

Reaction Mechanism of Intramolecular C-C Coupling Catalyzed by the Non-heme Deoxypodophyllotoxin Synthase

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Table S1. Calculated spin populations of key atoms or group of involved species for the formation of C ring and OH rebound at triplet and quintet states ((-)-yatein).

	Fe	O	C7'(Sub)	B ring	Owat
³ R / ⁵ R	1.51 / 3.15	0.49 / 0.61	0.00 / 0.00	0.00 / 0.00	0.00 / 0.00
³ TS / ⁵ TS	1.64 / 3.23	0.33 / 0.58	0.00 / 0.00	0.00 / 0.00	0.00 / 0.00
³ R' / ⁵ R'	1.32 / 3.21	0.71 / 0.51	0.00 / 0.00	0.00 / 0.00	0.00 / 0.07
³ TS1 / ⁵ TS1	2.81 / 4.19	-0.46 / -0.21	-0.30 / -0.24	0.00 / 0.00	0.03 / 0.00
³ IM1 / ⁵ IM1	2.78 / 4.25	0.04 / 0.24	-0.61 / -0.61	0.00 / 0.00	0.07 / 0.00
⁵ TS2	4.29	0.11	-0.60	-0.02	0.15
⁵ IM2	4.23	0.05	-0.60	-0.02	0.31
⁵ TS3	4.08	0.07	-0.32	-0.48	0.33
⁵ IM3	4.23	0.07	-0.05	-0.82	0.33
⁵ TS4	4.28	0.11	-0.05	-0.83	0.15
⁵ IM4	4.14	0.36	-0.06	-0.83	0.09
⁵ TS5	3.92	0.25	-0.04	-0.45	0.07
⁵ Pa	3.67	0.04	0.00	0.00	0.04
⁵ TS _{OH}	4.10	0.19	-0.42	0.00	0.06
⁵ IM _{OH}	3.70	0.00	0.00	0.00	0.04

Table S2. Comparison of the calculated barriers for the hydrogen abstraction (⁵R' to ⁵IM1) and C-C coupling (⁵IM2 to ⁵IM3) by using different sizes of QM region models. QM represents the model shown in Figure 2 of the main text, whereas QM-I contains the additional R249, and QM-II contains additional Y169, R249 and S251.

Barriers	QM	QM1	QM2
Hydrogen abstraction	13.4	15.7	15.7
C-C coupling	24.2	25.4	26.3

Table S3. Relative energies of the hydrogen abstraction from $^5R'$ to 5IM1 with B3LYP, M06, TPSSH and PBE0 functionals.

	B3LYP	M06	TPSSH	PBE0
$^5R'$	0.0	0.0	0.0	0.0
5TS1	13.4	12.8	17.1	11.0
5IM1	-12.7	-17.2	-5.6	-17.9

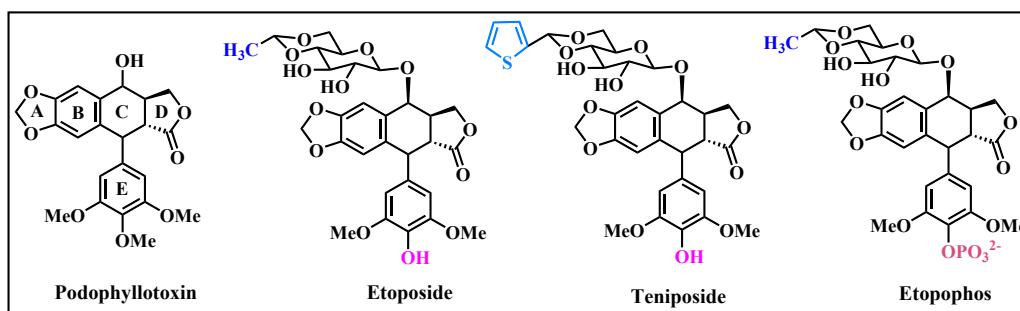


Figure S1. Structures of podophyllotoxin and its three derivatives etoposide, teniposide and etopophos.

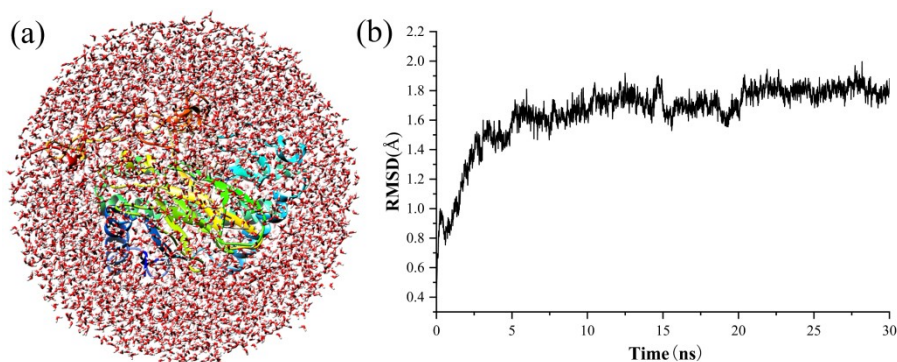


Figure S2. (a) The constructed solvation model. (b) RMSDs of 30 ns MD simulations for the backbone atoms of DPS in complex with the substrate.

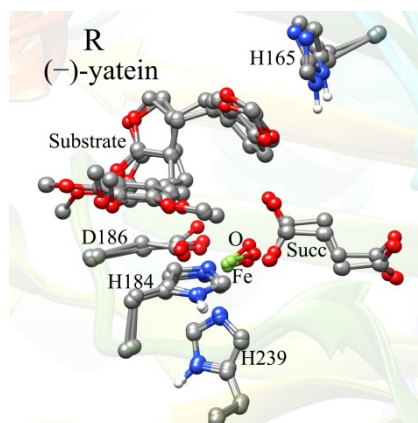


Figure S3. Overlap of active site pockets of three QM/MM-optimized reactants, which were derived from the MD trajectory from 28, 29 and 30 ns.

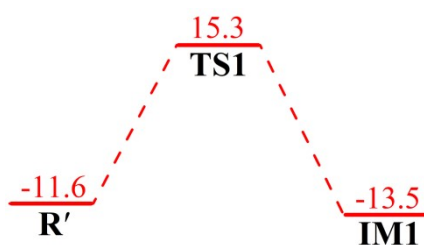


Figure S4. Calculated energy profiles for the hydrogen atom abstraction from C7'-position ((-)-yatein, π -pathway).

Electron affinity (IM1)	Fe(III)–(2His–1Asp–1Succ–H ₂ O)–OH: -0.68 eV
	Fe(III)–(2His–1Asp–1Succ–H ₂ O–OH)–T191: -1.03 eV
	Fe(III)–(2His–1Asp–1Succ–H ₂ O–OH)–(T191–S253): -1.22 eV
	Fe(III)–(2His–1Asp–1Succ–H ₂ O–OH)–(Y169–R249–S251): -0.53 eV
	Fe(III)–(2His–1Asp–1Succ–H ₂ O–OH)–(Y169–R249–S251–T191): -0.86 eV
	Fe(III)–(2His–1Asp–1Succ–H ₂ O–OH)–(Y169–R249–S251–T191–S253): -1.00 eV

Figure S5. The electron affinities of iron center in intermediate IM1, in which different surrounding residues were included.

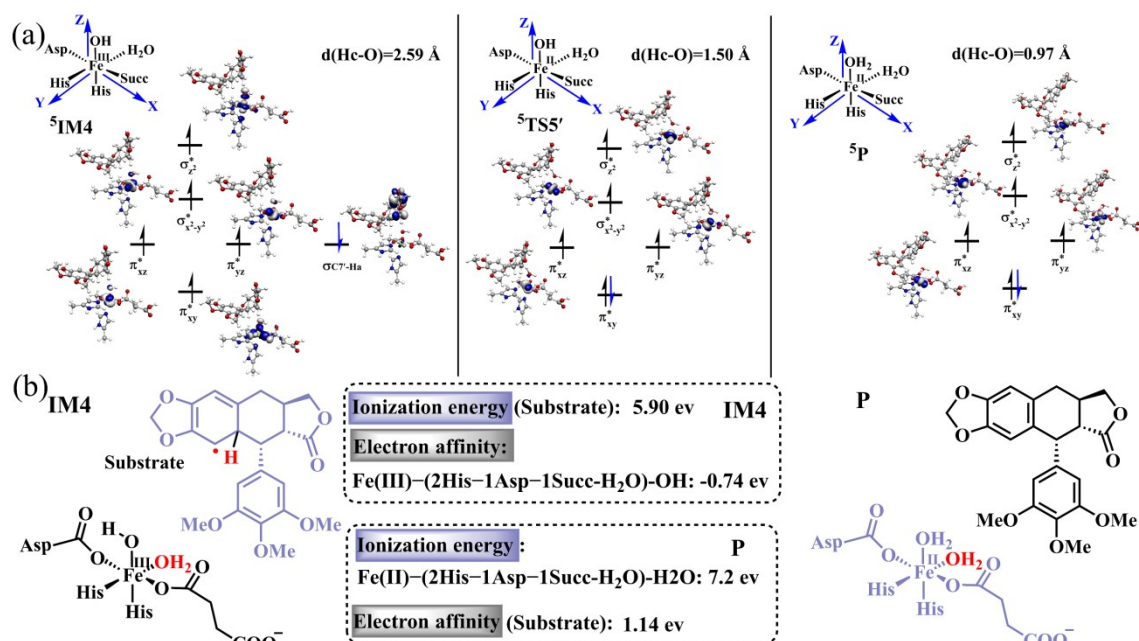


Figure S6. (a) Valence electron orbital diagrams of $^5\text{IM4}$, $^5\text{TS5'}$ and ^5P . (b) The ionization energy or electron affinity of the Fe^{3+} - and Fe^{2+} -coordinate fragments, substrate radical and the deoxypodophyllotoxin in IM4 and P.

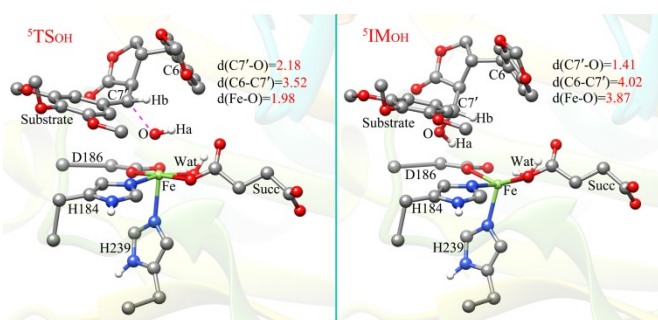


Figure S7. Optimized structures of involved species in the reaction of OH rebound ((-)-yatein). All distances are given in Å.

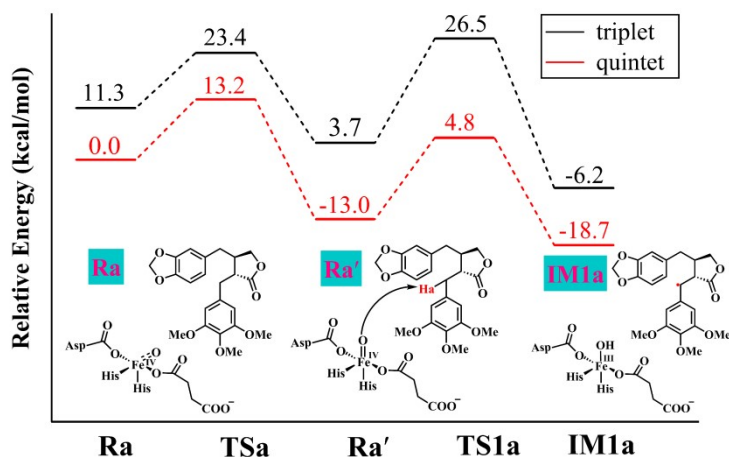


Figure S8. Calculated energy profiles for the isomerization of Fe(IV)=O species and H-abstraction in the penta-coordinate model ((-)-yatein, σ -pathway).

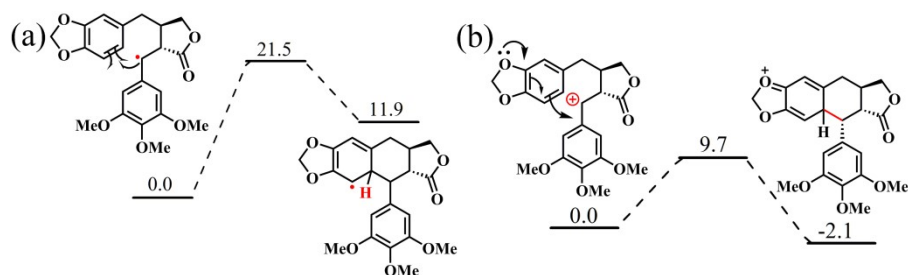


Figure S9. QM-only calculated energy profiles for C-C bond formation ((-)-yatein) driven by a carbon radical (a) or a carbocation (b).

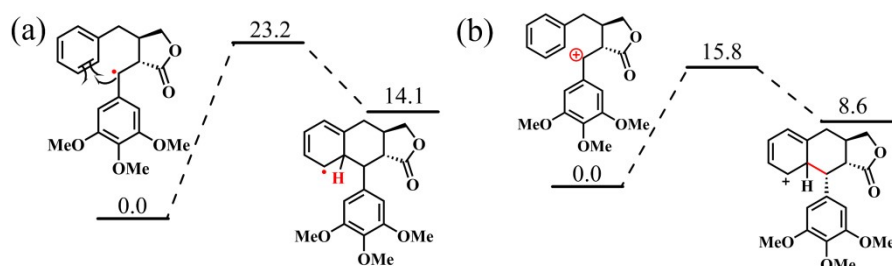


Figure S10. QM-only calculated energy profiles for C-C bond formation driven by a carbon radical (a) or a carbocation (b). Note that the ring A in IM1 was removed for comparison.

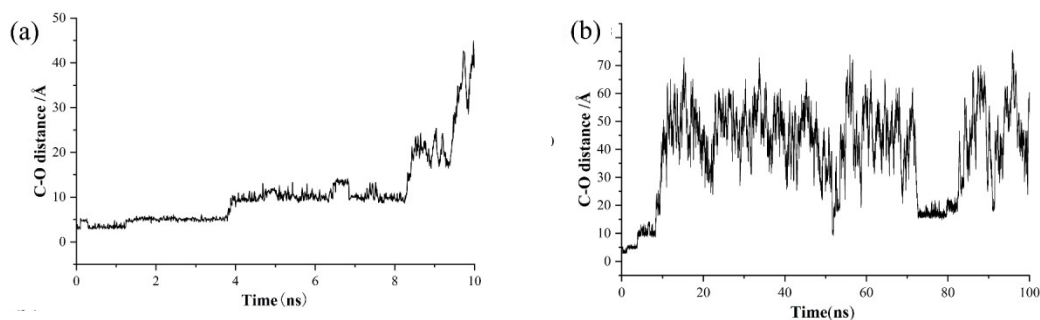


Figure S11. The time courses of distance between CO₂ and the iron center during 100 ns of MD simulations. (a) the zoom of 10 ns MD simulations, (b) the result of whole 100 ns. Note that the C-O distance refers that from the carbon of CO₂ and O atom in Fe(IV)=O.

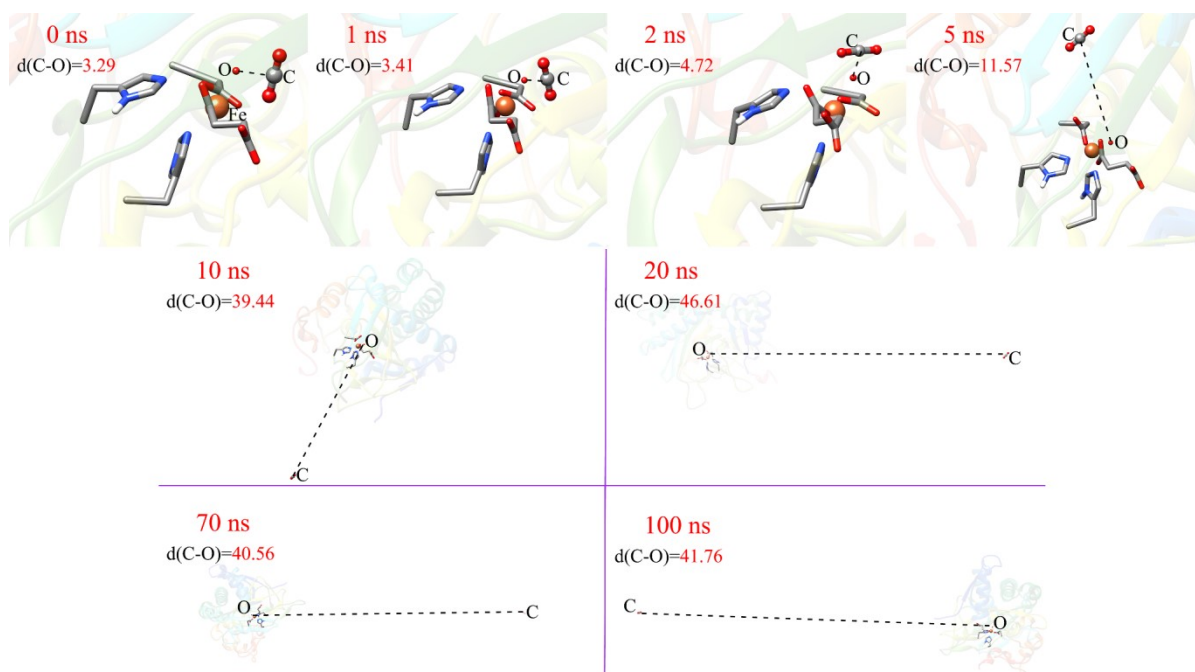


Figure S12. Different distances between the CO₂ and the Fe(IV)=O during MD simulations. All distances are given in Å.

Details of MD simulation with Amber22 package.¹ Firstly, the protonation state of all titratable residues was assigned according to calculated pK_a values by the PROPKA program,² which were conformed with careful visual inspection of the local hydrogen-bonded networks. The force field parameters of Fe(IV)=O, CO₂ and substrate were prepared with the “MCPB.py” modeling tool of AmberTools23,^{3,4} and the parameters of substrate were derived from the parmchk utility of AmberTools23, in which the general AMBER force field (gaff)⁵ was used. For the protein residues, the Amber ff19SB force field was employed.⁶ The partial atomic charges were obtained from RESP method⁷ at HF/6-31G(d) level of theory by Gaussian 09 package.⁸ All crystal water molecules were retained in their original positions. The whole system was solvated in a rectangular TIP3P waters box with a minimum distance of 10 Å from the protein surface. A few ions were added to the protein by using the keywords “addIonsRand” and “separation” to neutralize the total charge of the system.

The system is respectively subjected to minimization of water molecules, and minimization of steepest descent and conjugate gradient. Under the canonical ensemble (NVT), the weak constraint on the protein backbone atoms was set to be 5 kcal · mol⁻¹ · Å⁻², and the system was gradually heated from 0 to 300K in a time step of 1fs for 100 ps. Subsequently, the density equilibration for 1 ns was

performed under the isobaric ensemble (NPT) at a target temperature of 300 K and target pressure of 1.0 atm to achieve a uniform density. Subsequently, the system was further equilibrated under NPT ensemble for 1 ns with a restraint on the protein. Afterward, the system was further equilibrated in an NPT ensemble for 4 ns without protein constraints to achieve stable pressure and temperature. Finally, a 100 ns productive MD simulation was performed. The SHAKE algorithm⁴³ was used with a step integral of 2 fs to constrain covalent bonds containing hydrogen, and Particle Mesh Ewald (PME)⁴⁴ method with a cutoff value of 10 Å was implemented to non-bonding interactions.

References:

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Cartesian coordinates of QM regions of optimized species

³R

C	8.379000	1.776000	-1.408000	N	-0.026000	4.420000	4.719000
H	7.711000	1.624000	-2.230000	C	0.251000	4.379000	6.074000
H	7.885000	1.518000	-0.494000	H	1.271000	4.399000	6.419000
N	8.394000	4.091000	-0.372000	Fe	1.296000	4.793000	3.339000
H	7.824000	3.852000	0.457000	O	1.886000	3.501000	2.608000
C	8.796000	3.215000	-1.362000	C	6.629000	2.705000	6.717000
C	8.857000	5.326000	-0.697000	O	7.593000	3.341000	7.237000
H	8.682000	6.192000	-0.075000	O	6.141000	1.632000	7.175000
N	9.533000	5.310000	-1.838000	C	6.036000	3.274000	5.427000
C	9.496000	3.996000	-2.253000	H	6.069000	2.495000	4.657000
H	9.963000	3.684000	-3.174000	H	6.648000	4.113000	5.081000
C	-0.841000	9.960000	4.061000	C	4.585000	3.705000	5.621000
H	-1.279000	10.036000	3.088000	H	4.490000	4.416000	6.452000
H	-0.300000	10.857000	4.280000	H	3.966000	2.836000	5.870000
N	1.139000	8.629000	5.000000	C	3.944000	4.319000	4.383000
H	1.391000	9.254000	5.770000	O	2.748000	4.802000	4.637000
C	0.093000	8.792000	4.098000	O	4.508000	4.324000	3.284000
C	1.704000	7.425000	4.776000	C	8.301000	10.291000	1.085000
H	2.514000	7.005000	5.348000	H	8.181000	11.344000	1.345000
N	1.091000	6.805000	3.772000	H	9.356000	10.024000	0.948000
C	0.090000	7.650000	3.342000	O	7.586000	10.011000	-0.137000
H	-0.564000	7.369000	2.533000	O	7.721000	9.477000	2.110000
C	-1.698000	4.213000	0.339000	C	6.942000	8.814000	0.090000
H	-2.486000	3.492000	0.396000	C	7.030000	8.487000	1.442000
H	-1.188000	4.111000	-0.596000	C	6.423000	7.354000	1.951000
C	-0.710000	3.982000	1.487000	H	6.481000	7.093000	3.002000
O	-0.118000	5.026000	2.016000	C	5.719000	6.542000	1.040000
O	-0.517000	2.816000	1.819000	H	5.233000	5.650000	1.425000
C	-1.188000	4.310000	8.243000	C	5.634000	6.861000	-0.320000
H	-0.325000	3.926000	8.746000	C	6.263000	8.027000	-0.813000
H	-2.026000	3.674000	8.436000	H	6.217000	8.289000	-1.866000
N	-1.923000	4.366000	5.802000	C	4.900000	5.970000	-1.298000
H	-2.928000	4.422000	5.952000	H	4.717000	4.989000	-0.847000
C	-0.927000	4.357000	6.772000	H	5.556000	5.795000	-2.162000
C	-1.352000	4.415000	4.586000	C	3.570000	6.540000	-1.829000
H	-1.920000	4.435000	3.673000	H	3.668000	7.625000	-1.970000

C	3.185000	5.897000	-3.166000	H	4.779000	11.430000	3.779000
H	3.381000	4.817000	-3.149000	C	1.747000	11.342000	0.676000
H	3.672000	6.333000	-4.041000	O	1.587000	12.689000	0.932000
O	1.753000	6.096000	-3.299000	C	2.418000	13.537000	0.130000
C	1.209000	6.321000	-2.083000	H	2.245000	13.352000	-0.937000
O	0.016000	6.505000	-1.949000	H	3.479000	13.384000	0.363000
C	2.293000	6.268000	-1.010000	H	2.137000	14.565000	0.365000
H	2.315000	5.204000	-0.718000	C	0.916000	10.685000	-0.246000
C	1.992000	7.040000	0.287000	O	0.028000	11.490000	-0.902000
H	2.723000	6.705000	1.029000	C	-0.993000	10.867000	-1.666000
H	1.024000	6.669000	0.640000	H	-1.590000	10.189000	-1.043000
C	1.968000	8.562000	0.308000	H	-0.581000	10.302000	-2.512000
C	2.824000	9.229000	1.196000	H	-1.627000	11.673000	-2.043000
H	3.556000	8.657000	1.754000	C	1.016000	9.296000	-0.418000
C	2.702000	10.609000	1.394000	H	0.330000	8.774000	-1.072000
O	3.433000	11.348000	2.284000	O	2.172000	1.658000	4.802000
C	4.355000	10.668000	3.124000	H	2.136000	2.067000	3.922000
H	5.163000	10.201000	2.551000	H	1.411000	2.046000	5.249000
H	3.855000	9.904000	3.733000				
³ TS							
C	8.382000	1.776000	-1.409000	C	0.093000	7.580000	3.376000
H	7.714000	1.624000	-2.231000	H	-0.557000	7.293000	2.566000
H	7.888000	1.518000	-0.496000	C	-1.719000	4.192000	0.354000
N	8.396000	4.090000	-0.372000	H	-2.499000	3.464000	0.432000
H	7.827000	3.852000	0.457000	H	-1.224000	4.085000	-0.589000
C	8.797000	3.215000	-1.363000	C	-0.710000	3.982000	1.487000
C	8.857000	5.326000	-0.697000	O	-0.118000	5.026000	2.016000
H	8.683000	6.191000	-0.075000	O	-0.466000	2.819000	1.813000
N	9.533000	5.310000	-1.838000	C	-1.221000	4.314000	8.291000
C	9.496000	3.996000	-2.254000	H	-0.357000	3.929000	8.791000
H	9.962000	3.685000	-3.176000	H	-2.063000	3.687000	8.499000
C	-0.810000	9.913000	4.062000	N	-1.970000	4.342000	5.849000
H	-1.238000	9.986000	3.084000	H	-2.975000	4.407000	5.998000
H	-0.258000	10.804000	4.277000	C	-0.973000	4.343000	6.819000
N	1.149000	8.567000	5.027000	C	-1.394000	4.373000	4.633000
H	1.406000	9.203000	5.786000	H	-1.961000	4.384000	3.718000
C	0.109000	8.730000	4.118000	N	-0.069000	4.377000	4.761000
C	1.702000	7.353000	4.826000	C	0.202000	4.356000	6.118000
H	2.506000	6.932000	5.405000	H	1.222000	4.380000	6.466000
N	1.084000	6.731000	3.827000	Fe	1.296000	4.793000	3.339000

O	2.178000	4.028000	2.268000	O	1.746000	6.090000	-3.291000
C	6.641000	2.693000	6.747000	C	1.204000	6.315000	-2.074000
O	7.602000	3.332000	7.266000	O	0.010000	6.497000	-1.940000
O	6.157000	1.615000	7.199000	C	2.288000	6.266000	-1.003000
C	6.039000	3.264000	5.467000	H	2.312000	5.205000	-0.701000
H	6.086000	2.498000	4.685000	C	1.990000	7.041000	0.293000
H	6.628000	4.122000	5.130000	H	2.718000	6.704000	1.034000
C	4.579000	3.655000	5.671000	H	1.023000	6.669000	0.647000
H	4.464000	4.348000	6.516000	C	1.964000	8.563000	0.311000
H	3.984000	2.766000	5.905000	C	2.821000	9.230000	1.200000
C	3.939000	4.283000	4.442000	H	3.553000	8.658000	1.756000
O	2.709000	4.679000	4.679000	C	2.700000	10.611000	1.397000
O	4.551000	4.370000	3.373000	O	3.431000	11.349000	2.286000
C	8.300000	10.288000	1.086000	C	4.355000	10.669000	3.123000
H	8.181000	11.342000	1.345000	H	5.162000	10.202000	2.548000
H	9.356000	10.021000	0.950000	H	3.857000	9.904000	3.733000
O	7.586000	10.008000	-0.136000	H	4.781000	11.430000	3.779000
O	7.720000	9.476000	2.111000	C	1.745000	11.344000	0.678000
C	6.941000	8.811000	0.092000	O	1.587000	12.691000	0.933000
C	7.028000	8.485000	1.444000	C	2.419000	13.537000	0.130000
C	6.419000	7.354000	1.953000	H	2.246000	13.351000	-0.936000
H	6.474000	7.094000	3.005000	H	3.479000	13.383000	0.364000
C	5.713000	6.542000	1.043000	H	2.139000	14.566000	0.364000
H	5.222000	5.653000	1.430000	C	0.914000	10.686000	-0.244000
C	5.631000	6.859000	-0.317000	O	0.026000	11.491000	-0.901000
C	6.262000	8.024000	-0.811000	C	-0.993000	10.868000	-1.667000
H	6.216000	8.285000	-1.865000	H	-1.591000	10.189000	-1.044000
C	4.896000	5.968000	-1.295000	H	-0.579000	10.303000	-2.512000
H	4.713000	4.989000	-0.843000	H	-1.627000	11.673000	-2.044000
H	5.551000	5.794000	-2.160000	C	1.013000	9.298000	-0.415000
C	3.564000	6.538000	-1.824000	H	0.328000	8.775000	-1.069000
H	3.663000	7.623000	-1.967000	O	2.169000	1.677000	4.522000
C	3.178000	5.893000	-3.160000	H	2.184000	2.050000	3.631000
H	3.376000	4.814000	-3.143000	H	1.459000	2.168000	4.954000
H	3.664000	6.329000	-4.035000				
³ R'							
C	8.397000	1.835000	-1.416000	H	7.849000	3.882000	0.456000
H	7.709000	1.700000	-2.224000	C	8.827000	3.268000	-1.360000
H	7.922000	1.569000	-0.495000	C	8.878000	5.374000	-0.680000
N	8.421000	4.135000	-0.364000	H	8.698000	6.236000	-0.054000

N	9.556000	5.368000	-1.820000	H	3.535000	2.174000	6.233000
C	9.525000	4.056000	-2.244000	H	4.752000	1.530000	5.137000
H	9.994000	3.753000	-3.167000	C	3.570000	3.057000	4.279000
C	-0.591000	9.565000	4.054000	O	2.661000	3.947000	4.551000
H	-0.984000	9.644000	3.062000	O	3.882000	2.650000	3.138000
H	0.037000	10.407000	4.257000	C	8.287000	10.274000	1.077000
N	1.225000	8.081000	5.097000	H	8.189000	11.327000	1.345000
H	1.487000	8.702000	5.860000	H	9.337000	9.987000	0.936000
C	0.210000	8.303000	4.176000	O	7.564000	10.018000	-0.145000
C	1.712000	6.831000	4.896000	O	7.693000	9.464000	2.097000
H	2.492000	6.371000	5.480000	C	6.889000	8.837000	0.076000
N	1.076000	6.250000	3.891000	C	6.975000	8.497000	1.424000
C	0.140000	7.152000	3.435000	C	6.348000	7.373000	1.926000
H	-0.523000	6.898000	2.625000	H	6.412000	7.108000	2.976000
C	-2.024000	3.992000	0.373000	C	5.619000	6.586000	1.011000
H	-2.868000	3.430000	0.714000	H	5.109000	5.698000	1.375000
H	-1.788000	3.706000	-0.631000	C	5.533000	6.918000	-0.345000
C	-0.830000	3.712000	1.275000	C	6.188000	8.073000	-0.831000
O	-0.413000	4.578000	2.119000	H	6.144000	8.343000	-1.882000
O	-0.338000	2.567000	1.108000	C	4.778000	6.051000	-1.327000
C	-1.288000	4.324000	8.380000	H	4.599000	5.062000	-0.895000
H	-0.428000	3.933000	8.882000	H	5.419000	5.892000	-2.205000
H	-2.149000	3.748000	8.647000	C	3.438000	6.627000	-1.831000
N	-2.096000	4.285000	5.957000	H	3.540000	7.708000	-1.993000
H	-3.084000	4.471000	6.117000	C	3.032000	5.955000	-3.150000
C	-1.078000	4.250000	6.902000	H	3.252000	4.880000	-3.120000
C	-1.540000	4.178000	4.730000	H	3.493000	6.386000	-4.041000
H	-2.121000	4.206000	3.822000	O	1.596000	6.122000	-3.258000
N	-0.223000	4.050000	4.825000	C	1.074000	6.370000	-2.037000
C	0.070000	4.087000	6.171000	O	-0.119000	6.534000	-1.882000
H	1.092000	4.010000	6.508000	C	2.176000	6.370000	-0.984000
Fe	1.235000	4.333000	3.275000	H	2.219000	5.323000	-0.643000
O	2.219000	4.691000	2.029000	C	1.864000	7.170000	0.292000
C	6.348000	2.596000	6.929000	H	2.537000	6.807000	1.067000
O	7.518000	3.090000	7.034000	H	0.869000	6.836000	0.607000
O	5.988000	1.503000	7.433000	C	1.883000	8.687000	0.295000
C	5.334000	3.374000	6.088000	C	2.741000	9.334000	1.196000
H	5.882000	3.918000	5.310000	H	3.442000	8.743000	1.771000
H	4.865000	4.139000	6.719000	C	2.658000	10.719000	1.378000
C	4.274000	2.450000	5.478000	O	3.399000	11.440000	2.275000

C	4.296000	10.732000	3.120000	O	0.036000	11.647000	-0.964000
H	5.086000	10.233000	2.548000	C	-0.987000	11.030000	-1.732000
H	3.768000	9.990000	3.734000	H	-1.592000	10.357000	-1.111000
H	4.747000	11.481000	3.771000	H	-0.575000	10.461000	-2.576000
C	1.734000	11.472000	0.639000	H	-1.615000	11.838000	-2.111000
O	1.610000	12.823000	0.886000	C	0.967000	9.440000	-0.453000
C	2.457000	13.642000	0.073000	H	0.279000	8.929000	-1.115000
H	2.279000	13.449000	-0.991000	O	1.264000	2.403000	2.971000
H	3.515000	13.470000	0.307000	H	2.195000	2.270000	2.686000
H	2.198000	14.679000	0.296000	H	0.652000	2.312000	2.160000
C	0.899000	10.830000	-0.291000				
³ TS1							
C	8.415000	1.832000	-1.387000	C	-1.127000	4.301000	8.196000
H	7.723000	1.698000	-2.192000	H	-0.255000	3.930000	8.694000
H	7.948000	1.554000	-0.466000	H	-1.959000	3.662000	8.409000
N	8.375000	4.138000	-0.351000	N	-1.895000	4.374000	5.768000
H	7.783000	3.890000	0.459000	H	-2.892000	4.480000	5.934000
C	8.832000	3.268000	-1.321000	C	-0.885000	4.328000	6.721000
C	8.824000	5.381000	-0.663000	C	-1.329000	4.379000	4.543000
H	8.611000	6.246000	-0.051000	H	-1.903000	4.439000	3.634000
N	9.544000	5.374000	-1.777000	N	-0.008000	4.311000	4.646000
C	9.551000	4.058000	-2.187000	C	0.278000	4.271000	5.996000
H	10.061000	3.753000	-3.088000	H	1.302000	4.217000	6.333000
C	-0.760000	9.865000	4.098000	Fe	1.392000	4.755000	3.149000
H	-1.167000	9.945000	3.112000	O	2.480000	5.226000	1.809000
H	-0.202000	10.749000	4.326000	C	6.413000	2.645000	6.903000
N	1.177000	8.491000	5.078000	O	7.593000	3.107000	7.043000
H	1.418000	9.101000	5.864000	O	6.014000	1.550000	7.376000
C	0.142000	8.673000	4.171000	C	5.450000	3.482000	6.067000
C	1.750000	7.289000	4.826000	H	6.043000	4.066000	5.354000
H	2.564000	6.862000	5.391000	H	4.963000	4.214000	6.724000
N	1.148000	6.703000	3.803000	C	4.394000	2.643000	5.338000
C	0.144000	7.547000	3.391000	H	3.590000	2.366000	6.023000
H	-0.512000	7.283000	2.576000	H	4.847000	1.722000	4.963000
C	-2.023000	4.066000	0.285000	C	3.825000	3.420000	4.162000
H	-2.838000	3.457000	0.617000	O	2.955000	4.326000	4.461000
H	-1.768000	3.803000	-0.720000	O	4.234000	3.141000	3.007000
C	-0.818000	3.841000	1.191000	C	8.294000	10.284000	1.066000
O	-0.323000	4.798000	1.878000	H	8.172000	11.342000	1.310000
O	-0.372000	2.666000	1.172000	H	9.347000	10.027000	0.899000

O	7.541000	9.976000	-0.126000	C	1.684000	8.401000	0.365000
O	7.759000	9.487000	2.127000	C	2.571000	8.975000	1.285000
C	6.866000	8.808000	0.160000	H	3.236000	8.334000	1.849000
C	7.005000	8.510000	1.514000	C	2.549000	10.361000	1.502000
C	6.390000	7.408000	2.077000	O	3.311000	11.029000	2.416000
H	6.497000	7.175000	3.131000	C	4.126000	10.269000	3.299000
C	5.618000	6.596000	1.222000	H	4.898000	9.711000	2.760000
H	5.114000	5.726000	1.633000	H	3.525000	9.572000	3.896000
C	5.484000	6.884000	-0.141000	H	4.602000	10.994000	3.961000
C	6.125000	8.018000	-0.692000	C	1.671000	11.181000	0.774000
H	6.049000	8.251000	-1.750000	O	1.617000	12.532000	1.050000
C	4.720000	5.958000	-1.061000	C	2.448000	13.341000	0.208000
H	4.480000	5.035000	-0.529000	H	2.179000	13.206000	-0.846000
H	5.395000	5.674000	-1.881000	H	3.508000	13.102000	0.354000
C	3.429000	6.526000	-1.694000	H	2.266000	14.380000	0.493000
H	3.508000	7.616000	-1.792000	C	0.808000	10.608000	-0.174000
C	3.200000	5.912000	-3.083000	O	0.001000	11.487000	-0.839000
H	3.422000	4.837000	-3.074000	C	-1.023000	10.951000	-1.663000
H	3.764000	6.381000	-3.891000	H	-1.689000	10.298000	-1.084000
O	1.786000	6.079000	-3.362000	H	-0.610000	10.384000	-2.507000
C	1.109000	6.222000	-2.205000	H	-1.591000	11.803000	-2.041000
O	-0.098000	6.345000	-2.182000	C	0.803000	9.221000	-0.363000
C	2.084000	6.181000	-1.021000	H	0.104000	8.761000	-1.052000
H	2.122000	5.118000	-0.737000	O	1.601000	2.767000	2.714000
C	1.555000	6.907000	0.211000	H	2.490000	2.723000	2.312000
H	2.105000	6.208000	1.184000	H	0.871000	2.581000	2.037000
H	0.521000	6.589000	0.367000				
³ IM1							
C	8.417000	1.831000	-1.402000	H	-1.083000	9.813000	3.090000
H	7.731000	1.701000	-2.213000	H	-0.110000	10.636000	4.285000
H	7.941000	1.553000	-0.485000	N	1.195000	8.367000	5.144000
N	8.393000	4.132000	-0.352000	H	1.414000	8.991000	5.922000
H	7.805000	3.882000	0.459000	C	0.203000	8.550000	4.190000
C	8.839000	3.264000	-1.331000	C	1.749000	7.145000	4.937000
C	8.844000	5.375000	-0.662000	H	2.528000	6.723000	5.553000
H	8.636000	6.238000	-0.046000	N	1.188000	6.545000	3.900000
N	9.555000	5.371000	-1.781000	C	0.226000	7.410000	3.427000
C	9.554000	4.057000	-2.198000	H	-0.385000	7.152000	2.575000
H	10.054000	3.754000	-3.105000	C	-1.982000	3.951000	0.364000
C	-0.681000	9.755000	4.080000	H	-2.825000	3.381000	0.696000

H	-1.739000	3.676000	-0.641000	C	5.536000	6.886000	-0.484000
C	-0.789000	3.669000	1.270000	C	6.146000	8.076000	-0.943000
O	-0.377000	4.552000	2.100000	H	6.084000	8.374000	-1.985000
O	-0.302000	2.521000	1.145000	C	4.783000	6.020000	-1.472000
C	-1.210000	4.341000	8.346000	H	4.643000	5.018000	-1.057000
H	-0.345000	3.964000	8.850000	H	5.400000	5.899000	-2.373000
H	-2.056000	3.731000	8.585000	C	3.418000	6.570000	-1.923000
N	-1.991000	4.361000	5.919000	H	3.525000	7.632000	-2.181000
H	-2.984000	4.508000	6.082000	C	2.870000	5.814000	-3.132000
C	-0.978000	4.314000	6.871000	H	3.035000	4.734000	-3.024000
C	-1.431000	4.312000	4.694000	H	3.269000	6.147000	-4.092000
H	-2.003000	4.355000	3.782000	O	1.442000	6.061000	-3.131000
N	-0.111000	4.210000	4.798000	C	1.032000	6.460000	-1.901000
C	0.180000	4.204000	6.145000	O	-0.131000	6.730000	-1.693000
H	1.203000	4.134000	6.481000	C	2.219000	6.447000	-0.936000
Fe	1.251000	4.407000	3.268000	H	2.222000	5.424000	-0.526000
O	2.305000	4.655000	1.849000	C	2.266000	7.351000	0.251000
C	6.362000	2.574000	6.943000	H	3.135000	4.185000	2.086000
O	7.535000	3.058000	7.064000	H	2.698000	6.867000	1.120000
O	5.986000	1.480000	7.434000	C	2.043000	8.750000	0.366000
C	5.368000	3.366000	6.095000	C	2.694000	9.399000	1.454000
H	5.930000	4.058000	5.458000	H	3.321000	8.801000	2.103000
H	4.746000	3.983000	6.756000	C	2.571000	10.766000	1.643000
C	4.477000	2.440000	5.255000	O	3.203000	11.477000	2.627000
H	3.732000	1.962000	5.897000	C	4.129000	10.774000	3.445000
H	5.082000	1.653000	4.799000	H	4.923000	10.309000	2.847000
C	3.781000	3.202000	4.145000	H	3.631000	10.005000	4.048000
O	2.845000	4.008000	4.496000	H	4.572000	11.518000	4.106000
O	4.156000	2.996000	2.953000	C	1.739000	11.526000	0.799000
C	8.181000	10.300000	1.012000	O	1.577000	12.868000	1.054000
H	8.047000	11.343000	1.306000	C	2.348000	13.721000	0.199000
H	9.241000	10.055000	0.862000	H	2.103000	13.539000	-0.853000
O	7.462000	10.049000	-0.214000	H	3.422000	13.573000	0.361000
O	7.620000	9.445000	2.014000	H	2.078000	14.747000	0.456000
C	6.827000	8.840000	-0.020000	C	1.045000	10.888000	-0.251000
C	6.933000	8.473000	1.319000	O	0.213000	11.701000	-0.971000
C	6.356000	7.310000	1.794000	C	-0.779000	11.075000	-1.774000
H	6.438000	7.018000	2.835000	H	-1.338000	10.330000	-1.194000
C	5.654000	6.521000	0.862000	H	-0.340000	10.585000	-2.652000
H	5.189000	5.603000	1.208000	H	-1.454000	11.867000	-2.103000

C	1.217000	9.526000	-0.492000	H	2.166000	2.044000	2.732000
H	0.658000	9.035000	-1.276000	H	0.661000	2.182000	2.302000
O	1.285000	2.229000	3.094000				
⁵ R							
C	8.415000	1.773000	-1.487000	N	-0.062000	4.274000	4.872000
H	7.762000	1.617000	-2.320000	C	0.190000	4.322000	6.229000
H	7.901000	1.528000	-0.581000	H	1.201000	4.348000	6.606000
N	8.500000	4.068000	-0.420000	Fe	1.416000	4.734000	3.343000
H	7.961000	3.808000	0.424000	O	1.876000	3.252000	2.832000
C	8.840000	3.210000	-1.447000	C	6.612000	2.632000	6.680000
C	8.952000	5.306000	-0.744000	O	7.517000	3.332000	7.224000
H	8.815000	6.162000	-0.099000	O	6.140000	1.562000	7.158000
N	9.568000	5.307000	-1.919000	C	6.081000	3.114000	5.326000
C	9.497000	4.003000	-2.359000	H	6.024000	2.256000	4.647000
H	9.905000	3.709000	-3.313000	H	6.785000	3.837000	4.902000
C	-0.849000	9.908000	4.082000	C	4.690000	3.738000	5.443000
H	-1.283000	9.969000	3.106000	H	4.679000	4.543000	6.189000
H	-0.303000	10.805000	4.287000	H	3.952000	2.993000	5.770000
N	1.126000	8.592000	5.045000	C	4.164000	4.299000	4.132000
H	1.374000	9.228000	5.806000	O	3.048000	5.001000	4.269000
C	0.078000	8.735000	4.143000	O	4.733000	4.129000	3.055000
C	1.703000	7.391000	4.830000	C	8.300000	10.327000	1.066000
H	2.534000	6.999000	5.392000	H	8.150000	11.371000	1.347000
N	1.094000	6.753000	3.837000	H	9.363000	10.096000	0.920000
C	0.082000	7.582000	3.403000	O	7.587000	10.049000	-0.157000
H	-0.567000	7.289000	2.594000	O	7.752000	9.476000	2.079000
C	-1.591000	4.204000	0.339000	C	6.970000	8.835000	0.054000
H	-2.365000	3.465000	0.357000	C	7.076000	8.485000	1.398000
H	-1.066000	4.148000	-0.592000	C	6.500000	7.330000	1.889000
C	-0.616000	3.950000	1.491000	H	6.572000	7.052000	2.935000
O	0.063000	4.972000	1.974000	C	5.805000	6.519000	0.968000
O	-0.501000	2.791000	1.872000	H	5.343000	5.607000	1.338000
C	-1.260000	4.358000	8.394000	C	5.699000	6.864000	-0.383000
H	-0.406000	3.979000	8.916000	C	6.299000	8.052000	-0.860000
H	-2.111000	3.746000	8.609000	H	6.237000	8.334000	-1.907000
N	-1.978000	4.295000	5.947000	C	4.964000	5.981000	-1.369000
H	-2.982000	4.375000	6.086000	H	4.797000	4.992000	-0.932000
C	-0.993000	4.341000	6.924000	H	5.611000	5.829000	-2.244000
C	-1.382000	4.263000	4.735000	C	3.622000	6.547000	-1.874000
H	-1.943000	4.206000	3.816000	H	3.714000	7.632000	-2.015000

C	3.219000	5.903000	-3.205000	H	4.797000	11.416000	3.811000
H	3.420000	4.824000	-3.192000	C	1.789000	11.334000	0.685000
H	3.691000	6.341000	-4.086000	O	1.618000	12.678000	0.949000
O	1.784000	6.095000	-3.315000	C	2.433000	13.538000	0.145000
C	1.258000	6.317000	-2.091000	H	2.250000	13.360000	-0.922000
O	0.067000	6.494000	-1.938000	H	3.497000	13.394000	0.366000
C	2.359000	6.269000	-1.035000	H	2.146000	14.563000	0.390000
H	2.391000	5.204000	-0.745000	C	0.967000	10.677000	-0.245000
C	2.072000	7.037000	0.269000	O	0.074000	11.480000	-0.897000
H	2.817000	6.707000	0.999000	C	-0.946000	10.858000	-1.661000
H	1.112000	6.658000	0.635000	H	-1.538000	10.172000	-1.039000
C	2.033000	8.559000	0.297000	H	-0.535000	10.300000	-2.512000
C	2.879000	9.226000	1.195000	H	-1.586000	11.662000	-2.029000
H	3.613000	8.655000	1.752000	C	1.078000	9.291000	-0.427000
C	2.747000	10.604000	1.402000	H	0.398000	8.768000	-1.088000
O	3.469000	11.340000	2.299000	O	2.104000	1.802000	5.264000
C	4.383000	10.657000	3.146000	H	2.027000	2.069000	4.332000
H	5.200000	10.195000	2.580000	H	1.234000	2.014000	5.624000
H	3.877000	9.889000	3.745000				
⁵ TS							
C	8.408000	1.772000	-1.469000	C	0.079000	7.619000	3.406000
H	7.756000	1.620000	-2.304000	H	-0.557000	7.331000	2.584000
H	7.895000	1.518000	-0.565000	C	-1.615000	4.186000	0.361000
N	8.465000	4.072000	-0.402000	H	-2.390000	3.450000	0.411000
H	7.914000	3.823000	0.437000	H	-1.113000	4.111000	-0.581000
C	8.827000	3.210000	-1.418000	C	-0.616000	3.950000	1.491000
C	8.920000	5.310000	-0.724000	O	0.063000	4.972000	1.974000
H	8.769000	6.168000	-0.085000	O	-0.444000	2.791000	1.866000
N	9.557000	5.308000	-1.888000	C	-1.243000	4.347000	8.366000
C	9.498000	4.001000	-2.322000	H	-0.383000	3.979000	8.886000
H	9.926000	3.703000	-3.266000	H	-2.089000	3.735000	8.599000
C	-0.863000	9.940000	4.087000	N	-1.988000	4.249000	5.927000
H	-1.293000	10.001000	3.109000	H	-2.989000	4.351000	6.072000
H	-0.320000	10.839000	4.295000	C	-0.990000	4.308000	6.894000
N	1.097000	8.619000	5.071000	C	-1.405000	4.164000	4.712000
H	1.338000	9.252000	5.838000	H	-1.978000	4.084000	3.801000
C	0.067000	8.770000	4.150000	N	-0.081000	4.152000	4.834000
C	1.668000	7.413000	4.865000	C	0.183000	4.241000	6.189000
H	2.479000	7.011000	5.449000	H	1.200000	4.267000	6.547000
N	1.077000	6.783000	3.858000	Fe	1.416000	4.734000	3.343000

O	2.281000	3.796000	2.313000	O	1.768000	6.087000	-3.296000
C	6.604000	2.609000	6.753000	C	1.245000	6.310000	-2.071000
O	7.529000	3.294000	7.281000	O	0.053000	6.485000	-1.916000
O	6.143000	1.528000	7.218000	C	2.347000	6.269000	-1.017000
C	6.024000	3.127000	5.439000	H	2.383000	5.207000	-0.716000
H	6.001000	2.307000	4.714000	C	2.061000	7.043000	0.283000
H	6.669000	3.915000	5.040000	H	2.803000	6.710000	1.013000
C	4.602000	3.656000	5.623000	H	1.102000	6.665000	0.650000
H	4.551000	4.382000	6.446000	C	2.025000	8.564000	0.305000
H	3.909000	2.844000	5.870000	C	2.870000	9.232000	1.203000
C	4.054000	4.324000	4.375000	H	3.601000	8.661000	1.763000
O	2.846000	4.843000	4.564000	C	2.739000	10.611000	1.407000
O	4.689000	4.383000	3.325000	O	3.462000	11.348000	2.304000
C	8.305000	10.321000	1.073000	C	4.374000	10.663000	3.152000
H	8.160000	11.368000	1.346000	H	5.190000	10.200000	2.586000
H	9.366000	10.081000	0.935000	H	3.867000	9.897000	3.751000
O	7.598000	10.041000	-0.153000	H	4.790000	11.423000	3.816000
O	7.743000	9.481000	2.087000	C	1.784000	11.341000	0.687000
C	6.970000	8.832000	0.061000	O	1.615000	12.686000	0.948000
C	7.063000	8.490000	1.408000	C	2.433000	13.542000	0.142000
C	6.471000	7.345000	1.903000	H	2.250000	13.362000	-0.924000
H	6.529000	7.072000	2.952000	H	3.496000	13.395000	0.365000
C	5.775000	6.535000	0.983000	H	2.147000	14.568000	0.385000
H	5.297000	5.635000	1.357000	C	0.963000	10.683000	-0.243000
C	5.685000	6.870000	-0.373000	O	0.072000	11.486000	-0.898000
C	6.300000	8.049000	-0.852000	C	-0.948000	10.863000	-1.662000
H	6.247000	8.324000	-1.902000	H	-1.540000	10.178000	-1.040000
C	4.952000	5.986000	-1.358000	H	-0.537000	10.303000	-2.512000
H	4.787000	4.997000	-0.922000	H	-1.588000	11.667000	-2.032000
H	5.598000	5.836000	-2.234000	C	1.073000	9.296000	-0.423000
C	3.607000	6.548000	-1.861000	H	0.393000	8.773000	-1.083000
H	3.697000	7.633000	-2.005000	O	2.064000	1.795000	4.519000
C	3.203000	5.900000	-3.190000	H	2.203000	2.047000	3.593000
H	3.408000	4.822000	-3.176000	H	1.145000	2.053000	4.672000
H	3.671000	6.339000	-4.073000				
⁵ R'							
C	8.459000	1.760000	-1.494000	H	7.993000	3.768000	0.421000
H	7.792000	1.609000	-2.317000	C	8.878000	3.197000	-1.449000
H	7.963000	1.504000	-0.581000	C	8.959000	5.292000	-0.736000
N	8.524000	4.046000	-0.420000	H	8.810000	6.144000	-0.088000

N	9.578000	5.307000	-1.909000	H	4.335000	4.223000	6.530000
C	9.527000	4.003000	-2.355000	H	4.084000	2.479000	6.409000
H	9.941000	3.721000	-3.310000	C	3.602000	3.508000	4.636000
C	-0.775000	9.880000	4.110000	O	2.584000	4.297000	4.798000
H	-1.172000	9.945000	3.118000	O	3.862000	2.844000	3.615000
H	-0.203000	10.759000	4.323000	C	8.293000	10.251000	1.081000
N	1.112000	8.490000	5.156000	H	8.181000	11.306000	1.337000
H	1.360000	9.122000	5.919000	H	9.346000	9.978000	0.941000
C	0.104000	8.674000	4.218000	O	7.571000	9.970000	-0.137000
C	1.633000	7.252000	4.971000	O	7.713000	9.445000	2.113000
H	2.413000	6.819000	5.577000	C	6.897000	8.793000	0.104000
N	1.033000	6.643000	3.961000	C	6.989000	8.472000	1.457000
C	0.082000	7.515000	3.485000	C	6.364000	7.356000	1.977000
H	-0.564000	7.245000	2.664000	H	6.432000	7.106000	3.031000
C	-2.002000	3.987000	0.418000	C	5.628000	6.557000	1.077000
H	-2.844000	3.416000	0.750000	H	5.115000	5.678000	1.457000
H	-1.740000	3.691000	-0.576000	C	5.534000	6.872000	-0.283000
C	-0.820000	3.740000	1.351000	C	6.190000	8.018000	-0.788000
O	-0.446000	4.648000	2.176000	H	6.140000	8.275000	-1.842000
O	-0.294000	2.609000	1.246000	C	4.767000	5.996000	-1.249000
C	-1.412000	4.411000	8.438000	H	4.563000	5.022000	-0.794000
H	-0.564000	3.989000	8.936000	H	5.413000	5.801000	-2.116000
H	-2.285000	3.839000	8.673000	C	3.444000	6.590000	-1.779000
N	-2.187000	4.437000	6.000000	H	3.562000	7.671000	-1.933000
H	-3.185000	4.581000	6.148000	C	3.056000	5.930000	-3.109000
C	-1.184000	4.388000	6.962000	H	3.261000	4.852000	-3.082000
C	-1.605000	4.416000	4.781000	H	3.539000	6.360000	-3.989000
H	-2.164000	4.458000	3.860000	O	1.624000	6.116000	-3.243000
N	-0.287000	4.335000	4.902000	C	1.081000	6.361000	-2.031000
C	-0.016000	4.310000	6.252000	O	-0.113000	6.535000	-1.896000
H	1.001000	4.250000	6.606000	C	2.163000	6.344000	-0.957000
Fe	1.175000	4.544000	3.410000	H	2.186000	5.295000	-0.620000
O	2.233000	4.756000	2.190000	C	1.838000	7.151000	0.312000
C	6.648000	2.544000	6.805000	H	2.503000	6.793000	1.098000
O	7.634000	3.189000	7.261000	H	0.839000	6.824000	0.620000
O	6.202000	1.460000	7.280000	C	1.865000	8.670000	0.306000
C	5.942000	3.095000	5.570000	C	2.720000	9.318000	1.208000
H	5.991000	2.340000	4.778000	H	3.414000	8.727000	1.792000
H	6.445000	4.002000	5.217000	C	2.639000	10.703000	1.387000
C	4.469000	3.357000	5.874000	O	3.376000	11.425000	2.285000

C	4.256000	10.717000	3.148000	O	0.028000	11.631000	-0.967000
H	5.048000	10.204000	2.591000	C	-0.999000	11.016000	-1.730000
H	3.713000	9.987000	3.762000	H	-1.605000	10.346000	-1.104000
H	4.707000	11.469000	3.797000	H	-0.593000	10.443000	-2.573000
C	1.719000	11.456000	0.643000	H	-1.626000	11.825000	-2.109000
O	1.592000	12.807000	0.888000	C	0.954000	9.423000	-0.449000
C	2.443000	13.628000	0.080000	H	0.267000	8.911000	-1.112000
H	2.273000	13.433000	-0.986000	O	1.239000	2.427000	3.295000
H	3.499000	13.459000	0.321000	H	0.735000	2.315000	2.438000
H	2.180000	14.664000	0.299000	H	2.205000	2.344000	3.127000
C	0.888000	10.813000	-0.290000				
⁵ TS1							
C	8.453000	1.743000	-1.404000	C	-1.299000	4.391000	8.295000
H	7.768000	1.590000	-2.212000	H	-0.440000	3.983000	8.786000
H	7.984000	1.470000	-0.482000	H	-2.152000	3.779000	8.502000
N	8.396000	4.051000	-0.377000	N	-2.061000	4.498000	5.859000
H	7.821000	3.787000	0.439000	H	-3.059000	4.612000	6.015000
C	8.851000	3.186000	-1.353000	C	-1.059000	4.429000	6.821000
C	8.827000	5.300000	-0.694000	C	-1.474000	4.518000	4.641000
H	8.609000	6.162000	-0.080000	H	-2.035000	4.586000	3.723000
N	9.532000	5.301000	-1.817000	N	-0.156000	4.443000	4.754000
C	9.549000	3.985000	-2.228000	C	0.110000	4.384000	6.106000
H	10.049000	3.687000	-3.137000	H	1.126000	4.327000	6.464000
C	-0.871000	10.041000	4.157000	Fe	1.430000	4.881000	3.227000
H	-1.274000	10.101000	3.168000	O	2.482000	5.449000	1.884000
H	-0.336000	10.941000	4.379000	C	6.685000	2.586000	6.771000
N	1.069000	8.710000	5.184000	O	7.623000	3.253000	7.294000
H	1.300000	9.328000	5.967000	O	6.201000	1.515000	7.240000
C	0.059000	8.874000	4.246000	C	6.099000	3.105000	5.463000
C	1.636000	7.497000	4.980000	H	6.121000	2.303000	4.718000
H	2.432000	7.085000	5.579000	H	6.702000	3.937000	5.085000
N	1.060000	6.886000	3.959000	C	4.651000	3.535000	5.665000
C	0.080000	7.728000	3.494000	H	4.573000	4.369000	6.372000
H	-0.549000	7.453000	2.661000	H	4.096000	2.698000	6.108000
C	-1.976000	4.034000	0.416000	C	3.928000	3.905000	4.383000
H	-2.786000	3.446000	0.795000	O	2.881000	4.646000	4.574000
H	-1.743000	3.720000	-0.580000	O	4.313000	3.462000	3.282000
C	-0.750000	3.848000	1.309000	C	8.306000	10.253000	1.045000
O	-0.271000	4.830000	1.970000	H	8.177000	11.311000	1.287000
O	-0.269000	2.686000	1.309000	H	9.360000	10.005000	0.872000

O	7.547000	9.935000	-0.141000	C	1.682000	8.441000	0.285000
O	7.786000	9.454000	2.112000	C	2.561000	9.008000	1.218000
C	6.879000	8.765000	0.154000	H	3.213000	8.360000	1.790000
C	7.031000	8.473000	1.507000	C	2.536000	10.392000	1.446000
C	6.424000	7.370000	2.079000	O	3.293000	11.053000	2.370000
H	6.536000	7.145000	3.134000	C	4.114000	10.287000	3.243000
C	5.645000	6.555000	1.233000	H	4.884000	9.734000	2.695000
H	5.138000	5.693000	1.655000	H	3.517000	9.584000	3.837000
C	5.494000	6.840000	-0.129000	H	4.593000	11.008000	3.908000
C	6.130000	7.973000	-0.689000	C	1.660000	11.215000	0.721000
H	6.041000	8.206000	-1.746000	O	1.595000	12.561000	1.014000
C	4.711000	5.911000	-1.032000	C	2.443000	13.384000	0.203000
H	4.421000	5.023000	-0.468000	H	2.200000	13.263000	-0.859000
H	5.388000	5.567000	-1.827000	H	3.500000	13.147000	0.371000
C	3.455000	6.510000	-1.711000	H	2.250000	14.418000	0.497000
H	3.560000	7.599000	-1.800000	C	0.807000	10.649000	-0.240000
C	3.250000	5.910000	-3.110000	O	-0.001000	11.530000	-0.902000
H	3.444000	4.830000	-3.104000	C	-1.039000	10.990000	-1.705000
H	3.846000	6.372000	-3.900000	H	-1.687000	10.328000	-1.115000
O	1.846000	6.112000	-3.425000	H	-0.641000	10.430000	-2.561000
C	1.142000	6.266000	-2.285000	H	-1.622000	11.839000	-2.066000
O	-0.063000	6.411000	-2.288000	C	0.807000	9.263000	-0.444000
C	2.083000	6.198000	-1.079000	H	0.115000	8.805000	-1.141000
H	2.084000	5.135000	-0.797000	O	1.653000	2.812000	2.963000
C	1.556000	6.945000	0.141000	H	0.970000	2.615000	2.242000
H	2.093000	6.370000	1.084000	H	2.570000	2.752000	2.637000
H	0.521000	6.634000	0.300000				
⁵ IM1							
C	8.475000	1.732000	-1.437000	H	-1.247000	10.009000	3.114000
H	7.806000	1.582000	-2.259000	H	-0.281000	10.839000	4.310000
H	7.986000	1.460000	-0.525000	N	1.102000	8.589000	5.109000
N	8.442000	4.034000	-0.387000	H	1.323000	9.204000	5.895000
H	7.871000	3.773000	0.433000	C	0.101000	8.769000	4.162000
C	8.876000	3.173000	-1.377000	C	1.681000	7.387000	4.881000
C	8.875000	5.282000	-0.702000	H	2.467000	6.961000	5.483000
H	8.670000	6.141000	-0.080000	N	1.124000	6.796000	3.835000
N	9.564000	5.287000	-1.835000	C	0.141000	7.645000	3.378000
C	9.565000	3.975000	-2.256000	H	-0.470000	7.387000	2.527000
H	10.047000	3.680000	-3.175000	C	-1.957000	3.956000	0.446000
C	-0.825000	9.943000	4.095000	H	-2.786000	3.363000	0.772000

H	-1.676000	3.663000	-0.544000	C	5.574000	6.824000	-0.513000
C	-0.779000	3.746000	1.392000	C	6.169000	8.020000	-0.974000
O	-0.324000	4.720000	2.083000	H	6.091000	8.323000	-2.014000
O	-0.317000	2.579000	1.425000	C	4.801000	5.960000	-1.490000
C	-1.349000	4.412000	8.400000	H	4.641000	4.967000	-1.060000
H	-0.493000	4.003000	8.894000	H	5.411000	5.817000	-2.393000
H	-2.208000	3.814000	8.621000	C	3.445000	6.533000	-1.940000
N	-2.118000	4.475000	5.965000	H	3.575000	7.583000	-2.231000
H	-3.117000	4.598000	6.119000	C	2.859000	5.757000	-3.118000
C	-1.115000	4.422000	6.925000	H	3.002000	4.677000	-2.983000
C	-1.533000	4.489000	4.746000	H	3.250000	6.055000	-4.094000
H	-2.096000	4.543000	3.828000	O	1.437000	6.033000	-3.102000
N	-0.214000	4.425000	4.859000	C	1.055000	6.471000	-1.875000
C	0.054000	4.380000	6.210000	O	-0.102000	6.758000	-1.653000
H	1.071000	4.332000	6.566000	C	2.257000	6.468000	-0.933000
Fe	1.335000	4.718000	3.269000	H	2.252000	5.461000	-0.481000
O	2.470000	4.786000	1.809000	C	2.352000	7.410000	0.220000
C	6.674000	2.545000	6.819000	H	3.341000	4.484000	2.156000
O	7.595000	3.227000	7.352000	H	2.839000	6.952000	1.072000
O	6.199000	1.468000	7.280000	C	2.101000	8.803000	0.333000
C	6.097000	3.059000	5.504000	C	2.768000	9.464000	1.404000
H	6.139000	2.258000	4.759000	H	3.427000	8.879000	2.032000
H	6.694000	3.898000	5.134000	C	2.612000	10.825000	1.609000
C	4.643000	3.476000	5.693000	O	3.249000	11.546000	2.583000
H	4.546000	4.258000	6.456000	C	4.196000	10.855000	3.386000
H	4.067000	2.618000	6.063000	H	4.995000	10.412000	2.780000
C	3.965000	3.963000	4.428000	H	3.718000	10.070000	3.986000
O	2.853000	4.588000	4.624000	H	4.627000	11.602000	4.052000
O	4.469000	3.718000	3.304000	C	1.739000	11.568000	0.791000
C	8.188000	10.269000	0.973000	O	1.547000	12.903000	1.058000
H	8.037000	11.308000	1.270000	C	2.317000	13.777000	0.224000
H	9.251000	10.044000	0.816000	H	2.092000	13.601000	-0.834000
O	7.467000	10.008000	-0.250000	H	3.391000	13.645000	0.401000
O	7.648000	9.401000	1.975000	H	2.027000	14.796000	0.486000
C	6.851000	8.789000	-0.055000	C	1.039000	10.920000	-0.249000
C	6.973000	8.419000	1.283000	O	0.177000	11.720000	-0.947000
C	6.418000	7.246000	1.758000	C	-0.796000	11.081000	-1.762000
H	6.510000	6.950000	2.797000	H	-1.339000	10.314000	-1.195000
C	5.716000	6.452000	0.830000	H	-0.342000	10.613000	-2.645000
H	5.266000	5.530000	1.181000	H	-1.489000	11.861000	-2.083000

C	1.235000	9.563000	-0.501000	H	0.751000	2.399000	2.570000
H	0.670000	9.062000	-1.274000	H	2.292000	2.331000	2.921000
O	1.429000	2.540000	3.309000				
⁵ TS2							
C	8.479000	1.740000	-1.435000	N	-0.228000	4.350000	4.936000
H	7.814000	1.589000	-2.259000	C	0.035000	4.336000	6.289000
H	7.985000	1.473000	-0.524000	H	1.051000	4.307000	6.651000
N	8.467000	4.046000	-0.387000	Fe	1.272000	4.672000	3.422000
H	7.902000	3.796000	0.441000	O	2.561000	4.573000	1.763000
C	8.886000	3.181000	-1.379000	C	6.626000	2.549000	6.824000
C	8.904000	5.291000	-0.709000	O	7.552000	3.228000	7.355000
H	8.710000	6.153000	-0.088000	O	6.156000	1.469000	7.284000
N	9.582000	5.290000	-1.850000	C	6.048000	3.076000	5.513000
C	9.571000	3.977000	-2.267000	H	6.063000	2.272000	4.769000
H	10.041000	3.678000	-3.191000	H	6.671000	3.893000	5.139000
C	-0.863000	9.943000	4.080000	C	4.612000	3.556000	5.698000
H	-1.298000	10.007000	3.104000	H	4.536000	4.259000	6.539000
H	-0.316000	10.839000	4.286000	H	3.955000	2.715000	5.949000
N	1.087000	8.610000	5.065000	C	4.041000	4.246000	4.475000
H	1.318000	9.235000	5.839000	O	2.852000	4.748000	4.645000
C	0.063000	8.770000	4.137000	O	4.695000	4.322000	3.418000
C	1.668000	7.410000	4.843000	C	8.184000	10.254000	0.985000
H	2.472000	6.999000	5.432000	H	8.036000	11.292000	1.289000
N	1.091000	6.796000	3.819000	H	9.246000	10.025000	0.827000
C	0.092000	7.634000	3.371000	O	7.461000	10.002000	-0.238000
H	-0.532000	7.359000	2.534000	O	7.643000	9.382000	1.983000
C	-1.930000	3.995000	0.470000	C	6.855000	8.776000	-0.052000
H	-2.769000	3.397000	0.757000	C	6.978000	8.397000	1.283000
H	-1.628000	3.733000	-0.522000	C	6.434000	7.215000	1.748000
C	-0.774000	3.747000	1.436000	H	6.519000	6.905000	2.784000
O	-0.287000	4.718000	2.135000	C	5.740000	6.424000	0.811000
O	-0.360000	2.574000	1.472000	H	5.305000	5.494000	1.157000
C	-1.376000	4.413000	8.466000	C	5.597000	6.804000	-0.528000
H	-0.524000	4.007000	8.971000	C	6.180000	8.010000	-0.979000
H	-2.241000	3.827000	8.697000	H	6.100000	8.321000	-2.017000
N	-2.136000	4.422000	6.022000	C	4.828000	5.940000	-1.507000
H	-3.137000	4.549000	6.165000	H	4.684000	4.940000	-1.086000
C	-1.139000	4.390000	6.992000	H	5.429000	5.815000	-2.418000
C	-1.549000	4.410000	4.808000	C	3.460000	6.504000	-1.934000
H	-2.104000	4.439000	3.883000	H	3.577000	7.559000	-2.213000

C	2.871000	5.735000	-3.115000	H	4.639000	11.553000	4.083000
H	3.021000	4.655000	-2.990000	C	1.759000	11.509000	0.817000
H	3.253000	6.045000	-4.091000	O	1.567000	12.845000	1.081000
O	1.448000	6.004000	-3.085000	C	2.331000	13.718000	0.238000
C	1.074000	6.424000	-1.851000	H	2.096000	13.540000	-0.818000
O	-0.082000	6.708000	-1.619000	H	3.406000	13.585000	0.406000
C	2.282000	6.416000	-0.917000	H	2.043000	14.737000	0.501000
H	2.290000	5.403000	-0.478000	C	1.062000	10.860000	-0.224000
C	2.370000	7.349000	0.245000	O	0.206000	11.663000	-0.928000
H	3.438000	4.717000	2.182000	C	-0.765000	11.027000	-1.747000
H	2.869000	6.895000	1.092000	H	-1.317000	10.265000	-1.181000
C	2.119000	8.742000	0.364000	H	-0.308000	10.552000	-2.625000
C	2.783000	9.404000	1.437000	H	-1.450000	11.811000	-2.075000
H	3.441000	8.820000	2.067000	C	1.255000	9.502000	-0.473000
C	2.627000	10.766000	1.640000	H	0.692000	9.002000	-1.247000
O	3.259000	11.488000	2.616000	O	1.778000	2.755000	3.007000
C	4.211000	10.803000	3.418000	H	0.977000	2.402000	2.552000
H	5.013000	10.365000	2.810000	H	2.320000	3.442000	2.153000
H	3.740000	10.015000	4.018000				

⁵IM2

C	8.483000	1.739000	-1.435000	C	0.098000	7.574000	3.383000
H	7.819000	1.589000	-2.261000	H	-0.532000	7.294000	2.553000
H	7.987000	1.473000	-0.525000	C	-1.926000	3.991000	0.460000
N	8.473000	4.045000	-0.384000	H	-2.762000	3.393000	0.758000
H	7.910000	3.795000	0.443000	H	-1.638000	3.730000	-0.537000
C	8.891000	3.179000	-1.378000	C	-0.756000	3.741000	1.410000
C	8.911000	5.290000	-0.707000	O	-0.267000	4.701000	2.117000
H	8.718000	6.151000	-0.084000	O	-0.330000	2.569000	1.414000
N	9.586000	5.289000	-1.848000	C	-1.422000	4.429000	8.508000
C	9.574000	3.976000	-2.267000	H	-0.573000	4.010000	9.007000
H	10.041000	3.677000	-3.192000	H	-2.294000	3.855000	8.744000
C	-0.844000	9.900000	4.072000	N	-2.192000	4.440000	6.064000
H	-1.280000	9.960000	3.097000	H	-3.194000	4.571000	6.208000
H	-0.290000	10.794000	4.271000	C	-1.194000	4.405000	7.032000
N	1.100000	8.566000	5.062000	C	-1.605000	4.437000	4.848000
H	1.332000	9.196000	5.831000	H	-2.159000	4.466000	3.923000
C	0.074000	8.720000	4.137000	N	-0.286000	4.378000	4.977000
C	1.674000	7.359000	4.848000	C	-0.021000	4.357000	6.328000
H	2.479000	6.955000	5.440000	H	0.995000	4.325000	6.690000
N	1.093000	6.733000	3.834000	Fe	1.236000	4.529000	3.486000

O	2.727000	4.687000	1.728000	O	1.456000	6.030000	-3.126000
C	6.650000	2.534000	6.822000	C	1.079000	6.454000	-1.893000
O	7.563000	3.226000	7.358000	O	-0.078000	6.733000	-1.659000
O	6.179000	1.456000	7.285000	C	2.288000	6.450000	-0.959000
C	6.077000	3.046000	5.504000	H	2.294000	5.436000	-0.527000
H	6.077000	2.232000	4.771000	C	2.379000	7.381000	0.204000
H	6.703000	3.854000	5.115000	H	3.553000	4.701000	2.296000
C	4.648000	3.538000	5.707000	H	2.893000	6.931000	1.043000
H	4.593000	4.250000	6.541000	C	2.118000	8.770000	0.332000
H	3.992000	2.703000	5.981000	C	2.779000	9.425000	1.412000
C	4.043000	4.213000	4.495000	H	3.436000	8.837000	2.039000
O	2.869000	4.710000	4.677000	C	2.620000	10.785000	1.625000
O	4.679000	4.273000	3.413000	O	3.250000	11.501000	2.606000
C	8.184000	10.253000	0.986000	C	4.196000	10.808000	3.410000
H	8.032000	11.288000	1.300000	H	4.999000	10.370000	2.805000
H	9.246000	10.032000	0.821000	H	3.717000	10.019000	4.003000
O	7.457000	10.009000	-0.238000	H	4.622000	11.554000	4.081000
O	7.650000	9.369000	1.977000	C	1.751000	11.530000	0.806000
C	6.856000	8.780000	-0.061000	O	1.560000	12.865000	1.075000
C	6.986000	8.388000	1.270000	C	2.328000	13.740000	0.239000
C	6.448000	7.200000	1.725000	H	2.099000	13.567000	-0.818000
H	6.538000	6.880000	2.758000	H	3.403000	13.605000	0.412000
C	5.755000	6.415000	0.782000	H	2.041000	14.758000	0.505000
H	5.326000	5.477000	1.114000	C	1.054000	10.888000	-0.240000
C	5.602000	6.809000	-0.551000	O	0.194000	11.692000	-0.936000
C	6.180000	8.021000	-0.993000	C	-0.776000	11.056000	-1.757000
H	6.094000	8.343000	-2.026000	H	-1.322000	10.288000	-1.195000
C	4.830000	5.954000	-1.535000	H	-0.320000	10.591000	-2.640000
H	4.675000	4.955000	-1.114000	H	-1.467000	11.839000	-2.078000
H	5.435000	5.822000	-2.443000	C	1.251000	9.532000	-0.498000
C	3.469000	6.528000	-1.972000	H	0.689000	9.036000	-1.276000
H	3.595000	7.581000	-2.252000	O	1.619000	2.752000	3.180000
C	2.879000	5.760000	-3.153000	H	0.886000	2.398000	2.620000
H	3.027000	4.679000	-3.027000	H	2.547000	3.727000	1.693000
H	3.263000	6.067000	-4.128000				
⁵ TS3							
C	8.469000	1.793000	-1.462000	H	7.846000	3.825000	0.411000
H	7.797000	1.657000	-2.284000	C	8.880000	3.229000	-1.386000
H	7.981000	1.513000	-0.552000	C	8.867000	5.335000	-0.705000
N	8.428000	4.087000	-0.401000	H	8.649000	6.194000	-0.087000

N	9.577000	5.344000	-1.825000	H	3.846000	1.901000	5.613000
C	9.586000	4.033000	-2.250000	H	5.269000	1.802000	4.570000
H	10.086000	3.741000	-3.160000	C	3.898000	3.335000	4.027000
C	-0.686000	9.653000	4.080000	O	4.263000	3.237000	2.825000
H	-1.107000	9.690000	3.097000	O	2.982000	4.142000	4.442000
H	-0.092000	10.527000	4.247000	C	8.119000	9.902000	1.050000
N	1.174000	8.260000	5.160000	H	8.175000	10.961000	1.311000
H	1.398000	8.897000	5.922000	H	9.098000	9.412000	1.148000
C	0.175000	8.432000	4.210000	O	7.663000	9.761000	-0.307000
C	1.722000	7.033000	4.968000	O	7.158000	9.250000	1.889000
H	2.511000	6.621000	5.579000	C	6.755000	8.726000	-0.278000
N	1.149000	6.413000	3.948000	C	6.429000	8.426000	1.054000
C	0.187000	7.278000	3.468000	C	5.521000	7.459000	1.383000
H	-0.432000	7.007000	2.626000	H	5.326000	7.181000	2.414000
C	-2.119000	3.761000	0.705000	C	4.812000	6.805000	0.294000
H	-2.845000	3.286000	1.331000	H	4.516000	5.781000	0.518000
H	-2.094000	3.273000	-0.247000	C	5.296000	7.021000	-1.064000
C	-0.743000	3.668000	1.361000	C	6.218000	8.024000	-1.350000
O	-0.490000	4.424000	2.365000	H	6.525000	8.228000	-2.372000
O	0.077000	2.838000	0.894000	C	4.634000	6.236000	-2.166000
C	-1.462000	4.463000	8.664000	H	4.674000	5.159000	-1.950000
H	-0.627000	4.047000	9.188000	H	5.141000	6.396000	-3.122000
H	-2.349000	3.923000	8.921000	C	3.167000	6.668000	-2.263000
N	-2.221000	4.364000	6.222000	H	3.129000	7.728000	-2.547000
H	-3.218000	4.529000	6.352000	C	2.290000	5.866000	-3.216000
C	-1.227000	4.363000	7.194000	H	2.505000	4.794000	-3.139000
C	-1.630000	4.288000	5.010000	H	2.339000	6.176000	-4.262000
H	-2.175000	4.282000	4.079000	O	0.935000	6.096000	-2.753000
N	-0.313000	4.217000	5.146000	C	0.946000	6.504000	-1.450000
C	-0.053000	4.263000	6.496000	O	-0.088000	6.782000	-0.891000
H	0.959000	4.237000	6.871000	C	2.392000	6.486000	-0.945000
Fe	1.152000	4.165000	3.569000	H	2.529000	5.439000	-0.633000
O	2.237000	4.386000	1.650000	C	2.831000	7.301000	0.255000
C	6.360000	2.568000	6.899000	H	3.079000	3.941000	1.972000
O	7.535000	3.047000	7.027000	H	2.620000	6.768000	1.179000
O	5.983000	1.467000	7.376000	C	2.562000	8.747000	0.387000
C	5.367000	3.378000	6.067000	C	3.005000	9.373000	1.568000
H	5.918000	4.165000	5.541000	H	3.535000	8.784000	2.300000
H	4.660000	3.878000	6.740000	C	2.773000	10.727000	1.795000
C	4.592000	2.494000	5.076000	O	3.220000	11.411000	2.890000

C	4.113000	10.721000	3.756000	O	0.695000	11.616000	-1.053000
H	4.979000	10.332000	3.208000	C	-0.267000	10.943000	-1.856000
H	3.610000	9.899000	4.280000	H	-0.751000	10.134000	-1.296000
H	4.452000	11.455000	4.486000	H	0.186000	10.524000	-2.764000
C	2.006000	11.474000	0.886000	H	-1.009000	11.693000	-2.141000
O	1.706000	12.782000	1.185000	C	1.826000	9.508000	-0.540000
C	2.408000	13.745000	0.387000	H	1.432000	9.051000	-1.437000
H	2.179000	13.611000	-0.675000	O	1.264000	2.336000	3.422000
H	3.490000	13.671000	0.547000	H	0.793000	2.001000	2.641000
H	2.058000	14.727000	0.708000	H	1.695000	3.696000	1.204000
C	1.506000	10.843000	-0.263000				

⁵IM3

C	8.476000	1.789000	-1.468000	C	-1.459000	4.464000	8.670000
H	7.808000	1.658000	-2.294000	H	-0.623000	4.049000	9.193000
H	7.981000	1.509000	-0.562000	H	-2.346000	3.924000	8.929000
N	8.454000	4.077000	-0.392000	N	-2.221000	4.361000	6.230000
H	7.869000	3.816000	0.419000	H	-3.218000	4.527000	6.360000
C	8.893000	3.223000	-1.386000	C	-1.226000	4.362000	7.200000
C	8.900000	5.324000	-0.692000	C	-1.631000	4.283000	5.017000
H	8.693000	6.180000	-0.066000	H	-2.177000	4.277000	4.087000
N	9.602000	5.336000	-1.816000	N	-0.314000	4.213000	5.151000
C	9.599000	4.027000	-2.249000	C	-0.052000	4.260000	6.500000
H	10.090000	3.738000	-3.165000	H	0.960000	4.235000	6.874000
C	-0.695000	9.648000	4.076000	Fe	1.145000	4.161000	3.567000
H	-1.121000	9.684000	3.095000	O	2.217000	4.394000	1.646000
H	-0.101000	10.523000	4.239000	C	6.352000	2.571000	6.894000
N	1.165000	8.253000	5.154000	O	7.529000	3.048000	7.020000
H	1.388000	8.889000	5.918000	O	5.976000	1.471000	7.372000
C	0.167000	8.429000	4.202000	C	5.360000	3.381000	6.062000
C	1.712000	7.027000	4.960000	H	5.909000	4.173000	5.541000
H	2.500000	6.613000	5.572000	H	4.649000	3.875000	6.734000
N	1.141000	6.410000	3.938000	C	4.592000	2.499000	5.064000
C	0.181000	7.276000	3.457000	H	3.848000	1.899000	5.595000
H	-0.434000	7.011000	2.610000	H	5.272000	1.813000	4.554000
C	-2.148000	3.738000	0.730000	C	3.894000	3.340000	4.017000
H	-2.865000	3.270000	1.372000	O	4.257000	3.247000	2.814000
H	-2.136000	3.237000	-0.215000	O	2.974000	4.143000	4.437000
C	-0.762000	3.655000	1.368000	C	8.207000	9.566000	0.976000
O	-0.506000	4.409000	2.372000	H	8.339000	10.620000	1.232000
O	0.062000	2.837000	0.887000	H	9.147000	9.009000	1.089000

O	7.771000	9.456000	-0.392000	C	2.648000	8.774000	0.340000
O	7.188000	8.993000	1.797000	C	3.085000	9.404000	1.514000
C	6.744000	8.542000	-0.381000	H	3.628000	8.829000	2.247000
C	6.369000	8.263000	0.954000	C	2.822000	10.751000	1.754000
C	5.357000	7.425000	1.278000	O	3.259000	11.433000	2.855000
H	5.135000	7.163000	2.306000	C	4.144000	10.742000	3.727000
C	4.509000	6.850000	0.167000	H	5.021000	10.361000	3.189000
H	4.432000	5.765000	0.346000	H	3.640000	9.911000	4.236000
C	5.106000	7.035000	-1.221000	H	4.468000	11.470000	4.469000
C	6.152000	7.898000	-1.471000	C	2.026000	11.483000	0.861000
H	6.526000	8.045000	-2.481000	O	1.696000	12.783000	1.170000
C	4.435000	6.258000	-2.321000	C	2.387000	13.765000	0.388000
H	4.498000	5.178000	-2.114000	H	2.175000	13.633000	-0.679000
H	4.918000	6.435000	-3.286000	H	3.469000	13.714000	0.559000
C	2.962000	6.669000	-2.344000	H	2.012000	14.737000	0.709000
H	2.902000	7.722000	-2.653000	C	1.527000	10.845000	-0.282000
C	1.989000	5.858000	-3.191000	O	0.695000	11.599000	-1.066000
H	2.177000	4.782000	-3.097000	C	-0.229000	10.906000	-1.895000
H	1.949000	6.134000	-4.247000	H	-0.695000	10.072000	-1.358000
O	0.688000	6.151000	-2.612000	H	0.256000	10.517000	-2.800000
C	0.835000	6.597000	-1.324000	H	-0.990000	11.635000	-2.184000
O	-0.131000	6.946000	-0.688000	C	1.874000	9.514000	-0.562000
C	2.308000	6.514000	-0.963000	H	1.485000	9.058000	-1.462000
H	2.429000	5.458000	-0.676000	O	1.259000	2.332000	3.416000
C	2.941000	7.284000	0.206000	H	0.788000	1.996000	2.636000
H	3.065000	3.958000	1.962000	H	1.681000	3.697000	1.203000
H	2.557000	6.816000	1.119000				
⁵ TS4							
C	8.408000	1.772000	-1.469000	H	-1.293000	10.001000	3.109000
H	7.756000	1.620000	-2.304000	H	-0.320000	10.839000	4.295000
H	7.895000	1.518000	-0.565000	N	1.097000	8.619000	5.071000
N	8.465000	4.072000	-0.402000	H	1.338000	9.252000	5.838000
H	7.914000	3.823000	0.437000	C	0.067000	8.770000	4.150000
C	8.827000	3.210000	-1.418000	C	1.668000	7.413000	4.865000
C	8.920000	5.310000	-0.724000	H	2.479000	7.011000	5.449000
H	8.769000	6.168000	-0.085000	N	1.077000	6.783000	3.858000
N	9.557000	5.308000	-1.888000	C	0.079000	7.619000	3.406000
C	9.498000	4.001000	-2.322000	H	-0.557000	7.331000	2.584000
H	9.926000	3.703000	-3.266000	C	-1.615000	4.186000	0.361000
C	-0.863000	9.940000	4.087000	H	-2.390000	3.450000	0.411000

H	-1.113000	4.111000	-0.581000	C	5.685000	6.870000	-0.373000
C	-0.616000	3.950000	1.491000	C	6.300000	8.049000	-0.852000
O	0.063000	4.972000	1.974000	H	6.247000	8.324000	-1.902000
O	-0.444000	2.791000	1.866000	C	4.952000	5.986000	-1.358000
C	-1.243000	4.347000	8.366000	H	4.787000	4.997000	-0.922000
H	-0.383000	3.979000	8.886000	H	5.598000	5.836000	-2.234000
H	-2.089000	3.735000	8.599000	C	3.607000	6.548000	-1.861000
N	-1.988000	4.249000	5.927000	H	3.697000	7.633000	-2.005000
H	-2.989000	4.351000	6.072000	C	3.203000	5.900000	-3.190000
C	-0.990000	4.308000	6.894000	H	3.408000	4.822000	-3.176000
C	-1.405000	4.164000	4.712000	H	3.671000	6.339000	-4.073000
H	-1.978000	4.084000	3.801000	O	1.768000	6.087000	-3.296000
N	-0.081000	4.152000	4.834000	C	1.245000	6.310000	-2.071000
C	0.183000	4.241000	6.189000	O	0.053000	6.485000	-1.916000
H	1.200000	4.267000	6.547000	C	2.347000	6.269000	-1.017000
Fe	1.416000	4.734000	3.343000	H	2.383000	5.207000	-0.716000
O	2.281000	3.796000	2.313000	C	2.061000	7.043000	0.283000
C	6.604000	2.609000	6.753000	H	2.803000	6.710000	1.013000
O	7.529000	3.294000	7.281000	H	1.102000	6.665000	0.650000
O	6.143000	1.528000	7.218000	C	2.025000	8.564000	0.305000
C	6.024000	3.127000	5.439000	C	2.870000	9.232000	1.203000
H	6.001000	2.307000	4.714000	H	3.601000	8.661000	1.763000
H	6.669000	3.915000	5.040000	C	2.739000	10.611000	1.407000
C	4.602000	3.656000	5.623000	O	3.462000	11.348000	2.304000
H	4.551000	4.382000	6.446000	C	4.374000	10.663000	3.152000
H	3.909000	2.844000	5.870000	H	5.190000	10.200000	2.586000
C	4.054000	4.324000	4.375000	H	3.867000	9.897000	3.751000
O	2.846000	4.843000	4.564000	H	4.790000	11.423000	3.816000
O	4.689000	4.383000	3.325000	C	1.784000	11.341000	0.687000
C	8.305000	10.321000	1.073000	O	1.615000	12.686000	0.948000
H	8.160000	11.368000	1.346000	C	2.433000	13.542000	0.142000
H	9.366000	10.081000	0.935000	H	2.250000	13.362000	-0.924000
O	7.598000	10.041000	-0.153000	H	3.496000	13.395000	0.365000
O	7.743000	9.481000	2.087000	H	2.147000	14.568000	0.385000
C	6.970000	8.832000	0.061000	C	0.963000	10.683000	-0.243000
C	7.063000	8.490000	1.408000	O	0.072000	11.486000	-0.898000
C	6.471000	7.345000	1.903000	C	-0.948000	10.863000	-1.662000
H	6.529000	7.072000	2.952000	H	-1.540000	10.178000	-1.040000
C	5.775000	6.535000	0.983000	H	-0.537000	10.303000	-2.512000
H	5.297000	5.635000	1.357000	H	-1.588000	11.667000	-2.032000

C	1.073000	9.296000	-0.423000	H	2.203000	2.047000	3.593000
H	0.393000	8.773000	-1.083000	H	1.145000	2.053000	4.672000
O	2.064000	1.795000	4.519000				
⁵ IM4							
C	8.463000	1.790000	-1.482000	N	-0.194000	4.180000	4.870000
H	7.818000	1.661000	-2.326000	C	0.093000	4.200000	6.218000
H	7.943000	1.511000	-0.590000	H	1.114000	4.136000	6.563000
N	8.448000	4.073000	-0.387000	Fe	1.301000	4.432000	3.226000
H	7.863000	3.814000	0.424000	O	2.390000	4.704000	1.756000
C	8.880000	3.224000	-1.388000	C	6.352000	2.569000	6.953000
C	8.896000	5.321000	-0.681000	O	7.517000	3.066000	7.091000
H	8.696000	6.172000	-0.048000	O	5.982000	1.468000	7.436000
N	9.593000	5.337000	-1.809000	C	5.358000	3.348000	6.096000
C	9.584000	4.032000	-2.249000	H	5.912000	4.077000	5.494000
H	10.071000	3.746000	-3.169000	H	4.690000	3.923000	6.750000
C	-0.714000	9.729000	4.070000	C	4.530000	2.409000	5.206000
H	-1.136000	9.780000	3.088000	H	3.794000	1.880000	5.819000
H	-0.138000	10.611000	4.257000	H	5.176000	1.660000	4.743000
N	1.138000	8.321000	5.148000	C	3.819000	3.165000	4.105000
H	1.348000	8.936000	5.934000	O	4.147000	2.935000	2.904000
C	0.170000	8.525000	4.172000	O	2.906000	3.996000	4.466000
C	1.695000	7.104000	4.937000	C	8.258000	9.351000	0.682000
H	2.459000	6.669000	5.564000	H	8.425000	10.410000	0.894000
N	1.158000	6.524000	3.875000	H	9.188000	8.779000	0.794000
C	0.210000	7.400000	3.387000	O	7.782000	9.203000	-0.670000
H	-0.371000	7.167000	2.507000	O	7.251000	8.836000	1.553000
C	-2.194000	3.803000	0.575000	C	6.694000	8.362000	-0.597000
H	-2.990000	3.302000	1.085000	C	6.355000	8.143000	0.758000
H	-2.101000	3.409000	-0.415000	C	5.313000	7.372000	1.142000
C	-0.890000	3.586000	1.333000	H	5.113000	7.152000	2.184000
O	-0.427000	4.490000	2.111000	C	4.395000	6.821000	0.080000
O	-0.348000	2.468000	1.154000	H	4.254000	5.749000	0.295000
C	-1.282000	4.367000	8.424000	C	4.941000	6.931000	-1.335000
H	-0.419000	3.982000	8.926000	C	6.029000	7.721000	-1.647000
H	-2.136000	3.774000	8.677000	H	6.376000	7.818000	-2.672000
N	-2.077000	4.350000	5.999000	C	4.183000	6.150000	-2.378000
H	-3.069000	4.510000	6.159000	H	4.229000	5.074000	-2.146000
C	-1.062000	4.318000	6.947000	H	4.621000	6.288000	-3.371000
C	-1.513000	4.280000	4.773000	C	2.720000	6.602000	-2.338000
H	-2.088000	4.310000	3.862000	H	2.673000	7.637000	-2.706000

C	1.663000	5.784000	-3.074000	H	4.696000	11.560000	4.284000
H	1.800000	4.708000	-2.909000	C	2.069000	11.562000	0.808000
H	1.581000	5.986000	-4.144000	O	1.748000	12.861000	1.128000
O	0.411000	6.197000	-2.456000	C	2.414000	13.841000	0.323000
C	0.660000	6.737000	-1.216000	H	2.176000	13.702000	-0.737000
O	-0.236000	7.241000	-0.584000	H	3.500000	13.797000	0.469000
C	2.132000	6.552000	-0.917000	H	2.042000	14.814000	0.647000
H	2.193000	5.504000	-0.576000	C	1.522000	10.922000	-0.312000
C	2.865000	7.339000	0.179000	O	0.662000	11.676000	-1.067000
H	3.195000	4.180000	1.961000	C	-0.320000	10.982000	-1.828000
H	2.520000	6.914000	1.126000	H	-0.764000	10.164000	-1.249000
C	2.640000	8.842000	0.283000	H	0.104000	10.571000	-2.754000
C	3.144000	9.481000	1.425000	H	-1.085000	11.717000	-2.086000
H	3.714000	8.906000	2.138000	C	1.845000	9.587000	-0.597000
C	2.905000	10.832000	1.665000	H	1.413000	9.130000	-1.476000
O	3.404000	11.519000	2.738000	O	1.314000	2.284000	3.045000
C	4.324000	10.826000	3.570000	H	0.670000	2.205000	2.266000
H	5.165000	10.424000	2.993000	H	2.192000	2.074000	2.686000
H	3.835000	10.009000	4.117000				

⁵TS5

C	8.526000	1.794000	-1.520000	C	0.287000	7.534000	3.264000
H	7.893000	1.675000	-2.375000	H	-0.307000	7.300000	2.392000
H	7.987000	1.521000	-0.637000	C	-2.093000	3.843000	0.531000
N	8.609000	4.049000	-0.371000	H	-2.835000	3.319000	1.097000
H	8.045000	3.784000	0.454000	H	-2.055000	3.445000	-0.461000
C	8.962000	3.220000	-1.417000	C	-0.727000	3.675000	1.201000
C	9.064000	5.295000	-0.661000	O	-0.161000	4.654000	1.800000
H	8.928000	6.135000	0.003000	O	-0.245000	2.520000	1.109000
N	9.693000	5.328000	-1.828000	C	-1.159000	4.325000	8.195000
C	9.629000	4.036000	-2.300000	H	-0.293000	3.944000	8.694000
H	10.047000	3.766000	-3.257000	H	-1.997000	3.694000	8.403000
C	-0.754000	9.780000	4.049000	N	-1.913000	4.429000	5.761000
H	-1.202000	9.833000	3.079000	H	-2.906000	4.576000	5.918000
H	-0.215000	10.684000	4.243000	C	-0.912000	4.355000	6.721000
N	1.191000	8.437000	5.046000	C	-1.330000	4.399000	4.540000
H	1.375000	9.026000	5.858000	H	-1.891000	4.470000	3.623000
C	0.187000	8.616000	4.102000	N	-0.015000	4.283000	4.648000
C	1.830000	7.275000	4.758000	C	0.252000	4.250000	6.000000
H	2.631000	6.863000	5.353000	H	1.267000	4.155000	6.357000
N	1.314000	6.708000	3.678000	Fe	1.541000	4.591000	3.018000

O	2.769000	4.729000	1.491000	O	0.088000	6.372000	-2.328000
C	6.375000	2.566000	6.954000	C	0.354000	6.981000	-1.119000
O	7.553000	3.037000	7.084000	O	-0.503000	7.616000	-0.557000
O	5.987000	1.472000	7.438000	C	1.794000	6.682000	-0.769000
C	5.397000	3.374000	6.105000	H	1.775000	5.652000	-0.374000
H	5.966000	4.127000	5.550000	C	2.560000	7.474000	0.296000
H	4.713000	3.920000	6.765000	H	3.507000	4.164000	1.818000
C	4.593000	2.478000	5.151000	H	2.168000	7.141000	1.261000
H	3.789000	1.979000	5.699000	C	2.445000	8.994000	0.320000
H	5.234000	1.700000	4.728000	C	2.990000	9.650000	1.432000
C	4.007000	3.280000	4.006000	H	3.524000	9.079000	2.174000
O	4.394000	3.005000	2.828000	C	2.817000	11.016000	1.623000
O	3.156000	4.190000	4.303000	O	3.363000	11.714000	2.665000
C	8.065000	9.098000	0.812000	C	4.250000	11.002000	3.519000
H	7.918000	10.186000	0.793000	H	5.055000	10.520000	2.951000
H	9.092000	8.842000	1.080000	H	3.719000	10.246000	4.111000
O	7.786000	8.570000	-0.509000	H	4.682000	11.744000	4.189000
O	7.146000	8.489000	1.715000	C	1.994000	11.748000	0.754000
C	6.577000	7.941000	-0.410000	O	1.718000	13.061000	1.049000
C	6.157000	7.918000	0.935000	C	2.381000	13.999000	0.196000
C	4.968000	7.387000	1.314000	H	2.133000	13.815000	-0.854000
H	4.676000	7.323000	2.356000	H	3.468000	13.952000	0.334000
C	4.052000	6.851000	0.277000	H	2.019000	14.987000	0.481000
H	3.699000	5.804000	0.681000	C	1.412000	11.094000	-0.340000
C	4.631000	6.756000	-1.092000	O	0.560000	11.841000	-1.106000
C	5.859000	7.310000	-1.423000	C	-0.477000	11.140000	-1.792000
H	6.247000	7.251000	-2.435000	H	-0.917000	10.365000	-1.155000
C	3.825000	6.031000	-2.143000	H	-0.105000	10.674000	-2.714000
H	3.770000	4.966000	-1.880000	H	-1.232000	11.886000	-2.053000
H	4.316000	6.101000	-3.120000	C	1.688000	9.741000	-0.587000
C	2.413000	6.611000	-2.175000	H	1.233000	9.277000	-1.448000
H	2.461000	7.623000	-2.602000	O	1.581000	2.395000	2.883000
C	1.314000	5.834000	-2.895000	H	0.879000	2.293000	2.172000
H	1.367000	4.759000	-2.678000	H	2.424000	2.180000	2.454000
H	1.268000	5.988000	-3.975000				
⁵ P							
C	8.460000	1.785000	-1.571000	H	8.098000	3.758000	0.445000
H	7.848000	1.659000	-2.439000	C	8.904000	3.210000	-1.477000
H	7.897000	1.528000	-0.698000	C	9.109000	5.264000	-0.685000
N	8.636000	4.025000	-0.395000	H	9.032000	6.092000	0.002000

N	9.671000	5.306000	-1.885000	H	3.921000	1.685000	5.727000
C	9.542000	4.027000	-2.380000	H	5.323000	1.623000	4.658000
H	9.898000	3.767000	-3.365000	C	3.865000	3.076000	4.102000
C	-0.727000	9.642000	4.148000	O	4.143000	2.854000	2.874000
H	-1.135000	9.666000	3.159000	O	2.997000	3.916000	4.503000
H	-0.140000	10.521000	4.313000	C	8.635000	9.141000	0.295000
N	1.051000	8.225000	5.330000	H	9.171000	10.085000	0.186000
H	1.203000	8.833000	6.132000	H	9.237000	8.416000	0.859000
C	0.138000	8.428000	4.303000	O	8.347000	8.595000	-1.012000
C	1.650000	7.025000	5.125000	O	7.391000	9.364000	0.955000
H	2.382000	6.598000	5.795000	C	7.043000	8.133000	-0.919000
N	1.198000	6.452000	4.020000	C	6.475000	8.618000	0.251000
C	0.254000	7.318000	3.503000	C	5.154000	8.405000	0.549000
H	-0.281000	7.082000	2.594000	H	4.733000	8.845000	1.440000
C	-2.159000	3.780000	0.599000	C	4.360000	7.661000	-0.353000
H	-2.960000	3.270000	1.093000	H	3.015000	5.491000	2.321000
H	-2.051000	3.397000	-0.394000	C	4.958000	7.104000	-1.502000
C	-0.860000	3.560000	1.374000	C	6.320000	7.358000	-1.797000
O	-0.438000	4.438000	2.197000	H	6.770000	6.960000	-2.698000
O	-0.288000	2.463000	1.151000	C	4.180000	6.215000	-2.461000
C	-1.438000	4.415000	8.590000	H	4.266000	5.164000	-2.154000
H	-0.587000	4.012000	9.098000	H	4.612000	6.282000	-3.465000
H	-2.314000	3.869000	8.873000	C	2.717000	6.624000	-2.451000
N	-2.249000	4.308000	6.163000	H	2.631000	7.640000	-2.863000
H	-3.239000	4.505000	6.307000	C	1.686000	5.735000	-3.139000
C	-1.236000	4.303000	7.115000	H	1.869000	4.672000	-2.940000
C	-1.679000	4.176000	4.942000	H	1.582000	5.896000	-4.215000
H	-2.249000	4.168000	4.025000	O	0.428000	6.119000	-2.521000
N	-0.364000	4.062000	5.049000	C	0.666000	6.715000	-1.307000
C	-0.082000	4.139000	6.395000	O	-0.238000	7.204000	-0.678000
H	0.936000	4.086000	6.750000	C	2.153000	6.611000	-1.026000
Fe	1.154000	4.248000	3.495000	H	2.288000	5.585000	-0.644000
O	2.665000	4.742000	1.818000	C	2.852000	7.522000	-0.007000
C	6.360000	2.485000	6.980000	H	3.288000	3.993000	2.066000
O	7.521000	2.993000	7.116000	H	2.800000	6.977000	0.938000
O	5.998000	1.385000	7.471000	C	2.257000	8.895000	0.298000
C	5.363000	3.244000	6.112000	C	2.444000	9.369000	1.602000
H	5.898000	4.025000	5.561000	H	2.828000	8.697000	2.357000
H	4.634000	3.751000	6.756000	C	2.180000	10.698000	1.928000
C	4.623000	2.299000	5.155000	O	2.428000	11.247000	3.157000

C	3.334000	10.546000	4.006000	O	0.517000	11.839000	-1.097000
H	4.313000	10.435000	3.524000	C	-0.464000	11.198000	-1.914000
H	2.952000	9.564000	4.295000	H	-0.917000	10.351000	-1.387000
H	3.433000	11.149000	4.906000	H	-0.029000	10.840000	-2.856000
C	1.601000	11.548000	0.976000	H	-1.225000	11.949000	-2.136000
O	1.353000	12.853000	1.317000	C	1.638000	9.724000	-0.638000
C	2.167000	13.800000	0.610000	H	1.434000	9.376000	-1.643000
H	1.981000	13.752000	-0.467000	O	1.331000	2.081000	3.109000
H	3.232000	13.628000	0.809000	H	0.714000	2.076000	2.317000
H	1.882000	14.785000	0.980000	H	2.212000	1.898000	2.749000
C	1.243000	11.019000	-0.275000				
⁵ TS _{OH}							
C	8.472000	1.743000	-1.468000	C	-1.250000	4.416000	8.315000
H	7.802000	1.590000	-2.288000	H	-0.382000	4.027000	8.804000
H	7.979000	1.488000	-0.553000	H	-2.087000	3.781000	8.516000
N	8.509000	4.047000	-0.420000	N	-2.017000	4.505000	5.887000
H	7.941000	3.798000	0.406000	H	-3.017000	4.587000	6.051000
C	8.891000	3.181000	-1.426000	C	-1.009000	4.470000	6.841000
C	8.963000	5.285000	-0.744000	C	-1.437000	4.559000	4.665000
H	8.799000	6.147000	-0.114000	H	-2.007000	4.614000	3.752000
N	9.618000	5.278000	-1.897000	N	-0.116000	4.538000	4.767000
C	9.572000	3.968000	-2.323000	C	0.157000	4.480000	6.117000
H	10.017000	3.667000	-3.258000	H	1.176000	4.462000	6.474000
C	-0.979000	10.200000	4.179000	Fe	1.371000	5.143000	3.122000
H	-1.415000	10.266000	3.204000	O	2.291000	5.736000	1.475000
H	-0.475000	11.116000	4.407000	C	6.612000	2.654000	6.615000
N	1.014000	8.903000	5.145000	O	7.531000	3.331000	7.163000
H	1.236000	9.500000	5.946000	O	6.127000	1.585000	7.086000
C	-0.001000	9.072000	4.212000	C	6.076000	3.165000	5.273000
C	1.604000	7.708000	4.905000	H	6.038000	2.330000	4.565000
H	2.410000	7.295000	5.489000	H	6.766000	3.916000	4.876000
N	1.043000	7.118000	3.864000	C	4.673000	3.759000	5.411000
C	0.048000	7.954000	3.422000	H	4.651000	4.539000	6.181000
H	-0.568000	7.696000	2.573000	H	3.977000	2.982000	5.751000
C	-1.996000	4.025000	0.480000	C	4.086000	4.353000	4.131000
H	-2.792000	3.447000	0.901000	O	3.049000	5.095000	4.316000
H	-1.782000	3.672000	-0.507000	O	4.583000	4.091000	3.008000
C	-0.750000	3.885000	1.352000	C	8.192000	10.241000	1.001000
O	-0.306000	4.897000	1.986000	H	8.010000	11.257000	1.355000
O	-0.226000	2.741000	1.370000	H	9.261000	10.053000	0.838000

O	7.485000	10.029000	-0.241000	C	2.101000	8.803000	0.333000
O	7.670000	9.302000	1.947000	C	2.790000	9.469000	1.382000
C	6.917000	8.779000	-0.122000	H	3.463000	8.890000	2.004000
C	7.042000	8.334000	1.193000	C	2.612000	10.825000	1.609000
C	6.530000	7.114000	1.590000	O	3.237000	11.541000	2.590000
H	6.618000	6.753000	2.609000	C	4.157000	10.841000	3.421000
C	5.865000	6.352000	0.608000	H	4.978000	10.408000	2.835000
H	5.452000	5.393000	0.906000	H	3.657000	10.051000	3.993000
C	5.709000	6.805000	-0.709000	H	4.565000	11.584000	4.106000
C	6.266000	8.046000	-1.092000	C	1.739000	11.568000	0.791000
H	6.173000	8.415000	-2.110000	O	1.552000	12.900000	1.054000
C	4.917000	6.008000	-1.725000	C	2.326000	13.776000	0.222000
H	4.761000	4.987000	-1.361000	H	2.110000	13.596000	-0.836000
H	5.501000	5.926000	-2.652000	H	3.399000	13.648000	0.410000
C	3.551000	6.617000	-2.107000	H	2.029000	14.793000	0.480000
H	3.694000	7.670000	-2.380000	C	1.039000	10.920000	-0.249000
C	2.919000	5.866000	-3.278000	O	0.199000	11.720000	-0.969000
H	3.085000	4.787000	-3.168000	C	-0.817000	11.086000	-1.737000
H	3.269000	6.187000	-4.262000	H	-1.376000	10.365000	-1.127000
O	1.497000	6.119000	-3.198000	H	-0.402000	10.566000	-2.610000
C	1.153000	6.534000	-1.950000	H	-1.486000	11.880000	-2.074000
O	-0.001000	6.789000	-1.680000	C	1.189000	9.541000	-0.459000
C	2.397000	6.532000	-1.068000	H	0.614000	9.041000	-1.225000
H	2.411000	5.518000	-0.638000	O	1.817000	3.010000	2.915000
C	2.551000	7.431000	0.125000	H	1.067000	2.755000	2.291000
H	3.216000	5.640000	1.769000	H	2.652000	2.979000	2.427000
H	3.521000	7.282000	0.563000				
⁵ IM _{OH}							
C	8.473000	1.727000	-1.440000	H	-1.227000	10.042000	3.171000
H	7.799000	1.576000	-2.257000	H	-0.294000	10.902000	4.373000
H	7.989000	1.459000	-0.524000	N	1.122000	8.680000	5.208000
N	8.456000	4.026000	-0.391000	H	1.349000	9.306000	5.984000
H	7.892000	3.756000	0.432000	C	0.114000	8.836000	4.264000
C	8.879000	3.168000	-1.387000	C	1.692000	7.468000	5.005000
C	8.889000	5.275000	-0.705000	H	2.497000	7.069000	5.603000
H	8.694000	6.132000	-0.077000	N	1.128000	6.845000	3.981000
N	9.567000	5.282000	-1.845000	C	0.146000	7.691000	3.514000
C	9.561000	3.971000	-2.271000	H	-0.446000	7.446000	2.647000
H	10.034000	3.679000	-3.196000	C	-1.814000	3.933000	0.484000
C	-0.823000	9.996000	4.161000	H	-2.627000	3.326000	0.825000

H	-1.561000	3.660000	-0.519000	C	5.603000	6.838000	-0.246000
C	-0.602000	3.718000	1.391000	C	6.207000	8.016000	-0.745000
O	-0.026000	4.713000	1.980000	H	6.125000	8.291000	-1.793000
O	-0.198000	2.541000	1.480000	C	4.857000	5.946000	-1.215000
C	-1.490000	4.459000	8.525000	H	4.599000	5.001000	-0.729000
H	-0.647000	4.028000	9.023000	H	5.543000	5.690000	-2.034000
H	-2.371000	3.902000	8.768000	C	3.591000	6.560000	-1.849000
N	-2.263000	4.456000	6.080000	H	3.740000	7.638000	-1.989000
H	-3.265000	4.598000	6.218000	C	3.303000	5.919000	-3.210000
C	-1.269000	4.422000	7.049000	H	3.462000	4.833000	-3.170000
C	-1.670000	4.425000	4.864000	H	3.888000	6.329000	-4.036000
H	-2.230000	4.439000	3.942000	O	1.904000	6.167000	-3.470000
N	-0.352000	4.351000	4.991000	C	1.241000	6.408000	-2.309000
C	-0.097000	4.346000	6.346000	O	0.043000	6.578000	-2.312000
H	0.914000	4.308000	6.725000	C	2.237000	6.351000	-1.140000
Fe	1.256000	4.690000	3.622000	H	2.192000	5.297000	-0.820000
O	0.559000	6.890000	0.521000	C	1.891000	7.164000	0.140000
C	6.661000	2.488000	6.695000	H	0.486000	6.047000	1.014000
O	7.508000	3.244000	7.254000	H	2.599000	6.812000	0.904000
O	6.208000	1.414000	7.186000	C	1.997000	8.686000	0.124000
C	6.144000	2.908000	5.318000	C	2.830000	9.303000	1.065000
H	5.960000	2.016000	4.713000	H	3.497000	8.696000	1.664000
H	6.897000	3.522000	4.813000	C	2.736000	10.683000	1.282000
C	4.839000	3.687000	5.463000	O	3.440000	11.383000	2.224000
H	4.991000	4.610000	6.034000	C	4.261000	10.652000	3.125000
H	4.124000	3.088000	6.043000	H	5.086000	10.148000	2.609000
C	4.134000	4.030000	4.157000	H	3.679000	9.912000	3.689000
O	3.131000	4.829000	4.291000	H	4.674000	11.389000	3.816000
O	4.495000	3.517000	3.073000	C	1.825000	11.450000	0.543000
C	8.288000	10.276000	1.113000	O	1.670000	12.787000	0.840000
H	8.155000	11.324000	1.387000	C	2.491000	13.655000	0.054000
H	9.344000	10.031000	0.945000	H	2.305000	13.506000	-1.017000
O	7.545000	9.996000	-0.093000	H	3.555000	13.493000	0.268000
O	7.752000	9.440000	2.144000	H	2.217000	14.677000	0.323000
C	6.911000	8.796000	0.144000	C	1.016000	10.831000	-0.427000
C	7.043000	8.456000	1.489000	O	0.149000	11.660000	-1.081000
C	6.465000	7.312000	2.003000	C	-0.915000	11.056000	-1.802000
H	6.562000	7.047000	3.051000	H	-1.480000	10.367000	-1.160000
C	5.739000	6.501000	1.105000	H	-0.552000	10.506000	-2.679000
H	5.288000	5.586000	1.482000	H	-1.567000	11.868000	-2.128000

C	1.101000	9.449000	-0.635000	H	0.422000	8.948000	-1.312000
O	1.778000	2.601000	3.224000	H	1.118000	2.397000	2.510000
H	2.670000	2.642000	2.835000				