

## SUPPORTING INFORMATION

for

### **Stabilising High-Spin, High-Valent Transition-Metal–Oxo Species in Cucurbit[5]uril: Correlating Structure, Spin State, and Reactivity**

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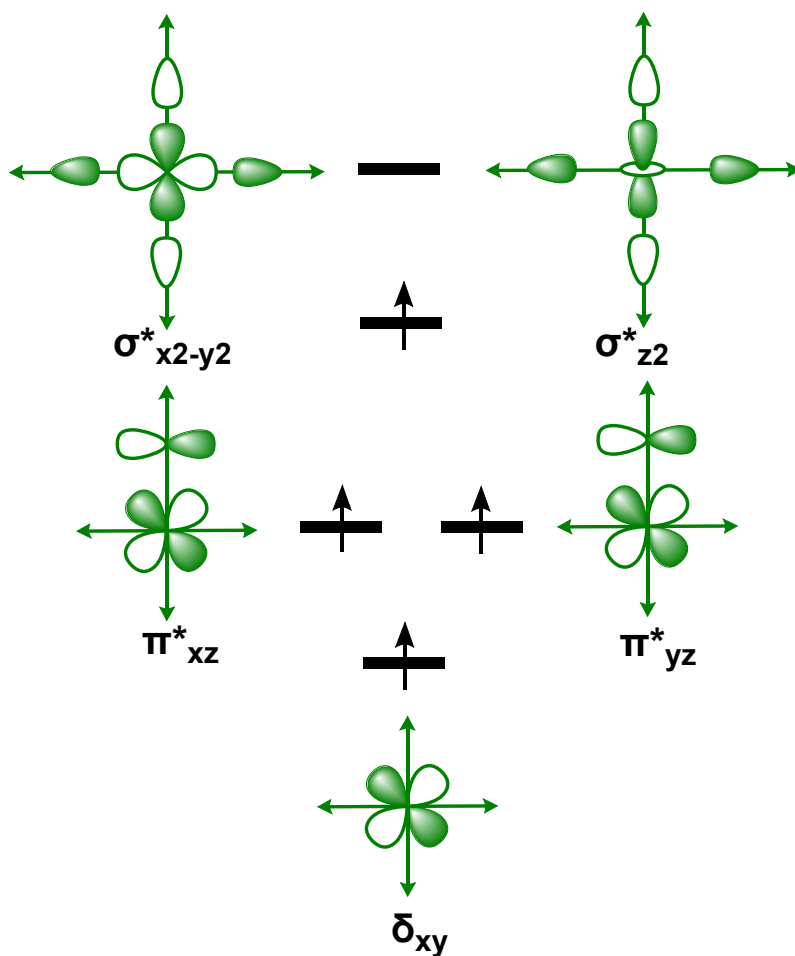
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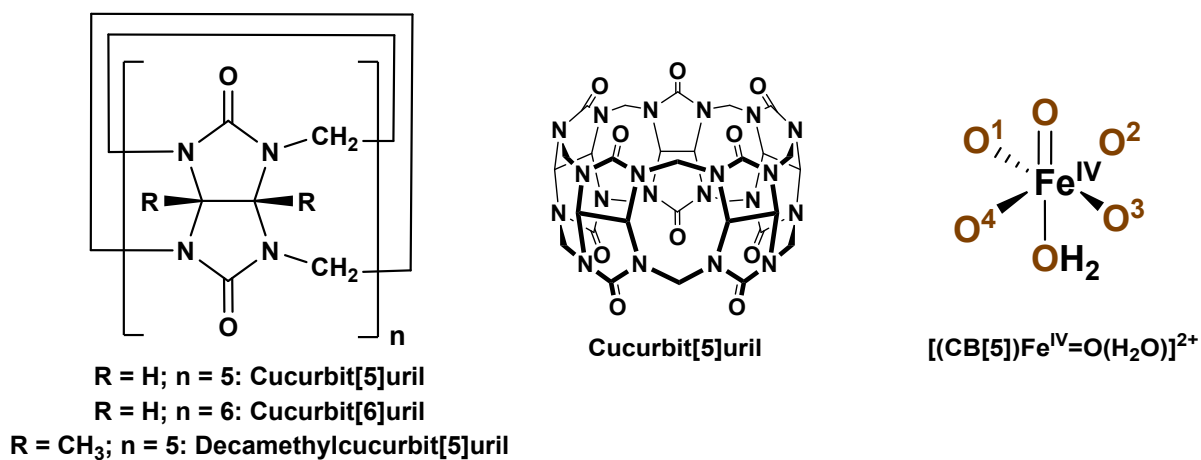
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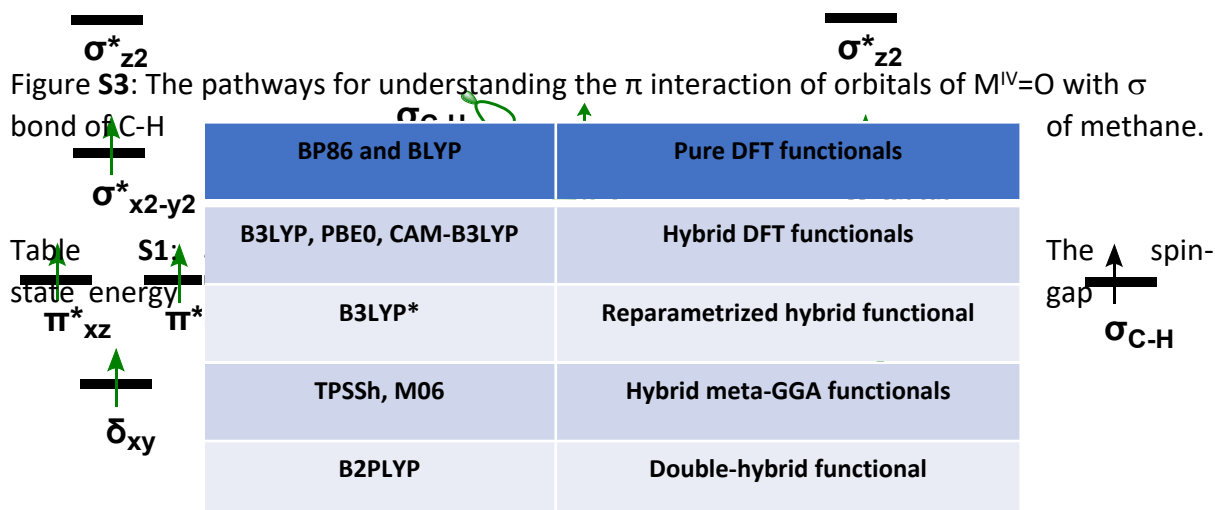


**Figure S1:** Qualitative molecular orbital (MO) diagram for a high-spin Iron(IV)=O species, a ChemDraw representation illustrating the key orbital interactions.

#### Architecture of Formation of $[(CB[5])M^{IV/V}=O(H_2O)]^{2/3+}$ ( $M = Mn, Fe, Co$ )



**Figure S2:** Schematic illustration of ligand–macromolecule assembly leading to high-valent metal–oxo complex formation.



benchmarking to evaluate **DFT functional performance** against **high-level ab initio (DLPNO-CCSD(T))** as reference data  $[(CB[5])M^{IV/V}=O(H_2O)]^{+2/+3}$ , (M = Mn, Fe, and Co; CB[5] = Cucurbit[5]uril). Note all are energy gap in kJ/mol. \*The values in parentheses are next gap.

Table S2: Various type of functional used in benchmarking of complexes against DLPNO-CCSD(T).

Complexes/Functionals	Mn <sup>IV</sup> =O	Mn <sup>V</sup> =O	Fe <sup>IV</sup> =O*	Fe <sup>V</sup> =O	Co <sup>IV</sup> =O*
DLPNO-CCSD	87.2	130.7	122 (258)	60.2	96.2
BP86	55.6	64.2	60.8 (95.9)	54.8	70.3
BLYP	57.4	47.4	63.4 (99.3)	56.8	59.4
OLYP	86.4	94.0	84.8	110.2	90.3
B3LYP	97.9	110.8	90.3 (216)	-5.7	102.9
CAM-B3LYP	19.4	40.2	84.7	123.1	37.2 (85.9)
PBE0	26.0	70.8	45.3	89.2	88.2
M06	55.2	88.2	56.2	59.3	-
TPSSh	-	70.2	33.2	66.7	76.2
B3LYP*	102.1	-	158 (298)	120.3	136.1
B2PLYP	178.2	-	195 (362)	175.6	248 (333)

Table S3: Summary of Functional Performance for benchmarking of complexes against DLPNO-CCSD(T).

Functional Category	Representative Functionals	Performance Summary
Pure GGA	BP86, BLYP	Large underestimation ( $\Delta E$ too small); LS over stabilized
Meta-GGA	OLYP	Best overall agreement (MAE $\approx$ 26 kJ mol <sup>-1</sup> ); balanced behaviour
Hybrid	B3LYP, PBE0, TPSSh	Reliable trends; moderate errors (25–35 kJ mol <sup>-1</sup> )
Meta-hybrid	M06	Slight overestimation; variable accuracy across metals
Range-separated hybrid	CAM-B3LYP	Excessive $\Delta E$ ; large scatter (MAE > 60 kJ mol <sup>-1</sup> )
Double-hybrid	B2PLYP	Drastically overestimated $\Delta E$ ; unsuitable for

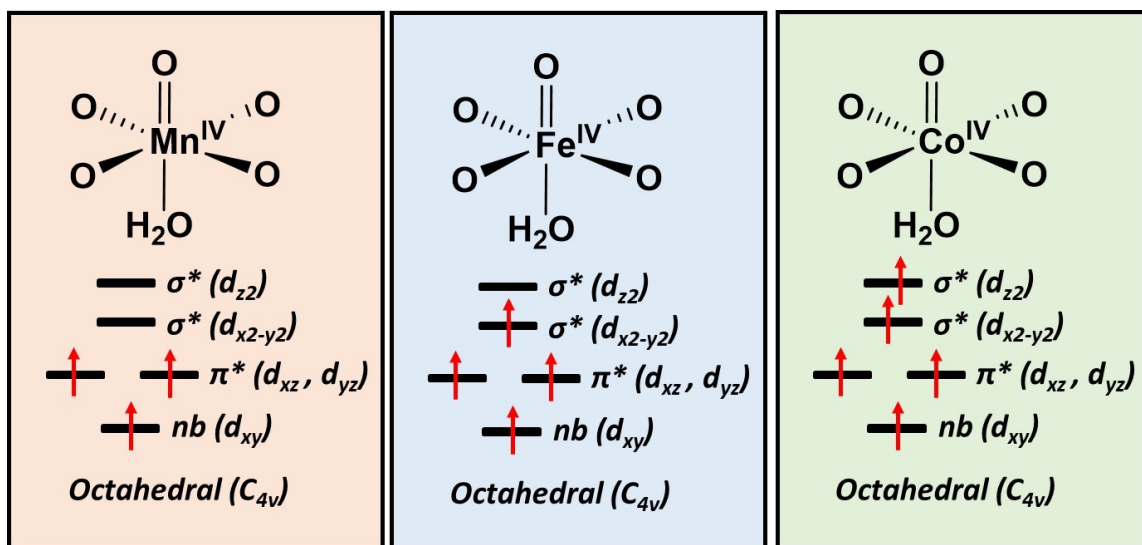


Figure S4: Crystal field splitting of d-orbitals in classical octahedral geometries of Mn<sup>IV</sup>=O, Fe<sup>IV</sup>=O, and Co<sup>IV</sup>=O complexes with Cucurbit[5]uril.

Table S4: Previous reports of C-H activation by Fe<sup>IV</sup>=O with DHA.

Complex	$\Delta G^\ddagger$ (kJ/mol)	References
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{CH}_3\text{CN})]^{2+}$	70.6	Siegbahn & Co-workers, <i>J. Phys. Chem. C</i> <b>2007</b> , <i>111</i> , 12397-12406
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{CF}_3\text{CO}_2)]^+$	60.6	
$[(\text{H}_3\text{buea})\text{Fe}^{\text{IV}}=\text{O}]^-$	109.1	Borovik, Shaik & Coworkers, <i>J. Am. Chem. Soc.</i> <b>2013</b> , <i>135</i> , 17090-17104
$[(\text{H1}^{\text{cyp}})\text{Fe}^{\text{IV}}=\text{O}]^-$	88.2	
$[(\text{N4Py})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$	36.8	
Cpd-I of HRP	59.4	Eldik & Coworkers, <i>Chem. Eur. J.</i> <b>2014</b> , <i>20</i> , 14437 – 14450
Cpd-II of HRP	68.6	
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{CH}_3\text{CN})]^{2+}$	108.3	Shaik & Coworker, <i>J. Am. Chem. Soc.</i> <b>2015</b> , <i>137</i> , 722-733
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{CH}_2\text{S})]^+$	110.4	
$[(\text{TMC})\text{Fe}^{\text{IV}}=\text{O}(\text{N}_3)]^+$	106.2	
Cpd I	38.9	Visser & Coworker <i>Chem. Eur. J.</i> <b>2015</b> , <i>21</i> , 9083-9092
$[(\text{Bn-TPEN})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$	60.2	Shaik & Coworker, <i>J. Am. Chem. Soc.</i> <b>2016</b> , <i>138</i> , 2094-2097
$[(\text{TMG3tren})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$	60.2	Que, Cramer & Coworker <i>Chem. Commun.</i> , <b>2016</b> , <i>52</i> , 10509-10512

[TMG <sub>2</sub> dien(MeCN)Fe <sup>IV</sup> =O] <sup>2+</sup>	45.6	
[(6-PhTPA)Fe <sup>IV</sup> =O] <sup>2+</sup>	58.3	Rajraman & Coworker <i>Chem. Commun.</i> <b>2017</b> , 53, 3193-3196
[(TPFPP)Fe <sup>IV</sup> =O] <sup>2+</sup>	73.6	Shaik & Coworker, <i>J. Am. Chem. Soc.</i> <b>2017</b> , 139, 11451-11459

Table S5: Reported Fe-O bond distance in Fe<sup>IV</sup>=O and Fe<sup>V</sup>=O moieties.

Species	Fe-O (Å)	Reference
CPO-I	1.65	<i>Proc. Natl. Acad. Sci. U.S.A</i> <b>2005</b> , 102 (46), 16563-16565.
TauD-J	1.62	<i>Inorg. Chem.</i> <b>2005</b> , 44 (4), 742-757.
[(H <sub>2</sub> O) <sub>5</sub> Fe <sup>IV</sup> =O] <sup>2+</sup>	1.62	<i>Angew. Chem. Int. Ed.</i> <b>2005</b> , 44, 6871–6874
[(TMG <sub>3</sub> tren)Fe <sup>IV</sup> =O] <sup>2+</sup>	1.66	<i>Angew. Chem. Int. Ed.</i> <b>2009</b> , 48, 3622–3626; <i>J. Am. Chem. Soc.</i> <b>2010</b> , 132, 8635–8644
[(H <sub>3</sub> buea)Fe <sup>IV</sup> =O] <sup>-</sup>	1.68	<i>J. Am. Chem. Soc.</i> <b>2010</b> , 132, 12188–12190
[(Me <sub>4</sub> cy)Fe <sup>IV</sup> =O(CH <sub>3</sub> CN)] <sup>2+</sup>	1.65	<i>Science</i> <b>2003</b> , 299, 1037–1039
[(Me <sub>4</sub> cyS)Fe <sup>IV</sup> =O] <sup>+</sup>	1.70	<i>Science</i> <b>2005</b> , 310, 1000–1002
[(TAML)Fe <sup>V</sup> =O] <sup>-</sup>	1.58	<i>Science</i> <b>2007</b> , 315, 835–838

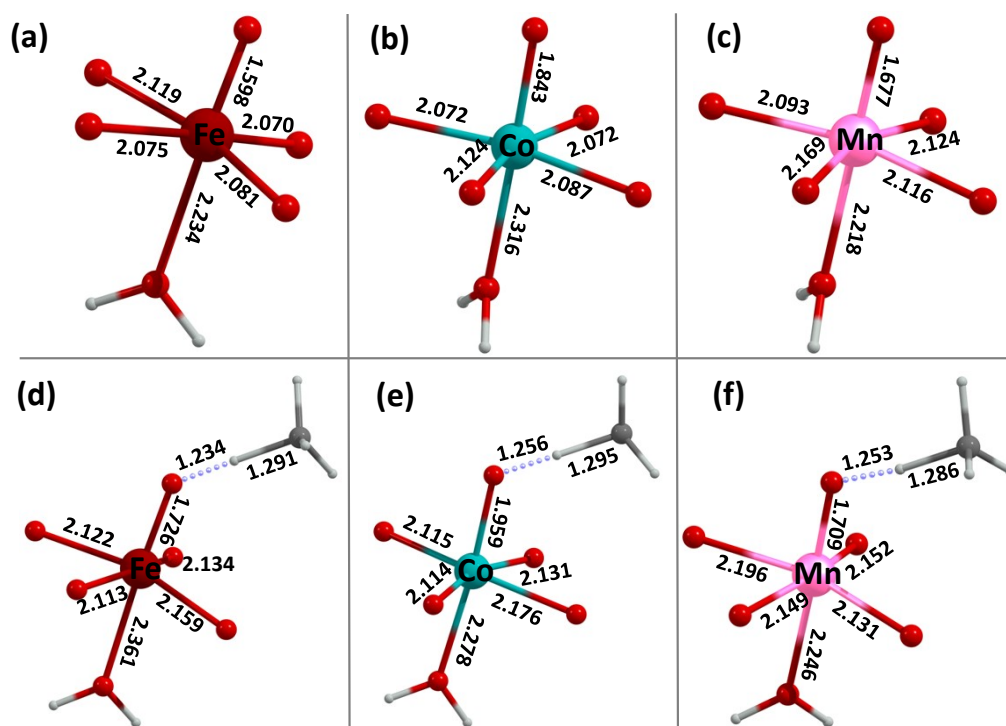


Figure S5: The optimised geometries of (a) Fe<sup>IV</sup>=O, (b) Co<sup>IV</sup>=O, and (c) Mn<sup>IV</sup>=O complexes in first row and below their crossponding transition state (d), (e), and (f) with methane along with their structure parameters. (only primary coordination has been taken for clarity).

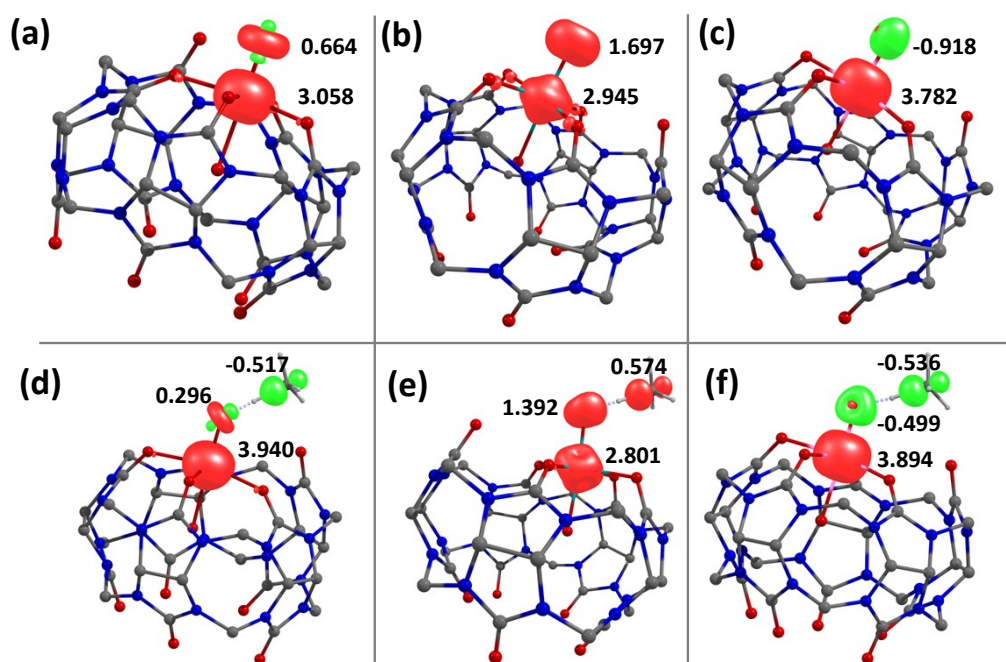


Figure S6: The spin density plots of optimised geometries of (a) Fe<sup>IV</sup>=O, (b) Co<sup>IV</sup>=O, and (c) Mn<sup>IV</sup>=O complexes and for transition state (d) Fe<sup>IV</sup>=O, (e) Co<sup>IV</sup>=O, and (f) Mn<sup>IV</sup>=O, with methane. (hydrogen atoms are omitted for clarity).

Table S6: Bond distance primary coordination sphere of Fe<sup>IV</sup>=O, Co<sup>IV</sup>=O, and Mn<sup>IV</sup>=O complexes and their corresponding transition state.

	rc_Mn <sup>IV</sup> =O	ts_Mn <sup>IV</sup> =O	rc_Fe <sup>IV</sup> =O	ts_Fe <sup>IV</sup> =O	rc_Co <sup>IV</sup> =O	ts_Co <sup>IV</sup> =O
Fe-O <sub>oxo</sub>	1.677	1.709	1.598	1.726	1.843	1.959
Fe-O <sub>1</sub>	2.093	2.196	2.119	2.122	2.072	2.115
Fe-O <sub>2</sub>	2.124	2.152	2.070	2.134	2.072	2.131
Fe-O <sub>3</sub>	2.116	2.131	2.081	2.159	2.087	2.176
Fe-O <sub>4</sub>	2.169	2.149	2.075	2.113	2.124	2.114
Fe-O <sub>H2O</sub>	2.218	2.246	2.234	2.361	2.316	2.278

Table S7: Energy calculated for def2-TZVP optimisations for checking basis set dependency of spin state and energy barrier.

Species	Relative energies (kJ/mol)
<sup>4</sup> rc_Mn <sup>IV</sup> =O	0.0
<sup>2</sup> rc_Mn <sup>IV</sup> =O	115
<sup>4</sup> ts_Mn <sup>IV</sup> =O	54.8
<sup>6</sup> rc_Co <sup>IV</sup> =O	0.0
<sup>4</sup> rc_Co <sup>IV</sup> =O	100.3

${}^6t_{s\_Co^{IV}=O}$	43.68
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Table  
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S8:

Functional	Mn <sup>V</sup> =O		Fe <sup>V</sup> =O	
	$\langle S^2 \rangle_{BS}$	$\langle S^2 \rangle_{HS}$	$\langle S^2 \rangle_{BS}$	$\langle S^2 \rangle_{HS}$
<b>BP86</b>	0.263	2.098	2.089	3.794
<b>BLYP</b>	0.288	2.122	1.954	3.798
<b>OLYP</b>	0.190	2.221	2.194	3.982
<b>B3LYP</b>	0.040	2.329	2.470	3.898
<b>CAM-B3LYP</b>	0.324	2.168	2.094	3.938
<b>PBE0</b>	0.495	2.295	2.304	4.021
<b>M06</b>	0.489	2.066	0.829	3.979
<b>TPSSH</b>	0.203	2.303	0.859	3.911
<b>B3LYP*</b>	--	--	2.206	3.692
<b>B2PLYP</b>	--	--	2.049	3.632

computed spin-expectation ( $\langle S^2 \rangle$ ) value for Mn<sup>V</sup>=O and Fe<sup>V</sup>=O species.

**Table S9:** Optimised geometries (in Angstroms) of all catalytic species in the DFT model were obtained using the unrestricted B3LYP-D3 functional with the LanL2DZ for metal and 6-31g\* for other atoms, basis set.

<sup>5</sup> Fe <sup>IV</sup> =O Species			
Fe	-0.066979000	-0.474808000	-2.543355000
C	0.870636000	3.612044000	-1.813407000
N	2.017321000	3.627438000	-1.027354000
C	1.771777000	4.080424000	0.337397000
C	0.236508000	4.443087000	0.322804000
N	-0.161291000	4.140348000	-1.047548000
N	-0.326839000	3.559477000	1.318332000
C	0.604963000	2.636279000	1.785176000
N	1.860880000	3.041085000	1.337723000
C	3.087606000	2.635165000	2.012847000
N	3.665080000	1.397282000	1.536298000
C	3.541964000	0.222402000	2.278666000
N	3.964313000	-0.828580000	1.447951000
C	4.336193000	-0.372027000	0.134156000
C	4.199214000	1.186929000	0.216591000
N	3.273029000	1.512956000	-0.874038000
C	2.731008000	0.389013000	-1.416431000
N	3.385526000	-0.712101000	-0.928273000
C	3.811164000	-2.206962000	1.865810000
N	2.575720000	-2.861880000	1.417824000
C	1.394984000	-2.742380000	2.147510000
N	0.356886000	-3.331485000	1.365078000
C	0.937323000	-4.179969000	0.331051000
C	2.414464000	-3.656392000	0.228698000
N	0.386600000	-3.917263000	-0.995716000
C	1.173397000	-3.017804000	-1.660926000
N	2.371244000	-2.913161000	-1.041531000
C	-0.902412000	-3.688432000	2.045298000
N	-2.055528000	-3.007709000	1.507777000
C	-2.570295000	-1.865669000	2.141561000
N	-3.611177000	-1.385815000	1.344085000
C	-3.823909000	-2.190054000	0.170061000
C	-2.771720000	-3.359932000	0.310344000
N	-3.418616000	-1.564280000	-1.100999000
C	-2.321253000	-2.142440000	-1.634458000
N	-1.980976000	-3.253665000	-0.926944000
C	-4.435132000	-0.254748000	1.780072000
N	-3.960652000	1.053970000	1.376738000
C	-3.122284000	1.802555000	2.217997000
N	-2.680128000	2.898364000	1.473572000
C	-3.230232000	2.945454000	0.144332000
C	-4.042652000	1.609335000	0.052481000
N	-2.237898000	2.820644000	-0.927002000
C	-2.221729000	1.561197000	-1.444027000
N	-3.306333000	0.863861000	-0.975109000
C	3.375411000	-2.012206000	-1.562968000
C	-0.980766000	-4.199040000	-1.401946000
C	-3.876854000	-0.296820000	-1.628419000
O	1.250546000	-2.231237000	3.226308000
O	-2.187265000	-1.409176000	3.189146000
O	-2.868806000	1.568216000	3.372652000
O	0.855139000	-2.378225000	-2.685025000
O	1.798448000	0.374924000	-2.254290000
O	-1.729350000	-1.712887000	-2.651130000
O	-1.354611000	1.131955000	-2.239890000
C	-1.620246000	3.747925000	1.967293000
C	3.154699000	2.867634000	-1.452867000
C	-1.511962000	3.972621000	-1.496875000
O	3.181798000	0.127656000	3.425025000
O	0.366150000	1.649842000	2.457174000
O	0.791391000	3.225648000	-2.960677000
O	-0.022584000	-0.271272000	-4.128334000
O	-0.138326000	-0.678087000	-0.319539000
H	-0.091241000	-1.494905000	0.224241000
H	-0.019042000	0.061684000	0.306953000
H	-0.802495000	-3.369126000	3.086198000
H	-1.049077000	-4.774373000	2.002596000
H	-5.456238000	-0.410363000	1.416833000
H	-4.431562000	-0.253669000	2.872090000
H	3.791219000	-2.194563000	2.957574000
H	4.660816000	-2.804454000	1.521072000



O	-1.910277000	-1.576808000	-2.670346000	H	5.186144000	1.872459000	0.548502000
O	0.979579000	-1.403327000	-2.164217000	H	2.273162000	4.904475000	-0.057904000
O	-2.197252000	1.027742000	-2.634397000	H	4.597866000	-2.666217000	-1.224849000
O	0.612055000	1.529501000	-2.150195000	H	3.690300000	-1.909274000	-2.559486000
C	2.975937000	2.817130000	1.947812000	H	3.103552000	2.681404000	-2.598436000
C	3.802838000	-1.957170000	-1.474804000	H	3.806634000	3.665013000	-1.288697000
C	3.205604000	2.779291000	-1.516050000				
O	1.235857000	-2.956242000	3.403066000			<b><sup>1</sup>FeIV=O</b>	
O	1.700704000	0.231903000	2.447019000	Fe	-0.585662000	-0.097840000	-2.465227000
O	3.383797000	0.381922000	-2.996761000	C	3.745537000	0.454581000	-1.839414000
O	-0.324755000	-0.062089000	-4.050766000	N	4.150238000	-0.615094000	-1.047537000
O	-0.794446000	-0.091388000	-0.264714000	C	4.466582000	-0.228034000	0.322127000
H	-1.510242000	-0.445519000	0.308513000	C	4.268139000	1.336834000	0.307226000
H	-0.021748000	0.033362000	0.318458000	N	3.853959000	1.603955000	-1.065327000
H	-3.442661000	-0.427004000	3.085864000	N	3.240109000	1.554060000	1.299777000
H	-4.849692000	-0.676018000	2.004909000	C	2.698496000	0.359087000	1.763864000
H	-2.260574000	4.962334000	1.424184000	N	3.511905000	-0.677000000	1.311312000
H	-1.749763000	4.050658000	2.873404000	C	3.558589000	-1.966058000	1.989426000
H	-0.733407000	-4.331418000	2.925665000	N	2.600321000	-2.938122000	1.509909000
H	-1.004884000	-5.346327000	1.480548000	C	1.462948000	-3.247286000	2.254342000
H	-3.066016000	-4.513196000	0.138679000	N	0.629467000	-4.014156000	1.421152000
H	-4.623506000	-2.640661000	0.556700000	C	1.171830000	-4.156202000	0.094722000
H	-5.212345000	1.520168000	0.386064000	C	2.587880000	-3.498596000	0.182177000
H	-4.061610000	3.683834000	0.109672000	N	2.576782000	-2.505405000	-0.894443000
H	-0.131872000	5.320773000	-0.304281000	C	1.319034000	-2.323847000	-1.392040000
H	-5.316760000	-0.633663000	-1.043600000	N	0.511236000	-3.338173000	-0.924818000
H	-4.293793000	-0.505001000	-2.493224000	C	-0.717010000	-4.349877000	1.831432000
H	-1.510074000	3.259735000	-2.685629000	N	-1.763788000	-3.415492000	1.387586000
H	-1.906541000	4.550616000	-1.531284000	C	-2.082161000	-2.284726000	2.136252000
H	-0.656247000	-3.554793000	-2.651097000	N	-3.004932000	-1.515273000	1.361358000
H	-0.752524000	-4.892844000	-1.484487000	C	-3.588136000	-2.348322000	0.317677000
H	3.323069000	-1.842629000	3.046937000	C	-2.571553000	-3.541593000	0.203422000
H	4.569140000	-2.376087000	1.886972000	N	-3.529776000	-1.720546000	-1.002298000
H	3.868467000	3.441818000	1.829688000	C	-2.405937000	-2.127414000	-1.659224000
H	2.792082000	2.649867000	3.011539000	N	-1.898660000	-3.225770000	-1.070391000
H	1.165580000	-5.210352000	-0.224267000	C	-3.779118000	-0.459875000	2.043631000
H	3.395476000	-4.215676000	0.024388000	N	-3.543444000	0.860672000	1.508018000
H	5.481805000	-0.560515000	0.580959000	C	-2.636363000	1.733486000	2.133822000

N	-2.560076000	2.884053000	1.347400000	H	-1.768191000	4.041477000	2.874022000
C	-3.397471000	2.812674000	0.180833000	H	-0.716689000	-4.335345000	2.923345000
C	-4.130838000	1.418565000	0.319158000	H	-0.982756000	-5.350881000	1.477667000
N	-2.675493000	2.651157000	-1.097153000	H	-3.045119000	-4.526314000	0.135208000
C	-2.826329000	1.421129000	-1.615660000	H	-4.611102000	-2.661183000	0.552568000
N	-3.761128000	0.720423000	-0.926264000	H	-5.221376000	1.497164000	0.384760000
C	-1.777602000	4.047820000	1.782052000	H	-4.079353000	3.665942000	0.109218000
N	-0.389318000	4.059111000	1.370598000	H	-0.156426000	5.318097000	-0.303071000
C	0.613574000	3.548507000	2.211313000	H	-5.314012000	-0.657957000	-1.046284000
N	1.789126000	3.517139000	1.459435000	H	-4.291144000	-0.521950000	-2.495315000
C	1.628215000	4.029330000	0.122658000	H	-1.525770000	3.251817000	-2.685486000
C	0.092608000	4.306772000	0.038366000	H	-1.926573000	4.541246000	-1.531001000
N	1.859232000	3.044413000	-0.935913000	H	-0.636701000	-3.553759000	-2.652673000
C	0.684411000	2.542491000	-1.416979000	H	-0.727259000	-4.893647000	-1.487801000
N	-0.350701000	3.330826000	-0.962619000	H	3.327968000	-1.827176000	3.048082000
C	-0.678647000	-3.805674000	-1.591994000	H	4.578227000	-2.354911000	1.890090000
C	-4.287556000	-0.547761000	-1.404491000	H	3.852336000	3.458496000	1.831407000
C	-1.623127000	3.494984000	-1.626686000	H	2.779232000	2.661714000	3.012887000
O	-1.661752000	-1.981024000	3.220451000	H	1.188206000	-5.203633000	-0.227461000
O	-2.057566000	1.519906000	3.168846000	H	3.414253000	-4.200530000	0.024710000
O	0.489659000	3.240669000	3.370013000	H	5.483982000	-0.536770000	0.585248000
O	-1.902093000	-1.585246000	-2.674453000	H	5.178217000	1.895119000	0.551478000
O	0.986630000	-1.390038000	-2.154679000	H	2.250403000	4.913154000	-0.057232000
O	-2.198489000	1.016093000	-2.629867000	H	4.610077000	-2.646377000	-1.222920000
O	0.607314000	1.533174000	-2.154261000	H	3.700149000	-1.892503000	-2.557654000
C	2.962648000	2.829724000	1.949199000	H	3.093198000	2.694586000	-2.596870000
C	3.812817000	-1.939896000	-1.472958000	H	3.790293000	3.681726000	-1.286549000
C	3.194074000	2.792892000	-1.514412000				
O	1.247088000	-2.952417000	3.403237000			<sup>5</sup> Fe <sup>IV</sup> =O (ts)	
O	1.693788000	0.239110000	2.440871000	Fe	-0.344063000	-0.261542000	2.550831000
O	3.385807000	0.396956000	-2.995411000	C	3.159974000	1.945620000	1.550840000
O	-0.324480000	-0.064172000	-4.051111000	N	2.781537000	3.033027000	0.776247000
O	-0.793477000	-0.092140000	-0.261877000	C	3.264552000	2.958296000	-0.597674000
H	-1.507517000	-0.453806000	0.308897000	C	4.095527000	1.619275000	-0.610097000
H	-0.023904000	0.039269000	0.324155000	N	3.959095000	1.134002000	0.757711000
H	-3.442966000	-0.445015000	3.083947000	N	3.435365000	0.820173000	-1.618461000
H	-4.848020000	-0.700375000	2.001958000	C	2.331572000	1.467010000	-2.175916000
H	-2.282522000	4.951436000	1.424987000	N	2.247155000	2.734675000	-1.600826000

C	1.435355000	3.780141000	-2.213350000	C	0.997207000	-3.811258000	1.452258000
N	0.093340000	3.892256000	-1.681392000	O	-2.647098000	0.459682000	-3.267937000
C	-1.009586000	3.420948000	-2.396529000	O	-0.806233000	-2.522094000	-3.308264000
N	-2.114707000	3.497928000	-1.532742000	O	2.241681000	-2.203913000	-3.594368000
C	-1.757465000	3.979313000	-0.225836000	O	-2.415047000	0.043471000	2.599924000
C	-0.240167000	4.346652000	-0.356335000	O	-0.160910000	1.799085000	2.094473000
N	0.389752000	3.586023000	0.724079000	O	-1.019577000	-2.267798000	2.622919000
C	-0.477556000	2.694478000	1.282409000	O	1.582890000	-1.014564000	2.106592000
N	-1.745960000	2.958718000	0.827760000	C	4.010822000	-0.357742000	-2.255522000
C	-3.380325000	2.893510000	-1.893078000	C	1.732306000	3.888105000	1.245275000
N	-3.581044000	1.522013000	-1.415922000	C	4.264728000	-0.191823000	1.204853000
C	-3.212932000	0.430079000	-2.203621000	O	-1.023198000	3.057501000	-3.545563000
N	-3.645599000	-0.726883000	-1.538276000	O	1.583803000	1.010584000	-3.013938000
C	-4.363105000	-0.444517000	-0.323163000	O	2.865764000	1.751284000	2.713481000
C	-4.276804000	1.128881000	-0.217838000	O	-0.105247000	-0.116510000	4.196252000
N	-3.695857000	-0.901675000	0.905856000	O	-0.596648000	-0.410095000	0.201422000
C	-3.144932000	0.139531000	1.589686000	H	-1.163941000	-0.991945000	-0.346300000
N	-3.527881000	1.312970000	1.036263000	H	-0.000436000	0.037313000	-0.423178000
C	-3.332716000	-2.034182000	-2.064200000	H	-3.072826000	-1.896880000	-3.117241000
N	-2.170098000	-2.661014000	-1.414550000	H	-4.204071000	-2.694591000	-1.979299000
C	-1.034335000	-2.970752000	-2.215388000	H	1.260034000	-5.298499000	-1.633665000
N	-0.250865000	-3.863860000	-1.488298000	H	1.027393000	-4.258513000	-3.068428000
C	-0.891815000	-4.303870000	-0.276329000	H	-3.399966000	2.863741000	-2.984567000
C	-2.314422000	-3.641127000	-0.347199000	H	-4.207220000	3.511383000	-1.527581000
N	-0.365691000	-3.735197000	0.974152000	H	-5.253022000	1.618292000	-0.135092000
C	-1.268022000	-2.949736000	1.607877000	H	-5.389166000	-0.828309000	-0.347459000
N	-2.476177000	-3.034974000	0.971723000	H	-3.122445000	-4.354129000	-0.544838000
C	1.069872000	-4.276786000	-1.977366000	H	-0.913728000	-5.396530000	-0.204616000
N	2.165665000	-3.408955000	-1.600114000	H	3.266745000	-4.291138000	-0.034454000
C	2.590984000	-2.376185000	-2.453569000	H	-4.536304000	-2.796548000	1.078858000
N	3.523776000	-1.622057000	-1.741107000	H	-3.611041000	-2.230436000	2.489869000
C	3.788662000	-2.140629000	-0.423856000	H	0.974568000	-3.579866000	2.518214000
C	2.788876000	-3.342123000	-0.304109000	H	1.367902000	-4.832190000	1.318383000
N	3.393870000	-1.254040000	0.674317000	H	-2.732438000	2.406707000	2.576153000
C	2.231689000	-1.662614000	1.257348000	H	-3.690727000	3.350335000	1.412553000
N	1.909282000	-2.909904000	0.784464000	H	1.314115000	3.550577000	-3.274423000
C	-2.952214000	2.550057000	1.517342000	H	1.967764000	4.731885000	-2.102994000
C	-3.634625000	-2.268519000	1.399821000	H	5.100489000	-0.303219000	-2.151955000



			<b><sup>4</sup>Fe<sup>III</sup>-OH</b>				
O	-0.554020000	-1.946120000	2.798410000				
O	-0.937844000	-3.031971000	-2.977319000	Fe	0.145591000	0.483631000	-2.477427000
O	-0.010945000	0.091136000	-4.393251000	C	-1.295635000	-3.345280000	-1.865171000
O	0.190800000	0.679019000	-0.279195000	N	-2.444455000	-3.246571000	-1.094854000
H	0.193597000	1.473311000	0.294615000	C	-2.286707000	-3.788903000	0.250465000
H	0.036081000	-0.072593000	0.318775000	C	-0.814246000	-4.346573000	0.237531000
H	0.999739000	3.339289000	3.137683000	N	-0.356029000	-4.030709000	-1.111448000
H	1.334391000	4.721297000	2.047822000	N	-0.162292000	-3.609797000	1.297029000
H	5.444968000	0.090519000	1.492443000	C	-1.010599000	-2.683216000	1.904254000
H	4.381418000	-0.017109000	2.924536000	N	-2.269043000	-2.805959000	1.311550000
H	-3.630018000	2.377250000	2.997826000	C	-3.454216000	-2.250006000	1.955748000
H	-4.479195000	3.054606000	1.579072000	N	-3.827993000	-0.926306000	1.498278000
H	-2.901577000	4.622396000	0.221247000	C	-3.561036000	0.206051000	2.270420000
H	-0.562893000	5.296878000	0.613066000	N	-3.852428000	1.323702000	1.468093000
H	3.479512000	4.163798000	0.427669000	C	-4.268298000	0.951493000	0.141829000
H	4.997698000	2.244894000	0.171217000	C	-4.347959000	-0.614472000	0.191708000
H	4.993570000	-2.028341000	-0.216516000	N	-3.488219000	-1.033388000	-0.918450000
H	1.550328000	5.127254000	-0.986070000	C	-2.775480000	0.012223000	-1.416377000
H	1.253305000	4.147026000	-2.440589000	N	-3.264513000	1.183050000	-0.902737000
H	3.682663000	0.096497000	-2.650324000	C	-3.486288000	2.658511000	1.896350000
H	5.006382000	-0.011580000	-1.468937000	N	-2.172547000	3.127254000	1.434333000
H	-3.081849000	2.120688000	-2.598910000	C	-1.020313000	2.846538000	2.161382000
H	-4.215789000	2.758253000	-1.386414000	N	0.089512000	3.309927000	1.389117000
H	-3.072949000	-2.369408000	3.051340000	C	-0.377066000	4.253934000	0.375978000
H	-4.047834000	-3.248554000	1.838870000	C	-1.909233000	3.932160000	0.266358000
H	1.633893000	-4.950507000	1.782915000	N	0.136620000	3.956418000	-0.955354000
H	1.324964000	-3.688914000	3.010335000	C	-0.762804000	3.187037000	-1.651185000
H	-5.301993000	1.041666000	-0.103994000	N	-1.967500000	3.232338000	-1.023109000
H	-5.250249000	-1.407995000	0.063970000	C	1.370994000	3.517168000	2.094505000
H	-2.697807000	-4.775292000	0.477060000	N	2.447289000	2.714790000	1.570963000
H	-0.355660000	-5.475080000	0.448210000	C	2.777347000	1.493372000	2.175820000
H	3.621874000	-4.056543000	-0.019164000	N	3.744340000	0.883026000	1.376373000
H	-4.259656000	-3.129619000	-1.233506000	C	4.087699000	1.676628000	0.222738000
H	-3.238871000	-2.535933000	-2.567724000	C	3.197720000	2.974347000	0.369820000
H	1.269916000	-3.874696000	-2.610857000	N	3.631271000	1.135141000	-1.066170000
H	1.819866000	-4.943420000	-1.295878000	C	2.610348000	1.849937000	-1.598503000
H	-0.309228000	-0.799504000	-4.663870000	N	2.397455000	2.979130000	-0.865653000
				C	4.412091000	-0.345061000	1.817956000

N	3.785077000	-1.582595000	1.396389000	H	4.828369000	-2.380854000	-0.250524000
C	2.833856000	-2.221884000	2.209677000	H	1.930656000	5.005122000	-0.976030000
N	2.251276000	-3.227783000	1.433460000	H	1.566288000	4.049463000	-2.432977000
C	2.831603000	-3.339201000	0.120481000	H	3.678128000	-0.154764000	-2.657332000
C	3.811549000	-2.117865000	0.063146000	H	4.991750000	-0.380086000	-1.480046000
N	1.900056000	-3.076174000	-0.978486000	H	-2.904429000	2.331335000	-2.605374000
C	2.047212000	-1.814488000	-1.466035000	H	-4.004844000	3.048349000	-1.404735000
N	3.192414000	-1.260325000	-0.957095000	H	-3.253851000	-2.146496000	3.024553000
C	-3.082464000	2.474720000	-1.538398000	H	-4.284326000	-2.949466000	1.805171000
C	1.535038000	4.054318000	-1.342503000	H	1.264931000	-5.050755000	1.754990000
C	3.922847000	-0.177855000	-1.594531000	H	1.048996000	-3.771049000	2.983741000
O	-0.944265000	2.299651000	3.230120000	H	-5.210717000	1.434485000	-0.140447000
O	2.315635000	1.070807000	3.206750000	H	-5.358152000	-1.012461000	0.043590000
O	2.596426000	-1.975994000	3.364964000	H	-3.042224000	-4.560233000	0.438474000
O	-0.529856000	2.534904000	-2.683183000	H	-0.756455000	-5.426755000	0.413508000
O	-1.835343000	-0.089814000	-2.237072000	H	3.319107000	-4.308216000	-0.036156000
O	1.974616000	1.511654000	-2.617580000	H	-4.479449000	-2.813910000	-1.262821000
O	1.257989000	-1.269046000	-2.272254000	H	-3.422844000	-2.282975000	-2.595337000
C	1.108653000	-3.977401000	1.912653000	H	0.984802000	-3.958966000	-2.639038000
C	-3.506106000	-2.380219000	-1.511577000	H	1.446649000	-5.062564000	-1.319535000
C	1.004663000	-4.089871000	-1.555896000	H	-0.173074000	-0.747805000	-4.349800000
O	-3.188295000	0.227355000	3.416197000				
O	-0.710972000	-1.912189000	2.789948000				<b><sup>2</sup>Fe<sup>III</sup>-OH</b>
O	-1.147869000	-2.928391000	-3.000015000	Fe	0.632166000	0.106034000	-2.450203000
O	0.028298000	0.205008000	-4.208737000	C	-3.690385000	-0.301523000	-1.889170000
O	0.251879000	0.716726000	-0.331312000	N	-4.053312000	0.784485000	-1.100155000
H	0.299253000	1.533423000	0.218597000	C	-4.444076000	0.408945000	0.252675000
H	0.021121000	-0.009492000	0.274322000	C	-4.307797000	-1.162027000	0.240518000
H	1.218104000	3.204971000	3.130887000	N	-3.872436000	-1.445606000	-1.120564000
H	1.639737000	4.579553000	2.061870000	N	-3.320034000	-1.423371000	1.265123000
H	5.450804000	-0.318434000	1.472684000	C	-2.796746000	-0.252353000	1.808813000
H	4.389271000	-0.352252000	2.909699000	N	-3.523993000	0.817655000	1.290451000
H	-3.453974000	2.630657000	2.987511000	C	-3.527473000	2.119253000	1.943373000
H	-4.241751000	3.379716000	1.569660000	N	-2.502555000	3.031382000	1.478780000
H	-2.548702000	4.820853000	0.238783000	C	-1.380927000	3.307747000	2.258287000
H	-0.166102000	5.292444000	0.653186000	N	-0.496876000	4.045754000	1.449756000
H	3.778613000	3.900778000	0.436084000	C	-0.999533000	4.218419000	0.111582000
H	5.161945000	1.883561000	0.175854000	C	-2.441662000	3.611864000	0.160628000

N	-2.445363000	2.639453000	-0.934079000	O	2.239234000	-1.086612000	-2.619586000
C	-1.189873000	2.429450000	-1.422548000	O	-0.622600000	-1.563510000	-2.189965000
N	-0.345419000	3.387810000	-0.902441000	C	-3.105318000	-2.717796000	1.901359000
C	0.854546000	4.312471000	1.889886000	C	-3.684297000	2.099773000	-1.527738000
N	1.862605000	3.330751000	1.456628000	C	-3.286258000	-2.673879000	-1.567050000
C	2.093628000	2.170400000	2.189272000	O	-1.209107000	3.009766000	3.413709000
N	2.999396000	1.365502000	1.427417000	O	-1.873341000	-0.175734000	2.594757000
C	3.667733000	2.193738000	0.429599000	O	-3.309266000	-0.259248000	-3.038785000
C	2.710586000	3.431677000	0.298037000	O	0.399288000	0.088454000	-4.163502000
N	3.646180000	1.598268000	-0.904735000	O	0.776043000	0.088194000	-0.321286000
C	2.565913000	2.063287000	-1.602212000	H	1.499567000	0.400222000	0.269837000
N	2.065158000	3.160952000	-0.999325000	H	-0.023011000	0.011839000	0.231180000
C	3.713206000	0.281407000	2.131911000	H	3.341690000	0.272199000	3.160268000
N	3.448575000	-1.024504000	1.580513000	H	4.790474000	0.486211000	2.127720000
C	2.504179000	-1.873695000	2.182207000	H	2.058538000	-5.067589000	1.430673000
N	2.394653000	-3.006799000	1.375083000	H	1.560337000	-4.157177000	2.885177000
C	3.258133000	-2.949578000	0.226036000	H	0.831035000	4.289022000	2.981391000
C	4.041887000	-1.589537000	0.398889000	H	1.177302000	5.301638000	1.550724000
N	2.573141000	-2.744850000	-1.065324000	H	3.230276000	4.394543000	0.257839000
C	2.805030000	-1.524468000	-1.583518000	H	4.689933000	2.456856000	0.721890000
N	3.736019000	-0.861626000	-0.846933000	H	5.126555000	-1.713362000	0.491229000
C	1.576700000	-4.153759000	1.793330000	H	3.907966000	-3.828012000	0.156890000
N	0.192572000	-4.122697000	1.371691000	H	-0.069521000	-5.351625000	-0.319136000
C	-0.794595000	-3.551667000	2.194591000	H	5.364618000	0.430979000	-0.890518000
N	-1.950062000	-3.444592000	1.420308000	H	4.394446000	0.369298000	-2.378727000
C	-1.799930000	-3.983750000	0.091689000	H	1.416114000	-3.300518000	-2.665906000
C	-0.275773000	-4.332486000	0.027968000	H	1.778968000	-4.610942000	-1.521435000
N	-1.974280000	-3.006044000	-0.981770000	H	0.849439000	3.562518000	-2.601715000
C	-0.773217000	-2.550915000	-1.442317000	H	0.981552000	4.887055000	-1.422105000
N	0.226547000	-3.366852000	-0.954527000	H	-3.336555000	1.984429000	3.010393000
C	0.882845000	3.803418000	-1.538153000	H	-4.520670000	2.561219000	1.805060000
C	4.348206000	0.383962000	-1.289151000	H	-4.015380000	-3.312644000	1.762614000
C	1.500788000	-3.556604000	-1.609066000	H	-2.931131000	-2.566189000	2.969055000
O	1.621360000	1.866981000	3.252161000	H	-0.972145000	5.269312000	-0.199047000
O	1.922927000	-1.655624000	3.214867000	H	-3.237628000	4.347617000	-0.000646000
O	-0.673068000	-3.253555000	3.356156000	H	-5.460787000	0.755578000	0.468971000
O	2.090862000	1.553934000	-2.642748000	H	-5.247673000	-1.681228000	0.458976000
O	-0.870800000	1.526058000	-2.222982000	H	-2.459401000	-4.841655000	-0.081520000



H	4.194412000	-1.127215000	2.999167000	C	2.335214000	-2.717815000	2.245403000
H	5.202537000	-1.536421000	1.582116000	N	1.734370000	-3.688466000	1.424396000
H	4.166536000	-3.537380000	0.268704000	C	2.283961000	-3.693107000	0.093096000
H	2.124875000	-4.851602000	0.701244000	C	3.462841000	-2.665087000	0.161108000
H	-2.048053000	-5.009887000	0.460040000	N	3.163697000	-1.724553000	-0.919701000
H	-4.082176000	-3.659128000	0.161156000	C	1.903826000	-1.912396000	-1.410663000
H	-5.378327000	0.420284000	-0.286736000	N	1.415459000	-3.105410000	-0.928418000
H	0.073190000	-5.370817000	-0.935547000	C	0.527608000	-4.366514000	1.845447000
H	0.075437000	-4.367124000	-2.404820000	N	-0.730387000	-3.748984000	1.397597000
H	-3.457264000	-1.229374000	-2.676229000	C	-1.338474000	-2.742332000	2.141090000
H	-4.763791000	-1.517896000	-1.506002000	N	-2.447958000	-2.265580000	1.375075000
H	3.594173000	-1.128243000	-2.596608000	C	-2.790439000	-3.240624000	0.345551000
H	4.867164000	-1.362709000	-1.376862000	C	-1.485787000	-4.105072000	0.223559000
H	2.213068000	3.212147000	3.010429000	N	-2.931860000	-2.643538000	-0.979038000
H	2.871399000	4.335291000	1.786375000	C	-1.749468000	-2.734164000	-1.668679000
H	-3.068387000	4.225318000	1.723124000	N	-0.943552000	-3.633298000	-1.060167000
H	-2.399496000	3.119098000	2.957126000	C	-3.484020000	-1.484966000	2.076898000
H	5.368310000	0.617255000	-0.129657000	N	-3.649330000	-0.149046000	1.553091000
H	4.570301000	2.934385000	0.024519000	C	-3.010675000	0.939775000	2.168216000
H	1.116066000	5.374598000	0.420909000	N	-3.263249000	2.065935000	1.381574000
H	-1.326749000	5.327677000	0.398011000	C	-4.053057000	1.761481000	0.220859000
H	-4.690503000	2.769476000	-0.074914000	C	-4.369955000	0.218683000	0.364789000
H	3.107670000	4.261907000	-1.289335000	N	-3.319219000	1.802799000	-1.061518000
H	2.302041000	3.381244000	-2.614277000	C	-3.132678000	0.576598000	-1.576285000
H	-2.377011000	3.307333000	-2.666577000	N	-3.824025000	-0.355149000	-0.881324000
H	-3.236842000	4.160814000	-1.358666000	C	-2.820785000	3.398280000	1.807690000
		<b><sup>2</sup>Mn<sup>IV</sup>=O</b>		N	-1.490716000	3.781066000	1.380341000
Mn	-0.546708000	-0.178916000	-2.588964000	C	-0.376379000	3.562527000	2.209447000
C	3.417309000	1.443159000	-1.863149000	N	0.755033000	3.850120000	1.443943000
N	4.118740000	0.534799000	-1.081687000	C	0.443678000	4.316991000	0.118755000
C	4.353137000	1.005117000	0.278517000	C	-1.112091000	4.171045000	0.050592000
C	3.725819000	2.452225000	0.269087000	N	0.919264000	3.443757000	-0.959051000
N	3.221733000	2.583692000	-1.093199000	C	-0.084241000	2.667813000	-1.450313000
N	2.706487000	2.383866000	1.291810000	N	-1.285884000	3.128305000	-0.969557000
C	2.569834000	1.101691000	1.821292000	C	0.382693000	-3.874847000	-1.583323000
N	3.597397000	0.317010000	1.302387000	C	-3.984718000	-1.725026000	-1.362055000
C	4.009623000	-0.919798000	1.956250000	C	-2.566828000	2.915883000	-1.604741000
N	3.333993000	-2.110276000	1.485129000	O	-1.005344000	-2.321550000	3.217162000



C	-3.761070000	1.170170000	-1.983502000	H	-3.464853000	1.181973000	-3.035689000
N	-3.723173000	-0.205878000	-1.554686000	H	-4.776474000	1.570713000	-1.878841000
C	-2.973649000	-1.150444000	-2.268862000	H	-3.060679000	-4.421963000	-1.790916000
N	-3.028854000	-2.347227000	-1.553399000	H	-2.462442000	-3.483031000	-3.188784000
C	-3.816623000	-2.238916000	-0.352408000	H	-0.203815000	4.580480000	-2.765731000
C	-4.333271000	-0.746186000	-0.367813000	H	-0.281617000	5.551360000	-1.267735000
N	-3.058929000	-2.290845000	0.906707000	H	-2.393031000	4.948401000	0.113210000
C	-3.026136000	-1.094581000	1.546937000	H	-4.213945000	3.356139000	-0.354645000
N	-3.819756000	-0.195203000	0.895501000	H	-5.425445000	-0.660406000	-0.389062000
C	-2.443825000	-3.571832000	-2.100506000	H	-4.621746000	-2.980999000	-0.326929000
N	-1.059809000	-3.810025000	-1.741342000	H	-0.965447000	-5.262314000	-0.220559000
C	-0.015188000	-3.368037000	-2.569943000	H	-5.167022000	1.370316000	1.162563000
N	1.170262000	-3.545124000	-1.851979000	H	-4.128723000	0.997851000	2.560044000
C	0.968354000	-4.179683000	-0.575910000	H	-2.014216000	-3.219289000	2.403811000
C	-0.591267000	-4.259968000	-0.460178000	H	-2.645588000	-4.313058000	1.151672000
N	1.351942000	-3.367507000	0.581205000	H	-0.084233000	3.550312000	2.769162000
C	0.267319000	-2.812541000	1.192285000	H	-0.053029000	4.947465000	1.666977000
N	-0.875152000	-3.356352000	0.664643000	H	3.526540000	1.630503000	-3.183360000
C	-0.126377000	3.856736000	1.722821000	H	4.823800000	1.893449000	-1.981284000
C	-4.154482000	1.101089000	1.474374000	H	3.199963000	-3.848005000	-2.287597000
C	-2.166845000	-3.345856000	1.331349000	H	2.259738000	-2.830938000	-3.418567000
O	-1.445675000	2.386202000	-3.124091000	H	1.918312000	5.057082000	0.316541000
O	-2.407704000	-0.957118000	-3.316204000	H	3.963037000	3.749486000	-0.045390000
O	-0.119380000	-2.954453000	-3.696824000	H	5.439237000	-0.179400000	-0.809645000
O	-1.674132000	1.771636000	2.782629000	H	4.778076000	-2.525516000	-0.921424000
O	1.256916000	1.326971000	2.241826000	H	1.467210000	-5.154198000	-0.517104000
O	-2.369701000	-0.870066000	2.580737000	H	4.958421000	1.890394000	1.075356000
O	0.322254000	-1.956521000	2.106066000	H	3.973394000	1.241155000	2.411075000
C	2.436938000	-3.064830000	-2.366198000	H	2.700278000	-3.271142000	2.175401000
C	4.045051000	1.342724000	1.326917000	H	3.232784000	-4.202955000	0.754642000
C	2.729976000	-3.288791000	1.085250000	C	1.355510000	-1.814353000	5.303423000
O	1.547469000	2.983495000	-3.383063000	H	0.566277000	-0.986217000	4.714872000
O	1.931662000	-0.333589000	-3.136909000	H	2.238485000	-1.782834000	4.667628000
O	3.205791000	-0.998693000	2.689310000	H	1.465180000	-1.352289000	6.284798000
O	-0.202131000	-0.105056000	4.261819000	H	0.799465000	-2.751493000	5.305715000
O	-0.691795000	0.183612000	0.347174000				
H	-1.393890000	0.649259000	-0.157719000			<sup>5</sup> Mn <sup>III</sup> -OH	
H	0.052475000	0.069098000	-0.268305000	Mn	0.016311000	-0.491103000	-2.563597000

C	0.309337000	3.526645000	-1.868047000	N	-3.073415000	2.474968000	1.421389000
N	1.438214000	3.756308000	-1.097551000	C	-3.672467000	2.422216000	0.112153000
C	1.134782000	4.256305000	0.239123000	C	-4.274694000	0.974655000	0.057968000
C	-0.433738000	4.383198000	0.221614000	N	-2.712870000	2.427278000	-0.992383000
N	-0.783869000	3.934263000	-1.121566000	C	-2.496147000	1.171759000	-1.469348000
N	-0.858948000	3.511339000	1.294504000	N	-3.439510000	0.319777000	-0.958898000
C	0.214809000	2.891009000	1.936407000	C	3.675621000	-1.541253000	-1.519384000
N	1.389383000	3.327971000	1.318449000	C	-0.341247000	-4.321971000	-1.334470000
C	2.685657000	3.122380000	1.954493000	C	-3.826731000	-0.925217000	-1.601899000
N	3.404096000	1.948279000	1.497852000	O	1.538072000	-1.939848000	3.240026000
C	3.462198000	0.790166000	2.275488000	O	-1.932949000	-1.661132000	3.203500000
N	4.060886000	-0.204157000	1.481328000	O	-3.052911000	1.179517000	3.354697000
C	4.375262000	0.266185000	0.158644000	O	1.236589000	-2.309478000	-2.676487000
C	4.009531000	1.792129000	0.200147000	O	1.802727000	0.577023000	-2.279620000
N	3.084832000	1.948372000	-0.925527000	O	-1.481972000	-2.025359000	-2.642995000
C	2.710155000	0.744621000	-1.434191000	O	-1.580970000	0.864589000	-2.263865000
N	3.495223000	-0.241002000	-0.900881000	C	-2.187478000	3.516895000	1.899543000
C	4.084668000	-1.585638000	1.917105000	C	2.708590000	3.241925000	-1.514858000
N	2.957481000	-2.406635000	1.455135000	C	-2.113067000	3.637682000	-1.569032000
C	1.767793000	-2.449960000	2.174990000	O	3.102859000	0.669792000	3.419402000
N	0.834012000	-3.204575000	1.401646000	O	0.142679000	2.116216000	2.864203000
C	1.546183000	-3.985508000	0.393731000	O	0.286550000	3.072562000	-2.999467000
C	2.931158000	-3.254565000	0.288694000	O	0.039626000	-0.111331000	-4.271761000
N	0.976430000	-3.844483000	-0.940899000	O	-0.018825000	-0.743605000	-0.362318000
C	1.635728000	-2.863298000	-1.638040000	H	0.146826000	-1.537298000	0.197381000
N	2.801003000	-2.568018000	-1.003106000	H	-0.049761000	0.017530000	0.243084000
C	-0.344628000	-3.753048000	2.102015000	H	-0.288944000	-3.408446000	3.137902000
N	-1.595986000	-3.277455000	1.569932000	H	-0.311950000	-4.848534000	2.072084000
C	-2.254220000	-2.195105000	2.170790000	H	-5.328701000	-1.219141000	1.466291000
N	-3.346994000	-1.875187000	1.364352000	H	-4.320346000	-0.884776000	2.903075000
C	-3.455367000	-2.740469000	0.215303000	H	4.041430000	-1.562726000	3.007998000
C	-2.240060000	-3.737484000	0.367463000	H	5.013999000	-2.066411000	1.596501000
N	-3.171002000	-2.101279000	-1.077315000	H	3.790553000	-3.933094000	0.265868000
C	-1.993732000	-2.509428000	-1.614960000	H	1.628282000	-5.041390000	0.673510000
N	-1.467565000	-3.522830000	-0.866576000	H	-2.540083000	-4.789029000	0.435494000
C	-4.341642000	-0.894437000	1.811344000	H	-4.429452000	-3.239152000	0.173055000
N	-4.100851000	0.472905000	1.393610000	H	-5.324445000	0.944048000	-0.255657000
C	-3.355838000	1.349892000	2.201045000	H	-0.462459000	-5.343909000	-0.965814000



C	-2.570685000	-3.240405000	1.907385000	H	-2.644873000	-3.111199000	-2.640314000
C	-4.011713000	1.422174000	-1.509847000	H	-3.244148000	-4.154119000	-1.327359000
C	-2.738208000	-3.211588000	-1.557622000	H	-0.705657000	-0.156919000	-4.324751000
O	-1.681539000	2.729265000	3.406010000				
O	-1.883173000	-0.541057000	2.698374000			<b><sup>6</sup>Co<sup>IV</sup>=O</b>	
O	-3.139797000	-0.814256000	-3.017745000	Co	-0.097188000	-0.413318000	-2.500858000
O	0.231858000	0.097555000	-4.185868000	C	1.125810000	3.545914000	-1.775414000
O	0.802943000	0.228598000	-0.290343000	N	2.273591000	3.488048000	-0.994027000
H	1.459288000	0.677101000	0.292156000	C	2.057135000	3.942295000	0.375781000
H	0.053029000	-0.017390000	0.279547000	C	0.551769000	4.414120000	0.362389000
H	3.315295000	0.900038000	3.120074000	N	0.135320000	4.149461000	-1.011252000
H	4.680298000	1.356408000	2.052960000	N	-0.074809000	3.562529000	1.347023000
H	2.943197000	-4.589906000	1.454811000	C	0.780968000	2.553370000	1.778584000
H	2.289504000	-3.755185000	2.893024000	N	2.067306000	2.884418000	1.360197000
H	0.096189000	4.365939000	2.960261000	C	3.257404000	2.390569000	2.044513000
H	0.234299000	5.427205000	1.529664000	N	3.757851000	1.122587000	1.564474000
H	2.397863000	4.902335000	0.203805000	C	3.528390000	-0.049261000	2.287701000
H	4.193903000	3.263117000	0.628265000	N	3.873873000	-1.118725000	1.448014000
H	5.377623000	-0.769395000	0.436965000	C	4.304065000	-0.677407000	0.146061000
H	4.546278000	-3.070974000	0.159470000	C	4.275282000	0.887302000	0.242828000
H	0.910441000	-5.264182000	-0.300225000	N	3.374475000	1.287814000	-0.845050000
H	5.192661000	1.388049000	-0.983151000	C	2.770339000	0.206947000	-1.410713000
H	4.212728000	1.121822000	-2.444632000	N	3.355405000	-0.937995000	-0.938139000
H	1.989826000	-3.014589000	-2.668195000	C	3.631565000	-2.488186000	1.856820000
H	2.569796000	-4.236179000	-1.515196000	N	2.359888000	-3.060323000	1.403599000
H	0.169334000	3.644165000	-2.622687000	C	1.189314000	-2.884293000	2.140061000
H	0.077182000	4.976869000	-1.448935000	N	0.120096000	-3.399235000	1.354503000
H	-3.617669000	1.358366000	3.020831000	C	0.639208000	-4.243556000	0.288569000
H	-4.889466000	1.721638000	1.820091000	C	2.147834000	-3.815904000	0.197375000
H	-3.350116000	-3.995453000	1.753787000	N	0.107248000	-3.902875000	-1.028463000
H	-2.435880000	-3.069957000	2.977927000	C	0.956379000	-3.050918000	-1.679322000
H	-1.884325000	5.016720000	-0.200640000	N	2.158519000	-3.046130000	-1.056725000
H	-3.960258000	3.721862000	0.030012000	C	-1.169628000	-3.664617000	2.011851000
H	-5.492763000	-0.225328000	0.473034000	N	-2.258504000	-2.879718000	1.477052000
H	-4.855102000	-2.586143000	0.436386000	C	-2.691246000	-1.716264000	2.131927000
H	-1.534427000	-5.207372000	-0.064939000	N	-3.696697000	-1.150543000	1.344970000
H	-4.921368000	1.974759000	-1.256035000	C	-3.967043000	-1.915992000	0.157131000
H	-3.893303000	1.406445000	-2.594617000	C	-3.001956000	-3.160424000	0.276689000

N	-3.520165000	-1.300545000	-1.104152000	H	2.844148000	-4.657746000	0.119489000
C	-2.466275000	-1.947260000	-1.650767000	H	0.496492000	-5.309809000	0.496312000
N	-2.211843000	-3.093451000	-0.962089000	H	-3.526354000	-4.121192000	0.326363000
C	-4.426467000	0.036855000	1.792809000	H	-5.025417000	-2.185642000	0.077149000
N	-3.853141000	1.307622000	1.394196000	H	-4.951648000	2.105814000	-0.217144000
C	-2.970445000	1.993131000	2.241059000	H	-1.603739000	-5.076745000	-1.103927000
N	-2.470514000	3.074840000	1.511195000	H	-1.287119000	-4.069311000	-2.535163000
C	-3.011009000	3.165374000	0.181232000	H	-3.658949000	0.000597000	-2.683309000
C	-3.918751000	1.891947000	0.081142000	H	-4.985687000	0.116683000	-1.506405000
N	-2.027419000	2.974883000	-0.890309000	H	3.056980000	-2.097962000	-2.638258000
C	-2.123401000	1.731725000	-1.437287000	H	4.184540000	-2.763634000	-1.435252000
N	-3.257181000	1.117133000	-0.973246000	H	3.027179000	2.231535000	3.100395000
C	3.237342000	-2.232749000	-1.570901000	H	4.029183000	3.163353000	1.956748000
C	-1.271593000	-4.092698000	-1.444598000	H	-1.540782000	4.912211000	1.903784000
C	-3.904648000	-0.005437000	-1.620680000	H	-1.268565000	3.586107000	3.064693000
O	1.080092000	-2.384863000	3.228995000	H	5.285185000	-1.088430000	-0.118165000
O	-2.277699000	-1.306089000	3.187248000	H	5.254270000	1.357142000	0.095258000
O	-2.724690000	1.728280000	3.390905000	H	2.764240000	4.736764000	0.636315000
O	0.687159000	-2.377808000	-2.695482000	H	0.420650000	5.472834000	0.609248000
O	1.849222000	0.255296000	-2.258456000	H	-3.548707000	4.106377000	0.018333000
O	-1.842666000	-1.547522000	-2.658737000	H	4.318714000	3.100880000	-1.158039000
O	-1.312015000	1.249148000	-2.261296000	H	3.276395000	2.568179000	-2.502686000
C	-1.348387000	3.838208000	2.004820000	H	-1.187867000	3.957374000	-2.540994000
C	3.356436000	2.648996000	-1.417254000	H	-1.761559000	4.999211000	-1.213076000
C	-1.225812000	4.076767000	-1.456829000				
O	3.147165000	-0.127685000	3.428681000			<b><sup>4</sup>Co<sup>IV</sup>=O</b>	
O	0.462039000	1.555624000	2.401461000	Co	-0.465933000	-0.475975000	-2.478414000
O	1.015735000	3.158238000	-2.920984000	C	2.767947000	2.341297000	-1.934818000
O	-0.012486000	-0.170883000	-4.326401000	N	3.708390000	1.685626000	-1.149534000
O	-0.176988000	-0.610385000	-0.194539000	C	3.838334000	2.248816000	0.187713000
H	-0.217980000	-1.442410000	0.319719000	C	2.812475000	3.444603000	0.171454000
H	-0.012769000	0.087821000	0.470695000	N	2.258839000	3.385669000	-1.174679000
H	-1.056186000	-3.376592000	3.060428000	N	1.890582000	3.115880000	1.238080000
H	-1.406342000	-4.733328000	1.943987000	C	2.209332000	1.914032000	1.870301000
H	-5.459145000	-0.035186000	1.435784000	N	3.361152000	1.408315000	1.264419000
H	-4.415658000	0.030348000	2.884791000	C	4.134427000	0.349809000	1.897698000
H	3.609159000	-2.481490000	2.948587000	N	3.803711000	-0.988402000	1.443937000
H	4.443920000	-3.134860000	1.510478000	C	3.071766000	-1.862340000	2.246820000

N	2.781431000	-2.992144000	1.457714000	O	-1.314349000	3.069384000	3.333932000
C	3.273953000	-2.856769000	0.113428000	O	-0.820500000	-2.558528000	-2.648024000
C	4.095154000	-1.524578000	0.137805000	O	1.608981000	-0.778867000	-2.262266000
N	3.532501000	-0.757146000	-0.974927000	O	-2.524316000	-0.452796000	-2.612894000
C	2.386274000	-1.321626000	-1.445269000	O	-0.453470000	1.650467000	-2.255148000
N	2.243685000	-2.574662000	-0.894082000	C	0.954898000	4.055091000	1.845141000
C	1.834036000	-3.986129000	1.912318000	C	4.202991000	0.412529000	-1.573551000
N	0.443907000	-3.771072000	1.477816000	C	1.081839000	4.065811000	-1.625030000
C	-0.406157000	-2.939752000	2.198794000	O	2.771427000	-1.705669000	3.403350000
N	-1.616870000	-2.815161000	1.442834000	O	1.599972000	1.400935000	2.783707000
C	-1.695519000	-3.906005000	0.473153000	O	2.466762000	2.065308000	-3.077117000
C	-0.201852000	-4.367273000	0.336346000	O	-0.319580000	-0.349773000	-4.063128000
N	-2.041502000	-3.441000000	-0.866050000	O	-0.609457000	-0.526733000	-0.408597000
C	-0.900135000	-3.214865000	-1.589272000	H	-0.974489000	-1.220402000	0.194002000
N	0.154189000	-3.800531000	-0.974965000	H	0.017110000	0.008427000	0.109803000
C	-2.822312000	-2.363177000	2.172491000	H	-2.507714000	-2.130369000	3.193334000
N	-3.397457000	-1.161346000	1.628770000	H	-3.564895000	-3.169727000	2.187097000
C	-3.104452000	0.085510000	2.203354000	H	-4.617713000	2.930340000	1.449851000
N	-3.687254000	1.060736000	1.394555000	H	-3.665308000	2.490958000	2.896290000
C	-4.375679000	0.497256000	0.262415000	H	1.842409000	-3.940590000	3.003337000
C	-4.213301000	-1.063460000	0.448277000	H	2.141941000	-4.983524000	1.584012000
N	-3.723909000	0.719463000	-1.040909000	H	-0.070827000	-5.454168000	0.319120000
C	-3.206176000	-0.413045000	-1.561166000	H	-2.372627000	-4.702747000	0.798866000
N	-3.545408000	-1.487408000	-0.795622000	H	-5.164954000	-1.596121000	0.552422000
C	-3.689355000	2.471167000	1.804755000	H	-5.417898000	0.828642000	0.210709000
N	-2.551969000	3.250749000	1.364128000	H	-3.079986000	4.384598000	-0.330219000
C	-1.404258000	3.366893000	2.169628000	H	-4.119762000	-3.488540000	-0.833206000
N	-0.409382000	3.934592000	1.371967000	H	-3.376454000	-2.873012000	-2.328355000
C	-0.871849000	4.287674000	0.052661000	H	-3.127130000	1.830802000	-2.656612000
C	-2.313410000	3.680449000	0.013599000	H	-4.169692000	2.696511000	-1.505328000
N	-0.183494000	3.596686000	-1.036281000	H	1.370424000	-3.436196000	-2.583268000
C	-0.900412000	2.527124000	-1.485195000	H	2.041364000	-4.574102000	-1.391765000
N	-2.173686000	2.592587000	-0.963917000	H	3.926105000	0.356630000	2.970031000
C	1.485647000	-3.639801000	-1.517578000	H	5.198208000	0.553276000	1.729973000
C	-3.323810000	-2.859139000	-1.238921000	H	1.329197000	5.070517000	1.670888000
C	-3.332671000	1.998350000	-1.598508000	H	0.912610000	3.861185000	2.919419000
O	-0.185329000	-2.397399000	3.248672000	H	3.858760000	-3.730821000	-0.195650000
O	-2.480391000	0.260039000	3.219889000	H	5.170766000	-1.663020000	-0.019768000

H	4.871583000	2.567750000	0.367575000	C	-3.176195000	0.303588000	2.151372000
H	3.282308000	4.419358000	0.346835000	N	-3.625996000	1.358657000	1.352227000
H	-0.840332000	5.369536000	-0.119668000	C	-4.322516000	0.904656000	0.178602000
H	5.266491000	0.305618000	-1.338706000	C	-4.320559000	-0.669878000	0.317257000
H	4.066113000	0.372286000	-2.655693000	N	-3.599619000	1.101162000	-1.091667000
H	1.036865000	3.919979000	-2.705784000	C	-3.158278000	-0.057869000	-1.615692000
H	1.141186000	5.136576000	-1.407221000	N	-3.653469000	-1.108015000	-0.918333000
				C	-3.479167000	2.753631000	1.779471000
		<b><sup>2</sup>Co<sup>IV</sup>=O</b>		N	-2.253612000	3.409426000	1.365457000
Co	-0.399233000	-0.375769000	-2.456437000	C	-1.127902000	3.420740000	2.203620000
C	3.071504000	2.117382000	-1.821017000	N	-0.071832000	3.940923000	1.451547000
N	3.938803000	1.378626000	-1.026818000	C	-0.452529000	4.321687000	0.116805000
C	4.049740000	1.884217000	0.336661000	C	-1.945610000	3.865474000	0.035713000
C	3.136208000	3.170312000	0.310844000	N	0.205023000	3.553263000	-0.946539000
N	2.638662000	3.194369000	-1.060656000	C	-0.619076000	2.588269000	-1.447951000
N	2.129526000	2.884918000	1.307449000	N	-1.891835000	2.811345000	-0.981390000
C	2.216554000	1.579932000	1.783621000	C	1.198796000	-3.691548000	-1.573097000
N	3.425438000	1.049361000	1.339569000	C	-3.512348000	-2.460532000	-1.418345000
C	4.069517000	-0.067386000	2.020629000	C	-3.092993000	2.340353000	-1.630690000
N	3.675776000	-1.376638000	1.545830000	O	-0.578608000	-2.541204000	3.243054000
C	2.799359000	-2.173963000	2.285717000	O	-2.586542000	0.386245000	3.199154000
N	2.415283000	-3.238114000	1.451841000	O	-1.091807000	3.092876000	3.362738000
C	3.001414000	-3.139609000	0.141106000	O	-0.885863000	-2.164058000	-2.632628000
C	3.935039000	-1.885420000	0.225380000	O	1.570455000	-0.903353000	-2.228070000
N	3.458741000	-1.021282000	-0.862915000	O	-2.419842000	-0.152974000	-2.622028000
C	2.297996000	-1.492453000	-1.395174000	O	-0.261176000	1.674401000	-2.230731000
N	2.068557000	-2.751490000	-0.916525000	C	1.284109000	3.885419000	1.947372000
C	1.380878000	-4.170531000	1.855468000	C	4.280519000	0.056455000	-1.447298000
N	0.021598000	-3.839721000	1.404053000	C	1.508465000	3.943236000	-1.519731000
C	-0.797017000	-2.992402000	2.150091000	O	2.465667000	-2.006921000	3.431841000
N	-1.960838000	-2.731684000	1.365090000	O	1.384218000	1.003240000	2.458941000
C	-2.068001000	-3.723058000	0.299754000	O	2.762988000	1.874224000	-2.968362000
C	-0.614725000	-4.300020000	0.196705000	O	-0.254791000	-0.319299000	-4.135153000
N	-2.289278000	-3.126376000	-1.015684000	O	-0.571820000	-0.411389000	-0.246350000
C	-1.092539000	-2.916824000	-1.650354000	H	-1.077172000	-1.040485000	0.307599000
N	-0.146637000	-3.680785000	-1.055300000	H	0.013267000	0.074723000	0.365364000
C	-3.148317000	-2.174348000	2.042073000	H	-2.870947000	-2.018120000	3.088054000
N	-3.553675000	-0.890987000	1.514918000	H	-3.979701000	-2.886865000	1.980714000



C	4.370144000	-0.617815000	0.621528000	H	-4.080642000	3.584557000	-1.290068000
C	1.866262000	3.512178000	1.297729000	H	-3.238436000	2.805353000	-2.660600000
O	1.076279000	-1.889769000	-3.588892000	H	-1.308908000	-5.252536000	0.078563000
O	1.541785000	1.573069000	-3.541399000	H	-3.510729000	-4.179397000	0.227170000
O	-0.988351000	3.300565000	-3.333202000	H	-5.548145000	-0.455765000	0.143339000
O	2.265260000	-1.724757000	2.260164000	H	-5.205733000	1.962512000	0.171130000
O	-0.698893000	-1.654991000	2.258163000	H	-2.218576000	4.976223000	0.302391000
O	2.592460000	0.965399000	2.226632000	H	-4.473209000	-2.595420000	1.700494000
O	-0.230729000	1.717834000	2.268156000	H	-3.338717000	-1.919526000	2.898916000
C	-3.247360000	2.932186000	-1.575636000	H	-2.680202000	2.705556000	2.939015000
C	-3.606984000	-1.941391000	1.841169000	H	-3.584127000	3.690012000	1.758499000
C	-2.929711000	2.821584000	1.882836000	C	3.002249000	-0.391164000	5.402254000
O	-1.836455000	-2.827792000	-3.377522000	H	3.548353000	0.474114000	5.028168000
O	-2.445572000	0.363119000	-2.623493000	H	1.842373000	-0.270918000	4.838620000
O	-2.807818000	0.360753000	3.278236000	H	3.353700000	-1.354338000	5.033852000
O	0.709123000	-0.156553000	4.307453000	H	2.748539000	-0.360895000	6.461628000
O	0.663824000	-0.092699000	0.074068000				
H	1.300334000	-0.427582000	-0.592165000			<b><sup>5</sup>Co<sup>III</sup>-OH</b>	
H	-0.161624000	0.078105000	-0.411038000	Co	-0.006176000	-0.542765000	-2.569815000
H	2.899532000	-0.405173000	-3.689213000	C	0.304967000	3.467276000	-1.829593000
H	4.435805000	-0.700813000	-2.815934000	N	1.432176000	3.694223000	-1.069408000
H	2.068510000	4.958512000	-1.802680000	C	1.132340000	4.211299000	0.263951000
H	1.335980000	4.068943000	-3.168729000	C	-0.433665000	4.337570000	0.248530000
H	0.166255000	-4.233523000	-3.239293000	N	-0.786548000	3.861804000	-1.087633000
H	0.623645000	-5.307670000	-1.886396000	N	-0.857310000	3.492437000	1.340150000
H	2.865264000	-4.538667000	-0.819492000	C	0.221348000	2.915439000	2.017688000
H	4.373110000	-2.682007000	-1.406233000	N	1.392570000	3.301339000	1.355568000
H	5.058641000	1.456805000	-1.227222000	C	2.696650000	3.102813000	1.981588000
H	3.999339000	3.626798000	-0.771044000	N	3.416500000	1.932164000	1.520568000
H	0.197475000	5.390405000	0.186490000	C	3.454862000	0.763759000	2.284543000
H	5.328806000	-0.724574000	0.106902000	N	4.071029000	-0.221313000	1.494674000
H	4.541398000	-0.616895000	1.698359000	C	4.416527000	0.261198000	0.182470000
H	1.909677000	3.273470000	2.361093000	C	4.041499000	1.788397000	0.229308000
H	2.200672000	4.543667000	1.150989000	N	3.135430000	1.946120000	-0.909329000
H	0.924118000	-3.725599000	2.312804000	C	2.775996000	0.741261000	-1.438585000
H	0.870963000	-4.999563000	1.071720000	N	3.567238000	-0.238591000	-0.901152000
H	-3.881206000	-1.759339000	-2.699239000	C	4.082746000	-1.607718000	1.915847000
H	-4.910589000	-2.299702000	-1.341696000	N	2.955601000	-2.418145000	1.436642000

C	1.773183000	-2.494060000	2.168648000	O	3.064899000	0.630651000	3.417443000
N	0.844187000	-3.241511000	1.389410000	O	0.155633000	2.214196000	3.000376000
C	1.546492000	-3.981840000	0.349436000	O	0.282384000	3.031938000	-2.978315000
C	2.929722000	-3.247385000	0.256948000	O	0.084019000	0.551544000	-4.167805000
N	0.969162000	-3.796691000	-0.977426000	O	-0.052165000	-0.678708000	-0.349900000
C	1.636430000	-2.814078000	-1.662223000	H	0.126065000	-1.453174000	0.225479000
N	2.803842000	-2.539644000	-1.024396000	H	-0.033896000	0.102948000	0.226707000
C	-0.338039000	-3.798500000	2.070078000	H	-0.283797000	-3.480186000	3.114392000
N	-1.586418000	-3.302970000	1.545831000	H	-0.313528000	-4.893242000	2.013340000
C	-2.237822000	-2.227966000	2.166318000	H	-5.314630000	-1.242746000	1.508271000
N	-3.330938000	-1.888493000	1.367531000	H	-4.282936000	-0.919102000	2.931103000
C	-3.452528000	-2.741258000	0.210422000	H	4.028692000	-1.597706000	3.006436000
C	-2.234533000	-3.736286000	0.336527000	H	5.013470000	-2.088199000	1.598590000
N	-3.189968000	-2.087598000	-1.080016000	H	3.790385000	-3.924183000	0.222343000
C	-2.015036000	-2.478867000	-1.634041000	H	1.630761000	-5.047811000	0.588442000
N	-1.472033000	-3.492422000	-0.897674000	H	-2.530725000	-4.790290000	0.382224000
C	-4.323118000	-0.917267000	1.839860000	H	-4.426318000	-3.241509000	0.175566000
N	-4.095798000	0.454676000	1.431094000	H	-5.369853000	0.952213000	-0.171229000
C	-3.335095000	1.324012000	2.229742000	H	-0.457452000	-5.304839000	-1.029932000
N	-3.074469000	2.460027000	1.457924000	H	-0.369177000	-4.264667000	-2.471589000
C	-3.695618000	2.417328000	0.157680000	H	-3.671313000	-0.858330000	-2.648812000
C	-4.309444000	0.971014000	0.105567000	H	-4.963766000	-1.068832000	-1.444827000
N	-2.759375000	2.421403000	-0.965539000	H	3.539767000	-1.443860000	-2.594491000
C	-2.571491000	1.167541000	-1.470385000	H	4.746709000	-1.877298000	-1.360382000
N	-3.514065000	0.324245000	-0.943887000	H	2.538830000	2.954636000	3.052382000
C	3.719171000	-1.536923000	-1.522253000	H	3.301272000	4.002618000	1.819696000
C	-0.343463000	-4.275744000	-1.381185000	H	-2.640039000	4.487769000	1.762667000
C	-3.888026000	-0.923766000	-1.581571000	H	-2.081645000	3.333875000	3.010249000
O	1.550980000	-2.013698000	3.249283000	H	5.469846000	0.072579000	-0.054508000
O	-1.913367000	-1.714827000	3.208539000	H	4.901595000	2.457550000	0.113183000
O	-3.002492000	1.141137000	3.373631000	H	1.645130000	5.168757000	0.414043000
O	1.236096000	-2.256028000	-2.702618000	H	-0.789369000	5.366172000	0.381370000
O	1.890262000	0.568134000	-2.293227000	H	-4.434462000	3.216372000	0.027852000
O	-1.512460000	-1.996014000	-2.670008000	H	3.494607000	3.958229000	-1.227879000
O	-1.694402000	0.859206000	-2.295807000	H	2.687151000	3.121007000	-2.574331000
C	-2.190819000	3.503056000	1.936466000	H	-2.086056000	3.498400000	-2.620088000
C	2.725216000	3.225125000	-1.488897000	H	-2.773480000	4.462789000	-1.292361000
C	-2.130538000	3.611365000	-1.535791000	H	0.166640000	1.506262000	-3.854754000

<sup>3</sup> Co <sup>III</sup> -OH							
			N	-4.088471000	0.433101000	1.423169000	
Co	-0.002450000	-0.544694000	-2.558372000	C	-3.338805000	1.299926000	2.233931000
C	0.301044000	3.513834000	-1.799191000	N	-3.076525000	2.441833000	1.471423000
N	1.427278000	3.722677000	-1.035521000	C	-3.689703000	2.406797000	0.167548000
C	1.125908000	4.222992000	0.304797000	C	-4.301005000	0.960938000	0.101869000
C	-0.441391000	4.346873000	0.289980000	N	-2.747729000	2.422272000	-0.951439000
N	-0.792682000	3.891553000	-1.054548000	C	-2.564015000	1.174588000	-1.475960000
N	-0.863790000	3.482779000	1.365946000	N	-3.505302000	0.325693000	-0.954146000
C	0.214349000	2.884591000	2.025089000	C	3.715590000	-1.524140000	-1.534225000
N	1.386043000	3.299684000	1.383652000	C	-0.336499000	-4.276537000	-1.405773000
C	2.689384000	3.089965000	2.006894000	C	-3.878387000	-0.921632000	-1.593739000
N	3.405809000	1.923441000	1.532190000	O	1.558633000	-2.039689000	3.241331000
C	3.448373000	0.749287000	2.287136000	O	-1.913661000	-1.737797000	3.194719000
N	4.057165000	-0.229750000	1.485110000	O	-3.015238000	1.111523000	3.379501000
C	4.403973000	0.265401000	0.177892000	O	1.241283000	-2.245996000	-2.714422000
C	4.025324000	1.790260000	0.237605000	O	1.888605000	0.585810000	-2.310329000
N	3.115561000	1.956129000	-0.897548000	O	-1.509132000	-1.988740000	-2.682923000
C	2.767399000	0.755598000	-1.446782000	O	-1.690302000	0.872968000	-2.308410000
N	3.560699000	-0.225898000	-0.914011000	C	-2.197052000	3.481803000	1.962387000
C	4.085585000	-1.617054000	1.902492000	C	2.715535000	3.244665000	-1.462931000
N	2.964019000	-2.436238000	1.427516000	C	-2.132875000	3.626133000	-1.508405000
C	1.780964000	-2.514711000	2.158282000	O	3.067408000	0.608494000	3.422158000
N	0.852329000	-3.257063000	1.374692000	O	0.147114000	2.145950000	2.980413000
C	1.553311000	-3.988809000	0.328097000	O	0.280799000	3.105042000	-2.958159000
C	2.935621000	-3.251513000	0.238945000	O	0.094388000	0.700955000	-4.197693000
N	0.974104000	-3.795496000	-0.996824000	O	-0.042513000	-0.664063000	-0.312438000
C	1.639726000	-2.807852000	-1.675312000	H	0.133005000	-1.444654000	0.254452000
N	2.804577000	-2.530775000	-1.034921000	H	-0.061636000	0.104582000	0.281539000
C	-0.333132000	-3.814329000	2.048330000	H	-0.281716000	-3.500480000	3.094168000
N	-1.578853000	-3.313581000	1.521651000	H	-0.311055000	-4.908946000	1.987197000
C	-2.236773000	-2.247535000	2.150340000	H	-5.315677000	-1.259365000	1.488727000
N	-3.334602000	-1.912231000	1.356443000	H	-4.290387000	-0.944175000	2.917985000
C	-3.449341000	-2.753300000	0.191049000	H	4.037600000	-1.610518000	2.993400000
C	-2.229089000	-3.746640000	0.313010000	H	5.019149000	-2.087682000	1.578768000
N	-3.182625000	-2.087204000	-1.092323000	H	3.796826000	-3.927042000	0.194181000
C	-2.010084000	-2.479193000	-1.649967000	H	1.639697000	-5.056349000	0.559376000
N	-1.469502000	-3.499920000	-0.921921000	H	-2.523674000	-4.801127000	0.358166000
C	-4.324606000	-0.938991000	1.826544000	H	-4.421638000	-3.255731000	0.147306000



O	-2.090346000	1.105968000	-2.621939000	H	4.504884000	-2.835536000	-1.179267000
O	0.705069000	1.468939000	-2.093866000	H	3.638055000	-2.055297000	-2.525420000
C	3.063707000	2.695063000	1.981985000	H	3.226643000	2.579360000	-2.560544000
C	3.739017000	-2.098886000	-1.439580000	H	3.956921000	3.519441000	-1.236073000
C	3.322875000	2.660772000	-1.476450000	H	0.723116000	0.044817000	-4.175498000
O	1.090934000	-2.991640000	3.413707000				
O	1.650504000	0.159368000	2.404354000				
O	3.385146000	0.255346000	-2.959014000	Co	-0.047625000	-0.471225000	2.418127000
O	-0.249284000	-0.037518000	-4.099986000	C	-0.457122000	3.493602000	1.686920000
O	-0.811434000	-0.042365000	-0.174571000	N	-1.554196000	3.685163000	0.866506000
H	-1.554004000	-0.395835000	0.363675000	C	-1.205178000	4.183995000	-0.460030000
H	-0.051613000	0.036161000	0.434801000	C	0.354556000	4.354459000	-0.373339000
H	-3.520268000	-0.305011000	3.055672000	N	0.656856000	3.915341000	0.985971000
H	-4.914930000	-0.496185000	1.947528000	N	0.851647000	3.500320000	-1.427615000
H	-2.084634000	5.030693000	1.427658000	C	-0.176117000	2.867199000	-2.131205000
H	-1.622517000	4.090415000	2.874795000	N	-1.388144000	3.245660000	-1.544931000
H	-0.929015000	-4.292250000	2.918486000	C	-2.650462000	3.010539000	-2.239842000
H	-1.221732000	-5.299260000	1.472113000	N	-3.370144000	1.829155000	-1.807685000
H	-3.236949000	-4.396172000	0.106250000	C	-3.340907000	0.652204000	-2.558848000
H	-4.734667000	-2.469919000	0.496819000	N	-3.966212000	-0.341191000	-1.786755000
H	-5.161160000	1.718184000	0.326950000	C	-4.376120000	0.143047000	-0.493848000
H	-3.919778000	3.835906000	0.087728000	C	-4.037698000	1.678246000	-0.539309000
H	0.062733000	5.307308000	-0.290978000	N	-3.177545000	1.868023000	0.629408000
H	-5.323828000	-0.427466000	-1.108077000	C	-2.811296000	0.676699000	1.183160000
H	-4.268687000	-0.335344000	-2.538077000	N	-3.559836000	-0.326095000	0.626992000
H	-1.352091000	3.304084000	-2.684082000	C	-3.913091000	-1.732715000	-2.187273000
H	-1.701702000	4.614507000	-1.535194000	N	-2.787101000	-2.500069000	-1.640768000
H	-0.760955000	-3.503319000	-2.655618000	C	-1.573144000	-2.559467000	-2.318670000
H	-0.908699000	-4.846735000	-1.499208000	N	-0.661883000	-3.273591000	-1.487087000
H	3.222690000	-1.961967000	3.073880000	C	-1.396390000	-4.021339000	-0.472210000
H	4.459921000	-2.543686000	1.928615000	C	-2.799411000	-3.322348000	-0.454216000
H	3.982578000	3.282636000	1.876308000	N	-0.890363000	-3.815870000	0.878368000
H	2.865072000	2.527050000	3.042965000	C	-1.619709000	-2.852278000	1.536262000
H	0.956928000	-5.237255000	-0.221727000	N	-2.759102000	-2.610376000	0.826726000
H	3.228343000	-4.344500000	0.050954000	C	0.558914000	-3.814973000	-2.111424000
H	5.451778000	-0.771155000	0.626254000	N	1.774590000	-3.289685000	-1.541821000
H	5.248759000	1.675125000	0.595816000	C	2.419503000	-2.196711000	-2.136773000
H	2.452598000	4.818406000	-0.021593000	N	3.465333000	-1.821651000	-1.292387000

<sup>4</sup>Co<sup>II</sup>-OH(CH<sub>3</sub>)

C	3.553250000	-2.657656000	-0.120197000	H	-3.805718000	-1.734819000	-3.273971000
C	2.375373000	-3.694723000	-0.297711000	H	-4.843146000	-2.238184000	-1.908952000
N	3.201132000	-1.999017000	1.145336000	H	-3.642549000	-4.022112000	-0.463701000
C	2.009971000	-2.423280000	1.638422000	H	-1.443133000	-5.090440000	-0.708469000
N	1.546758000	-3.468980000	0.895714000	H	2.708519000	-4.738240000	-0.322436000
C	4.448457000	-0.822885000	-1.722675000	H	4.539485000	-3.125410000	-0.029038000
N	4.161078000	0.545199000	-1.338106000	H	5.330030000	1.080742000	0.330311000
C	3.425170000	1.389963000	-2.185208000	H	0.559451000	-5.297922000	0.998084000
N	3.097508000	2.525854000	-1.439123000	H	0.393127000	-4.249566000	2.427331000
C	3.651286000	2.510230000	-0.108464000	H	3.538981000	-0.737608000	2.724324000
C	4.287257000	1.077306000	-0.007827000	H	4.909908000	-0.910146000	1.603704000
N	2.659351000	2.509470000	0.965383000	H	-3.589722000	-1.507790000	2.337571000
C	2.463448000	1.257997000	1.469116000	H	-4.728260000	-1.980023000	1.053217000
N	3.444756000	0.423805000	1.000177000	H	-2.432399000	2.855514000	-3.298975000
C	-3.715220000	-1.620296000	1.259814000	H	-3.281894000	3.898494000	-2.120310000
C	0.411218000	-4.268914000	1.336937000	H	2.622400000	4.537431000	-1.787247000
C	3.822954000	-0.805176000	1.673128000	H	2.150831000	3.354223000	-3.042849000
O	-1.313650000	-2.089440000	-3.395800000	H	-5.433296000	-0.070490000	-0.298427000
O	2.126486000	-1.696273000	-3.194655000	H	-4.917645000	2.326790000	-0.459839000
O	3.160650000	1.190403000	-3.344000000	H	-1.735244000	5.123469000	-0.656809000
O	-1.304354000	-2.288199000	2.596551000	H	0.688053000	5.389596000	-0.513129000
O	-1.958563000	0.527722000	2.076212000	H	4.367425000	3.324886000	0.049123000
O	1.433100000	-1.940807000	2.633144000	H	-3.630915000	3.863556000	0.925234000
O	1.547896000	0.946062000	2.252521000	H	-2.850027000	3.061958000	2.309730000
C	2.207747000	3.538810000	-1.967600000	H	1.893915000	3.593081000	2.574974000
C	-2.843491000	3.164261000	1.223537000	H	2.622756000	4.554165000	1.266104000
C	1.982729000	3.695700000	1.492352000	H	-0.218222000	1.405556000	4.003206000
O	-2.897071000	0.518339000	-3.671754000	C	-1.258429000	0.195708000	5.218460000
O	-0.042960000	2.129491000	-3.080911000	H	-1.071330000	0.794722000	6.112713000
O	-0.477816000	3.065125000	2.833600000	H	-2.242198000	0.427200000	4.800719000
O	-0.220233000	0.453522000	4.246512000	H	-1.196478000	-0.863352000	5.468430000
O	0.072507000	-0.720909000	0.193335000				
H	-0.058173000	-1.521535000	-0.359744000				
							<sup>2</sup> Co <sup>II</sup> -OH(CH <sub>3</sub> )
H	0.084063000	0.032747000	-0.419856000	Co	-0.260512000	-0.529846000	2.298503000
H	0.541942000	-3.509386000	-3.160735000	C	0.619196000	3.441316000	1.821747000
H	0.553199000	-4.909256000	-2.042550000	N	-0.372700000	3.964124000	1.007429000
H	5.431590000	-1.115599000	-1.339420000	C	0.113214000	4.388921000	-0.300725000
H	4.462952000	-0.832944000	-2.814514000	C	1.653775000	4.087698000	-0.218599000

N	1.811963000	3.549846000	1.128299000	C	2.691827000	0.454401000	1.483081000
N	1.877147000	3.148084000	-1.296075000	N	3.383686000	-0.627112000	0.993391000
C	0.712055000	2.876564000	-2.016614000	C	-4.021060000	-0.477686000	1.226349000
N	-0.332548000	3.588443000	-1.418892000	C	-0.895772000	-4.239864000	1.184873000
C	-1.606680000	3.751928000	-2.108033000	C	3.373096000	-1.924930000	1.641887000
N	-2.636243000	2.813287000	-1.704576000	O	-1.842674000	-1.442900000	-3.437053000
C	-2.975264000	1.722693000	-2.507488000	O	1.555527000	-2.121869000	-3.251738000
N	-3.870557000	0.932246000	-1.764924000	O	3.413831000	0.324335000	-3.306377000
C	-4.103821000	1.460755000	-0.446817000	O	-1.967870000	-1.905573000	2.517699000
C	-3.327506000	2.825502000	-0.440252000	O	-1.681158000	1.029438000	2.121547000
N	-2.459087000	2.711749000	0.732667000	O	0.761132000	-2.337402000	2.571342000
C	-2.454024000	1.445963000	1.234881000	O	1.695839000	0.412390000	2.224274000
N	-3.452408000	0.720096000	0.637551000	C	3.185981000	2.802368000	-1.845915000
C	-4.242256000	-0.392052000	-2.219362000	C	-1.754782000	3.834715000	1.362421000
N	-3.404338000	-1.486966000	-1.711932000	C	3.006382000	2.917928000	1.614076000
C	-2.248096000	-1.865153000	-2.385874000	O	-2.603087000	1.512187000	-3.634416000
N	-1.593855000	-2.848187000	-1.582153000	O	0.620885000	2.160226000	-2.987839000
C	-2.538860000	-3.401267000	-0.614783000	O	0.467890000	3.001152000	2.951464000
C	-3.674171000	-2.319293000	-0.563657000	O	-0.097403000	0.063656000	4.184624000
N	-2.018618000	-3.424479000	0.746097000	O	-0.187103000	-0.777569000	0.204286000
C	-2.432596000	-2.313278000	1.441551000	H	-0.565919000	-1.478048000	-0.375995000
N	-3.437862000	-1.707773000	0.748332000	H	0.027680000	-0.021265000	-0.366928000
C	-0.583672000	-3.703157000	-2.239527000	H	-0.500159000	-3.359691000	-3.273856000
N	0.726690000	-3.589791000	-1.654407000	H	-0.919443000	-4.746659000	-2.219484000
C	1.674992000	-2.718516000	-2.209991000	H	4.861493000	-2.623248000	-1.375842000
N	2.773007000	-2.697025000	-1.350405000	H	4.039815000	-2.015492000	-2.842045000
C	2.593765000	-3.561672000	-0.208215000	H	-4.137251000	-0.382908000	-3.306255000
C	1.163846000	-4.195424000	-0.423455000	H	-5.282445000	-0.603041000	-1.952500000
N	2.437276000	-2.873092000	1.078898000	H	-4.685881000	-2.737553000	-0.603462000
C	1.169230000	-2.939921000	1.559573000	H	-2.893971000	-4.393809000	-0.913131000
N	0.422168000	-3.773343000	0.774440000	H	1.172615000	-5.289472000	-0.484193000
C	4.018931000	-2.032597000	-1.750432000	H	3.395709000	-4.304137000	-0.134238000
N	4.161211000	-0.654375000	-1.325079000	H	5.397169000	-0.556073000	0.377797000
C	3.716576000	0.398766000	-2.141916000	H	-1.038067000	-5.256106000	0.807435000
N	3.736523000	1.555524000	-1.357809000	H	-0.921189000	-4.255270000	2.275158000
C	4.245723000	1.331165000	-0.026748000	H	3.100581000	-1.799307000	2.690738000
C	4.411433000	-0.229486000	0.026574000	H	4.382425000	-2.343501000	1.582152000
N	3.289282000	1.600149000	1.043036000	H	-3.868564000	-0.454491000	2.306099000

H	-5.095502000	-0.479424000	1.017210000
H	-1.444587000	3.575112000	-3.173800000
H	-1.955063000	4.779844000	-1.954526000
H	3.875828000	3.628156000	-1.636375000
H	3.079628000	2.678855000	-2.926147000
H	-5.174459000	1.560962000	-0.233889000
H	-3.975529000	3.703156000	-0.334826000
H	-0.114802000	5.449716000	-0.459206000
H	2.278252000	4.980758000	-0.339915000
H	5.175012000	1.882575000	0.156360000
H	-2.306472000	4.741320000	1.094321000
H	-1.789404000	3.701275000	2.444737000
H	2.886952000	2.811353000	2.693463000
H	3.879203000	3.546191000	1.411462000
H	0.145305000	1.009296000	4.088737000
C	-1.173401000	-0.078760000	5.144009000
H	-0.831070000	0.301341000	6.109204000
H	-2.063187000	0.460529000	4.809070000
H	-1.380848000	-1.145257000	5.217656000

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