.043445000	-0.495702000	2.639505000	O	-2.706584000	2.978691000	-1.868431000
N	0.132960000	0.099092000	-1.694582000	O	0.046963000	-2.235841000	0.320823000
C	0.622506000	-1.873664000	2.703121000	C	5.736299000	-4.054859000	-1.253712000

C	5.806106000	-2.807323000	-1.877921000	H	-1.143888000	0.673279000	3.093337000
C	5.423832000	-1.644961000	-1.200941000	N	-1.950645000	-0.049059000	0.553033000
C	4.974858000	-1.741357000	0.134962000	C	-3.096026000	-0.036780000	0.713826000
C	4.908302000	-3.003394000	0.755887000	C	-4.530671000	-0.023023000	0.928698000
C	5.286111000	-4.153408000	0.069267000	H	-4.963454000	-0.949917000	0.532985000
C	5.463391000	-0.295002000	-1.881628000	H	-4.961774000	0.854157000	0.430634000
C	4.566107000	-0.514575000	0.860436000	H	-4.731513000	0.038455000	2.004021000
C	5.183361000	0.753726000	0.403112000	O	-5.242536000	-3.270863000	0.082678000
C	5.633561000	0.868779000	-0.930844000	O	-4.372758000	-5.378869000	-0.950095000
C	6.214690000	2.068412000	-1.353745000	C	-2.900271000	-4.167700000	0.849789000
H	6.575059000	2.153980000	-2.376230000	F	-1.721796000	-4.660724000	0.421061000
C	6.341342000	3.149877000	-0.478993000	F	-3.378275000	-5.005084000	1.787449000
C	5.891054000	3.039574000	0.842990000	F	-2.655863000	-2.984267000	1.448515000
C	5.316412000	1.849051000	1.278091000	S	-4.104715000	-3.979007000	-0.555114000
H	6.247651000	-0.277966000	-2.646881000	O	-3.347741000	-3.174968000	-1.544277000
H	6.039026000	-4.947545000	-1.794367000	O	-4.649145000	5.216733000	-1.377992000
H	6.165372000	-2.733426000	-2.901691000	O	-5.317759000	3.080921000	-0.257933000
H	4.568785000	-3.068385000	1.786975000	C	-3.047521000	4.199371000	0.432803000
H	5.238954000	-5.121387000	0.560365000	F	-2.696094000	3.065875000	1.069064000
H	3.361615000	-0.393410000	0.679363000	F	-3.574468000	5.033092000	1.347173000
H	6.797424000	4.073747000	-0.824298000	F	-1.922082000	4.770575000	-0.043436000
H	5.996862000	3.875777000	1.528548000	S	-4.254947000	3.860667000	-0.939552000
H	4.976395000	1.748981000	2.306155000	O	-3.445214000	3.092618000	-1.916057000
H	4.585137000	-0.633542000	1.949100000	O	-0.049795000	2.028453000	-0.161587000
H	4.516160000	-0.157057000	-2.431036000	O	-0.504612000	-0.104109000	-1.834840000
		<b>NO<sub>3</sub></b>		O	0.259389000	-2.115380000	0.258021000
Fe	0.218660000	-0.029115000	0.124745000	C	6.217943000	3.645273000	0.578693000
O	1.857238000	0.068246000	-0.298185000	C	6.404127000	2.369657000	1.115261000
N	0.631685000	-0.106852000	2.226131000	C	5.802562000	1.250656000	0.529828000
C	1.453794000	-1.357360000	2.278442000	C	5.010630000	1.420696000	-0.626601000
H	1.641433000	-1.643601000	3.321535000	C	4.828971000	2.710523000	-1.160959000
H	2.406641000	-1.144897000	1.793649000	C	5.426858000	3.816811000	-0.564999000
C	0.758670000	-2.523350000	1.565287000	C	5.973895000	-0.127427000	1.128598000
H	-0.105387000	-2.895918000	2.117313000	C	4.363662000	0.240311000	-1.256754000
H	1.473815000	-3.340101000	1.439736000	C	5.020196000	-1.071213000	-1.017211000
C	0.832342000	-2.796930000	-0.895709000	C	5.810802000	-1.257837000	0.137546000
H	0.741587000	-3.870345000	-0.708062000	C	6.421048000	-2.497738000	0.353543000
H	1.892248000	-2.529932000	-0.968238000	H	7.042694000	-2.638605000	1.234692000
C	0.062080000	-2.441845000	-2.165637000	C	6.245855000	-3.548855000	-0.548992000
H	0.447735000	-3.111336000	-2.945727000	C	5.457275000	-3.367324000	-1.692698000
H	-0.997921000	-2.685127000	-2.028222000	C	4.849979000	-2.136299000	-1.922142000
C	0.194158000	-1.022996000	-2.717308000	H	6.944288000	-0.203110000	1.632403000
H	1.239317000	-0.708930000	-2.811358000	H	6.694296000	4.503094000	1.045618000
H	-0.291334000	-0.965265000	-3.696038000	H	7.026802000	2.238743000	1.997194000
C	-0.797526000	1.241090000	-2.306212000	H	4.224427000	2.831728000	-2.056717000
H	-0.621387000	1.297886000	-3.383764000	H	5.287513000	4.806831000	-0.990264000
H	-1.853416000	1.418592000	-2.096447000	H	3.269181000	0.161814000	-0.786280000
C	0.063488000	2.270222000	-1.588808000	H	6.729556000	-4.504643000	-0.366310000
H	-0.310600000	3.275269000	-1.806380000	H	5.326906000	-4.179910000	-2.402004000
H	1.117468000	2.193249000	-1.875045000	H	4.247681000	-1.981289000	-2.814120000
C	0.834219000	2.851448000	0.649847000	H	4.121239000	0.404837000	-2.312718000
H	0.495028000	3.885218000	0.535736000	H	5.222894000	-0.254465000	1.927362000
H	1.852454000	2.760118000	0.255375000			<b>O<sub>4</sub></b>	
C	0.768243000	2.448819000	2.122238000	Fe	-0.176110000	0.172641000	0.665949000
H	-0.270175000	2.502387000	2.465641000	O	-1.839661000	0.373233000	0.641891000
H	1.304854000	3.239658000	2.660923000	C	-0.491513000	1.554762000	3.122866000
C	1.435398000	1.122401000	2.538595000	H	-0.260202000	1.708300000	4.181724000
H	2.399229000	1.021301000	2.036295000	H	-1.569405000	1.649851000	2.958296000
H	1.614857000	1.138132000	3.621206000	C	0.303423000	2.540605000	2.275350000
C	-0.516257000	-0.213913000	3.164000000	H	1.361211000	2.524730000	2.541288000
H	-0.133835000	-0.307133000	4.188540000	H	-0.094618000	3.549145000	2.410584000
H	-1.124192000	-1.085994000	2.926534000	C	-0.490245000	3.040029000	-0.053960000



H	1.845741000	-1.022902000	-1.969417000	N	0.508311000	0.170188000	-1.857191000
C	0.807216000	-2.337975000	1.812075000	C	0.643782000	-2.181350000	2.516443000
H	0.678913000	-3.133665000	2.559889000	H	0.537471000	-2.670256000	3.498921000
H	1.534799000	-1.617718000	2.184910000	H	1.698996000	-2.000001000	2.317929000
H	1.197112000	-2.784059000	0.901129000	C	0.080148000	-3.135686000	1.447326000
C	0.320231000	1.688457000	2.702587000	H	-0.927496000	-3.445699000	1.733945000
H	0.037900000	2.145136000	3.661655000	H	0.696816000	-4.045440000	1.440987000
H	0.865944000	2.419934000	2.105422000	C	1.165117000	-2.945022000	-0.776909000
H	0.976051000	0.839220000	2.893429000	H	1.137910000	-4.036128000	-0.937837000
N	1.648709000	0.282275000	0.310702000	H	2.058631000	-2.705018000	-0.200445000
C	2.795660000	0.386214000	0.431992000	C	1.266522000	-2.272684000	-2.165963000
C	4.230762000	0.512505000	0.599071000	H	2.106265000	-2.780244000	-2.659828000
H	4.588508000	-0.335193000	1.192859000	H	0.390738000	-2.522226000	-2.774114000
H	4.455117000	1.467772000	1.087632000	C	1.590962000	-0.764793000	-2.282577000
H	4.712297000	0.479744000	-0.382518000	H	2.461587000	-0.542221000	-1.665567000
O	4.542813000	-2.731212000	1.359155000	H	1.839716000	-0.556457000	-3.337225000
O	3.158864000	-4.286631000	-0.027840000	C	0.947368000	1.599466000	-1.865350000
C	5.771845000	-4.476393000	-0.171681000	H	1.638010000	1.788255000	-2.701695000
F	5.715794000	-5.132806000	-1.344888000	H	0.054301000	2.206804000	-2.030097000
F	5.817000000	-5.392254000	0.812819000	C	1.600300000	2.093923000	-0.577292000
F	6.922981000	-3.780657000	-0.142316000	H	1.714978000	3.183067000	-0.642783000
S	3.549278000	4.644413000	0.799973000	H	2.583010000	1.642812000	-0.407999000
O	2.132620000	4.229163000	0.966413000	C	1.168859000	2.271600000	1.800527000
O	4.537506000	3.773586000	1.482042000	H	1.004368000	3.356363000	1.806907000
O	3.795398000	6.096917000	0.919978000	H	2.248220000	2.094863000	1.914280000
C	3.869863000	4.308890000	-0.999134000	C	0.397922000	1.628844000	2.956402000
F	5.112183000	4.682461000	-1.348149000	H	-0.676561000	1.764623000	2.789507000
F	2.999905000	4.976017000	-1.778543000	H	0.644484000	2.231134000	3.840505000
F	3.742869000	2.994033000	-1.279699000	C	0.722853000	0.158582000	3.306637000
S	4.307575000	-3.351034000	0.031027000	H	1.790082000	-0.021042000	3.155018000
O	4.428356000	-2.427757000	-1.121921000	H	0.517867000	-0.004434000	4.376553000
C	-5.866125000	-4.242256000	0.626175000	C	-1.403386000	-0.965956000	3.026927000
C	-6.152799000	-3.026980000	1.255916000	H	-1.400152000	-1.369276000	4.052564000
C	-6.110436000	-1.818797000	0.557041000	H	-2.002614000	-1.620470000	2.393457000
C	-5.760746000	-1.827322000	-0.824146000	H	-1.881160000	0.015049000	3.041758000
C	-5.478309000	-3.070272000	-1.450375000	C	-1.268287000	-3.012309000	-0.558012000
C	-5.530059000	-4.259384000	-0.736547000	H	-1.297592000	-4.110752000	-0.640088000
C	-6.447383000	-0.520733000	1.261202000	H	-1.376971000	-2.591283000	-1.556531000
C	-5.691250000	-0.602427000	-1.552555000	H	-2.117917000	-2.682101000	0.039652000
C	-5.957741000	0.662675000	-0.949402000	C	-0.652028000	0.056943000	-2.766539000
C	-6.313570000	0.737139000	0.428215000	H	-0.364471000	0.309283000	-3.800143000
C	-6.553554000	1.986897000	1.002813000	H	-1.438320000	0.741130000	-2.445512000
H	-6.824935000	2.042070000	2.055229000	H	-1.052552000	-0.956010000	-2.759405000
C	-6.458409000	3.163061000	0.252205000	N	-1.917164000	0.273637000	0.200361000
C	-6.117200000	3.096855000	-1.107764000	C	-2.995342000	0.697280000	0.190048000
C	-5.870604000	1.865772000	-1.699236000	C	-4.351649000	1.219489000	0.187495000
H	-7.478109000	-0.583321000	1.644244000	H	-5.010837000	0.516591000	-0.335782000
H	-5.907321000	-5.169260000	1.191424000	H	-4.368871000	2.199589000	-0.303823000
H	-6.418724000	-3.018718000	2.311116000	H	-4.697015000	1.329411000	1.221254000
H	-5.220416000	-3.075120000	-2.506954000	O	0.734961000	1.766154000	0.525414000
H	-5.313082000	-5.201453000	-1.233341000	O	-6.262913000	-1.339107000	-1.000209000
H	-3.001526000	-0.173806000	-0.703352000	O	-6.897605000	-3.753304000	-0.856001000
H	-6.652362000	4.123532000	0.721743000	C	-5.287866000	-2.773915000	0.963459000
H	-6.048543000	4.006979000	-1.697865000	F	-4.801178000	-3.979095000	1.308847000
H	-5.608445000	1.805492000	-2.753122000	F	-6.313583000	-2.490490000	1.784549000
H	-5.436284000	-0.635355000	-2.609141000	F	-4.315682000	-1.861946000	1.198495000
H	-5.825761000	-0.426044000	2.163803000	S	-5.817335000	-2.743087000	-0.816725000
		<b>N<sub>3</sub>O</b>		O	-4.577822000	-3.110167000	-1.539396000
Fe	0.315454000	-0.367817000	0.329468000	O	-2.361686000	5.927661000	-2.125484000
O	2.275086000	-0.632207000	0.604309000	O	-4.067054000	4.411136000	-1.095580000
N	-0.026995000	-0.852794000	2.510104000	C	-1.752851000	4.688994000	0.104131000
N	-0.006505000	-2.561065000	0.065153000	F	-2.001112000	3.599920000	0.856730000

F	-2.125477000	5.768564000	0.814910000	C	0.697266000	0.755029000	3.356559000
F	-0.420234000	4.763936000	-0.086137000	H	1.751511000	0.570859000	3.138601000
S	-2.658722000	4.612685000	-1.517370000	H	0.576397000	0.728435000	4.450948000
O	-2.041113000	3.447025000	-2.195259000	C	-1.430031000	-0.412489000	3.363870000
C	5.682793000	1.904823000	2.550702000	H	-1.355364000	-0.629843000	4.441263000
C	5.230240000	0.620664000	2.316025000	H	-2.037923000	-1.184056000	2.890073000
C	5.483346000	-0.006069000	1.065771000	H	-1.940978000	0.542823000	3.234882000
C	6.207105000	0.683736000	0.051289000	C	-1.073203000	-0.246843000	-2.448144000
C	6.647791000	1.982792000	0.309361000	H	-0.879083000	-0.259827000	-3.532705000
C	6.389545000	2.584670000	1.540649000	H	-1.834069000	0.505601000	-2.240113000
C	5.035330000	-1.326701000	0.827232000	H	-1.466156000	-1.218787000	-2.147374000
C	6.474816000	0.026181000	-1.269477000	N	-2.081040000	0.178791000	0.431292000
C	6.079107000	-1.415055000	-1.390116000	C	-3.221533000	0.374390000	0.392106000
C	5.352818000	-2.053085000	-0.342982000	C	-4.654310000	0.610010000	0.343966000
C	4.973719000	-3.417480000	-0.462759000	H	-5.138884000	-0.228367000	-0.170656000
H	4.427707000	-3.883180000	0.352187000	H	-4.851277000	1.550943000	-0.183787000
C	5.306966000	-4.131097000	-1.597582000	H	-5.044944000	0.679927000	1.364948000
C	6.019035000	-3.493340000	-2.631057000	O	0.467407000	2.013748000	0.400441000
C	6.399487000	-2.155191000	-2.528855000	O	-5.665498000	-2.447757000	-0.864705000
H	4.494058000	-1.836454000	1.617010000	O	-5.102995000	-4.843773000	-1.313457000
H	5.499313000	2.388361000	3.504965000	C	-4.020723000	-3.674009000	0.767249000
H	4.686695000	0.070362000	3.078690000	F	-2.965233000	-4.507953000	0.839741000
H	7.200569000	2.523185000	-0.453962000	F	-4.988577000	-4.165349000	1.560650000
H	6.745283000	3.594576000	1.724200000	F	-3.636099000	-2.486464000	1.281472000
H	5.949124000	0.596046000	-2.053460000	S	-4.612905000	-3.487212000	-0.984817000
H	5.026243000	-5.174954000	-1.694931000	O	-3.391283000	-3.062852000	-1.707515000
H	6.282023000	-4.054166000	-3.523562000	O	-3.336745000	5.494646000	-2.220275000
H	6.953010000	-1.685016000	-3.336760000	O	-4.748842000	3.788347000	-1.052502000
H	7.537836000	0.137543000	-1.525680000	C	-2.457978000	4.469020000	0.027407000
H	2.652232000	0.088619000	1.128673000	F	-2.528986000	3.401018000	0.845265000
		<b>N<sub>2</sub>O<sub>2</sub></b>		F	-2.948619000	5.527162000	0.698133000
Fe	0.183211000	-0.112704000	0.529301000	F	-1.156608000	4.711108000	-0.225326000
O	2.144764000	-0.287457000	0.747071000	S	-3.405396000	4.179854000	-1.546195000
N	-0.087452000	-0.361570000	2.754301000	O	-2.643899000	3.091221000	-2.205765000
N	0.163470000	0.078914000	-1.700477000	O	0.080263000	-2.265783000	0.542635000
C	0.590290000	-1.679842000	2.899777000	C	5.744680000	-3.653058000	-2.236693000
H	0.478598000	-2.074510000	3.922776000	C	6.077064000	-2.314771000	-2.447637000
H	1.647756000	-1.521896000	2.688292000	C	5.837587000	-1.363119000	-1.455766000
C	0.045253000	-2.725933000	1.916457000	C	5.242453000	-1.787417000	-0.231708000
H	-0.999480000	-2.972916000	2.119962000	C	4.912419000	-3.155790000	-0.032294000
H	0.634155000	-3.644900000	2.010477000	C	5.163965000	-4.079991000	-1.027353000
C	1.141501000	-2.805488000	-0.285680000	C	6.184606000	0.079637000	-1.670298000
H	1.061225000	-3.899360000	-0.257506000	C	4.998833000	-0.841071000	0.788294000
H	2.101718000	-2.497760000	0.133641000	C	5.391575000	0.514536000	0.700617000
C	1.007557000	-2.341970000	-1.739679000	C	5.988244000	0.996377000	-0.500264000
H	1.771934000	-2.910936000	-2.286237000	C	6.374639000	2.336060000	-0.564645000
H	0.044981000	-2.680887000	-2.137204000	H	6.830859000	2.720120000	-1.472697000
C	1.256516000	-0.858089000	-2.093615000	C	6.184956000	3.178888000	0.530237000
H	2.167100000	-0.519793000	-1.597451000	C	5.603731000	2.706890000	1.722634000
H	1.399431000	-0.789085000	-3.184717000	C	5.207384000	1.386360000	1.808325000
C	0.510224000	1.511858000	-1.956391000	H	7.223022000	0.156534000	-2.023314000
H	1.126310000	1.609450000	-2.862946000	H	5.942106000	-4.379454000	-3.019923000
H	-0.428340000	2.041674000	-2.133031000	H	6.529501000	-2.009596000	-3.386977000
C	1.223961000	2.226301000	-0.807855000	H	4.468012000	-3.455710000	0.912081000
H	1.260785000	3.299338000	-1.033636000	H	4.918975000	-5.127299000	-0.882347000
H	2.246150000	1.862202000	-0.660581000	H	2.565991000	0.546012000	0.999429000
C	0.976128000	2.681705000	1.571078000	H	6.496445000	4.217368000	0.462241000
H	0.773962000	3.754146000	1.461314000	H	5.472630000	3.377890000	2.565550000
H	2.065990000	2.546966000	1.621495000	H	4.760633000	0.992770000	2.716804000
C	0.307819000	2.164499000	2.849011000	H	4.546574000	-1.186401000	1.712241000
H	-0.778541000	2.258979000	2.742398000	H	5.586816000	0.459488000	-2.515021000
H	0.596406000	2.876479000	3.633153000			<b>NO<sub>3</sub></b>	

Fe	0.210453000	0.092210000	-0.080145000	C	5.654597000	4.130535000	0.160150000
O	2.055411000	0.399369000	-0.689920000	C	6.066359000	2.998046000	0.862325000
N	0.785814000	-0.119507000	2.037333000	C	5.747556000	1.721389000	0.395851000
C	1.784179000	-1.213209000	1.875001000	C	4.989669000	1.602010000	-0.802895000
H	2.151513000	-1.566627000	2.851520000	C	4.579991000	2.764847000	-1.507827000
H	2.618062000	-0.798790000	1.308350000	C	4.911752000	4.018570000	-1.029850000
C	1.220811000	-2.417220000	1.102224000	C	6.177115000	0.495968000	1.147466000
H	0.489591000	-2.979676000	1.688268000	C	4.669668000	0.315000000	-1.303730000
H	2.047731000	-3.088929000	0.850453000	C	5.174906000	-0.879589000	-0.734818000
C	1.060928000	-2.485261000	-1.365571000	C	5.935931000	-0.819330000	0.467251000
H	1.092904000	-3.579544000	-1.310749000	C	6.439318000	-2.006737000	1.001087000
H	2.076748000	-2.103220000	-1.506316000	H	7.022221000	-1.978715000	1.917458000
C	0.150883000	-2.078344000	-2.530060000	C	6.207697000	-3.223853000	0.360053000
H	0.506353000	-2.656541000	-3.393884000	C	5.467233000	-3.288328000	-0.834682000
H	-0.871575000	-2.417021000	-2.324998000	C	4.953022000	-2.126272000	-1.377868000
C	0.124559000	-0.612602000	-2.983055000	H	7.238459000	0.582006000	1.417872000
H	1.135882000	-0.198182000	-3.053826000	H	5.917652000	5.115195000	0.536227000
H	-0.365620000	-0.547791000	-3.961704000	H	6.645003000	3.106412000	1.775467000
C	-1.009920000	1.523590000	-2.380659000	H	4.012162000	2.648265000	-2.426713000
H	-0.872973000	1.698726000	-3.453091000	H	4.607350000	4.911300000	-1.566974000
H	-2.069264000	1.627006000	-2.133535000	H	2.221633000	1.338678000	-0.859026000
C	-0.203627000	2.556179000	-1.590914000	H	6.613466000	-4.136204000	0.788011000
H	-0.668956000	3.541409000	-1.715841000	H	5.305602000	-4.243765000	-1.323703000
H	0.836506000	2.608750000	-1.935617000	H	4.381586000	-2.144963000	-2.301098000
C	0.510803000	3.022919000	0.700562000	H	4.111858000	0.247289000	-2.230454000
H	0.018391000	4.002010000	0.726167000	H	5.651175000	0.484510000	2.116737000
H	1.529692000	3.160553000	0.312486000				
C	0.537628000	2.430247000	2.114187000				
H	-0.493474000	2.257803000	2.441695000	Fe	0.280415000	0.299450000	-0.151847000
H	0.926453000	3.232791000	2.754317000	O	2.192434000	0.511842000	-0.076313000
C	1.422536000	1.187682000	2.376833000	C	0.549010000	1.052906000	2.609522000
H	2.335799000	1.266264000	1.782614000	H	0.280479000	1.601935000	3.521462000
H	1.712559000	1.179920000	3.439045000	H	1.640551000	1.048055000	2.506848000
C	-0.219861000	-0.486054000	3.052567000	C	-0.005488000	-0.370019000	2.705357000
H	0.259334000	-0.641539000	4.031732000	H	-1.073775000	-0.341544000	2.939975000
H	-0.736720000	-1.402475000	2.762100000	H	0.517116000	-0.910347000	3.501102000
H	-0.966295000	0.303916000	3.148785000	C	1.058792000	-2.170865000	1.347915000
N	-1.997356000	-0.188256000	0.493054000	H	0.854024000	-2.878189000	2.160030000
C	-3.120420000	-0.343442000	0.727339000	H	2.078424000	-1.785796000	1.471352000
C	-4.529071000	-0.538318000	1.027953000	C	0.894145000	-2.894688000	0.004506000
H	-4.867318000	-1.482740000	0.586532000	H	1.513157000	-3.798758000	0.083649000
H	-5.102865000	0.305705000	0.627545000	H	-0.143306000	-3.234545000	-0.102675000
H	-4.665457000	-0.582012000	2.113903000	C	1.334414000	-2.197646000	-1.291109000
O	-4.824695000	-3.944302000	0.139180000	H	2.306111000	-1.708803000	-1.170862000
O	-3.685970000	-5.894996000	-0.939397000	H	1.391203000	-2.942116000	-2.094200000
C	-2.338998000	-4.462130000	0.793213000	C	0.511399000	-0.543078000	-2.953046000
F	-1.121111000	-4.775909000	0.309629000	H	1.151196000	-1.139770000	-3.612050000
F	-2.640963000	-5.355551000	1.753192000	H	-0.491995000	-0.493815000	-3.386975000
F	-2.248976000	-3.251409000	1.379442000	C	1.092773000	0.865267000	-2.820521000
S	-3.621445000	-4.468080000	-0.553301000	H	1.042311000	1.364938000	-3.796778000
O	-3.044933000	-3.562370000	-1.574322000	H	2.128887000	0.835001000	-2.470666000
O	-5.401632000	4.876026000	-0.861305000	C	0.817480000	2.894837000	-1.492675000
O	-5.643293000	2.602764000	0.155187000	H	0.660421000	3.564635000	-2.347419000
C	-3.474060000	3.982048000	0.677365000	H	1.892422000	2.804053000	-1.302384000
F	-2.902551000	2.871395000	1.177753000	C	0.089337000	3.458753000	-0.264129000
F	-3.993517000	4.673744000	1.708002000	H	-0.992964000	3.341211000	-0.385830000
F	-2.498744000	4.735780000	0.128499000	H	0.277233000	4.540716000	-0.280184000
S	-4.781268000	3.563583000	-0.576607000	C	0.525174000	2.991043000	1.131841000
O	-3.999341000	2.981184000	-1.693238000	H	1.617956000	2.931031000	1.195904000
O	-0.230707000	2.177284000	-0.201788000	H	0.163637000	3.705141000	1.882120000
O	-0.650701000	0.165505000	-2.044400000	N	-1.979627000	0.213130000	-0.289846000
O	0.547473000	-1.992149000	-0.106974000	C	-3.135589000	0.193911000	-0.222491000
				C	-4.585458000	0.178967000	-0.139449000

**O<sub>4</sub>**

H	-4.961766000	-0.658046000	-0.735871000
H	-4.984151000	1.134357000	-0.499788000
H	-4.884364000	0.031986000	0.903200000
O	-4.452245000	-2.980240000	-1.344557000
O	-2.453335000	-4.292052000	-0.605089000
C	-4.833579000	-5.136236000	0.100618000
F	-4.334021000	-5.888711000	1.098602000
F	-4.945167000	-5.918343000	-0.988957000
F	-6.072097000	-4.749347000	0.457820000
S	-4.395740000	4.388011000	-0.638480000
O	-3.237473000	4.063224000	-1.503959000
O	-5.513628000	3.412754000	-0.693819000
O	-4.802933000	5.810330000	-0.631883000
C	-3.721711000	4.139520000	1.075383000
F	-4.637129000	4.452797000	2.009152000
F	-2.635678000	4.908470000	1.288807000
F	-3.355910000	2.856990000	1.275343000
S	-3.746822000	-3.668028000	-0.235606000
O	-3.753338000	-2.945131000	1.057399000
C	5.375914000	-4.064015000	-0.061060000
C	5.669682000	-3.022501000	-0.941931000
C	5.951932000	-1.746493000	-0.454496000
C	5.933190000	-1.536137000	0.957664000
C	5.632189000	-2.610012000	1.841265000
C	5.355391000	-3.862950000	1.333228000
C	6.264150000	-0.613905000	-1.383904000
C	6.213799000	-0.253539000	1.468664000
C	6.520948000	0.861589000	0.665410000
C	6.557378000	0.713437000	-0.754622000
C	6.866831000	1.828037000	-1.533315000
H	6.900666000	1.736162000	-2.615091000
C	7.132725000	3.057206000	-0.929113000
C	7.096702000	3.210637000	0.470812000
C	6.793427000	2.123356000	1.264049000
H	7.111370000	-0.901128000	-2.025793000
H	5.160010000	-5.051047000	-0.460225000
H	5.680458000	-3.204397000	-2.012796000
H	5.627257000	-2.421569000	2.910895000
H	5.125331000	-4.689893000	1.997182000
H	2.627058000	0.187154000	0.724831000
H	7.372629000	3.913855000	-1.552603000
H	7.307013000	4.177581000	0.916330000
H	6.757973000	2.208215000	2.346201000
H	6.191068000	-0.116362000	2.548182000
H	5.426788000	-0.494164000	-2.089164000
O	-0.029882000	1.694243000	1.456619000
O	0.300318000	1.591306000	-1.855078000
O	0.349285000	-1.206373000	-1.677879000
O	0.109227000	-1.084162000	1.452216000