

Supporting Information:

A general mechanism for B12-dependent reductive dehalogenation

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Table S1. Gas-phase BDEs for the C-X bond of interest for this study ground state and 1-electron reduced substrates.

Substrate	Charge	BDE / kJ mol ⁻¹
TCE	0	916.7
	-1	109.1
TBE	0	820.5
	-1	105.7
DBMP	-1	342.1
	-2	-285.0
DCMP	-1	381.5
	-2	-310.0

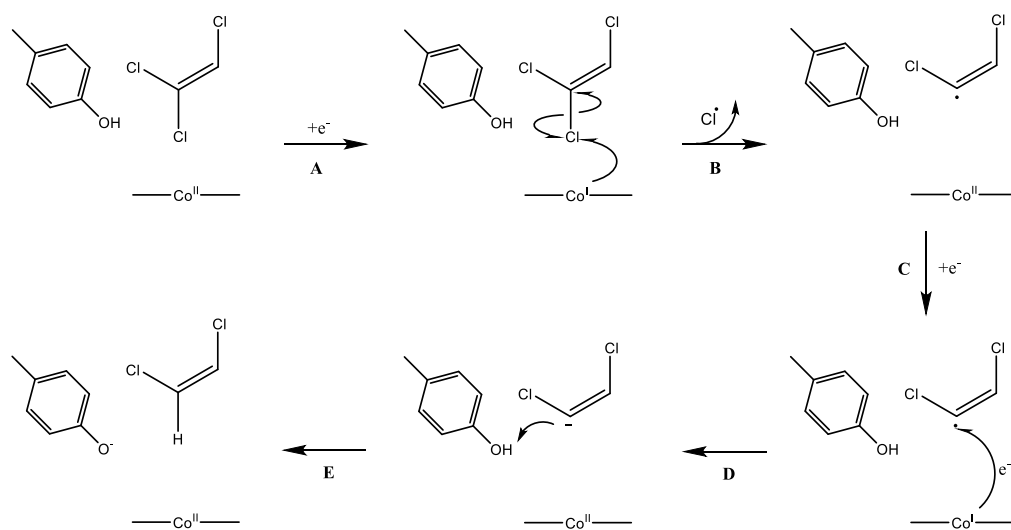
BDEs were calculated from the equation:

$$\text{BDE} = E(\text{RX}) - [E(\text{R}^+) + E(\text{X}^-)]$$

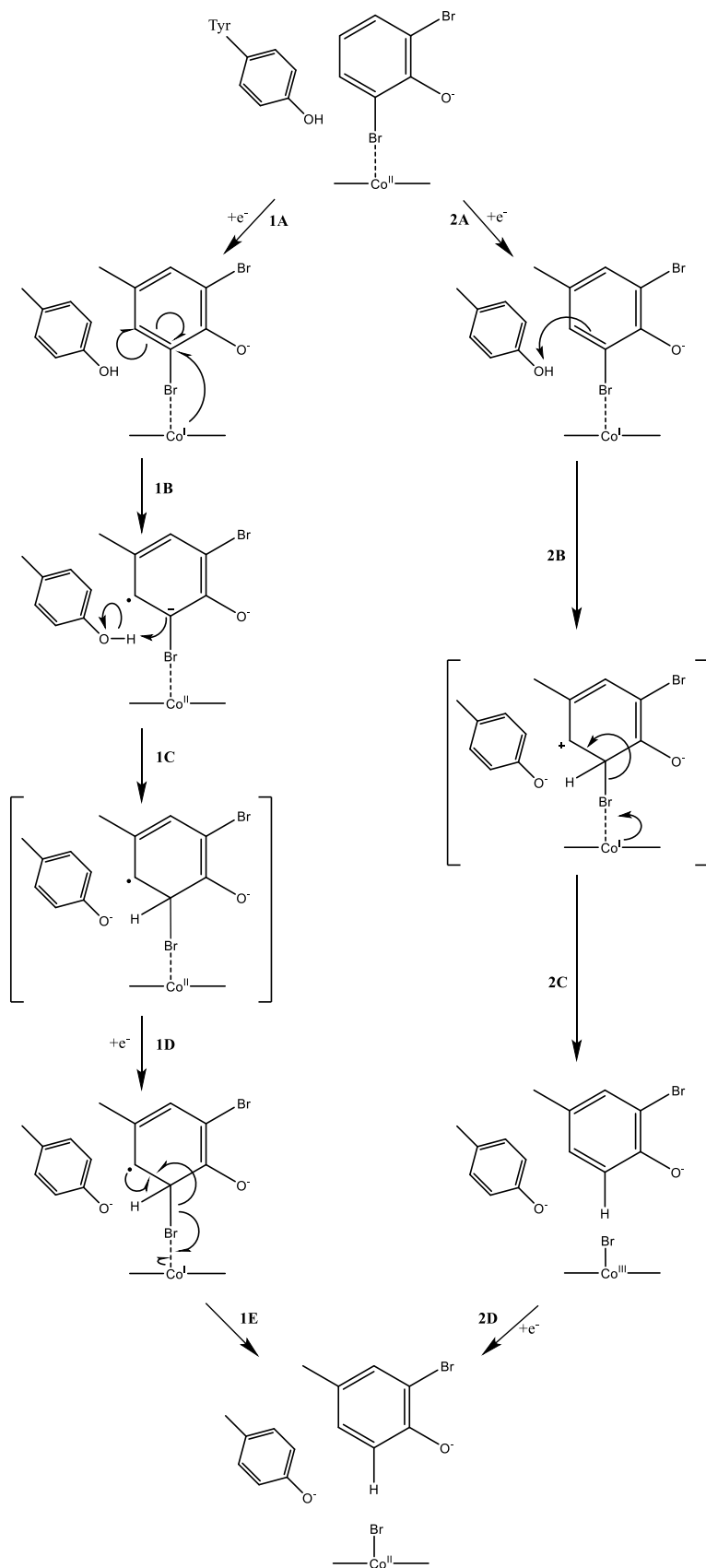
where E is the potential energy, R^+ is the substrate without the halide X^- and $E(\text{RX})$ includes the correction for basis set superposition error using the counterpoise method.

Table S2. HOMO and LUMO energies for the substrates in the gas phase

Substrate	HOMO / eV	LUMO / eV
TCE	-0.00789	3.17
TBE	0.220	3.42
DBMP	-6.10	-1.82
DCMP	-6.13	-1.52



Scheme S1. Dissociative electron transfer mechanism for dehalogenation proposed by Bommer *et al.*^[1]



Scheme S2. Homolytic (A) and heterolytic (B) dehalogenation mechanisms proposed by Payne *et al.*^[2] The concerted mechanism proposed by Liao *et al.* corresponds to the heterolytic mechanism with steps **2B** and **2C** combined.^[3]

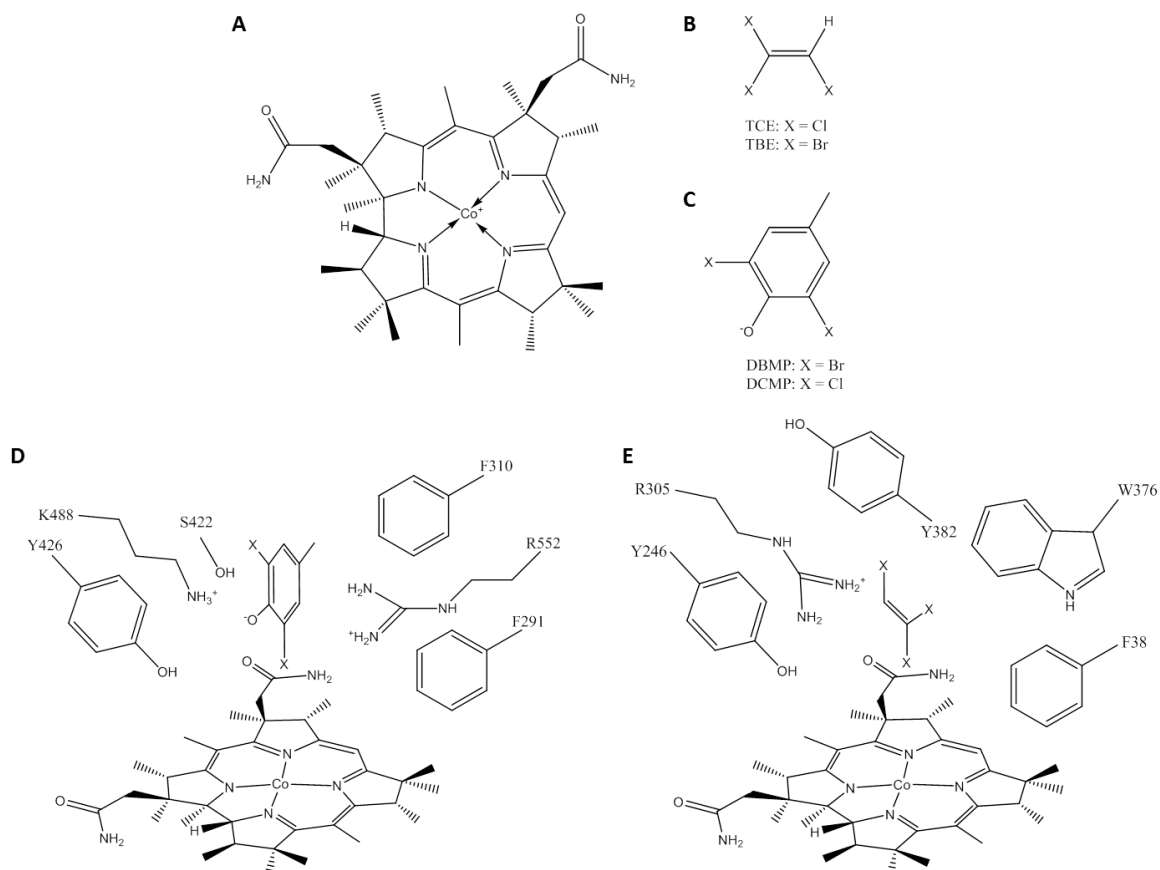


Figure S1. Structures used in DFT models: (A) cobalamin, (B) trihaloethylene, (C) 2,6-dihalo-4-methylphenolate, (D) NpRdhA active site with bound substrate, (E) PceA active site with bound substrate.

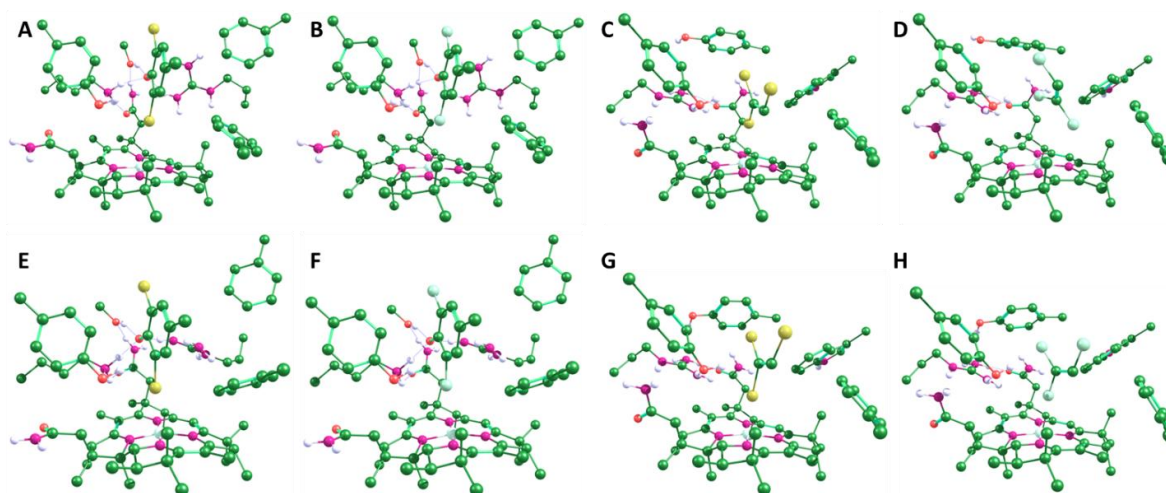


Figure S2. Optimised active site models, with non-polar hydrogens removed for clarity: (A-D) Co^{II} active site models and (E-F) Co^{I} active site models for (A,E) DBMP, (B,F) DCMP, (C,G) TBE and (D,H) TCE.

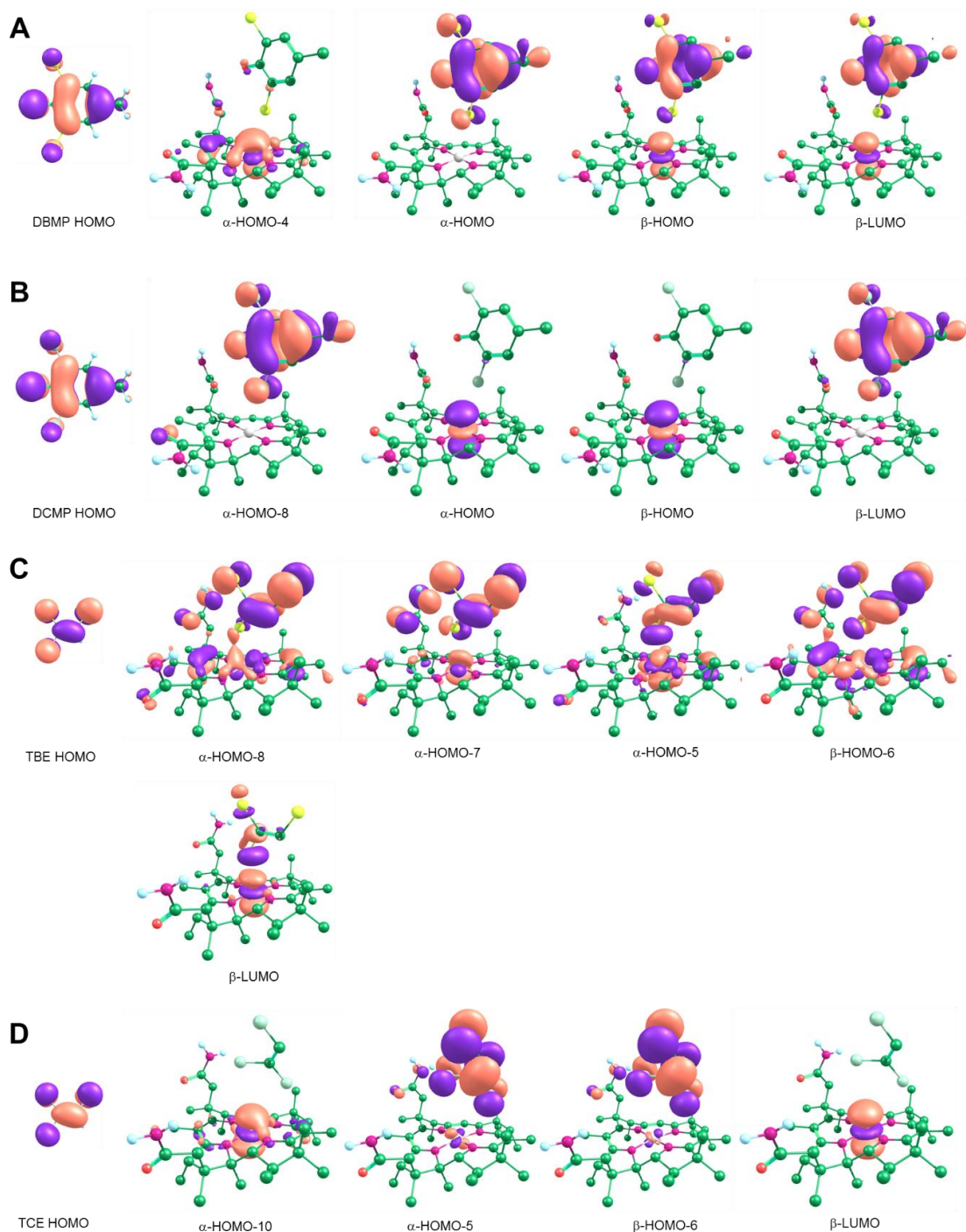


Figure S3. Molecular orbitals for the Co^{II} optimised active site models corresponding to the $\text{Co } d_z^2$ orbitals; the HOMO of the substrate is shown for comparison on the far left. **(A)** NpRdhA/DBMP: half a charge is transferred (Table 2 in the main text) so that the SOMO and LUMO are both delocalised across the substrate HOMO and $\text{Co } d_z^2$ orbitals. **(B)** NpRdhA/DCMP: DCMP fully reduces the cobalamin (the spin density is fully localised on the substrate, see Table 2 in the main text) so that the HOMO of the substrate is split into highest singly-occupied MO (SOMO) and lowest unoccupied MO (LUMO). **(C)** PceA/TBE: the HOMO of the substrate is delocalised with bonding orbitals of the cobalamin, so that the unoccupied $\text{Co } d_z^2$ orbital is delocalised with the C-Br anti-bonding orbital in the LUMO, hence TBE has very little spin density. **(D)** PceA/TCE: there is no delocalisation of the TCE HOMO and $\text{Co } d_z^2$ orbitals.

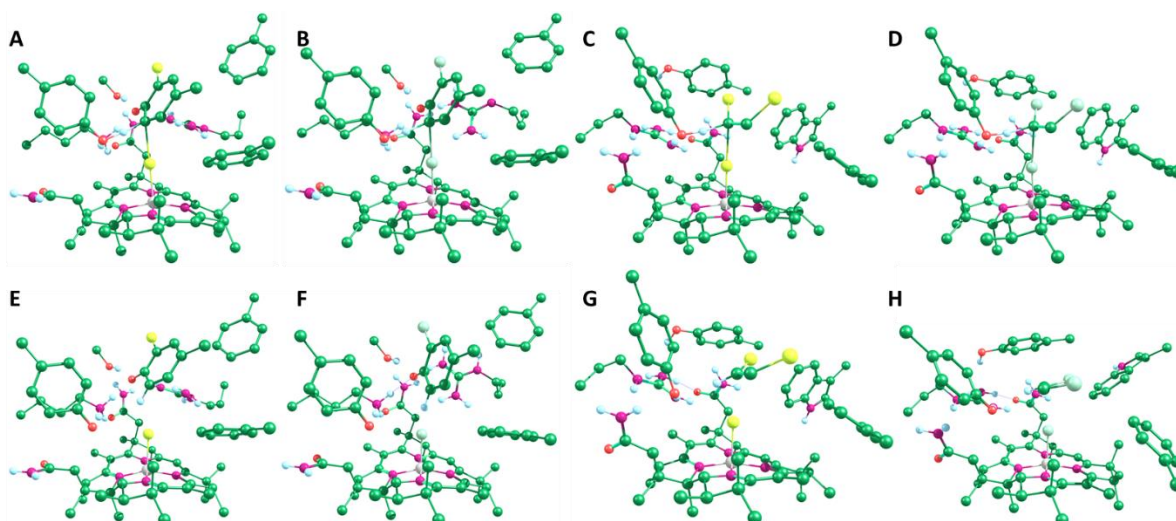


Figure S4. (A-D) Transition state and (E-H) product geometries, truncated for clarity (most amino acids and non-polar hydrogens removed) for dehalogenation in Co^{I} active site models: (A,E) DBMP, (B,F) DCMP, (C,G) TBE and (D,H) TCE.

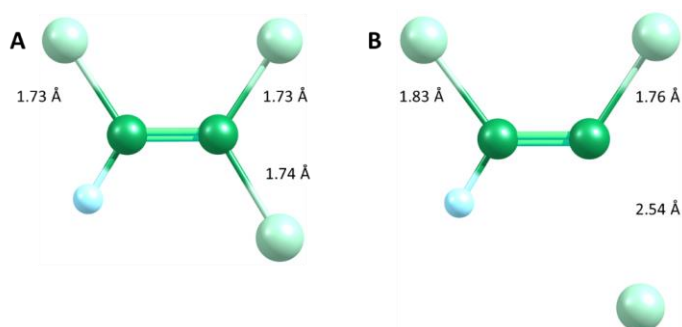


Figure S5. Optimised gas phase geometry of TCE (A) before and (B) after 1-electron reduction.

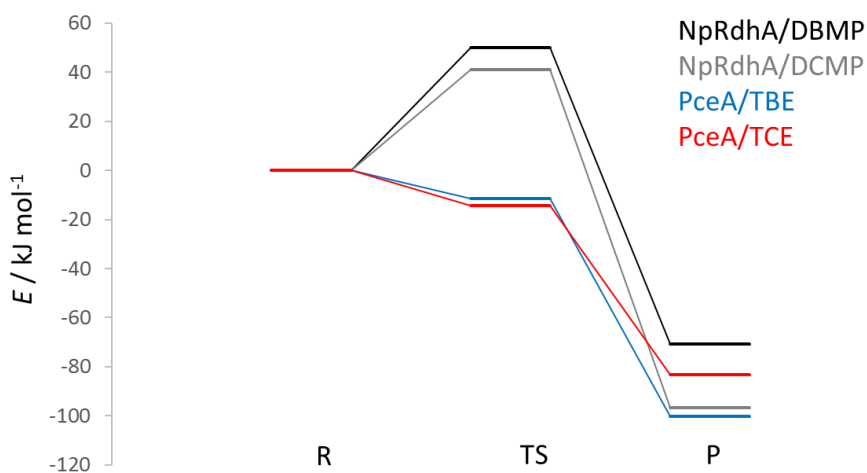


Figure S6. Calculated Gibbs free energy diagram for Co^{I} -catalysed dehalogenation in NpRdhA and PceA models.

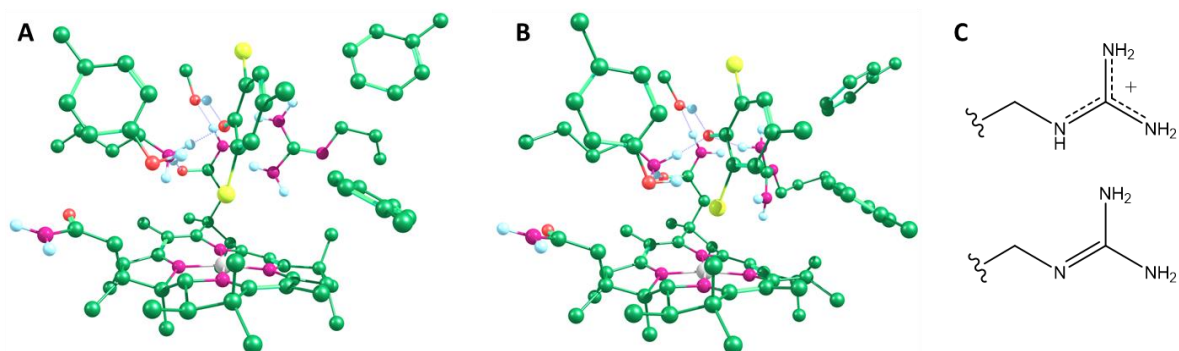


Figure S7. Optimised (A) Co^{II} and (B) Co^I NpRdhA/DBMP active site models with a neutralised R552 analogue, with non-polar hydrogens removed for clarity. (C) The chemical structure of protonated arginine, top, and the neutral form, bottom.

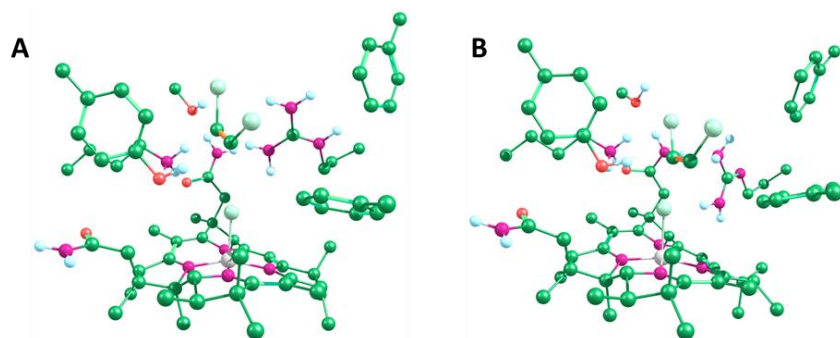


Figure S8. Optimised Co^I active site models for (A) NpRdhA/TCE and (B) NpRdhA/TCE with a neutralized R552.

References

1. Bommer, M., et al., *Structural basis for organohalide respiration*. *Science*, 2014. **346**(6208): p. 455-8.
2. Payne, K.A., et al., *Reductive dehalogenase structure suggests a mechanism for B12-dependent dehalogenation*. *Nature*, 2015. **517**(7535): p. 513-6.
3. Liao, R.-Z., S.-L. Chen, and P.E.M. Siegbahn, *Which Oxidation State Initiates Dehalogenation in the B12-Dependent Enzyme NpRdhA: CoII, CoI, or Co0?* *ACS Catal.*, 2015. **5**(12): p. 7350-7358.

Cartesian coordinates of optimised structures

1A. NpRdhA/DBMP, Co^{II}
1B. NpRdhA/DBMP, Co^I
1C. NpRdhA/DBMP, Co^I → Co^{III} Transition State
1D. NpRdhA/DBMP, Co^{III}

2A. NpRdhA/DCMP, Co^{II}
2B. NpRdhA/DCMP, Co^I
2C. NpRdhA/DCMP, Co^I → Co^{III} Transition State
2D. NpRdhA/DCMP, Co^{III}

3A. PceA/TCE, Co^{II}
3B. PceA/TCE, Co^I
3C. PceA/TCE, Co^I → Co^{III} Transition State
3D. PceA/TCE, Co^{III}

4A. PceA/TBE, Co^{II}
4B. PceA/TBE, Co^I
4C. PceA/TBE, Co^I → Co^{III} Transition State
4D. PceA/TBE, Co^{III}

5A. NpRdhA/DBMP with neutralized R552, Co^{II}
5B. NpRdhA/DBMP with neutralized R552, Co^I

6A. NpRdhA/TCE, Co^I
6B. NpRdhA/TCE with neutralized R552, Co^I

1A. NpRdhA/DBMP, Co^{II} (Charge = 2, Multiplicity = 2)

C	2.767042000	7.745209000	-1.375468000
C	6.234703000	4.776158000	2.000383000
C	-6.250795000	-2.553039000	3.470035000
C	-10.122743000	1.914071000	0.835203000
C	-0.160317000	5.144444000	3.344998000
C	-4.351732000	-2.447006000	-5.147355000
Co	1.968360000	-2.807275000	0.307740000
C	-1.522924000	2.439099000	-0.134346000
C	-1.270962000	1.440318000	-1.108282000
C	-1.783610000	1.474046000	-2.403861000
C	-2.631821000	2.511591000	-2.808358000
C	-2.922424000	3.515993000	-1.875231000
C	-2.379875000	3.474066000	-0.596416000
O	-1.006038000	2.402438000	1.072781000
Br	-0.147602000	-0.038732000	-0.600571000
Br	-2.763883000	4.893973000	0.626378000
C	-3.252553000	2.519016000	-4.184396000
H	-2.671596000	1.909869000	-4.883281000
H	-4.270855000	2.111626000	-4.149933000
H	-3.317445000	3.533828000	-4.587436000
H	-1.534470000	0.674788000	-3.094200000
H	-3.573719000	4.339884000	-2.150346000
C	-4.439443000	-2.476168000	-3.638193000
C	-3.841416000	-1.460918000	-2.864051000
C	-3.887252000	-1.489255000	-1.463398000
C	-4.551630000	-2.537930000	-0.809296000
C	-5.153059000	-3.558107000	-1.562346000
C	-5.094381000	-3.526648000	-2.963984000
H	-5.185432000	-2.996161000	-5.614477000
H	-3.412242000	-2.920851000	-5.493007000
H	-4.357929000	-1.412904000	-5.531752000
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H	-3.424285000	-0.680075000	-0.888607000
H	-4.624664000	-2.545595000	0.281031000
H	-5.683808000	-4.373640000	-1.058909000
H	-5.574017000	-4.322843000	-3.544214000
C	2.420073000	6.316347000	-1.713079000
C	3.424088000	5.390539000	-2.034756000
C	3.125808000	4.066773000	-2.345269000
C	1.796901000	3.640112000	-2.336120000
C	0.774993000	4.540865000	-2.034204000
C	1.094640000	5.865562000	-1.726620000
O	1.552933000	2.299135000	-2.590623000
H	0.586986000	2.157250000	-2.588645000
H	3.154000000	8.274275000	-2.254202000

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H	1.891915000	8.292837000	-1.014920000
H	4.463919000	5.708846000	-2.040471000
H	3.913573000	3.367423000	-2.600003000
H	-0.261307000	4.212640000	-2.039329000
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C	4.010670000	3.666098000	1.362945000
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N	1.783476000	2.648839000	0.791487000
H	1.920887000	1.876819000	1.506571000
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C	1.553530000	0.556969000	3.808074000
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N	1.157990000	1.611345000	4.541840000
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H	-1.182321000	-5.244947000	-3.330418000
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H	-0.240749000	-6.869645000	0.029063000
H	-1.229523000	-6.689655000	-1.427656000
H	-1.769621000	-5.758760000	3.539943000
H	-1.037763000	-6.850716000	2.353979000
H	-2.767793000	-6.464954000	2.269902000
H	-2.332647000	-2.865209000	1.239031000
H	-2.328422000	-3.370650000	2.960517000
H	-3.509127000	-4.061419000	1.819617000
H	0.136737000	-4.617048000	3.792802000
H	1.660705000	-3.203564000	5.281023000
H	3.077154000	-5.196988000	4.685209000
H	3.991020000	-4.021907000	5.642610000
H	4.247648000	-4.129963000	3.886662000
H	3.689422000	-1.621827000	6.243372000
H	4.171137000	-0.234863000	5.269476000
H	4.936100000	-1.808715000	5.002288000
H	1.483619000	-0.701143000	5.577618000
H	0.740620000	-1.328887000	4.106765000
H	0.824821000	2.473577000	4.075226000
H	0.930708000	1.485605000	5.518811000
H	2.450883000	-0.893285000	-2.208687000

1B. NpRdhA/DBMP, Co^I (Charge = 1, Multiplicity = 1)

C	2.767042000	7.745209000	-1.375468000
C	6.234703000	4.776158000	2.000383000
C	-6.250795000	-2.553039000	3.470035000
C	-10.122743000	1.914071000	0.835203000
C	-0.160317000	5.144444000	3.344998000
C	-4.351732000	-2.447006000	-5.147355000
Co	1.968360000	-2.807275000	0.307740000
C	-1.522924000	2.439099000	-0.134346000
C	-1.270962000	1.440318000	-1.108282000
C	-1.783610000	1.474046000	-2.403861000
C	-2.631821000	2.511591000	-2.808358000
C	-2.922424000	3.515993000	-1.875231000
C	-2.379875000	3.474066000	-0.596416000
O	-1.006038000	2.402438000	1.072781000
Br	-0.147602000	-0.038732000	-0.600571000
Br	-2.763883000	4.893973000	0.626378000
C	-3.252553000	2.519016000	-4.184396000
H	-2.671596000	1.909869000	-4.883281000
H	-4.270855000	2.111626000	-4.149933000
H	-3.317445000	3.533828000	-4.587436000
H	-1.534470000	0.674788000	-3.094200000
H	-3.573719000	4.339884000	-2.150346000
C	-4.439443000	-2.476168000	-3.638193000
C	-3.841416000	-1.460918000	-2.864051000
C	-3.887252000	-1.489255000	-1.463398000
C	-4.551630000	-2.537930000	-0.809296000
C	-5.153059000	-3.558107000	-1.562346000
C	-5.094381000	-3.526648000	-2.963984000
H	-5.185432000	-2.996161000	-5.614477000
H	-3.412242000	-2.920851000	-5.493007000
H	-4.357929000	-1.412904000	-5.531752000

H	-3.349810000	-0.624894000	-3.371880000
H	-3.424285000	-0.680075000	-0.888607000
H	-4.624664000	-2.545595000	0.281031000
H	-5.683808000	-4.373640000	-1.058909000
H	-5.574017000	-4.322843000	-3.544214000
C	2.420073000	6.316347000	-1.713079000
C	3.424088000	5.390539000	-2.034756000
C	3.125808000	4.066773000	-2.345269000
C	1.796901000	3.640112000	-2.336120000
C	0.774993000	4.540865000	-2.034204000
C	1.094640000	5.865562000	-1.726620000
O	1.552933000	2.299135000	-2.590623000
H	0.586986000	2.157250000	-2.588645000
H	3.154000000	8.274275000	-2.254202000
H	3.541750000	7.792203000	-0.601652000
H	1.891915000	8.292837000	-1.014920000
H	4.463919000	5.708846000	-2.040471000
H	3.913573000	3.367423000	-2.600003000
H	-0.261307000	4.212640000	-2.039329000
H	0.289754000	6.557288000	-1.489896000
C	4.745016000	4.977946000	1.692787000
C	4.010670000	3.666098000	1.362945000
C	2.518643000	3.906439000	1.152842000
N	1.783476000	2.648839000	0.791487000
H	1.920887000	1.876819000	1.506571000
H	0.738877000	2.766223000	0.796519000
H	2.051056000	2.299698000	-0.140189000
H	6.753324000	4.303398000	1.147320000
H	6.373154000	4.123388000	2.881677000
H	6.729676000	5.738524000	2.213869000
H	4.629785000	5.672946000	0.838714000
H	4.249443000	5.466779000	2.554703000
H	4.457431000	3.206848000	0.461998000
H	4.149479000	2.945685000	2.192524000
H	2.333202000	4.634654000	0.348067000
H	2.041731000	4.268457000	2.073669000
C	-6.632026000	-1.419490000	2.507326000
C	-5.790696000	-0.147585000	2.653903000
N	-4.363723000	-0.423658000	2.393011000
C	-3.404801000	0.513581000	2.275626000
N	-3.732770000	1.815753000	2.223840000
N	-2.099085000	0.179528000	2.258616000
H	-4.048775000	-1.382568000	2.533452000
H	-2.987298000	2.484572000	2.001576000
H	-4.688567000	2.093933000	2.001199000
H	-1.836256000	-0.797976000	2.160054000
H	-1.442623000	0.894896000	1.864452000
H	-6.931671000	-3.411460000	3.346884000
H	-6.307222000	-2.224263000	4.522716000
H	-5.226436000	-2.935464000	3.292734000
H	-7.681053000	-1.122858000	2.679737000
H	-6.580861000	-1.760889000	1.457280000
H	-6.144063000	0.599297000	1.922901000
H	-5.898682000	0.277196000	3.671137000
C	-8.672684000	1.791622000	0.405680000
C	-8.212433000	0.649279000	-0.285082000
C	-6.894279000	0.562434000	-0.760341000
C	-5.998435000	1.623981000	-0.552797000
C	-6.433439000	2.763353000	0.147591000
C	-7.752960000	2.839749000	0.626539000
H	-10.721879000	2.367545000	0.023597000
H	-10.230135000	2.557836000	1.724053000
H	-10.563708000	0.928162000	1.058552000
H	-8.905373000	-0.180492000	-0.467550000
H	-6.566064000	-0.331302000	-1.301592000
H	-4.975205000	1.570651000	-0.940914000
H	-5.752181000	3.610584000	0.296335000
H	-8.082574000	3.739774000	1.158447000
O	-0.005593000	3.741166000	3.133987000
H	0.069223000	5.724846000	2.430645000
H	0.546265000	5.440494000	4.137497000
H	-1.185575000	5.398778000	3.675347000
H	-0.575117000	3.432597000	2.379466000
C	0.846343000	-3.908690000	-4.829403000
C	1.055394000	-2.785041000	-3.798146000
C	0.211286000	-1.543864000	-4.168816000
C	2.584005000	-2.443204000	-3.721083000
C	3.085495000	-1.494462000	-4.808531000
C	2.746951000	-1.947102000	-2.282889000
C	4.061669000	-2.146701000	-1.489845000
C	5.199012000	-1.059734000	-1.592319000
C	5.667537000	-0.922329000	-0.099946000
C	4.441727000	-1.345938000	0.675021000
C	4.221965000	-1.087289000	2.070183000
C	5.069138000	-0.009752000	2.715365000
C	6.911107000	-1.726069000	0.330488000
C	4.590212000	0.309148000	-2.028962000
C	5.599350000	1.452174000	-2.011453000
N	6.074987000	1.846382000	-3.224174000
O	5.953720000	2.001284000	-0.966554000
C	6.335720000	-1.434221000	-2.550322000
C	4.573979000	-3.586212000	-1.668103000
N	3.589407000	-1.992871000	-0.079890000
N	1.719909000	-2.725320000	-1.539125000
C	0.769711000	-3.165603000	-2.335169000

C	-0.372108000	-3.877443000	-1.839231000
C	-1.452834000	-4.325556000	-2.799420000
C	-0.499374000	-4.192110000	-0.501999000
N	0.364350000	-3.810943000	0.520606000
C	-1.561263000	-5.127657000	0.053933000
C	-1.230043000	-6.580884000	-0.340710000
C	-1.492522000	-4.851409000	1.580845000
C	-1.775632000	-6.055895000	2.485995000
C	-2.478911000	-3.706279000	1.927444000
C	-0.094901000	-4.274864000	1.711532000
C	0.572947000	-4.140984000	2.921508000
C	1.713542000	-3.376244000	3.122248000
N	2.350653000	-2.671074000	2.159039000
C	2.378145000	-3.152606000	4.454305000
C	3.496744000	-4.186989000	4.681639000
C	2.884511000	-1.687620000	4.247302000
C	3.232772000	-1.757546000	2.750614000
C	3.992786000	-1.311177000	5.237252000
C	1.619436000	-0.794641000	4.494484000
C	1.553530000	0.556969000	3.808074000
O	1.787673000	0.632931000	2.586876000
N	1.157990000	1.611345000	4.541840000
H	1.233250000	-4.864002000	-4.460539000
H	1.393772000	-3.654956000	-5.743886000
H	-0.200486000	-4.040017000	-5.107587000
H	-0.854656000	-1.742646000	-4.026095000
H	0.370107000	-1.280077000	-5.219088000
H	0.478264000	-0.682920000	-3.548530000
H	3.111465000	-3.400751000	-3.814582000
H	4.176613000	-1.415919000	-4.785247000
H	2.666197000	-0.489445000	-4.693342000
H	2.814156000	-1.861801000	-5.803396000
H	5.889137000	0.131281000	0.090716000
H	4.466951000	0.603844000	3.386084000
H	5.476074000	0.660081000	1.955719000
H	5.913451000	-0.410556000	3.286378000
H	7.114207000	-1.550450000	1.390711000
H	7.789493000	-1.398866000	-0.231854000
H	6.788095000	-2.803311000	0.189702000
H	3.786798000	0.591914000	-1.341071000
H	4.151491000	0.216004000	-3.025359000
H	5.810597000	1.390948000	-4.085634000
H	6.777465000	2.574782000	-3.259737000
H	6.806951000	-2.381576000	-2.283291000
H	7.112740000	-0.664217000	-2.535105000
H	5.972411000	-1.518811000	-3.580013000
H	3.755932000	-4.291705000	-1.487633000
H	5.372343000	-3.806356000	-0.957605000
H	4.954245000	-3.753289000	-2.678616000
H	-2.395785000	-4.499201000	-2.280657000
H	-1.182321000	-5.244947000	-3.330418000
H	-1.652138000	-3.558931000	-3.549232000
H	-2.553290000	-4.869962000	-0.330769000
H	-1.970549000	-7.274045000	0.067367000
H	-0.240749000	-6.869645000	0.029063000
H	-1.229523000	-6.689655000	-1.427656000
H	-1.769621000	-5.758760000	3.539943000
H	-1.037763000	-6.850716000	2.353979000
H	-2.767793000	-6.464954000	2.269902000
H	-2.332647000	-2.865209000	1.239031000
H	-2.328422000	-3.370650000	2.960517000
H	-3.509127000	-4.061419000	1.819617000
H	0.136737000	-4.617048000	3.792802000
H	1.660705000	-3.203564000	5.281023000
H	3.077154000	-5.196988000	4.685209000
H	3.991020000	-4.021907000	5.642610000
H	4.247648000	-4.129963000	3.886662000
H	3.689422000	-1.621827000	6.243372000
H	4.171137000	-0.234863000	5.269476000
H	4.936100000	-1.808715000	5.002288000
H	1.483619000	-0.701143000	5.577618000
H	0.740620000	-1.328887000	4.106765000
H	0.824821000	2.473577000	4.075226000
H	0.930708000	1.485605000	5.518811000
H	2.450883000	-0.893285000	-2.208687000

1C. NpRdhA/DBMP, Co^I → Co^{III} Transition State (Charge = 1, Multiplicity = 1)

C	3.611124000	7.387625000	-2.898475000
C	6.624390000	4.621247000	1.038851000
C	-6.742569000	-0.640476000	3.362143000
C	-9.960615000	3.769895000	-0.113838000
C	0.327426000	6.052666000	2.106595000
C	-4.785496000	-2.281967000	-5.084501000
Co	1.389795000	-2.515155000	0.540481000
C	-1.103218000	2.687613000	-0.405383000
C	-0.609541000	1.797778000	-1.405656000
C	-1.415895000	1.456725000	-2.502772000
C	-2.670827000	2.030923000	-2.723706000
C	-3.122796000	2.981816000	-1.790939000
C	-2.353586000	3.304120000	-0.681066000
O	-0.473119000	2.884063000	0.736803000
Br	0.393192000	-0.381811000	-0.213758000
Br	-3.045133000	4.563544000	0.598703000
C	-3.530620000	1.657937000	-3.908074000
H	-2.923981000	1.247116000	-4.720825000

H	-4.272223000	0.898444000	-3.627938000
H	-4.076241000	2.524550000	-4.294023000
H	-1.018058000	0.759960000	-3.238885000
H	-4.091293000	3.454592000	-1.923543000
C	-4.228912000	-2.341746000	-3.683887000
C	-2.952213000	-1.808930000	-3.411393000
C	-2.393751000	-1.886086000	-2.132949000
C	-3.113611000	-2.497365000	-1.093302000
C	-4.395995000	-3.011310000	-1.337790000
C	-4.947659000	-2.932190000	-2.626372000
H	-5.829802000	-2.631898000	-5.126240000
H	-4.189518000	-2.912784000	-5.769581000
H	-4.751551000	-1.251451000	-5.481708000
H	-2.390231000	-1.327703000	-4.218966000
H	-1.398968000	-1.480552000	-1.928919000
H	-2.646345000	-2.588277000	-0.106910000
H	-4.968335000	-3.485323000	-0.531986000
H	-5.946420000	-3.341169000	-2.816229000
C	3.142111000	5.959014000	-2.723714000
C	4.053336000	4.893961000	-2.690623000
C	3.632787000	3.576511000	-2.533551000
C	2.267936000	3.258817000	-2.396104000
C	1.342293000	4.317558000	-2.466861000
C	1.783805000	5.633714000	-2.617742000
O	1.921153000	1.972116000	-2.144232000
H	0.736170000	1.846522000	-1.751021000
H	3.852461000	7.602496000	-3.947519000
H	4.513950000	7.584368000	-2.309392000
H	2.839676000	8.098074000	-2.585401000
H	5.119483000	5.099271000	-2.775312000
H	4.361120000	2.773742000	-2.494949000
H	0.280325000	4.112520000	-2.382965000
H	1.042563000	6.430384000	-2.650583000
C	5.104958000	4.811450000	1.011994000
C	4.354557000	3.474746000	0.954368000
C	2.844278000	3.658022000	0.893794000
N	2.142396000	2.367142000	0.624720000
H	2.356735000	1.666234000	1.350354000
H	1.077527000	2.505654000	0.674212000
H	2.326287000	1.999996000	-0.336733000
H	6.967166000	4.057574000	0.153270000
H	6.938871000	4.048962000	1.930696000
H	7.150674000	5.591644000	1.058484000
H	4.817797000	5.415128000	0.129317000
H	4.776370000	5.383782000	1.901583000
H	4.694093000	2.914542000	0.065424000
H	4.615939000	2.857615000	1.835069000
H	2.561325000	4.343215000	0.078599000
H	2.435528000	4.040601000	1.840632000
C	-5.741889000	-1.729246000	2.967253000
C	-4.722020000	-1.266677000	1.925666000
N	-3.870581000	-0.193520000	2.451058000
C	-3.017503000	0.535173000	1.692028000
N	-2.965098000	0.320381000	0.375188000
N	-2.241584000	1.466989000	2.267642000
H	-3.739479000	-0.149793000	3.459581000
H	-2.297679000	0.852641000	-0.195538000
H	-3.287020000	-0.556176000	-0.036193000
H	-2.540386000	1.870066000	3.150935000
H	-1.537867000	2.030504000	1.714573000
H	-7.473781000	-1.022257000	4.094193000
H	-7.296564000	-0.275271000	2.479305000
H	-6.238548000	0.231752000	3.815612000
H	-6.272194000	-2.598446000	2.538536000
H	-5.203799000	-2.113078000	3.857525000
H	-4.090552000	-2.119095000	1.614757000
H	-5.247125000	-0.885168000	1.031862000
C	-8.761627000	2.862659000	-0.326663000
C	-8.854311000	1.721259000	-1.151118000
C	-7.737706000	0.907792000	-1.396837000
C	-6.497035000	1.216742000	-0.816616000
C	-6.389791000	2.339423000	0.019572000
C	-7.510928000	3.150235000	0.259737000
H	-10.020475000	4.526827000	-0.918671000
H	-9.892320000	4.311173000	0.844795000
H	-10.904989000	3.199685000	-0.126869000
H	-9.816360000	1.470824000	-1.613846000
H	-7.835394000	0.032324000	-2.040905000
H	-5.616160000	0.599224000	-1.026155000
H	-5.426584000	2.596252000	0.474213000
H	-7.409392000	4.029534000	0.906923000
O	0.047349000	4.738290000	2.565522000
H	1.095437000	6.060873000	1.307352000
H	0.711495000	6.634339000	2.961310000
H	-0.581770000	6.554298000	1.719679000
H	-0.277396000	4.179781000	1.805058000
C	1.593832000	-4.556082000	-4.483314000
C	1.557455000	-3.322633000	-3.567318000
C	0.793641000	-2.158906000	-4.240329000
C	3.022961000	-2.910699000	-3.199130000
C	3.741397000	-2.081098000	-4.263176000
C	2.850899000	-2.230493000	-1.839221000
C	3.917339000	-2.359505000	-0.731548000
C	5.155095000	-1.397623000	-0.731404000
C	5.302745000	-1.058007000	0.796249000
C	3.892111000	-1.251773000	1.317198000
C	3.411431000	-0.759697000	2.579812000
C	4.340127000	0.153845000	3.353777000
C	6.350716000	-1.859877000	1.590603000
C	4.813780000	-0.076913000	-1.479548000
C	6.012378000	0.863851000	-1.563500000

N	6.437702000	1.150702000	-2.827800000
O	6.584538000	1.316884000	-0.572993000
C	6.415410000	-2.017308000	-1.348700000
C	4.304067000	-3.838652000	-0.536991000
N	3.145867000	-1.922530000	0.474078000
N	1.662587000	-2.897174000	-1.258920000
C	0.959687000	-3.530554000	-2.166664000
C	-0.206392000	-4.288766000	-1.823073000
C	-1.060270000	-4.893919000	-2.916953000
C	-0.585295000	-4.451901000	-0.506148000
N	-0.098271000	-3.717780000	0.571403000
C	-1.648736000	-5.440761000	-0.048795000
C	-1.404145000	-6.892208000	-0.494650000
C	-1.707285000	-5.240070000	1.499343000
C	-1.139462000	-6.429058000	2.311283000
C	-3.145399000	-4.963345000	1.970694000
C	-0.772927000	-4.059120000	1.698197000
C	-0.562307000	-3.477641000	2.938608000
C	0.434155000	-2.565068000	3.254596000
N	1.342604000	-2.064713000	2.389593000
C	0.741050000	-2.135718000	4.663999000
C	1.572195000	-3.227997000	5.366776000
C	1.507262000	-0.804755000	4.409035000
C	2.180626000	-1.156585000	3.061500000
C	2.387520000	-0.413563000	5.602049000
C	0.395428000	0.267794000	4.206134000
C	0.865777000	1.686572000	3.929092000
O	1.888061000	1.914744000	3.275974000
N	0.085049000	2.687522000	4.395706000
H	1.925679000	-5.444904000	-3.936445000
H	2.305722000	-4.375400000	-5.296572000
H	0.628196000	-4.770505000	-4.944215000
H	-0.257685000	-2.422975000	-4.379370000
H	1.217462000	-1.944206000	-5.226549000
H	0.836856000	-1.248118000	-3.633261000
H	3.573847000	-3.848279000	-3.051717000
H	4.801706000	-1.967141000	-4.018480000
H	3.301279000	-1.082994000	-4.357790000
H	3.688781000	-2.569460000	-5.242090000
H	5.591342000	-0.005568000	0.870349000
H	3.787694000	0.973377000	3.804825000
H	5.087111000	0.593443000	2.690980000
H	4.880355000	-0.386036000	4.139610000
H	6.351201000	-1.543498000	2.636835000
H	7.349663000	-1.672133000	1.188163000
H	6.162587000	-2.936736000	1.569691000
H	4.001276000	0.448635000	-0.965755000
H	4.453579000	-0.294630000	-2.486264000
H	5.907657000	0.881849000	-3.644116000
H	7.184341000	1.824878000	-2.941498000
H	6.715045000	-2.935077000	-0.839680000
H	7.252021000	-1.315304000	-1.286148000
H	6.256540000	-2.253619000	-2.406149000
H	3.398047000	-4.444020000	-0.441898000
H	4.894863000	-3.969047000	0.371226000
H	4.887062000	-4.212532000	-1.382309000
H	-2.084723000	-5.040199000	-2.567169000
H	-0.680149000	-5.851316000	-3.289166000
H	-1.121934000	-4.210103000	-3.765732000
H	-2.610292000	-5.119561000	-0.473435000
H	-2.157905000	-7.552398000	-0.054187000
H	-0.415495000	-7.245299000	-0.189158000
H	-1.476702000	-6.995115000	-1.577497000
H	-1.151722000	-6.183427000	3.377762000
H	-0.105991000	-6.651651000	2.030865000
H	-1.744034000	-7.329105000	2.166340000
H	-3.575105000	-4.110227000	1.438593000
H	-3.184577000	-4.755370000	3.045275000
H	-3.776082000	-5.837747000	1.775415000
H	-1.170884000	-3.834215000	3.764227000
H	-0.173215000	-1.956963000	5.242130000
H	1.010197000	-4.166560000	5.391485000
H	1.807930000	-2.943620000	6.396011000
H	2.509565000	-3.406979000	4.829327000
H	1.786316000	-0.481093000	6.516758000
H	2.751012000	0.611282000	5.522000000
H	3.246523000	-1.077995000	5.715520000
H	-0.246553000	0.255386000	5.097583000
H	-0.235427000	-0.013611000	3.351978000
H	0.174082000	3.619413000	3.955151000
H	-0.740377000	2.482226000	4.939545000
H	2.591515000	-1.170948000	-1.955725000

1D. NpRdhA/DBMP, Co^{III} (Charge = 1, Multiplicity = 1)

C	3.065540000	7.687582000	-2.534524000
C	6.355525000	4.898666000	1.157835000
C	-6.571715000	-1.379632000	3.445425000
C	-10.161934000	3.005105000	0.319097000
C	0.008059000	5.836930000	2.449612000
C	-4.731049000	-2.376045000	-5.127243000
Co	1.590294000	-2.530719000	0.335880000
C	-1.656435000	2.922223000	-0.365370000
C	-1.373881000	2.205978000	-1.555490000
C	-2.306476000	2.087305000	-2.583970000
C	-3.578872000	2.664088000	-2.494835000
C	-3.874630000	3.396882000	-1.338187000
C	-2.940428000	3.523938000	-0.314296000
O	-0.816085000	2.919946000	0.660529000

Br	0.236945000	-0.545006000	0.212685000
Br	-3.435739000	4.479524000	1.272924000
C	-4.600737000	2.513070000	-3.596169000
H	-4.417907000	1.600846000	-4.174198000
H	-5.614828000	2.459420000	-3.187411000
H	-4.565750000	3.360062000	-4.293021000
H	-2.038485000	1.516401000	-3.470030000
H	-4.853991000	3.850697000	-1.221065000
C	-4.117037000	-2.334198000	-3.751822000
C	-2.967595000	-1.555738000	-3.503104000
C	-2.328152000	-1.588051000	-2.259579000
C	-2.842409000	-2.392488000	-1.229150000
C	-4.018936000	-3.128123000	-1.443482000
C	-4.646988000	-3.101485000	-2.696937000
H	-5.770729000	-2.742043000	-5.101255000
H	-4.156091000	-3.054659000	-5.785653000
H	-4.725706000	-1.380258000	-5.603757000
H	-2.562234000	-0.929165000	-4.305938000
H	-1.424455000	-0.999562000	-2.075440000
H	-2.299115000	-2.447193000	-0.279017000
H	-4.449489000	-3.737157000	-0.641340000
H	-5.555212000	-3.691715000	-2.862656000
C	2.915696000	6.190435000	-2.594439000
C	4.038208000	5.352663000	-2.746031000
C	3.925863000	3.973598000	-2.705687000
C	2.668839000	3.331271000	-2.464534000
C	1.526073000	4.194483000	-2.407356000
C	1.658722000	5.572765000	-2.459370000
O	2.582197000	2.055654000	-2.226912000
H	-0.407376000	1.715807000	-1.632161000
H	3.832972000	8.043609000	-3.230735000
H	3.369754000	8.010356000	-1.528524000
H	2.124580000	8.194077000	-2.770519000
H	5.019590000	5.805378000	-2.880371000
H	4.808556000	3.346969000	-2.786213000
H	0.546672000	3.742548000	-2.284114000
H	0.769571000	6.195879000	-2.376993000
C	4.817315000	4.948157000	1.195556000
C	4.127299000	3.615801000	0.842718000
C	2.603758000	3.756914000	0.848095000
N	1.886805000	2.508047000	0.431519000
H	2.041399000	1.755074000	1.124498000
H	0.831124000	2.658502000	0.437277000
H	2.154093000	2.187822000	-0.544322000
H	6.715034000	4.632983000	0.147478000
H	6.750941000	4.138734000	1.853717000
H	6.785811000	5.878248000	1.428696000
H	4.460309000	5.722222000	0.487890000
H	4.482432000	5.272344000	2.200622000
H	4.454382000	3.296948000	-0.162154000
H	4.439098000	2.825609000	1.551533000
H	2.290871000	4.544839000	0.145084000
H	2.220620000	4.009475000	1.848869000
C	-5.432414000	-2.297501000	2.989407000
C	-4.514383000	-1.686694000	1.923977000
N	-3.713899000	-0.574607000	2.455044000
C	-3.051687000	0.327750000	1.685249000
N	-3.196399000	0.290384000	0.355022000
N	-2.287085000	1.265283000	2.253522000
H	-3.406417000	-0.652390000	3.422887000
H	-2.689875000	0.976503000	-0.220187000
H	-3.425266000	-0.584470000	-0.117721000
H	-2.421400000	1.498673000	3.231982000
H	-1.677735000	1.918898000	1.679549000
H	-7.199062000	-1.878183000	4.203024000
H	-7.215349000	-1.098210000	2.593591000
H	-6.183282000	-0.444536000	3.887009000
H	-5.846872000	-3.226790000	2.557783000
H	-4.817150000	-2.619216000	3.854431000
H	-3.839526000	-2.467326000	1.524314000
H	-5.120822000	-1.299447000	1.086275000
C	-8.906559000	2.224972000	-0.020173000
C	-8.913497000	1.258906000	-1.048259000
C	-7.746072000	0.565979000	-1.401055000
C	-6.541543000	0.823679000	-0.728029000
C	-6.518987000	1.772651000	0.306135000
C	-7.690619000	2.463342000	0.654022000
H	-10.272296000	3.875443000	-0.355254000
H	-10.132671000	3.389070000	1.352641000
H	-11.066214000	2.383485000	0.203323000
H	-9.847886000	1.051441000	-1.583175000
H	-7.774546000	-0.174104000	-2.208898000
H	-5.622943000	0.304917000	-1.021097000
H	-5.582997000	1.990093000	0.831783000
H	-7.657737000	3.208767000	1.457438000
O	-0.097152000	4.440856000	2.702017000
H	0.684391000	6.054008000	1.597662000
H	0.425329000	6.314792000	3.351965000
H	-0.979936000	6.288831000	2.234669000
H	-0.503912000	3.994102000	1.903035000
C	1.883508000	-3.293896000	-5.023646000
C	1.792103000	-2.337264000	-3.824683000
C	0.957234000	-1.083465000	-4.177634000
C	3.241571000	-1.948869000	-3.364806000
C	3.894676000	-0.825870000	-4.172469000

C	3.059330000	-1.641267000	-1.876485000
C	4.126191000	-2.039730000	-0.826018000
C	5.370536000	-1.121241000	-0.565748000
C	5.478397000	-1.151446000	1.001190000
C	4.047129000	-1.405844000	1.418337000
C	3.493539000	-1.117125000	2.710455000
C	4.323196000	-0.253250000	3.637148000
C	6.457390000	-2.154306000	1.639896000
C	5.058337000	0.349044000	-0.965377000
C	6.261621000	1.259961000	-0.747826000
N	6.822112000	1.763688000	-1.883928000
O	6.729207000	1.506155000	0.364082000
C	6.643599000	-1.588483000	-1.281409000
C	4.508963000	-3.522994000	-0.994848000
N	3.331580000	-1.893267000	0.434343000
N	1.894355000	-2.471746000	-1.489675000
C	1.225914000	-2.922117000	-2.519593000
C	0.121095000	-3.828334000	-2.357610000
C	-0.693952000	-4.227248000	-3.567939000
C	-0.231233000	-4.320338000	-1.115315000
N	0.219253000	-3.820040000	0.100472000
C	-1.240641000	-5.435496000	-0.882116000
C	-0.952217000	-6.739397000	-1.644042000
C	-1.277568000	-5.589566000	0.674246000
C	-0.563471000	-6.862389000	1.191824000
C	-2.717775000	-5.571850000	1.211922000
C	-0.453031000	-4.399123000	1.124706000
C	-0.354632000	-3.998857000	2.451395000
C	0.546596000	-3.070920000	2.960443000
N	1.508495000	-2.465801000	2.237368000
C	0.665067000	-2.710539000	4.420234000
C	1.421380000	-3.819583000	5.177648000
C	1.428211000	-1.350814000	4.330824000
C	2.246661000	-1.596387000	3.050752000
C	2.158617000	-1.009538000	5.634148000
C	0.339477000	-0.267525000	4.046489000
C	0.835203000	1.143192000	3.746425000
O	1.784441000	1.342152000	2.982264000
N	0.140003000	2.162671000	4.302681000
H	2.263398000	-4.275636000	-4.721475000
H	2.580398000	-2.875262000	-5.758252000
H	0.926571000	-3.431240000	-5.530990000
H	-0.085977000	-1.358533000	-4.358885000
H	1.344839000	-0.617447000	-5.088831000
H	0.986047000	-0.342745000	-3.371792000
H	3.843423000	-2.861485000	-3.464685000
H	4.962207000	-0.758095000	-3.937758000
H	3.433035000	0.143183000	-3.953867000
H	3.817456000	-1.019469000	-5.247900000
H	5.801715000	-0.156437000	1.318678000
H	3.720431000	0.551105000	4.054828000
H	5.143101000	0.216156000	3.092904000
H	4.761423000	-0.832424000	4.457186000
H	6.411501000	-2.069268000	2.730110000
H	7.481698000	-1.927230000	1.332470000
H	6.235388000	-3.192347000	1.377655000
H	4.237462000	0.731911000	-0.351993000
H	4.720545000	0.414368000	-1.999545000
H	6.410935000	1.617260000	-2.794055000
H	7.605147000	2.399038000	-1.799485000
H	6.929420000	-2.603834000	-0.999621000
H	7.479888000	-0.928573000	-1.032216000
H	6.511752000	-1.562665000	-2.368812000
H	3.604684000	-4.133866000	-1.063346000
H	5.090426000	-3.873271000	-0.140820000
H	5.102045000	-3.675894000	-1.899893000
H	-1.707226000	-4.513693000	-3.276146000
H	-0.248365000	-5.051171000	-4.136110000
H	-0.795256000	-3.376202000	-4.243378000
H	-2.221500000	-5.065240000	-1.209955000
H	-1.666241000	-7.513721000	-1.345641000
H	0.057901000	-7.106525000	-1.444164000
H	-1.053410000	-6.602978000	-2.721067000
H	-0.544100000	-6.850049000	2.286178000
H	0.470192000	-6.915722000	0.837857000
H	-1.090519000	-7.766037000	0.871769000
H	-3.217031000	-4.630452000	0.967587000
H	-2.742168000	-5.701684000	2.299059000
H	-3.292422000	-6.391631000	0.767150000
H	-1.000899000	-4.496965000	3.167795000
H	-0.322036000	-2.573651000	4.878201000
H	0.885536000	-4.768871000	5.081383000
H	1.509239000	-3.584772000	6.242050000
H	2.426366000	-3.953723000	4.763671000
H	1.457262000	-1.119971000	6.469781000
H	2.516599000	0.021129000	5.641736000
H	3.007358000	-1.671122000	5.818669000
H	-0.351940000	-0.262139000	4.900208000
H	-0.231187000	-0.555889000	3.151703000
H	0.221007000	3.113848000	3.905428000
H	-0.599050000	1.980780000	4.966108000
H	2.779825000	-0.591229000	-1.722094000

2A. NpRdhA/DCMP, Co^{II} (Charge = 2, Multiplicity = 2)

C	3.111172000	7.726287000	-1.171983000
C	6.404368000	4.460264000	2.102812000
C	-6.487214000	-2.164915000	3.398524000
C	-10.094830000	2.597627000	0.910011000
C	0.044287000	5.162693000	3.479714000
C	-4.599918000	-1.914854000	-5.218469000
Co	1.697445000	-2.806538000	0.201814000
C	-1.393458000	2.626038000	-0.058047000
C	-1.163730000	1.663162000	-1.071291000
C	-1.637057000	1.794421000	-2.376263000
C	-2.413688000	2.897631000	-2.747003000
C	-2.681896000	3.865209000	-1.769761000
C	-2.183460000	3.727526000	-0.479775000
O	-0.914796000	2.501576000	1.162117000
Cl	-0.232463000	0.229953000	-0.643212000
Cl	-2.510279000	4.970684000	0.708181000
C	-2.984442000	3.016382000	-4.139172000
H	-2.430082000	2.394498000	-4.848259000
H	-4.032662000	2.692724000	-4.156122000
H	-2.954144000	4.050314000	-4.495333000
H	-1.415453000	1.014534000	-3.097131000
H	-3.280995000	4.737470000	-2.013157000
C	-4.655451000	-1.874780000	-3.708881000
C	-3.939677000	-0.903644000	-2.981913000
C	-3.967788000	-0.876497000	-1.580091000
C	-4.728739000	-1.823085000	-0.880353000
C	-5.446061000	-2.801803000	-1.586593000
C	-5.407331000	-2.826452000	-2.987996000
H	-5.995690000	-2.081824000	-5.654767000
H	-3.955174000	-2.745306000	-5.564727000
H	-4.193864000	-0.978081000	-5.634741000
H	-3.366408000	-0.146475000	-3.526917000
H	-3.415928000	-0.100817000	-1.039349000
H	-4.788493000	-1.775926000	0.209146000
H	-6.051855000	-3.537426000	-1.045824000
H	-5.977378000	-3.587413000	-3.532928000
C	2.744111000	6.306139000	-1.524143000
C	3.736502000	5.355739000	-1.807470000
C	3.417795000	4.039971000	-2.133242000
C	2.079028000	3.650518000	-2.179023000
C	1.068289000	4.576203000	-1.920254000
C	1.408906000	5.890809000	-1.594945000
O	1.805638000	2.312242000	-2.433595000
H	0.836856000	2.207522000	-2.482735000
H	3.496477000	8.260879000	-2.048324000
H	3.893145000	7.755036000	-0.404987000
H	2.245619000	8.280284000	-0.798259000
H	4.783340000	5.647514000	-1.769668000
H	4.197552000	3.318805000	-2.351040000
H	0.024836000	4.274859000	-1.968623000
H	0.613383000	6.603155000	-1.389845000
C	4.915407000	4.718375000	1.837776000
C	4.132577000	3.444813000	1.472411000
C	2.648819000	3.747560000	1.286113000
N	1.862079000	2.538073000	0.874345000
H	1.958208000	1.736437000	1.560761000
H	0.820873000	2.700156000	0.891879000
H	2.110745000	2.213612000	-0.072063000
H	6.888342000	4.000655000	1.222901000
H	6.542642000	3.773453000	2.957775000
H	6.933433000	5.399310000	2.337570000
H	4.802919000	5.449039000	1.013573000
H	4.452917000	5.187808000	2.728338000
H	4.554844000	3.002499000	0.551746000
H	4.255932000	2.689318000	2.273064000
H	2.486796000	4.518212000	0.516342000
H	2.190232000	4.086283000	2.225290000
C	-6.776211000	-0.953999000	2.500028000
C	-5.830341000	0.234653000	2.705524000
N	-4.431757000	-0.145977000	2.423896000
C	-3.404083000	0.713731000	2.291091000
N	-3.621817000	2.038852000	2.275311000
N	-2.131582000	0.273740000	2.217298000
H	-4.190464000	-1.127780000	2.551392000
H	-2.826048000	2.645574000	2.043454000
H	-4.560029000	2.405021000	2.116501000
H	-1.950761000	-0.717973000	2.083770000
H	-1.427547000	0.954021000	1.846043000
H	-7.239851000	-2.954562000	3.238433000
H	-6.508993000	-1.888703000	4.467523000
H	-5.500885000	-2.623588000	3.189441000
H	-7.795926000	-0.580156000	2.696871000
H	-6.759001000	-1.243356000	1.433391000
H	-6.120675000	1.043757000	2.013681000
H	-5.902777000	0.616090000	3.742916000
C	-8.640929000	2.440225000	0.507084000
C	-8.212649000	1.322940000	-0.242779000
C	-6.889634000	1.210122000	-0.697133000
C	-5.955588000	2.217970000	-0.406436000
C	-6.357964000	3.328452000	0.356713000
C	-7.683946000	3.431860000	0.812309000
H	-10.660122000	3.099389000	0.102563000
H	-10.200545000	3.212844000	1.818999000
H	-10.573885000	1.620217000	1.088219000
H	-8.935152000	0.536343000	-0.490513000

H	-6.587816000	0.340033000	-1.289269000
H	-4.927946000	2.145969000	-0.780067000
H	-5.645544000	4.134438000	0.572550000
H	-7.988310000	4.310590000	1.392624000
O	0.122879000	3.750800000	3.274169000
H	0.361003000	5.726409000	2.580630000
H	0.721771000	5.415254000	4.311357000
H	-0.980567000	5.479530000	3.751797000
H	-0.433770000	3.480119000	2.496314000
C	0.671264000	-3.467212000	-5.033117000
C	0.948001000	-2.442377000	-3.918559000
C	0.243854000	-1.102238000	-4.228915000
C	2.498065000	-2.257760000	-3.769092000
C	3.133642000	-1.302240000	-4.777701000
C	2.648403000	-1.862886000	-2.299087000
C	3.909151000	-2.221787000	-1.475474000
C	5.136162000	-1.230918000	-1.475198000
C	5.548315000	-1.205765000	0.040217000
C	4.261744000	-1.570351000	0.744158000
C	4.003502000	-1.370327000	2.142927000
C	4.906542000	-0.406008000	2.885965000
C	6.704726000	-2.126985000	0.477241000
C	4.663750000	0.204060000	-1.860158000
C	5.771245000	1.249535000	-1.776197000
N	6.285248000	1.668488000	-2.965276000
O	6.166943000	1.705229000	-0.702160000
C	6.278050000	-1.654396000	-2.406207000
C	4.305135000	-3.688140000	-1.721767000
N	3.394455000	-2.108470000	-0.076599000
N	1.528276000	-2.588140000	-1.641014000
C	0.573363000	-2.888925000	-2.494013000
C	-0.643227000	-3.528472000	-2.083563000
C	-1.724499000	-3.806833000	-3.105667000
C	-0.846029000	-3.921048000	-0.776371000
N	0.006589000	-3.679354000	0.296818000
C	-1.996730000	-4.805546000	-0.323510000
C	-1.779903000	-6.241816000	-0.842343000
C	-1.950587000	-4.670174000	1.223239000
C	-2.315231000	-5.935940000	2.009088000
C	-2.886245000	-3.513558000	1.657453000
C	-0.527326000	-4.187513000	1.437117000
C	0.095510000	-4.167306000	2.678212000
C	1.275708000	-3.497473000	2.969139000
N	2.010761000	-2.801087000	2.071933000
C	1.887601000	-3.386516000	4.340297000
C	2.903647000	-4.520660000	4.574158000
C	2.521676000	-1.962016000	4.226785000
C	2.934680000	-1.991741000	2.745559000
C	3.606153000	-1.722929000	5.282932000
C	1.324048000	-0.974477000	4.458442000
C	1.404109000	0.399689000	3.821556000
O	1.657947000	0.488998000	2.605050000
N	1.115616000	1.465135000	4.588777000
H	0.948273000	-4.479220000	-4.720964000
H	1.275946000	-3.208614000	-5.909393000
H	-0.371853000	-3.473357000	-5.353428000
H	-0.842752000	-1.214024000	-4.173883000
H	0.498000000	-0.767505000	-5.239344000
H	0.540956000	-0.324931000	-3.518509000
H	2.933052000	-3.256150000	-3.903258000
H	4.225406000	-1.343851000	-4.717495000
H	2.819531000	-0.267169000	-4.607134000
H	2.859854000	-1.574891000	-5.801816000
H	5.843707000	-0.183120000	0.291228000
H	4.318639000	0.266966000	3.513023000
H	5.458934000	0.220065000	2.183457000
H	5.639848000	-0.910102000	3.523669000
H	6.875276000	-2.018342000	1.552235000
H	7.629403000	-1.846520000	-0.033541000
H	6.501650000	-3.182756000	0.278040000
H	3.875996000	0.527709000	-1.172039000
H	4.238225000	0.197055000	-2.866279000
H	5.991878000	1.281461000	-3.850520000
H	7.052809000	2.328947000	-2.958781000
H	6.654534000	-2.651503000	-2.171840000
H	7.117485000	-0.957841000	-2.319659000
H	5.954877000	-1.655539000	-3.452666000
H	3.423819000	-4.329732000	-1.613880000
H	5.052509000	-4.016172000	-0.997274000
H	4.712192000	-3.830250000	-2.725819000
H	-2.696238000	-3.937012000	-2.628424000
H	-1.515314000	-4.701596000	-3.702214000
H	-1.831945000	-2.968689000	-3.795353000
H	-2.953346000	-4.431511000	-0.703352000
H	-2.586961000	-6.902261000	-0.513834000
H	-0.828736000	-6.648391000	-0.483514000
H	-1.760460000	-6.252319000	-1.934369000
H	-2.321028000	-5.734672000	3.085265000
H	-1.614322000	-6.752427000	1.820519000
H	-3.320358000	-6.272609000	1.736074000
H	-2.678320000	-2.617918000	1.060661000
H	-2.748018000	-3.291387000	2.722507000
H	-3.930678000	-3.796261000	1.488819000
H	-0.409180000	-4.658077000	3.503377000
H	1.126761000	-3.412110000	5.128433000

H	2.402397000	-5.490687000	4.510955000
H	3.358704000	-4.438047000	5.564869000
H	3.697386000	-4.494752000	3.820333000
H	3.223715000	-2.039837000	6.259713000
H	3.878915000	-0.669319000	5.365282000
H	4.510750000	-2.297778000	5.073726000
H	1.148446000	-0.910161000	5.537837000
H	0.422930000	-1.417470000	4.012169000
H	0.875469000	2.373481000	4.155372000
H	0.866177000	1.330036000	5.559081000
H	2.442771000	-0.792764000	-2.174656000

2B. NpRdhA/DCMP, Co^I (Charge = 1, Multiplicity = 1)

C	3.771046000	7.438651000	-2.150048000
C	6.596248000	4.258353000	1.610062000
C	-6.993244000	-0.685864000	3.230348000
C	-9.977384000	4.102677000	0.059071000
C	0.329501000	5.826102000	2.663556000
C	-4.900861000	-1.714085000	-5.280349000
Co	1.132021000	-2.620616000	0.430163000
C	-0.925349000	2.551894000	-0.489718000
C	-0.603507000	1.452060000	-1.322823000
C	-0.926983000	1.404531000	-2.675898000
C	-1.630849000	2.449299000	-3.286542000
C	-1.985794000	3.544871000	-2.493186000
C	-1.635633000	3.586172000	-1.146624000
O	-0.603713000	2.600559000	0.793205000
Cl	0.193196000	0.028736000	-0.587297000
Cl	-2.063312000	5.001328000	-0.198019000
C	-2.037025000	2.360398000	-4.737529000
H	-1.246201000	1.905165000	-5.342593000
H	-2.936268000	1.740858000	-4.848012000
H	-2.257770000	3.348586000	-5.150512000
H	-0.650849000	0.528217000	-3.253436000
H	-2.531227000	4.380155000	-2.921889000
C	-4.495373000	-1.619939000	-3.827689000
C	-3.151727000	-1.376483000	-3.480438000
C	-2.738659000	-1.356811000	-2.143785000
C	-3.675258000	-1.554901000	-1.120786000
C	-5.021293000	-1.779243000	-1.444117000
C	-5.426130000	-1.813398000	-2.787727000
H	-5.991668000	-1.616798000	-5.407950000
H	-4.600775000	-2.691001000	-5.704387000
H	-4.410549000	-0.932050000	-5.886443000
H	-2.416345000	-1.215971000	-4.276965000
H	-1.687612000	-1.209917000	-1.890025000
H	-3.338150000	-1.556509000	-0.080961000
H	-5.763238000	-1.945040000	-0.653795000
H	-6.477968000	-1.998473000	-3.033531000
C	3.413600000	5.971151000	-2.161668000
C	4.408439000	4.983567000	-2.110261000
C	4.096804000	3.626326000	-2.142167000
C	2.760420000	3.233537000	-2.224583000
C	1.749586000	4.192878000	-2.290856000
C	2.083248000	5.547374000	-2.254331000
O	2.483219000	1.876700000	-2.195338000
H	1.519252000	1.759361000	-2.302668000
H	4.160467000	7.756168000	-3.125341000
H	4.544690000	7.654212000	-1.404959000
H	2.897869000	8.057775000	-1.923936000
H	5.452611000	5.280013000	-2.039492000
H	4.877910000	2.874709000	-2.097514000
H	0.710075000	3.884504000	-2.363632000
H	1.285514000	6.285387000	-2.299844000
C	5.081652000	4.488413000	1.565175000
C	4.298457000	3.173435000	1.443447000
C	2.802454000	3.406941000	1.280323000
N	2.072240000	2.120679000	1.037720000
H	2.151544000	1.508946000	1.880935000
H	1.026293000	2.287658000	0.920992000
H	2.409900000	1.630480000	0.196063000
H	6.941052000	3.731017000	0.703534000
H	6.878029000	3.633767000	2.476712000
H	7.143293000	5.213938000	1.689376000
H	4.828231000	5.133903000	0.701952000
H	4.750334000	5.034194000	2.470099000
H	4.682972000	2.605171000	0.577466000
H	4.476693000	2.543488000	2.334929000
H	2.588691000	4.065627000	0.422366000
H	2.346398000	3.835873000	2.184340000
C	-5.578964000	-1.182026000	3.558819000
C	-4.586302000	-1.016005000	2.399724000
N	-4.400243000	0.394038000	2.040854000
C	-3.229935000	1.034529000	1.864916000
N	-2.051728000	0.381967000	1.847759000
N	-3.205546000	2.373389000	1.760504000
H	-5.245903000	0.946267000	1.886348000
H	-1.239686000	0.950048000	1.542752000
H	-2.007822000	-0.618585000	1.656729000
H	-4.067358000	2.910620000	1.703744000
H	-2.308389000	2.808109000	1.475228000
H	-7.680686000	-0.878180000	4.070714000
H	-7.398425000	-1.197023000	2.338169000
H	-7.022249000	0.402452000	3.035660000

H	-5.610497000	-2.258919000	3.805294000
H	-5.183883000	-0.661297000	4.450887000
H	-3.607392000	-1.441701000	2.673609000
H	-4.949475000	-1.569996000	1.516749000
C	-8.598365000	3.472753000	-0.032238000
C	-8.438661000	2.070889000	-0.070393000
C	-7.173930000	1.486152000	-0.243384000
C	-6.031168000	2.294271000	-0.374988000
C	-6.168517000	3.691469000	-0.305227000
C	-7.437243000	4.268629000	-0.134079000
H	-10.399836000	4.244940000	-0.953390000
H	-9.938389000	5.092467000	0.543881000
H	-10.677325000	3.463076000	0.622613000
H	-9.322535000	1.427801000	0.015152000
H	-7.081850000	0.395840000	-0.308359000
H	-5.051888000	1.841308000	-0.570585000
H	-5.287422000	4.335364000	-0.414465000
H	-7.531007000	5.360298000	-0.098275000
O	-0.056698000	4.460164000	2.744272000
H	1.223754000	5.970734000	2.024499000
H	0.575728000	6.156864000	3.685490000
H	-0.486366000	6.464989000	2.272443000
H	-0.301408000	4.080767000	1.863027000
C	1.422730000	-4.239413000	-4.712263000
C	1.453887000	-3.058693000	-3.726559000
C	0.904471000	-1.778412000	-4.394756000
C	2.923128000	-2.853069000	-3.230072000
C	3.820585000	-2.066860000	-4.186387000
C	2.727079000	-2.239342000	-1.843016000
C	3.705028000	-2.542334000	-0.690300000
C	5.023002000	-1.699672000	-0.551230000
C	5.107534000	-1.476780000	0.998531000
C	3.654292000	-1.580937000	1.426439000
C	3.149080000	-1.161881000	2.697098000
C	4.100157000	-0.380282000	3.584856000
C	6.028966000	-2.429596000	1.784750000
C	4.838556000	-0.307006000	-1.221106000
C	6.081722000	0.567833000	-1.148936000
N	6.722465000	0.767517000	-2.339030000
O	6.487430000	1.084368000	-0.107977000
C	6.263650000	-2.382547000	-1.141450000
C	3.954433000	-4.059524000	-0.595236000
N	2.895562000	-2.129033000	0.495436000
N	1.435892000	-2.798197000	-1.373875000
C	0.731369000	-3.276166000	-2.386038000
C	-0.540183000	-3.890133000	-2.185913000
C	-1.366413000	-4.304170000	-3.386769000
C	-1.056854000	-4.073057000	-0.916127000
N	-0.538255000	-3.518528000	0.253166000
C	-2.334067000	-4.854329000	-0.622720000
C	-2.434489000	-6.261576000	-1.235621000
C	-2.415329000	-4.850381000	0.934556000
C	-1.980350000	-6.191049000	1.578721000
C	-3.831073000	-4.506566000	1.420736000
C	-1.355496000	-3.825428000	1.297066000
C	-1.136061000	-3.413757000	2.605808000
C	-0.030321000	-2.713985000	3.064617000
N	0.976294000	-2.238820000	2.283281000
C	0.300200000	-2.538709000	4.524402000
C	1.016064000	-3.797348000	5.051063000
C	1.193447000	-1.265250000	4.462108000
C	1.865521000	-1.501732000	3.086962000
C	2.086935000	-1.120546000	5.699372000
C	0.159310000	-0.108377000	4.431918000
C	0.625825000	1.303827000	4.136995000
O	1.729881000	1.568046000	3.636383000
N	-0.268495000	2.274755000	4.420457000
H	1.584077000	-5.188167000	-4.190469000
H	2.226198000	-4.116830000	-5.448275000
H	0.485979000	-4.306345000	-5.268669000
H	-0.165830000	-1.878680000	-4.597175000
H	1.408115000	-1.584096000	-5.347812000
H	1.046122000	-0.908522000	-3.744646000
H	3.341274000	-3.859419000	-3.104449000
H	4.866091000	-2.110577000	-3.865292000
H	3.524703000	-1.013564000	-4.243847000
H	3.779344000	-2.484791000	-5.198231000
H	5.485965000	-0.464461000	1.170353000
H	3.582285000	0.429174000	4.094602000
H	4.895194000	0.069275000	2.986026000
H	4.582989000	-1.014276000	4.337144000
H	5.999114000	-2.179427000	2.848459000
H	7.065482000	-2.325443000	1.450133000
H	5.733529000	-3.477425000	1.683700000
H	4.027507000	0.229253000	-0.719693000
H	4.542386000	-0.424406000	-2.264735000
H	6.435999000	0.300900000	-3.187225000
H	7.592096000	1.285161000	-2.340795000
H	6.455191000	-3.355093000	-0.684924000
H	7.153252000	-1.764065000	-0.983914000
H	6.150607000	-2.536518000	-2.220133000
H	2.992833000	-4.579520000	-0.603373000
H	4.461010000	-4.306694000	0.339023000
H	4.564535000	-4.422532000	-1.427126000
H	-2.432261000	-4.267936000	-3.152570000

H	-1.126677000	-5.308409000	-3.754330000
H	-1.211111000	-3.609729000	-4.214477000
H	-3.178620000	-4.261371000	-1.006017000
H	-3.303375000	-6.783287000	-0.820325000
H	-1.542456000	-6.857112000	-1.022358000
H	-2.567165000	-6.230985000	-2.316672000
H	-1.971326000	-6.085545000	2.668319000
H	-0.971914000	-6.474450000	1.262623000
H	-2.670243000	-7.001399000	1.323679000
H	-4.183125000	-3.576876000	0.966269000
H	-3.867644000	-4.402886000	2.511348000
H	-4.529741000	-5.303546000	1.140341000
H	-1.831506000	-3.770337000	3.361146000
H	-0.594148000	-2.356877000	5.133581000
H	0.365265000	-4.669487000	4.935656000
H	1.270034000	-3.697912000	6.110983000
H	1.935606000	-3.983209000	4.485977000
H	1.472415000	-1.266265000	6.596281000
H	2.535485000	-0.128257000	5.764387000
H	2.886103000	-1.864746000	5.715265000
H	-0.365729000	-0.106493000	5.397304000
H	-0.604150000	-0.338331000	3.677878000
H	-0.139443000	3.203570000	3.991556000
H	-1.188618000	2.026146000	4.756408000
H	2.596754000	-1.152305000	-1.915035000

2C. NpRdhA/DCMP, Co^I → Co^{III} Transition State (Charge = 1, Multiplicity = 1)

C	3.489726000	7.396796000	-2.945973000
C	6.626146000	4.564186000	0.845344000
C	-6.692857000	-0.585823000	3.643859000
C	-9.999033000	3.888545000	0.336225000
C	0.390946000	6.048147000	2.171985000
C	-5.084931000	-2.167849000	-4.887295000
Co	1.302934000	-2.514615000	0.488897000
C	-1.008507000	2.584828000	-0.224530000
C	-0.506931000	1.697444000	-1.215868000
C	-1.240590000	1.444169000	-2.381411000
C	-2.401099000	2.151289000	-2.703469000
C	-2.823338000	3.140189000	-1.799149000
C	-2.140896000	3.350574000	-0.607952000
O	-0.449404000	2.712821000	0.969055000
Cl	0.375504000	-0.441376000	-0.134072000
Cl	-2.690035000	4.653633000	0.455031000
C	-3.164728000	1.908793000	-3.983634000
H	-2.537198000	1.403528000	-4.724229000
H	-4.044719000	1.276236000	-3.805448000
H	-3.518453000	2.847205000	-4.422732000
H	-0.838571000	0.737971000	-3.106182000
H	-3.686183000	3.758134000	-2.029690000
C	-4.555154000	-2.158033000	-3.470101000
C	-3.295858000	-1.594727000	-3.175874000
C	-2.758398000	-1.645372000	-1.882759000
C	-3.489120000	-2.258142000	-0.852745000
C	-4.759255000	-2.795823000	-1.116513000
C	-5.285479000	-2.743911000	-2.415569000
H	-6.173082000	-2.342426000	-4.914315000
H	-4.603193000	-2.972495000	-5.474305000
H	-4.871875000	-1.215420000	-5.403282000
H	-2.721808000	-1.118503000	-3.977766000
H	-1.768036000	-1.228970000	-1.672693000
H	-3.046191000	-2.354254000	0.144620000
H	-5.334975000	-3.271304000	-0.314307000
H	-6.272272000	-3.175220000	-2.619178000
C	3.081353000	5.959598000	-2.681948000
C	4.027358000	4.925122000	-2.644238000
C	3.660078000	3.601424000	-2.410771000
C	2.315718000	3.244719000	-2.196187000
C	1.353228000	4.270620000	-2.266709000
C	1.742127000	5.592849000	-2.495558000
O	2.022809000	1.951205000	-1.891130000
H	0.844711000	1.782233000	-1.528858000
H	3.599055000	7.587379000	-4.021388000
H	4.449831000	7.628919000	-2.472650000
H	2.741351000	8.096796000	-2.561320000
H	5.081350000	5.158577000	-2.787166000
H	4.418633000	2.826539000	-2.374461000
H	0.302607000	4.039023000	-2.128756000
H	0.971254000	6.361054000	-2.527697000
C	5.108985000	4.706077000	1.017097000
C	4.389679000	3.349766000	1.018569000
C	2.874443000	3.492324000	1.107273000
N	2.185917000	2.183683000	0.876245000
H	2.459032000	1.485276000	1.583258000
H	1.123713000	2.298013000	0.956059000
H	2.349126000	1.839025000	-0.099616000
H	6.869438000	4.052808000	-0.102694000
H	7.066690000	3.963014000	1.661150000
H	7.122030000	5.550561000	0.844676000
H	4.697826000	5.321443000	0.193684000
H	4.881381000	5.246651000	1.956568000
H	4.650140000	2.810089000	0.091028000
H	4.756339000	2.728941000	1.857906000
H	2.499935000	4.176826000	0.329532000
H	2.543505000	3.853542000	2.091669000

C	-5.831796000	-1.055875000	2.460318000
C	-5.540354000	0.044535000	1.424289000
N	-4.658352000	1.115101000	1.916957000
C	-3.310679000	1.138993000	1.852454000
N	-2.641567000	0.148282000	1.235225000
N	-2.609541000	2.112389000	2.467822000
H	-5.109794000	1.944606000	2.296367000
H	-1.634296000	0.246871000	1.043024000
H	-3.135199000	-0.434689000	0.559376000
H	-3.138321000	2.924050000	2.785464000
H	-1.684369000	2.374013000	2.010888000
H	-6.880745000	-1.411571000	4.350356000
H	-7.670022000	-0.206234000	3.295305000
H	-6.193117000	0.225203000	4.204606000
H	-6.348984000	-1.873818000	1.924505000
H	-4.872614000	-1.475890000	2.819225000
H	-5.099733000	-0.386608000	0.508613000
H	-6.471949000	0.535587000	1.099774000
C	-8.706532000	3.248049000	-0.128162000
C	-8.718101000	2.084022000	-0.925720000
C	-7.526920000	1.527101000	-1.415893000
C	-6.292149000	2.122503000	-1.113829000
C	-6.260964000	3.270377000	-0.305961000
C	-7.456288000	3.822991000	0.181090000
H	-10.401239000	4.556843000	-0.448436000
H	-9.846884000	4.497870000	1.242917000
H	-10.772887000	3.131483000	0.549808000
H	-9.677129000	1.615004000	-1.175872000
H	-7.562388000	0.625982000	-2.038769000
H	-5.359936000	1.693216000	-1.496841000
H	-5.303979000	3.745644000	-0.063801000
H	-7.420360000	4.728535000	0.798714000
O	0.055132000	4.749400000	2.641473000
H	1.290220000	6.040760000	1.523249000
H	0.605287000	6.677952000	3.051320000
H	-0.442825000	6.507118000	1.604764000
H	-0.192244000	4.158384000	1.879521000
C	1.240537000	-4.252022000	-4.651856000
C	1.317842000	-3.089556000	-3.650307000
C	0.613087000	-1.830487000	-4.206045000
C	2.818078000	-2.799828000	-3.302243000
C	3.565959000	-1.967394000	-4.343205000
C	2.719841000	-2.180540000	-1.905845000
C	3.807576000	-2.399402000	-0.831198000
C	5.084522000	-1.488362000	-0.813463000
C	5.265834000	-1.207420000	0.722961000
C	3.856571000	-1.362117000	1.257013000
C	3.409199000	-0.885118000	2.539887000
C	4.379435000	-0.029156000	3.329542000
C	6.285980000	-2.079869000	1.478573000
C	4.789566000	-0.129737000	-1.511740000
C	6.012237000	0.781606000	-1.558805000
N	6.442496000	1.112414000	-2.810790000
O	6.594051000	1.183344000	-0.551858000
C	6.312499000	-2.132826000	-1.469395000
C	4.138499000	-3.899367000	-0.710627000
N	3.076522000	-1.982060000	0.406527000
N	1.519084000	-2.827588000	-1.327643000
C	0.748823000	-3.355110000	-2.247636000
C	-0.457585000	-4.053573000	-1.914096000
C	-1.374638000	-4.541467000	-3.016033000
C	-0.812736000	-4.270639000	-0.597173000
N	-0.245785000	-3.637820000	0.503620000
C	-1.921190000	-5.219116000	-0.160292000
C	-1.781032000	-6.652657000	-0.701524000
C	-1.915120000	-5.111897000	1.398619000
C	-1.390230000	-6.380326000	2.113839000
C	-3.313297000	-4.780864000	1.953448000
C	-0.905698000	-4.003003000	1.631434000
C	-0.636309000	-3.493753000	2.891531000
C	0.393966000	-2.624210000	3.216764000
N	1.304517000	-2.128834000	2.351342000
C	0.724003000	-2.225781000	4.628311000
C	1.541263000	-3.345116000	5.304371000
C	1.514089000	-0.905107000	4.385829000
C	2.172643000	-1.255655000	3.030384000
C	2.401005000	-0.550849000	5.585489000
C	0.420193000	0.188320000	4.180193000
C	0.903389000	1.624713000	4.031779000
O	2.031197000	1.902994000	3.608927000
N	0.012821000	2.580840000	4.380213000
H	1.513617000	-5.201044000	-4.178799000
H	1.945924000	-4.068025000	-5.470005000
H	0.250926000	-4.358441000	-5.099901000
H	-0.462763000	-2.004935000	-4.295212000
H	0.996244000	-1.581715000	-5.200877000
H	0.761927000	-0.970009000	-3.545544000
H	3.302974000	-3.780885000	-3.216870000
H	4.637928000	-1.940915000	-4.125130000
H	3.195740000	-0.937230000	-4.373522000
H	3.452699000	-2.397626000	-5.343946000
H	5.599882000	-0.171372000	0.828881000
H	3.861562000	0.797753000	3.809167000
H	5.141592000	0.395349000	2.673847000
H	4.899216000	-0.612591000	4.097841000

H	6.311324000	-1.795530000	2.533893000
H	7.288317000	-1.924799000	1.070578000
H	6.048790000	-3.146150000	1.427626000
H	3.992326000	0.404419000	-0.983952000
H	4.425662000	-0.301161000	-2.526193000
H	5.911629000	0.881571000	-3.637987000
H	7.207492000	1.769615000	-2.898104000
H	6.583139000	-3.080110000	-0.999596000
H	7.176145000	-1.465660000	-1.391507000
H	6.133095000	-2.322158000	-2.533157000
H	3.211829000	-4.471632000	-0.611485000
H	4.751710000	-4.091797000	0.171352000
H	4.678903000	-4.257797000	-1.590620000
H	-2.397028000	-4.650086000	-2.646765000
H	-1.060847000	-5.495130000	-3.454414000
H	-1.417350000	-3.806762000	-3.822832000
H	-2.873750000	-4.816159000	-0.528995000
H	-2.559849000	-7.292535000	-0.274901000
H	-0.807070000	-7.081770000	-0.452149000
H	-1.893750000	-6.683531000	-1.785481000
H	-1.338436000	-6.196675000	3.191410000
H	-0.387157000	-6.651296000	1.772419000
H	-2.058576000	-7.230760000	1.949345000
H	-3.690872000	-3.835344000	1.555253000
H	-3.299816000	-4.708329000	3.046030000
H	-4.017743000	-5.574552000	1.680438000
H	-1.245787000	-3.852717000	3.715132000
H	-0.180283000	-2.038974000	5.218537000
H	0.962924000	-4.274065000	5.314027000
H	1.787174000	-3.084756000	6.337497000
H	2.472653000	-3.529955000	4.758376000
H	1.792869000	-0.609820000	6.496263000
H	2.797499000	0.461239000	5.516443000
H	3.236095000	-1.246035000	5.695454000
H	-0.278283000	0.132438000	5.024901000
H	-0.159630000	-0.045248000	3.276557000
H	0.156971000	3.528143000	3.999369000
H	-0.942611000	2.307643000	4.569106000
H	2.499922000	-1.107031000	-1.967194000

2D. NpRdhA/DCMP, Co^{III} (Charge = 1, Multiplicity = 1)

C	2.702132000	7.845233000	-2.101449000
C	6.212818000	4.923418000	1.270919000
C	-6.456406000	-1.803485000	3.718372000
C	-10.278293000	2.668945000	1.020584000
C	-0.091000000	5.623031000	2.886035000
C	-4.972181000	-2.237659000	-4.969415000
Co	1.584936000	-2.560582000	0.200498000
C	-1.694211000	2.812446000	-0.182785000
C	-1.423505000	1.999925000	-1.305919000
C	-2.110635000	2.146077000	-2.505509000
C	-3.121606000	3.101975000	-2.664588000
C	-3.394877000	3.934689000	-1.573947000
C	-2.700313000	3.789859000	-0.376473000
O	-1.051350000	2.643095000	0.971499000
Cl	0.387494000	-0.633160000	0.326356000
Cl	-3.068000000	4.900282000	0.943886000
C	-3.909640000	3.221602000	-3.947255000
H	-3.371201000	2.763150000	-4.782788000
H	-4.883301000	2.720329000	-3.862118000
H	-4.104687000	4.268179000	-4.203304000
H	-1.845418000	1.506422000	-3.344561000
H	-4.156654000	4.705638000	-1.650115000
C	-4.428696000	-2.239330000	-3.555920000
C	-3.333097000	-1.426799000	-3.195370000
C	-2.747799000	-1.512218000	-1.923495000
C	-3.275719000	-2.399545000	-0.972235000
C	-4.405759000	-3.171049000	-1.291912000
C	-4.969973000	-3.094708000	-2.573500000
H	-6.016008000	-2.590818000	-5.004837000
H	-4.371313000	-2.910376000	-5.610547000
H	-4.928006000	-1.230921000	-5.419034000
H	-2.916756000	-0.730948000	-3.932464000
H	-1.871283000	-0.905604000	-1.675805000
H	-2.778927000	-2.522386000	-0.001447000
H	-4.838938000	-3.851475000	-0.550607000
H	-5.836560000	-3.718366000	-2.821066000
C	2.600561000	6.342514000	-2.160784000
C	3.738895000	5.547718000	-2.403208000
C	3.678464000	4.165185000	-2.379245000
C	2.464373000	3.473961000	-2.067867000
C	1.299574000	4.292391000	-1.912079000
C	1.380483000	5.676429000	-1.944387000
O	2.439097000	2.189688000	-1.857129000
H	-0.628896000	1.265097000	-1.210297000
H	3.318569000	8.239385000	-2.917614000
H	3.169711000	8.170263000	-1.161412000
H	1.715447000	8.314588000	-2.159545000
H	4.692300000	6.037074000	-2.597140000
H	4.574794000	3.572264000	-2.533578000
H	0.348377000	3.798425000	-1.738323000
H	0.477077000	6.264028000	-1.787872000
C	4.683826000	4.897887000	1.471008000
C	4.007914000	3.555192000	1.121367000

C	2.484406000	3.639449000	1.266469000
N	1.774116000	2.401661000	0.799211000
H	1.990518000	1.602497000	1.421783000
H	0.723036000	2.508481000	0.854188000
H	2.006669000	2.169377000	-0.217448000
H	6.469660000	4.733953000	0.212840000
H	6.711883000	4.146468000	1.874893000
H	6.626228000	5.907103000	1.552456000
H	4.224939000	5.688947000	0.845747000
H	4.445795000	5.158092000	2.521110000
H	4.252172000	3.291055000	0.077862000
H	4.407475000	2.747672000	1.762916000
H	2.091122000	4.468285000	0.656652000
H	2.179887000	3.797922000	2.311751000
C	-5.546602000	-1.918113000	2.483668000
C	-5.581208000	-0.693981000	1.548897000
N	-4.954672000	0.518702000	2.104245000
C	-3.652043000	0.855894000	1.985455000
N	-2.774430000	0.015122000	1.404589000
N	-3.174401000	1.996530000	2.511556000
H	-5.585434000	1.265028000	2.391751000
H	-1.828269000	0.363045000	1.204064000
H	-3.112369000	-0.716061000	0.781326000
H	-3.838280000	2.706931000	2.813990000
H	-2.281722000	2.362280000	2.061350000
H	-6.389621000	-2.709212000	4.344149000
H	-7.511986000	-1.671779000	3.420173000
H	-6.169990000	-0.939505000	4.345234000
H	-5.852525000	-2.791045000	1.876389000
H	-4.499587000	-2.106569000	2.790231000
H	-5.104391000	-0.931811000	0.580600000
H	-6.619997000	-0.417113000	1.307423000
C	-8.877829000	2.396927000	0.505551000
C	-8.629072000	1.350292000	-0.407549000
C	-7.349190000	1.143456000	-0.947254000
C	-6.283008000	1.979737000	-0.581520000
C	-6.509495000	3.017091000	0.338467000
C	-7.790747000	3.216783000	0.878479000
H	-10.819821000	3.337283000	0.324844000
H	-10.259164000	3.164380000	2.005950000
H	-10.866141000	1.739389000	1.107752000
H	-9.455648000	0.697084000	-0.711918000
H	-7.184062000	0.327608000	-1.660553000
H	-5.285599000	1.836575000	-1.011463000
H	-5.686055000	3.683624000	0.620261000
H	-7.957642000	4.040118000	1.583557000
O	-0.246762000	4.211381000	2.943497000
H	0.540401000	5.937227000	2.030461000
H	0.404919000	5.943479000	3.817579000
H	-1.064510000	6.145507000	2.807187000
H	-0.645744000	3.855173000	2.098876000
C	1.619445000	-2.646003000	-5.220740000
C	1.603083000	-1.858357000	-3.901237000
C	0.764888000	-0.563736000	-4.039791000
C	3.079039000	-1.543401000	-3.469356000
C	3.704986000	-0.332081000	-4.162453000
C	2.967904000	-1.422769000	-1.946522000
C	4.079558000	-1.930429000	-0.990849000
C	5.323324000	-1.030421000	-0.663093000
C	5.479569000	-1.234082000	0.887166000
C	4.061622000	-1.538889000	1.313341000
C	3.529478000	-1.360751000	2.636733000
C	4.376225000	-0.584309000	3.621171000
C	6.472938000	-2.301470000	1.383340000
C	4.983757000	0.470525000	-0.885518000
C	6.172333000	1.377673000	-0.585786000
N	6.698909000	2.023101000	-1.664799000
O	6.652717000	1.510515000	0.540068000
C	6.578270000	-1.393648000	-1.465515000
C	4.468857000	-3.377100000	-1.348194000
N	3.329292000	-1.941031000	0.304256000
N	1.822539000	-2.302243000	-1.616227000
C	1.092295000	-2.604577000	-2.657956000
C	-0.023299000	-3.506952000	-2.556642000
C	-0.888339000	-3.757786000	-3.771243000
C	-0.329982000	-4.144116000	-1.368143000
N	0.185611000	-3.803055000	-0.125042000
C	-1.336870000	-5.278380000	-1.224672000
C	-1.126573000	-6.469749000	-2.173249000
C	-1.267891000	-5.648363000	0.293764000
C	-0.497508000	-6.962060000	0.577287000
C	-2.667019000	-5.742626000	0.924364000
C	-0.428468000	-4.516317000	0.851698000
C	-0.267889000	-4.280620000	2.210263000
C	0.630925000	-3.385127000	2.780791000
N	1.560814000	-2.699417000	2.091589000
C	0.764371000	-3.124850000	4.259850000
C	1.592285000	-4.239056000	4.929038000
C	1.458435000	-1.724817000	4.243772000
C	2.288466000	-1.870041000	2.955826000
C	2.159370000	-1.407824000	5.567910000
C	0.315278000	-0.691809000	3.988488000
C	0.736257000	0.764286000	3.805295000
O	1.831926000	1.079989000	3.321945000
N	-0.178163000	1.685140000	4.176562000

H	2.000331000	-3.662331000	-5.074074000
H	2.283534000	-2.136972000	-5.928005000
H	0.636169000	-2.706170000	-5.691093000
H	-0.294041000	-0.808887000	-4.170301000
H	1.088847000	0.003607000	-4.918065000
H	0.865532000	0.080565000	-3.160543000
H	3.662536000	-2.441621000	-3.709447000
H	4.784137000	-0.299951000	-3.977962000
H	3.265302000	0.603190000	-3.799184000
H	3.569625000	-0.387066000	-5.248163000
H	5.812444000	-0.280802000	1.305869000
H	3.768807000	0.140332000	4.157797000
H	5.157575000	-0.026162000	3.103541000
H	4.866586000	-1.245807000	4.344698000
H	6.472511000	-2.321047000	2.477654000
H	7.486696000	-2.053974000	1.056594000
H	6.227821000	-3.307991000	1.032959000
H	4.168699000	0.770086000	-0.220700000
H	4.625260000	0.645791000	-1.899881000
H	6.279940000	1.963851000	-2.581008000
H	7.465070000	2.667773000	-1.519333000
H	6.880223000	-2.432457000	-1.317724000
H	7.416784000	-0.759252000	-1.162398000
H	6.414063000	-1.236968000	-2.537474000
H	3.568181000	-3.990983000	-1.437364000
H	5.100930000	-3.812817000	-0.573039000
H	5.012641000	-3.415343000	-2.295512000
H	-1.886457000	-4.085978000	-3.474304000
H	-0.465150000	-4.503273000	-4.453756000
H	-1.019473000	-2.832397000	-4.334955000
H	-2.332418000	-4.860888000	-1.424314000
H	-1.817237000	-7.278215000	-1.912840000
H	-0.105720000	-6.856806000	-2.114505000
H	-1.324106000	-6.198647000	-3.210569000
H	-0.403862000	-7.101151000	1.658916000
H	0.510216000	-6.937275000	0.152136000
H	-1.029109000	-7.826594000	0.168672000
H	-3.190003000	-4.783957000	0.872782000
H	-2.611551000	-6.048083000	1.974554000
H	-3.264607000	-6.491765000	0.393181000
H	-0.878606000	-4.864099000	2.892209000
H	-0.218479000	-3.067673000	4.741876000
H	1.107409000	-5.208372000	4.777063000
H	1.683941000	-4.069408000	6.005496000
H	2.596943000	-4.289434000	4.495686000
H	1.458090000	-1.596154000	6.389544000
H	2.458889000	-0.360459000	5.624411000
H	3.041464000	-2.030976000	5.729184000
H	-0.398625000	-0.771239000	4.818502000
H	-0.219476000	-0.966191000	3.068496000
H	-0.062457000	2.669978000	3.892802000
H	-1.104751000	1.394674000	4.457513000
H	2.689484000	-0.401042000	-1.657725000

3A. PccA/TCE, Co^{II} (Charge = 2, Multiplicity = 2)

Co	0.647996000	-2.232535000	-1.444288000
C	-1.664623000	-3.757968000	-0.866276000
C	-3.232620000	-3.616792000	-0.965339000
C	-3.398072000	-2.817196000	-2.312142000
C	-2.077026000	-2.089043000	-2.447117000
C	-1.832690000	-0.984029000	-3.336258000
C	-0.544896000	-0.542459000	-3.562014000
C	-0.055128000	0.584554000	-4.493454000
C	1.305249000	-0.035374000	-4.942366000
C	1.699435000	-0.753178000	-3.679468000
C	3.007097000	-0.999085000	-3.298140000
C	3.404059000	-1.664190000	-2.144387000
C	4.845586000	-1.754106000	-1.686493000
C	4.748799000	-2.855350000	-0.593166000
C	3.267681000	-2.880017000	-0.258246000
C	2.735052000	-3.518641000	0.845858000
C	1.319501000	-3.701735000	0.995930000
C	0.593899000	-4.401446000	2.157446000
C	-0.798562000	-4.692998000	1.500111000
C	-0.948531000	-3.552687000	0.492038000
C	-1.135054000	-5.031940000	-1.551339000
N	-1.167085000	-2.581076000	-1.644080000
N	0.595789000	-1.123776000	-2.984268000
N	2.547567000	-2.244178000	-1.266374000
N	0.457177000	-3.228420000	0.123584000
C	-3.961219000	-4.968275000	-0.944367000
C	-3.764946000	-2.729286000	0.181156000
C	-5.244420000	-2.349416000	0.088122000
O	-5.995236000	-2.659447000	-0.825290000
N	-5.692473000	-1.532047000	1.119555000
C	-3.748047000	-3.643314000	-3.564661000
C	-3.038942000	-0.381746000	-4.030707000
C	-0.915757000	1.009157000	-5.688683000
C	0.358766000	1.834609000	-3.656493000
C	-0.673398000	2.491719000	-2.756123000
O	-1.900170000	2.300448000	-2.865258000
N	-0.163054000	3.316915000	-1.826115000
C	5.214773000	-0.402838000	-1.027136000
C	5.835183000	-2.044887000	-2.824701000

C	5.193007000	-4.261481000	-1.047885000
C	3.676383000	-4.046409000	1.908854000
C	0.478278000	-3.397391000	3.329005000
C	1.202532000	-5.729154000	2.640514000
C	-1.956016000	-4.854377000	2.484451000
C	1.199732000	-1.031897000	-6.112398000
H	-4.204503000	-2.091642000	-2.188244000
H	2.025018000	0.749672000	-5.200911000
H	3.787709000	-0.616535000	-3.946245000
H	5.342497000	-2.561524000	0.278417000
H	-0.675813000	-5.629554000	0.942618000
H	-1.367480000	-2.662986000	0.979415000
H	-0.040578000	-5.030064000	-1.537803000
H	-1.459643000	-5.074836000	-2.592099000
H	-1.484796000	-5.934166000	-1.044985000
H	-3.646953000	-5.619179000	-1.761641000
H	-5.037992000	-4.814998000	-1.032478000
H	-3.767151000	-5.495269000	-0.003947000
H	-3.191728000	-1.797677000	0.243872000
H	-3.621197000	-3.226790000	1.146976000
H	-6.701264000	-1.523069000	1.241656000
H	-5.159994000	-1.465179000	1.983046000
H	-3.827858000	-2.990890000	-4.437963000
H	-4.713886000	-4.134095000	-3.423280000
H	-2.995493000	-4.404675000	-3.785174000
H	-3.165312000	-0.774204000	-5.045355000
H	-2.955081000	0.700284000	-4.089773000
H	-3.952758000	-0.611066000	-3.479272000
H	-0.283874000	1.568860000	-6.388069000
H	-1.733525000	1.663568000	-5.387402000
H	-1.327594000	0.152044000	-6.224726000
H	0.696648000	2.604545000	-4.364011000
H	1.230095000	1.587794000	-3.038161000
H	-0.771499000	3.900949000	-1.256872000
H	0.836756000	3.456153000	-1.721723000
H	2.167026000	-1.515062000	-6.276536000
H	0.912815000	-0.522956000	-7.036444000
H	0.460965000	-1.811437000	-5.897677000
H	5.128901000	0.420617000	-1.741539000
H	6.246617000	-0.445510000	-0.665748000
H	4.563836000	-0.183271000	-0.176306000
H	5.879828000	-1.197934000	-3.516701000
H	5.566497000	-2.937884000	-3.394972000
H	6.842134000	-2.181516000	-2.418614000
H	6.254842000	-4.268837000	-1.307413000
H	4.618904000	-4.592429000	-1.919330000
H	5.037218000	-4.987542000	-0.246483000
H	4.650305000	-3.561198000	1.847186000
H	3.829855000	-5.128094000	1.832061000
H	3.290921000	-3.838774000	2.909455000
H	1.468995000	-3.077069000	3.663167000
H	-0.028762000	-3.865285000	4.178573000
H	-0.082301000	-2.502059000	3.038729000
H	1.515715000	-6.353576000	1.797707000
H	0.441572000	-6.282168000	3.201962000
H	2.054131000	-5.589105000	3.307468000
H	-1.712742000	-5.587159000	3.260265000
H	-2.855460000	-5.214674000	1.976601000
H	-2.197758000	-3.907304000	2.979155000
C	0.680485000	0.862167000	3.495269000
C	0.898321000	0.640037000	2.192860000
CI	2.060824000	-0.505127000	1.661447000
CI	0.031851000	1.458121000	0.927656000
CI	-0.495086000	1.956985000	4.098452000
H	1.253714000	0.331767000	4.246788000
C	5.552285000	-3.051710000	5.267355000
C	5.672340000	-1.924132000	4.270462000
C	6.619269000	-1.983430000	3.237701000
C	4.877261000	-0.775586000	4.371876000
C	6.772291000	-0.926065000	2.341228000
C	5.027489000	0.285331000	3.476136000
C	5.975410000	0.215095000	2.455985000
H	5.703259000	-4.025224000	4.789013000
H	4.572345000	-3.053489000	5.755350000
H	6.310883000	-2.955068000	6.053501000
H	7.254530000	-2.862260000	3.147680000
H	4.146226000	-0.705591000	5.175524000
H	7.526702000	-0.987072000	1.560894000
H	4.408601000	1.173390000	3.581162000
H	6.092286000	1.040654000	1.760422000
C	-6.662172000	2.281366000	5.299433000
C	-5.616458000	1.651628000	4.410355000
C	-5.174518000	0.337565000	4.622129000
C	-5.023137000	2.381191000	3.370278000
C	-4.163734000	-0.228168000	3.839746000
C	-4.028235000	1.824364000	2.568644000
C	-3.597351000	0.522557000	2.812341000
O	-2.631810000	-0.083827000	1.995211000
H	-7.375853000	1.538350000	5.667351000
H	-7.216461000	3.062456000	4.770945000
H	-6.192364000	2.746545000	6.174705000
H	-5.608885000	-0.249577000	5.427548000
H	-5.334813000	3.404209000	3.175751000
H	-3.793840000	-1.230667000	4.041170000
H	-3.588250000	2.403719000	1.762959000

H	-1.902380000	0.551832000	1.855405000
C	-8.433753000	0.038240000	-1.015280000
C	-7.964670000	1.478245000	-1.257590000
C	-6.911882000	1.957513000	-0.246075000
N	-5.655900000	1.195240000	-0.290313000
C	-4.579367000	1.516806000	-1.003161000
N	-4.588881000	2.512347000	-1.903125000
N	-3.433400000	0.832095000	-0.819602000
H	-7.617522000	-0.682446000	-1.130759000
H	-9.217659000	-0.236036000	-1.726276000
H	-8.852394000	-0.066656000	-0.006491000
H	-7.565239000	1.572446000	-2.276788000
H	-8.815070000	2.167640000	-1.191399000
H	-7.292338000	1.857337000	0.775690000
H	-6.667492000	3.015890000	-0.388554000
H	-5.595655000	0.341199000	0.273105000
H	-5.457923000	2.842129000	-2.295936000
H	-3.709395000	2.736072000	-2.373932000
H	-3.250566000	0.385065000	0.076867000
H	-2.644386000	1.076489000	-1.413972000
C	7.318474000	5.612016000	0.827149000
C	6.462767000	5.142901000	-0.313895000
C	6.603888000	5.475127000	-1.640103000
C	5.345378000	4.237619000	-0.249949000
N	5.641691000	4.830081000	-2.403067000
C	4.857789000	4.054124000	-1.581205000
C	4.711278000	3.550683000	0.799227000
C	3.795257000	3.192806000	-1.876384000
C	3.650425000	2.700236000	0.511032000
C	3.203603000	2.512498000	-0.813050000
H	6.723993000	6.143316000	1.580046000
H	8.100746000	6.290213000	0.476576000
H	7.804261000	4.767556000	1.330698000
H	7.324413000	6.127699000	-2.114086000
H	5.556392000	4.903717000	-3.406069000
H	5.054106000	3.675296000	1.823172000
H	3.467935000	3.033601000	-2.901859000
H	3.173599000	2.150509000	1.315703000
H	2.416205000	1.787327000	-1.004742000
C	1.226249000	5.750891000	0.175051000
C	-0.252031000	5.592165000	0.436874000
C	-0.713078000	4.909452000	1.572338000
C	-1.213035000	6.123700000	-0.434183000
C	-2.071428000	4.756806000	1.832469000
C	-2.581289000	5.959986000	-0.201808000
C	-3.011099000	5.274920000	0.936565000
O	-4.345015000	5.064181000	1.221007000
H	1.659166000	6.520166000	0.825755000
H	1.418989000	6.056015000	-0.858455000
H	1.775817000	4.823113000	0.368329000
H	0.005868000	4.497444000	2.275570000
H	-0.891103000	6.674402000	-1.315177000
H	-2.413115000	4.255013000	2.731682000
H	-3.306498000	6.380630000	-0.895748000
H	-4.883236000	5.641680000	0.655422000

3B. PceA/TCE, Co^I (Charge = 1, Multiplicity = 1)

Co	0.497713000	-2.087840000	-1.604582000
C	-1.812028000	-3.597697000	-1.036794000
C	-3.379027000	-3.411394000	-1.030589000
C	-3.601784000	-2.495514000	-2.288346000
C	-2.261738000	-1.805529000	-2.451272000
C	-2.028074000	-0.660467000	-3.277455000
C	-0.734234000	-0.252404000	-3.558169000
C	-0.287779000	0.912914000	-4.464313000
C	1.080686000	0.361334000	-4.952982000
C	1.500402000	-0.437042000	-3.746708000
C	2.814414000	-0.723270000	-3.430009000
C	3.236406000	-1.496706000	-2.357170000
C	4.695931000	-1.648582000	-1.967460000
C	4.612297000	-2.793688000	-0.920771000
C	3.139887000	-2.807556000	-0.542039000
C	2.641531000	-3.488169000	0.552545000
C	1.238604000	-3.694004000	0.719693000
C	0.539149000	-4.434497000	1.870693000
C	-0.863446000	-4.699435000	1.228566000
C	-1.025039000	-3.505002000	0.288589000
C	-1.361631000	-4.838457000	-1.829319000
N	-1.306246000	-2.385502000	-1.752183000
N	0.412993000	-0.869841000	-3.048967000
N	2.392021000	-2.126998000	-1.498787000
N	0.363359000	-3.199322000	-0.136351000
C	-4.145467000	-4.742490000	-1.075351000
C	-3.819363000	-2.622219000	0.219965000
C	-5.284357000	-2.195973000	0.265692000
O	-6.127633000	-2.429106000	-0.587943000
N	-5.617541000	-1.420782000	1.377926000
C	-4.072683000	-3.207418000	-3.569719000
C	-3.247092000	0.020828000	-3.876244000
C	-1.183741000	1.351064000	-5.629750000
C	0.071561000	2.148693000	-3.566895000
C	-0.989776000	2.544296000	-2.568646000
O	-2.117240000	2.948497000	-2.921743000
N	-0.653760000	2.422111000	-1.269126000

C	5.157223000	-0.352057000	-1.266059000
C	5.619287000	-1.924560000	-3.163430000
C	5.020291000	-4.185591000	-1.444025000
C	3.613435000	-4.055062000	1.566966000
C	0.443941000	-3.483480000	3.086301000
C	1.155443000	-5.779937000	2.292045000
C	-1.996328000	-4.922617000	2.229109000
C	0.993292000	-0.549858000	-6.191743000
H	-4.372046000	-1.757750000	-2.046817000
H	1.775853000	1.184895000	-5.159845000
H	3.579423000	-0.292101000	-4.068152000
H	5.242044000	-2.545857000	-0.059627000
H	-0.749815000	-5.603562000	0.617127000
H	-1.385048000	-2.629812000	0.847055000
H	-0.269948000	-4.844513000	-1.887037000
H	-1.750781000	-4.808047000	-2.849036000
H	-1.699405000	-5.764617000	-1.356572000
H	-3.895158000	-5.332927000	-1.958034000
H	-5.221555000	-4.559377000	-1.086217000
H	-3.910395000	-5.348580000	-0.193437000
H	-3.206763000	-1.722071000	0.336676000
H	-3.637010000	-3.213730000	1.124309000
H	-6.609841000	-1.407755000	1.595949000
H	-5.008988000	-1.426301000	2.192323000
H	-4.179652000	-2.486172000	-4.384470000
H	-5.047227000	-3.675866000	-3.406552000
H	-3.364974000	-3.972927000	-3.898563000
H	-3.451823000	-0.312586000	-4.900075000
H	-3.133385000	1.103165000	-3.899684000
H	-4.138559000	-0.203080000	-3.284159000
H	-0.579271000	1.939834000	-6.329837000
H	-2.005843000	1.985027000	-5.297836000
H	-1.589477000	0.494918000	-6.173543000
H	0.241103000	3.010613000	-4.222930000
H	1.006665000	1.939381000	-3.038125000
H	-1.228880000	2.864088000	-0.560595000
H	0.271239000	2.122815000	-0.990018000
H	1.972836000	-0.995293000	-6.388798000
H	0.685873000	0.008057000	-7.081654000
H	0.279520000	-1.363348000	-6.022772000
H	5.067227000	0.510993000	-1.932306000
H	6.204173000	-0.448907000	-0.958266000
H	4.556190000	-0.154119000	-0.374603000
H	5.653531000	-1.053549000	-3.826491000
H	5.289755000	-2.784766000	-3.752460000
H	6.642396000	-2.108922000	-2.818570000
H	6.071024000	-4.200085000	-1.749409000
H	4.404310000	-4.476581000	-2.301232000
H	4.884950000	-4.938635000	-0.663134000
H	4.587104000	-3.571002000	1.493923000
H	3.764463000	-5.134712000	1.450518000
H	3.261130000	-3.884607000	2.587831000
H	1.444725000	-3.216252000	3.438623000
H	-0.081998000	-3.965017000	3.918116000
H	-0.079299000	-2.555764000	2.830999000
H	1.447749000	-6.370239000	1.417514000
H	0.411750000	-6.356468000	2.854714000
H	2.026551000	-5.661623000	2.938906000
H	-1.726274000	-5.689396000	2.963123000
H	-2.905543000	-5.267006000	1.726741000
H	-2.234843000	-4.004275000	2.777472000
C	1.691179000	0.160306000	2.977920000
C	0.885577000	0.618967000	2.017287000
Cl	0.669633000	-0.295130000	0.493704000
Cl	-0.040094000	2.088054000	2.158530000
Cl	1.929676000	0.935252000	4.501228000
H	2.264446000	-0.747845000	2.831328000
C	5.661267000	-3.575418000	4.790350000
C	5.847616000	-2.399571000	3.855992000
C	6.800180000	-2.452852000	2.816477000
C	5.099972000	-1.215935000	4.009299000
C	7.003786000	-1.358010000	1.964611000
C	5.304336000	-0.115986000	3.160217000
C	6.256486000	-0.181395000	2.134278000
H	5.608744000	-4.527178000	4.232137000
H	4.740084000	-3.474871000	5.388517000
H	6.510543000	-3.657286000	5.493951000
H	7.393177000	-3.364708000	2.677777000
H	4.358139000	-1.146147000	4.814127000
H	7.752997000	-1.421544000	1.167690000
H	4.723202000	0.799704000	3.311148000
H	6.412642000	0.678217000	1.475112000
C	-6.401265000	2.000579000	5.810263000
C	-5.392443000	1.456020000	4.825101000
C	-4.855822000	0.169267000	4.975753000
C	-4.929584000	2.236016000	3.755960000
C	-3.878404000	-0.320376000	4.106008000
C	-3.963069000	1.758671000	2.871709000
C	-3.436003000	0.482103000	3.055998000
O	-2.512411000	-0.055348000	2.150336000
H	-7.056672000	1.210436000	6.189302000
H	-7.022831000	2.777389000	5.355076000
H	-5.893095000	2.448313000	6.673248000
H	-5.191439000	-0.456930000	5.799068000
H	-5.326875000	3.236359000	3.599487000

H	-3.439905000	-1.304820000	4.248128000
H	-3.631104000	2.379854000	2.046694000
H	-1.766671000	0.574512000	2.062482000
C	-8.496830000	0.335872000	-0.583737000
C	-7.912570000	1.732564000	-0.829052000
C	-6.774222000	2.114267000	0.134008000
N	-5.572655000	1.278427000	0.014628000
C	-4.495893000	1.564192000	-0.725833000
N	-4.514235000	2.574565000	-1.632782000
N	-3.352985000	0.887459000	-0.522477000
H	-7.743339000	-0.457874000	-0.732999000
H	-9.332235000	0.134963000	-1.274656000
H	-8.889393000	0.252324000	0.446879000
H	-7.551949000	1.810696000	-1.874060000
H	-8.700926000	2.500016000	-0.718060000
H	-7.110887000	2.024250000	1.181554000
H	-6.476253000	3.166739000	-0.008284000
H	-5.529232000	0.411802000	0.578148000
H	-5.381673000	2.743242000	-2.140785000
H	-3.616534000	2.772533000	-2.143676000
H	-3.174290000	0.386733000	0.358582000
H	-2.611963000	0.877927000	-1.225766000
C	7.456268000	5.390808000	1.011354000
C	6.506934000	5.051198000	-0.105679000
C	6.538935000	5.544400000	-1.397572000
C	5.393851000	4.127789000	-0.062234000
N	5.518938000	4.983721000	-2.153151000
C	4.801955000	4.103471000	-1.369591000
C	4.839133000	3.306797000	0.945782000
C	3.712667000	3.273087000	-1.688465000
C	3.752334000	2.484297000	0.634869000
C	3.202768000	2.459737000	-0.670916000
H	6.921766000	5.816228000	1.881171000
H	8.208739000	6.126696000	0.683777000
H	7.992991000	4.492050000	1.368460000
H	7.225828000	6.263268000	-1.846789000
H	5.346210000	5.175976000	-3.134987000
H	5.263283000	3.307467000	1.955909000
H	3.296073000	3.244712000	-2.701344000
H	3.329521000	1.828660000	1.400963000
H	2.405075000	1.743147000	-0.896572000
C	1.347169000	5.716634000	0.645316000
C	-0.144317000	5.490165000	0.691091000
C	-0.803073000	5.191587000	1.903381000
C	-0.922883000	5.509278000	-0.480174000
C	-2.160477000	4.848795000	1.942054000
C	-2.286180000	5.178519000	-0.462588000
C	-2.900461000	4.808377000	0.746391000
O	-4.212507000	4.397533000	0.802066000
H	1.705306000	6.248595000	1.543231000
H	1.641659000	6.301936000	-0.241758000
H	1.890916000	4.753430000	0.597410000
H	-0.234654000	5.206728000	2.840171000
H	-0.455291000	5.767457000	-1.436868000
H	-2.652920000	4.607057000	2.888700000
H	-2.864549000	5.195335000	-1.392247000
H	-4.494915000	4.196034000	-0.113605000

3C. PceA/TCE, Co^I → Co^{III} Transition State (Charge = 1, Multiplicity = 1)

Co	0.592538000	-2.197466000	-1.353774000
C	-1.709092000	-3.870215000	-1.150728000
C	-3.268320000	-3.640741000	-1.201260000
C	-3.416969000	-2.670329000	-2.426576000
C	-2.066837000	-1.985116000	-2.477189000
C	-1.789356000	-0.781732000	-3.216383000
C	-0.491594000	-0.346004000	-3.379893000
C	0.020435000	0.863353000	-4.187384000
C	1.424282000	0.326507000	-4.598074000
C	1.749859000	-0.533862000	-3.407458000
C	3.037145000	-0.844626000	-3.005697000
C	3.379265000	-1.609562000	-1.899011000
C	4.808816000	-1.937397000	-1.532249000
C	4.639864000	-2.409138000	-0.057721000
C	3.161889000	-2.776612000	0.008620000
C	2.562748000	-3.512050000	1.011831000
C	1.189291000	-3.909936000	0.921932000
C	0.426118000	-4.814867000	1.905310000
C	-0.844171000	-5.160690000	1.053635000
C	-1.009254000	-3.889158000	0.221604000
C	-1.224301000	-5.051050000	-2.008408000
N	-1.170162000	-2.612109000	-1.760153000
N	0.619129000	-0.987448000	-2.819445000
N	2.488664000	-2.205494000	-1.071150000
N	0.394103000	-3.484606000	-0.032514000
C	-4.071431000	-4.941504000	-1.336680000
C	-3.712420000	-2.874380000	0.063754000
C	-5.167050000	-2.409071000	0.100805000
O	-6.004885000	-2.613170000	-0.769816000
N	-5.475791000	-1.672803000	1.229101000
C	-3.826254000	-3.306627000	-3.767395000
C	-2.970082000	-0.067020000	-3.842489000
C	-0.781117000	1.347052000	-5.402476000
C	0.308314000	2.041458000	-3.196792000
C	-0.870060000	2.542443000	-2.385906000

O	-1.936587000	2.902018000	-2.925352000
N	-0.693638000	2.588560000	-1.055289000
C	5.781622000	-0.756906000	-1.647473000
C	5.257816000	-3.083587000	-2.474463000
C	5.693458000	-3.444913000	0.360782000
C	3.364581000	-3.857115000	2.249176000
C	0.034220000	-3.997169000	3.159209000
C	1.155207000	-6.111032000	2.294121000
C	-2.060147000	-5.601948000	1.865561000
C	1.431734000	-0.526777000	-5.881438000
H	-4.184598000	-1.930643000	-2.185491000
H	2.137306000	1.152200000	-4.706532000
H	3.849699000	-0.437975000	-3.598871000
H	4.763924000	-1.522482000	0.582859000
H	-0.550971000	-5.975963000	0.379638000
H	-1.433073000	-3.086665000	0.836225000
H	-0.130037000	-5.076943000	-1.997455000
H	-1.549946000	-4.942822000	-3.044721000
H	-1.600412000	-6.002481000	-1.623959000
H	-3.793201000	-5.508311000	-2.227527000
H	-5.138098000	-4.717566000	-1.393486000
H	-3.906032000	-5.585330000	-0.467498000
H	-3.081709000	-1.990322000	0.220340000
H	-3.571506000	-3.503378000	0.950392000
H	-6.457436000	-1.607632000	1.474854000
H	-4.807836000	-1.606167000	1.990632000
H	-3.869156000	-2.545437000	-4.550904000
H	-4.820395000	-3.751742000	-3.679029000
H	-3.124360000	-4.078781000	-4.092604000
H	-3.117175000	-0.356940000	-4.889049000
H	-2.843177000	1.012606000	-3.809891000
H	-3.890385000	-0.305671000	-3.306054000
H	-0.126953000	1.971784000	-6.021920000
H	-1.632529000	1.959403000	-5.111239000
H	-1.129189000	0.512473000	-6.015847000
H	0.666596000	2.894512000	-3.787052000
H	1.117363000	1.752427000	-2.518693000
H	-1.349251000	3.091936000	-0.465247000
H	0.153042000	2.261248000	-0.607773000
H	2.418789000	-0.977325000	-6.022372000
H	1.204487000	0.080291000	-6.761962000
H	0.695354000	-1.334570000	-5.812638000
H	5.917138000	-0.451335000	-2.691579000
H	6.764635000	-1.051497000	-1.264590000
H	5.434684000	0.101390000	-1.067556000
H	5.212991000	-2.744291000	-3.514413000
H	4.609546000	-3.960077000	-2.372504000
H	6.287444000	-3.383578000	-2.259173000
H	6.669789000	-3.128144000	-0.020463000
H	5.474804000	-4.438418000	-0.041898000
H	5.794308000	-3.515863000	1.442378000
H	4.065571000	-3.052911000	2.478949000
H	3.928798000	-4.790699000	2.148890000
H	2.715480000	-3.960427000	3.117966000
H	0.916304000	-3.617669000	3.679792000
H	-0.517842000	-4.629596000	3.861498000
H	-0.592983000	-3.138697000	2.897956000
H	1.594991000	-6.590929000	1.413660000
H	0.437223000	-6.809624000	2.738108000
H	1.944941000	-5.948991000	3.029454000
H	-1.798444000	-6.421748000	2.542709000
H	-2.858052000	-5.966092000	1.213289000
H	-2.463639000	-4.784127000	2.471020000
C	0.372420000	0.089850000	3.380544000
C	-0.359536000	0.691664000	2.435124000
Cl	0.061536000	-0.657452000	0.226688000
Cl	-0.238090000	2.421186000	2.209390000
Cl	1.412924000	0.864380000	4.556952000
H	0.344266000	-0.986484000	3.500563000
C	5.896732000	-2.430497000	5.094444000
C	5.831870000	-1.434784000	3.954704000
C	6.941392000	-1.209474000	3.113842000
C	4.669477000	-0.666582000	3.737348000
C	6.900485000	-0.228862000	2.109730000
C	4.623026000	0.312000000	2.734195000
C	5.743483000	0.544064000	1.921221000
H	6.598045000	-3.254582000	4.877587000
H	4.904586000	-2.864365000	5.308823000
H	6.245094000	-1.936756000	6.021173000
H	7.854356000	-1.799601000	3.257992000
H	3.790297000	-0.822909000	4.372656000
H	7.780427000	-0.061255000	1.478424000
H	3.712993000	0.901701000	2.593322000
H	5.709268000	1.325521000	1.154951000
C	-6.249448000	3.050461000	5.349938000
C	-5.362806000	2.199466000	4.469282000
C	-5.158432000	0.841110000	4.746072000
C	-4.680442000	2.750769000	3.374650000
C	-4.300423000	0.061803000	3.968985000
C	-3.822875000	1.982475000	2.590413000
C	-3.629763000	0.624532000	2.876894000
O	-2.838479000	-0.173753000	2.078240000
H	-7.055359000	2.459251000	5.796078000
H	-6.697947000	3.874650000	4.786024000
H	-5.671588000	3.492168000	6.171639000

H	-5.666374000	0.386378000	5.594060000
H	-4.820539000	3.798747000	3.118922000
H	-4.124825000	-0.983476000	4.215407000
H	-3.297086000	2.436693000	1.756751000
H	-1.758258000	0.141275000	2.150007000
C	-8.426859000	0.230737000	-0.595997000
C	-7.808556000	1.614023000	-0.848724000
C	-6.632811000	1.957528000	0.085015000
N	-5.459882000	1.093612000	-0.074463000
C	-4.346114000	1.398320000	-0.762262000
N	-4.333311000	2.402278000	-1.657604000
N	-3.238891000	0.667904000	-0.530241000
H	-7.697873000	-0.580451000	-0.773401000
H	-9.286744000	0.058200000	-1.264444000
H	-8.790854000	0.149864000	0.445243000
H	-7.472272000	1.686661000	-1.902077000
H	-8.574792000	2.400144000	-0.712512000
H	-6.944449000	1.874773000	1.141244000
H	-6.300910000	3.001308000	-0.054376000
H	-5.411926000	0.232399000	0.487754000
H	-5.210227000	2.737775000	-2.045214000
H	-3.439855000	2.688581000	-2.120314000
H	-3.083556000	0.275449000	0.431147000
H	-2.389092000	0.858151000	-1.059343000
C	7.453199000	5.736520000	-0.269408000
C	6.588269000	4.645985000	-0.848843000
C	6.789412000	3.990249000	-2.049487000
C	5.388910000	4.064615000	-0.276932000
N	5.792485000	3.045181000	-2.257453000
C	4.915125000	3.065536000	-1.190722000
C	4.669293000	4.273804000	0.922707000
C	3.769676000	2.289106000	-0.933202000
C	3.531554000	3.503335000	1.184257000
C	3.087581000	2.517580000	0.267651000
H	6.876636000	6.667450000	-0.115278000
H	8.299398000	5.967196000	-0.936995000
H	7.864681000	5.442554000	0.714010000
H	7.582270000	4.125852000	-2.786719000
H	5.724593000	2.434624000	-3.065243000
H	5.006528000	5.026026000	1.643868000
H	3.437584000	1.514461000	-1.632359000
H	2.973445000	3.647977000	2.115040000
H	2.218231000	1.900831000	0.522471000
C	1.333540000	5.896561000	-0.559632000
C	-0.140293000	5.742932000	-0.257787000
C	-0.587343000	5.448559000	1.047052000
C	-1.114091000	5.821613000	-1.271732000
C	-1.937381000	5.206004000	1.330923000
C	-2.471662000	5.584651000	-1.007996000
C	-2.888005000	5.266699000	0.296966000
O	-4.200928000	5.007646000	0.617980000
H	1.877164000	6.346066000	0.287858000
H	1.500606000	6.524580000	-1.451217000
H	1.801376000	4.911422000	-0.747224000
H	0.140872000	5.395979000	1.864125000
H	-0.811067000	6.054737000	-2.298495000
H	-2.265089000	4.972828000	2.347937000
H	-3.204147000	5.639119000	-1.822245000
H	-4.754307000	5.212123000	-0.156349000

3D. PceA/TCE, Co^{III} (Charge = 1, Multiplicity = 1)

Co	0.526287000	-1.996342000	-1.658297000
C	-1.833570000	-3.487363000	-1.073070000
C	-3.395743000	-3.269462000	-1.116050000
C	-3.569086000	-2.402981000	-2.417526000
C	-2.218071000	-1.742899000	-2.572631000
C	-1.949516000	-0.600216000	-3.405794000
C	-0.652330000	-0.262373000	-3.721751000
C	-0.153691000	0.892393000	-4.607774000
C	1.177902000	0.268222000	-5.129454000
C	1.564824000	-0.578852000	-3.947437000
C	2.870643000	-0.906207000	-3.620585000
C	3.271732000	-1.639800000	-2.512609000
C	4.722404000	-1.808279000	-2.107275000
C	4.610314000	-2.927955000	-1.035501000
C	3.143586000	-2.880766000	-0.646455000
C	2.620545000	-3.501227000	0.467679000
C	1.204510000	-3.600779000	0.677701000
C	0.483319000	-4.222062000	1.882292000
C	-0.952027000	-4.433598000	1.288075000
C	-1.064000000	-3.306380000	0.258487000
C	-1.388146000	-4.782468000	-1.778226000
N	-1.296148000	-2.333370000	-1.861936000
N	0.469400000	-0.959038000	-3.254117000
N	2.419258000	-2.203855000	-1.621516000
N	0.343058000	-3.099981000	-0.171211000
C	-4.178203000	-4.591076000	-1.127413000
C	-3.855249000	-2.406787000	0.074515000
C	-5.333562000	-2.012493000	0.063549000
O	-6.110026000	-2.224188000	-0.867066000
N	-5.737746000	-1.324519000	1.179311000
C	-4.008414000	-3.139726000	-3.695652000
C	-3.144890000	0.166544000	-3.931580000
C	-1.036333000	1.392447000	-5.756823000

C	0.290951000	2.065686000	-3.673289000
C	-0.766030000	2.696987000	-2.782148000
O	-1.850909000	3.119173000	-3.228799000
N	-0.439408000	2.814290000	-1.482343000
C	5.158142000	-0.489813000	-1.422726000
C	5.665499000	-2.110807000	-3.279591000
C	4.968188000	-4.342219000	-1.535500000
C	3.561632000	-4.120929000	1.470697000
C	0.493905000	-3.159253000	3.006738000
C	1.015106000	-5.570775000	2.394443000
C	-2.068375000	-4.486497000	2.330253000
C	1.029989000	-0.607258000	-6.388532000
H	-4.330246000	-1.645638000	-2.222613000
H	1.922057000	1.050229000	-5.319044000
H	3.649606000	-0.515070000	-4.266018000
H	5.245153000	-2.681543000	-0.178218000
H	-0.920022000	-5.391120000	0.752399000
H	-1.391122000	-2.371030000	0.731184000
H	-0.295917000	-4.825223000	-1.817509000
H	-1.764431000	-4.815596000	-2.802612000
H	-1.752381000	-5.666967000	-1.250791000
H	-3.923173000	-5.221331000	-1.981630000
H	-5.249170000	-4.386107000	-1.166137000
H	-3.971572000	-5.161959000	-0.215056000
H	-3.276182000	-1.478916000	0.138443000
H	-3.663865000	-2.922103000	1.019617000
H	-6.735911000	-1.208752000	1.309033000
H	-5.150638000	-1.242612000	2.007035000
H	-4.078606000	-2.437638000	-4.531692000
H	-4.996708000	-3.579819000	-3.542654000
H	-3.309299000	-3.930398000	-3.981727000
H	-3.415744000	-0.142608000	-4.947644000
H	-2.951352000	1.237370000	-3.944940000
H	-4.015470000	-0.005071000	-3.295657000
H	-0.410746000	1.969562000	-6.447564000
H	-1.825131000	2.054723000	-5.404856000
H	-1.478448000	0.563551000	-6.314952000
H	0.674010000	2.871416000	-4.313369000
H	1.121750000	1.721344000	-3.048883000
H	-0.979545000	3.430714000	-0.877723000
H	0.400752000	2.396218000	-1.102505000
H	1.979889000	-1.103172000	-6.609302000
H	0.751381000	-0.003548000	-7.256336000
H	0.268312000	-1.380235000	-6.240656000
H	5.112746000	0.351440000	-2.120327000
H	6.185588000	-0.588449000	-1.057077000
H	4.511288000	-0.260385000	-0.573415000
H	5.722472000	-1.251425000	-3.955391000
H	5.345445000	-2.980690000	-3.859602000
H	6.678121000	-2.294959000	-2.906885000
H	6.019109000	-4.396182000	-1.832821000
H	4.348475000	-4.624643000	-2.393070000
H	4.803484000	-5.077748000	-0.744308000
H	4.572046000	-3.728300000	1.365800000
H	3.604883000	-5.211968000	1.375750000
H	3.246357000	-3.887933000	2.488256000
H	1.519004000	-2.917983000	3.300948000
H	-0.027548000	-3.537874000	3.891455000
H	0.016252000	-2.228530000	2.686548000
H	1.254091000	-6.247640000	1.567401000
H	0.237343000	-6.046323000	3.002158000
H	1.897053000	-5.465348000	3.027984000
H	-1.826719000	-5.199472000	3.125521000
H	-3.009593000	-4.815530000	1.879948000
H	-2.230763000	-3.506361000	2.789365000
C	-0.185016000	0.260153000	4.182266000
C	-0.105133000	0.966415000	3.056459000
Cl	0.423028000	-0.189306000	-0.385785000
Cl	1.309772000	1.795063000	2.515180000
Cl	1.109064000	0.017311000	5.304313000
H	-1.116944000	-0.219971000	4.457631000
C	5.506137000	-4.090543000	4.712130000
C	5.540877000	-2.832983000	3.874032000
C	6.573082000	-2.622233000	2.936780000
C	4.516663000	-1.869210000	3.966105000
C	6.575927000	-1.487402000	2.112673000
C	4.510043000	-0.735680000	3.138890000
C	5.542905000	-0.541430000	2.209503000
H	5.057677000	-4.927836000	4.141963000
H	4.904181000	-3.953153000	5.625961000
H	6.519842000	-4.408724000	5.009756000
H	7.385277000	-3.354507000	2.856892000
H	3.710995000	-2.004304000	4.697657000
H	7.395536000	-1.332759000	1.401680000
H	3.701359000	-0.002507000	3.231242000
H	5.556100000	0.348742000	1.574566000
C	-6.431696000	1.715893000	5.897969000
C	-5.484220000	1.253955000	4.817895000
C	-4.859556000	-0.000816000	4.861256000
C	-5.166782000	2.090354000	3.732690000
C	-3.968021000	-0.413373000	3.870267000
C	-4.283463000	1.700217000	2.737803000
C	-3.656340000	0.423023000	2.763043000
O	-2.857550000	0.011637000	1.799889000
H	-6.714897000	0.891404000	6.559411000

H	-7.348428000	2.139803000	5.471539000
H	-5.974168000	2.497337000	6.518575000
H	-5.073875000	-0.670771000	5.692283000
H	-5.618785000	3.079684000	3.671228000
H	-3.489143000	-1.389695000	3.929622000
H	-4.059854000	2.382796000	1.925758000
H	-0.959749000	1.024676000	2.390052000
C	-8.424881000	0.585419000	-0.643867000
C	-7.775603000	1.922442000	-1.023701000
C	-6.582286000	2.318187000	-0.138811000
N	-5.400995000	1.452118000	-0.268159000
C	-4.234209000	1.801477000	-0.847506000
N	-4.225145000	2.839063000	-1.747171000
N	-3.116744000	1.170572000	-0.498868000
H	-7.729845000	-0.260771000	-0.790318000
H	-9.316059000	0.391773000	-1.264210000
H	-8.749947000	0.596003000	0.413370000
H	-7.453488000	1.899611000	-2.083503000
H	-8.519829000	2.736808000	-0.942464000
H	-6.873241000	2.298284000	0.926895000
H	-6.272971000	3.353839000	-0.353445000
H	-5.359629000	0.633849000	0.353118000
H	-5.058110000	2.939919000	-2.327973000
H	-3.332209000	3.019078000	-2.256137000
H	-3.004758000	0.692103000	0.508260000
H	-2.257986000	1.368748000	-1.013786000
C	7.610757000	5.079008000	1.649422000
C	6.710669000	5.076578000	0.444612000
C	6.779021000	5.923558000	-0.646865000
C	5.611642000	4.175676000	0.178539000
N	5.794262000	5.599634000	-1.569664000
C	5.064527000	4.527321000	-1.100442000
C	5.033816000	3.100492000	0.890690000
C	3.993488000	3.823547000	-1.680493000
C	3.969513000	2.398768000	0.317610000
C	3.461624000	2.750718000	-0.957023000
H	7.036606000	5.233146000	2.582019000
H	8.366092000	5.879011000	1.581295000
H	8.144561000	4.115859000	1.753049000
H	7.467870000	6.746646000	-0.842742000
H	5.644237000	6.074234000	-2.454623000
H	5.418099000	2.820972000	1.877718000
H	3.596653000	4.100372000	-2.663644000
H	3.516875000	1.557662000	0.850107000
H	2.649836000	2.151268000	-1.383475000
C	1.521902000	5.594694000	1.183934000
C	0.034225000	5.362917000	1.074362000
C	-0.689489000	4.775489000	2.134932000
C	-0.675798000	5.681565000	-0.097499000
C	-2.051302000	4.479655000	2.025475000
C	-2.043316000	5.382651000	-0.232368000
C	-2.732600000	4.764606000	0.827570000
O	-4.060373000	4.430740000	0.734932000
H	1.803501000	5.939844000	2.193507000
H	1.870733000	6.344395000	0.453959000
H	2.084163000	4.661165000	0.990135000
H	-0.169803000	4.530196000	3.067142000
H	-0.152843000	6.158578000	-0.934426000
H	-2.593301000	4.016250000	2.854415000
H	-2.576595000	5.640942000	-1.154513000
H	-4.277588000	4.330811000	-0.216563000

4A. PceA/TBE, Co^{II} (Charge = 2, Multiplicity = 2)

Co	0.565510000	-2.281429000	-1.446735000
C	-1.790319000	-3.767958000	-0.903352000
C	-3.353088000	-3.587408000	-1.024662000
C	-3.481647000	-2.790673000	-2.377342000
C	-2.138139000	-2.103286000	-2.501447000
C	-1.843937000	-1.027887000	-3.413077000
C	-0.535719000	-0.682435000	-3.677690000
C	0.018332000	0.356995000	-4.670518000
C	1.317674000	-0.394431000	-5.112065000
C	1.689048000	-1.059970000	-3.812136000
C	2.981204000	-1.352998000	-3.410617000
C	3.345339000	-1.944218000	-2.202984000
C	4.780133000	-2.041652000	-1.723567000
C	4.635498000	-3.000373000	-0.506021000
C	3.147733000	-2.957751000	-0.204604000
C	2.575693000	-3.492199000	0.936051000
C	1.158397000	-3.694787000	1.041335000
C	0.407180000	-4.419101000	2.173100000
C	-0.959088000	-4.725793000	1.466684000
C	-1.091595000	-3.576899000	0.465550000
C	-1.280700000	-5.055734000	-1.576821000
N	-1.255609000	-2.607165000	-1.679025000
N	0.572072000	-1.313820000	-3.087171000
N	2.465240000	-2.409505000	-1.283968000
N	0.320406000	-3.255415000	0.129229000
C	-4.118752000	-4.917791000	-1.007518000
C	-3.870675000	-2.676504000	0.109572000
C	-5.338167000	-2.257808000	0.004844000
O	-6.091424000	-2.547872000	-0.912976000
N	-5.765377000	-1.420236000	1.028904000
C	-3.843144000	-3.611836000	-3.629627000

C	-3.025728000	-0.359124000	-4.086751000
C	-0.843567000	0.780711000	-5.863704000
C	0.543854000	1.616791000	-3.912920000
C	-0.395910000	2.354137000	-2.971973000
O	-1.631106000	2.187600000	-2.969445000
N	0.205006000	3.218419000	-2.138678000
C	5.194632000	-0.637851000	-1.221336000
C	5.762498000	-2.501219000	-2.811045000
C	5.069885000	-4.455742000	-0.779013000
C	3.483778000	-3.936994000	2.062916000
C	0.223166000	-3.451134000	3.364178000
C	1.035823000	-5.740603000	2.647396000
C	-2.144324000	-4.917798000	2.411466000
C	1.095194000	-1.450055000	-6.211493000
H	-4.267670000	-2.040863000	-2.264959000
H	2.087559000	0.314229000	-5.437540000
H	3.781772000	-1.063172000	-4.082403000
H	5.213938000	-2.612007000	0.339028000
H	-0.803869000	-5.653131000	0.902133000
H	-1.512727000	-2.688493000	0.954227000
H	-0.186905000	-5.079181000	-1.544241000
H	-1.587528000	-5.092379000	-2.623322000
H	-1.661340000	-5.947915000	-1.074972000
H	-3.809615000	-5.581226000	-1.816779000
H	-5.189551000	-4.735956000	-1.112633000
H	-3.953612000	-5.444869000	-0.061940000
H	-3.275211000	-1.757921000	0.159463000
H	-3.743799000	-3.165825000	1.082102000
H	-6.773959000	-1.366095000	1.139345000
H	-5.240671000	-1.374406000	1.898041000
H	-3.894823000	-2.961080000	-4.506437000
H	-4.824201000	-4.074021000	-3.497196000
H	-3.110344000	-4.395431000	-3.838743000
H	-3.212515000	-0.760547000	-5.088572000
H	-2.866508000	0.712882000	-4.169272000
H	-3.934698000	-0.514507000	-3.501631000
H	-0.199266000	1.267372000	-6.604943000
H	-1.610611000	1.498246000	-5.570691000
H	-1.324587000	-0.071807000	-6.347036000
H	0.879642000	2.339355000	-4.669033000
H	1.438317000	1.348666000	-3.336770000
H	-0.354931000	3.746149000	-1.474772000
H	1.215020000	3.291385000	-2.065992000
H	2.010791000	-2.028315000	-6.363517000
H	0.829807000	-0.977373000	-7.160910000
H	0.295270000	-2.142519000	-5.928368000
H	5.174403000	0.095716000	-2.032242000
H	6.209912000	-0.681592000	-0.814618000
H	4.523710000	-0.291013000	-0.431006000
H	5.832255000	-1.751057000	-3.605185000
H	5.467409000	-3.451000000	-3.264016000
H	6.764795000	-2.614268000	-2.386679000
H	6.131335000	-4.498326000	-1.036188000
H	4.494531000	-4.889572000	-1.603175000
H	4.913534000	-5.075917000	0.106120000
H	4.438212000	-3.411875000	2.025486000
H	3.685835000	-5.013179000	2.039581000
H	3.044942000	-3.707630000	3.036018000
H	1.188188000	-3.099479000	3.739774000
H	-0.286233000	-3.959677000	4.188560000
H	-0.372283000	-2.574485000	3.086794000
H	1.392148000	-6.337330000	1.801646000
H	0.274168000	-6.325888000	3.174164000
H	1.863329000	-5.589914000	3.342151000
H	-1.914518000	-5.659590000	3.182890000
H	-3.022738000	-5.280994000	1.870352000
H	-2.415213000	-3.982920000	2.913847000
C	0.926221000	-0.079682000	2.346448000
C	0.472322000	0.722799000	1.379477000
Br	0.536481000	0.134356000	-0.443814000
Br	-0.259548000	2.452633000	1.592667000
Br	0.831709000	0.340588000	4.174729000
H	1.378974000	-1.039330000	2.121470000
C	5.325265000	-3.147094000	5.362410000
C	5.441016000	-2.097843000	4.278665000
C	6.528269000	-2.114994000	3.378625000
C	4.479270000	-1.078803000	4.135872000
C	6.655305000	-1.139750000	2.379344000
C	4.603008000	-0.099872000	3.136258000
C	5.694198000	-0.122355000	2.256347000
H	5.332084000	-4.166024000	4.933656000
H	4.398363000	-3.025629000	5.946968000
H	6.177466000	-3.087502000	6.063097000
H	7.291897000	-2.895978000	3.472270000
H	3.630237000	-1.041013000	4.828502000
H	7.519174000	-1.162292000	1.705714000
H	3.855944000	0.698705000	3.063277000
H	5.803228000	0.656291000	1.494941000
C	-6.764112000	2.458538000	5.118434000
C	-5.696668000	1.792579000	4.282357000
C	-5.306561000	0.469243000	4.536599000
C	-5.037427000	2.485915000	3.257029000
C	-4.287619000	-0.141866000	3.803194000
C	-4.026013000	1.885206000	2.506563000
C	-3.656633000	0.572458000	2.787301000

O	-2.695892000	-0.092929000	1.993956000
H	-7.568053000	1.760164000	5.370056000
H	-7.199330000	3.317090000	4.599577000
H	-6.339833000	2.822060000	6.062248000
H	-5.793200000	-0.088784000	5.332807000
H	-5.305381000	3.514651000	3.030809000
H	-3.965059000	-1.156011000	4.026646000
H	-3.529170000	2.442122000	1.718603000
H	-1.828377000	0.326908000	2.138468000
C	-8.468993000	0.196355000	-1.207832000
C	-7.785747000	1.529732000	-1.554128000
C	-6.735649000	2.012546000	-0.532704000
N	-5.497335000	1.218975000	-0.474358000
C	-4.355297000	1.514171000	-1.109322000
N	-4.304563000	2.464424000	-2.067338000
N	-3.215229000	0.872267000	-0.783009000
H	-7.753165000	-0.644831000	-1.201698000
H	-9.249522000	-0.039317000	-1.949548000
H	-8.956632000	0.252832000	-0.217091000
H	-7.317329000	1.465029000	-2.556167000
H	-8.547764000	2.328283000	-1.622209000
H	-7.161076000	2.001241000	0.486305000
H	-6.444460000	3.058243000	-0.737037000
H	-5.489018000	0.389017000	0.140229000
H	-5.139344000	2.686972000	-2.604038000
H	-3.385448000	2.637102000	-2.502358000
H	-3.083588000	0.470420000	0.155650000
H	-2.382540000	1.068636000	-1.346218000
C	7.368418000	5.432681000	0.878230000
C	6.636662000	5.002779000	-0.363390000
C	6.924937000	5.377625000	-1.663620000
C	5.514824000	4.096061000	-0.454808000
N	6.054596000	4.759733000	-2.549670000
C	5.182802000	3.958818000	-1.846841000
C	4.761785000	3.371715000	0.497566000
C	4.161129000	3.102162000	-2.293561000
C	3.736722000	2.527208000	0.058931000
C	3.451744000	2.383018000	-1.322710000
H	6.692732000	5.940775000	1.590878000
H	8.187362000	6.128476000	0.635130000
H	7.805585000	4.564622000	1.405373000
H	7.702595000	6.047619000	-2.033130000
H	6.079550000	4.866374000	-3.559662000
H	4.988237000	3.462489000	1.565385000
H	3.950512000	2.976668000	-3.361869000
H	3.161463000	1.944280000	0.786232000
H	2.702940000	1.646360000	-1.632082000
C	1.293963000	5.701979000	0.111258000
C	-0.199168000	5.647424000	0.354415000
C	-0.721492000	5.427375000	1.651125000
C	-1.126971000	5.748250000	-0.700947000
C	-2.091103000	5.228948000	1.872695000
C	-2.502913000	5.546039000	-0.499305000
C	-2.986764000	5.257293000	0.786694000
O	-4.307905000	4.993111000	1.043531000
H	1.800428000	6.361470000	0.836951000
H	1.526893000	6.070756000	-0.901390000
H	1.751901000	4.699457000	0.220479000
H	-0.039715000	5.412528000	2.509040000
H	-0.773875000	5.993960000	-1.709413000
H	-2.481154000	5.058834000	2.880638000
H	-3.197333000	5.617661000	-1.344904000
H	-4.838913000	5.218060000	0.258158000

4B. PceA/TBE, Co^I (Charge = 1, Multiplicity = 1)

Co	0.508003000	-2.467660000	-1.341659000
C	-1.767986000	-3.938808000	-0.509657000
C	-3.332509000	-3.748939000	-0.490704000
C	-3.592451000	-3.076020000	-1.885070000
C	-2.267917000	-2.403068000	-2.184157000
C	-2.071414000	-1.406433000	-3.195836000
C	-0.793861000	-1.054257000	-3.585189000
C	-0.382141000	-0.096954000	-4.722399000
C	0.976584000	-0.738979000	-5.124621000
C	1.436649000	-1.262575000	-3.789990000
C	2.762480000	-1.446457000	-3.446061000
C	3.220637000	-1.981544000	-2.249155000
C	4.686684000	-2.008037000	-1.857889000
C	4.656208000	-2.962731000	-0.634085000
C	3.188955000	-2.969173000	-0.237571000
C	2.724313000	-3.493703000	0.951828000
C	1.329174000	-3.722022000	1.164796000
C	0.667341000	-4.290815000	2.429781000
C	-0.745921000	-4.673124000	1.873743000
C	-0.946158000	-3.643180000	0.761486000
C	-1.332214000	-5.287155000	-1.112029000
N	-1.296294000	-2.848795000	-1.421476000
N	0.372284000	-1.554279000	-2.996152000
N	2.409985000	-2.470749000	-1.277106000
N	0.427965000	-3.395869000	0.262594000
C	-4.094864000	-5.063316000	-0.268415000
C	-3.728282000	-2.733597000	0.602918000
C	-5.192894000	-2.299393000	0.615546000
O	-6.062526000	-2.684601000	-0.153335000

N	-5.487756000	-1.331879000	1.573217000
C	-4.064453000	-4.005351000	-3.019172000
C	-3.314172000	-0.824243000	-3.843112000
C	-1.317087000	0.079425000	-5.925477000
C	-0.003805000	1.293600000	-4.108511000
C	-1.057705000	1.928190000	-3.232412000
O	-2.172026000	2.280156000	-3.671999000
N	-0.732101000	2.085925000	-1.933782000
C	5.084632000	-0.589443000	-1.391836000
C	5.618517000	-2.439234000	-3.000615000
C	5.115780000	-4.405840000	-0.925449000
C	3.723237000	-3.863629000	2.028275000
C	0.577530000	-3.155895000	3.476469000
C	1.323141000	-5.540490000	3.041495000
C	-1.848726000	-4.735962000	2.930255000
C	0.855177000	-1.895774000	-6.134615000
H	-4.371963000	-2.319164000	-1.766673000
H	1.660553000	0.019937000	-5.523796000
H	3.506223000	-1.130818000	-4.170378000
H	5.277958000	-2.550429000	0.167557000
H	-0.636791000	-5.664040000	1.414852000
H	-1.294423000	-2.692727000	1.186374000
H	-0.242136000	-5.304402000	-1.196250000
H	-1.749929000	-5.422649000	-2.111269000
H	-1.650777000	-6.125605000	-0.487090000
H	-3.876852000	-5.799671000	-1.043823000
H	-5.170959000	-4.880917000	-0.266182000
H	-3.819045000	-5.504660000	0.695213000
H	-3.115942000	-1.828234000	0.523194000
H	-3.512802000	-3.142989000	1.596494000
H	-6.471378000	-1.265886000	1.818200000
H	-4.847045000	-1.181394000	2.347438000
H	-4.184448000	-3.437088000	-3.945596000
H	-5.033610000	-4.444014000	-2.767257000
H	-3.353780000	-4.812180000	-3.215873000
H	-3.590722000	-1.347246000	-4.765755000
H	-3.183159000	0.228095000	-4.086957000
H	-4.167450000	-0.900588000	-3.164178000
H	-0.742436000	0.510592000	-6.753721000
H	-2.138680000	0.762746000	-5.711334000
H	-1.725174000	-0.877004000	-6.261096000
H	0.191912000	1.988807000	-4.933532000
H	0.921694000	1.182903000	-3.534354000
H	-1.259370000	2.737433000	-1.359151000
H	0.169394000	1.801832000	-1.570315000
H	1.829325000	-2.376009000	-6.265282000
H	0.515459000	-1.538238000	-7.111013000
H	0.149457000	-2.650927000	-5.772049000
H	4.989121000	0.132768000	-2.207349000
H	6.124484000	-0.592553000	-1.047461000
H	4.450144000	-0.252905000	-0.567930000
H	5.609169000	-1.693054000	-3.802038000
H	5.330892000	-3.402465000	-3.430537000
H	6.650029000	-2.512438000	-2.640116000
H	6.165687000	-4.429508000	-1.231657000
H	4.510767000	-4.855669000	-1.719540000
H	5.010438000	-5.025350000	-0.031449000
H	4.670881000	-3.345759000	1.881108000
H	3.925462000	-4.940496000	2.063365000
H	3.363576000	-3.566356000	3.015899000
H	1.576192000	-2.788495000	3.730747000
H	0.109653000	-3.515146000	4.398950000
H	-0.005319000	-2.310292000	3.094934000
H	1.604446000	-6.258513000	2.264196000
H	0.605834000	-6.030240000	3.710281000
H	2.208337000	-5.306179000	3.635171000
H	-1.556005000	-5.382310000	3.764535000
H	-2.773034000	-5.148260000	2.514682000
H	-2.070167000	-3.743486000	3.338034000
C	1.021419000	0.690115000	2.914339000
C	0.429836000	1.069216000	1.783967000
Br	0.374681000	-0.426113000	0.207829000
Br	-0.198750000	2.824054000	1.437091000
Br	1.348106000	1.777190000	4.453401000
H	1.406197000	-0.315956000	3.034159000
C	5.628889000	-2.635759000	5.255219000
C	5.671538000	-1.657161000	4.102840000
C	6.692490000	-1.740995000	3.132604000
C	4.717793000	-0.628840000	3.976915000
C	6.765554000	-0.818340000	2.079834000
C	4.789284000	0.297678000	2.924711000
C	5.815567000	0.210602000	1.974388000
H	5.717760000	-3.678575000	4.900375000
H	4.690708000	-2.545880000	5.828066000
H	6.467156000	-2.458971000	5.954337000
H	7.444792000	-2.535034000	3.210929000
H	3.916692000	-0.538408000	4.720987000
H	7.574232000	-0.895162000	1.344231000
H	4.044857000	1.097112000	2.858325000
H	5.873468000	0.942440000	1.162934000
C	-6.430150000	3.036489000	5.050317000
C	-5.366711000	2.288182000	4.280966000
C	-4.884933000	1.054537000	4.740526000
C	-4.809499000	2.813449000	3.106220000
C	-3.895695000	0.357987000	4.044887000

C	-3.820771000	2.129030000	2.399552000
C	-3.377775000	0.892364000	2.866031000
O	-2.519390000	0.096828000	2.091549000
H	-7.137839000	2.348628000	5.523344000
H	-6.989287000	3.715289000	4.399507000
H	-5.978348000	3.641134000	5.846468000
H	-5.286584000	0.630433000	5.657868000
H	-5.153805000	3.769951000	2.719546000
H	-3.519882000	-0.595685000	4.407637000
H	-3.403160000	2.558132000	1.494976000
H	-1.586669000	0.408210000	2.139202000
C	-8.488556000	0.116075000	-0.889390000
C	-7.791451000	1.423575000	-1.289780000
C	-6.700593000	1.898260000	-0.309320000
N	-5.485363000	1.070689000	-0.270343000
C	-4.383660000	1.279209000	-1.005332000
N	-4.418740000	2.125485000	-2.069965000
N	-3.232297000	0.683281000	-0.658378000
H	-7.776308000	-0.726837000	-0.828548000
H	-9.265464000	-0.152772000	-1.624107000
H	-8.980212000	0.222474000	0.095028000
H	-7.357444000	1.321762000	-2.304740000
H	-8.535508000	2.238942000	-1.358037000
H	-7.096356000	1.912168000	0.720827000
H	-6.398387000	2.934952000	-0.536842000
H	-5.424530000	0.330241000	0.448247000
H	-5.294639000	2.172926000	-2.590392000
H	-3.550347000	2.227006000	-2.655737000
H	-3.044811000	0.389976000	0.316517000
H	-2.410883000	0.735938000	-1.265005000
C	7.462959000	5.382145000	-0.244389000
C	6.529317000	4.737561000	-1.234523000
C	6.626790000	4.797085000	-2.612884000
C	5.365495000	3.921924000	-0.954885000
N	5.601464000	4.070763000	-3.201563000
C	4.811296000	3.516279000	-2.215643000
C	4.732989000	3.482384000	0.231156000
C	3.682000000	2.683423000	-2.310716000
C	3.607667000	2.656432000	0.140565000
C	3.095095000	2.252514000	-1.116555000
H	6.927059000	6.090975000	0.414083000
H	8.264165000	5.937558000	-0.758805000
H	7.938050000	4.627789000	0.410195000
H	7.364751000	5.309576000	-3.231933000
H	5.462403000	3.961703000	-4.201239000
H	5.123800000	3.779306000	1.210423000
H	3.292349000	2.363790000	-3.283822000
H	3.111356000	2.305887000	1.050270000
H	2.253098000	1.551374000	-1.141454000
C	1.356844000	5.629971000	-0.708212000
C	-0.149017000	5.558021000	-0.622158000
C	-0.829897000	5.723228000	0.605757000
C	-0.924123000	5.213593000	-1.743330000
C	-2.193902000	5.428545000	0.741520000
C	-2.293900000	4.927070000	-1.631675000
C	-2.918347000	4.967354000	-0.371852000
O	-4.218044000	4.558861000	-0.190900000
H	1.772672000	6.378391000	-0.012277000
H	1.696183000	5.879386000	-1.727609000
H	1.803640000	4.653385000	-0.443381000
H	-0.269292000	6.047315000	1.489716000
H	-0.446666000	5.130210000	-2.726212000
H	-2.694628000	5.513305000	1.710656000
H	-2.865872000	4.649030000	-2.523058000
H	-4.475612000	4.053449000	-0.989592000

4C. PceA/TBE, Co^I → Co^{III} Transition State (Charge = 1, Multiplicity = 1)

Co	-0.575686000	-2.561256000	1.099065000
C	1.706959000	-4.136609000	0.434340000
C	3.268830000	-3.934907000	0.484638000
C	3.466862000	-3.265410000	1.891409000
C	2.127200000	-2.602121000	2.139441000
C	1.885912000	-1.604125000	3.146731000
C	0.597888000	-1.220442000	3.456552000
C	0.128642000	-0.244922000	4.554694000
C	-1.269417000	-0.856284000	4.867937000
C	-1.644046000	-1.397662000	3.514956000
C	-2.946937000	-1.597481000	3.095606000
C	-3.335123000	-2.102997000	1.862088000
C	-4.781280000	-2.342750000	1.490985000
C	-4.672675000	-2.537198000	-0.050214000
C	-3.196257000	-2.849295000	-0.253062000
C	-2.639050000	-3.333124000	-1.420043000
C	-1.261954000	-3.718373000	-1.482175000
C	-0.532597000	-4.344195000	-2.682873000
C	0.763388000	-4.879390000	-1.983270000
C	0.963574000	-3.840306000	-0.880216000
C	1.236661000	-5.480260000	1.017089000
N	1.200052000	-3.045681000	1.329035000
N	-0.537823000	-1.703459000	2.796063000
N	-2.479581000	-2.513803000	0.896006000
N	-0.429019000	-3.514057000	-0.486859000
C	4.054351000	-5.240938000	0.303031000
C	3.689594000	-2.912339000	-0.594129000

C	5.152194000	-2.473656000	-0.575228000
O	6.006973000	-2.876051000	0.205409000
N	5.450157000	-1.512020000	-1.522409000
C	3.901072000	-4.194903000	3.040073000
C	3.094309000	-1.055676000	3.878670000
C	0.979165000	-0.082344000	5.820208000
C	-0.178637000	1.144007000	3.902912000
C	0.961209000	1.797366000	3.148818000
O	2.062456000	2.041920000	3.684199000
N	0.705769000	2.109062000	1.869095000
C	-5.729882000	-1.189499000	1.846434000
C	-5.221562000	-3.631713000	2.230695000
C	-5.717800000	-3.513116000	-0.610424000
C	-3.492466000	-3.401653000	-2.668218000
C	-0.184652000	-3.223789000	-3.693156000
C	-1.264483000	-5.506850000	-3.372085000
C	1.949191000	-5.108838000	-2.917818000
C	-1.253025000	-1.994660000	5.906592000
H	4.238706000	-2.495903000	1.802337000
H	-1.965867000	-0.076566000	5.198011000
H	-3.734215000	-1.329374000	3.792823000
H	-4.847145000	-1.554945000	-0.515649000
H	0.489682000	-5.833016000	-1.513205000
H	1.370192000	-2.914901000	-1.305554000
H	0.142819000	-5.496338000	1.046659000
H	1.606481000	-5.617882000	2.034826000
H	1.581516000	-6.318506000	0.406308000
H	3.788486000	-5.987547000	1.053847000
H	5.125044000	-5.045054000	0.378447000
H	3.856701000	-5.673883000	-0.682503000
H	3.075776000	-2.004792000	-0.534326000
H	3.508586000	-3.328251000	-1.591843000
H	6.428230000	-1.407791000	-1.769479000
H	4.775153000	-1.271432000	-2.241863000
H	3.983681000	-3.631896000	3.973344000
H	4.881606000	-4.624344000	2.820249000
H	3.190674000	-5.009372000	3.205264000
H	3.286219000	-1.591030000	4.815534000
H	2.969348000	-0.001608000	4.115902000
H	3.989792000	-1.150432000	3.261202000
H	0.358963000	0.376525000	6.598921000
H	1.831855000	0.575068000	5.655839000
H	1.332521000	-1.046106000	6.194863000
H	-0.468668000	1.833887000	4.705211000
H	-1.038060000	1.041820000	3.232073000
H	1.338522000	2.704680000	1.345191000
H	-0.170659000	1.875740000	1.418944000
H	-2.245300000	-2.450577000	5.974232000
H	-0.981179000	-1.620619000	6.897416000
H	-0.539456000	-2.773877000	5.618322000
H	-5.820508000	-1.062459000	2.931258000
H	-6.731090000	-1.408836000	1.459772000
H	-5.393368000	-0.248594000	1.404630000
H	-5.140805000	-3.480909000	3.312034000
H	-4.590788000	-4.483921000	1.957741000
H	-6.261818000	-3.878074000	1.999814000
H	-6.687955000	-3.298555000	-0.150534000
H	-5.460127000	-4.554779000	-0.397494000
H	-5.853141000	-3.397072000	-1.684279000
H	-4.219718000	-2.588322000	-2.674208000
H	-4.031252000	-4.350239000	-2.769204000
H	-2.881582000	-3.275608000	-3.561588000
H	-1.087530000	-2.752538000	-4.088586000
H	0.371112000	-3.640093000	-4.539121000
H	0.421278000	-2.439753000	-3.226420000
H	-1.666983000	-6.209122000	-2.634574000
H	-0.556424000	-6.051212000	-4.006779000
H	-2.081754000	-5.172664000	-4.013082000
H	1.666214000	-5.752794000	-3.757001000
H	2.769999000	-5.605342000	-2.393888000
H	2.328495000	-4.168728000	-3.330569000
C	-0.468239000	0.948772000	-3.074449000
C	0.337196000	1.255840000	-2.053537000
Br	-0.127555000	-0.601926000	-0.219845000
Br	0.444878000	3.042332000	-1.382789000
Br	-1.547357000	2.136739000	-4.120283000
H	-0.561998000	-0.073941000	-3.421820000
C	-5.974032000	-1.618152000	-5.204792000
C	-5.900180000	-0.846232000	-3.903206000
C	-6.957980000	-0.878626000	-2.971611000
C	-4.780265000	-0.041484000	-3.605327000
C	-6.909485000	-0.114562000	-1.793828000
C	-4.725269000	0.717808000	-2.428635000
C	-5.794924000	0.693678000	-1.519900000
H	-6.659172000	-2.479525000	-5.128708000
H	-4.979957000	-1.989542000	-5.509742000
H	-6.344954000	-0.970429000	-6.021301000
H	-7.837116000	-1.500756000	-3.177568000
H	-3.940288000	0.001510000	-4.308757000
H	-7.750093000	-0.146169000	-1.091445000
H	-3.849533000	1.338842000	-2.223441000
H	-5.752669000	1.307443000	-0.613826000
C	6.283174000	3.597066000	-4.759342000
C	5.364494000	2.681786000	-3.989222000
C	4.980708000	1.437681000	-4.505081000

C	4.825465000	3.075928000	-2.755785000
C	4.083396000	0.616134000	-3.821876000
C	3.934548000	2.262447000	-2.062135000
C	3.557997000	1.018232000	-2.587840000
O	2.717875000	0.175083000	-1.900093000
H	6.934738000	3.035547000	-5.436295000
H	6.913685000	4.188685000	-4.087565000
H	5.706105000	4.303481000	-5.369779000
H	5.374818000	1.113246000	-5.465918000
H	5.090255000	4.040360000	-2.327662000
H	3.761514000	-0.332818000	-4.246372000
H	3.512018000	2.602561000	-1.122638000
H	1.636885000	0.580624000	-1.919695000
C	8.482519000	-0.212838000	0.597248000
C	7.899982000	1.062459000	1.226552000
C	6.718191000	1.673264000	0.449009000
N	5.511434000	0.841163000	0.414975000
C	4.408344000	1.022437000	1.161989000
N	4.437638000	1.798124000	2.264476000
N	3.267699000	0.422063000	0.779696000
H	7.742428000	-1.032707000	0.575547000
H	9.354587000	-0.566775000	1.171861000
H	8.820359000	-0.018477000	-0.437809000
H	7.583124000	0.856276000	2.268032000
H	8.683192000	1.841216000	1.288835000
H	7.005054000	1.858863000	-0.601592000
H	6.436229000	2.654868000	0.869635000
H	5.428784000	0.145138000	-0.339876000
H	5.321710000	1.955142000	2.741133000
H	3.556810000	1.973670000	2.798423000
H	3.067895000	0.263634000	-0.243801000
H	2.441468000	0.491486000	1.372167000
C	-7.277616000	5.571573000	1.466370000
C	-6.449538000	4.374664000	1.860199000
C	-6.664544000	3.552470000	2.951558000
C	-5.276009000	3.846540000	1.191741000
N	-5.698731000	2.555262000	3.003169000
C	-4.828896000	2.708032000	1.941355000
C	-4.556948000	4.207646000	0.028113000
C	-3.707981000	1.945195000	1.563225000
C	-3.444916000	3.450783000	-0.354445000
C	-3.025309000	2.328036000	0.402659000
H	-6.668890000	6.494690000	1.454647000
H	-8.112281000	5.723720000	2.170038000
H	-7.703572000	5.450379000	0.453105000
H	-7.446298000	3.601809000	3.711106000
H	-5.641988000	1.830910000	3.711779000
H	-4.873015000	5.068410000	-0.570850000
H	-3.392043000	1.069182000	2.140613000
H	-2.884963000	3.718182000	-1.256234000
H	-2.172762000	1.733943000	0.053478000
C	-1.152346000	5.564735000	1.672176000
C	0.316886000	5.571846000	1.311702000
C	0.753959000	5.917552000	0.014257000
C	1.298657000	5.162397000	2.233076000
C	2.094923000	5.798167000	-0.372252000
C	2.646498000	5.028000000	1.863166000
C	3.044556000	5.321634000	0.547325000
O	4.337867000	5.157014000	0.111707000
H	-1.708016000	6.350775000	1.133627000
H	-1.304511000	5.714177000	2.754774000
H	-1.617445000	4.599576000	1.396728000
H	0.022763000	6.271035000	-0.721430000
H	1.010512000	4.915136000	3.260900000
H	2.415175000	6.050643000	-1.387021000
H	3.383899000	4.687734000	2.599719000
H	4.892461000	4.912950000	0.873915000

4D. PceA/TBE, Co^{III} (Charge = 1, Multiplicity = 1)

Co	0.463728000	-2.414674000	-1.297323000
C	-1.879629000	-3.979682000	-0.863746000
C	-3.433226000	-3.766457000	-1.022532000
C	-3.525775000	-3.001150000	-2.390816000
C	-2.175183000	-2.322994000	-2.484607000
C	-1.858840000	-1.231681000	-3.369356000
C	-0.545976000	-0.875082000	-3.589864000
C	0.015353000	0.206511000	-4.529941000
C	1.395134000	-0.437323000	-4.876226000
C	1.686393000	-1.170168000	-3.594415000
C	2.958942000	-1.482949000	-3.143518000
C	3.268479000	-2.082759000	-1.929933000
C	4.682238000	-2.411606000	-1.506723000
C	4.495481000	-2.650747000	0.022123000
C	2.998228000	-2.896963000	0.149528000
C	2.359994000	-3.387458000	1.272077000
C	0.962488000	-3.707071000	1.255049000
C	0.145425000	-4.355478000	2.384437000
C	-1.123330000	-4.822280000	1.588886000
C	-1.230958000	-3.738909000	0.515215000
C	-1.368794000	-5.296567000	-1.471227000
N	-1.305497000	-2.848798000	-1.662663000
N	0.540382000	-1.496607000	-2.960106000
N	2.353314000	-2.490821000	-1.017842000
N	0.192144000	-3.424260000	0.231761000

C	-4.233821000	-5.074194000	-0.985855000
C	-3.922942000	-2.803589000	0.074475000
C	-5.386627000	-2.356930000	0.004317000
O	-6.202754000	-2.723446000	-0.837859000
N	-5.699104000	-1.478261000	1.006401000
C	-3.846827000	-3.840947000	-3.641467000
C	-3.020262000	-0.551011000	-4.062896000
C	-0.772294000	0.581565000	-5.791061000
C	0.364344000	1.470016000	-3.676825000
C	-0.774763000	2.136906000	-2.927320000
O	-1.869925000	2.390551000	-3.468780000
N	-0.514137000	2.463765000	-1.653639000
C	5.699971000	-1.296418000	-1.784277000
C	5.088623000	-3.696860000	-2.271999000
C	5.468120000	-3.692586000	0.593834000
C	3.141920000	-3.546501000	2.555865000
C	-0.222806000	-3.258227000	3.413197000
C	0.800367000	-5.565768000	3.069149000
C	-2.369764000	-5.041222000	2.444137000
C	1.368753000	-1.423316000	-6.059487000
H	-4.316616000	-2.251039000	-2.306818000
H	2.143089000	0.340589000	-5.069356000
H	3.789424000	-1.205145000	-3.784327000
H	4.693672000	-1.693091000	0.527720000
H	-0.851658000	-5.767919000	1.101294000
H	-1.656103000	-2.824348000	0.943664000
H	-0.276140000	-5.325916000	-1.414129000
H	-1.657437000	-5.380475000	-2.520541000
H	-1.769668000	-6.158492000	-0.932429000
H	-3.919843000	-5.772663000	-1.764678000
H	-5.294909000	-4.859019000	-1.121960000
H	-4.109885000	-5.573060000	-0.019124000
H	-3.307624000	-1.896272000	0.092737000
H	-3.797764000	-3.262910000	1.060054000
H	-6.674683000	-1.315939000	1.222160000
H	-4.963571000	-1.180436000	1.657417000
H	-3.866201000	-3.204244000	-4.530602000
H	-4.833136000	-4.298947000	-3.535110000
H	-3.109448000	-4.630345000	-3.811598000
H	-3.199410000	-0.962994000	-5.062658000
H	-2.846774000	0.518527000	-4.161313000
H	-3.936741000	-0.686801000	-3.485152000
H	-0.099127000	1.108785000	-6.477192000
H	-1.600580000	1.251991000	-5.569016000
H	-1.153232000	-0.303716000	-6.306273000
H	0.780192000	2.227660000	-4.354216000
H	1.150890000	1.210174000	-2.961400000
H	-1.142817000	3.070236000	-1.134096000
H	0.361321000	2.216629000	-1.212224000
H	2.340039000	-1.918639000	-6.152648000
H	1.158563000	-0.905452000	-6.999012000
H	0.607293000	-2.195457000	-5.906916000
H	5.845234000	-1.143011000	-2.859765000
H	6.671098000	-1.574441000	-1.360755000
H	5.388009000	-0.353134000	-1.330224000
H	5.064202000	-3.506112000	-3.349780000
H	4.405607000	-4.525041000	-2.056942000
H	6.103916000	-4.002937000	-2.004857000
H	6.466527000	-3.507477000	0.184561000
H	5.175269000	-4.714042000	0.333765000
H	5.559542000	-3.617422000	1.676084000
H	3.909607000	-2.774908000	2.630184000
H	3.623310000	-4.526641000	2.644499000
H	2.490105000	-3.421241000	3.419822000
H	0.671630000	-2.816812000	3.858985000
H	-0.821953000	-3.690629000	4.220713000
H	-0.790561000	-2.445979000	2.948584000
H	1.254747000	-6.237650000	2.333482000
H	0.033158000	-6.128542000	3.612033000
H	1.563130000	-5.280534000	3.795891000
H	-2.159167000	-5.728730000	3.269984000
H	-3.177705000	-5.483039000	1.854473000
H	-2.735311000	-4.102868000	2.872250000
C	-0.192976000	0.465292000	4.335198000
C	-0.573751000	0.925156000	3.148783000
Br	0.080801000	-0.444964000	-0.071482000
Br	0.245220000	2.358895000	2.225656000
Br	1.255695000	1.094813000	5.369758000
H	-0.736045000	-0.346419000	4.806302000
C	5.810762000	-1.988216000	5.105080000
C	5.719923000	-1.134988000	3.856688000
C	6.786606000	-1.066854000	2.937840000
C	4.571352000	-0.355800000	3.598511000
C	6.719194000	-0.229883000	1.812092000
C	4.496930000	0.476114000	2.472390000
C	5.576809000	0.551001000	1.577460000
H	4.854245000	-2.497541000	5.317714000
H	6.048449000	-1.363737000	5.986736000
H	6.599428000	-2.754458000	5.017963000
H	7.687388000	-1.666649000	3.114287000
H	3.724516000	-0.393159000	4.293464000
H	7.566654000	-0.181516000	1.119156000
H	3.595886000	1.072593000	2.297050000
H	5.523862000	1.217877000	0.711239000
C	-6.062788000	4.045836000	4.615090000

C	-5.338117000	2.952111000	3.875600000
C	-5.467849000	1.605439000	4.251924000
C	-4.477239000	3.247666000	2.806738000
C	-4.784762000	0.595211000	3.585253000
C	-3.779484000	2.252707000	2.138152000
C	-3.932762000	0.885594000	2.487468000
O	-3.344259000	-0.086016000	1.801369000
H	-7.022741000	3.696215000	5.009865000
H	-6.251240000	4.908020000	3.966873000
H	-5.472406000	4.404866000	5.469126000
H	-6.118705000	1.347392000	5.085681000
H	-4.364303000	4.277009000	2.474641000
H	-4.893194000	-0.442065000	3.897800000
H	-3.120200000	2.517948000	1.318014000
H	-1.417076000	0.495618000	2.610814000
C	-8.424816000	0.522709000	-0.867013000
C	-7.776617000	1.873100000	-1.193076000
C	-6.572507000	2.205224000	-0.298190000
N	-5.463512000	1.251385000	-0.414482000
C	-4.308360000	1.455022000	-1.067072000
N	-4.240528000	2.428773000	-2.028646000
N	-3.243025000	0.730671000	-0.718684000
H	-7.726418000	-0.317268000	-1.033404000
H	-9.310835000	0.346443000	-1.499618000
H	-8.756636000	0.492669000	0.187586000
H	-7.462547000	1.893252000	-2.255746000
H	-8.513631000	2.688638000	-1.072288000
H	-6.869413000	2.211054000	0.765472000
H	-6.185107000	3.214697000	-0.513388000
H	-5.477547000	0.424064000	0.197203000
H	-5.080098000	2.552866000	-2.595795000
H	-3.343604000	2.501954000	-2.564949000
H	-3.189982000	0.349465000	0.302259000
H	-2.372619000	0.813400000	-1.243132000
C	7.697749000	5.257383000	-1.362868000
C	6.785008000	4.150164000	-1.821309000
C	6.963424000	3.349870000	-2.934943000
C	5.557824000	3.694709000	-1.198282000
N	5.926725000	2.431357000	-3.041318000
C	5.046368000	2.616001000	-1.994026000
C	4.840206000	4.073187000	-0.039407000
C	3.869000000	1.923188000	-1.659603000
C	3.671829000	3.383187000	0.299932000
C	3.192828000	2.314218000	-0.497905000
H	7.166916000	6.226645000	-1.324385000
H	8.558126000	5.368361000	-2.042744000
H	8.088701000	5.060519000	-0.347388000
H	7.765848000	3.362872000	-3.674078000
H	5.832787000	1.737758000	-3.776252000
H	5.204104000	4.890124000	0.592617000
H	3.508162000	1.086557000	-2.266815000
H	3.123775000	3.657909000	1.207380000
H	2.309503000	1.751067000	-0.174696000
C	1.589826000	5.665850000	-1.656868000
C	0.142317000	5.545316000	-1.251569000
C	-0.221934000	5.330323000	0.093305000
C	-0.885677000	5.550538000	-2.214445000
C	-1.547470000	5.064449000	0.463198000
C	-2.216916000	5.293121000	-1.863697000
C	-2.550113000	5.015362000	-0.523147000
O	-3.828134000	4.694596000	-0.142588000
H	2.201826000	6.121855000	-0.861015000
H	1.706289000	6.270523000	-2.572558000
H	2.025672000	4.667956000	-1.855919000
H	0.553260000	5.343343000	0.868243000
H	-0.640243000	5.732215000	-3.266781000
H	-1.813440000	4.866780000	1.505329000
H	-2.998988000	5.289429000	-2.630213000
H	-4.230876000	4.190555000	-0.882260000

5A. NpRdhA/DBMP with neutralized R552, Co^{II} (Charge = 1, Multiplicity = 2)

C	3.032077000	7.671627000	-1.417080000
C	6.307168000	4.575109000	2.035657000
C	-6.524037000	-2.159147000	3.366956000
C	-10.145216000	2.458704000	0.637244000
C	-0.083840000	5.248630000	3.277189000
C	-4.490884000	-2.214045000	-5.220015000
Co	1.721874000	-2.818189000	0.335838000
C	-1.226236000	2.387838000	-0.211288000
C	-0.933204000	1.471682000	-1.251803000
C	-1.457243000	1.548098000	-2.540254000
C	-2.372984000	2.552548000	-2.871907000
C	-2.722315000	3.468653000	-1.870233000
C	-2.164999000	3.384134000	-0.601315000
O	-0.699735000	2.313149000	0.979487000
Br	0.247495000	0.006686000	-0.834549000
Br	-2.647641000	4.683063000	0.714896000
C	-3.014307000	2.608553000	-4.237200000
H	-2.428853000	2.047771000	-4.972272000
H	-4.021887000	2.175162000	-4.207805000
H	-3.107872000	3.639923000	-4.591182000
H	-1.183483000	0.795358000	-3.273258000
H	-3.440722000	4.254475000	-2.082660000
C	-4.455535000	-2.111348000	-3.709635000

C	-3.687095000	-1.122789000	-3.066427000
C	-3.666110000	-1.011837000	-1.667629000
C	-4.423865000	-1.886636000	-0.877147000
C	-5.181395000	-2.890908000	-1.504033000
C	-5.195499000	-3.002533000	-2.902924000
H	-5.527298000	-2.166257000	-5.599350000
H	-4.065219000	-3.175044000	-5.565304000
H	-3.917563000	-1.399233000	-5.693173000
H	-3.112968000	-0.416750000	-3.676143000
H	-3.074377000	-0.224274000	-1.191003000
H	-4.437490000	-1.752294000	0.211375000
H	-5.782507000	-3.578143000	-0.897566000
H	-5.802896000	-3.781509000	-3.379302000
C	2.686613000	6.252097000	-1.805230000
C	3.678332000	5.367468000	-2.254816000
C	3.375422000	4.067564000	-2.651271000
C	2.052457000	3.620762000	-2.605644000
C	1.045957000	4.477434000	-2.154317000
C	1.371410000	5.776224000	-1.758044000
O	1.797586000	2.324559000	-3.003468000
H	0.841375000	2.160906000	-2.895673000
H	3.365040000	8.247632000	-2.288699000
H	3.843734000	7.696031000	-0.680365000
H	2.167756000	8.185663000	-0.986742000
H	4.712205000	5.703086000	-2.300792000
H	4.153632000	3.396113000	-2.999144000
H	0.014811000	4.135255000	-2.114489000
H	0.574798000	6.431118000	-1.412071000
C	4.891160000	4.695209000	1.465706000
C	4.110224000	3.384578000	1.619421000
C	2.685599000	3.476658000	1.085275000
N	1.969520000	2.179267000	1.294234000
H	2.049751000	1.872176000	2.307258000
H	0.921753000	2.231258000	1.078910000
H	2.364718000	1.427172000	0.715161000
H	6.872545000	3.783996000	1.511470000
H	6.282114000	4.319313000	3.110742000
H	6.866896000	5.520642000	1.929112000
H	4.934542000	4.967145000	0.394244000
H	4.343661000	5.513168000	1.973734000
H	4.652723000	2.583040000	1.083920000
H	4.073212000	3.098369000	2.688158000
H	2.657392000	3.716104000	0.010229000
H	2.095377000	4.229758000	1.626583000
C	-6.526286000	-0.935333000	2.444945000
C	-5.333854000	0.006078000	2.665650000
N	-4.065176000	-0.619683000	2.298159000
C	-3.003001000	0.114233000	2.337387000
N	-2.924339000	1.444895000	2.752549000
N	-1.741520000	-0.441239000	2.058479000
H	-2.183406000	1.987992000	2.288570000
H	-3.817116000	1.938094000	2.753814000
H	-1.817795000	-1.309008000	1.528713000
H	-1.096667000	0.220610000	1.611935000
H	-7.381301000	-2.823835000	3.158948000
H	-6.580787000	-1.856829000	4.429129000
H	-5.593983000	-2.740593000	3.234155000
H	-7.454759000	-0.352002000	2.590439000
H	-6.528757000	-1.253118000	1.385694000
H	-5.512148000	0.927187000	2.067384000
H	-5.319060000	0.321077000	3.734457000
C	-8.702849000	2.203327000	0.241901000
C	-8.340587000	1.033577000	-0.459336000
C	-7.016198000	0.805914000	-0.860762000
C	-6.018747000	1.748419000	-0.565986000
C	-6.359845000	2.915133000	0.134962000
C	-7.687576000	3.136608000	0.534721000
H	-10.722675000	2.847017000	-0.223080000
H	-10.216524000	3.202095000	1.448756000
H	-10.640834000	1.530720000	0.971609000
H	-9.110154000	0.287623000	-0.691856000
H	-6.755142000	-0.113142000	-1.396593000
H	-4.982322000	1.566507000	-0.868883000
H	-5.587553000	3.654643000	0.375676000
H	-7.941466000	4.051512000	1.083420000
O	0.090619000	3.872178000	2.966112000
H	0.251332000	5.900289000	2.446046000
H	0.533090000	5.466062000	4.164490000
H	-1.137936000	5.493953000	3.511454000
H	-0.428430000	3.607842000	2.159699000
C	1.082750000	-3.948873000	-4.869423000
C	1.256306000	-2.815100000	-3.843790000
C	0.547772000	-1.529637000	-4.328997000
C	2.787161000	-2.568612000	-3.602101000
C	3.467684000	-1.686852000	-4.648002000
C	2.808917000	-2.036926000	-2.168492000
C	4.015036000	-2.235422000	-1.222317000
C	5.174272000	-1.170453000	-1.220716000
C	5.484794000	-1.019354000	0.312838000
C	4.176131000	-1.415389000	0.965695000
C	3.825254000	-1.149262000	2.335555000
C	4.745436000	-0.223450000	3.106896000
C	6.673855000	-1.829971000	0.865370000
C	4.647497000	0.199843000	-1.746679000
C	5.708199000	1.294889000	-1.718171000

N	6.202155000	1.665696000	-2.933022000
O	6.106022000	1.811512000	-0.674359000
C	6.397132000	-1.587441000	-2.046866000
C	4.515715000	-3.688474000	-1.308668000
N	3.389602000	-2.040353000	0.121919000
N	1.683321000	-2.766411000	-1.529035000
C	0.791029000	-3.153836000	-2.416402000
C	-0.431527000	-3.796802000	-2.041263000
C	-1.472197000	-4.121397000	-3.093974000
C	-0.682802000	-4.151765000	-0.729303000
N	0.091349000	-3.813933000	0.374009000
C	-1.804703000	-5.086862000	-0.307981000
C	-1.519232000	-6.508762000	-0.833879000
C	-1.820051000	-4.957597000	1.242789000
C	-2.017591000	-6.273952000	2.011507000
C	-2.920873000	-3.957272000	1.668885000
C	-0.473896000	-4.311073000	1.504259000
C	0.067242000	-4.164832000	2.774357000
C	1.152791000	-3.367380000	3.097091000
N	1.888130000	-2.650526000	2.213707000
C	1.660876000	-3.145202000	4.493796000
C	2.738786000	-4.188730000	4.844458000
C	2.193846000	-1.682836000	4.356406000
C	2.720058000	-1.755029000	2.904977000
C	3.170368000	-1.318697000	5.479022000
C	0.907390000	-0.804571000	4.447068000
C	1.044931000	0.676353000	4.150160000
O	2.137568000	1.183098000	3.810283000
N	-0.070274000	1.408074000	4.254806000
H	1.373301000	-4.915002000	-4.443859000
H	1.729790000	-3.750891000	-5.731538000
H	0.060641000	-4.025969000	-5.243606000
H	-0.538380000	-1.650995000	-4.307214000
H	0.842015000	-1.302421000	-5.358554000
H	0.800993000	-0.673583000	-3.697107000
H	3.262403000	-3.557847000	-3.606193000
H	4.551717000	-1.671520000	-4.499305000
H	3.100557000	-0.656181000	-4.607369000
H	3.287613000	-2.068865000	-5.658208000
H	5.701772000	0.034672000	0.508611000
H	4.171366000	0.445082000	3.743298000
H	5.327910000	0.396006000	2.422745000
H	5.455625000	-0.779452000	3.729384000
H	6.771205000	-1.660060000	1.940637000
H	7.605179000	-1.506008000	0.393235000
H	6.558627000	-2.905630000	0.706825000
H	3.812100000	0.542225000	-1.126600000
H	4.266058000	0.083750000	-2.763372000
H	5.881310000	1.254919000	-3.797396000
H	6.921121000	2.377036000	-2.970051000
H	6.817249000	-2.537163000	-1.711362000
H	7.185259000	-0.832263000	-1.969878000
H	6.137263000	-1.688769000	-3.105635000
H	3.666450000	-4.371459000	-1.200197000
H	5.227943000	-3.906295000	-0.510942000
H	4.997310000	-3.889302000	-2.269250000
H	-2.467411000	-4.183520000	-2.650657000
H	-1.269607000	-5.062908000	-3.616885000
H	-1.523438000	-3.332622000	-3.845565000
H	-2.762927000	-4.746704000	-0.715204000
H	-2.300981000	-7.204584000	-0.517023000
H	-0.556086000	-6.877640000	-0.466312000
H	-1.487654000	-6.514709000	-1.925438000
H	-2.059820000	-6.081362000	3.088137000
H	-1.214999000	-6.992287000	1.824433000
H	-2.970414000	-6.731815000	1.728585000
H	-2.865219000	-3.033853000	1.090126000
H	-2.842761000	-3.699107000	2.728291000
H	-3.908067000	-4.396508000	1.489149000
H	-0.449450000	-4.646758000	3.596887000
H	0.851660000	-3.197034000	5.229794000
H	2.318368000	-5.196796000	4.781237000
H	3.110890000	-4.037410000	5.861350000
H	3.583716000	-4.124714000	4.150247000
H	2.715442000	-1.595094000	6.437622000
H	3.373101000	-0.248378000	5.503607000
H	4.116891000	-1.856577000	5.389715000
H	0.503482000	-0.917064000	5.461688000
H	0.129396000	-1.184558000	3.768531000
H	-0.041424000	2.396041000	3.951933000
H	-0.981665000	0.968355000	4.327120000
H	2.536355000	-0.974138000	-2.162083000

5B. NpRdhA/DBMP with neutralized R552, Co^I (Charge = 0, Multiplicity = 1)

C	3.049661000	7.685182000	-1.683509000
C	6.323233000	4.510081000	1.698554000
C	-6.640384000	-1.896372000	3.331152000
C	-10.205012000	2.809020000	0.677444000
C	-0.018779000	5.346281000	3.084093000
C	-4.805143000	-2.010768000	-5.299651000
Co	1.514942000	-2.766596000	0.114633000
C	-0.959755000	2.471564000	-0.449104000
C	-0.631073000	1.414439000	-1.335693000
C	-1.003016000	1.382470000	-2.676323000

C	-1.757416000	2.419300000	-3.234183000
C	-2.137370000	3.471333000	-2.387730000
C	-1.751428000	3.486789000	-1.053817000
O	-0.589281000	2.498152000	0.803982000
Br	0.323435000	-0.157465000	-0.613430000
Br	-2.295266000	4.950444000	0.054878000
C	-2.184130000	2.394560000	-4.683246000
H	-1.707609000	1.565552000	-5.215934000
H	-3.270746000	2.272381000	-4.775163000
H	-1.913608000	3.324627000	-5.196348000
H	-0.719005000	0.525530000	-3.280716000
H	-2.738925000	4.289884000	-2.772652000
C	-4.820413000	-1.785540000	-3.800101000
C	-4.019725000	-0.784031000	-3.209757000
C	-4.077091000	-0.525562000	-1.832437000
C	-4.939117000	-1.270321000	-1.012158000
C	-5.722958000	-2.284326000	-1.580039000
C	-5.661216000	-2.540226000	-2.959193000
H	-5.260304000	-2.979147000	-5.567876000
H	-3.775283000	-1.992212000	-5.700070000
H	-5.372082000	-1.217362000	-5.822309000
H	-3.348774000	-0.189644000	-3.840007000
H	-3.450987000	0.258912000	-1.395327000
H	-4.993448000	-1.059626000	0.059155000
H	-6.390606000	-2.877784000	-0.945605000
H	-6.283489000	-3.332359000	-3.392887000
C	2.946713000	6.179680000	-1.753839000
C	4.083440000	5.365306000	-1.654439000
C	3.996243000	3.975630000	-1.717529000
C	2.747291000	3.372664000	-1.879104000
C	1.604360000	4.161763000	-2.019527000
C	1.711655000	5.549003000	-1.944183000
O	2.690260000	1.992819000	-1.860124000
H	1.753398000	1.716158000	-1.908320000
H	3.279395000	8.114049000	-2.667770000
H	3.843950000	7.998440000	-0.997338000
H	2.109404000	8.129585000	-1.342407000
H	5.059433000	5.823931000	-1.508285000
H	4.882169000	3.355813000	-1.616495000
H	0.635135000	3.695677000	-2.167263000
H	0.806538000	6.146605000	-2.026239000
C	4.803261000	4.544520000	1.907074000
C	4.127719000	3.180483000	1.689008000
C	2.606504000	3.302499000	1.680183000
N	1.922481000	1.991141000	1.470462000
H	1.872772000	1.443127000	2.368004000
H	0.890781000	2.135095000	1.163017000
H	2.370030000	1.424489000	0.737499000
H	6.566905000	4.213757000	0.661902000
H	6.805528000	3.774960000	2.365871000
H	6.773586000	5.500554000	1.886750000
H	4.354960000	5.276227000	1.207432000
H	4.568654000	4.906152000	2.926845000
H	4.456060000	2.765401000	0.719591000
H	4.453869000	2.462054000	2.464112000
H	2.278233000	3.973961000	0.869214000
H	2.213052000	3.694790000	2.629050000
C	-5.412127000	-2.054916000	4.240359000
C	-4.066642000	-1.876075000	3.510902000
N	-3.830801000	-0.486838000	3.149303000
C	-3.098739000	-0.222720000	2.106014000
N	-2.442865000	-1.150413000	1.317301000
N	-3.003868000	1.087358000	1.647400000
H	-1.813839000	-0.824284000	0.583834000
H	-2.180853000	-2.052192000	1.713460000
H	-3.508821000	1.737489000	2.249146000
H	-2.066571000	1.441742000	1.400507000
H	-7.580503000	-2.010073000	3.899631000
H	-6.636648000	-2.655006000	2.525459000
H	-6.647181000	-0.902778000	2.851100000
H	-5.426066000	-3.059151000	4.707620000
H	-5.455659000	-1.316919000	5.063420000
H	-3.254542000	-2.237298000	4.182633000
H	-4.055011000	-2.556801000	2.628474000
C	-8.717526000	2.578540000	0.485602000
C	-8.057748000	3.060168000	-0.664068000
C	-6.677615000	2.879837000	-0.836282000
C	-5.924226000	2.211366000	0.140240000
C	-6.565653000	1.722270000	1.288535000
C	-7.948080000	1.904259000	1.455574000
H	-10.398395000	3.819499000	1.086400000
H	-10.639253000	2.078694000	1.381509000
H	-10.750868000	2.733586000	-0.279418000
H	-8.636956000	3.582052000	-1.436088000
H	-6.186032000	3.258566000	-1.739848000
H	-4.847406000	2.060440000	0.014300000
H	-5.984973000	1.189635000	2.051392000
H	-8.439284000	1.511248000	2.354440000
O	-0.267650000	3.951488000	3.002839000
H	0.771908000	5.672716000	2.376787000
H	0.323030000	5.564407000	4.110249000
H	-0.927585000	5.948135000	2.881540000
H	-0.556122000	3.685352000	2.086003000
C	2.228034000	-3.176522000	-5.173098000
C	2.244242000	-2.219204000	-3.968408000

C	1.895232000	-0.779352000	-4.410067000
C	3.660271000	-2.261126000	-3.296161000
C	4.719761000	-1.385877000	-3.966033000
C	3.331039000	-1.920384000	-1.843894000
C	4.195343000	-2.400516000	-0.660070000
C	5.423775000	-1.532155000	-0.197475000
C	5.314626000	-1.609719000	1.364349000
C	3.831975000	-1.838730000	1.574409000
C	3.137300000	-1.622980000	2.806922000
C	3.891108000	-0.900690000	3.907411000
C	6.177613000	-2.669539000	2.076218000
C	5.208402000	-0.045092000	-0.605498000
C	6.367349000	0.869673000	-0.225338000
N	6.971022000	1.496224000	-1.282441000
O	6.741150000	1.067052000	0.928893000
C	6.777074000	-2.008210000	-0.738263000
C	4.536686000	-3.890622000	-0.835760000
N	3.234699000	-2.263007000	0.476241000
N	2.004234000	-2.551117000	-1.637562000
C	1.357486000	-2.656741000	-2.787239000
C	-0.009981000	-3.067335000	-2.840435000
C	-0.783914000	-2.927030000	-4.137866000
C	-0.673454000	-3.517248000	-1.712226000
N	-0.152165000	-3.500128000	-0.418472000
C	-2.118004000	-4.016609000	-1.665239000
C	-2.675600000	-4.859532000	-2.820953000
C	-2.166702000	-4.766504000	-0.301457000
C	-1.785417000	-6.260864000	-0.439645000
C	-3.539210000	-4.635488000	0.368251000
C	-1.038743000	-4.078085000	0.436276000
C	-0.907550000	-4.076909000	1.818716000
C	0.094266000	-3.427407000	2.525775000
N	1.143805000	-2.776225000	1.963124000
C	0.176058000	-3.365721000	4.027773000
C	0.937485000	-4.586215000	4.577640000
C	0.924998000	-2.007944000	4.205267000
C	1.841453000	-2.077035000	2.962342000
C	1.553006000	-1.873248000	5.595980000
C	-0.184174000	-0.935989000	4.009029000
C	0.204442000	0.529956000	4.033061000
O	1.384162000	0.916712000	3.906732000
N	-0.821700000	1.389447000	4.161760000
H	2.328904000	-4.215550000	-4.842156000
H	3.070482000	-2.944491000	-5.836326000
H	1.314722000	-3.093514000	-5.766267000
H	0.862347000	-0.709917000	-4.759277000
H	2.543261000	-0.461318000	-5.234234000
H	2.015668000	-0.070674000	-3.585494000
H	3.989650000	-3.307458000	-3.334369000
H	5.707159000	-1.563975000	-3.528795000
H	4.486835000	-0.320831000	-3.860052000
H	4.794480000	-1.607744000	-5.036675000
H	5.622729000	-0.640995000	1.765903000
H	3.243081000	-0.187252000	4.412446000
H	4.730815000	-0.338958000	3.491191000
H	4.302475000	-1.591841000	4.653318000
H	5.997801000	-2.619359000	3.154230000
H	7.242294000	-2.479568000	1.907129000
H	5.947212000	-3.687762000	1.750083000
H	4.309285000	0.338259000	-0.111253000
H	5.030619000	0.031957000	-1.679715000
H	6.723793000	1.290864000	-2.239400000
H	7.775781000	2.081859000	-1.100972000
H	6.980067000	-3.048230000	-0.475820000
H	7.585972000	-1.397009000	-0.323814000
H	6.818978000	-1.923498000	-1.829254000
H	3.614511000	-4.438207000	-1.051199000
H	4.968179000	-4.303329000	0.077946000
H	5.244405000	-4.044586000	-1.656029000
H	-1.791189000	-2.553852000	-3.935635000
H	-0.874447000	-3.866778000	-4.694579000
H	-0.309704000	-2.204665000	-4.800923000
H	-2.753503000	-3.123014000	-1.558169000
H	-3.580080000	-5.375324000	-2.479736000
H	-1.959661000	-5.615178000	-3.159142000
H	-2.971377000	-4.250612000	-3.674629000
H	-1.674439000	-6.702711000	0.556099000
H	-0.834775000	-6.374704000	-0.971449000
H	-2.557969000	-6.821161000	-0.977095000
H	-3.792120000	-3.584725000	0.532880000
H	-3.569480000	-5.161881000	1.328784000
H	-4.313812000	-5.074186000	-0.271679000
H	-1.667771000	-4.592298000	2.398159000
H	-0.818035000	-3.322989000	4.488945000
H	0.419557000	-5.506450000	4.289448000
H	1.002253000	-4.557138000	5.670126000
H	1.952550000	-4.623645000	4.167149000
H	0.796635000	-2.128877000	6.348619000
H	1.885316000	-0.853377000	5.792597000
H	2.401962000	-2.548041000	5.728922000
H	-0.970555000	-1.104449000	4.755955000
H	-0.657697000	-1.098472000	3.032967000
H	-0.661084000	2.385821000	3.964301000
H	-1.773438000	1.033954000	4.141491000
H	3.173781000	-0.838760000	-1.739378000

6A. NpRdhA/TCE, Co^I

C	4.269647000	7.450288000	-1.481652000
C	6.961186000	3.759508000	1.889917000
C	-6.890955000	-0.406400000	3.472000000
C	-9.616953000	4.838883000	0.835781000
C	0.843893000	5.633808000	3.270004000
C	-5.081174000	-0.785702000	-5.156324000
Co	1.012592000	-2.607719000	0.263555000
Cl	-1.206069000	4.827364000	0.162811000
C	-0.550669000	3.145245000	-0.023456000
C	-0.945258000	2.511759000	-1.136407000
Cl	-1.971817000	3.084282000	-2.465911000
Cl	0.142107000	-0.579683000	0.373993000
H	-0.636458000	1.480464000	-1.290966000
C	-4.596706000	-0.932676000	-3.732367000
C	-3.421579000	-0.279847000	-3.307473000
C	-2.904206000	-0.485296000	-2.022159000
C	-3.568688000	-1.326041000	-1.120907000
C	-4.766353000	-1.947202000	-1.508082000
C	-5.270437000	-1.755721000	-2.805021000
H	-6.171496000	-0.929881000	-5.234652000
H	-4.602604000	-1.543693000	-5.805324000
H	-4.829328000	0.205876000	-5.567982000
H	-2.903568000	0.397573000	-3.995106000
H	-1.973430000	-0.003051000	-1.717758000
H	-3.134879000	-1.493720000	-0.130791000
H	-5.308221000	-2.594563000	-0.808375000
H	-6.197594000	-2.256770000	-3.105529000
C	3.683292000	6.086796000	-1.754453000
C	4.505019000	4.959767000	-1.905239000
C	3.972596000	3.692771000	-2.133506000
C	2.589376000	3.533885000	-2.217917000
C	1.749526000	4.642716000	-2.115522000
C	2.301754000	5.901839000	-1.878229000
O	2.090849000	2.243394000	-2.363835000
H	1.118488000	2.306676000	-2.326376000
H	4.844894000	7.812412000	-2.341879000
H	4.951865000	7.424084000	-0.624139000
H	3.486523000	8.183671000	-1.271148000
H	5.584508000	5.070166000	-1.832724000
H	4.623087000	2.832041000	-2.239664000
H	0.673833000	4.527868000	-2.209038000
H	1.635512000	6.755986000	-1.786506000
C	5.519986000	4.259958000	1.704221000
C	4.521019000	3.126341000	1.413848000
C	3.096577000	3.642634000	1.212728000
N	2.147634000	2.527520000	0.886667000
H	2.082647000	1.870071000	1.704263000
H	1.130685000	2.839604000	0.665238000
H	2.454984000	2.006740000	0.052521000
H	7.310257000	3.218274000	0.992978000
H	7.032637000	3.064951000	2.746642000
H	7.650049000	4.599956000	2.079666000
H	5.481887000	4.986914000	0.870204000
H	5.194723000	4.812010000	2.607659000
H	4.849667000	2.578433000	0.511663000
H	4.530143000	2.398634000	2.247983000
H	3.043127000	4.375727000	0.392465000
H	2.705098000	4.108849000	2.126258000
C	-5.366033000	-0.577124000	3.508636000
C	-4.689457000	-0.497542000	2.129081000
N	-4.735777000	0.830482000	1.511088000
C	-3.700682000	1.662062000	1.284167000
N	-2.432834000	1.332199000	1.616582000
N	-3.945801000	2.876559000	0.768813000
H	-5.650289000	1.154901000	1.179850000
H	-1.667571000	1.908440000	1.207210000
H	-2.187023000	0.346007000	1.688843000
H	-4.885774000	3.125358000	0.451937000
H	-3.173642000	3.485858000	0.482476000
H	-7.320217000	-0.509300000	4.482100000
H	-7.360452000	-1.169678000	2.825282000
H	-7.182182000	0.589189000	3.090199000
H	-5.117147000	-1.569631000	3.929466000
H	-4.906187000	0.175055000	4.176498000
H	-3.636217000	-0.808830000	2.213587000
H	-5.170061000	-1.204982000	1.429982000
C	-8.613221000	3.837843000	0.295057000
C	-8.709832000	2.463560000	0.599505000
C	-7.836987000	1.524179000	0.022757000
C	-6.833674000	1.939688000	-0.870968000
C	-6.704909000	3.311583000	-1.160655000
C	-7.581634000	4.243439000	-0.580977000
H	-10.432453000	4.988663000	0.103875000
H	-9.150586000	5.822019000	1.015149000
H	-10.073711000	4.487931000	1.775631000
H	-9.498227000	2.118495000	1.278284000
H	-7.968335000	0.458308000	0.245978000
H	-6.176003000	1.206844000	-1.354232000
H	-5.937755000	3.651540000	-1.866524000
H	-7.480705000	5.305170000	-0.833971000
O	0.387982000	4.329766000	2.885671000
H	1.347097000	6.147266000	2.429382000

H	1.566976000	5.496622000	4.089478000
H	0.012111000	6.266670000	3.632485000
H	-0.227098000	4.431380000	2.125293000
C	0.377926000	-3.495739000	-5.039964000
C	0.648418000	-2.490956000	-3.908302000
C	0.046527000	-1.110081000	-4.253266000
C	2.193490000	-2.403187000	-3.653973000
C	2.953175000	-1.500181000	-4.624967000
C	2.272196000	-1.996739000	-2.180524000
C	3.409726000	-2.494472000	-1.262423000
C	4.774684000	-1.715032000	-1.212160000
C	5.091699000	-1.702114000	0.327817000
C	3.720284000	-1.813891000	0.951828000
C	3.401482000	-1.487070000	2.315092000
C	4.447013000	-0.734263000	3.105416000
C	6.062513000	-2.771707000	0.865245000
C	4.570663000	-0.239077000	-1.666167000
C	5.857969000	0.576950000	-1.582896000
N	6.427184000	0.909477000	-2.772802000
O	6.353183000	0.915191000	-0.507297000
C	5.884444000	-2.353181000	-2.056978000
C	3.594682000	-4.015606000	-1.409667000
N	2.824323000	-2.230027000	0.092566000
N	1.047470000	-2.598579000	-1.597381000
C	0.152001000	-2.889724000	-2.508983000
C	-1.093214000	-3.516633000	-2.168358000
C	-2.129028000	-3.751336000	-3.242049000
C	-1.348690000	-3.947629000	-0.880129000
N	-0.592405000	-3.641531000	0.243389000
C	-2.466458000	-4.909887000	-0.517662000
C	-2.219859000	-6.284420000	-1.172392000
C	-2.465552000	-4.911044000	1.043593000
C	-2.477729000	-6.305649000	1.698105000
C	-3.669988000	-4.101938000	1.576400000
C	-1.185034000	-4.156094000	1.352363000
C	-0.713683000	-3.973086000	2.644501000
C	0.410239000	-3.244464000	3.009599000
N	1.263603000	-2.659484000	2.144360000
C	0.860285000	-3.018117000	4.429154000
C	1.746497000	-4.184714000	4.907185000
C	1.616643000	-1.660369000	4.261050000
C	2.190907000	-1.877908000	2.849551000
C	2.564903000	-1.371700000	5.427839000
C	0.494863000	-0.576276000	4.205271000
C	0.917623000	0.829226000	3.797034000
O	1.980624000	1.030595000	3.186079000
N	0.053506000	1.815383000	4.086708000
H	0.570387000	-4.523936000	-4.716913000
H	1.051238000	-3.276135000	-5.875491000
H	-0.640875000	-3.431986000	-5.425568000
H	-1.042361000	-1.168434000	-4.305293000
H	0.411749000	-0.771923000	-5.227542000
H	0.307414000	-0.356447000	-3.502883000
H	2.574030000	-3.427606000	-3.750295000
H	4.033647000	-1.624518000	-4.504949000
H	2.707480000	-0.444225000	-4.471537000
H	2.717240000	-1.756551000	-5.662556000
H	5.530634000	-0.727990000	0.565647000
H	3.983904000	0.038066000	3.713809000
H	5.157729000	-0.244516000	2.437833000
H	5.018084000	-1.404323000	3.757884000
H	6.185842000	-2.651805000	1.945157000
H	7.046863000	-2.649881000	0.406512000
H	5.714582000	-3.791471000	0.679740000
H	3.835243000	0.249747000	-1.018729000
H	4.176127000	-0.211071000	-2.683626000
H	6.030561000	0.638596000	-3.660790000
H	7.296145000	1.429443000	-2.770408000
H	6.089496000	-3.384584000	-1.765540000
H	6.815278000	-1.789488000	-1.945369000
H	5.620752000	-2.349768000	-3.120084000
H	2.625443000	-4.517426000	-1.333927000
H	4.239709000	-4.404552000	-0.620317000
H	4.042125000	-4.267003000	-2.373924000
H	-3.115029000	-3.908636000	-2.804469000
H	-1.893585000	-4.611733000	-3.876439000
H	-2.209858000	-2.872798000	-3.885052000
H	-3.424300000	-4.520786000	-0.880910000
H	-3.001355000	-6.994015000	-0.889369000
H	-1.250978000	-6.695651000	-0.874437000
H	-2.227908000	-6.196210000	-2.260282000
H	-2.478654000	-6.212018000	2.788580000
H	-1.610446000	-6.904868000	1.411176000
H	-3.385050000	-6.848587000	1.417772000
H	-3.690677000	-3.103710000	1.133626000
H	-3.625134000	-3.998652000	2.665668000
H	-4.602577000	-4.614853000	1.318696000
H	-1.284343000	-4.424871000	3.449189000
H	0.005765000	-2.909450000	5.105947000
H	1.184835000	-5.122633000	4.871647000
H	2.075696000	-4.024832000	5.936952000
H	2.629873000	-4.289291000	4.268396000
H	2.020784000	-1.525681000	6.366707000
H	2.916688000	-0.339257000	5.417406000
H	3.432348000	-2.034410000	5.431206000

H	0.003516000	-0.551155000	5.185946000
H	-0.265417000	-0.882508000	3.472488000
H	0.212953000	2.777360000	3.741679000
H	-0.808270000	1.618080000	4.576014000
H	2.173441000	-0.909530000	-2.068290000

6B. NpRdhA/TCE with neutralized R552, Co^I

C	4.749722000	7.165579000	-1.815771000
C	7.116805000	3.540453000	1.857182000
C	-7.004504000	0.324308000	3.270314000
C	-9.328946000	5.546954000	0.234062000
C	1.092617000	5.863043000	2.932234000
C	-4.992437000	-0.708815000	-5.259584000
Co	0.830172000	-2.547090000	0.445585000
Cl	-0.620627000	3.393537000	-0.622911000
C	-0.313543000	1.764423000	-1.234311000
C	-0.796706000	1.410918000	-2.427898000
Cl	-1.690593000	2.407564000	-3.563150000
Cl	0.381172000	-0.339689000	-0.140211000
H	-0.657959000	0.396102000	-2.782455000
C	-4.967070000	-0.731694000	-3.748330000
C	-3.739435000	-0.736872000	-3.056288000
C	-3.695891000	-0.793477000	-1.657172000
C	-4.889625000	-0.836610000	-0.917379000
C	-6.119249000	-0.815568000	-1.590791000
C	-6.155129000	-0.766115000	-2.992482000
H	-5.988564000	-0.436507000	-5.645669000
H	-4.735607000	-1.703033000	-5.673034000
H	-4.257884000	0.011661000	-5.660861000
H	-2.804967000	-0.689954000	-3.626837000
H	-2.730257000	-0.806152000	-1.142923000
H	-4.858892000	-0.869063000	0.175185000
H	-7.055195000	-0.825698000	-1.022028000
H	-7.121471000	-0.745573000	-3.509335000
C	4.186830000	5.776102000	-2.030469000
C	5.020009000	4.645868000	-2.025059000
C	4.507081000	3.355300000	-2.131461000
C	3.126732000	3.161423000	-2.251436000
C	2.284495000	4.271807000	-2.349162000
C	2.817596000	5.558096000	-2.224012000
O	2.660669000	1.861669000	-2.222820000
H	1.676102000	1.848206000	-2.182387000
H	5.555436000	7.383876000	-2.525506000
H	5.169173000	7.265669000	-0.807016000
H	3.975735000	7.928663000	-1.937038000
H	6.094396000	4.773098000	-1.912094000
H	5.166688000	2.495479000	-2.091245000
H	1.218645000	4.135549000	-2.502432000
H	2.142944000	6.409704000	-2.278026000
C	5.753219000	4.171931000	1.579976000
C	4.651858000	3.114580000	1.429527000
C	3.325961000	3.758500000	1.061302000
N	2.241335000	2.735747000	0.908784000
H	2.025545000	2.314659000	1.864654000
H	1.365100000	3.171616000	0.565571000
H	2.483542000	1.989879000	0.237355000
H	7.402953000	2.850437000	1.044658000
H	7.099827000	2.956212000	2.795473000
H	7.903198000	4.308803000	1.955995000
H	5.798971000	4.773939000	0.652522000
H	5.482239000	4.873852000	2.392857000
H	4.949133000	2.385404000	0.654099000
H	4.542707000	2.551979000	2.375666000
H	3.394926000	4.320406000	0.118587000
H	2.985363000	4.444398000	1.846883000
C	-5.905514000	-0.252246000	4.169664000
C	-4.638604000	-0.581982000	3.367297000
N	-4.213245000	0.585294000	2.620608000
C	-3.255374000	0.474483000	1.769915000
N	-2.542485000	-0.667407000	1.458617000
N	-2.826641000	1.627532000	1.085993000
H	-1.654560000	-0.595201000	0.949414000
H	-2.596800000	-1.455494000	2.098915000
H	-3.566445000	2.334564000	1.072344000
H	-2.465377000	1.453995000	0.142890000
H	-7.929686000	0.520296000	3.840272000
H	-7.255462000	-0.372791000	2.448231000
H	-6.662232000	1.269331000	2.820480000
H	-6.256623000	-1.166499000	4.684726000
H	-5.647841000	0.482614000	4.955464000
H	-3.837757000	-0.946891000	4.054398000
H	-4.867206000	-1.434312000	2.684803000
C	-8.151393000	4.687652000	-0.192696000
C	-7.755231000	3.556923000	0.550911000
C	-6.690890000	2.743229000	0.127351000
C	-5.994477000	3.047433000	-1.051926000
C	-6.368983000	4.176491000	-1.797733000
C	-7.433619000	4.983844000	-1.371237000
H	-10.235971000	5.279262000	-0.340401000
H	-9.131012000	6.617730000	0.053012000
H	-9.560519000	5.412240000	1.303977000
H	-8.288764000	3.304721000	1.475473000
H	-6.403151000	1.868014000	0.719771000
H	-5.175785000	2.402719000	-1.392037000

H	-5.832021000	4.427507000	-2.719581000
H	-7.717123000	5.861018000	-1.965581000
O	0.563026000	5.023082000	1.895961000
H	1.818234000	6.595205000	2.529285000
H	1.608856000	5.195817000	3.640396000
H	0.292225000	6.401229000	3.473250000
H	0.027716000	5.564250000	1.288190000
C	0.869206000	-4.341421000	-4.635856000
C	1.116089000	-3.164340000	-3.677649000
C	0.810165000	-1.814294000	-4.368368000
C	2.598891000	-3.210935000	-3.167493000
C	3.634689000	-2.647398000	-4.138740000
C	2.494802000	-2.502780000	-1.815970000
C	3.435605000	-2.821155000	-0.631580000
C	4.809216000	-2.062426000	-0.512774000
C	4.873561000	-1.725551000	1.020468000
C	3.410485000	-1.683718000	1.410454000
C	2.890567000	-1.077568000	2.608789000
C	3.849369000	-0.234195000	3.423147000
C	5.684756000	-2.681674000	1.916323000
C	4.738143000	-0.716641000	-1.293327000
C	6.026137000	0.091102000	-1.213173000
N	6.741067000	0.171303000	-2.370495000
O	6.407759000	0.646010000	-0.181287000
C	6.012192000	-2.871875000	-1.010508000
C	3.559876000	-4.343172000	-0.447694000
N	2.654375000	-2.271578000	0.518877000
N	1.144762000	-2.888942000	-1.344352000
C	0.358042000	-3.226148000	-2.339638000
C	-1.017893000	-3.573390000	-2.138765000
C	-1.923072000	-3.758308000	-3.338662000
C	-1.535864000	-3.729458000	-0.866774000
N	-0.885842000	-3.360413000	0.308819000
C	-2.917552000	-4.280854000	-0.531950000
C	-3.464574000	-5.456744000	-1.353726000
C	-2.798833000	-4.601957000	0.988803000
C	-2.363744000	-6.065020000	1.256745000
C	-4.106202000	-4.301245000	1.730718000
C	-1.635224000	-3.720503000	1.384203000
C	-1.353592000	-3.357130000	2.693776000
C	-0.281605000	-2.567772000	3.099593000
N	0.721762000	-2.166438000	2.295123000
C	-0.061914000	-2.088370000	4.509818000
C	0.607517000	-3.192955000	5.349883000
C	0.835565000	-0.831900000	4.253701000
C	1.590693000	-1.316406000	3.001351000
C	1.628815000	-0.438458000	5.505355000
C	-0.165867000	0.299796000	3.864135000
C	0.390759000	1.595552000	3.303211000
O	1.601365000	1.914707000	3.412178000
N	-0.490621000	2.410150000	2.711718000
H	0.884732000	-5.295446000	-4.098545000
H	1.664350000	-4.364660000	-5.389419000
H	-0.078203000	-4.260786000	-5.171184000
H	-0.256877000	-1.713878000	-4.583548000
H	1.347457000	-1.744615000	-5.319360000
H	1.107485000	-0.967699000	-3.740832000
H	2.823478000	-4.269630000	-2.984778000
H	4.649681000	-2.831845000	-3.773472000
H	3.511823000	-1.568580000	-4.280448000
H	3.553577000	-3.126896000	-5.119772000
H	5.323863000	-0.734504000	1.124768000
H	3.346821000	0.647301000	3.814687000
H	4.684533000	0.103911000	2.806711000
H	4.272379000	-0.796524000	4.263631000
H	5.635374000	-2.345857000	2.955925000
H	6.737027000	-2.681908000	1.619089000
H	5.312031000	-3.709187000	1.881423000
H	3.934649000	-0.091473000	-0.891421000
H	4.499134000	-0.908791000	-2.341182000
H	6.437982000	-0.272274000	-3.224943000
H	7.616327000	0.679417000	-2.370840000
H	6.117378000	-3.822132000	-0.484153000
H	6.938126000	-2.307238000	-0.862927000
H	5.923255000	-3.089358000	-2.080227000
H	2.561084000	-4.790317000	-0.438012000
H	4.046748000	-4.583403000	0.498983000
H	4.137807000	-4.795152000	-1.257918000
H	-2.938224000	-3.439816000	-3.098446000
H	-1.956177000	-4.792641000	-3.697638000
H	-1.592846000	-3.133490000	-4.168747000
H	-3.615253000	-3.434377000	-0.629991000
H	-4.294723000	-5.919991000	-0.810178000
H	-2.703478000	-6.223524000	-1.525877000
H	-3.859242000	-5.140839000	-2.318720000
H	-2.153725000	-6.195533000	2.323030000
H	-1.457930000	-6.320515000	0.696957000
H	-3.156289000	-6.766003000	0.979017000
H	-4.390140000	-3.251926000	1.610479000
H	-4.028305000	-4.524149000	2.799997000
H	-4.913240000	-4.921282000	1.325410000
H	-2.042693000	-3.686757000	3.464646000
H	-1.007433000	-1.797996000	4.982774000
H	-0.029088000	-4.082770000	5.370918000
H	0.765284000	-2.863387000	6.380356000

H	1.574444000	-3.475776000	4.919984000
H	0.938541000	-0.407133000	6.356767000
H	2.074713000	0.550069000	5.404658000
H	2.414110000	-1.161514000	5.736701000
H	-0.738731000	0.561599000	4.764343000
H	-0.897171000	-0.084966000	3.145938000
H	-0.170830000	3.334309000	2.409013000
H	-1.396078000	2.098411000	2.332807000
H	2.467273000	-1.414376000	-1.951209000