Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

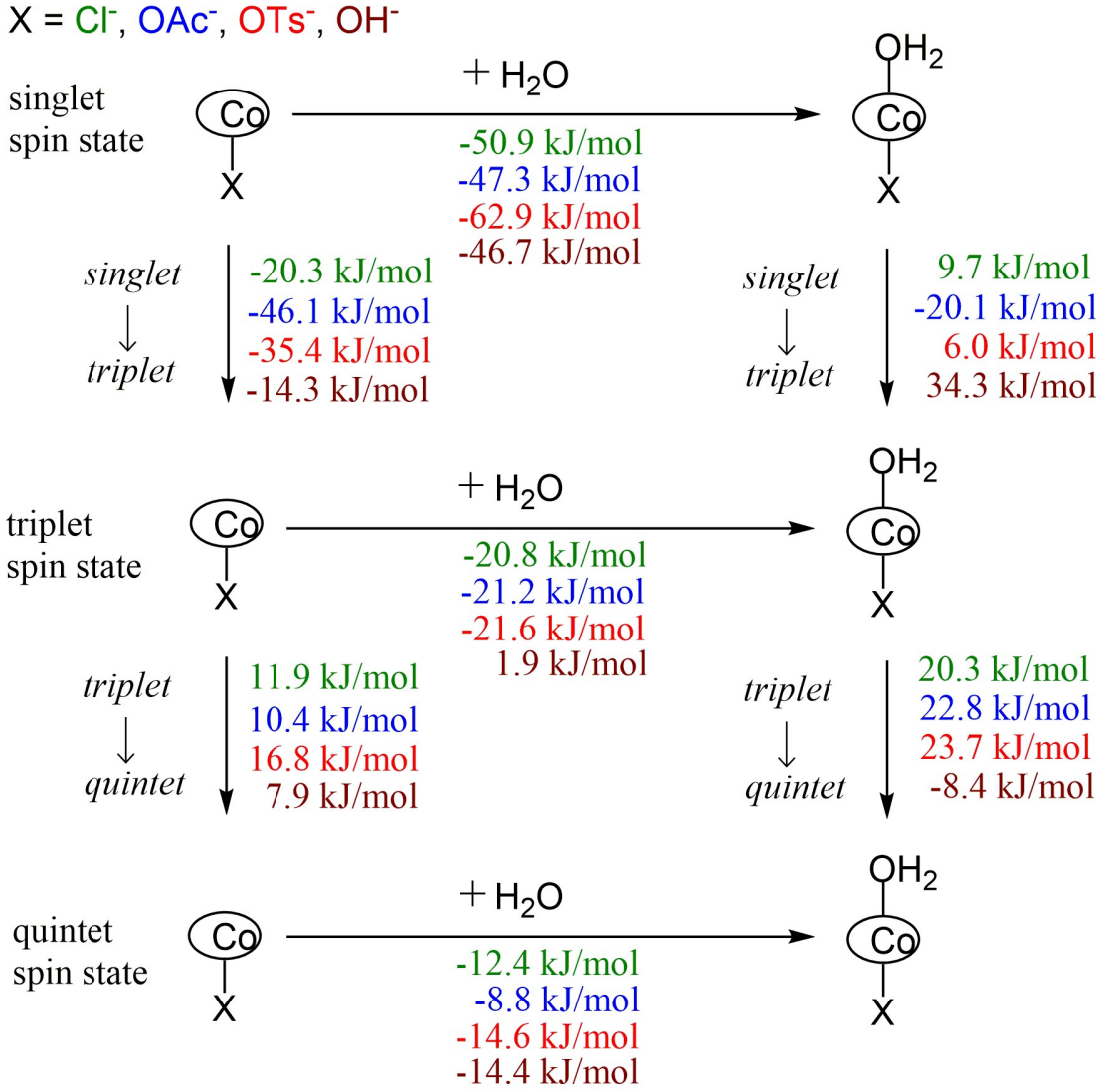


Fig. S1 The spin state of five-coordinated Co^{III}(salen)-X (X = Cl^-, OAc^-, OTs^-, OH^-) and six-coordinate H_2O-Co^{III}-X (X = Cl^-, OAc^-, OTs^-, OH^-) calculated at the B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level in the gas phase. The structures of salen complexes are complete or unsimplified, that is, -$C(CH_3)_3$ groups in salen-complexes are not replaced by H atoms in calculations (see computational details).

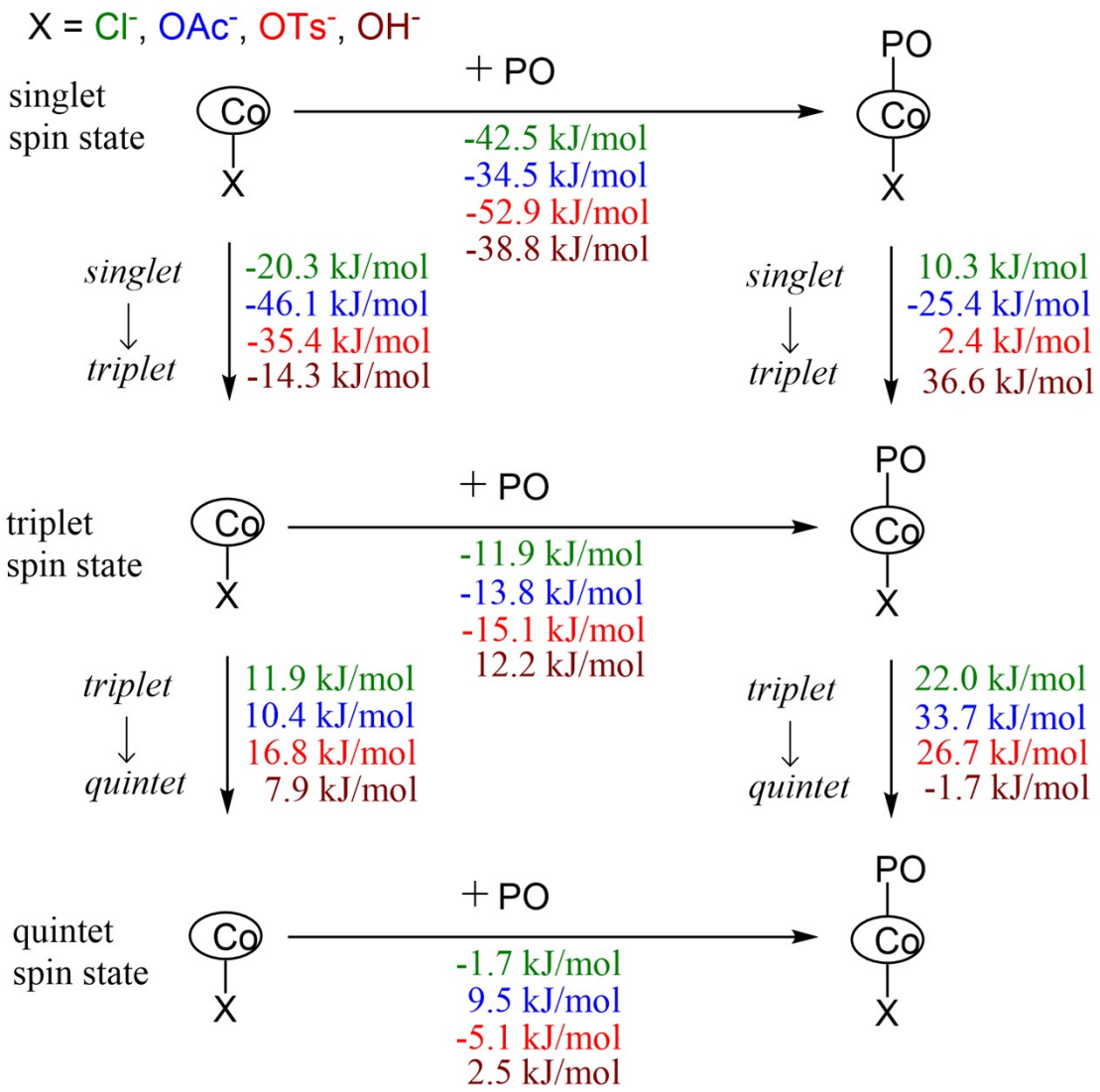
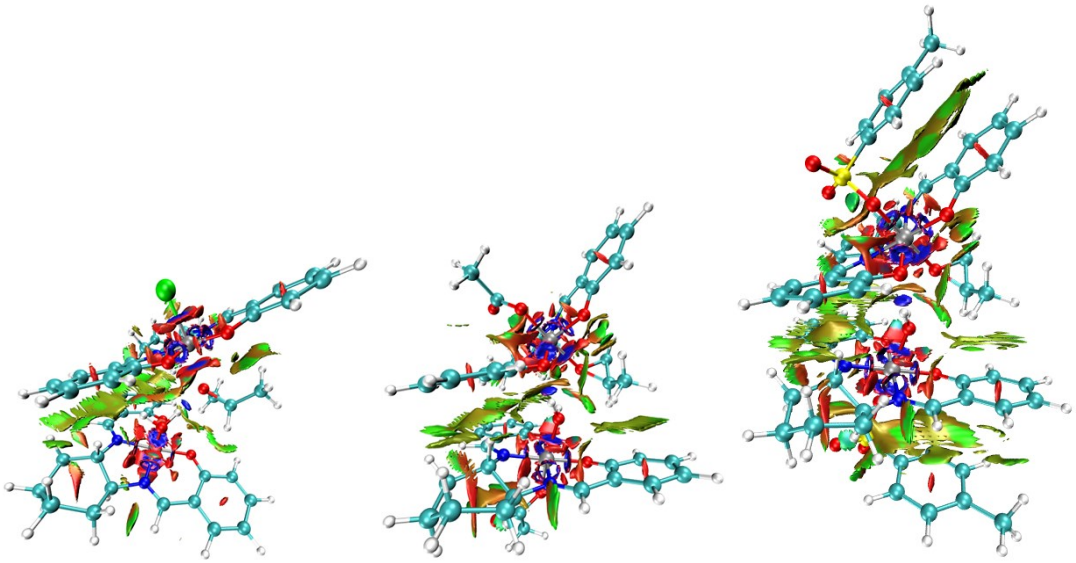
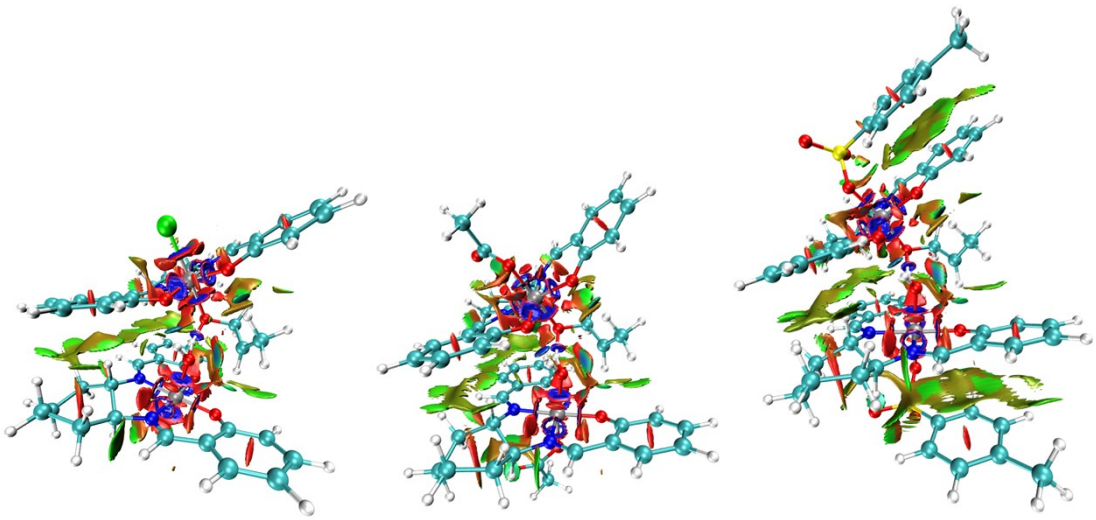


Fig. S2 The spin state of five-coordinated Co^{III}(salen)-X (X = Cl^-, OAc^-, OTs^-, OH^-) and six-coordinate PO-Co^{III}-X (X = Cl^-, OAc^-, OTs^-, OH^-) calculated at the B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level in the gas phase. The structures of Co^{III}(salen) are unsimplified.



Int-Cl Int-OAc Int-OTs



TS-Cl TS-OAc TS-OTs

Fig. S3 NCI plots for the three transition states and precursors of route IV-m, blue regions representing strong electrostatic interactions and green regions representing more dispersive attractive interactions and red regions representing repulsive interactions. The sign(λ_2)ρ is ranging from -0.09 to 0.09 a.u..

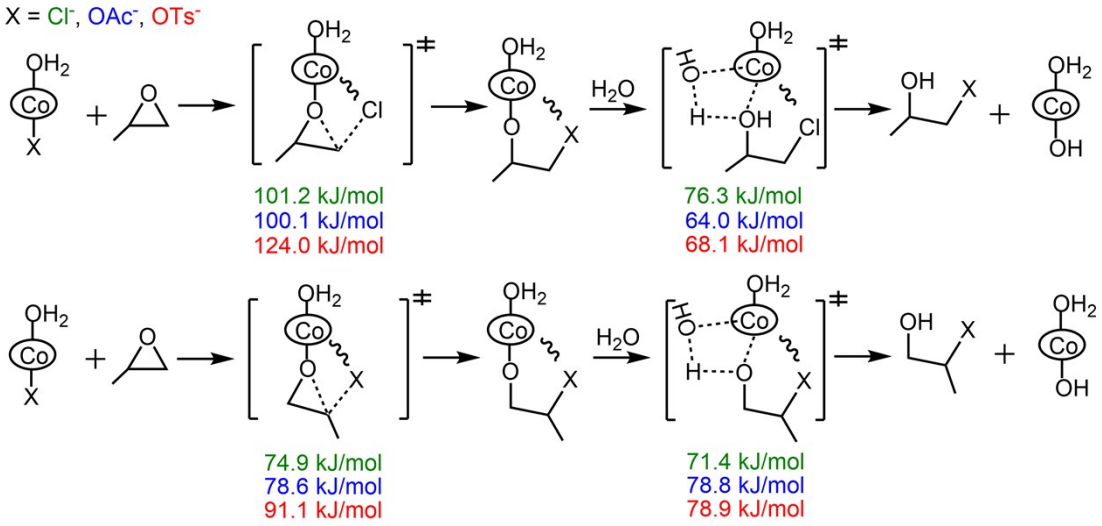


Fig. S4 The two pathways of respectively attacking the terminal or middle carbon of PO and the subsequent hydrolysis to form six-coordinated nucleophile H_2O-Co^{III}-OH calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level. The hydrogen bond interaction of X with H atoms of Co^{III}(salen) ligand was signed with a wavy line. The free energy barriers were listed under the corresponding transition state structures.

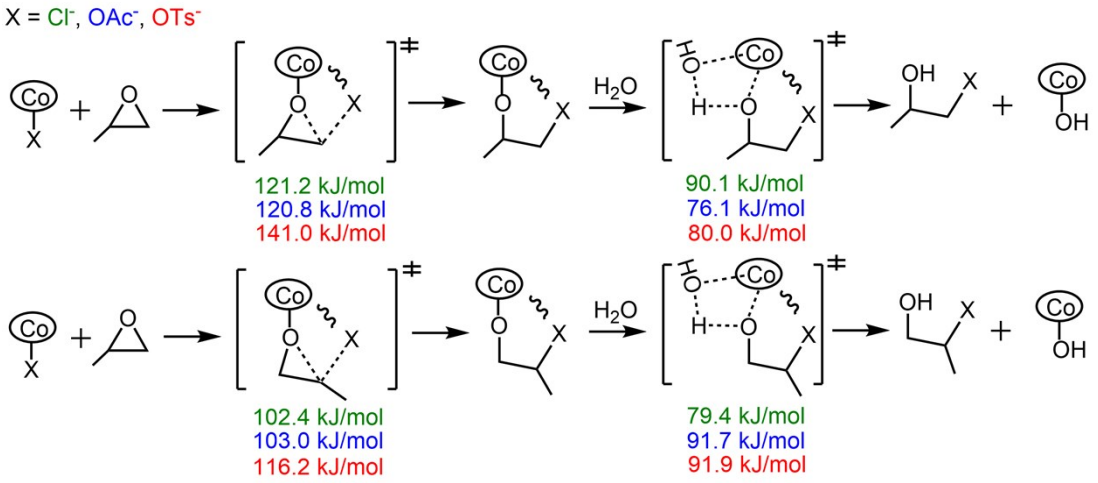


Fig. S5 The two pathways of respectively attacking the terminal or middle carbon of PO and the subsequent hydrolysis to form five-coordinated Co^{III}(salen)-OH calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level. The hydrogen bond interaction of X between H of Co^{III}(salen) ligand was denoted with wavy line. The free energy barriers were listed under the corresponding transition state structures.

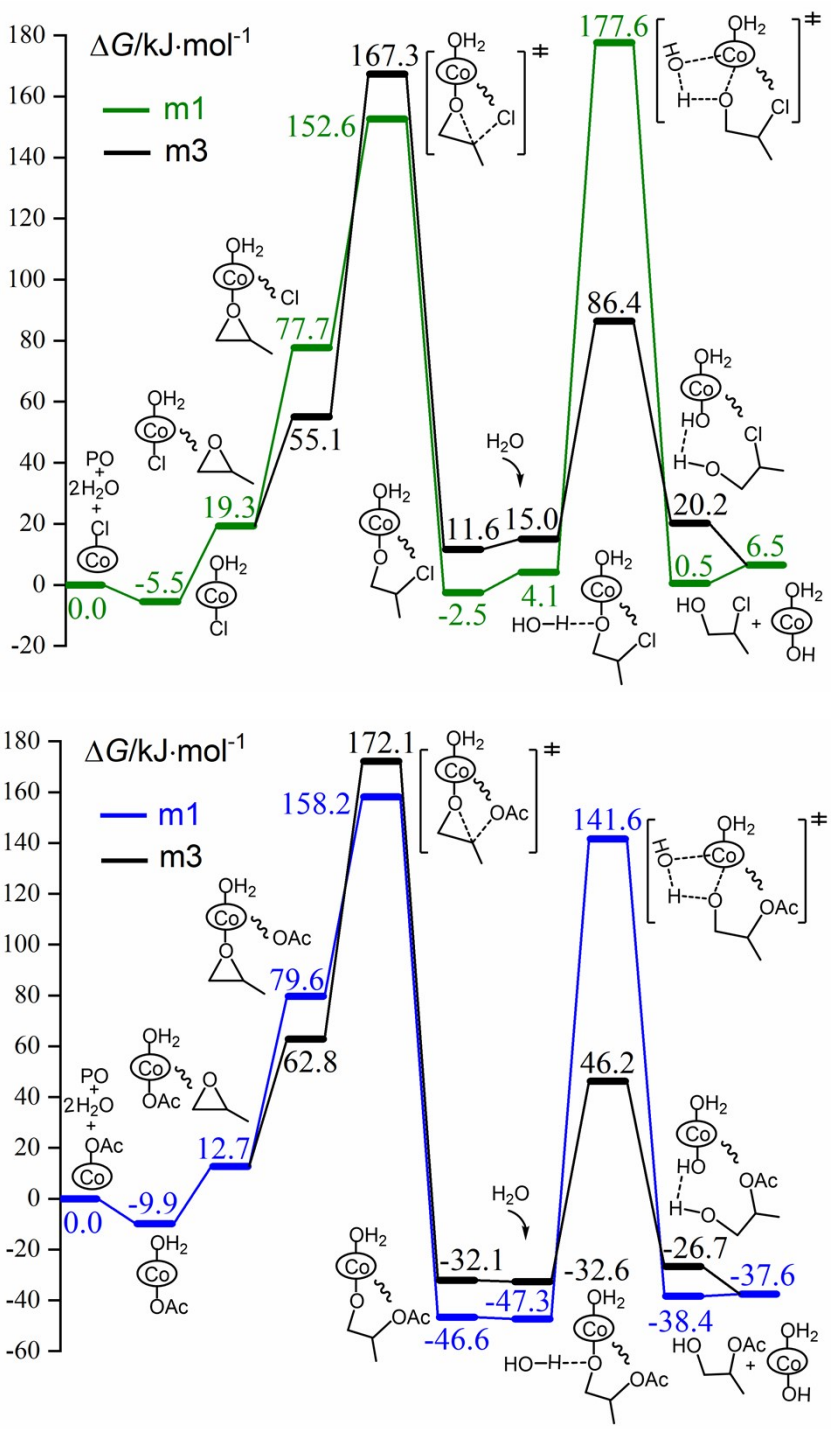


Fig. S6 Potential relative free energy profiles and sketch structures of transition states and intermediates for the formation of six-coordinated nucleophile H_2O-Co^{III}-OH calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level.

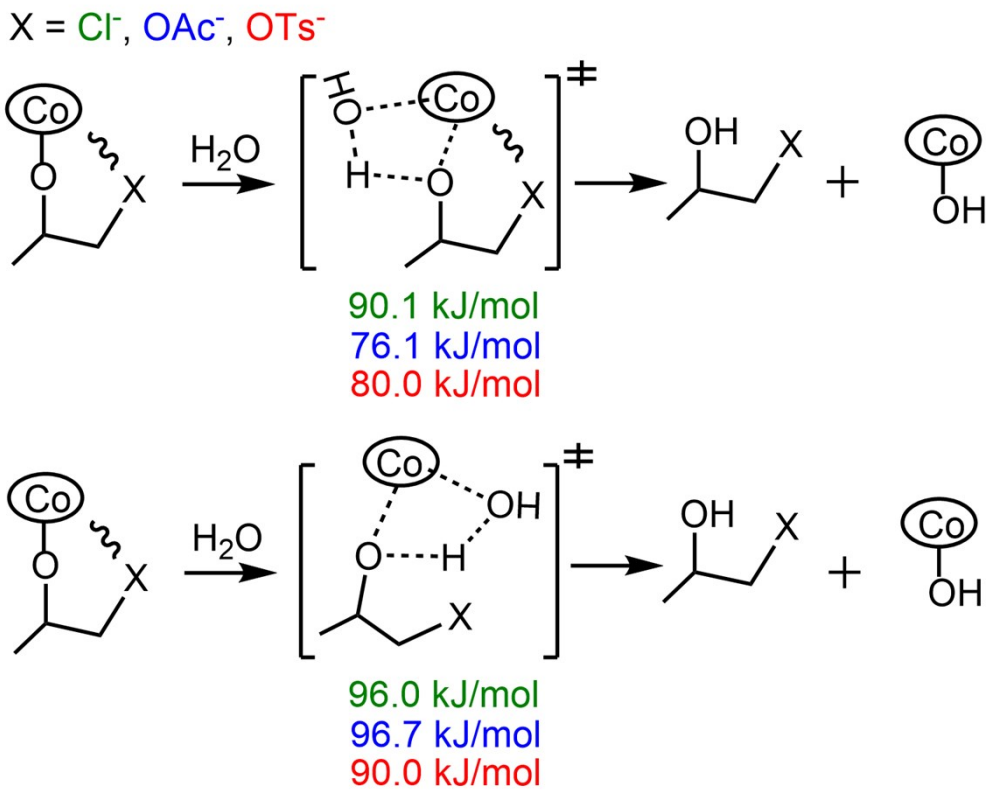


Fig. S7 The two pathways of hydrolysis after counterion addition step to form five-coordinated Co^{III}(salen)-OH calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level. The hydrogen bond interaction of X with H atoms of Co^{III}(salen) ligand was denoted with a wavy line. The free energy barriers were listed under the corresponding transition state structures.

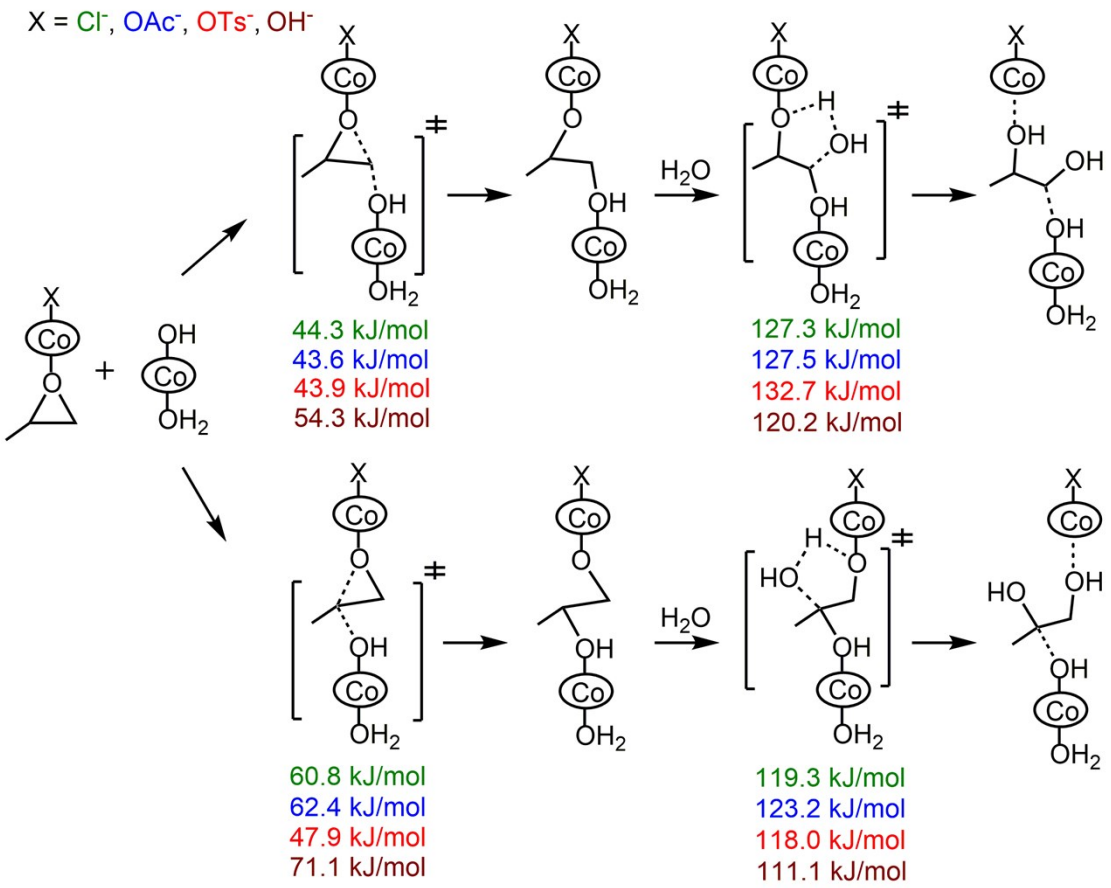


Fig. S8 The stepwise pathways of ring-opening through H_2O-Co^{III}-OH attacking the terminal or middle carbon of PO activated by Co^{III}(salen)-X from the back and the subsequent hydration reaction calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level. The free energy barriers were listed under the corresponding transition state structures.

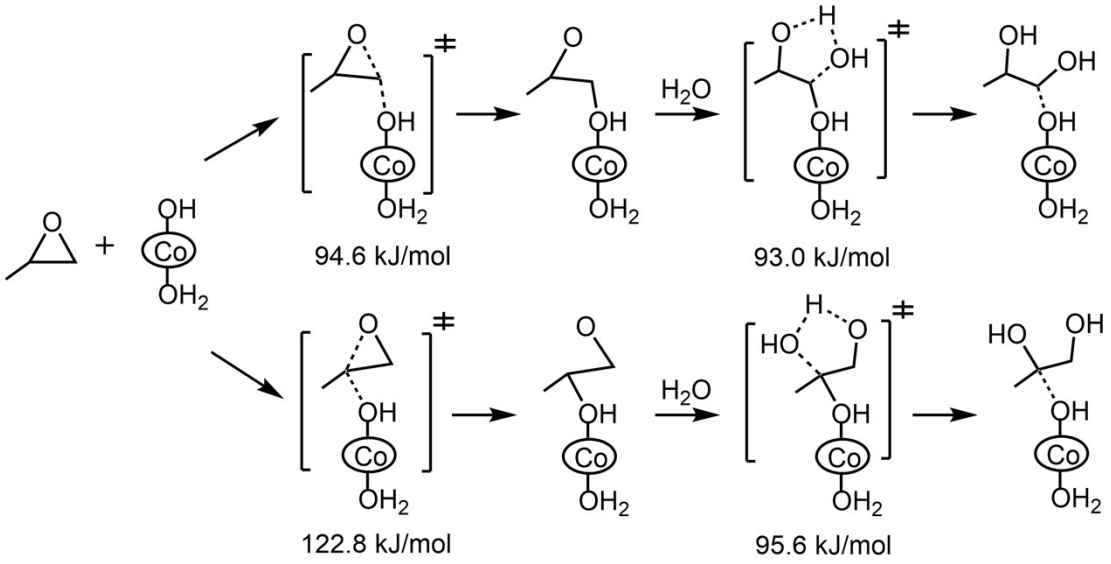


Fig. S9 The stepwise pathways of ring-opening through H_2O-Co^{III}-OH attacking the terminal or middle carbon of unactivated PO from the back and the subsequent hydration reaction calculated at the B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level. The free energy barriers were listed under the corresponding transition state structures.

Table S1 The free energy barriers (kJ/mol) of the bimetallic ring-opening for the

different counterions based on the different basis sets.

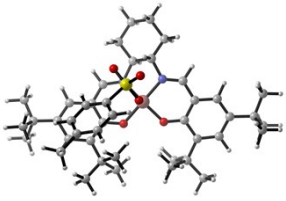
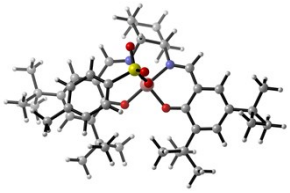
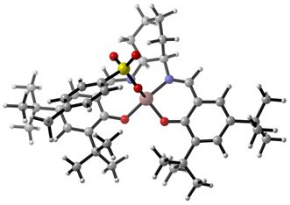
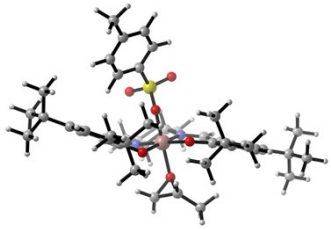
	PO-Co^{III}-Cl + H_2O-Co^{III}-OH	PO-Co^{III}-OAc + H_2O-Co^{III}-OH	PO-Co^{III}-OTs + H_2O-Co^{III}-OH
B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/ LanL2TZ(f)~6-31G(d,p)	44.3	43.6	43.9
B3LYP-D3BJ/def2TZVP (SMD)//B3LYP-D3BJ/ LanL2TZ(f)~6-311G(d,p)	45.0	45.5	43.9

Table S2 The free energy barriers of different routes catalyzed by Co^{III}(salen)-Cl of simplified and unsimplified catalyst structures calculated at the B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level in the gas phase.

	Unsimplified structure (S,S)		Simplified structure (S,S)	
	terminal carbon	middle carbon	terminal carbon	middle carbon
PO + H_2O	206.9	193.9	206.9	193.9
PO + H_2O-Co^{III}-Cl	196.1	152.6	194.3	178.1
PO-Co^{III}-Cl + H_2O	163.4	134.2	164.0	133.6
PO + H_2O-Co^{III}-OH	135.9	160.0	137.7	160.1
PO-Co^{III}-Cl + H_2O-Co^{III}-OH	42.4	--	39.0	--

Table S3 The geometry structures and relative free energy difference ΔG of four

Co^{III}(salen)-OTs and two PO-Co^{III}-OTs calculated at the B3LYP-D3BJ/LanL2TZ(f) (for Co) 6-31G(d,p) (for all non-metal atoms) level in the gas phase. The catalyst structures used are unsimplified.

Catalyst structures	ΔG (kJ/mol)
 Co^{III}(salen)(S,S)-OTs	0.0
 Co^{III}(salen)(R,S)-OTs	3.0
 Co^{III}(salen)(S,R)-OTs	22.7
 Co^{III}(salen)(R,R)-OTs	23.6
 PO(R)-Co^{III}(S,S)-OTs	0.0

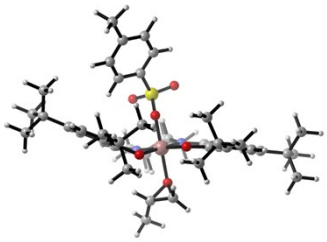
	1.9
PO(S)-Co^{III}(S,S)-OTs	

Table S4 The spin multiplicity of low-lying states of all the species studied.*

singlet state	triplet state
H_2O-Co^{III}-Cl	Co^{III}(salen)-Cl
PO-Co^{III}-Cl	Co^{III}(salen)-OTs
H_2O-Co^{III}-OTs	Co^{III}(salen)-OH
PO-Co^{III}-OTs	Co^{III}(salen)-OAc
H_2O-Co^{III}-OH	H_2O-Co^{III}-OAc
PO-Co^{III}-OH	PO-Co^{III}-OAc
PO~H_2O-Co^{III}-X	
[PO~H_2O-Co^{III}-X]$^{\neq}$	
PG~Co^{III}(salen)-X	
X-Co^{III}-PO~H_2O	
[X-Co^{III}-PO~H_2O]$^{\neq}$	
X-Co^{III}-PO~H_2O-Co^{III}-X	
[X-Co^{III}-PO~H_2O-Co^{III}-X]$^{\neq}$	
Co^{III}(salen)-X~PG~Co^{III}(salen)-X	
H_2O-Co^{III}-X~PO	Co^{III}(salen)-PO~X
[H_2O-Co^{III}-PO~X]$^{\neq}$	[Co^{III}(salen)-PO~X]$^{\neq}$
H_2O-Co^{III}-PO-X	Co^{III}(salen)-PO-X
H_2O-Co^{III}-PO-X~H_2O	Co^{III}(salen)-PO-X~H_2O
H_2O-Co^{III}-OH~$CH_3CHOHCH_2X$	[Co^{III}(salen)-PO-X~H_2O]$^{\neq}$
	Co^{III}(salen)-OH~$CH_3CHOHCH_2X$
	H_2O-Co^{III}-PO~X
PO-Co^{III}-X~H_2O-Co^{III}-OH	[H_2O-Co^{III}-PO-X~H_2O]$^{\neq}$
[PO-Co^{III}-X~H_2O-Co^{III}-OH]$^{\neq}$	
X-Co^{III}-PO-OH-Co^{III}-H_2O	
X-Co^{III}-PO-OH-Co^{III}-H_2O~H_2O	
[X-Co^{III}-PO-OH-Co^{III}-H_2O~H_2O]$^{\neq}$	
Co^{III}(salen)-X~PG~OH-Co^{III}-H_2O	

*: This table shows that the ground states of all the six-coordinated speceis, except the four marked light blue, are in singlet states. All the five-coordinated ones are in triplet states. X = Cl^-, OAc^- and OTs^-.

Table S5 The important bond lengths (in Å) and charges (e) of some atoms of transition states in route IV-m.*

			TS-Cl	TS-OAc	TS-OTs
bond	Co1⋯O1		1.958	1.965	1.933
	O2-H1⋯O1		1.470	1.489	1.453
	O2⋯C2		2.425	2.402	2.423
	Co2⋯O2		1.958	1.964	1.938
charges	Co1	NPA	0.441	0.611	0.623
		ADCH	0.225	0.257	0.242
		Hirshfeld	0.199	0.237	0.240
	O1	NPA	-0.655	-0.662	-0.647
		ADCH	-0.245	-0.252	-0.249
		Hirshfeld	-0.201	-0.203	-0.195
	H1	NPA	0.542	0.542	0.544
		ADCH	0.146	0.145	0.146
		Hirshfeld	0.107	0.107	0.107
	O2	NPA	-0.858	-0.860	-0.851
		ADCH	-0.255	-0.262	-0.270
		Hirshfeld	-0.181	-0.181	-0.179
	Co2	NPA	0.435	0.612	0.619
		ADCH	0.184	0.223	0.247
		Hirshfeld	0.207	0.248	0.249
	C2	NPA	0.238	0.232	0.240
		ADCH	0.099	0.094	0.096
		Hirshfeld	0.198	0.196	0.199
	C1	NPA	-0.160	-0.159	-0.160
		ADCH	-0.060	-0.063	-0.056
		Hirshfeld	0.026	0.027	0.029

*: The atomic numbering (O1 etc.) is marked on the route IV-m in Fig. 1.

Table S6 The ADCH and Hirshfeld charge (e) of metal Co in five-coordinated complexes.

		Co^{III}(salen)-Cl	Co^{III}(salen)-OAc	Co^{III}(salen)-OTs
Co	ADCH	0.330	0.309	0.395
	Hirshfeld	0.280	0.325	0.329

The structures of transition states (t), corresponding reactant complexes (r) and product complexes (p) in all the routes where the substrate is PO.
Et, Er and Ep denote the single point energies of transition states, reactants (or reactant complexes) and products (or product complexes) calculated at at B3PLY-D3BJ/ def2TZVP respectively. Frequencies are in unit of cm^{-1}.

I-t (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.403532
Thermal correction to Gibbs Free Energy (a.u.): 0.079054
Imaginary frequencies: -515.92
Calculation of single point energy based on the optimized structure, Et = -269.6079696 a.u.

C	-0.65587800	-0.02462000	0.39589200
C	0.26935600	0.98525600	-0.14568900
O	0.02916000	-1.08001200	-0.19960000
H	-0.62899600	-0.03891600	1.50074400
H	0.82753200	1.70613000	0.43742000
H	0.25905800	1.10801000	-1.22308300
C	-2.10150900	0.09709500	-0.08148900
H	-2.62568700	-0.82328700	0.19380600
H	-2.61970500	0.94970100	0.37068700
H	-2.13176000	0.18862200	-1.17122800
O	2.19520800	-0.00792400	0.14264700
H	1.45577000	-0.73178700	0.07323700
H	2.59703200	-0.00136700	-0.73824800

I-t (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.482347
Thermal correction to Gibbs Free Energy (a.u.): 0.079395
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -269.6834746 a.u.

C	-0.66606100	-0.26602500	0.27113600
C	-0.14797000	1.10286500	0.37276300
O	0.03682200	0.34020700	-0.84006900
H	-0.08347600	-1.04431200	0.76385100
H	0.76763300	1.27981800	0.93210300
H	-0.83206500	1.94465200	0.27900200
C	-2.12311200	-0.56172200	0.04395500
H	-2.24335500	-1.45354400	-0.57895300
H	-2.62741000	-0.74534300	0.99861500
H	-2.61442600	0.27680700	-0.45683100
O	2.49427700	-0.54710100	0.14996800
H	1.79297200	-0.31342000	-0.48499300
H	3.21419500	0.05978400	-0.05911100

I-t (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.509266
Thermal correction to Gibbs Free Energy (a.u.): 0.084762
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -269.7148076 a.u.

C	-0.46858300	0.05322900	-0.34353100
C	0.71243100	-0.74494100	0.19744400
O	-0.42498500	1.37300500	0.18064300
H	-0.37638200	0.07726500	-1.44311800
H	0.72199700	-1.75820400	-0.23113600
H	0.61563200	-0.82753300	1.28981500
C	-1.80449400	-0.56264400	0.03938100
H	-2.62175600	0.05278700	-0.34451300
H	-1.90515400	-1.57102400	-0.37411200
H	-1.90133800	-0.61453000	1.12839500

O	1.88860400	-0.01677900	-0.16158300
H	0.49875200	1.65104900	0.08559400
H	2.62317300	-0.33348400	0.37683400

I-m (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.408511
Thermal correction to Gibbs Free Energy (a.u.): 0.078456
Imaginary frequencies: -483.25
Calculation of single point energy based on the optimized structure, Et = -269.6150501 a.u.

C	-0.54090300	-0.16734400	0.61635800
C	-0.19115600	1.25759700	0.42049200
O	0.52308400	1.07319500	-0.74888800
H	-0.24415300	-0.72553500	1.49842500
H	0.37983600	1.66952500	1.27387000
H	-1.10239400	1.87762700	0.30437700
C	-1.45327300	-0.85177100	-0.32296100
H	-1.00155300	-1.77775700	-0.69012400
H	-2.35619800	-1.14284600	0.23631000
H	-1.71242600	-0.21220300	-1.16587600
O	1.44162300	-1.07760100	0.00669100
H	1.30228700	-0.16910600	-0.47166500
H	2.12893700	-0.91534600	0.66892400

I-m (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.482355
Thermal correction to Gibbs Free Energy (a.u.): 0.079388
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -269.6834841 a.u.

C	-0.66618900	0.26583500	-0.27113100
C	-0.14818800	-1.10304900	-0.37302900
O	0.03685000	-0.34067800	0.84010800
H	-0.08327900	1.04407200	-0.76351300
H	0.76739300	-1.27999600	-0.93243200
H	-0.83215300	-1.94494800	-0.27931200
C	-2.12301400	0.56220300	-0.04379800
H	-2.24251200	1.45370400	0.57971100
H	-2.62710200	0.74689200	-0.99835900
H	-2.61499300	-0.27629600	0.45637800
O	2.49407100	0.54709800	-0.15009400
H	1.79300700	0.31130400	0.48442200
H	3.21661500	-0.05602800	0.06073700

I-m (PO + H_2O)
PO + H_2O = PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.508860
Thermal correction to Gibbs Free Energy (a.u.): 0.085339
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -269.7139385 a.u.

C	0.54691800	0.10176100	0.48918800
C	-0.94735500	-0.18892800	0.66539100
O	-1.59739600	-0.26706800	-0.58848400
H	1.00490600	0.25425600	1.47861700
H	-1.39335500	0.59938200	1.29920600
H	-1.09826700	-1.14428000	1.17947300
C	1.27874400	-1.00598800	-0.25196600
H	2.31297500	-0.71345000	-0.44753800
H	1.27728600	-1.92515000	0.34133600
H	0.78085200	-1.20914500	-1.20295000
O	0.68268000	1.29183100	-0.30895100
H	-1.21766300	0.45903200	-1.10856700
H	0.38114900	2.04018000	0.22422000

II-t (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.771747
Thermal correction to Gibbs Free Energy (a.u.): 0.421124
Imaginary frequencies: -514.07
Calculation of single point energy based on the optimized structure, Et = -3147.4758658 a.u.

C	-2.77185500	-2.17986100	1.87962800
C	-1.38676000	-2.61649200	1.69405900
O	-2.29650200	-1.22122600	2.84206100
H	-3.19633500	-1.70217700	0.99581800
H	-0.79827900	-2.45434900	0.79349600
H	-0.93559300	-3.13513700	2.53581100
C	-3.74245400	-3.14043600	2.53545500
H	-4.62515100	-2.58099800	2.85670000
H	-4.05638500	-3.91290000	1.82806300
H	-3.29193500	-3.61385400	3.41209500
O	-0.37048500	-0.33501600	1.61656000
H	-1.59510400	-0.62271700	2.35737800
H	0.42320100	-0.59460000	2.10281000
C	-4.95349600	-0.46255700	-1.59110800
C	-5.14232600	0.92271200	-1.41939800
C	-3.71864900	-1.04721400	-1.38515300
H	-5.79011500	-1.08374400	-1.90042500
C	-4.05876100	1.69497400	-1.05056700
H	-6.11421300	1.37334600	-1.58753500
C	-2.58693600	-0.27992900	-0.98092400
H	-3.56341400	-2.11027600	-1.53994800
C	-2.78162800	1.13219800	-0.82623000
H	-4.17387100	2.76994500	-0.92920000
O	-1.47532200	-0.90405000	-0.75107900
C	-1.70780900	2.01937900	-0.48993400
Co	0.16850100	-0.11341400	-0.22520800
N	-0.49179900	1.67528200	-0.23643600
H	-1.96099600	3.08046300	-0.47855200
N	1.81348300	0.64233400	0.37993100
Cl	0.80564200	0.18888800	-2.38356300
C	0.59176400	2.65328900	-0.07649700
C	2.96816200	0.06952400	0.29032900
C	1.61555500	2.00830300	0.87275700
C	0.19227100	4.04727600	0.40939900
H	3.85675700	0.64092900	0.56201000
C	3.19347300	-1.28144300	-0.12553500
C	2.86310100	2.87759500	1.02107600
C	1.43900500	4.92863700	0.57665700
H	-0.34038300	3.95911300	1.36583700
H	-0.49195000	4.52178100	-0.30090100
C	4.52952000	-1.72195700	-0.26931000
C	2.11216100	-2.19991000	-0.33003000
C	2.47145500	4.28096300	1.50602500
H	3.56493600	2.42418200	1.72943900
H	3.37482600	2.94522100	0.05220800
H	1.14794000	5.91280200	0.95875100
H	1.89381900	5.09535700	-0.40861100
C	4.82830800	-3.02366800	-0.61569200
H	5.32953200	-1.00355400	-0.10401900
C	2.45081700	-3.53528800	-0.67500200
O	0.85766100	-1.89095000	-0.17410300
H	2.05331900	4.20795000	2.51903000
H	3.36467800	4.91011700	1.58002800
C	3.76721500	-3.92955100	-0.81580900
H	5.85749700	-3.34509100	-0.73234300
H	1.63260100	-4.22807000	-0.84151500
H	3.98658100	-4.95753100	-1.09237900
H	1.12448100	1.91404900	1.85233800
H	1.07070700	2.72818000	-1.06234600

II-t (PO + H_2O-Co^{III}-Cl)
PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
Charge: 0

Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.845770
Thermal correction to Gibbs Free Energy (a.u.): 0.422903
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -3147.5449871 a.u.

C	-3.45234700	-2.13268500	1.63625200
C	-2.31201300	-2.95085700	1.20720100
O	-2.16626200	-1.98935400	2.29142600
H	-3.70770800	-1.27826500	1.01426400
H	-1.76115100	-2.68644600	0.30999200
H	-2.25388000	-3.98491000	1.54319100
C	-4.55563500	-2.67898600	2.50032100
H	-4.93113300	-1.90982200	3.18277600
H	-5.39145100	-3.01306000	1.87616700
H	-4.20154000	-3.52603400	3.09423000
O	-0.29448600	-0.20160000	1.82462400
H	-1.12853300	-0.75108800	1.89910900
H	0.38774600	-0.82735200	2.11158300
C	-4.89337600	0.70051700	-1.55498400
C	-4.78213600	2.09805600	-1.41019800
C	-3.82810500	-0.13525900	-1.28238000
H	-5.83077200	0.27031200	-1.89774100
C	-3.57347700	2.62430400	-1.00388700
H	-5.62422100	2.74495200	-1.62999400
C	-2.57828300	0.37624500	-0.83184500
H	-3.90465200	-1.20907300	-1.41510100
C	-2.46067000	1.79903700	-0.71547500
H	-3.45322100	3.70101500	-0.90609500
O	-1.63914100	-0.46941900	-0.53157300
C	-1.22893200	2.43564900	-0.36374000
Co	0.15939100	-0.04665300	-0.13070500
N	-0.11438700	1.84135500	-0.09676000
H	-1.24796200	3.52635000	-0.35870700
N	1.95231300	0.34446100	0.40051500
Cl	0.71084900	0.13371100	-2.29961800
C	1.15174800	2.57537000	0.04272100
C	2.96316600	-0.44314200	0.22257100
C	2.06028400	1.70771700	0.92836000
C	1.06003400	4.00207100	0.58755600
H	3.96284400	-0.06717900	0.44369800
C	2.88229500	-1.79655900	-0.23013500
C	3.46429300	2.30055800	1.03471100
C	2.46439900	4.61055900	0.71857400
H	0.56052700	3.98335200	1.56524600
H	0.45611500	4.63119200	-0.07346700
C	4.08567500	-2.49250300	-0.49182100
C	1.62330700	-2.47067700	-0.35359400
C	3.38624500	3.73581700	1.57562000
H	4.08968900	1.68970200	1.69466200
H	3.93565700	2.29866900	0.04322600
H	2.39292000	5.61726200	1.14349900
H	2.90021900	4.72204700	-0.28298900
C	4.08172900	-3.81563400	-0.88120000
H	5.02610300	-1.95641400	-0.38463300
C	1.65198000	-3.83487500	-0.74475700
O	0.47459300	-1.92054600	-0.07823200
H	3.00898200	3.71119500	2.60670300
H	4.39039100	4.17028200	1.61935800
C	2.84488400	-4.48162500	-1.00286900
H	5.01025400	-4.33576100	-1.08954900
H	0.69920900	-4.34362900	-0.84421700
H	2.82746400	-5.52386700	-1.31042400
H	1.60597200	1.68921900	1.92970200
H	1.60063100	2.59196300	-0.96022900

II-t (PO + H_2O-Co^{III}-Cl)
PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.866311

Thermal correction to Gibbs Free Energy (a.u.): 0.426227
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -3147.5708739 a.u.

C	-2.19259400	0.74069800	2.42065100
C	-1.26119100	-0.44591200	2.62097800
O	-1.52753800	1.95280100	2.78219200
H	-2.46654000	0.77702200	1.35997800
H	-1.68493400	-1.36619200	2.21506200
H	-1.03236100	-0.57108400	3.68564300
C	-3.45416700	0.60814200	3.25877300
H	-4.08637300	1.48855100	3.11843600
H	-4.02419400	-0.27733700	2.96056200
H	-3.20612400	0.53282400	4.32211500
O	-0.02391000	-0.13268800	1.93881800
H	-0.58785700	1.80354400	2.60674300
H	0.65226600	-0.82512600	2.10468300
C	-4.14834900	-3.29925000	-0.80279300
C	-4.80433200	-2.20814100	-1.41342500
C	-2.85652200	-3.18834900	-0.33198500
H	-4.66797900	-4.24887900	-0.70669900
C	-4.12901300	-1.01370600	-1.53187500
H	-5.81814800	-2.31232100	-1.78387100
C	-2.13135200	-1.96912500	-0.44310500
H	-2.34464900	-4.02730000	0.12690500
C	-2.80274900	-0.85970400	-1.05538300
H	-4.61017600	-0.15710900	-1.99857600
O	-0.92804400	-1.92524000	0.04176500
C	-2.18456400	0.41783700	-1.19508400
Co	0.27782500	-0.48749100	-0.09015300
N	-1.00532800	0.74609500	-0.77197600
H	-2.78157200	1.18012300	-1.69771600
N	1.48012000	0.99257600	-0.06433300
Cl	0.84979200	-0.97606800	-2.18765700
C	-0.41762500	2.05860500	-1.08656100
C	2.76771200	0.90111000	-0.06462900
C	0.74880200	2.25847300	-0.10816000
C	-1.37152100	3.25379900	-0.99931000
H	3.35714100	1.81352900	-0.16363700
C	3.50412300	-0.32041900	0.07525000
C	1.53987100	3.52244500	-0.43727900
C	-0.61364200	4.55367500	-1.31037200
H	-1.79583500	3.28741800	0.01275000
H	-2.20366600	3.14512400	-1.70125000
C	4.90492500	-0.28756100	-0.10571700
C	2.86368400	-1.53909800	0.46130700
C	0.60265500	4.73957100	-0.39503700
H	2.35658700	3.66238300	0.27890000
H	1.99065800	3.42297300	-1.43325500
H	-1.29122300	5.40848000	-1.21500500
H	-0.28046100	4.53137000	-2.35650200
C	5.67772400	-1.41906900	0.06551100
H	5.36839000	0.65364800	-0.39234600
C	3.67919600	-2.68085900	0.64054900
O	1.57685500	-1.63849900	0.70366700
H	0.25884600	4.88841900	0.63688900
H	1.15506900	5.64225300	-0.67585800
C	5.04745400	-2.61959500	0.44400700
H	6.75087200	-1.38489500	-0.08740600
H	3.18771900	-3.60442700	0.92625800
H	5.64406000	-3.51742900	0.58061500
H	0.29493200	2.38392300	0.88403600
H	0.00421300	1.98282700	-2.09839300

II-m (PO + H_2O-Co^{III}-Cl)
PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.776794
Thermal correction to Gibbs Free Energy (a.u.): 0.421278

Imaginary frequencies: -411.84
Calculation of single point energy based on the optimized structure, Et = -3147.4843703 a.u.

C	-4.54210800	-2.13410800	-1.55910500
C	-5.00770000	-0.82847900	-1.82712600
C	-3.25802500	-2.35633400	-1.10546900
H	-5.20347700	-2.98129700	-1.72126100
C	-4.14520100	0.23218900	-1.64177700
C	-2.35056800	-1.28002800	-0.87688800
C	-2.82357800	0.04619200	-1.16809800
H	-4.47538700	1.24612700	-1.85683200
O	-1.19903700	-1.55032400	-0.35691700
C	-2.00141000	1.21124300	-0.99743300
Co	0.24923700	-0.32354800	-0.13183500
N	-0.79105400	1.22634000	-0.55573600
H	-2.45978400	2.15553400	-1.29695900
N	1.68853100	0.88554200	0.15024400
C	0.03517700	2.44369100	-0.60684100
C	2.93933300	0.57287700	0.11034800
C	1.18410100	2.23528900	0.39216500
C	-0.68591200	3.76623200	-0.33747400
H	3.68061100	1.36872000	0.19549700
C	3.44816800	-0.75925800	-0.01895400
C	2.19325900	3.38009400	0.31976100
C	0.31307000	4.93225600	-0.38643500
H	-1.16531500	3.71759400	0.64924900
H	-1.47671400	3.93864600	-1.07408100
C	4.83838000	-0.93560100	-0.20010500
C	2.59100200	-1.90009800	0.10851900
C	1.48499100	4.71814800	0.57847800
H	2.98954300	3.23439200	1.05739200
H	2.66434300	3.39013600	-0.67191600
H	-0.20206500	5.87099900	-0.15651200
H	0.69972700	5.02794600	-1.40967300
C	5.40173800	-2.19346800	-0.27560100
H	5.46434300	-0.04998400	-0.28636900
C	3.20014000	-3.18012300	0.03946700
O	1.30823700	-1.82846600	0.33594900
H	1.11175400	4.73221000	1.61121300
H	2.20230800	5.54117000	0.49277900
C	4.56189800	-3.31806900	-0.15104100
H	4.99104800	-4.31500700	-0.20998700
H	0.73962500	2.20976500	1.39670900
H	0.47873700	2.45922300	-1.61211300
Cl	0.77779900	-0.44762900	-2.34251200
O	-0.14653600	-0.20080000	1.74866300
H	0.50254300	-0.85474400	2.05179000
H	-0.95828200	0.26903200	2.84826800
C	-2.43381000	-1.34541600	2.40892800
C	-1.95279200	-1.11897200	3.78858600
O	-1.69414500	0.26456000	3.58993300
H	-1.80987700	-1.83014100	1.65811400
H	-1.06513100	-1.70007800	4.05823400
H	-2.73312200	-1.24307400	4.54518600
C	-3.71523000	-0.80065000	1.97357500
H	-3.55489400	-0.12115000	1.12178700
H	-4.28959000	-1.61956400	1.51426300
H	-4.27537100	-0.30548000	2.76675300
H	6.46881000	-2.31576200	-0.42673000
H	2.55017100	-4.04391400	0.12912300
H	-2.88996300	-3.35798400	-0.90910000
H	-6.01661400	-0.66640100	-2.19003600

II-m (PO + H_2O-Co^{III}-Cl)
PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.844620
Thermal correction to Gibbs Free Energy (a.u.): 0.423647
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -3147.5464894 a.u.

C	-4.44784100	-1.68413600	-1.83735800
C	-4.81508400	-0.33989200	-2.05918600
C	-3.22604000	-2.01062700	-1.28451900
H	-5.13745400	-2.47895900	-2.10923400
C	-3.91598900	0.65319400	-1.72758300
C	-2.28306900	-1.00779600	-0.91866300
C	-2.65050600	0.35532800	-1.16794900
H	-4.16723800	1.69673500	-1.90417700
O	-1.18189300	-1.37806300	-0.34333600
C	-1.76009900	1.44374000	-0.90719300
Co	0.35406700	-0.29232000	-0.09888100
N	-0.55474000	1.34929700	-0.45039800
H	-2.14126600	2.43482400	-1.15866300
N	1.87630600	0.78374700	0.27854000
C	0.36521200	2.49843200	-0.44610100
C	3.09690200	0.36615600	0.27444700
C	1.47869600	2.16356300	0.55818800
C	-0.25140400	3.86356100	-0.13364000
H	3.89894300	1.09214200	0.41456400
C	3.49644400	-1.00086400	0.12025900
C	2.57944500	3.22303400	0.53792400
C	0.83847600	4.94637200	-0.13120700
H	-0.74614600	3.81750200	0.84547600
H	-1.01677400	4.12463900	-0.87080100
C	4.87252900	-1.28890500	-0.02155400
C	2.54549700	-2.06880500	0.18760600
C	1.97861700	4.60506200	0.83536600
H	3.35028400	2.98863500	1.27966700
H	3.06377300	3.22649100	-0.44734300
H	0.39783000	5.91474200	0.12837500
H	1.24331700	5.04714600	-1.14688700
C	5.33036100	-2.58793900	-0.11436300
H	5.57308900	-0.45777100	-0.06255600
C	3.04490800	-3.39264300	0.10228600
O	1.26249800	-1.89278800	0.37007200
H	1.59643200	4.61492700	1.86484200
H	2.76150700	5.36897700	0.78410100
C	4.39666500	-3.64054300	-0.04797100
H	4.74286800	-4.66817200	-0.12077500
H	1.01945200	2.14629100	1.55688200
H	0.82453400	2.52026300	-1.44443400
Cl	0.91532100	-0.39124700	-2.26881900
O	-0.05023300	-0.24125500	1.86438100
H	0.28186600	-1.14368400	2.01841900
H	-1.03230000	-0.24320200	2.02222400
C	-3.45714600	-1.29157100	2.11849300
C	-2.96815900	-1.14261000	3.49476500
O	-2.62884500	-0.15608800	2.49340600
H	-2.92858700	-1.99065900	1.47471600
H	-2.13287200	-1.74677200	3.84584100
H	-3.63965900	-0.77828100	4.26967100
C	-4.86766300	-0.95573500	1.72710000
H	-4.89051700	-0.51049500	0.72988500
H	-5.47531900	-1.86621300	1.70327700
H	-5.31061600	-0.25544700	2.44092100
H	6.38801800	-2.79592700	-0.23457100
H	2.32192600	-4.19994500	0.14687900
H	-2.93583500	-3.04286500	-1.11918600
H	-5.77722500	-0.09510700	-2.49544900

II-m (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.862846

Thermal correction to Gibbs Free Energy (a.u.): 0.426928

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5697367 a.u.

C	-4.61029100	-2.66542500	-0.99851900
C	-5.21535400	-1.43721900	-1.34426800

C	-3.27873900	-2.73593600	-0.64601900
H	-5.20292800	-3.57620000	-1.01647200
C	-4.44855100	-0.29363900	-1.32126800
C	-2.45936100	-1.57303900	-0.61639100
C	-3.07811200	-0.32524300	-0.95944100
H	-4.88900600	0.66580100	-1.58317600
O	-1.21949500	-1.70634600	-0.25738600
C	-2.36199200	0.90770400	-0.93646800
Co	0.09208000	-0.36193000	-0.25342700
N	-1.12650800	1.06550300	-0.58089900
H	-2.92757000	1.78954100	-1.24071400
N	1.42020100	0.99663500	-0.07648900
C	-0.43782600	2.35662700	-0.73768300
C	2.69061300	0.81834400	-0.21689600
C	0.79690700	2.29683000	0.17466700
C	-1.27018500	3.60474000	-0.43320700
H	3.34696000	1.68940100	-0.20147500
C	3.32805000	-0.45561000	-0.37931000
C	1.67468100	3.53577800	0.00870600
C	-0.40591600	4.86651900	-0.57772800
H	-1.66675300	3.52875700	0.58782400
H	-2.12805100	3.67568100	-1.10853000
C	4.70542600	-0.48576000	-0.69131600
C	2.61877400	-1.67802800	-0.16624100
C	0.85077200	4.79946900	0.29781900
H	2.53382100	3.49082800	0.68658800
H	2.06768600	3.56962900	-1.01583000
H	-0.99845000	5.75158200	-0.32373700
H	-0.10924300	4.97775600	-1.62900600
C	5.38698600	-1.68051200	-0.81580000
H	5.22393700	0.45846500	-0.84105800
C	3.34132700	-2.88701200	-0.29014300
O	1.35372000	-1.73120000	0.18683700
H	0.55679000	4.80147000	1.35588400
H	1.47002400	5.68901500	0.14291000
C	4.68795400	-2.88460700	-0.60944500
H	5.21232400	-3.83136500	-0.70599600
H	0.42873800	2.25797000	1.21022200
H	-0.07676100	2.39537700	-1.77496200
Cl	0.44213200	-0.49535500	-2.45131100
O	0.02643100	-0.36109700	1.83649000
H	0.70003500	-1.07474900	1.74409100
H	0.60597100	0.31678300	4.02329300
C	-1.09347700	-0.88069700	2.61223200
C	-0.54124900	-1.22637600	3.99479200
O	-0.00141200	-0.09504800	4.65404600
H	-1.46163500	-1.78329900	2.11566200
H	0.20840700	-2.02966000	3.89257200
H	-1.34936200	-1.61084700	4.62518600
C	-2.16810000	0.18859700	2.65377900
H	-2.50051700	0.44278200	1.64858600
H	-3.02898000	-0.18176100	3.21802100
H	-1.79075700	1.08362900	3.15460700
H	6.44190800	-1.69232200	-1.06717900
H	2.79639500	-3.81173900	-0.13513300
H	-2.80713300	-3.67901000	-0.39178100
H	-6.26210500	-1.39883100	-1.62487500

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.778325

Thermal correction to Gibbs Free Energy (a.u.): 0.421456

Imaginary frequencies: -382.38

Calculation of single point energy based on the optimized structure, Et = -3147.4855152 a.u.

C	-4.90592200	-2.32219900	-0.62976100
C	-5.49478200	-1.04773500	-0.49446900
C	-3.53579100	-2.47393300	-0.69753000

H	-5.54110400	-3.20233400	-0.68651800
C	-4.67068600	0.05690300	-0.43408100
H	-6.57288600	-0.93979200	-0.44768900
C	-2.65815900	-1.35400700	-0.62678900
H	-3.07806100	-3.45093000	-0.81131900
C	-3.26166100	-0.06018000	-0.48868400
H	-5.09966900	1.05230300	-0.34045000
O	-1.38121600	-1.57555200	-0.68095200
C	-2.48656500	1.14236800	-0.43965800
Co	-0.02148100	-0.29129700	-0.35868100
N	-1.19887800	1.20874800	-0.40173200
H	-3.05551800	2.07314000	-0.44790000
N	1.34109500	0.98152100	0.06809000
C	-0.45668500	2.47111900	-0.48022300
C	2.60994100	0.75428100	-0.00394700
C	0.77878800	2.29018200	0.41786800
C	-1.22002400	3.74630300	-0.12494400
H	3.29868200	1.57897800	0.18107000
C	3.21565400	-0.50666700	-0.30700800
C	1.71731500	3.49279900	0.32079000
C	-0.28420800	4.96087700	-0.21362300
H	-1.62865500	3.65864200	0.89122700
H	-2.06642600	3.88866000	-0.80443400
C	4.62281700	-0.55376000	-0.44139700
C	2.44631900	-1.70946300	-0.42998700
C	0.95881200	4.78302100	0.66527600
H	2.56514300	3.37299800	1.00308900
H	2.12094200	3.55300200	-0.69809900
H	-0.82604100	5.86840700	0.07303700
H	0.02694100	5.09620300	-1.25762500
C	5.28611800	-1.73594900	-0.69881000
H	5.18095800	0.37448200	-0.34036100
C	3.15727400	-2.91262700	-0.68881800
O	1.15740600	-1.77481400	-0.26416800
H	0.65543000	4.75064600	1.72060900
H	1.62679000	5.64413700	0.55837200
C	4.53236300	-2.92079700	-0.82014100
H	6.36506600	-1.75492100	-0.80702000
H	2.57177700	-3.81988600	-0.79320500
H	5.04010100	-3.85925100	-1.02713700
C	-0.63487200	-1.80172900	2.00506500
C	0.65563300	-1.85678700	2.68743100
O	-0.43609200	-0.47052800	1.53298700
H	-0.65390600	-2.49036300	1.14780300
H	1.54097900	-1.88805800	2.06516600
H	0.77583900	-1.95414700	3.76075000
C	-1.88993200	-1.92739900	2.84869100
H	-2.76424600	-1.73723200	2.22240900
H	-1.97417700	-2.93650900	3.26660100
H	-1.88362300	-1.20287700	3.66982700
O	1.18088600	0.32442300	3.32887500
H	0.52016800	0.32213900	2.58252500
H	0.67455000	0.56320700	4.11821300
Cl	0.37537300	0.00624200	-2.56500600
H	-0.09411000	2.53473800	-1.51471900
H	0.41982300	2.21567400	1.45531500

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.840795

Thermal correction to Gibbs Free Energy (a.u.): 0.423365

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5454006 a.u.

C	-4.53023100	-2.70269300	-0.75852100
C	-5.19973500	-1.46058800	-0.77412900
C	-3.15191100	-2.77552600	-0.74439600
H	-5.10948900	-3.62225000	-0.76253500
C	-4.44607200	-0.30597900	-0.78277600

H	-6.28308700	-1.41756100	-0.79106800
C	-2.34431900	-1.60108200	-0.73238200
H	-2.63409100	-3.72879800	-0.74287300
C	-3.02991300	-0.34066800	-0.75380600
H	-4.93546100	0.66544400	-0.81384500
O	-1.05700100	-1.74382100	-0.68922300
C	-2.32780400	0.90635100	-0.76635200
Co	0.19203000	-0.36326200	-0.35491000
N	-1.05302000	1.05230400	-0.63365200
H	-2.94373500	1.79792700	-0.88149000
N	1.41580000	1.00962100	0.14784400
C	-0.39325500	2.36300200	-0.66696100
C	2.70044000	0.86932100	0.19590700
C	0.72806200	2.28362100	0.38469800
C	-1.28865800	3.57648100	-0.41494000
H	3.31401900	1.75056800	0.38644300
C	3.40321100	-0.36526400	0.03229300
C	1.58410400	3.54854800	0.38299500
C	-0.44559900	4.86001000	-0.39354600
H	-1.81049700	3.43575700	0.54044500
H	-2.04902500	3.65903500	-1.19869400
C	4.81739500	-0.33454900	-0.00217100
C	2.71370900	-1.61972900	-0.03493900
C	0.69484600	4.77704900	0.62735900
H	2.35577900	3.49253200	1.15839600
H	2.09664100	3.63820600	-0.58365300
H	-1.08780500	5.71924800	-0.17389000
H	-0.02402300	5.02951600	-1.39321700
C	5.55975700	-1.49168600	-0.11147000
H	5.31444700	0.63133500	0.05417700
C	3.50427100	-2.79401700	-0.13822700
O	1.41854300	-1.74353400	0.04674600
H	0.27262000	4.71809100	1.63916300
H	1.30379900	5.68644900	0.59260700
C	4.88340400	-2.72726000	-0.17729100
H	6.64304400	-1.45447700	-0.14634800
H	2.97950800	-3.74137300	-0.19722400
H	5.45676400	-3.64612500	-0.26633400
C	-0.65154900	-1.77264300	2.19178200
C	0.38095000	-0.86068300	2.69804600
O	-0.46377000	-0.44214700	1.58521100
H	-0.30788900	-2.54448200	1.50973700
H	1.41313900	-1.03009200	2.41234200
H	0.19949300	-0.27948700	3.59855600
C	-1.98247600	-1.96318300	2.85815000
H	-2.73823400	-2.21858200	2.10966100
H	-1.92196100	-2.78783800	3.57584000
H	-2.29352200	-1.05397400	3.37922200
O	-2.55588200	1.37665400	2.30380200
H	-1.81590000	0.82477400	2.00147100
H	-3.31177700	0.98881100	1.84445400
Cl	0.82736300	-0.22155000	-2.48641600
H	0.08604300	2.44134100	-1.65159000
H	0.23487100	2.19675100	1.36431600

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.863516

Thermal correction to Gibbs Free Energy (a.u.): 0.427445

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.572434 a.u.

C	-4.80836600	-2.34221600	-0.82316900
C	-5.44083800	-1.12773600	-0.48205800
C	-3.44039100	-2.41734700	-0.98740400
H	-5.40916700	-3.23703100	-0.96372500
C	-4.66145500	-0.00229700	-0.31884700
H	-6.51750500	-1.08099800	-0.36090800
C	-2.60584900	-1.27612600	-0.80994500

H	-2.95151600	-3.34693700	-1.25885800
C	-3.25382000	-0.04339900	-0.46575300
H	-5.12378900	0.95014700	-0.06822300
O	-1.32701300	-1.42603500	-0.96388000
C	-2.52445600	1.17636400	-0.30698700
Co	-0.01438600	-0.16508800	-0.45631300
N	-1.23849500	1.28912700	-0.31363400
H	-3.12507600	2.07818400	-0.17987500
N	1.29244400	1.07909300	0.18692100
C	-0.53749100	2.57373300	-0.25141000
C	2.57297200	0.89631800	0.11925600
C	0.68656800	2.33522800	0.65038300
C	-1.34390900	3.78418500	0.21557000
H	3.23044000	1.71560700	0.41164600
C	3.22352500	-0.30131900	-0.30285900
C	1.59229600	3.56619000	0.69033400
C	-0.44221200	5.02659400	0.26316700
H	-1.76445100	3.58649900	1.21124600
H	-2.18432800	3.96676800	-0.46191200
C	4.63815600	-0.30106300	-0.37497700
C	2.49306200	-1.49876200	-0.60281700
C	0.79175400	4.79654100	1.14308000
H	2.43323000	3.40580500	1.37315100
H	2.01039300	3.73421500	-0.31038200
H	-1.01368700	5.88636300	0.62832500
H	-0.11935800	5.27289700	-0.75665100
C	5.34305500	-1.42960900	-0.73308100
H	5.16528900	0.62127500	-0.14101100
C	3.24934800	-2.64880900	-0.96205600
O	1.20241500	-1.61098500	-0.52056400
H	0.47336500	4.65489900	2.18485300
H	1.43753200	5.68073600	1.13144900
C	4.62729800	-2.61039100	-1.02503200
H	6.42589500	-1.41341800	-0.79012800
H	2.69454800	-3.55085900	-1.19657900
H	5.17043200	-3.50721300	-1.31128100
C	-0.53264600	-2.07672200	1.80101500
C	0.77047900	-2.41262700	2.53105800
O	-0.46144200	-0.66484600	1.45419100
H	-0.57944500	-2.61860300	0.85650700
H	1.59088000	-2.44182700	1.81490100
H	0.69676200	-3.38565100	3.03188400
C	-1.79549000	-2.29896600	2.62044800
H	-2.66867100	-1.96448800	2.05622700
H	-1.91765400	-3.36282100	2.84891500
H	-1.76550800	-1.74187300	3.56487600
O	1.10148500	-1.36652800	3.45827300
H	0.19020900	-0.29037700	2.07816900
H	0.51095100	-1.43986800	4.21988300
Cl	0.42613600	0.41996300	-2.57404800
H	-0.15791800	2.75499900	-1.26530300
H	0.30153800	2.15459500	1.66742500

III-m (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.784816

Thermal correction to Gibbs Free Energy (a.u.): 0.420367

Imaginary frequencies: -274.43

Calculation of single point energy based on the optimized structure, Et = -3147.4955817 a.u.

C	-4.71906500	-2.86520400	-0.33612200
C	-5.42406600	-1.64318900	-0.32839600
C	-3.34124000	-2.89595900	-0.39807100
H	-5.27019400	-3.80131200	-0.29769700
C	-4.70622700	-0.46674600	-0.38687500
C	-2.57024000	-1.69832900	-0.45399300
C	-3.29227700	-0.45705000	-0.44179600
H	-5.22648200	0.48888000	-0.39213800

O	-1.28109000	-1.80726000	-0.51001600
C	-2.63518800	0.81224400	-0.51594300
Co	-0.05471100	-0.37566900	-0.34897500
N	-1.35928800	1.00334300	-0.50643400
H	-3.29076500	1.68089300	-0.59476000
N	1.19749900	1.04287800	-0.07158300
C	-0.73768000	2.31981800	-0.67857600
C	2.47653100	0.93221600	-0.19816300
C	0.51978800	2.31142400	0.21088300
C	-1.61300100	3.53818400	-0.38625800
H	3.09086000	1.82994500	-0.11707100
C	3.18510500	-0.29207200	-0.43248600
C	1.33834100	3.58856900	0.02542100
C	-0.79770700	4.82851800	-0.55658100
H	-2.00065500	3.47084900	0.63953300
H	-2.47608100	3.56106500	-1.05931600
C	4.57952900	-0.22419500	-0.65557200
C	2.52873100	-1.56602200	-0.39777000
C	0.46545600	4.81900900	0.31180100
H	2.20505200	3.58933300	0.69506400
H	1.71888200	3.62840500	-1.00347800
H	-1.42064600	5.69553300	-0.31233100
H	-0.51141600	4.93356700	-1.61121500
C	5.33623700	-1.36148900	-0.85264600
H	5.05148900	0.75581900	-0.67482400
C	3.33405000	-2.71886200	-0.59850500
O	1.26360500	-1.72590100	-0.13559200
H	0.17795200	4.81628600	1.37180500
H	1.04708900	5.73210200	0.14679500
C	4.69354800	-2.61557000	-0.82042000
H	5.27597700	-3.51939500	-0.97899700
H	0.18337000	2.25939700	1.25659700
H	-0.39347900	2.35298900	-1.72094400
Cl	0.28451900	-0.25502100	-2.58402800
O	-0.34337200	1.02792300	3.64129700
H	-1.21506400	1.14418200	4.04219800
H	-0.51998000	0.70324700	2.71397100
C	0.44605400	-1.28654500	3.28534700
C	-0.44851800	-1.64893200	2.17594600
O	-0.48555500	-0.39649700	1.53443100
H	0.09245500	-1.29209500	4.31380000
H	-1.44150000	-1.98914600	2.49385200
H	0.01029700	-2.40926400	1.52160200
C	1.85760200	-0.94579600	3.07185200
H	2.07536500	0.03202300	3.51567500
H	2.45783100	-1.67329800	3.64269000
H	2.13475600	-0.96718300	2.02173600
H	6.40383200	-1.29338000	-1.03131200
H	2.83295200	-3.68076800	-0.58157000
H	-2.79453500	-3.83284600	-0.41652600
H	-6.50774100	-1.63120900	-0.28564500

III-m (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.835694

Thermal correction to Gibbs Free Energy (a.u.): 0.422326

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5408912 a.u.

C	-4.51277400	-3.10400200	-0.31008200
C	-5.25792600	-1.91511500	-0.46721600
C	-3.13425300	-3.08691000	-0.27065400
H	-5.03404900	-4.05383700	-0.22414500
C	-4.57826000	-0.72242000	-0.58539300
C	-2.40179800	-1.86941900	-0.37977200
C	-3.16305700	-0.66316300	-0.53942300
H	-5.12672800	0.20759400	-0.72067600
O	-1.10870100	-1.92832200	-0.31802500
C	-2.54204000	0.61608000	-0.68026900

Co	0.06936500	-0.45547400	-0.26515200
N	-1.27588200	0.85629800	-0.59221200
H	-3.21473200	1.45253400	-0.87254200
N	1.24789200	1.02584300	-0.04211200
C	-0.70066500	2.18998200	-0.81267300
C	2.53452200	0.95996200	-0.14607800
C	0.50685200	2.27857200	0.13730100
C	-1.64240400	3.37749600	-0.60800000
H	3.10820100	1.88726900	-0.12515400
C	3.29057200	-0.24831100	-0.26701000
C	1.28172200	3.57914500	-0.06220200
C	-0.87648400	4.69630000	-0.78917700
H	-2.06764400	3.31140400	0.40077200
H	-2.46804100	3.34009800	-1.32648100
C	4.68494800	-0.15011300	-0.48414500
C	2.68034300	-1.53605500	-0.11188000
C	0.34255900	4.77827800	0.13668500
H	2.11636000	3.64099500	0.64491000
H	1.70785900	3.59809500	-1.07386400
H	-1.54850300	5.54105100	-0.60469600
H	-0.54433500	4.78054600	-1.83255200
C	5.48226400	-1.27295400	-0.56170600
H	5.12168900	0.83989800	-0.59518700
C	3.52769800	-2.67236200	-0.18544300
O	1.41584800	-1.71523900	0.15036900
H	0.00430400	4.79951700	1.18079200
H	0.89106400	5.70996900	-0.03742600
C	4.88482100	-2.54063900	-0.40671000
H	5.50170600	-3.43324500	-0.46757400
H	0.10233800	2.26410200	1.15953200
H	-0.31001400	2.18905900	-1.83913800
Cl	0.49088600	-0.53517300	-2.45025400
O	-2.22059700	1.73829100	2.41893800
H	-3.17020100	1.61301200	2.30430500
H	-1.82266400	0.96129600	1.99096200
C	0.18709600	-0.39072400	3.02806300
C	-0.44997300	-1.60646900	2.50153700
O	-0.50932100	-0.37474500	1.73152100
H	-0.38494300	0.19929400	3.74250200
H	-1.41968800	-1.92806900	2.87016800
H	0.17016300	-2.35642100	2.02024300
C	1.67277200	-0.18635000	3.04411500
H	1.91982000	0.86355100	2.86473900
H	2.05284700	-0.45605600	4.03538100
H	2.16445500	-0.80194400	2.29381800
H	6.54874300	-1.18473400	-0.73783300
H	3.06230300	-3.64562200	-0.07345700
H	-2.55793500	-3.99949200	-0.16196600
H	-6.34141000	-1.94382000	-0.50337900

III-m (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.859912

Thermal correction to Gibbs Free Energy (a.u.): 0.427643

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5705219 a.u.

C	-4.67925300	-2.86914100	-0.58824100
C	-5.42144300	-1.70097500	-0.30903700
C	-3.31037900	-2.82805100	-0.75016500
H	-5.19608100	-3.82068900	-0.68305000
C	-4.74876600	-0.50315000	-0.20349100
C	-2.58326200	-1.60746500	-0.63571500
C	-3.34210300	-0.42221100	-0.35219500
H	-5.29685400	0.41467700	-0.00089500
O	-1.29839200	-1.64824600	-0.79517300
C	-2.73198000	0.86576500	-0.25750300
Co	-0.10963200	-0.23012800	-0.43179500
N	-1.46213600	1.10397100	-0.28995000

H	-3.41574200	1.71027300	-0.15940500
N	1.10154900	1.16833900	0.06395900
C	-0.89225100	2.45381700	-0.30945500
C	2.38315000	1.12321000	-0.11822400
C	0.39930200	2.37263600	0.52420000
C	-1.79074100	3.59307000	0.17011400
H	2.96855000	2.02184200	0.07893200
C	3.12205100	-0.01911300	-0.55022600
C	1.17446100	3.68921100	0.47760600
C	-1.01960600	4.92100800	0.13432900
H	-2.13542000	3.38491500	1.19245600
H	-2.68048400	3.67002200	-0.46291800
C	4.51540100	0.12644300	-0.75887300
C	2.50464600	-1.30301800	-0.71675200
C	0.27816800	4.84505200	0.94653500
H	2.06568400	3.63491500	1.11168500
H	1.51409800	3.86857100	-0.55049200
H	-1.65559400	5.72946500	0.50984700
H	-0.78037500	5.16686500	-0.90841600
C	5.30528400	-0.94142500	-1.12572500
H	4.95642200	1.11161100	-0.62345100
C	3.34721500	-2.38645200	-1.08872500
O	1.24901300	-1.54419700	-0.49555400
H	0.03458600	4.70354800	2.00826400
H	0.82739300	5.78960900	0.87528700
C	4.70105100	-2.20674000	-1.28685100
H	5.31216200	-3.05693000	-1.57829300
H	0.09433400	2.19145600	1.56842800
H	-0.59043500	2.63785000	-1.34892900
Cl	0.14682900	0.27734400	-2.59682500
O	0.50633700	-0.88268700	3.96736200
H	-0.30451500	-1.09337300	4.45106300
H	-0.11859300	-0.10257800	2.20683200
C	0.81315100	-1.99309500	3.09646400
C	-0.24449900	-2.03450400	1.98973600
O	-0.46262800	-0.69247100	1.51221600
H	0.76792800	-2.93707000	3.65734200
H	-1.20157700	-2.40679900	2.37537800
H	0.06463300	-2.63834500	1.13742800
C	2.22820700	-1.76015900	2.59426500
H	2.91968500	-1.72011100	3.43936400
H	2.53355700	-2.55880300	1.91548100
H	2.29303500	-0.81810900	2.04663500
H	6.36994400	-0.81474500	-1.28857000
H	2.87693100	-3.35490300	-1.22083200
H	-2.73821700	-3.72153400	-0.97614000
H	-6.49841700	-1.74667400	-0.18981400

IV-t (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3548.156311

Thermal correction to Gibbs Free Energy (a.u.): 0.769711

Imaginary frequencies: -384.92

Calculation of single point energy based on the optimized structure, Et = -6025.3483821 a.u.

C	1.17380300	1.51447200	-1.78326900
C	0.27651800	2.29099100	-0.91828100
O	1.29645300	0.44381300	-0.84703300
H	0.62915400	1.12897600	-2.64903100
H	-0.76268100	2.49133500	-1.17788500
H	0.71915000	2.65879300	0.00626000
C	2.44784000	2.21160300	-2.23973000
H	3.10107600	1.47893800	-2.72139200
H	2.19420800	2.97521700	-2.98259000
H	2.98055800	2.68003400	-1.41553800
O	-1.01058400	0.57192400	-0.00461300
H	-0.15986700	0.18859600	-0.39697400
H	-0.77711500	0.66693600	0.94190900

C	0.75556900	-2.33345800	-4.20423200
C	0.63120100	-3.53319300	-3.47275100
C	0.03163600	-1.20920900	-3.86223600
H	1.41873700	-2.29692600	-5.06476800
C	-0.23401500	-3.56226300	-2.39715500
H	1.19075500	-4.41669300	-3.76032900
C	-0.86143400	-1.20399200	-2.75060100
H	0.10023500	-0.29749700	-4.44628500
C	-0.98175100	-2.42641300	-2.00956400
H	-0.36019300	-4.47909700	-1.82518300
O	-1.49096200	-0.10504900	-2.47471400
C	-1.89754700	-2.56887000	-0.91686300
Co	-2.67297300	0.18120100	-1.00719700
N	-2.64783900	-1.63879100	-0.43270100
H	-1.97033300	-3.56820700	-0.48654200
N	-3.73089500	0.50084900	0.54594700
Cl	-4.50107500	-0.25979800	-2.22225300
C	-3.68438500	-1.89318300	0.57600100
C	-4.45317000	1.55503100	0.73896400
C	-3.71194100	-0.64340000	1.46865000
C	-3.54725200	-3.17126400	1.40024500
H	-5.09482900	1.58838400	1.61979600
C	-4.48938300	2.71038300	-0.10332900
C	-4.84674800	-0.71693500	2.48978800
C	-4.68414200	-3.25151300	2.43018000
H	-2.57740200	-3.17687300	1.91111700
H	-3.58710400	-4.05073900	0.74879200
C	-5.41352900	3.73499400	0.20924400
C	-3.59057100	2.87284600	-1.20558600
C	-4.73048600	-2.00422000	3.31941500
H	-4.81851200	0.15127500	3.15696100
H	-5.80897000	-0.69368500	1.96156500
H	-4.56045500	-4.14911100	3.04540700
H	-5.64119400	-3.35999500	1.90300200
C	-5.48070600	4.89703200	-0.53098000
H	-6.08195200	3.58618200	1.05433400
C	-3.67745500	4.08158100	-1.94522400
O	-2.67576500	2.00573800	-1.53691000
H	-3.81564500	-1.95909700	3.92075200
H	-5.57054100	-2.06707700	4.01922100
C	-4.59604200	5.05946400	-1.61618600
H	-6.19908800	5.67117800	-0.28471700
H	-3.00466200	4.19788500	-2.78835300
H	-4.63954700	5.96828900	-2.21051400
C	-1.16954900	-1.37391000	4.38350300
C	-0.91295300	-2.72292000	4.07789000
C	-0.59065900	-0.35234500	3.65021700
H	-1.82475900	-1.12599200	5.21413000
C	-0.05248000	-3.01371000	3.03452000
H	-1.36850400	-3.51749200	4.65844200
C	0.30074500	-0.62465600	2.58049000
H	-0.77337100	0.68977700	3.89112300
C	0.57196600	-1.99570200	2.28100900
H	0.17535700	-4.04892300	2.79084900
O	0.77250900	0.38289700	1.89061300
C	1.53056500	-2.39329500	1.28660100
Co	2.38223900	0.30261300	0.81637300
N	2.29889800	-1.60725300	0.61588200
H	1.64737300	-3.46992100	1.15175500
N	3.92395400	0.20610900	-0.27696600
C	3.44699900	-2.13190900	-0.14690900
C	4.88929400	1.06088900	-0.26357000
C	3.88816000	-1.00701200	-1.09248900
C	3.20905400	-3.43192100	-0.91477500
H	5.78141900	0.85144200	-0.85524100
C	4.86710600	2.30505300	0.44706000
C	5.15525500	-1.37810000	-1.85636800
C	4.45962300	-3.81249200	-1.72168700
H	2.35382000	-3.29754000	-1.58431500

H	2.96212500	-4.24873300	-0.22863900
C	6.04602400	3.08437200	0.47703400
C	3.66549900	2.80320400	1.05020500
C	4.90928600	-2.67354200	-2.64477800
H	5.43805200	-0.56998200	-2.54031500
H	5.98740100	-1.51804500	-1.15367700
H	4.25572500	-4.71512100	-2.30751400
H	5.27678000	-4.06283600	-1.03189300
C	6.07760200	4.32033000	1.09005100
H	6.94116400	2.68438300	0.00616400
C	3.72456400	4.08184700	1.65967300
O	2.51845600	2.17781500	1.01715100
H	4.13151100	-2.49131000	-3.39802500
H	5.81712000	-2.95807200	-3.18681200
C	4.89735300	4.81304800	1.68073500
H	6.99145200	4.90367000	1.11517600
H	2.81666300	4.45507000	2.12128700
H	4.90770500	5.78475600	2.16710400
Cl	3.63091300	-0.06518400	2.66375300
H	4.25178100	-2.27052100	0.58894200
H	3.06992500	-0.86004600	-1.81014900
H	-4.63139500	-1.91261300	0.02045400
H	-2.75504400	-0.60705500	2.00834200

IV-t (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3548.217020

Thermal correction to Gibbs Free Energy (a.u.): 0.771611

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6025.4125713 a.u.

C	1.45353500	0.44593400	-2.28235800
C	1.29891800	1.75781800	-1.65034800
O	1.31672300	0.55481100	-0.80287700
H	0.54279300	0.00201800	-2.68023900
H	0.32960300	2.23601000	-1.66292600
H	2.17702200	2.37032700	-1.47949200
C	2.75786900	-0.06425500	-2.81467000
H	2.83886200	-1.14442100	-2.66181600
H	2.78642000	0.12100500	-3.89415900
H	3.60841800	0.43275900	-2.35059800
O	-1.04281400	-0.25658700	0.13588000
H	-0.19619700	-0.00051500	-0.31457100
H	-1.16786800	0.43889300	0.80289800
C	0.54279600	-4.19696900	-2.81218500
C	-0.06980100	-5.09818500	-1.91761700
C	0.10529200	-2.89190700	-2.92580500
H	1.36736700	-4.53594900	-3.43388800
C	-1.12508800	-4.64764300	-1.14927600
H	0.27304400	-6.12428500	-1.84447000
C	-0.97966900	-2.39475400	-2.14477600
H	0.55702100	-2.21209300	-3.63984000
C	-1.59388700	-3.31622800	-1.23172500
H	-1.62376500	-5.32551800	-0.45988100
O	-1.34420600	-1.16132500	-2.31185400
C	-2.72360200	-2.95416000	-0.42540000
Co	-2.52215600	-0.20663500	-1.15561100
N	-3.23248900	-1.77470800	-0.33216400
H	-3.18056400	-3.76582500	0.14240800
N	-3.55586700	0.74938500	0.13741900
Cl	-4.22874700	-0.20226400	-2.61230700
C	-4.41954500	-1.46441300	0.46931900
C	-3.76622800	2.02580400	0.12716000
C	-4.09522500	-0.13689800	1.17541800
C	-4.88078400	-2.52651700	1.46493200
H	-4.40785600	2.45058200	0.89801400
C	-3.21886200	2.95334000	-0.80864100
C	-5.29082300	0.38533400	1.97049600
C	-6.08746700	-2.00862400	2.26156200

H	-4.05807800	-2.77041500	2.15146400
H	-5.15222500	-3.44883500	0.94083400
C	-3.60774000	4.31000000	-0.70359200
C	-2.25593400	2.55963100	-1.79264300
C	-5.77168000	-0.68289700	2.96335400
H	-5.01615100	1.29391100	2.51591200
H	-6.09823200	0.64868800	1.27547000
H	-6.39929700	-2.76121800	2.99319900
H	-6.93337900	-1.86462900	1.57707400
C	-3.09274700	5.27672000	-1.54100500
H	-4.33318400	4.57900700	0.06093700
C	-1.75677800	3.57516400	-2.65398100
O	-1.77255400	1.35775100	-1.91136000
H	-4.99099300	-0.84931600	3.71831000
H	-6.65263300	-0.31719900	3.50083600
C	-2.16058500	4.88960500	-2.52551900
H	-3.40198800	6.31215400	-1.45124700
H	-1.05348200	3.27381700	-3.42292700
H	-1.75502400	5.63728800	-3.20177900
C	-1.50329500	3.60864500	2.38952200
C	-2.04174200	2.55162500	3.15835200
C	-0.28935100	3.48415900	1.74941000
H	-2.05688900	4.53823100	2.29371000
C	-1.33589500	1.36993000	3.24191400
H	-2.98563500	2.67211300	3.67912700
C	0.47471400	2.28072400	1.82233600
H	0.12452900	4.29555000	1.16122600
C	-0.09888400	1.19238100	2.56790600
H	-1.72924200	0.53644800	3.82018200
O	1.60642700	2.23133100	1.20196300
C	0.48439300	-0.11790200	2.56942600
Co	2.62490800	0.67091300	0.84501500
N	1.47754900	-0.49715900	1.84002900
H	-0.01828700	-0.85900800	3.19167500
N	3.53307800	-0.90985700	0.31759200
C	1.98272800	-1.87889300	1.87047200
C	4.75764300	-0.95635100	-0.09409600
C	2.69865000	-2.09553500	0.52751200
C	0.93292600	-2.97134300	2.09065400
H	5.21318300	-1.93212100	-0.26415100
C	5.57360800	0.18231700	-0.37697600
C	3.39853400	-3.45243500	0.48953400
C	1.59986000	-4.35457400	2.04469600
H	0.16539000	-2.88821200	1.31067600
H	0.43539700	-2.84531400	3.05756900
C	6.93119600	-0.02668500	-0.71688700
C	5.03064500	1.50802200	-0.38623700
C	2.37814000	-4.57166000	0.74221600
H	3.87754600	-3.60727700	-0.48337900
H	4.18829000	-3.47469700	1.25205000
H	0.83779700	-5.13294700	2.15900700
H	2.28057500	-4.45163600	2.90103600
C	7.75840200	1.02505500	-1.04981800
H	7.31564100	-1.04406900	-0.70619300
C	5.90284800	2.56939400	-0.74221800
O	3.77979500	1.78386600	-0.14335200
H	1.67344300	-4.60676500	-0.09528900
H	2.89185800	-5.53876900	0.76594800
C	7.22535500	2.33078200	-1.06079600
H	8.79956100	0.85383000	-1.30030000
H	5.49019600	3.57236000	-0.74226000
H	7.86781800	3.16787100	-1.32029400
Cl	3.87455100	0.86322300	2.68117300
H	2.74476300	-1.92021500	2.66048800
H	1.92775400	-2.07856900	-0.25787500
H	-5.22030700	-1.26091900	-0.25303600
H	-3.27347200	-0.33766400	1.88084300

IV-t (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3548.260459
Thermal correction to Gibbs Free Energy (a.u.): 0.778490
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -6025.4560489 a.u.

C	0.42571900	2.08962900	-0.76689900
C	-0.47221700	2.14979000	0.47438800
O	1.16001700	0.83709200	-0.80651900
H	-0.21869200	2.05744200	-1.64477900
H	-1.24723600	2.90264900	0.32361000
H	0.11724200	2.37575600	1.36302900
C	1.37342800	3.26994300	-0.86514500
H	1.99284600	3.17941800	-1.76186900
H	0.79170000	4.19363100	-0.95120500
H	2.02169500	3.35008000	0.00620500
O	-1.14724900	0.90028500	0.72116500
H	0.48370700	0.15879000	-1.08339600
H	-0.45996600	0.23618900	1.02213000
C	0.31892400	-3.66790800	-2.98405200
C	-0.31281300	-4.65897900	-2.21270000
C	0.08306200	-2.32362100	-2.75012800
H	0.99307300	-3.95746700	-3.78589300
C	-1.17678700	-4.26722600	-1.20667000
H	-0.13178000	-5.71022300	-2.40837600
C	-0.79588900	-1.90084200	-1.72681200
H	0.54941900	-1.55339900	-3.35460000
C	-1.43248100	-2.90576400	-0.94037100
H	-1.66711500	-5.01331700	-0.58822200
O	-0.94905000	-0.61256900	-1.52259400
C	-2.32749800	-2.58989000	0.13484900
Co	-2.46313100	0.15627900	-0.61196900
N	-2.74233800	-1.41178600	0.45890000
H	-2.70315300	-3.44507700	0.69714500
N	-3.82106700	0.95360100	0.44527600
Cl	-3.98676900	-0.68912800	-2.03462700
C	-3.86777900	-1.24536800	1.39746400
C	-4.53517200	1.97425700	0.10524900
C	-3.95352600	0.25109900	1.72324200
C	-3.81133200	-2.07268800	2.68378000
H	-5.33254400	2.29677600	0.77559700
C	-4.35746200	2.74518000	-1.08541800
C	-5.19368800	0.56020600	2.56061400
C	-5.04830200	-1.77881200	3.54475700
H	-2.89901500	-1.81717900	3.23305700
H	-3.75992800	-3.14258500	2.46090600
C	-5.29563900	3.76178400	-1.37955700
C	-3.22291400	2.55049300	-1.93638100
C	-5.18002300	-0.28094700	3.84645400
H	-5.22739500	1.62423100	2.81754600
H	-6.09465300	0.33601200	1.97450600
H	-4.99544200	-2.34954000	4.47785600
H	-5.94627800	-2.12334700	3.01479400
C	-5.15369300	4.57431300	-2.48512300
H	-6.14424700	3.89009400	-0.71126300
C	-3.09798100	3.40706400	-3.06199100
O	-2.28356600	1.67757400	-1.71317300
H	-4.33588000	0.03699400	4.47256200
H	-6.08969600	-0.08736900	4.42433300
C	-4.03729100	4.38481400	-3.32523200
H	-5.88430400	5.34496500	-2.70510100
H	-2.24297500	3.25321500	-3.71160300
H	-3.91361300	5.01712600	-4.20046800
C	-0.40459000	-3.77487100	2.81477300
C	0.22733500	-4.74239000	2.01481800
C	-0.17360800	-2.42388500	2.61595300
H	-1.07546000	-4.08809700	3.61036000
C	1.09319900	-4.32128400	1.02192900
H	0.04846400	-5.79905500	2.18108000

C	0.69811700	-1.97161600	1.60156800
H	-0.63913700	-1.67062600	3.24135100
C	1.34747800	-2.95272400	0.79570700
H	1.59000900	-5.04914400	0.38713000
O	0.84473300	-0.67755300	1.42531100
C	2.27061100	-2.60594400	-0.24644700
Co	2.39632500	0.10531200	0.61499800
N	2.71355600	-1.42143000	-0.50163100
H	2.64964500	-3.44143500	-0.83599900
N	3.82701600	0.91870700	-0.32314300
C	3.86366000	-1.22466800	-1.40200000
C	4.55527300	1.88459300	0.12685800
C	4.00177400	0.28713400	-1.63068300
C	3.80874700	-1.96029500	-2.74281200
H	5.40508500	2.21877000	-0.46962800
C	4.32261100	2.58222300	1.35411700
C	5.28129300	0.60722200	-2.40074000
C	5.07654100	-1.65245800	-3.55360900
H	2.91682700	-1.63535000	-3.29036800
H	3.71554000	-3.04045100	-2.59529400
C	5.28102900	3.52896200	1.78426600
C	3.11806000	2.39061800	2.10701600
C	5.27725400	-0.14305800	-3.74235300
H	5.36063700	1.68461600	-2.58114800
H	6.15369000	0.31003300	-1.80402300
H	5.02540100	-2.15089300	-4.52731500
H	5.94657500	-2.07148300	-3.03073800
C	5.09424400	4.27322500	2.93053800
H	6.18241400	3.65757100	1.18920600
C	2.94849100	3.17903100	3.27494500
O	2.15344900	1.58917700	1.75227000
H	4.46724100	0.25310600	-4.36892300
H	6.21200900	0.05129900	-4.27838700
C	3.91007000	4.08753500	3.67249900
H	5.84121100	4.98933200	3.25507700
H	2.03943900	3.02921700	3.84744600
H	3.74992900	4.66731000	4.57765400
Cl	3.82661600	-0.81197000	2.08976300
H	4.75004400	-1.55094100	-0.83939200
H	3.13669200	0.60386700	-2.22826800
H	-4.77382900	-1.50649600	0.83235800
H	-3.05607000	0.51172600	2.30080300

IV-m (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3548.162706

Thermal correction to Gibbs Free Energy (a.u.): 0.770148

Imaginary frequencies: -261.98

Calculation of single point energy based on the optimized structure, Et = -6025.3545631 a.u.

N	-2.31690700	1.50967200	-0.36802200
N	-3.72287500	-0.59853300	0.14509600
C	-1.59602700	2.48881000	-0.79912000
H	-1.62431100	3.42829100	-0.24508500
C	-4.11335200	-1.78965100	0.45371600
H	-4.80647800	-1.90623800	1.28792300
C	-0.74348700	2.47113700	-1.95031400
C	-0.07730600	3.66900600	-2.29717400
C	-0.54030300	1.28922700	-2.73539100
C	0.79181500	3.73624200	-3.36796400
H	-0.27090600	4.55560900	-1.69692200
C	0.36941900	1.38563900	-3.82687800
C	1.01266400	2.56955100	-4.12945700
H	1.28862800	4.66563200	-3.62370400
H	0.51481100	0.49444000	-4.42840300
H	1.68893500	2.60510900	-4.97960700
C	-3.73130100	-2.99630300	-0.21776300
C	-4.15086700	-4.22813900	0.33671600

C	-2.99799600	-2.97976900	-1.45019700
C	-3.86365700	-5.43375700	-0.27028500
H	-4.71263800	-4.20754300	1.26795400
C	-2.74294400	-4.23837300	-2.06763100
C	-3.15665900	-5.42293900	-1.48984700
H	-4.18698200	-6.36938100	0.17219200
H	-2.21527700	-4.22624800	-3.01597100
H	-2.93762100	-6.36252900	-1.99032700
O	-1.10648300	0.14714900	-2.50529700
O	-2.55433700	-1.90925100	-2.03286900
H	-2.47160200	1.34112200	1.68921000
C	-3.12192600	1.63259800	0.85594700
C	-3.69798600	3.03723100	1.12191300
C	-4.25896400	0.60812200	0.77975600
C	-4.99624800	2.96547900	1.95834800
H	-2.95030100	3.63808200	1.64763200
H	-3.90639100	3.52349700	0.16325900
C	-4.88763700	0.42398100	2.16837600
H	-5.00184400	0.99420900	0.07244600
C	-4.97560500	1.77453800	2.92354700
H	-5.13026400	3.90067700	2.51087000
H	-5.86044800	2.87633000	1.28986200
H	-4.27783500	-0.27637000	2.75088600
H	-5.88352700	-0.01877100	2.06329400
H	-4.10858300	1.87587600	3.58326900
H	-5.86265600	1.78480100	3.56421000
Co	-2.46541800	-0.19229700	-1.21639700
Cl	-4.08920100	0.63671600	-2.52919700
H	-0.12081300	-0.48111300	-0.41571900
O	1.30704200	-0.38479800	-0.75189900
C	1.63309700	-1.42537800	-1.65167300
C	0.45564200	-2.32752000	-1.46477100
H	2.57357600	-1.92151600	-1.39397800
H	1.67724800	-1.03747700	-2.67591300
H	-0.43672000	-2.13127700	-2.06269200
C	0.47377700	-3.43946900	-0.53072600
H	0.91346000	-3.09207700	0.42008400
H	1.23033400	-4.15432600	-0.90194800
H	-0.49262800	-3.92520100	-0.41447500
O	-1.00556500	-0.92199300	-0.13472400
H	-0.90797200	-0.92962700	0.83909700
N	1.87343600	1.70120900	0.70223900
N	3.82291700	0.11013600	0.04434300
C	1.04198800	2.42470200	1.36534200
H	0.98639800	3.49078300	1.14254800
C	4.75129200	-0.77469000	-0.10507700
H	5.67660800	-0.46845000	-0.59712500
C	0.16571600	1.94823000	2.40098400
C	-0.54253200	2.89803000	3.16736100
C	-0.02974300	0.55257100	2.63925700
C	-1.41480900	2.51504600	4.17051000
H	-0.37805600	3.95357800	2.96259700
C	-0.93960200	0.18531200	3.66406600
C	-1.60407100	1.14159300	4.41284500
H	-1.93816600	3.25740900	4.76286700
H	-1.07416600	-0.87453900	3.85349600
H	-2.27857800	0.82381600	5.20326500
C	4.69546000	-2.14030100	0.32280800
C	5.82086700	-2.96138200	0.07528500
C	3.54295700	-2.68741000	0.97350000
C	5.84242000	-4.29082800	0.44363300
H	6.68349200	-2.51718200	-0.41623500
C	3.59396400	-4.05920400	1.34213800
C	4.70999500	-4.83202800	1.08422500
H	6.71425600	-4.90614400	0.25109500
H	2.72927100	-4.47059900	1.85220500
H	4.71451800	-5.87515400	1.38895400
O	0.52389600	-0.39245400	1.92373800
O	2.44685600	-2.02412100	1.20239800

H	2.18838900	1.93126500	-1.30935200
C	2.69765500	2.23063600	-0.38616900
C	2.92789100	3.74860700	-0.37893100
C	4.05035600	1.51230400	-0.33036300
C	4.15242100	4.13290400	-1.24870400
H	2.03248000	4.24860500	-0.75327000
H	3.09173900	4.08169800	0.65210300
C	4.80085400	1.71145900	-1.66368800
H	4.61852700	1.95707300	0.49694000
C	4.44724800	3.06860800	-2.31233700
H	3.98034700	5.10479600	-1.72103200
H	5.03548900	4.25257400	-0.60975800
H	4.53431000	0.89559200	-2.34475500
H	5.88043600	1.64944500	-1.49160800
H	3.56574600	2.95219000	-2.95083500
H	5.26606700	3.39236700	-2.96243100
Co	2.19376400	-0.15940600	0.97963500
Cl	3.28509800	0.31815000	2.90062100

IV-m (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3548.198662

Thermal correction to Gibbs Free Energy (a.u.): 0.771839

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6025.3937321 a.u.

N	3.02964000	-1.11890700	0.20897300
N	3.70097000	1.38212600	-0.00083600
C	2.82066800	-2.37384000	-0.01208900
H	3.26481300	-3.10291200	0.66653700
C	3.88681000	2.64122500	-0.21610900
H	4.67394100	3.14766900	0.34531400
C	2.06131200	-2.90845600	-1.10445000
C	2.08773900	-4.30498200	-1.32326600
C	1.29076100	-2.06430600	-1.96915500
C	1.41786700	-4.88397900	-2.38436300
H	2.66831400	-4.92383100	-0.64272300
C	0.63046300	-2.68574200	-3.06384800
C	0.69846500	-4.05149000	-3.26536200
H	1.45944400	-5.95503000	-2.54785800
H	0.08905400	-2.03951800	-3.74661800
H	0.18817100	-4.48892700	-4.11921600
C	3.16058400	3.45848700	-1.13881000
C	3.50046400	4.82998100	-1.21659000
C	2.11702700	2.93605900	-1.96939700
C	2.84997100	5.69274900	-2.07422200
H	4.29856200	5.19812400	-0.57579200
C	1.46970300	3.84762000	-2.84984700
C	1.82549300	5.18137200	-2.89569100
H	3.12371700	6.74092900	-2.12077600
H	0.69416200	3.44710400	-3.49439000
H	1.30898000	5.84512100	-3.58409300
O	1.12836800	-0.79055300	-1.77614400
O	1.70731700	1.70318600	-1.95722400
H	3.06232400	-0.30450300	2.10582400
C	3.79728500	-0.62822600	1.35676700
C	4.74764700	-1.63850800	2.01517400
C	4.56948000	0.61702100	0.90167300
C	5.83299300	-0.91952500	2.85336800
H	4.16523300	-2.31215900	2.65125900
H	5.22472400	-2.24675400	1.23929000
C	5.07269200	1.39460300	2.13700900
H	5.41466900	0.27043500	0.29328000
C	5.34882800	0.45359400	3.33178800
H	6.12091400	-1.54546500	3.70336600
H	6.73705900	-0.78638900	2.24748500
H	4.31817600	2.13541600	2.42211400
H	5.98381100	1.94350500	1.87779700
H	4.43283800	0.32570200	3.92075600

H	6.08528600	0.91116900	3.99933700
Co	2.42920000	0.30783200	-0.91381300
Cl	4.00732700	-0.19133900	-2.43342600
H	0.19945800	0.89416900	0.12112400
O	-1.37330200	1.03237500	-0.46795100
C	-1.41805100	0.99464700	-1.93023900
C	-1.42374600	2.28964200	-1.23920000
H	-2.36627300	0.61544200	-2.30241300
H	-0.50190300	0.60660800	-2.36478300
H	-0.46594700	2.79734700	-1.17133000
C	-2.63992600	3.15664800	-1.13353200
H	-2.68776700	3.64351500	-0.15818600
H	-3.56067800	2.59251100	-1.28588200
H	-2.57087600	3.93013700	-1.90649700
O	1.12393300	0.83698800	0.47095500
H	1.07149800	0.16866600	1.17240000
N	-1.50350400	-1.54595100	0.57037000
N	-3.76464400	-0.61989800	-0.31995900
C	-0.52132800	-2.00133900	1.27225300
H	-0.04845100	-2.93098900	0.95845800
C	-4.92160200	-0.08507500	-0.56552100
H	-5.58677800	-0.60626300	-1.25689900
C	0.03587700	-1.37081100	2.43401900
C	1.06738300	-2.04709400	3.13184500
C	-0.39527800	-0.07044100	2.87010500
C	1.69118600	-1.48136600	4.22404700
H	1.35991800	-3.03471900	2.78321200
C	0.28151000	0.49130800	3.99303200
C	1.28663300	-0.19355200	4.64379200
H	2.47135900	-2.01430500	4.75656500
H	-0.03386200	1.47826100	4.31254100
H	1.77179600	0.26488200	5.50135300
C	-5.42936100	1.11895800	-0.00021600
C	-6.71365700	1.56393200	-0.40718600
C	-4.68621300	1.87124600	0.97073000
C	-7.27231700	2.71325800	0.10405400
H	-7.25614300	0.96929900	-1.13879000
C	-5.29451600	3.05240900	1.48351000
C	-6.54285900	3.45565900	1.06022800
H	-8.25582900	3.04166900	-0.21334100
H	-4.73321900	3.61585900	2.22086300
H	-6.97649900	4.36158900	1.47526900
O	-1.28527100	0.64227500	2.25985300
O	-3.49066300	1.57627600	1.36746400
H	-1.45347000	-1.75738100	-1.47718100
C	-1.96838100	-2.23783300	-0.63691600
C	-1.70543800	-3.74990300	-0.67699700
C	-3.47137200	-1.98887800	-0.77192900
C	-2.58764300	-4.44240000	-1.74761200
H	-0.65262600	-3.93904800	-0.88712300
H	-1.92840300	-4.16594000	0.31184600
C	-3.93459700	-2.32913200	-2.20301000
H	-3.96830300	-2.65180300	-0.05230200
C	-3.07243500	-3.45574500	-2.81740900
H	-2.02226600	-5.25385900	-2.21496300
H	-3.45923400	-4.90383300	-1.26852900
H	-3.87100400	-1.43082800	-2.82823900
H	-4.98665700	-2.63164000	-2.18613600
H	-2.20026700	-3.02192200	-3.31660000
H	-3.64471200	-3.97892500	-3.58978300
Co	-2.54311300	0.00068500	0.99478500
Cl	-3.64864600	-1.16283000	2.53755500

IV-m (PO-Co^{III}-Cl + H_2O-Co^{III}-Cl)

PO-Co^{III}-Cl + H_2O-Co^{III}-Cl = PG + 2Co^{III}(salen)-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3548.247752

Thermal correction to Gibbs Free Energy (a.u.): 0.778607

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6025.4414365 a.u.

N	2.42689100	-1.44419400	0.27563100
N	3.83341200	0.73560900	0.10539600
C	1.91146200	-2.58696500	-0.01458500
H	2.09561100	-3.43287000	0.64641600
C	4.46588600	1.82881700	-0.16720400
H	5.37472200	2.04870500	0.39642900
C	1.10100800	-2.84783200	-1.17781000
C	0.82959400	-4.18678700	-1.51781100
C	0.54747200	-1.79131700	-1.95771400
C	0.06375800	-4.50760000	-2.62700000
H	1.24375400	-4.97397800	-0.89312500
C	-0.21606200	-2.13838100	-3.09332500
C	-0.44514300	-3.46639000	-3.42184100
H	-0.12202700	-5.54324500	-2.88980600
H	-0.59187100	-1.32973200	-3.71100600
H	-1.02115500	-3.70247100	-4.31256000
C	4.10048700	2.79005300	-1.16039100
C	4.93159100	3.92455700	-1.32625900
C	2.93425700	2.63527900	-1.97871900
C	4.64991400	4.89663100	-2.26219200
H	5.81164800	4.01424300	-0.69334200
C	2.66984400	3.65371900	-2.93494500
C	3.50266100	4.74634700	-3.06889900
H	5.29776200	5.75821600	-2.38007900
H	1.79146000	3.53040300	-3.55946200
H	3.27004800	5.50236600	-3.81413300
O	0.68617100	-0.52162000	-1.63753700
O	2.08737100	1.65516700	-1.87543300
H	2.60364800	-0.68611500	2.17355700
C	3.25252200	-1.20878100	1.46032100
C	3.85444000	-2.45398000	2.12587900
C	4.37596000	-0.24513200	1.05305200
C	5.05611000	-2.07732200	3.02912000
H	3.07940100	-2.95967100	2.70704800
H	4.18659300	-3.15074400	1.34843700
C	5.02172300	0.36136900	2.31654800
H	5.11473100	-0.83386400	0.49356300
C	4.96839300	-0.62312800	3.50737600
H	5.10702100	-2.75944600	3.88314100
H	5.99157400	-2.21018600	2.47283400
H	4.49411500	1.28596200	2.57446300
H	6.06152500	0.63040600	2.10433300
H	4.03294400	-0.48298700	4.06195700
H	5.77751100	-0.39924400	4.20921300
Co	2.29551500	0.11981300	-0.80961200
Cl	3.64170600	-0.82369500	-2.34059200
H	-0.51656800	0.36689900	-1.01551700
O	-1.16688400	0.99730400	-0.58472600
C	-0.52800600	2.27896200	-0.44046500
C	0.66703300	2.27842000	0.55004900
H	-1.29518300	2.98561500	-0.12840800
H	-0.15778600	2.54490300	-1.43183600
H	1.45891700	2.87492500	0.09812800
C	0.39376800	2.80629400	1.95165600
H	-0.31556100	2.17138800	2.48047000
H	-0.02996500	3.81416500	1.89174100
H	1.33565300	2.86089100	2.50649300
O	1.20744600	0.94463700	0.65850300
H	0.48817200	0.36746000	1.05673100
N	-2.31722700	-1.50365300	-0.21276100
N	-3.84948900	0.59765500	-0.30273400
C	-1.74421100	-2.58851100	0.17833900
H	-1.85391500	-3.48803600	-0.42565700
C	-4.51562200	1.70189500	-0.22027500
H	-5.36912400	1.83514400	-0.88710300
C	-0.95907800	-2.72602200	1.37850700
C	-0.57745600	-4.02045000	1.78236800
C	-0.52189800	-1.59471100	2.12334600

C	0.20290200	-4.22385200	2.90844700
H	-0.90916700	-4.86673700	1.18654000
C	0.27368500	-1.82097400	3.26855500
C	0.62040800	-3.10727700	3.65366700
H	0.47522200	-5.22678000	3.21866700
H	0.57993200	-0.95440100	3.84487800
H	1.21663900	-3.25187700	4.55064000
C	-4.26336800	2.77505600	0.68777100
C	-5.09959400	3.91605700	0.62562600
C	-3.22310500	2.70395300	1.66857000
C	-4.93995800	4.97590400	1.49241700
H	-5.88394600	3.93874400	-0.12767100
C	-3.09193200	3.80571300	2.55950100
C	-3.92293800	4.90401500	2.46738400
H	-5.58758600	5.84371900	1.43414400
H	-2.31700500	3.74536700	3.31510800
H	-3.79221400	5.72695400	3.16510200
O	-0.77711600	-0.35475400	1.75874400
O	-2.38256700	1.72086400	1.77651100
H	-2.48426700	-0.96140700	-2.18886300
C	-3.12364000	-1.43619400	-1.43383900
C	-3.64895300	-2.77734500	-1.96821600
C	-4.30737000	-0.50163000	-1.15915000
C	-4.84524900	-2.56889700	-2.93059300
H	-2.83880800	-3.30659600	-2.47423500
H	-3.96543700	-3.39585600	-1.12134400
C	-4.94903900	-0.06977300	-2.49409300
H	-5.02831400	-1.07001400	-0.55760200
C	-4.81875700	-1.17480300	-3.56714800
H	-4.83910800	-3.34370300	-3.70321000
H	-5.78672100	-2.68885500	-2.38162700
H	-4.46119700	0.84623300	-2.84471400
H	-6.00576000	0.16713300	-2.33322200
H	-3.87842900	-1.04831500	-4.11683700
H	-5.62101500	-1.07154300	-4.30409600
Co	-2.36393500	0.13309700	0.77920600
Cl	-3.76997800	-0.83597300	2.23900400

II-t (PO + H_2O-Co^{III}-OAc)
PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1677.011706
Thermal correction to Gibbs Free Energy (a.u.): 0.466720
Imaginary frequencies: -516.22
Calculation of single point energy based on the optimized structure, Et = -2915.8164024 a.u.

C	3.21794900	-1.79449800	-2.02757400
C	1.86146400	-2.34272200	-2.08088200
O	2.79328400	-0.75928200	-2.93193700
H	3.48230900	-1.40301500	-1.04494200
H	1.15772700	-2.33742900	-1.25223700
H	1.56336200	-2.78189800	-3.02914600
C	4.33905600	-2.60198700	-2.64953400
H	5.20657700	-1.95026000	-2.78387900
H	4.62327500	-3.43255900	-1.99755200
H	4.04347400	-2.99345700	-3.62675700
O	0.66231400	-0.16018700	-1.88851500
H	1.98020200	-0.27802600	-2.48829600
H	-0.05578700	-0.46009600	-2.46145800
C	4.77191000	-0.47517900	2.14255300
C	4.84265600	0.92464800	2.27657100
C	3.67582400	-1.08288800	1.55983000
H	5.58836200	-1.09152500	2.51003300
C	3.78711100	1.68632400	1.81409300
H	5.70486500	1.39311200	2.73823800
C	2.57468000	-0.32364500	1.06932400
H	3.60742600	-2.16295700	1.47507800
C	2.65033200	1.10058200	1.21282700
H	3.81597700	2.76960100	1.90973500

O	1.59897100	-0.95573700	0.49523300
C	1.60851400	1.97435800	0.75504100
Co	-0.04342100	-0.18875900	-0.08373600
N	0.50370200	1.61776800	0.19549300
H	1.78689400	3.03961400	0.91392300
N	-1.67018600	0.54547900	-0.72725400
C	-0.55404100	2.59128000	-0.12668800
C	-2.81293300	-0.04165400	-0.63484500
C	-1.47279500	1.92625400	-1.16574900
C	-0.09703900	3.96046600	-0.63132600
H	-3.71568700	0.52294300	-0.86889000
C	-2.99103000	-1.41168500	-0.24031300
C	-2.72213800	2.77161200	-1.39605600
C	-1.32640500	4.84131600	-0.90854300
H	0.50044800	3.83476900	-1.54441300
H	0.54032200	4.45897000	0.10574800
C	-4.29877600	-1.87761200	0.01337600
C	-1.88168000	-2.31740800	-0.17551800
C	-2.30888900	4.17118800	-1.87786500
H	-3.37469300	2.30136300	-2.14051500
H	-3.28489300	2.84135300	-0.45713500
H	-1.00767100	5.81135700	-1.30511100
H	-1.83853600	5.04072100	0.04163800
C	-4.54306500	-3.19735500	0.34375200
H	-5.12066900	-1.16784800	-0.04720300
C	-2.16491100	-3.66871600	0.14609900
O	-0.65351400	-1.96666000	-0.44544600
H	-1.83872500	4.08350900	-2.86676100
H	-3.19771800	4.79772200	-2.00797300
C	-3.45728600	-4.09113000	0.40249800
H	-5.55124300	-3.53945100	0.55076100
H	-1.32587300	-4.35462600	0.19979900
H	-3.63418200	-5.13218300	0.66008600
H	-0.90261800	1.85973800	-2.10323400
H	-1.14779800	2.69104500	0.78820900
C	-1.95445000	-0.46473200	3.63536100
H	-1.06230000	-0.81193200	4.16179700
H	-2.54884100	-1.34820900	3.37862400
H	-2.54470900	0.19497500	4.27303100
C	-1.57315400	0.25278700	2.34435800
O	-0.65313700	-0.39496800	1.69198500
O	-2.14003600	1.29943700	2.01583800

II-t (PO + H_2O-Co^{III}-OAc)

PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.086444

Thermal correction to Gibbs Free Energy (a.u.): 0.469106

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8859665 a.u.

C	3.85553000	-1.56271700	-1.86944700
C	2.76552500	-2.54259300	-1.79614000
O	2.67102200	-1.39487300	-2.68755000
H	3.91615300	-0.83746500	-1.06254200
H	2.07020900	-2.51350400	-0.96198000
H	2.87341500	-3.48841500	-2.32473600
C	5.12717800	-1.82919500	-2.62743700
H	5.50790200	-0.90873200	-3.08152600
H	5.89630100	-2.21313300	-1.94858200
H	4.96169100	-2.56340400	-3.42064300
O	0.44995800	-0.07254400	-2.13187600
H	1.39249400	-0.38778500	-2.22198700
H	-0.05327100	-0.86321400	-2.38887100
C	4.59918800	0.62383100	2.20130200
C	4.33291700	1.99257000	2.39969300
C	3.72707900	-0.18051900	1.49208300
H	5.50202000	0.18727000	2.62039600
C	3.17171400	2.52266000	1.87369200
H	5.02288800	2.61401700	2.95981200

C	2.52751700	0.33870300	0.93219000
H	3.92062400	-1.23923000	1.35583500
C	2.25427100	1.72855700	1.14790300
H	2.93912100	3.57547900	2.01759500
O	1.77297500	-0.45572400	0.23129400
C	1.07500300	2.35990200	0.63504400
Co	-0.04548800	-0.11800600	-0.17904300
N	0.10990700	1.77375800	0.00991500
H	0.99544000	3.43476600	0.81325100
N	-1.83802100	0.22663200	-0.70496400
C	-1.12694300	2.50044700	-0.33128400
C	-2.81974800	-0.58040700	-0.49586000
C	-1.96005000	1.58188600	-1.23892400
C	-0.95545500	3.86362100	-1.00309900
H	-3.83730700	-0.23148000	-0.67476900
C	-2.66220700	-1.93493300	-0.04299100
C	-3.36455300	2.15049200	-1.41954600
C	-2.34326200	4.48218700	-1.24231300
H	-0.41783300	3.73991400	-1.95235300
H	-0.35929100	4.53812100	-0.38028500
C	-3.80647900	-2.65587700	0.35954900
C	-1.38230100	-2.57910400	-0.07561600
C	-3.26156500	3.55114900	-2.04741100
H	-3.96597000	1.50068600	-2.06522400
H	-3.86207400	2.20187400	-0.44327700
H	-2.24077000	5.44383800	-1.75645900
H	-2.80679700	4.69166100	-0.26948900
C	-3.72234100	-3.97980100	0.74807400
H	-4.76536100	-2.14274200	0.36757600
C	-1.33005700	-3.94107200	0.30849300
O	-0.28872400	-1.98840500	-0.48869000
H	-2.86907600	3.45244000	-3.06837400
H	-4.25971200	3.99265800	-2.13724400
C	-2.46808600	-4.61713700	0.71291500
H	-4.60627400	-4.51974300	1.06969400
H	-0.36139900	-4.42888000	0.28432900
H	-2.38835100	-5.65863800	1.01306300
H	-1.46082700	1.55433200	-2.21731700
H	-1.67911500	2.60143000	0.60786700
C	-1.46381000	-0.51766200	3.71763100
H	-0.47013500	-0.64449500	4.15368600
H	-1.89471200	-1.51571400	3.58624000
H	-2.10165900	0.06911800	4.37989500
C	-1.36884700	0.15521200	2.35320200
O	-0.42916200	-0.38430600	1.62619300
O	-2.13539800	1.06600300	2.03759300

II-t (PO + H_2O-Co^{III}-OAc)

PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.105958

Thermal correction to Gibbs Free Energy (a.u.): 0.473695

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.913349 a.u.

C	2.70548900	0.82840700	-2.22338100
C	1.59872900	-0.04538600	-2.79151000
O	2.37374000	2.20930400	-2.37917400
H	2.80903600	0.59048500	-1.15786800
H	1.78281600	-1.10229100	-2.59131400
H	1.49144400	0.13304700	-3.86742300
C	4.03050200	0.57503700	-2.92415800
H	4.79586600	1.24159100	-2.51893400
H	4.35564700	-0.45854400	-2.77116100
H	3.94405300	0.76794900	-3.99807400
O	0.35946000	0.35787400	-2.15493100
H	1.42086200	2.27695100	-2.22898800
H	-0.39109500	-0.15221200	-2.52756600
C	3.72297200	-3.74125900	0.74789300
C	4.27577600	-2.86988900	1.71037800

C	2.61964600	-3.37964100	0.00164700
H	4.17026100	-4.71963900	0.59341200
C	3.69636600	-1.63269100	1.89212100
H	5.14074300	-3.16887800	2.29211500
C	1.98989300	-2.11656500	0.17679400
H	2.18589500	-4.05058800	-0.73213200
C	2.56281900	-1.22682200	1.14571000
H	4.10795500	-0.93761600	2.62048600
O	0.96416700	-1.83008600	-0.56701700
C	2.06107300	0.09527200	1.34902900
Co	-0.20019500	-0.37082300	-0.29168400
N	1.04656500	0.62466700	0.74527200
H	2.60707800	0.70979500	2.06829200
N	-1.32429200	1.15396400	-0.13417900
C	0.58598700	1.97931000	1.09881800
C	-2.61078200	1.11280800	-0.14643000
C	-0.52768500	2.35251200	0.10935800
C	1.65478700	3.07488400	1.08265000
H	-3.16990000	2.01386400	0.10785000
C	-3.37368400	-0.05748000	-0.48636000
C	-1.23963500	3.62053500	0.57019500
C	1.00747100	4.40470800	1.50558000
H	2.08709000	3.14469400	0.07614500
H	2.47249700	2.83414400	1.76972700
C	-4.76453300	-0.05611000	-0.24910400
C	-2.75943700	-1.17647500	-1.13359100
C	-0.21068500	4.76360400	0.64073500
H	-2.04210600	3.89197000	-0.12466100
H	-1.69466700	3.44364900	1.55220700
H	1.74660700	5.21144600	1.45992500
H	0.69175300	4.32413800	2.55400200
C	-5.55566300	-1.13029300	-0.61231900
H	-5.20660800	0.81005000	0.23763400
C	-3.59427600	-2.25306100	-1.51137600
O	-1.47947900	-1.22680300	-1.42883000
H	0.12747900	4.99453000	-0.37828000
H	-0.68962200	5.67073200	1.02386100
C	-4.95454600	-2.22936100	-1.25213300
H	-6.62162700	-1.12456900	-0.41226400
H	-3.12520700	-3.09998900	-2.00038700
H	-5.56580800	-3.07864300	-1.54525400
H	-0.04234600	2.57001900	-0.85229500
H	0.12439700	1.89926000	2.08691900
C	-2.04027400	-1.83336100	3.13273500
H	-1.39980300	-2.71620300	3.19366600
H	-2.97691700	-2.13917400	2.65518900
H	-2.25121300	-1.44173900	4.12857900
C	-1.38657000	-0.75384400	2.27839700
O	-0.89732800	-1.26128000	1.17769300
O	-1.38276700	0.42531000	2.62905100

II-m (PO + H_2O-Co^{III}-OAc)
PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1677.018211
Thermal correction to Gibbs Free Energy (a.u.): 0.466294
Imaginary frequencies: -407.07
Calculation of single point energy based on the optimized structure, Et = -2915.8264927 a.u.

C	-4.09643400	-2.93280900	-1.42765500
C	-4.49259500	-1.84912100	-2.23946000
C	-2.99206000	-2.84258000	-0.60422000
H	-4.66522400	-3.85857900	-1.45616800
C	-3.74998600	-0.68624200	-2.20090300
C	-2.20781900	-1.65489900	-0.53595000
C	-2.61380500	-0.55410900	-1.36800200
H	-4.03458700	0.16200200	-2.81949400
O	-1.23543800	-1.60457900	0.31655300
C	-1.93055100	0.71183700	-1.35731400

Co	0.15795500	-0.28634000	0.29315500
N	-0.88150900	0.99853600	-0.66809200
H	-2.35503500	1.48438500	-2.00359400
N	1.51535900	1.03105800	0.29712700
C	-0.19012900	2.28853100	-0.84695600
C	2.77576700	0.77473200	0.30174700
C	0.92374100	2.36103100	0.20856600
C	-1.05996800	3.54304300	-0.76213900
H	3.48115400	1.59430400	0.15885200
C	3.32693700	-0.53777600	0.49760100
C	1.84890900	3.53812000	-0.08680300
C	-0.17955900	4.77770000	-1.01957700
H	-1.52444300	3.60011300	0.23127000
H	-1.87112300	3.51254200	-1.49716200
C	4.70456500	-0.73889300	0.26827400
C	2.51773200	-1.60780700	1.00478500
C	1.02556300	4.83788000	-0.06901800
H	2.64871800	3.59909500	0.65963900
H	2.31977800	3.39346800	-1.06703300
H	-0.77730900	5.69079100	-0.92518100
H	0.18094800	4.74119000	-2.05586000
C	5.30353600	-1.96202700	0.50459100
H	5.29249700	0.09433800	-0.11033600
C	3.16525300	-2.84367200	1.25891300
O	1.24781000	-1.48712900	1.28737600
H	0.66773300	5.01416400	0.95424600
H	1.66543900	5.68825600	-0.32783300
C	4.51536100	-3.01350400	1.00969400
H	4.97339700	-3.98002400	1.20386400
H	0.44286300	2.51810600	1.18318500
H	0.30141400	2.22040500	-1.82224100
O	-0.44529400	0.37382800	1.99976400
H	0.18275100	-0.08984800	2.57373000
H	-1.44168500	1.14352900	2.68924900
C	-2.82965700	-0.61731000	2.59175800
C	-2.61915600	0.12826100	3.85201200
O	-2.31312000	1.36470700	3.22514500
H	-2.09207200	-1.31613100	2.19842100
H	-1.80731900	-0.26324000	4.47377500
H	-3.53353100	0.23015500	4.44502700
C	-3.99933100	-0.34428100	1.76130000
H	-3.68139600	-0.02908500	0.75549500
H	-4.49757800	-1.30591600	1.56470900
H	-4.68542200	0.38283500	2.19566300
H	6.36061700	-2.10848500	0.31042400
H	2.55455200	-3.65392300	1.64294700
H	-2.67518700	-3.67626800	0.01395800
H	-5.35853500	-1.93274300	-2.88687400
C	1.94612000	-1.64956200	-3.24404500
H	2.82778500	-2.08300800	-2.75991200
H	2.23802900	-1.20466100	-4.19651300
H	1.22886700	-2.45873000	-3.40128800
C	1.36188500	-0.58491400	-2.32097000
O	0.76780800	-1.11608500	-1.29313500
O	1.50401800	0.61490700	-2.57330000

II-m (PO + H_2O-Co^{III}-OAc)

PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.085543

Thermal correction to Gibbs Free Energy (a.u.): 0.469571

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.888765 a.u.

C	-4.18812600	-2.24850000	-1.81260600
C	-4.49563600	-1.02238800	-2.43679700
C	-3.09586400	-2.37165600	-0.97621300
H	-4.81941500	-3.11457400	-1.99349400
C	-3.67227600	0.06180900	-2.20481900
C	-2.23278300	-1.27108200	-0.71173700

C	-2.54030000	-0.03024600	-1.36171300
H	-3.88391600	1.01773700	-2.67883100
O	-1.26439800	-1.43293100	0.13697700
C	-1.74670300	1.14741700	-1.16963600
Co	0.24652700	-0.28356000	0.26021300
N	-0.65487400	1.22385500	-0.48546600
H	-2.10558000	2.04964200	-1.67031900
N	1.71591200	0.88647200	0.49407800
C	0.16561200	2.44935500	-0.49265700
C	2.94565600	0.50985500	0.51998300
C	1.25609200	2.27050300	0.57481100
C	-0.57271200	3.76730000	-0.25614800
H	3.72957800	1.26804300	0.52267600
C	3.36581700	-0.86423500	0.56092400
C	2.30165100	3.37552000	0.45042000
C	0.43465900	4.92646800	-0.34053800
H	-1.05625300	3.74579200	0.72945900
H	-1.36259700	3.91656100	-0.99929700
C	4.73151800	-1.16352800	0.36949800
C	2.44115700	-1.90957400	0.88591900
C	1.61352900	4.74025200	0.62592500
H	3.08232700	3.25825900	1.21014900
H	2.78208700	3.30870800	-0.53341800
H	-0.07024600	5.87704000	-0.13735400
H	0.81715900	4.98495600	-1.36786500
C	5.20607500	-2.45786800	0.47008600
H	5.41113400	-0.34834300	0.13160000
C	2.95947400	-3.22285800	1.00268100
O	1.16956400	-1.70581000	1.12144000
H	1.24847300	4.82083500	1.65864500
H	2.34324300	5.54526800	0.48841900
C	4.30206300	-3.48632400	0.79538300
H	4.66189800	-4.50832300	0.88110200
H	0.76983500	2.35166500	1.55686000
H	0.67087000	2.45941700	-1.46301300
O	-0.31923700	0.16376600	2.13614400
H	0.01206500	-0.66886900	2.51476300
H	-1.31147200	0.16304600	2.19894700
C	-3.75448500	-0.85353600	2.13253400
C	-3.51122800	-0.42876100	3.51675500
O	-2.96076600	0.33198000	2.41796700
H	-3.14637700	-1.66829500	1.74753300
H	-2.77684400	-0.95228300	4.12716600
H	-4.29405600	0.08797400	4.06857200
C	-5.05846200	-0.60182500	1.43064700
H	-4.88593900	-0.37679900	0.37557300
H	-5.68969700	-1.49473800	1.48430600
H	-5.59130800	0.23479400	1.89149400
H	6.25575200	-2.67715900	0.30705800
H	2.25862200	-4.01356400	1.24829100
H	-2.85269300	-3.31456100	-0.49747400
H	-5.35546900	-0.93629800	-3.09199900
C	1.90565600	-1.29496000	-3.42216200
H	2.69779400	-1.93841200	-3.02541800
H	2.28286500	-0.74326100	-4.28424400
H	1.07428400	-1.94145400	-3.71307200
C	1.47207700	-0.32381800	-2.32972200
O	0.79998100	-0.93680400	-1.39474100
O	1.77805700	0.86818400	-2.38000600

II-m (PO + H_2O-Co^{III}-OAc)

PO + H_2O-Co^{III}-OAc = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.103566

Thermal correction to Gibbs Free Energy (a.u.): 0.472812

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9120222 a.u.

C	-4.29801100	-3.26411900	-0.44018200
C	-4.81827700	-2.36444400	-1.39502600

C	-3.11099500	-3.00823700	0.21551400
H	-4.83891800	-4.18057800	-0.21951300
C	-4.11957900	-1.20704900	-1.66190200
C	-2.35882800	-1.83030400	-0.04862900
C	-2.89684000	-0.91075300	-1.01051400
H	-4.50226400	-0.49201300	-2.38676700
O	-1.25666800	-1.64051300	0.61082600
C	-2.26528100	0.33760600	-1.30003400
Co	0.04330800	-0.34102000	0.19051700
N	-1.15471100	0.76388100	-0.79105000
H	-2.79004000	0.98721100	-2.00415000
N	1.31734600	1.04004100	-0.09270300
C	-0.55733800	2.03599800	-1.23526900
C	2.58848400	0.85542200	-0.16850200
C	0.63879500	2.31508600	-0.31307400
C	-1.48730600	3.25054400	-1.24265800
H	3.22503600	1.68345300	-0.48217300
C	3.23967300	-0.38845200	0.14490900
C	1.46334800	3.48076700	-0.85113700
C	-0.70873200	4.47513200	-1.75160500
H	-1.86670700	3.42725200	-0.22746900
H	-2.35657100	3.07679700	-1.88485500
C	4.59932900	-0.54938500	-0.19487100
C	2.55510100	-1.41977400	0.86236200
C	0.56820300	4.72927100	-0.93685400
H	2.31909000	3.68592500	-0.19820100
H	1.85601400	3.21888900	-1.84126100
H	-1.35010600	5.36255900	-1.72902800
H	-0.43814900	4.30737700	-2.80216900
C	5.28966500	-1.70178700	0.13335200
H	5.09775600	0.25310300	-0.73350700
C	3.28856300	-2.57940600	1.20114100
O	1.30341600	-1.31836000	1.25447200
H	0.29115600	5.03548000	0.08087000
H	1.13210000	5.56157400	-1.37080700
C	4.61916600	-2.71552600	0.84091100
H	5.15107800	-3.62488800	1.10723200
H	0.23206900	2.59511400	0.66916400
H	-0.15458200	1.85254400	-2.23564900
O	-0.24991700	0.49857500	2.07050300
H	0.47348400	-0.10670500	2.35264200
H	-0.04595200	2.13910500	3.75281200
C	-1.42988300	0.22817800	2.88663500
C	-1.05804200	0.60555100	4.31964900
O	-0.70699500	1.97242000	4.43947300
H	-1.65204600	-0.84060400	2.81677500
H	-0.24219300	-0.05212800	4.66582200
H	-1.91669100	0.43507200	4.97680400
C	-2.57871300	1.04885400	2.33300100
H	-2.79720300	0.76447400	1.30487000
H	-3.47327300	0.87541900	2.93839600
H	-2.33936500	2.11432500	2.37651100
H	6.33102100	-1.82074400	-0.14550900
H	2.76546000	-3.35978900	1.74316700
H	-2.70338300	-3.70191400	0.94307600
H	-5.75050200	-2.58059900	-1.90514800
C	1.44372400	-2.12129600	-3.29163400
H	2.36156100	-2.53386200	-2.86007300
H	1.63943200	-1.78900000	-4.31186100
H	0.69183000	-2.91370300	-3.28210000
C	0.99138200	-0.94178100	-2.43918800
O	0.51100600	-1.34947400	-1.29424200
O	1.11883800	0.21739600	-2.83152800

III-t (PO-Co^{III}-OAc + H_2O)
PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1677.017369

Thermal correction to Gibbs Free Energy (a.u.): 0.466953
Imaginary frequencies: -388.10
Calculation of single point energy based on the optimized structure, Et = -2915.8250707 a.u.

C	-4.96565200	-2.21737900	-1.05806700
C	-5.49774600	-0.91376300	-1.13269300
C	-3.61671800	-2.42830400	-0.85428900
H	-5.62706600	-3.07318500	-1.16537500
C	-4.63938600	0.15847400	-0.99968900
H	-6.55856400	-0.75880600	-1.29660400
C	-2.70710100	-1.34213600	-0.70782600
H	-3.20045900	-3.42903400	-0.80351400
C	-3.25258700	-0.01860800	-0.78289400
H	-5.02374800	1.17448500	-1.05953000
O	-1.45456200	-1.61506900	-0.50605700
C	-2.43861400	1.15459600	-0.66092200
Co	-0.08972400	-0.35682300	-0.08052600
N	-1.17309300	1.18166200	-0.41318800
H	-2.95927400	2.10351000	-0.79805000
N	1.26285900	0.88166100	0.42440600
C	-0.39532700	2.42773000	-0.37781700
C	2.52456000	0.62508500	0.38217400
C	0.71330200	2.21725800	0.66944400
C	-1.16420100	3.71856700	-0.10235100
H	3.23062000	1.43990700	0.53733700
C	3.09341100	-0.66757700	0.12541800
C	1.70126200	3.38149700	0.65046900
C	-0.19035800	4.90758300	-0.08916200
H	-1.68685500	3.64248200	0.86177200
H	-1.92534300	3.88854700	-0.87087200
C	4.48812400	-0.75959700	-0.07495200
C	2.28990400	-1.85305200	0.12036400
C	0.95437200	4.69832200	0.90906700
H	2.47384300	3.24144100	1.41433000
H	2.19499600	3.40649000	-0.32813900
H	-0.73342100	5.82990500	0.14390800
H	0.22830600	5.03201100	-1.09588800
C	5.10725300	-1.97529100	-0.29403900
H	5.07266500	0.15749000	-0.06343600
C	2.95399800	-3.08849400	-0.09248300
O	1.00564600	-1.85726700	0.35297700
H	0.54814900	4.68677500	1.92998300
H	1.65590300	5.53799400	0.86149500
C	4.32106700	-3.14325800	-0.29669000
H	6.17773700	-2.03026000	-0.45943100
H	2.34302900	-3.98497700	-0.10324500
H	4.79393300	-4.10668000	-0.46890000
C	-1.19204300	-1.60484500	2.26628200
C	-0.00789200	-1.73015200	3.11093500
O	-0.79347000	-0.33865600	1.74281300
H	-1.17585800	-2.35216200	1.45976600
H	0.93101700	-1.88353700	2.59230000
H	-0.02517900	-1.75946200	4.19470000
C	-2.55159600	-1.54286800	2.93653800
H	-3.31109300	-1.31783400	2.18427100
H	-2.79685300	-2.50356200	3.40221500
H	-2.57552500	-0.76068900	3.70256500
O	0.63897400	0.43843600	3.70853200
H	0.09470000	0.44428500	2.87552700
H	0.05470000	0.78500100	4.39764200
H	0.11820700	2.48297300	-1.34448100
H	0.23424000	2.18277500	1.65878500
C	1.80819800	-0.47844300	-3.80535800
H	2.59019200	-1.16770500	-3.46899800
H	2.23253600	0.23082300	-4.51745400
H	1.02525900	-1.07686600	-4.27683600
C	1.26225700	0.26003800	-2.58760000
O	0.50834500	-0.51302400	-1.86226500
O	1.57037500	1.43764500	-2.37641800

III-t (PO-Co^{III}-OAc + H_2O)

PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1677.079596
Thermal correction to Gibbs Free Energy (a.u.): 0.469443
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -2915.8856922 a.u.

C	-4.57560000	-2.68435300	-1.09253800
C	-5.19734300	-1.43230600	-1.28253100
C	-3.22061800	-2.78281600	-0.84742200
H	-5.17268100	-3.59111000	-1.14259600
C	-4.41978500	-0.29463800	-1.22456700
H	-6.26198400	-1.36840900	-1.47821200
C	-2.39195700	-1.62577800	-0.76695500
H	-2.73766700	-3.74438400	-0.70861200
C	-3.02829800	-0.35502200	-0.96470000
H	-4.87079900	0.68323500	-1.38082600
O	-1.13266700	-1.78884600	-0.50947200
C	-2.30449500	0.87986900	-0.90534600
Co	0.10211000	-0.41059000	-0.08469600
N	-1.05948600	1.01693700	-0.59510400
H	-2.88468300	1.77711300	-1.12028200
N	1.28709200	0.95154600	0.49772400
C	-0.40543800	2.33313200	-0.51852300
C	2.56494000	0.80327100	0.59282600
C	0.59495700	2.23468400	0.64891600
C	-1.32578000	3.53975900	-0.33514500
H	3.18223500	1.68255100	0.77481200
C	3.25123800	-0.45029500	0.47379500
C	1.46277500	3.48761000	0.72640200
C	-0.48395400	4.82002800	-0.21570100
H	-1.94733300	3.38833300	0.55698500
H	-2.00060800	3.64055900	-1.19212700
C	4.66281400	-0.44786300	0.41725900
C	2.53659500	-1.69197100	0.48121300
C	0.56287000	4.72077100	0.90022800
H	2.16343100	3.42090300	1.56640900
H	2.05200600	3.56830700	-0.19500300
H	-1.14080600	5.67879900	-0.04115000
H	0.02602700	5.00060800	-1.17088900
C	5.38152500	-1.62541100	0.35256000
H	5.17856500	0.50959400	0.41620900
C	3.30112000	-2.88497500	0.43028300
O	1.23738300	-1.77473500	0.58315500
H	0.05357200	4.65852100	1.87125000
H	1.17739100	5.62691400	0.92485900
C	4.68206600	-2.84805700	0.36446200
H	6.46451300	-1.61092800	0.29645700
H	2.75806500	-3.82397600	0.43306800
H	5.23614700	-3.78167500	0.31481200
C	-1.09844700	-1.66957200	2.38925300
C	-0.14241700	-0.73034000	2.98690200
O	-0.81881500	-0.37144600	1.74472000
H	-0.66473600	-2.47568100	1.80583400
H	0.91773700	-0.91583000	2.85467100
H	-0.44423500	-0.10126000	3.82041300
C	-2.51124000	-1.83127300	2.86775500
H	-3.15221600	-2.12834800	2.03240300
H	-2.55480200	-2.61921200	3.62683200
H	-2.89343800	-0.89918200	3.29142300
O	-3.03687800	1.41747000	2.08680000
H	-2.23469300	0.89707900	1.91725800
H	-3.68692500	0.99952000	1.50723700
H	0.19546900	2.42954200	-1.42823000
H	0.00501800	2.15812800	1.57467000
C	2.23511600	-0.54372500	-3.65255800
H	3.05467500	-1.16279600	-3.27258900
H	2.62989400	0.18035500	-4.36642600
H	1.51663400	-1.20990700	-4.13514500

C	1.59272300	0.18275900	-2.47615400
O	0.86049300	-0.63356800	-1.76764500
O	1.80871100	1.37840700	-2.27297600

III-t (PO-Co^{III}-OAc + H_2O)

PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.102502

Thermal correction to Gibbs Free Energy (a.u.): 0.473304

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9125099 a.u.

C	-4.96908200	-1.92688700	-1.36825700
C	-5.51698100	-0.65246600	-1.11193800
C	-3.60756400	-2.14613700	-1.31301700
H	-5.62991300	-2.75345900	-1.61640000
C	-4.66010200	0.38402900	-0.80615200
H	-6.58835900	-0.49178900	-1.16161000
C	-2.69776200	-1.09881500	-0.98852800
H	-3.18144400	-3.12298600	-1.51623400
C	-3.25919300	0.19520400	-0.73096800
H	-5.05500800	1.37922600	-0.61285300
O	-1.43247900	-1.37940000	-0.94022600
C	-2.44366000	1.33013700	-0.42099100
Co	-0.07995700	-0.25033500	-0.23728700
N	-1.16505400	1.32070200	-0.24350100
H	-2.97094200	2.28117900	-0.33352400
N	1.24503800	0.84495900	0.58355000
C	-0.38273200	2.53276300	0.02492300
C	2.51039200	0.58533300	0.55241900
C	0.69536700	2.12541000	1.04709400
C	-1.14836000	3.76488500	0.50203100
H	3.20770300	1.34944100	0.89346900
C	3.09171500	-0.63858700	0.09286200
C	1.69092900	3.26371500	1.26161800
C	-0.16546100	4.92079200	0.74550000
H	-1.69679300	3.53131200	1.42569400
H	-1.88785900	4.07132600	-0.24530300
C	4.50072600	-0.71876700	-0.00010700
C	2.28774200	-1.78618800	-0.21019800
C	0.94758800	4.52603700	1.72338500
H	2.44021100	2.98614600	2.01121600
H	2.21336500	3.44837800	0.31588300
H	-0.70673700	5.79607200	1.12038100
H	0.28315000	5.21152000	-0.21279000
C	5.13257400	-1.88205500	-0.38907100
H	5.08416100	0.16783700	0.23733400
C	2.96734600	-2.97375600	-0.59288400
O	0.99125200	-1.81211500	-0.10744800
H	0.51157100	4.34500600	2.71559800
H	1.65842800	5.35079100	1.84054800
C	4.34549000	-3.01467700	-0.68116800
H	6.21337300	-1.92710100	-0.46657300
H	2.35753500	-3.84037800	-0.82503700
H	4.83030100	-3.93777700	-0.98809500
C	-1.13552100	-2.07665700	1.89935100
C	0.00988000	-2.57726700	2.78261400
O	-0.84077600	-0.68399700	1.58902500
H	-1.12789700	-2.60741700	0.94767300
H	0.90207100	-2.70271000	2.17018700
H	-0.24788500	-3.53569600	3.24973000
C	-2.51251500	-2.13452300	2.54398700
H	-3.25444700	-1.69163900	1.87592200
H	-2.79781200	-3.17370100	2.73791300
H	-2.53628000	-1.58454200	3.49272900
O	0.34717900	-1.58545200	3.76533600
H	-0.22991200	-0.39955500	2.29633400
H	-0.34195900	-1.58414900	4.44303400
H	0.15841700	2.75645300	-0.90064700
H	0.17929200	1.92522300	2.00055200

C	1.84968500	0.42562600	-3.86835500
H	2.58739300	-0.37100000	-3.72553300
H	2.31741200	1.26473400	-4.38509600
H	1.03276600	0.01209200	-4.46403600
C	1.34627700	0.86965600	-2.49928000
O	0.54761000	-0.02083900	-1.98243200
O	1.71400900	1.94002000	-2.00716400

III-m (PO-Co^{III}-OAc + H_2O)

PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.023674

Thermal correction to Gibbs Free Energy (a.u.): 0.466096

Imaginary frequencies: -285.16

Calculation of single point energy based on the optimized structure, Et = -2915.8352559 a.u.

C	-4.76669500	-2.89689800	-0.55252100
C	-5.43191900	-1.68330800	-0.82474500
C	-3.40378000	-2.93290100	-0.34061100
H	-5.33569900	-3.82219000	-0.51182500
C	-4.69021400	-0.52109300	-0.87708100
C	-2.60984500	-1.75007100	-0.38779100
C	-3.29183900	-0.51679500	-0.66118600
H	-5.17922100	0.42736100	-1.08960900
O	-1.33620500	-1.86146000	-0.18024100
C	-2.61039300	0.74155800	-0.73214300
Co	-0.10933700	-0.42108400	-0.03945100
N	-1.35155100	0.93988900	-0.53123500
H	-3.23596500	1.60046300	-0.98083700
N	1.13193500	0.99850900	0.21150200
C	-0.71725700	2.25868500	-0.66791300
C	2.40841800	0.86471500	0.11070000
C	0.45095600	2.28800400	0.33715000
C	-1.61575300	3.48050600	-0.48272800
H	3.03294000	1.75788900	0.10808400
C	3.09276600	-0.39351800	-0.01393000
C	1.30036800	3.54065200	0.13447300
C	-0.78492700	4.76304900	-0.64746100
H	-2.08024900	3.45180400	0.51311100
H	-2.42628700	3.48294600	-1.21877100
C	4.47202300	-0.38377200	-0.31364000
C	2.41663100	-1.63741600	0.20614900
C	0.42172500	4.78999200	0.29833500
H	2.12071500	3.57104800	0.86037300
H	1.74155400	3.51090200	-0.86904100
H	-1.41852300	5.64058400	-0.47859300
H	-0.43088400	4.82286200	-1.68453800
C	5.19614200	-1.55666800	-0.41610100
H	4.95873700	0.57538200	-0.47547000
C	3.18747300	-2.82371800	0.10954500
O	1.15888400	-1.72047600	0.54680000
H	0.06825700	4.84520600	1.33695700
H	1.01975600	5.69049900	0.12211100
C	4.53601100	-2.78060200	-0.19668800
H	5.09276300	-3.71079200	-0.27535500
H	0.02479200	2.31236100	1.34983200
H	-0.25594000	2.26378000	-1.66171400
O	-0.81962000	1.45782700	3.70562900
H	-1.71682400	1.66101000	4.00188600
H	-0.92379400	1.03923000	2.80585900
C	-0.07068500	-0.89118700	3.68589600
C	-0.88660600	-1.35588700	2.55216200
O	-0.80247200	-0.19305000	1.76365300
H	-0.51008000	-0.75502000	4.67133300
H	-1.92029100	-1.60497400	2.82170300
H	-0.42333800	-2.21611100	2.04410900
C	1.36599500	-0.62325000	3.55622700
H	1.57565100	0.41163100	3.85076600
H	1.88383900	-1.25257400	4.29811600

H	1.72575100	-0.82764400	2.55107600
H	6.25270600	-1.53580200	-0.66034400
H	2.67261400	-3.76466600	0.27217600
H	-2.88507800	-3.86451100	-0.13984400
H	-6.50317600	-1.66647700	-0.99355700
C	1.59596700	-0.87444800	-3.83696100
H	2.47311200	-1.42062200	-3.47364400
H	1.88965000	-0.22679500	-4.66433400
H	0.86382000	-1.61461100	-4.16811600
C	1.03666600	-0.04077500	-2.68813900
O	0.43421200	-0.78671600	-1.80973700
O	1.20654100	1.18252500	-2.65917700

III-m (PO-Co^{III}-OAc + H_2O)

PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.075382

Thermal correction to Gibbs Free Energy (a.u.): 0.467577

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8828288 a.u.

C	-4.51310500	-3.15312800	-0.43591400
C	-5.21436400	-2.00066500	-0.85047700
C	-3.16227400	-3.10991600	-0.15894300
H	-5.04540300	-4.09533400	-0.33504700
C	-4.51959900	-0.81701500	-0.97959300
C	-2.41655600	-1.90146300	-0.27579000
C	-3.13245400	-0.73247900	-0.70002900
H	-5.03321500	0.08512700	-1.30541300
O	-1.15526400	-1.92862300	0.02042700
C	-2.50028400	0.54411700	-0.83888600
Co	0.02862300	-0.45088900	0.02724600
N	-1.26452600	0.81556700	-0.58221000
H	-3.14770300	1.35609300	-1.17026900
N	1.18511400	1.03774200	0.21369600
C	-0.71317600	2.17282800	-0.73932800
C	2.47016700	0.96646500	0.14261900
C	0.42605900	2.28631600	0.28939000
C	-1.70078700	3.32769100	-0.56603100
H	3.04619600	1.89078700	0.10026700
C	3.21370400	-0.25997000	0.12252900
C	1.19751500	3.58942100	0.10590500
C	-0.95903300	4.66767600	-0.69749800
H	-2.19784800	3.23458800	0.40809300
H	-2.48158200	3.28440200	-1.33268900
C	4.60091900	-0.20725700	-0.13983300
C	2.59017200	-1.51321600	0.43326100
C	0.23062000	4.77323100	0.26498800
H	2.00464300	3.66796800	0.84330900
H	1.65523100	3.59783800	-0.89077200
H	-1.65644000	5.49440700	-0.52569100
H	-0.59462000	4.77081700	-1.72797100
C	5.38081300	-1.34670100	-0.11870200
H	5.04696900	0.75759200	-0.36980700
C	3.41975700	-2.66303800	0.46544100
O	1.32691100	-1.63524100	0.74096400
H	-0.13958000	4.79522100	1.29878300
H	0.76616000	5.71460500	0.10280100
C	4.77277100	-2.57868900	0.19274600
H	5.37587400	-3.48251400	0.21425900
H	-0.04039000	2.29650300	1.28632500
H	-0.24187900	2.19979600	-1.72657600
O	-3.16143100	1.33218600	2.10001400
H	-3.83374500	0.81586200	1.63785200
H	-2.34159700	0.84887700	1.90612800
C	-0.17639800	-0.02903000	3.28468200
C	-0.80076600	-1.28012700	2.83188700
O	-0.74438600	-0.13829500	1.93131500
H	-0.79648000	0.63958800	3.88059100
H	-1.81346800	-1.52883400	3.13528500

H	-0.16429600	-2.09418700	2.50043500
C	1.30759600	0.14175500	3.42464300
H	1.60653100	1.16120200	3.16569800
H	1.58286200	-0.03407800	4.47018800
H	1.84095500	-0.56063600	2.78701000
H	6.44249200	-1.29529600	-0.33418400
H	2.94619400	-3.61035000	0.69990800
H	-2.61845500	-3.99536800	0.15287300
H	-6.27564500	-2.04864000	-1.06806000
C	1.66806600	-1.08307700	-3.73718300
H	2.58104500	-1.57586700	-3.38680600
H	1.89898100	-0.46973200	-4.60905300
H	0.95054800	-1.86538500	-3.99445900
C	1.12974200	-0.20512900	-2.61295600
O	0.58612500	-0.93452100	-1.67505200
O	1.25630800	1.01876800	-2.64399500

III-m (PO-Co^{III}-OAc + H_2O)

PO-Co^{III}-OAc + H_2O = PG + Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.099301

Thermal correction to Gibbs Free Energy (a.u.): 0.473275

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9110832 a.u.

C	-4.84971300	-2.65542000	-0.97420900
C	-5.54299700	-1.44222200	-0.77424700
C	-3.47166100	-2.70664900	-0.94768100
H	-5.41113000	-3.56823800	-1.15645300
C	-4.81217000	-0.29501900	-0.55227000
C	-2.68715700	-1.53976200	-0.71367100
C	-3.39622400	-0.30848300	-0.51153400
H	-5.32054200	0.65530300	-0.40287300
O	-1.39803300	-1.66376800	-0.69974900
C	-2.72249600	0.93304400	-0.29142100
Co	-0.16449700	-0.31312200	-0.21503600
N	-1.44586800	1.09919900	-0.17716900
H	-3.36494300	1.81203600	-0.22006000
N	1.07765700	0.99354000	0.40041300
C	-0.81975500	2.41844600	-0.02286500
C	2.35509700	0.90696400	0.22753800
C	0.40909600	2.20770200	0.88106600
C	-1.69845700	3.54788600	0.51171900
H	2.97208700	1.77643100	0.45107200
C	3.04728900	-0.25490500	-0.24074200
C	1.25074300	3.48039900	0.94988100
C	-0.87162100	4.83924100	0.61553800
H	-2.10313400	3.27333800	1.49628100
H	-2.55193200	3.72056900	-0.15197000
C	4.43648900	-0.15494100	-0.48766500
C	2.38199200	-1.51589000	-0.39284500
C	0.39020800	4.64422400	1.46459800
H	2.11085100	3.34009700	1.61380300
H	1.63262700	3.69744100	-0.05440800
H	-1.48818600	5.64273600	1.03251500
H	-0.58089100	5.15442600	-0.39456600
C	5.17914000	-1.24857900	-0.88244100
H	4.91361600	0.81446400	-0.36309400
C	3.17619100	-2.62709600	-0.78472900
O	1.12133000	-1.70551600	-0.14178100
H	0.10035400	4.44427400	2.50540700
H	0.98347300	5.56458900	1.47728500
C	4.53010700	-2.49236600	-1.02377000
H	5.10368500	-3.36245100	-1.33247700
H	0.03619500	1.98534500	1.89539700
H	-0.41908200	2.68226700	-1.00739400
O	0.08086500	-0.95527500	4.19581700
H	-0.75882700	-1.13949900	4.63939900
H	-0.42212000	-0.17291200	2.40429700
C	0.40388200	-2.08364600	3.35375200

C	-0.58727500	-2.09945400	2.18621700
O	-0.72654800	-0.75503600	1.68475500
H	0.29240600	-3.02004400	3.91811400
H	-1.57852700	-2.43037800	2.52008100
H	-0.25225700	-2.72394900	1.35952300
C	1.85464300	-1.90332300	2.93851000
H	2.49288000	-1.88273500	3.82525700
H	2.17082000	-2.71676400	2.28286000
H	1.98454800	-0.96786300	2.39146500
H	6.24187400	-1.15623300	-1.07794800
H	2.67117500	-3.58025800	-0.89983800
H	-2.93488400	-3.63546200	-1.10943000
H	-6.62685000	-1.41473100	-0.80135200
C	1.21552300	0.42312600	-4.07819200
H	2.07430100	-0.25242100	-4.00581800
H	1.48759300	1.29256800	-4.67810700
H	0.40145000	-0.13194700	-4.54977500
C	0.82345400	0.86191500	-2.67142100
O	0.23759100	-0.10702600	-2.02595000
O	1.08433400	1.99836900	-2.26792100

IV-t (PO-Co^{III}-OAc + H_2O-Co^{III}-OAc)

PO-Co^{III}-OAc + H_2O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3084.637713

Thermal correction to Gibbs Free Energy (a.u.): 0.861507

Imaginary frequencies: -378.12

Calculation of single point energy based on the optimized structure, Et = -5562.0327052 a.u.

C	0.89954800	1.20020300	-2.31699000
C	0.15241900	2.15233600	-1.48245200
O	1.17245900	0.32944900	-1.22110700
H	0.22001300	0.67025000	-2.99140300
H	-0.91538300	2.33155200	-1.60125900
H	0.74028400	2.69159900	-0.74222900
C	2.09383700	1.75140400	-3.08489200
H	2.65731900	0.91748100	-3.51268100
H	1.74103500	2.37797300	-3.91090800
H	2.74947200	2.33456300	-2.44231600
O	-0.93001500	0.71497800	-0.02319300
H	-0.20781400	0.20523500	-0.50681800
H	-0.45377500	0.95250200	0.81338600
C	-0.27757700	-3.40884000	-3.80140100
C	-0.45956300	-4.44987400	-2.86781900
C	-0.69854200	-2.12146400	-3.52985200
H	0.19269200	-3.62300100	-4.75770300
C	-1.05410500	-4.15250700	-1.65799400
H	-0.13544300	-5.45942700	-3.09508300
C	-1.34191000	-1.78913600	-2.30222500
H	-0.58350600	-1.32700500	-4.25985000
C	-1.49239100	-2.84476600	-1.34287100
H	-1.19361500	-4.93349400	-0.91379300
O	-1.73293000	-0.56684800	-2.11916500
C	-2.06743600	-2.62615700	-0.04799900
Co	-2.71573400	0.09305500	-0.61605200
N	-2.54415400	-1.51513100	0.40272600
H	-2.09621700	-3.49949000	0.60603700
N	-3.55057700	0.81464100	0.92100000
C	-3.20279100	-1.43134400	1.71964500
C	-4.41673000	1.76815800	0.89202700
C	-3.20272600	0.05160100	2.12157500
C	-2.60144800	-2.27783300	2.84087700
H	-4.95568000	2.01218000	1.80715000
C	-4.73517900	2.54959700	-0.26860000
C	-4.07291600	0.26446700	3.35800100
C	-3.41938100	-2.07668500	4.12703700
H	-1.55682400	-1.98954700	3.00281200
H	-2.61038900	-3.34084500	2.57835600
C	-5.83179000	3.43727600	-0.20530500

C	-3.92124400	2.49970600	-1.44617500
C	-3.53753700	-0.59675700	4.51288400
H	-4.06763000	1.31879900	3.65641000
H	-5.10712500	-0.00908400	3.11589800
H	-2.95919600	-2.63955400	4.94631700
H	-4.42350900	-2.49461600	3.97796800
C	-6.15520700	4.26018800	-1.26670900
H	-6.42871800	3.45655000	0.70360800
C	-4.26574400	3.36888200	-2.51264900
O	-2.86585600	1.74046200	-1.56358900
H	-2.54798000	-0.22477300	4.80059800
H	-4.18715100	-0.48650100	5.38789800
C	-5.35319800	4.21880300	-2.42340100
H	-7.00743200	4.92857000	-1.21017400
H	-3.65139500	3.32868300	-3.40608500
H	-5.59453600	4.86218500	-3.26548200
C	0.08445200	0.11647200	4.91525800
C	0.40048600	-1.24954500	5.00849300
C	0.32143000	0.82771500	3.74907300
H	-0.34564200	0.62840400	5.77171200
C	0.96245100	-1.87750600	3.91028200
H	0.21192900	-1.79908200	5.92404600
C	0.91227000	0.21228000	2.62018400
H	0.08921200	1.88513700	3.67617700
C	1.23365700	-1.17650300	2.71606200
H	1.21476000	-2.93415500	3.95747000
O	1.08002800	0.92310900	1.52638900
C	1.83526300	-1.90331800	1.62764900
Co	2.49850300	0.49285000	0.25350300
N	2.29108900	-1.38969200	0.54015500
H	1.94281500	-2.98143400	1.77301700
N	3.83181400	-0.00162400	-0.98403100
C	3.06942600	-2.21714600	-0.40002600
C	4.87449500	0.70451400	-1.24210800
C	3.51073000	-1.30642700	-1.55292500
C	2.33812100	-3.42640600	-0.97613300
H	5.65425200	0.27880100	-1.87537600
C	5.07275800	2.04582900	-0.76193000
C	4.54554500	-2.01430400	-2.41888300
C	3.28854400	-4.18784900	-1.91430100
H	1.45182100	-3.08729700	-1.51881700
H	1.99084900	-4.09329400	-0.17954100
C	6.33885500	2.64565100	-0.93524600
C	3.99369400	2.80241300	-0.19360800
C	3.88798700	-3.28079200	-3.00129500
H	4.88093700	-1.36427000	-3.23530100
H	5.42593500	-2.27215500	-1.81722300
H	2.75164100	-5.01967900	-2.38218600
H	4.10210300	-4.62547600	-1.32061000
C	6.57728400	3.95179500	-0.55228500
H	7.13597300	2.05054500	-1.37494200
C	4.26321300	4.14473600	0.17070300
O	2.77655900	2.34139100	-0.05222600
H	3.08694900	-2.97381600	-3.68656700
H	4.61724400	-3.83987400	-3.59702800
C	5.51958900	4.69846100	-0.00036400
H	7.55846500	4.39595500	-0.67957800
H	3.44746000	4.71601800	0.60097800
H	5.69128700	5.72805900	0.30210700
H	3.96824100	-2.51903500	0.14500800
H	2.61706300	-1.12761500	-2.16302500
H	-4.24874500	-1.70210700	1.54340200
H	-2.16764400	0.32448300	2.37407200
C	-6.50592100	-0.89827000	-2.02808700
H	-6.76647900	0.10587300	-2.37899600
H	-7.39621600	-1.38270600	-1.62496400
H	-6.11826900	-1.45490800	-2.88438700
C	-5.44319300	-0.77062700	-0.94242000
O	-4.28282800	-0.46576900	-1.45532100

O	-5.72750600	-0.92288900	0.24669900
C	5.49463700	0.50518700	3.16181800
H	6.27070400	-0.19331000	3.47702600
H	4.81429300	0.72063800	3.98966500
H	5.95324900	1.45245300	2.86032900
C	4.72359300	-0.06746800	1.97820300
O	3.67252400	0.65599700	1.70533700
O	5.11129300	-1.07620900	1.38815100

IV-t (PO-Co^{III}-OAc + H$_2$O-Co^{III}-OAc)

PO-Co^{III}-OAc + H$_2$O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3084.698173

Thermal correction to Gibbs Free Energy (a.u.): 0.861695

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5562.0951037 a.u.

C	1.14771700	-0.14735100	-2.70198300
C	0.89724300	1.24896500	-2.33172400
O	1.20289800	0.26579300	-1.28042400
H	0.26150300	-0.76100900	-2.84159800
H	-0.13213200	1.59348800	-2.29027200
H	1.69532400	1.97565500	-2.43877800
C	2.42015300	-0.59859000	-3.35455500
H	2.67805800	-1.61775300	-3.05318400
H	2.26436700	-0.60259600	-4.43913700
H	3.24703600	0.06943200	-3.11787000
O	-0.94922300	0.50740100	0.24324100
H	-0.18076900	0.18701200	-0.29114100
H	-0.94750500	1.46580100	0.10110600
C	-0.43138700	-4.88158400	-1.90603800
C	-0.94251400	-5.49392100	-0.74461000
C	-0.61770000	-3.53340400	-2.14606900
H	0.11601500	-5.47896000	-2.63042900
C	-1.64414700	-4.71635100	0.15528100
H	-0.79139300	-6.55250700	-0.56527600
C	-1.33937400	-2.70622600	-1.23929400
H	-0.23641600	-3.07041000	-3.05001700
C	-1.86126800	-3.33593900	-0.06139200
H	-2.04644700	-5.16282200	1.06182800
O	-1.45409300	-1.44105300	-1.50874400
C	-2.54681600	-2.59915100	0.96209100
Co	-2.58664800	-0.21365200	-0.58783100
N	-2.83981200	-1.34513000	0.92962400
H	-2.82715000	-3.17258800	1.84829700
N	-3.56926700	1.07693300	0.39171800
C	-3.59356000	-0.69950800	2.02073600
C	-4.30144000	1.99116400	-0.14454700
C	-3.45771800	0.81940100	1.82676700
C	-3.17199800	-1.06535800	3.44474800
H	-4.94733500	2.59108100	0.49709000
C	-4.31323900	2.28847900	-1.54939200
C	-4.40725200	1.56547500	2.75860000
C	-4.07206300	-0.31951900	4.44457000
H	-2.11949100	-0.78854500	3.59196500
H	-3.25293200	-2.14302400	3.61902600
C	-5.30233700	3.15965100	-2.05456100
C	-3.28394300	1.79255500	-2.41453300
C	-4.06447400	1.19804800	4.21219000
H	-4.30605900	2.64783600	2.62219200
H	-5.44319900	1.29263100	2.52219700
H	-3.75600300	-0.54363200	5.46917400
H	-5.09783000	-0.69668700	4.34121200
C	-5.31667000	3.53758300	-3.38373000
H	-6.06582600	3.52665400	-1.37253300
C	-3.31143200	2.21453400	-3.76651400
O	-2.30458200	1.02620900	-2.00628600
H	-3.06831000	1.59496000	4.44254800
H	-4.76735900	1.68621500	4.89555000
C	-4.30331500	3.05801100	-4.23499900

H	-6.08978800	4.19636200	-3.76387100
H	-2.53270500	1.83900400	-4.42198600
H	-4.30029600	3.35108100	-5.28152300
C	-0.42144000	3.96561600	2.87822100
C	-0.58863400	3.00180800	3.89331600
C	0.32245300	3.69300400	1.74559700
H	-0.87697200	4.94594200	2.99013500
C	-0.00631400	1.75977300	3.72704200
H	-1.15874200	3.23327100	4.78635800
C	0.95088800	2.42986900	1.55520600
H	0.46153100	4.43625500	0.96756400
C	0.75399300	1.44286000	2.57844700
H	-0.13508300	0.99141100	4.48630700
O	1.60106800	2.22487600	0.45002200
C	1.19691900	0.09126900	2.41903900
Co	2.70180900	0.71613000	0.08852600
N	1.85404500	-0.37866900	1.41216400
H	0.92043200	-0.59863900	3.21951700
N	3.65295200	-0.85319400	-0.37186000
C	2.31168500	-1.78110400	1.40088800
C	4.84798800	-0.86215100	-0.85241700
C	2.89141300	-2.04289500	0.00455900
C	1.24973700	-2.83386300	1.71671900
H	5.37103000	-1.81442000	-0.94360400
C	5.54251500	0.30984700	-1.30234900
C	3.60486100	-3.39071600	-0.03062600
C	1.88740500	-4.23181700	1.66381700
H	0.43502500	-2.76150500	0.98968400
H	0.81377700	-2.66748900	2.70766400
C	6.91007600	0.20105700	-1.64015300
C	4.85396400	1.55421600	-1.49134800
C	2.59544000	-4.49532100	0.32703600
H	4.02241100	-3.58182900	-1.02601300
H	4.43871500	-3.37831400	0.68209700
H	1.11656700	-4.99209400	1.82596000
H	2.61100200	-4.32474800	2.48448500
C	7.61592900	1.27777500	-2.13921900
H	7.40414000	-0.75631300	-1.49113900
C	5.60076800	2.63630800	-2.02349100
O	3.58072100	1.72270200	-1.25427000
H	1.84087600	-4.55616900	-0.46522900
H	3.10327300	-5.46534200	0.35664500
C	6.94144100	2.49948500	-2.33247800
H	8.66859400	1.18506400	-2.38322400
H	5.07896700	3.57657800	-2.16592600
H	7.48479800	3.35380600	-2.72742600
H	3.14309600	-1.83703000	2.10925800
H	2.04268900	-2.08672800	-0.69382500
H	-4.64366200	-0.95259300	1.84646900
H	-2.42894600	1.09089200	2.09874900
C	-6.18821100	-1.43807700	-2.27914500
H	-6.30469000	-0.59115100	-2.96353900
H	-7.16609400	-1.72916500	-1.89352900
H	-5.73864500	-2.25740000	-2.84509000
C	-5.27794700	-1.01468200	-1.13228600
O	-4.03738700	-0.91533900	-1.52381900
O	-5.73053800	-0.78316500	-0.01024300
C	5.75666900	1.66129200	2.74180100
H	6.29398200	1.13647600	3.53266900
H	5.23536400	2.53346700	3.14304500
H	6.47017000	2.02028000	1.99281600
C	4.77484100	0.71292400	2.06326000
O	3.93952400	1.37284900	1.30480600
O	4.83846300	-0.50356700	2.23314600

IV-t (PO-Co^{III}-OAc + H_2O-Co^{III}-OAc)

PO-Co^{III}-OAc + H_2O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3084.744917

Thermal correction to Gibbs Free Energy (a.u.): 0.870435
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -5562.1438352 a.u.

C	-0.33271400	-2.31695700	-0.58768800
C	0.39825100	-2.24588400	0.75960000
O	-1.04353900	-1.08172800	-0.86097100
H	0.41820800	-2.38594600	-1.37448100
H	1.18856400	-2.99797500	0.77540300
H	-0.30060500	-2.40010900	1.58191100
C	-1.28334200	-3.49808400	-0.66383500
H	-1.77359700	-3.52511300	-1.64102000
H	-0.71871600	-4.42881300	-0.54533900
H	-2.04346300	-3.44882600	0.11544100
O	1.03700700	-0.97298600	0.98158600
H	-0.33905600	-0.41304400	-1.09831700
H	0.32446200	-0.28154600	1.11277000
C	0.18068600	3.38208400	-3.19641600
C	0.72642400	4.40914400	-2.40874600
C	0.32459900	2.05244300	-2.83436400
H	-0.35319800	3.62885000	-4.11049400
C	1.41496600	4.06879900	-1.25771600
H	0.61372800	5.44804400	-2.69879800
C	1.01916900	1.68144900	-1.66148100
H	-0.08129000	1.25466900	-3.44517900
C	1.58029400	2.72487700	-0.86468200
H	1.83372300	4.84529400	-0.62397000
O	1.08221200	0.40901000	-1.33978400
C	2.28568400	2.46625100	0.36111500
Co	2.49159900	-0.29480200	-0.23175100
N	2.61477800	1.30510600	0.81206100
H	2.57843600	3.34729200	0.93495100
N	3.77501400	-0.99576600	0.96909600
C	3.52124600	1.17949900	1.97051600
C	4.66629500	-1.87173800	0.65832800
C	3.68478700	-0.31900500	2.26138800
C	3.11539200	1.90819400	3.25142900
H	5.44905000	-2.10258700	1.38123500
C	4.70018400	-2.58266700	-0.58704200
C	4.82208800	-0.53696800	3.25623300
C	4.22457100	1.71673400	4.29846700
H	2.17074600	1.49745500	3.62556000
H	2.95067000	2.97417000	3.06509600
C	5.82996400	-3.37213700	-0.89295900
C	3.57542200	-2.56386000	-1.47379100
C	4.51429900	0.23009500	4.55417700
H	4.94275400	-1.60291800	3.47935900
H	5.76150600	-0.18111300	2.81532600
H	3.94509900	2.21006900	5.23556000
H	5.13891300	2.20835400	3.94142700
C	5.88955600	-4.12449800	-2.05009900
H	6.66526400	-3.37138600	-0.19637000
C	3.65742200	-3.36016900	-2.64456200
O	2.47664900	-1.90236900	-1.23489100
H	3.64013700	-0.22770100	5.03610100
H	5.34952000	0.12334600	5.25433400
C	4.78393200	-4.11284800	-2.92241700
H	6.76794600	-4.71714100	-2.28130200
H	2.80703200	-3.34474100	-3.31811300
H	4.81626700	-4.70239100	-3.83493700
C	-0.14737200	3.98128400	2.42881700
C	-0.69675900	4.82928200	1.45320600
C	-0.27878900	2.60521100	2.33315800
H	0.37920300	4.40686600	3.27913600
C	-1.38414700	4.26427300	0.39314100
H	-0.59229200	5.90575700	1.53349600
C	-0.96073500	2.00565900	1.25231700
H	0.12809500	1.94550900	3.08942800
C	-1.53998800	2.86846300	0.27303800
H	-1.81396000	4.89820200	-0.37719900

O	-1.00503100	0.69457300	1.17714700
C	-2.27092300	2.36909400	-0.85999700
Co	-2.44640900	-0.20987300	0.29275100
N	-2.61865800	1.14314800	-1.04821200
H	-2.57469700	3.11447100	-1.59733600
N	-3.78068800	-1.13057800	-0.67874300
C	-3.55525800	0.78309100	-2.12941500
C	-4.64182900	-1.92936900	-0.15273000
C	-3.74363700	-0.74048700	-2.08584400
C	-3.17093600	1.20792400	-3.54649200
H	-5.45425900	-2.30840700	-0.77347700
C	-4.60252300	-2.37372900	1.21175500
C	-4.91779200	-1.14577500	-2.97233500
C	-4.30959200	0.81195500	-4.50128900
H	-2.23837100	0.71141000	-3.83960400
H	-2.99081600	2.28638200	-3.60069800
C	-5.70453200	-3.09456200	1.72233300
C	-3.44120100	-2.16659700	2.02706800
C	-4.63660100	-0.68702600	-4.41457700
H	-5.06087400	-2.23201400	-2.95472600
H	-5.83717500	-0.68311100	-2.59288500
H	-4.04618600	1.07749000	-5.53071500
H	-5.20469400	1.39289300	-4.24341000
C	-5.70294300	-3.59857100	3.00829700
H	-6.56843300	-3.24144800	1.07806100
C	-3.46134800	-2.71238200	3.33624100
O	-2.36064600	-1.56212500	1.61436600
H	-3.78726100	-1.26203900	-4.80706700
H	-5.49494300	-0.92208500	-5.05269300
C	-4.56181600	-3.40250800	3.81017700
H	-6.56059800	-4.13987800	3.39254300
H	-2.58288400	-2.55541800	3.95320900
H	-4.54513100	-3.79681400	4.82284700
H	-4.51212200	1.23074300	-1.84581700
H	-2.82610800	-1.19400700	-2.48253600
H	4.49194000	1.54176300	1.61955900
H	2.74581200	-0.67296600	2.70705000
C	5.64140600	1.03258500	-2.61969800
H	5.87559500	0.05955200	-3.06374800
H	6.56444400	1.59023600	-2.45658400
H	4.99031000	1.56337800	-3.31852900
C	4.92605100	0.80414600	-1.29334700
O	3.71778200	0.34969800	-1.48355700
O	5.48669800	1.01975200	-0.21841800
C	-5.49918400	1.61718600	2.46805900
H	-6.42961200	2.13112600	2.22377700
H	-4.82422600	2.28359200	3.01092200
H	-5.71162400	0.76380700	3.12011800
C	-4.83216300	1.10847300	1.19537000
O	-3.62538300	0.67604800	1.43876900
O	-5.42373000	1.11480700	0.11551200

IV-m (PO-Co^{III}-OAc + H$_2$O-Co^{III}-OAc)
PO-Co^{III}-OAc + H$_2$O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3084.644048
Thermal correction to Gibbs Free Energy (a.u.): 0.860419
Imaginary frequencies: -272.35
Calculation of single point energy based on the optimized structure, Et = -5562.0380295 a.u.

N	2.34044400	-1.31347800	0.11832500
N	3.58994200	0.88536300	0.66592900
C	1.77208300	-2.37109900	-0.34797700
H	1.70307800	-3.24376900	0.30208800
C	3.88579200	2.11820200	0.90941300
H	4.37617600	2.35175500	1.85537400
C	1.21630300	-2.52464800	-1.66229400
C	0.73339500	-3.79991900	-2.03333200
C	1.11267200	-1.42863000	-2.57892500

C	0.14485300	-4.02664500	-3.26233200
H	0.84283800	-4.61655300	-1.32307000
C	0.48380200	-1.68620000	-3.82925800
C	0.01961600	-2.94551100	-4.15817100
H	-0.21338300	-5.01359400	-3.53337000
H	0.40624200	-0.85600200	-4.52363400
H	-0.44104600	-3.10531500	-5.12955300
C	3.63919100	3.23475700	0.04413700
C	3.94016400	4.52900100	0.52846000
C	3.13977000	3.06978200	-1.28969800
C	3.75851400	5.65660100	-0.24693700
H	4.32281400	4.62170000	1.54250900
C	2.98510200	4.25000100	-2.07334300
C	3.28006900	5.49952900	-1.56330700
H	3.98957900	6.64171700	0.14291300
H	2.63159800	4.12436200	-3.09188600
H	3.14451800	6.37551500	-2.19235000
O	1.53001900	-0.22559800	-2.33235800
O	2.82049100	1.93122500	-1.82145600
H	1.98603200	-0.86844600	2.10384300
C	2.82329200	-1.24995100	1.50662000
C	3.30373200	-2.58953400	2.09630300
C	3.94635200	-0.20946500	1.57566100
C	4.37185500	-2.36549600	3.18973300
H	2.44706100	-3.12507400	2.51724700
H	3.73516300	-3.18685300	1.29036900
C	4.20513200	0.17915200	3.03718800
H	4.82910500	-0.68102200	1.13597000
C	4.12538100	-1.06357700	3.96128500
H	4.37851900	-3.21724600	3.87740700
H	5.36339500	-2.33469800	2.72429500
H	3.46047200	0.91834700	3.35668100
H	5.18983200	0.65120100	3.12188000
H	3.13104300	-1.11079700	4.41549400
H	4.84221600	-0.96193800	4.78219000
Co	2.62809800	0.28979100	-0.86100000
H	0.18533900	0.54625800	-0.56883800
O	-1.19040800	0.38945400	-1.11650300
C	-1.38594700	1.37112100	-2.11298200
C	-0.25237700	2.29470200	-1.80249700
H	-2.35613800	1.86938900	-2.02120900
H	-1.27636800	0.92759000	-3.11022200
H	0.72456500	2.06969500	-2.23499300
C	-0.42435200	3.48811200	-0.98792700
H	-1.08832500	3.26210900	-0.13980800
H	-1.01493000	4.18579000	-1.61164300
H	0.51594600	3.95482200	-0.70168600
O	0.96643000	1.05401400	-0.14635900
H	0.64092000	1.10511500	0.78355500
N	-1.88969000	-1.57765900	0.45706500
N	-3.76398700	-0.17889900	-0.64887900
C	-1.24451600	-2.20122200	1.37413400
H	-1.13158400	-3.28272400	1.29245400
C	-4.76497100	0.59356100	-0.90434400
H	-5.59325200	0.18041700	-1.48525100
C	-0.66266100	-1.57659400	2.53747300
C	-0.19862900	-2.40196100	3.58168500
C	-0.49539900	-0.15988900	2.62361800
C	0.39674800	-1.87192700	4.71399200
H	-0.32861500	-3.47751500	3.48733300
C	0.12631100	0.35753900	3.78561500
C	0.55373500	-0.47802600	4.80557800
H	0.73556200	-2.51941000	5.51516300
H	0.24197400	1.43438900	3.85151800
H	1.01435200	-0.04588200	5.68971600
C	-4.90184500	1.96183600	-0.49649700
C	-6.10393300	2.63597000	-0.81226200
C	-3.84610200	2.66187100	0.17206200
C	-6.29677200	3.96351500	-0.48593800

H	-6.88717700	2.07988200	-1.32250900
C	-4.06949300	4.02822600	0.48861800
C	-5.25968700	4.65500100	0.17002300
H	-7.22736000	4.46479000	-0.72816200
H	-3.27527600	4.55637600	1.00608300
H	-5.39747100	5.69937700	0.43728700
O	-0.81876100	0.66675100	1.65589500
O	-2.68978200	2.13482700	0.45885300
H	-1.71717800	-1.94260600	-1.54017300
C	-2.41903700	-2.21962000	-0.74551000
C	-2.58575800	-3.74145700	-0.70017900
C	-3.77918600	-1.58879700	-1.06759000
C	-3.52889100	-4.21165100	-1.84089600
H	-1.60866700	-4.21991700	-0.79876000
H	-3.01230300	-4.02150200	0.26851300
C	-4.09598700	-1.82284300	-2.55447900
H	-4.51659200	-2.07756200	-0.42712900
C	-3.57612600	-3.21066400	-3.00606200
H	-3.20758500	-5.19218700	-2.20551200
H	-4.54144200	-4.34645100	-1.44347400
H	-3.62372900	-1.03441200	-3.15189100
H	-5.17644500	-1.75079900	-2.71842400
H	-2.56880800	-3.10494200	-3.41894400
H	-4.20570100	-3.59992200	-3.81256900
Co	-2.31896900	0.27459200	0.48763100
C	-4.70005100	-0.59586100	3.80977400
H	-5.42532200	-1.37362600	4.05156000
H	-5.16793000	0.39071000	3.86417700
H	-3.88555100	-0.61045500	4.54089200
C	-4.12525800	-0.82985400	2.41664000
O	-3.35608500	0.15617600	2.04861200
O	-4.38320900	-1.85532300	1.78374300
C	5.82544100	-1.62011800	-2.74616400
H	6.28183200	-0.69374500	-3.10363200
H	5.22637200	-2.02630700	-3.56760500
H	6.59372600	-2.34129500	-2.46451300
C	4.91127400	-1.33917700	-1.55756500
O	4.13019900	-0.32443700	-1.79156500
O	4.96146100	-2.03748700	-0.54149300

IV-m (PO-Co^{III}-OAc + H_2O-Co^{III}-OAc)

PO-Co^{III}-OAc + H_2O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3084.678380

Thermal correction to Gibbs Free Energy (a.u.): 0.864548

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5562.0760329 a.u.

N	2.78699500	-0.82184300	0.67058500
N	3.28883800	1.69614900	0.32358500
C	2.66771900	-2.10316500	0.62661400
H	2.84168700	-2.66865400	1.54255900
C	3.14108900	2.95894600	0.09256500
H	3.43239900	3.66160100	0.87432700
C	2.33011300	-2.87948800	-0.53605800
C	2.36903100	-4.28842500	-0.43290100
C	1.91015400	-2.26712400	-1.76105200
C	2.02544800	-5.10451400	-1.49516400
H	2.68486800	-4.72742900	0.51086800
C	1.55977600	-3.13037100	-2.83539300
C	1.62200300	-4.50572700	-2.70486100
H	2.06974900	-6.18387800	-1.40102200
H	1.25525500	-2.66183700	-3.76535200
H	1.35609100	-5.13305800	-3.55154800
C	2.61963400	3.54321400	-1.10601100
C	2.40522700	4.94141000	-1.12686000
C	2.33667200	2.75651100	-2.27259600
C	1.91473100	5.58463100	-2.24479700
H	2.63182300	5.50948900	-0.22708200
C	1.85887900	3.45522900	-3.42073800

C	1.65009200	4.81976000	-3.40030600
H	1.74820700	6.65620500	-2.24138100
H	1.66661600	2.86530000	-4.31121500
H	1.27692100	5.31302400	-4.29435500
O	1.79138400	-0.98346000	-1.92748800
O	2.48648500	1.47453500	-2.34865700
H	2.12713800	0.17538900	2.34740000
C	3.09544400	-0.11414600	1.92065500
C	3.89557600	-0.92320100	2.95656000
C	3.84776700	1.17882900	1.57623900
C	4.67836700	0.01263400	3.90619100
H	3.20993500	-1.55108300	3.53346200
H	4.59910500	-1.56520500	2.42192300
C	3.80338300	2.12958000	2.78152400
H	4.87466900	0.88462100	1.34573200
C	3.94938200	1.34595900	4.11088100
H	4.83704000	-0.48547000	4.86806100
H	5.67319300	0.20278700	3.48796300
H	2.85090700	2.67314800	2.78474600
H	4.60187200	2.87382700	2.69127200
H	2.95442600	1.14262500	4.52069900
H	4.47243600	1.96164100	4.84941700
Co	2.66245500	0.32942500	-0.83837000
H	0.33530600	0.27204600	-1.04797900
O	-1.66311700	0.77616800	-1.48358100
C	-2.45901100	1.44031900	-2.49970900
C	-1.21909600	2.07967700	-2.04256000
H	-3.40639600	1.81771300	-2.13012800
H	-2.48703100	0.90117400	-3.44320700
H	-0.33068700	1.92462000	-2.64857100
C	-1.18713600	3.28094500	-1.14814100
H	-2.07150800	3.32584500	-0.51346700
H	-1.12114500	4.17285000	-1.78031300
H	-0.29089200	3.25084000	-0.52780500
O	0.81337600	0.87097700	-0.45408000
H	0.23338900	0.98716300	0.34464800
N	-1.42305000	-1.38909900	0.29416100
N	-3.72303000	-0.78953400	-0.71795900
C	-0.64586900	-1.76246200	1.24695700
H	-0.19226600	-2.75133400	1.19996100
C	-4.96808300	-0.47096200	-0.85656700
H	-5.62363200	-1.18508100	-1.36145000
C	-0.34830800	-0.95030100	2.40279500
C	0.24044100	-1.55441500	3.52915500
C	-0.61377100	0.45189500	2.40255900
C	0.54714000	-0.81368800	4.66041900
H	0.43956500	-2.62289400	3.50305500
C	-0.27261600	1.19082000	3.55320800
C	0.28559600	0.56609800	4.66103000
H	0.98493400	-1.29116500	5.53010800
H	-0.47711100	2.25581500	3.54480500
H	0.52043400	1.15625200	5.54234100
C	-5.57829900	0.74171500	-0.40528300
C	-6.97500100	0.89447900	-0.57980300
C	-4.81022300	1.80673600	0.17200200
C	-7.62720000	2.04863000	-0.20041100
H	-7.53187200	0.07125700	-1.02146300
C	-5.50847200	2.98684900	0.54283300
C	-6.87321400	3.09889700	0.36286200
H	-8.69871400	2.14940100	-0.33305200
H	-4.92602500	3.79043800	0.98058500
H	-7.37468000	4.01394700	0.66637900
O	-1.08444700	1.08133900	1.33583100
O	-3.51811700	1.77425200	0.32960300
H	-1.19266700	-1.73252800	-1.70382300
C	-1.72853700	-2.20954700	-0.87391500
C	-1.35264300	-3.69040000	-0.80573300
C	-3.23527600	-2.10993600	-1.14974800
C	-2.04707300	-4.46525300	-1.95944700

H	-0.27159600	-3.80850500	-0.86878000
H	-1.68527100	-4.08904900	0.15836600
C	-3.48254300	-2.45389100	-2.63010100
H	-3.72319700	-2.83527400	-0.49537000
C	-2.48030400	-3.53758000	-3.10650500
H	-1.36817700	-5.23362700	-2.34008600
H	-2.92902200	-4.98896100	-1.57304000
H	-3.37255200	-1.54817900	-3.23742500
H	-4.51145200	-2.80545400	-2.76061900
H	-1.58849300	-3.05718400	-3.52411300
H	-2.92400000	-4.12126900	-3.91896900
Co	-2.49017100	0.19564700	0.33171300
C	-4.10746300	-1.36739800	3.82000000
H	-4.58536300	-2.30747200	4.09761800
H	-4.78691800	-0.52779100	3.98419300
H	-3.22573700	-1.20450100	4.44855700
C	-3.66439100	-1.42036500	2.36357600
O	-3.29113400	-0.23744400	1.94687900
O	-3.65156700	-2.47378100	1.73029600
C	6.38174400	-1.18405700	-1.98322700
H	6.55837400	-0.41214000	-2.73634000
H	5.97909200	-2.05978400	-2.50248500
H	7.31410800	-1.45213200	-1.48466900
C	5.36037400	-0.70125100	-0.95792200
O	4.31704300	-0.18468200	-1.53844500
O	5.56752400	-0.83306800	0.25168100

IV-m (PO-Co^{III}-OAc + H_2O-Co^{III}-OAc)

PO-Co^{III}-OAc + H_2O-Co^{III}-OAc = PG + 2Co^{III}(salen)-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3084.733345

Thermal correction to Gibbs Free Energy (a.u.): 0.868561

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5562.1285283 a.u.

N	2.32605000	-1.24203500	0.69533800
N	3.77870900	0.90108900	0.63418700
C	1.88806300	-2.40235500	0.36450700
H	1.96808600	-3.22269800	1.07671400
C	4.54940500	1.89150000	0.33183800
H	5.38655500	2.10875400	0.99972800
C	1.31113200	-2.70970000	-0.92454000
C	1.15770600	-4.06020100	-1.28758600
C	0.86713000	-1.68188200	-1.80822000
C	0.62340100	-4.42051500	-2.51559600
H	1.47894900	-4.82491300	-0.58512500
C	0.34679500	-2.06870300	-3.06120100
C	0.23216200	-3.40837600	-3.40655600
H	0.52616300	-5.46514800	-2.79036000
H	0.05392900	-1.28155200	-3.74778400
H	-0.16342700	-3.67422400	-4.38308000
C	4.41644700	2.74629400	-0.80916100
C	5.39660500	3.74660400	-1.01221000
C	3.30932200	2.63837900	-1.71301600
C	5.32154400	4.62899500	-2.06986100
H	6.22406400	3.80635000	-0.30870600
C	3.25377900	3.56771500	-2.78718900
C	4.23120100	4.52831100	-2.95791900
H	6.08365500	5.38658200	-2.21577600
H	2.41613100	3.48372100	-3.47157700
H	4.15801400	5.21672100	-3.79574300
O	0.89029800	-0.40561500	-1.48021700
O	2.34120600	1.77953200	-1.58825200
H	2.10764900	-0.39944100	2.54107700
C	2.90150500	-0.92909600	2.00088300
C	3.39348800	-2.10976700	2.84349100
C	4.06539400	0.05039200	1.79785800
C	4.33468200	-1.60430400	3.96979800
H	2.53696700	-2.64037700	3.26682500
H	3.93489500	-2.80298900	2.19203900

C	4.30872900	0.80349700	3.11777500
H	4.93598500	-0.54794000	1.52072400
C	4.06522800	-0.13408800	4.32836000
H	4.22570200	-2.23532800	4.85728500
H	5.37723600	-1.70443000	3.64713000
H	3.63749300	1.66806700	3.16806900
H	5.33436100	1.18626000	3.14174700
H	3.02761200	-0.03391300	4.66837900
H	4.69309100	0.17315900	5.17037100
Co	2.37207500	0.26755800	-0.45971300
H	-0.37007700	0.50272300	-1.09866000
O	-1.08303500	1.14142700	-0.79513700
C	-0.48794400	2.43415400	-0.58757100
C	0.56399600	2.47664200	0.55609300
H	-1.30392500	3.12777500	-0.38915800
H	0.00753300	2.69437700	-1.52470700
H	1.41003600	3.05702100	0.18780100
C	0.09683200	3.05896100	1.88358600
H	-0.67402200	2.43551400	2.33472700
H	-0.32348600	4.05791500	1.72600400
H	0.95226900	3.14775600	2.56068900
O	1.08976600	1.15598100	0.79665900
H	0.32865700	0.57368500	1.10591800
N	-2.23154400	-1.34851500	-0.55461500
N	-3.78661100	0.70620900	-0.84750300
C	-1.75041500	-2.43538400	-0.06791000
H	-1.76609500	-3.33863400	-0.67616500
C	-4.58020900	1.72222800	-0.77028600
H	-5.35239500	1.82306500	-1.53623900
C	-1.19327100	-2.56087300	1.25886300
C	-0.93080900	-3.85112000	1.75674700
C	-0.84561200	-1.41807300	2.03565700
C	-0.36461500	-4.04062900	3.00785300
H	-1.18314600	-4.70623500	1.13513700
C	-0.27658000	-1.63116000	3.30979500
C	-0.04608200	-2.91460900	3.78474400
H	-0.18150500	-5.04073500	3.38539400
H	-0.04040700	-0.75595300	3.90583900
H	0.38205400	-3.04711400	4.77465000
C	-4.55716600	2.74167400	0.23235400
C	-5.53808900	3.76019400	0.17837700
C	-3.56482000	2.75886900	1.26381600
C	-5.57020100	4.78128400	1.10506600
H	-6.27816200	3.72061100	-0.61782300
C	-3.62215600	3.82390300	2.20500000
C	-4.59511900	4.80043100	2.12355800
H	-6.32998000	5.55341700	1.05440300
H	-2.87549100	3.83441400	2.99126800
H	-4.60972900	5.59690400	2.86293800
O	-0.98296800	-0.18392400	1.59203900
O	-2.60669700	1.88901000	1.37077800
H	-1.97938600	-0.76652300	-2.49654700
C	-2.77125200	-1.24905300	-1.90978900
C	-3.18655700	-2.56128600	-2.58433700
C	-3.98440900	-0.31281300	-1.88775800
C	-4.09703100	-2.27050800	-3.80771600
H	-2.29773600	-3.11573800	-2.89245400
H	-3.73106700	-3.16587300	-1.85272000
C	-4.21865800	0.22852400	-3.30969100
H	-4.83321300	-0.91313600	-1.55373800
C	-3.87739600	-0.85504400	-4.36359700
H	-3.91827300	-3.01508000	-4.58964900
H	-5.14798500	-2.37697300	-3.51573900
H	-3.59817200	1.11809900	-3.46637800
H	-5.26337400	0.53721500	-3.42056700
H	-2.83078800	-0.75100400	-4.67357200
H	-4.47915000	-0.70114700	-5.26463600
Co	-2.43808500	0.27788600	0.41461000
C	-5.14841000	-1.82795100	2.78035400

H	-5.97570900	-2.51272300	2.59075700
H	-5.49800300	-0.95186500	3.33263600
H	-4.39335100	-2.32334000	3.39893200
C	-4.51137200	-1.40141000	1.46237700
O	-3.61241800	-0.47536500	1.65311100
O	-4.83777200	-1.92367400	0.39583200
C	5.07178100	-1.92278900	-2.75181000
H	5.31754700	-1.10431300	-3.43329200
H	4.31996000	-2.54542200	-3.24729100
H	5.95946100	-2.51891600	-2.53739900
C	4.48509800	-1.37393100	-1.45624300
O	3.51382600	-0.53620400	-1.69718800
O	4.90661000	-1.73719600	-0.35766200

II-t (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.268435

Thermal correction to Gibbs Free Energy (a.u.): 0.540748

Imaginary frequencies: -481.36

Calculation of single point energy based on the optimized structure, Et = -3582.3351448 a.u.

C	3.91792600	-2.41233800	-1.77618900
C	2.64826900	-2.26296600	-2.49002700
O	4.31160300	-1.11951300	-2.27478800
H	3.79649200	-2.41682000	-0.69315900
H	1.68124500	-2.13210200	-2.01041300
H	2.70589000	-2.28798700	-3.57498100
C	4.88804600	-3.47008100	-2.26149000
H	5.87083300	-3.26854800	-1.82695000
H	4.56295900	-4.46470800	-1.94432300
H	4.97817300	-3.44874300	-3.35095000
O	2.22538900	0.12608300	-1.86003000
H	3.59415100	-0.44190400	-1.97190600
H	1.77080700	0.30576600	-2.69402800
C	3.51068700	-2.93446000	2.98827300
C	3.83903800	-1.79758200	3.75008200
C	2.80581700	-2.82240700	1.80405100
H	3.80542800	-3.91975600	3.33988700
C	3.44486200	-0.55662600	3.28959700
H	4.38420400	-1.89568300	4.68226000
C	2.38216400	-1.55870900	1.30896000
H	2.52659000	-3.69976000	1.22896500
C	2.72633900	-0.40382100	2.08269100
H	3.68280700	0.33690900	3.86178000
O	1.74842800	-1.52433300	0.17369500
C	2.38957700	0.92517400	1.66788300
Co	0.86188100	-0.00589000	-0.53721600
N	1.74123400	1.24982700	0.60014200
H	2.71885600	1.72615300	2.33283300
N	-0.01526700	1.49895000	-1.28481300
C	1.33911600	2.64461900	0.34560600
C	-1.24010700	1.47200200	-1.68475200
C	0.78288800	2.70598300	-1.08702900
C	2.42353100	3.70907800	0.51956800
H	-1.74728600	2.41409200	-1.89129900
C	-1.99564100	0.26682000	-1.88626900
C	0.10660400	4.05138900	-1.33109100
C	1.81365600	5.09530100	0.25076400
H	3.24921400	3.50687700	-0.17546000
H	2.83941200	3.68457900	1.53167000
C	-3.38530900	0.36636200	-2.10385100
C	-1.35655400	-1.01451700	-1.91462200
C	1.13723800	5.17462800	-1.12579400
H	-0.29977500	4.10094600	-2.34789000
H	-0.73004600	4.16426300	-0.63138000
H	2.58729300	5.86624900	0.33335500
H	1.07031100	5.30857600	1.02967300
C	-4.15719900	-0.75286000	-2.35194100

H	-3.84727500	1.34893000	-2.05246200
C	-2.16403600	-2.13851000	-2.21078800
O	-0.07149400	-1.17897800	-1.72203600
H	1.90353300	5.09975900	-1.90922300
H	0.65500400	6.14976600	-1.25189900
C	-3.52677600	-2.00786700	-2.41559600
H	-5.22895600	-0.66566700	-2.49154500
H	-1.68005700	-3.10932000	-2.23851100
H	-4.12102000	-2.89609800	-2.61360800
H	1.63996700	2.60479100	-1.76736800
H	0.50068900	2.85252600	1.01908900
S	-1.36606900	0.59846600	1.67884700
O	-0.96361000	0.46122700	3.08606500
O	-1.48437500	1.98876500	1.17269800
O	-0.50705900	-0.31451700	0.78244900
C	-2.98091900	-0.13726200	1.43339600
C	-3.10372400	-1.50937500	1.21673000
C	-4.10610700	0.68406000	1.45424000
C	-4.36706300	-2.05334800	1.00932400
H	-2.21410000	-2.12611300	1.17739700
C	-5.36522400	0.12300600	1.24918700
H	-3.98408700	1.75022500	1.60766900
C	-5.51400800	-1.24869600	1.01592600
H	-4.46430600	-3.11931100	0.82095800
H	-6.24461800	0.76183500	1.25785200
C	-6.86916500	-1.84487200	0.72839100
H	-7.67614700	-1.20029800	1.08788300
H	-7.01312700	-1.98258000	-0.35083400
H	-6.98312100	-2.82732500	1.19710400

II-t (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.341725

Thermal correction to Gibbs Free Energy (a.u.): 0.542564

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.4019147 a.u.

C	4.05525700	-2.88604900	-1.48937800
C	2.78968900	-3.05134100	-2.21362700
O	3.62787000	-1.88278700	-2.44639600
H	3.98719500	-2.54094500	-0.46142400
H	1.85153000	-2.82784400	-1.71371800
H	2.75496100	-3.72966600	-3.06443100
C	5.30142900	-3.63971500	-1.86445400
H	6.19139200	-3.02527600	-1.69519000
H	5.39329500	-4.54207100	-1.25046000
H	5.27826300	-3.93304100	-2.91752600
O	2.22524400	0.29151000	-2.01520500
H	2.84636400	-0.49392500	-1.97126400
H	1.64508700	0.05622400	-2.75911400
C	3.37393300	-2.61160100	3.17115600
C	3.60405100	-1.44700000	3.92757100
C	2.79099400	-2.54954300	1.91868900
H	3.64764200	-3.58015100	3.58126900
C	3.23313900	-0.22873100	3.39519600
H	4.05373500	-1.50817600	4.91234500
C	2.40162600	-1.31035900	1.34581100
H	2.59126900	-3.44847500	1.34512200
C	2.63501900	-0.12846500	2.11844800
H	3.38900800	0.68522500	3.96304400
O	1.89382700	-1.31421700	0.14409400
C	2.28973400	1.17433000	1.63950300
Co	0.88256600	0.10832100	-0.57575700
N	1.69439300	1.44116200	0.52333100
H	2.54792900	2.00863400	2.29507000
N	-0.07123400	1.54804600	-1.36509600
C	1.24530200	2.81094000	0.21302200
C	-1.29364200	1.44681600	-1.76062400
C	0.67328600	2.79584300	-1.21468500

C	2.29816700	3.91422000	0.32679600
H	-1.84929800	2.35477000	-1.99424700
C	-1.98062800	0.19532200	-1.91981900
C	-0.06155600	4.10288200	-1.49588000
C	1.63463100	5.26744300	0.01799300
H	3.11726200	3.71311000	-0.37589700
H	2.73256400	3.93900100	1.33129100
C	-3.37769500	0.20356200	-2.10956400
C	-1.26281600	-1.04355400	-1.92889700
C	0.92859700	5.27145100	-1.34666700
H	-0.48248600	4.10035700	-2.50782800
H	-0.89286700	4.20839400	-0.78860500
H	2.38162300	6.06752600	0.05479500
H	0.89983900	5.48485900	0.80392500
C	-4.08177300	-0.96933600	-2.30702400
H	-3.89944000	1.15647700	-2.07595000
C	-2.00254900	-2.22374200	-2.17233000
O	0.03755500	-1.12346400	-1.76311400
H	1.68203500	5.19899600	-2.14244800
H	0.40644000	6.22237200	-1.49594100
C	-3.37540000	-2.18406600	-2.34868800
H	-5.15952000	-0.95358400	-2.42536900
H	-1.45777900	-3.16179400	-2.18717200
H	-3.91684300	-3.11281800	-2.50787900
H	1.52500300	2.71242300	-1.90342800
H	0.41039100	3.02377200	0.88878200
S	-1.31725700	0.63749700	1.63351700
O	-0.85669700	0.54619900	3.02578200
O	-1.51316900	2.00673900	1.10068200
O	-0.44537700	-0.26238800	0.72247200
C	-2.89586400	-0.18641500	1.44714500
C	-2.95395600	-1.57035400	1.28415400
C	-4.05834800	0.58122700	1.45364400
C	-4.19207800	-2.18105600	1.11516700
H	-2.03697400	-2.14612600	1.25577500
C	-5.29127600	-0.04709700	1.28816400
H	-3.98619400	1.65707100	1.56481800
C	-5.37642400	-1.43212200	1.10803600
H	-4.24013700	-3.25684100	0.96893600
H	-6.20016300	0.54889000	1.28596600
C	-6.70471200	-2.10280400	0.86292700
H	-7.53702500	-1.48523800	1.21167700
H	-6.85623900	-2.28608000	-0.20837900
H	-6.76397700	-3.07199600	1.36775200

II-t (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.360180

Thermal correction to Gibbs Free Energy (a.u.): 0.547062

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4282134 a.u.

C	4.27238100	0.11135500	-1.51606700
C	3.17042700	-0.14391100	-2.53093300
O	4.52397600	1.51229300	-1.39983300
H	3.94092900	-0.28882500	-0.55039800
H	2.90014900	-1.19991900	-2.57251900
H	3.47180600	0.22355600	-3.51781900
C	5.56862800	-0.57029800	-1.92387900
H	6.35027800	-0.34006600	-1.19583800
H	5.43828500	-1.65604400	-1.96016700
H	5.90108300	-0.21638300	-2.90479700
O	2.01041600	0.63185400	-2.12098000
H	3.66148300	1.94826500	-1.42507100
H	1.29729900	0.54765800	-2.78969400
C	2.60715800	-4.81818000	0.47110100
C	3.04838800	-4.37660300	1.73576200
C	2.03980100	-3.94586300	-0.43666400
H	2.70669700	-5.86754700	0.20658000

C	2.91395600	-3.04279500	2.05448400
H	3.48288700	-5.07497300	2.44232100
C	1.87165200	-2.56967600	-0.12944100
H	1.68633000	-4.28494700	-1.40455500
C	2.34158900	-2.11807300	1.14730700
H	3.24755900	-2.67427300	3.02133300
O	1.33434300	-1.79883600	-1.03155300
C	2.29613300	-0.74476100	1.53032700
Co	0.71942100	-0.04988200	-0.70956400
N	1.82701200	0.22900800	0.81489800
H	2.71537000	-0.50337700	2.50905000
N	0.17147700	1.75225600	-0.45334300
C	1.76006100	1.59632500	1.36108900
C	-1.02243400	2.16900700	-0.69703100
C	1.20156700	2.50438500	0.25366100
C	3.08288300	2.17774900	1.86517300
H	-1.32362500	3.15020500	-0.33050100
C	-1.99733100	1.41286500	-1.43468000
C	0.84308800	3.87034700	0.82933100
C	2.82015800	3.58518700	2.42856100
H	3.80541000	2.20525500	1.03957400
H	3.51184300	1.54396000	2.64812400
C	-3.34246500	1.83403500	-1.41744700
C	-1.61451300	0.27392100	-2.20987800
C	2.11934100	4.50307100	1.41412800
H	0.42904900	4.52311000	0.05258400
H	0.07804500	3.74564300	1.60464700
H	3.76232700	4.03995800	2.75197300
H	2.19047400	3.49280600	3.32299200
C	-4.31183600	1.16368000	-2.14026500
H	-3.61063300	2.68934800	-0.80292300
C	-2.61616400	-0.37042000	-2.96779800
O	-0.37664900	-0.17431000	-2.26961200
H	2.81107200	4.72332600	0.58997000
H	1.87650700	5.46261100	1.88235100
C	-3.93160900	0.06285200	-2.92646300
H	-5.34808200	1.48054200	-2.09970600
H	-2.32118100	-1.23053000	-3.55915300
H	-4.68386700	-0.46942200	-3.50228200
H	2.00506500	2.64883400	-0.48210000
H	1.02119100	1.58159200	2.16847700
S	-1.29801800	-0.37140000	1.68933200
O	-0.90833900	-1.33394800	2.72790500
O	-1.11493400	1.06033200	2.02271100
O	-0.66919600	-0.77680500	0.32824900
C	-3.02996800	-0.56123600	1.27955500
C	-3.43960700	-1.55694100	0.39266900
C	-3.95290900	0.31211900	1.85047100
C	-4.78857000	-1.66296500	0.07131000
H	-2.70310300	-2.20895000	-0.06085700
C	-5.30157700	0.18817600	1.52158300
H	-3.60781000	1.08799400	2.52422700
C	-5.73769500	-0.79212300	0.62335700
H	-5.10971600	-2.42486100	-0.63383500
H	-6.02453500	0.87122300	1.95970500
C	-7.18720800	-0.88365000	0.21772600
H	-7.83981000	-0.39341400	0.94533600
H	-7.35095100	-0.39782400	-0.75251600
H	-7.51021200	-1.92429600	0.11614000

II-m (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.281598

Thermal correction to Gibbs Free Energy (a.u.): 0.542275

Imaginary frequencies: -390.99

Calculation of single point energy based on the optimized structure, Et = -3582.3547345 a.u.

C	4.63217700	-3.01620300	2.00521500

C	5.58388000	-2.00975500	1.74957000
C	3.29049500	-2.81514000	1.74231500
H	4.95488500	-3.96534100	2.42517500
C	5.14665500	-0.80204400	1.24280100
C	2.81033800	-1.59092500	1.19305300
C	3.78396200	-0.56467300	0.95013200
H	5.85779600	0.00081500	1.06135500
O	1.54019200	-1.47697600	0.95233600
C	3.41121900	0.74419800	0.48603600
Co	0.74895200	-0.08756400	-0.10106500
N	2.24192900	1.08128100	0.06490200
H	4.19532100	1.50222800	0.51085900
N	0.00329800	1.24717200	-1.23476500
C	1.86011600	2.45223500	-0.28378400
C	-1.15170100	1.18965800	-1.79916600
C	0.95656600	2.33242400	-1.51923400
C	2.98959500	3.45337800	-0.50873100
H	-1.45261300	2.01660400	-2.44194200
C	-2.10369600	0.12370900	-1.67945500
C	0.34875200	3.69117000	-1.87359500
C	2.39236400	4.82225600	-0.86933400
H	3.64659400	3.10240600	-1.31721400
H	3.60208300	3.54778700	0.39422000
C	-3.32202500	0.24179400	-2.38313800
C	-1.84228700	-1.04495400	-0.89805100
C	1.46245400	4.72781100	-2.08432200
H	-0.25026900	3.62271900	-2.78760100
H	-0.31531000	3.98755100	-1.05519500
H	3.19750700	5.53971100	-1.06033100
H	1.82637600	5.19919500	-0.00848900
C	-4.28200100	-0.75084900	-2.34707000
H	-3.49381800	1.14487400	-2.96426200
C	-2.85153100	-2.04661600	-0.87086600
O	-0.74192000	-1.25878000	-0.23848300
H	2.05164600	4.45259700	-2.97030000
H	1.01767100	5.70583400	-2.29607300
C	-4.02805700	-1.90450800	-1.58282000
H	-4.77164200	-2.69613400	-1.54203800
H	1.58288300	1.97847900	-2.35251300
H	1.22179900	2.80363900	0.53364600
O	1.50922400	-0.89185100	-1.65296100
H	1.07326800	-1.79699200	-2.72759900
C	0.98682200	-3.43909600	-1.30077400
C	0.06230700	-3.49128500	-2.44682300
O	0.91274800	-2.67578600	-3.25212200
H	0.75867500	-2.79782200	-0.44785600
H	-0.92150600	-3.05858900	-2.25886100
H	-0.02137800	-4.48042100	-2.90640700
C	2.22866400	-4.21363200	-1.27817300
H	2.06818400	-4.98574700	-0.50452000
H	2.46804900	-4.69096300	-2.22863500
H	3.06171700	-3.61645700	-0.89426200
H	-5.21092900	-0.64508900	-2.89643300
H	-2.66888600	-2.91769300	-0.25070700
H	2.55222400	-3.57959600	1.96363600
H	6.63386500	-2.17455100	1.96419000
S	-0.96178400	1.68887600	1.93031700
O	-0.80019000	2.06342100	3.34067100
O	-1.05005300	2.79623800	0.94976300
O	0.14328500	0.67053800	1.57686600
C	-2.47244400	0.74681800	1.78435600
C	-2.55894100	-0.49446300	2.41492500
C	-3.55510000	1.26780600	1.08193700
C	-3.74468200	-1.21638500	2.32924500
H	-1.69915800	-0.88851700	2.94433100
C	-4.73650000	0.53331300	1.00463700
H	-3.45594500	2.23260000	0.59863000
C	-4.84703400	-0.71725000	1.62135300
H	-3.81725900	-2.18761500	2.81189000

H	-5.57917600	0.92979600	0.44525200
C	-6.10618800	-1.53264400	1.47875400
H	-6.99727800	-0.89773200	1.46809300
H	-6.09551300	-2.09285900	0.53526000
H	-6.21175900	-2.25677600	2.29162900
H	2.47076800	-0.86619200	-1.56672100

II-m (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.341750

Thermal correction to Gibbs Free Energy (a.u.): 0.544847

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.4083557 a.u.

C	-4.41923800	-3.36519600	-1.65325100
C	-5.44626800	-2.41196100	-1.48641200
C	-3.10257200	-3.05533400	-1.38198400
H	-4.66678700	-4.36122600	-2.01063100
C	-5.10740400	-1.14496600	-1.06364700
C	-2.72301200	-1.76757500	-0.90516900
C	-3.76773300	-0.79234900	-0.76512200
H	-5.87484100	-0.38138300	-0.95798700
O	-1.47127900	-1.55468400	-0.63831900
C	-3.48938200	0.57185000	-0.42392300
Co	-0.77723600	-0.01453300	0.23661400
N	-2.34707900	1.02901000	-0.03316500
H	-4.32064300	1.27105900	-0.52419100
N	-0.13082700	1.47914800	1.22818000
C	-2.05402400	2.45230700	0.15746000
C	1.04173800	1.57639300	1.75323300
C	-1.15044100	2.52850000	1.39571300
C	-3.24588400	3.39855900	0.27229800
H	1.29306000	2.49452100	2.28292900
C	2.07204900	0.58325300	1.71484000
C	-0.63057200	3.95375200	1.59535300
C	-2.73794400	4.83413500	0.47587900
H	-3.88203000	3.09891000	1.11712100
H	-3.85939400	3.35185200	-0.63352500
C	3.30977500	0.88610400	2.32628500
C	1.87306400	-0.69128100	1.09929300
C	-1.80855100	4.93540300	1.69061100
H	-0.03354700	4.02526000	2.51034700
H	0.01888000	4.19913200	0.74851900
H	-3.58771300	5.51562300	0.58854900
H	-2.19452000	5.14845400	-0.42383800
C	4.34749600	-0.02344500	2.34936400
H	3.43145400	1.86566400	2.78266700
C	2.96118100	-1.60479400	1.12950000
O	0.76082700	-1.07388600	0.53901900
H	-2.38261300	4.72549200	2.60385700
H	-1.42660000	5.95682800	1.78957700
C	4.15524000	-1.27972300	1.74357800
H	4.96315100	-2.00662400	1.74887900
H	-1.75909200	2.23576200	2.26565900
H	-1.43847100	2.75155000	-0.69773300
O	-1.54936200	-0.71003400	1.93011200
H	-1.21823400	-1.65273500	2.07124400
C	-0.39940900	-3.93373000	1.21589800
C	0.37380400	-3.70306900	2.44221400
O	-0.98430500	-3.20900400	2.34243900
H	-0.19755900	-3.27361100	0.37584700
H	1.13968900	-2.93389300	2.45961000
H	0.48855600	-4.51142600	3.16211200
C	-1.04838500	-5.25662900	0.92012300
H	-0.41724300	-5.84104100	0.24194800
H	-1.20719400	-5.83324000	1.83574500
H	-2.01575500	-5.10144500	0.43360400
H	5.29147800	0.22276200	2.82284000
H	2.82336900	-2.55840100	0.63290500

H	-2.30964100	-3.77938300	-1.53265600
H	-6.47681100	-2.66721400	-1.70659300
S	0.84210000	1.60094800	-1.95725300
O	0.60221400	1.84923800	-3.38320100
O	0.93542300	2.78300700	-1.07303800
O	-0.23096900	0.58316400	-1.48471600
C	2.37501100	0.70063500	-1.80201300
C	2.44807100	-0.60120900	-2.29786600
C	3.48884800	1.31675100	-1.23891900
C	3.65571900	-1.28684900	-2.22032800
H	1.56351000	-1.06704800	-2.71648200
C	4.69119800	0.61695000	-1.16889400
H	3.39870800	2.32567600	-0.85426400
C	4.79130200	-0.69153800	-1.65363400
H	3.71951100	-2.30399400	-2.59801200
H	5.55966300	1.08783900	-0.71727000
C	6.07813000	-1.46354500	-1.51518800
H	6.95065600	-0.80943000	-1.60304400
H	6.13255300	-1.94725400	-0.53158000
H	6.16077800	-2.24841300	-2.27239000
H	-2.50047900	-0.80929900	1.77846900

II-m (PO + H_2O-Co^{III}-OTs)

PO + H_2O-Co^{III}-OTs = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.355883

Thermal correction to Gibbs Free Energy (a.u.): 0.548028

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4307041 a.u.

C	-4.37146000	-3.35281200	-2.10787400
C	-5.37348100	-2.36992400	-1.95192200
C	-3.04919200	-3.08188700	-1.82409500
H	-4.64525400	-4.34309500	-2.46173200
C	-5.00675700	-1.11696000	-1.51364400
C	-2.63682800	-1.80209000	-1.35061300
C	-3.66069900	-0.80441200	-1.19531000
H	-5.75535100	-0.33561300	-1.40324600
O	-1.38091600	-1.62224500	-1.08322700
C	-3.35403500	0.53886700	-0.79754000
Co	-0.69348300	-0.17897600	-0.05549500
N	-2.21488300	0.93472100	-0.33608200
H	-4.15846800	1.26897100	-0.89623000
N	-0.08986800	1.20034800	1.11419700
C	-1.88558100	2.32870400	-0.03053000
C	1.04620100	1.21510100	1.72786100
C	-1.07721900	2.28298200	1.27445200
C	-3.04669900	3.31412400	0.06125000
H	1.28799900	2.08334500	2.33975700
C	2.03474700	0.18344900	1.70006900
C	-0.52168900	3.66796800	1.61241200
C	-2.50183800	4.70995100	0.40090800
H	-3.75644900	2.98753300	0.83462600
H	-3.59053200	3.35178200	-0.88854000
C	3.21725500	0.37189000	2.45460200
C	1.84252000	-1.02958700	0.96653200
C	-1.66642400	4.69019900	1.68613500
H	0.00379000	3.65270600	2.57289400
H	0.20082000	3.94081500	0.83645500
H	-3.33121700	5.41841100	0.49699900
H	-1.87890500	5.05940600	-0.43169900
C	4.19619700	-0.59670400	2.51344000
H	3.33872400	1.30726200	2.99570600
C	2.86468800	-2.01269500	1.05072500
O	0.78588500	-1.30123800	0.25715800
H	-2.31747500	4.44556800	2.53706200
H	-1.25509600	5.68537500	1.88412100
C	3.99972100	-1.80073600	1.80651400
H	4.75835600	-2.57749700	1.85233900
H	-1.76749600	1.96410000	2.07250300

H	-1.19542100	2.65735800	-0.81432300
O	-1.70455600	-1.00542000	1.51038400
H	-1.57169200	-0.70583800	3.84703400
C	-1.35574300	-2.38137500	1.92525000
C	-0.56550900	-2.21563200	3.21774800
O	-1.32692300	-1.56299400	4.22199400
H	-0.72261600	-2.79139800	1.13722800
H	0.36722500	-1.67904600	3.00722500
H	-0.30244100	-3.20476400	3.60502500
C	-2.63805800	-3.17822800	2.09023700
H	-2.39357600	-4.21211600	2.35048100
H	-3.24637500	-2.76142400	2.89792500
H	-3.21118900	-3.19994200	1.15755500
H	5.09644400	-0.44128100	3.09761300
H	2.71843600	-2.92852200	0.48972700
H	-2.27571900	-3.83188700	-1.94953800
H	-6.40799500	-2.59625700	-2.18463200
S	1.13999500	1.53808600	-1.96777400
O	1.03004900	1.89524800	-3.38600900
O	1.19346700	2.64825900	-0.99233800
O	-0.01545500	0.53848900	-1.66848600
C	2.61691300	0.56442700	-1.74661800
C	2.68393300	-0.70467400	-2.32183700
C	3.69690600	1.09376300	-1.04588200
C	3.85146700	-1.44712600	-2.18197100
H	1.82337700	-1.10485900	-2.84505900
C	4.85931300	0.33750700	-0.91547300
H	3.61117600	2.07903400	-0.60327600
C	4.95166200	-0.94112800	-1.47551100
H	3.90912500	-2.44079600	-2.61807600
H	5.70006600	0.73899000	-0.35710600
C	6.18681200	-1.77954500	-1.27117700
H	7.08854700	-1.16203100	-1.22316700
H	6.12111100	-2.33391600	-0.32640600
H	6.31449000	-2.51155200	-2.07364500
H	-2.61421100	-1.02263600	1.17571600

III-t (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.274297

Thermal correction to Gibbs Free Energy (a.u.): 0.542911

Imaginary frequencies: -377.29

Calculation of single point energy based on the optimized structure, Et = -3582.3482958 a.u.

C	-4.41781900	-3.64830400	-1.55838400
C	-5.39993400	-2.63715600	-1.56766600
C	-3.09861900	-3.36217900	-1.26685700
H	-4.70033900	-4.67206600	-1.78919800
C	-5.01705400	-1.34214400	-1.28363700
H	-6.43189800	-2.87194300	-1.80412500
C	-2.67613300	-2.03863300	-0.95554900
H	-2.33753600	-4.13539400	-1.26666400
C	-3.67822600	-1.01377000	-0.96769400
H	-5.75231100	-0.54061700	-1.29908500
O	-1.42150900	-1.84864900	-0.67799300
C	-3.36142400	0.36175400	-0.72263300
Co	-0.68964900	-0.25471400	0.04421600
N	-2.21954700	0.81236900	-0.32982500
H	-4.16397200	1.07716400	-0.90768400
N	0.00036800	1.30203000	0.91407100
C	-1.88636300	2.23799400	-0.25978300
C	1.14430200	1.38548100	1.50077600
C	-0.97829000	2.40365700	0.96458900
C	-3.04825700	3.22748700	-0.22653300
H	1.41351500	2.32916500	1.97399800
C	2.11387900	0.33570700	1.62054000
C	-0.40535800	3.82095600	1.02430500
C	-2.49496700	4.65952600	-0.15879200

H	-3.68831400	3.02482200	0.64389800
H	-3.66940900	3.11941500	-1.12162400
C	3.30081500	0.60891300	2.33771300
C	1.89772100	-0.96856800	1.07000100
C	-1.54997400	4.84546100	1.03404400
H	0.20172000	3.95784300	1.92507300
H	0.24300700	3.96034200	0.15366300
H	-3.32243700	5.37495500	-0.10395600
H	-1.95090400	4.87187600	-1.08741200
C	4.26329000	-0.35919000	2.54308500
H	3.44181500	1.61178200	2.73386000
C	2.90286700	-1.94759900	1.30335900
O	0.83543600	-1.32256500	0.41078400
H	-2.12104300	4.74176600	1.96746100
H	-1.13528900	5.85897600	1.03254000
C	4.04339300	-1.64988000	2.02411000
H	5.16662100	-0.13419000	3.09926600
H	2.73967300	-2.93238300	0.88012100
H	4.78549400	-2.42701200	2.18696200
C	-1.33628000	-2.10940200	2.13549300
C	-0.46721400	-1.73267100	3.25059600
O	-1.52249800	-0.76146400	1.70962700
H	-0.77991600	-2.66188700	1.36492400
H	0.52268800	-1.34990300	3.03489200
H	-0.72709000	-1.88486100	4.29243500
C	-2.64904200	-2.78780600	2.48286000
H	-3.25543100	-2.89325900	1.58152500
H	-2.46445000	-3.78476500	2.89784200
H	-3.20951700	-2.19780900	3.21551400
O	-1.10432700	0.41685800	3.93143500
H	-1.41945100	0.24911600	3.00406900
H	-1.89823900	0.39629900	4.48427000
H	-1.26311100	2.44478700	-1.13624500
H	-1.59326700	2.22946600	1.86173000
S	0.97920100	1.13804400	-2.26882600
O	0.84414100	1.20124300	-3.72874500
O	1.01059900	2.42718300	-1.54033600
O	-0.11685100	0.18378800	-1.73733000
C	2.50599700	0.29355800	-1.89042200
C	2.63856600	-1.05266000	-2.23173800
C	3.55474000	0.98672000	-1.29334400
C	3.83659000	-1.70402800	-1.95973800
H	1.80308500	-1.57868400	-2.67872200
C	4.74953300	0.32069700	-1.02746500
H	3.41949000	2.03074100	-1.03629600
C	4.90560900	-1.03099800	-1.35079300
H	3.94423500	-2.75533600	-2.21332300
H	5.56639300	0.85376400	-0.54912100
C	6.17540600	-1.76167100	-0.99914000
H	6.12776300	-2.13649400	0.03105400
H	6.34112000	-2.62091200	-1.65531600
H	7.04842200	-1.10565700	-1.06602700

III-t (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.333730

Thermal correction to Gibbs Free Energy (a.u.): 0.544139

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.4053724 a.u.

C	-4.08362500	-3.89795100	-1.34547200
C	-5.09665000	-2.93262200	-1.52014300
C	-2.78845400	-3.53150100	-1.03596700
H	-4.32316200	-4.95173000	-1.46003400
C	-4.76683000	-1.59935300	-1.38871100
H	-6.10850600	-3.23267500	-1.76862600
C	-2.42225800	-2.16560100	-0.86546400
H	-2.00527700	-4.27155000	-0.90936600
C	-3.45335500	-1.18773600	-1.05599700

H	-5.52208000	-0.83168800	-1.54376500
O	-1.19309400	-1.89613100	-0.54484600
C	-3.18951100	0.21828200	-0.96358400
Co	-0.58417100	-0.22122200	0.09912000
N	-2.09284800	0.74358300	-0.53884100
H	-3.99586400	0.88102700	-1.27610300
N	-0.06387300	1.42173100	0.91674400
C	-1.82873900	2.18482700	-0.53334600
C	1.07210800	1.64538900	1.48790800
C	-1.09818400	2.46316900	0.78828800
C	-3.03697600	3.10292700	-0.70047100
H	1.27928300	2.65318500	1.84479900
C	2.10230400	0.68066900	1.72296600
C	-0.61884300	3.91362700	0.84581300
C	-2.58006300	4.56804700	-0.63506100
H	-3.76914600	2.88977300	0.09001500
H	-3.52571400	2.91685800	-1.66263000
C	3.28709700	1.11380900	2.36415800
C	1.94628000	-0.69654300	1.36757900
C	-1.81119600	4.86421800	0.65758000
H	-0.14034500	4.12797400	1.80741100
H	0.12877300	4.05873700	0.05810100
H	-3.44782100	5.23043200	-0.72028300
H	-1.93407400	4.77777900	-1.49691800
C	4.30460800	0.23441800	2.66754400
H	3.38090200	2.16797000	2.61398400
C	3.00590100	-1.58103300	1.70088700
O	0.88552200	-1.19009900	0.79265400
H	-2.49145200	4.76346100	1.51428300
H	-1.45703900	5.90033200	0.65831200
C	4.14524300	-1.12566600	2.33329600
H	5.20872900	0.57928300	3.15700400
H	2.88931100	-2.62178200	1.42133900
H	4.93734100	-1.83088800	2.57032600
C	-1.49968500	-1.99402500	2.37076900
C	-1.05472600	-0.79920700	3.09857500
O	-1.63862600	-0.65193500	1.76880400
H	-0.72324000	-2.55167700	1.85587400
H	0.00259500	-0.56483100	3.14230500
H	-1.68596000	-0.37148100	3.87323600
C	-2.80171100	-2.68507700	2.64997800
H	-3.17565500	-3.15820000	1.73776100
H	-2.64631200	-3.46640700	3.40121100
H	-3.55062200	-1.97725200	3.01394000
O	-4.39333600	0.18879800	1.88344500
H	-3.44265500	0.02307400	1.78511700
H	-4.78146700	-0.44378900	1.26508600
H	-1.10931700	2.37106500	-1.33831800
H	-1.82253700	2.28817500	1.59929200
S	1.32146400	1.00009200	-2.10110600
O	1.23224300	1.04571400	-3.56429700
O	1.36767400	2.29313400	-1.38586000
O	0.16514300	0.08241500	-1.60873900
C	2.79018000	0.09010700	-1.65600000
C	2.82829100	-1.28674300	-1.87760300
C	3.89329100	0.76549300	-1.14117500
C	3.99042300	-1.98717300	-1.57159500
H	1.94928100	-1.79448300	-2.25711500
C	5.04929400	0.04935800	-0.84048900
H	3.82981000	1.83330600	-0.96827500
C	5.11343600	-1.33313800	-1.04648600
H	4.02530900	-3.06148400	-1.73192600
H	5.90805100	0.56856600	-0.42454200
C	6.34369800	-2.11039700	-0.65442700
H	6.29210000	-2.40580500	0.40137900
H	6.44803800	-3.02464300	-1.24555800
H	7.25268600	-1.51493500	-0.78057800

III-t (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2343.358967
Thermal correction to Gibbs Free Energy (a.u.): 0.548689
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -3582.4340271 a.u.

C	-4.38511700	-3.35046700	-2.06573800
C	-5.38728300	-2.37180200	-1.90280500
C	-3.06253800	-3.07759400	-1.77824900
H	-4.65583000	-4.33877100	-2.42797400
C	-5.02005300	-1.12024500	-1.45416700
H	-6.42192100	-2.59673000	-2.13703400
C	-2.65526800	-1.80194500	-1.29478000
H	-2.28786600	-3.82559500	-1.90994100
C	-3.67698200	-0.80894400	-1.13553500
H	-5.76996500	-0.34124800	-1.33528600
O	-1.39536000	-1.62278900	-1.03150100
C	-3.37279200	0.52577400	-0.71577300
Co	-0.70319700	-0.17802900	-0.02632200
N	-2.22943600	0.92814000	-0.27647300
H	-4.18284400	1.25231100	-0.79448000
N	-0.08576200	1.21179500	1.13720600
C	-1.90256600	2.32547500	0.01191700
C	1.06286100	1.23085800	1.73005900
C	-1.06770700	2.30131100	1.29989000
C	-3.06431000	3.30917900	0.11848200
H	1.31593500	2.10319600	2.33172600
C	2.05072400	0.19941400	1.69127700
C	-0.50358300	3.69005700	1.60509300
C	-2.51513800	4.71072400	0.42662900
H	-3.75570200	2.99004700	0.91116600
H	-3.62952300	3.33333200	-0.81903100
C	3.23890300	0.39117600	2.43609700
C	1.85811700	-1.01374300	0.95454900
C	-1.64792600	4.71199100	1.69099500
H	0.04452200	3.68880500	2.55314300
H	0.20001000	3.95087200	0.80811400
H	-3.34354800	5.41896100	0.53355500
H	-1.91356200	5.05036900	-0.42553900
C	4.22270100	-0.57287400	2.48824000
H	3.36099300	1.32710300	2.97620900
C	2.88619600	-1.99367400	1.03512500
O	0.80430700	-1.28835800	0.24668500
H	-2.27745400	4.47937800	2.56139800
H	-1.23368400	5.71078000	1.86364200
C	4.02545800	-1.77805300	1.78339100
H	5.12676100	-0.41319600	3.06536600
H	2.74101300	-2.90853100	0.47205300
H	4.78762200	-2.55182700	1.82316900
C	-1.42739400	-2.43302700	1.82586100
C	-0.47883400	-2.52945100	3.02571100
O	-1.60216200	-1.01285500	1.55196400
H	-0.95884700	-2.85645900	0.93764100
H	0.54237300	-2.30400900	2.71986100
H	-0.50274000	-3.53726000	3.45713900
C	-2.80236100	-3.03952600	2.06548800
H	-3.44774300	-2.85946500	1.20380100
H	-2.71695900	-4.12085500	2.21447800
H	-3.28311600	-2.60422600	2.94996200
O	-0.81808400	-1.53012300	3.99970700
H	-1.37134000	-0.56334400	2.38854800
H	-1.61245800	-1.81879000	4.46852200
H	-1.22980100	2.65230000	-0.78756800
H	-1.74439600	2.00196800	2.11803800
S	1.08514400	1.54424500	-1.97805600
O	0.96121300	1.90391600	-3.39479200
O	1.15615400	2.65532900	-1.00362300
O	-0.06304600	0.54728300	-1.66041200
C	2.56771500	0.57305000	-1.77587400

C	2.62777500	-0.69968300	-2.34359200
C	3.65799400	1.10730200	-1.09500000
C	3.79824000	-1.44010000	-2.21702200
H	1.75927800	-1.10435500	-2.84998700
C	4.82338100	0.35330500	-0.97737500
H	3.57751900	2.09521800	-0.65726400
C	4.90860700	-0.92867600	-1.53065900
H	3.85025700	-2.43657600	-2.64757500
H	5.67207700	0.75913700	-0.43422800
C	6.14741800	-1.76492000	-1.33941900
H	6.09659900	-2.31339000	-0.39022400
H	6.26377100	-2.50192700	-2.13910600
H	7.04934900	-1.14648900	-1.30894800

III-m (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.280485

Thermal correction to Gibbs Free Energy (a.u.): 0.540555

Imaginary frequencies: -289.82

Calculation of single point energy based on the optimized structure, Et = -3582.3581384 a.u.

C	-4.06335400	-4.20309800	-1.09345600
C	-5.10799000	-3.28913800	-1.33936200
C	-2.78566800	-3.76855400	-0.80106100
H	-4.26363000	-5.27044600	-1.13909500
C	-4.82965900	-1.93831500	-1.28632300
C	-2.46863900	-2.38192200	-0.73146300
C	-3.53702700	-1.45605100	-0.97636700
H	-5.61466900	-1.21200600	-1.48612500
O	-1.24440700	-2.04848700	-0.45860100
C	-3.32932600	-0.03820400	-0.97263300
Co	-0.69506200	-0.31127700	0.06261000
N	-2.24882100	0.55919300	-0.60405300
H	-4.16403000	0.56967600	-1.32515200
N	-0.19364600	1.40994400	0.72209000
C	-2.02444000	2.00101000	-0.72196500
C	0.93967900	1.70571800	1.25556100
C	-1.26186700	2.40857800	0.54780700
C	-3.25314600	2.87948200	-0.94219900
H	1.12544900	2.74093100	1.53922800
C	2.00488900	0.78667100	1.53951000
C	-0.81832000	3.86983100	0.46581100
C	-2.82270500	4.35183500	-1.02214200
H	-3.96527300	2.73775700	-0.11695100
H	-3.76385600	2.59559200	-1.86825300
C	3.17620900	1.29691700	2.14419700
C	1.89541800	-0.61470300	1.26878000
C	-2.03448200	4.77598200	0.22224500
H	-0.32471400	4.17865500	1.39342900
H	-0.09223400	3.95956100	-0.34949300
H	-3.70356200	4.98988700	-1.15063100
H	-2.19663400	4.49026200	-1.91239200
C	4.22650200	0.47368500	2.49598900
H	3.23445600	2.36695100	2.32945100
C	2.99109100	-1.43853500	1.64428800
O	0.84987000	-1.18103100	0.73987400
H	-2.69512000	4.73825300	1.09959300
H	-1.70359900	5.81526400	0.12404500
C	4.11598300	-0.90800300	2.24339300
H	4.93352000	-1.56966100	2.51715700
H	-1.94591600	2.28124200	1.40124400
H	-1.32971200	2.13535200	-1.55824300
O	-2.90865000	0.61356400	3.55661200
H	-3.85419900	0.41422200	3.54531000
H	-2.57249400	0.33680900	2.66367400
C	-1.32300100	-1.31310500	3.69067600
C	-1.45683700	-1.85293000	2.32845400
O	-1.68415500	-0.62447200	1.67659600

H	-2.08680400	-1.51337200	4.43815400
H	-2.28660600	-2.55772800	2.20129200
H	-0.51901900	-2.31214600	1.97355200
C	-0.16978000	-0.52256600	4.13080000
H	-0.50886200	0.38222700	4.64562500
H	0.35293600	-1.12683500	4.89236800
H	0.52102100	-0.28080100	3.32709300
H	5.11909700	0.88032600	2.95866200
H	2.91031400	-2.49738700	1.42613800
H	-1.97564300	-4.46842700	-0.62412700
H	-6.10609100	-3.64162000	-1.57544700
S	1.09381000	0.83199500	-2.31834000
O	0.98732400	0.75355800	-3.78043000
O	1.08808600	2.18668600	-1.72000200
O	0.01115100	-0.09223300	-1.71588900
C	2.62463300	0.05044500	-1.83228700
C	2.74723700	-1.33381900	-1.95424800
C	3.68772000	0.82587300	-1.37808800
C	3.95204300	-1.93871400	-1.61121700
H	1.89862500	-1.92019100	-2.28681300
C	4.88756200	0.20542000	-1.03790700
H	3.55847000	1.89754700	-1.28244400
C	5.03577400	-1.18166000	-1.14550600
H	4.05215800	-3.01775100	-1.69469900
H	5.71528700	0.80453500	-0.66867800
C	6.31426700	-1.85162500	-0.71166900
H	6.29603000	-2.05462800	0.36684400
H	6.46200200	-2.80716800	-1.22293700
H	7.18590000	-1.22000000	-0.90767200

III-m (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.328107

Thermal correction to Gibbs Free Energy (a.u.): 0.542499

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.3996235 a.u.

C	-3.65769700	-4.59418500	-0.28799900
C	-4.71829700	-3.84126200	-0.83471000
C	-2.45252700	-4.00539900	0.03650900
H	-3.78807100	-5.66055600	-0.12353100
C	-4.52902000	-2.49219000	-1.04484700
C	-2.22861200	-2.61282300	-0.16018700
C	-3.31129000	-1.85017200	-0.71142900
H	-5.32466000	-1.89044700	-1.47912900
O	-1.07082700	-2.12817700	0.17069000
C	-3.19434200	-0.45011100	-0.98127700
Co	-0.63473900	-0.28807100	0.26439200
N	-2.20472500	0.30402100	-0.63943200
H	-4.02668000	0.00429000	-1.52010000
N	-0.26654400	1.56137200	0.53103600
C	-2.08701900	1.71361400	-1.03012200
C	0.87806600	2.04495600	0.88001700
C	-1.40636900	2.41340500	0.15609000
C	-3.38444500	2.42320800	-1.41359000
H	1.00595000	3.12600600	0.87372500
C	2.01336200	1.28753100	1.30818300
C	-1.08825400	3.86902700	-0.18191100
C	-3.09130500	3.89419200	-1.74403700
H	-4.08715200	2.34718800	-0.57424400
H	-3.84233500	1.94190400	-2.28421200
C	3.19559300	1.98761300	1.64233300
C	1.95939600	-0.13385000	1.45583600
C	-2.37569400	4.60203900	-0.58811600
H	-0.64132800	4.37749800	0.67948600
H	-0.35638100	3.88616400	-0.99807100
H	-4.02566300	4.41201400	-1.98540100
H	-2.46231100	3.93986200	-2.64228400
C	4.31133000	1.33081100	2.11719100

H	3.20809600	3.06721400	1.51314300
C	3.11841900	-0.78267600	1.95620000
O	0.90299400	-0.85688700	1.20347700
H	-3.04905800	4.65307900	0.27783700
H	-2.13859100	5.63464100	-0.86512800
C	4.25597500	-0.06829000	2.27560300
H	5.12753500	-0.59940100	2.64884500
H	-2.11756700	2.38118000	0.99397500
H	-1.38145900	1.74623200	-1.86881500
O	-4.19121600	1.08734700	1.80866800
H	-4.99834500	0.70169000	1.44790800
H	-3.49609100	0.44542900	1.59123100
C	-1.61662400	-0.01637100	3.39395300
C	-1.52262500	-1.41075500	2.93691800
O	-1.77013100	-0.35547900	1.96804800
H	-2.57992200	0.31935200	3.77344800
H	-2.36045700	-2.09268700	3.04846800
H	-0.53968300	-1.85448500	2.81206000
C	-0.42766700	0.78717200	3.82563700
H	-0.53582800	1.83058500	3.51872800
H	-0.37176500	0.76258100	4.91933000
H	0.49919700	0.39034300	3.41694400
H	5.21398500	1.87821500	2.36540400
H	3.07902200	-1.86117100	2.05741400
H	-1.63074300	-4.58394100	0.44516600
H	-5.65754500	-4.31773400	-1.09295500
S	1.16851200	0.34611000	-2.26773400
O	1.00672200	-0.03311100	-3.67556000
O	1.15962500	1.79025900	-1.95402400
O	0.10763800	-0.45648500	-1.46202200
C	2.71376000	-0.32617400	-1.68014300
C	2.81503700	-1.69999500	-1.45783200
C	3.81017000	0.51304900	-1.50286100
C	4.03476700	-2.22879600	-1.04843000
H	1.94051200	-2.32872700	-1.57786200
C	5.02367600	-0.03281100	-1.09220800
H	3.69763800	1.57809100	-1.66784300
C	5.15285500	-1.40601400	-0.85588500
H	4.11961200	-3.29632100	-0.86318100
H	5.87863900	0.61924600	-0.93683900
C	6.45128200	-1.97766200	-0.34635300
H	6.49154200	-1.92828900	0.74945500
H	6.56809600	-3.02734600	-0.63053500
H	7.31261300	-1.42151500	-0.72794000

III-m (PO-Co^{III}-OTs + H_2O)

PO-Co^{III}-OTs + H_2O = PG + Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.354911

Thermal correction to Gibbs Free Energy (a.u.): 0.548360

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.431336 a.u.

C	-4.16629000	-3.59956000	-2.18806900
C	-5.21718700	-2.66280900	-2.10092900
C	-2.87547300	-3.26514700	-1.83122900
H	-4.37346800	-4.60413600	-2.54764000
C	-4.93076600	-1.39050100	-1.65299000
C	-2.54967100	-1.96389800	-1.35362200
C	-3.62236800	-1.01554800	-1.26439900
H	-5.71906600	-0.64339200	-1.59047400
O	-1.31275900	-1.72078300	-1.04115400
C	-3.40233300	0.33704700	-0.85222600
Co	-0.73904600	-0.23004700	-0.02878000
N	-2.30371000	0.79949000	-0.35877200
H	-4.23971700	1.02372800	-0.98524600
N	-0.22902000	1.20797000	1.12554200
C	-2.05676200	2.21423300	-0.07649700
C	0.93034000	1.33474200	1.68335100
C	-1.27166800	2.24351100	1.24354100

C	-3.26976200	3.13913500	-0.02567100
H	1.13510200	2.24644000	2.24279500
C	1.99029600	0.37741600	1.65510100
C	-0.79474500	3.66233000	1.55752600
C	-2.80692500	4.56929500	0.29196900
H	-3.97539900	2.78996400	0.74136000
H	-3.79717600	3.12766600	-0.98514500
C	3.18274900	0.68650200	2.35307900
C	1.86210800	-0.88089800	0.98466100
C	-1.99265000	4.62379800	1.58985400
H	-0.28426000	3.69598500	2.52585700
H	-0.07492200	3.95583700	0.78610800
H	-3.67461400	5.23396700	0.35950400
H	-2.19000800	4.93456300	-0.53841900
C	4.23278900	-0.20358200	2.41719200
H	3.25385000	1.65349200	2.84553700
C	2.95919900	-1.78088400	1.07270500
O	0.80449500	-1.26346700	0.33435200
H	-2.64342000	4.36388700	2.43647500
H	-1.63789300	5.64378700	1.77067700
C	4.10219900	-1.45039200	1.77071800
H	4.92071400	-2.16400500	1.81583800
H	-1.96295500	1.91534000	2.03838200
H	-1.37073800	2.56659000	-0.85404300
O	-2.03334800	-1.74254000	4.01834500
H	-2.92336200	-2.11913600	3.97368200
H	-1.82231800	-0.65104800	2.32548900
C	-1.13634200	-2.61081700	3.29541300
C	-1.47021200	-2.50866900	1.80407800
O	-1.69267700	-1.12040200	1.48233900
H	-1.27902300	-3.65331400	3.61205500
H	-2.39171400	-3.05111400	1.56303800
H	-0.66200300	-2.86621200	1.16698200
C	0.27020300	-2.15423500	3.64509000
H	0.43148700	-2.23781100	4.72236500
H	1.01521600	-2.75779800	3.12235300
H	0.42485600	-1.11358800	3.35271800
H	5.14051300	0.04588900	2.95545100
H	2.86370400	-2.72856500	0.55522200
H	-2.06277400	-3.97964900	-1.90874900
H	-6.22577800	-2.93609300	-2.39093000
S	1.04269300	1.54258600	-1.95947200
O	0.89071500	1.91996500	-3.36900700
O	1.09728100	2.64210000	-0.97132000
O	-0.07356900	0.50941500	-1.64396000
C	2.54932800	0.60225200	-1.79071400
C	2.61015200	-0.68438700	-2.32603100
C	3.65696700	1.17642000	-1.17294200
C	3.80019200	-1.39840300	-2.23133400
H	1.72770500	-1.11974700	-2.78015800
C	4.84093000	0.44825000	-1.08659900
H	3.57506000	2.17284000	-0.75517900
C	4.92839000	-0.84696200	-1.60867000
H	3.85335100	-2.40552400	-2.63627900
H	5.70362200	0.88485100	-0.59136800
C	6.19109000	-1.65396100	-1.44817800
H	6.19289900	-2.17728200	-0.48338900
H	6.28813600	-2.41075500	-2.23179000
H	7.08088100	-1.01794200	-1.47366100

IV-t (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.150739

Thermal correction to Gibbs Free Energy (a.u.): 1.011164

Imaginary frequencies: -366.79

Calculation of single point energy based on the optimized structure, Et = -6895.0723022 a.u.

C	0.56740300	-0.53437100	-2.94229600

C	-0.27224100	0.55395200	-2.42007200
O	0.92902400	-0.97858600	-1.63562000
H	-0.04459800	-1.32653800	-3.38647200
H	-1.35389100	0.59803600	-2.52535600
H	0.25461300	1.36953600	-1.93015900
C	1.68971100	-0.16429900	-3.90243700
H	2.33756900	-1.03567700	-4.03384000
H	1.26569900	0.09235500	-4.87896600
H	2.28057200	0.66818700	-3.52969100
O	-1.14085000	-0.31898000	-0.47332300
H	-0.55323900	-1.04756900	-0.78855800
H	-0.48872600	0.22567200	0.09967900
C	-1.14224000	-4.24236200	-3.72041100
C	-0.78329100	-5.08498400	-2.64835000
C	-1.84615300	-3.07295900	-3.50806100
H	-0.87024600	-4.52086100	-4.73512400
C	-1.17379800	-4.72989000	-1.37233400
H	-0.24034400	-6.00660200	-2.82697900
C	-2.21667900	-2.65137900	-2.19670900
H	-2.14293100	-2.43315800	-4.33293800
C	-1.87607500	-3.53007600	-1.11412200
H	-0.94605300	-5.38168200	-0.53182300
O	-2.82306000	-1.51188800	-2.06444700
C	-2.29699100	-3.26671200	0.23314500
Co	-3.05279500	-0.59500300	-0.40335100
N	-2.83369500	-2.17085400	0.64428800
H	-2.15795600	-4.07773900	0.94941300
N	-3.07230900	0.32086500	1.27029100
C	-3.35853300	-1.96666200	1.99618400
C	-2.99997600	1.60244800	1.40417600
C	-2.87219200	-0.57862100	2.42460500
C	-3.01303000	-3.01261200	3.05100600
H	-2.92595300	2.00447400	2.41430600
C	-2.96460300	2.56707600	0.34655300
C	-3.53128600	-0.15260200	3.73749900
C	-3.67639000	-2.61462600	4.37966100
H	-1.92252600	-3.07356700	3.17633500
H	-3.36801500	-4.00202600	2.74278700
C	-2.80892400	3.92719800	0.69926700
C	-3.05709800	2.19481100	-1.03214300
C	-3.25678100	-1.20711100	4.82094700
H	-3.13094200	0.80971800	4.07215700
H	-4.60354600	-0.03528800	3.55803300
H	-3.42211900	-3.34574600	5.15460300
H	-4.76549000	-2.64909200	4.25324100
C	-2.72154200	4.91878300	-0.25660600
H	-2.75403300	4.18084700	1.75545700
C	-2.96819600	3.23724800	-1.99457200
O	-3.21086800	0.97553700	-1.45965400
H	-2.18458900	-1.20712900	5.05253700
H	-3.78123200	-0.93040800	5.74179400
C	-2.79406700	4.55434600	-1.61548100
H	-2.59246700	5.95646600	0.03042900
H	-3.05434800	2.95617500	-3.03869200
H	-2.71760500	5.32149300	-2.38153800
C	-0.09082300	1.20323800	4.11986100
C	0.26432000	-0.01237000	4.72506600
C	0.11987900	1.41221100	2.76393100
H	-0.52768600	1.99589300	4.72070800
C	0.82935000	-1.00912900	3.94735400
H	0.11177600	-0.16340300	5.78776000
C	0.70311900	0.41314100	1.96111100
H	-0.14546800	2.34784400	2.28365800
C	1.05941200	-0.82323900	2.56898800
H	1.12535200	-1.95127200	4.40048700
O	0.82035000	0.64005200	0.65741000
C	1.68568000	-1.89773000	1.83987400
Co	2.22515000	-0.21660200	-0.38913700
N	2.09997200	-1.84711200	0.62062900

H	1.85621900	-2.81823600	2.40336200
N	3.56982900	-1.09587900	-1.36423200
C	2.92705600	-2.93610900	0.06456900
C	4.60784400	-0.49514300	-1.82994400
C	3.32443500	-2.53441100	-1.36545600
C	2.28808900	-4.32378700	0.03801600
H	5.42540300	-1.09558500	-2.22907300
C	4.75837500	0.93370600	-1.86700900
C	4.41984300	-3.46084900	-1.87982900
C	3.31611600	-5.32569100	-0.51657300
H	1.39044600	-4.30047400	-0.59065500
H	1.97713200	-4.62875600	1.04340900
C	6.02515600	1.47260200	-2.17690800
C	3.64665900	1.80859500	-1.63807000
C	3.86704400	-4.89885700	-1.88722200
H	4.72342000	-3.17626300	-2.89384300
H	5.30265100	-3.38461200	-1.23371000
H	2.86415000	-6.32044600	-0.59201500
H	4.14718600	-5.40946500	0.19572100
C	6.22327800	2.83642200	-2.27193300
H	6.85634700	0.78764600	-2.32288000
C	3.86951200	3.19845000	-1.78015000
O	2.43615300	1.38846100	-1.35446500
H	3.06102700	-4.95973300	-2.63054700
H	4.64704600	-5.59612200	-2.21006400
C	5.12551100	3.69469400	-2.08269000
H	7.20673500	3.23815400	-2.48897700
H	3.02456100	3.85864300	-1.61549100
H	5.26606600	4.76939600	-2.16090500
H	3.84324600	-2.95246400	0.66341400
H	2.43240800	-2.66605500	-1.99001700
H	-4.44597400	-1.90576300	1.88860000
H	-1.78577300	-0.64321300	2.57613800
S	4.64738500	-0.08549200	1.65438000
O	4.31469900	-0.25212000	3.07708700
O	5.23809000	-1.26673800	0.98320800
O	3.43556500	0.51153000	0.89706000
C	5.82786800	1.24273600	1.44779500
C	5.39595200	2.56900400	1.43061300
C	7.17544900	0.92730900	1.29049100
C	6.32973300	3.58212400	1.24253400
H	4.34019300	2.79144600	1.52626400
C	8.09865700	1.95538800	1.10769800
H	7.48412700	-0.11180100	1.29220700
C	7.69057100	3.29336100	1.07248900
H	5.99524500	4.61546000	1.20855700
H	9.15036500	1.71398700	0.97833900
C	8.68009000	4.40036800	0.80947800
H	8.63941800	4.71638500	-0.24057000
H	8.46654000	5.28275500	1.42056700
H	9.70493700	4.08119800	1.01767200
S	-6.12823500	-0.36449800	0.19089200
O	-7.31859200	-1.07993900	-0.27988100
O	-5.93195100	-0.25946800	1.65377400
O	-4.90280900	-1.00315700	-0.51955600
C	-6.20078300	1.30468200	-0.43695600
C	-6.23225400	1.51115000	-1.81693900
C	-6.25411000	2.37692600	0.44805300
C	-6.29963900	2.81099200	-2.30336100
H	-6.17905900	0.66329200	-2.48979600
C	-6.32596500	3.67527500	-0.05533500
H	-6.23413200	2.18302500	1.51407100
C	-6.34045100	3.91127000	-1.43280700
H	-6.31179000	2.98142900	-3.37653200
H	-6.35710600	4.51659200	0.63127600
C	-6.34715100	5.31711200	-1.97326100
H	-6.84341500	6.00908600	-1.28673600
H	-5.31937500	5.67389300	-2.11300400
H	-6.85148600	5.37382400	-2.94238000

IV-t (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.205904

Thermal correction to Gibbs Free Energy (a.u.): 1.013272

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6895.1290144 a.u.

C	0.75532700	-0.42825500	-3.28498400
C	0.14875900	0.69432000	-2.56212200
O	0.77051700	-0.40948100	-1.80593000
H	0.08186500	-1.21817000	-3.60816600
H	-0.92743900	0.73656700	-2.41481100
H	0.72236800	1.61055200	-2.46666900
C	2.04519300	-0.31736800	-4.04226000
H	2.59358800	-1.26274800	-4.03341500
H	1.80116400	-0.08387500	-5.08469900
H	2.67526800	0.47210400	-3.63840200
O	-1.07778100	-0.74290400	0.04781200
H	-0.65525000	-1.08658100	-0.75988000
H	-0.60037300	0.11480800	0.16179400
C	-1.21220200	-4.50428100	-3.42984300
C	-1.25898600	-5.43365700	-2.37198000
C	-1.68720100	-3.21575800	-3.27122300
H	-0.81113900	-4.80758200	-4.39343500
C	-1.81000600	-5.03458000	-1.16910700
H	-0.89431800	-6.44576500	-2.50765700
C	-2.21895800	-2.76077100	-2.02952500
H	-1.69312600	-2.51170500	-4.09717200
C	-2.28379600	-3.71891300	-0.96446200
H	-1.87960100	-5.73892000	-0.34315000
O	-2.59737400	-1.52044100	-1.93657700
C	-2.84531600	-3.39680300	0.31956200
Co	-2.97945300	-0.61646700	-0.29168100
N	-3.20497100	-2.22480900	0.70734200
H	-2.97082900	-4.23355300	1.00796000
N	-3.10433100	0.27529500	1.38666700
C	-3.81752300	-1.94411800	2.00894700
C	-2.97962200	1.54534200	1.57371600
C	-3.12988200	-0.67009400	2.51686700
C	-3.76326800	-3.05543500	3.05325600
H	-3.01463500	1.91594300	2.59628800
C	-2.74875500	2.53268400	0.56468800
C	-3.78380900	-0.16634500	3.80304000
C	-4.41591900	-2.56620200	4.35545300
H	-2.71810300	-3.34005500	3.24151200
H	-4.28624500	-3.94713900	2.69114300
C	-2.59850600	3.87649800	0.97588500
C	-2.60594200	2.18857000	-0.81391200
C	-3.76109900	-1.27653900	4.86356500
H	-3.24258200	0.70214500	4.19082500
H	-4.80926400	0.14014300	3.57180300
H	-4.35527400	-3.35069900	5.11730700
H	-5.48166100	-2.38286000	4.17072900
C	-2.30038400	4.87924100	0.07656400
H	-2.71486900	4.10537400	2.03247800
C	-2.31128200	3.24230400	-1.72081900
O	-2.71251000	0.97854400	-1.28635500
H	-2.71807900	-1.48274600	5.14191300
H	-4.26516600	-0.92935400	5.77159500
C	-2.14919300	4.54204700	-1.28333800
H	-2.17921300	5.90476400	0.40755600
H	-2.22453700	2.98688600	-2.77113300
H	-1.90645600	5.31801300	-2.00443500
C	-0.16272800	2.14721800	3.73191000
C	-0.05788000	0.95510000	4.46932400
C	0.18768700	2.19620900	2.39068600
H	-0.52119600	3.04980100	4.21973500
C	0.41572300	-0.18176900	3.83737500

H	-0.32477800	0.93134300	5.52013300
C	0.65825400	1.04552500	1.72601000
H	0.08704000	3.10553900	1.80994800
C	0.78012100	-0.16318800	2.47545900
H	0.52623900	-1.11002600	4.39170200
O	0.86133700	1.09985600	0.41915500
C	1.23919100	-1.38560300	1.87586300
Co	2.19796600	-0.00503000	-0.41083700
N	1.69182700	-1.51127000	0.67310200
H	1.20771400	-2.27524600	2.50870500
N	3.34921400	-1.22422100	-1.27430900
C	2.26398100	-2.78912000	0.21398600
C	4.52251900	-0.90995800	-1.70192300
C	2.77326000	-2.56395700	-1.21871000
C	1.30670900	-3.98008500	0.22216500
H	5.19794200	-1.70483100	-2.01954700
C	4.99322700	0.44230500	-1.80377800
C	3.61402900	-3.75180500	-1.67133500
C	2.05207100	-5.22825200	-0.27898800
H	0.44640200	-3.76498200	-0.42008700
H	0.91708700	-4.15655300	1.23071700
C	6.36297400	0.66716700	-2.06141600
C	4.09348200	1.55452900	-1.69591800
C	2.71570500	-5.00404800	-1.64765600
H	4.00095400	-3.58973600	-2.68415500
H	4.47424400	-3.87423700	-1.00233300
H	1.35503200	-6.07005100	-0.34296300
H	2.82036000	-5.50320400	0.45540900
C	6.86428500	1.94388800	-2.21943700
H	7.02637100	-0.19214700	-2.11533300
C	4.62887400	2.84844400	-1.90306600
O	2.80800300	1.43424600	-1.46565300
H	1.92954200	-4.88856200	-2.40537600
H	3.29989700	-5.88621400	-1.92930200
C	5.97705200	3.03387500	-2.15084200
H	7.92227100	2.10447600	-2.39429100
H	3.94486800	3.68721800	-1.83068300
H	6.35842000	4.04316500	-2.28008100
H	3.13518100	-2.99016700	0.84527000
H	1.88615200	-2.52399400	-1.86543400
H	-4.86082100	-1.68104700	1.80595300
H	-2.07938800	-0.92013100	2.72481100
S	4.46910700	-0.25622800	1.75019200
O	4.04506300	-0.26183400	3.15696300
O	4.82537800	-1.56978200	1.16870600
O	3.43898900	0.53889700	0.89631300
C	5.90614400	0.78841500	1.54415200
C	5.76220200	2.17184100	1.43968100
C	7.16378400	0.19231300	1.48382100
C	6.89589900	2.95723600	1.26088700
H	4.77332300	2.61325000	1.46302500
C	8.28942100	0.99511500	1.30934300
H	7.24786300	-0.88616400	1.55328200
C	8.17266900	2.38419100	1.18687400
H	6.78735100	4.03366800	1.15969700
H	9.27227600	0.53456700	1.25545100
C	9.38391000	3.24539300	0.93237900
H	9.46933000	3.48967600	-0.13400000
H	9.32401100	4.19267300	1.47691500
H	10.30654400	2.73904300	1.22880200
S	-6.04754700	0.05106000	-0.13349600
O	-7.25793300	-0.55874500	-0.69492700
O	-5.98345800	0.19733300	1.33822100
O	-4.83240200	-0.72606200	-0.70669800
C	-5.87540800	1.68707200	-0.82522500
C	-5.65754000	1.82305000	-2.19676000
C	-5.98454800	2.80463300	-0.00351100
C	-5.53641500	3.09766600	-2.73794100
H	-5.55933200	0.93913300	-2.81606300

C	-5.86268100	4.07602900	-0.56118600
H	-6.15174500	2.66593000	1.05818000
C	-5.63037100	4.24061300	-1.93014000
H	-5.35480400	3.21251800	-3.80325100
H	-5.93298300	4.95165700	0.07790400
C	-5.42849900	5.61415600	-2.51453100
H	-6.01647400	6.36787500	-1.98258800
H	-4.37427200	5.90787700	-2.43774900
H	-5.70475700	5.64696000	-3.57238100

IV-t (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.255258

Thermal correction to Gibbs Free Energy (a.u.): 1.017265

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6895.1776404 a.u.

C	0.20885200	-2.14645600	0.53320700
C	0.53205300	-1.23454400	1.72357500
O	-0.53217700	-1.42188200	-0.48681900
H	1.14580000	-2.41116300	0.04326500
H	1.35790100	-1.66196800	2.29461700
H	-0.34584500	-1.11446700	2.35792500
C	-0.54079900	-3.39908100	0.94669100
H	-0.74382300	-4.02209200	0.07136000
H	0.07981300	-3.97989200	1.63695400
H	-1.48207500	-3.15591900	1.43867000
O	0.93845000	0.08779800	1.31886800
H	0.14160300	-0.81586500	-0.91749300
H	0.13835800	0.56118800	0.92791000
C	0.69426900	1.29528500	-4.61298000
C	0.84625000	2.68271700	-4.45675400
C	0.93579700	0.42790500	-3.55934100
H	0.39667600	0.89029500	-5.57653300
C	1.24723700	3.17318400	-3.22713300
H	0.66391100	3.35557700	-5.28730300
C	1.33167300	0.90887000	-2.29374700
H	0.83798500	-0.64492300	-3.67751600
C	1.49472800	2.31478700	-2.13602000
H	1.36862600	4.24208900	-3.07955300
O	1.49139700	0.04543400	-1.31161200
C	1.90849200	2.90915900	-0.89813600
Co	2.57644000	0.39809600	0.23940400
N	2.24766100	2.28510900	0.17874400
H	1.96734500	3.99761400	-0.90102800
N	3.42549000	0.72511200	1.90633100
C	2.94389000	3.00294800	1.26430500
C	4.11244900	-0.12610600	2.58841200
C	3.04259300	2.03889800	2.44651500
C	2.32762200	4.33021700	1.71010500
H	4.52726200	0.19705700	3.54249300
C	4.37002800	-1.48666000	2.22796700
C	3.94830200	2.62512900	3.53063900
C	3.21042800	4.95315900	2.80171000
H	1.31560300	4.15338600	2.09333000
H	2.23508700	5.02391400	0.86918900
C	5.16184900	-2.27270800	3.09630100
C	3.80423500	-2.07030300	1.05192600
C	3.40675700	3.99183000	3.98029500
H	3.99837900	1.96166800	4.40008800
H	4.96145100	2.71966700	3.12301900
H	2.76739300	5.89229300	3.14976000
H	4.18770300	5.20347900	2.36953800
C	5.40669300	-3.60587300	2.84065600
H	5.58005100	-1.79917500	3.98153400
C	4.07413600	-3.44451200	0.81215100
O	3.03706700	-1.43627300	0.21365200
H	2.44390400	3.84403000	4.48801700
H	4.08572400	4.43079700	4.71877800

C	4.84517200	-4.18580900	1.68554600
H	6.01466400	-4.19829600	3.51544200
H	3.65729200	-3.88367800	-0.08745000
H	5.02312600	-5.23674500	1.47335500
C	-1.07974300	4.63954200	-0.27655500
C	-1.49738600	4.75908700	-1.61180700
C	-1.01022200	3.40011500	0.34030900
H	-0.81797600	5.52982100	0.28903300
C	-1.84115900	3.61354900	-2.30705700
H	-1.56110800	5.73247600	-2.08538400
C	-1.34861200	2.22084400	-0.35373800
H	-0.70160400	3.29988600	1.37459200
C	-1.77613600	2.33988600	-1.70767100
H	-2.16809300	3.68005600	-3.34026200
O	-1.22245100	1.06305700	0.26561000
C	-2.13325400	1.20435700	-2.51034400
Co	-2.25262500	-0.46846200	-0.23572400
N	-2.23619300	-0.01342000	-2.09494600
H	-2.35688000	1.41274300	-3.55760700
N	-3.17715000	-2.02217200	-0.77715600
C	-2.82024800	-1.05851700	-2.95838600
C	-4.10831800	-2.57370700	-0.07930300
C	-2.83102800	-2.36797200	-2.15302100
C	-2.14652500	-1.29641000	-4.30941700
H	-4.71841000	-3.34972700	-0.54068600
C	-4.40024000	-2.23757700	1.28494100
C	-3.69314300	-3.40595600	-2.86522000
C	-2.95653900	-2.35437600	-5.07731800
H	-1.11829600	-1.64214200	-4.15348800
H	-2.08912700	-0.36906700	-4.88799800
C	-5.57933200	-2.74407700	1.87243000
C	-3.50074600	-1.43823100	2.06090300
C	-3.11637000	-3.65302000	-4.27102000
H	-3.71046600	-4.34631200	-2.30263600
H	-4.72361000	-3.03666500	-2.93061600
H	-2.47718700	-2.56874800	-6.03839400
H	-3.94927800	-1.94405300	-5.30306500
C	-5.88961900	-2.49205600	3.19441800
H	-6.25501100	-3.32870600	1.25332500
C	-3.82290000	-1.23126000	3.42442000
O	-2.38814500	-0.93334200	1.59233800
H	-2.13475700	-4.13495200	-4.16921200
H	-3.75516800	-4.35655400	-4.81504900
C	-4.98816200	-1.73954100	3.96940700
H	-6.80947000	-2.86827300	3.62816700
H	-3.13606400	-0.63367300	4.01450200
H	-5.21661400	-1.54001900	5.01299000
H	-3.86498100	-0.77203600	-3.11521000
H	-1.79694600	-2.73294000	-2.10692200
H	3.96720100	3.17208000	0.90852800
H	2.02865200	1.90472500	2.85091300
S	-5.14842600	0.71012400	-0.75896500
O	-5.21065800	2.03904000	-1.38387500
O	-5.44054400	-0.44047700	-1.64501000
O	-3.82352600	0.56316900	0.03232600
C	-6.32513900	0.60400000	0.58507500
C	-6.00479800	1.11153500	1.84384200
C	-7.55680600	-0.00387700	0.35137400
C	-6.92941700	0.99377400	2.87622000
H	-5.03141200	1.55604700	2.01144600
C	-8.47331800	-0.10934100	1.39562400
H	-7.77646100	-0.40433300	-0.63165700
C	-8.17124400	0.37783100	2.67229700
H	-6.67597000	1.36961800	3.86382400
H	-9.43253900	-0.58910700	1.21989900
C	-9.13549400	0.20096400	3.81802700
H	-8.86248000	-0.67267400	4.42338800
H	-9.13166100	1.06954400	4.48361800
H	-10.15824200	0.04771400	3.46268900

S	5.50661400	1.10377200	-0.69018500
O	6.01177800	1.78386000	-1.88781200
O	5.74377700	1.75785000	0.61480900
O	4.00792500	0.78567700	-0.94230200
C	6.24257800	-0.51987000	-0.60946800
C	5.95018500	-1.44286800	-1.61407100
C	7.09643300	-0.84862400	0.43873000
C	6.51602100	-2.71144800	-1.55192600
H	5.27143300	-1.17094800	-2.41409200
C	7.65596800	-2.12353800	0.48659300
H	7.30011800	-0.11219700	1.20710800
C	7.36914700	-3.07294000	-0.49979800
H	6.28472300	-3.43992400	-2.32447100
H	8.31073900	-2.39095900	1.31106600
C	7.92122600	-4.47125100	-0.39997900
H	8.92621400	-4.47703100	0.03246600
H	7.28462400	-5.08713400	0.24755700
H	7.96620500	-4.95797400	-1.37829900

IV-m (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.154924

Thermal correction to Gibbs Free Energy (a.u.): 1.011764

Imaginary frequencies: -254.30

Calculation of single point energy based on the optimized structure, Et = -6895.0817176 a.u.

N	2.28981000	-1.60597600	0.61426000
N	3.35330800	0.73827600	0.81877000
C	1.86590500	-2.78359000	0.30312300
H	1.80426600	-3.52906700	1.09666800
C	3.57249300	2.01042500	0.83064200
H	3.93673100	2.45940200	1.75395800
C	1.43828900	-3.21577400	-0.99452000
C	1.06030600	-4.56967700	-1.14804400
C	1.33453000	-2.31746000	-2.10490800
C	0.57239300	-5.05766600	-2.34396900
H	1.16735900	-5.23273600	-0.29249600
C	0.81834100	-2.84415200	-3.32064400
C	0.45094400	-4.17144300	-3.43345800
H	0.29435900	-6.10063400	-2.44654400
H	0.75135800	-2.16707300	-4.16573200
H	0.07537300	-4.53979600	-4.38437800
C	3.40862700	2.90603000	-0.27525600
C	3.66080000	4.27863000	-0.05541400
C	3.09286300	2.44026600	-1.59113100
C	3.60489600	5.20175500	-1.08141300
H	3.91496600	4.59872700	0.95225900
C	3.05114300	3.41122100	-2.63070500
C	3.29946100	4.74801800	-2.37977400
H	3.79801200	6.25228700	-0.89444800
H	2.83737100	3.05575200	-3.63374500
H	3.26243300	5.45835400	-3.20140300
O	1.64816700	-1.05799600	-2.06396600
O	2.85983800	1.19908900	-1.90012300
H	1.67751400	-0.83801900	2.43348000
C	2.60378100	-1.23913900	2.00463100
C	3.12427000	-2.39131900	2.88511900
C	3.63756700	-0.11109100	1.97801800
C	4.03623200	-1.85910700	4.01457700
H	2.27441800	-2.93239800	3.31235500
H	3.69931600	-3.07759100	2.25803100
C	3.69669800	0.58293200	3.34230000
H	4.59875200	-0.58179900	1.76551900
C	3.60574100	-0.46312000	4.48355900
H	4.02569000	-2.55964900	4.85533900
H	5.06978900	-1.82436000	3.65272400
H	2.87027200	1.29875900	3.43158500
H	4.63147200	1.14861200	3.41904600

H	2.57286900	-0.51743500	4.83972200
H	4.21555200	-0.13998100	5.33289900
Co	2.58802500	-0.21562900	-0.64555400
H	0.13339600	-0.01301800	-0.64763500
O	-1.10799100	-0.37426600	-1.31143100
C	-1.17345100	0.33555200	-2.53297000
C	-0.18275800	1.42825500	-2.27964100
H	-2.17289600	0.73181500	-2.73459200
H	-0.84857500	-0.31085600	-3.35469200
H	0.86098100	1.23906200	-2.53999000
C	-0.57112300	2.70603000	-1.71188800
H	-1.26272600	2.52791500	-0.86990800
H	-1.22305000	3.19830900	-2.45707200
H	0.27441400	3.34220000	-1.45761400
O	0.87187000	0.59919800	-0.26230100
H	0.47975800	0.82764400	0.60671200
N	-1.91600000	-2.07658900	0.47289000
N	-3.65973000	-1.07082400	-1.16654700
C	-1.35316800	-2.43818900	1.57085800
H	-1.17213900	-3.50039400	1.73747800
C	-4.53648100	-0.42995600	-1.86054700
H	-5.22858500	-1.01027000	-2.47100900
C	-0.93768600	-1.55264100	2.62625100
C	-0.52327500	-2.12084900	3.84860600
C	-0.89974400	-0.13570800	2.45281400
C	-0.09568700	-1.33466500	4.90399400
H	-0.55994100	-3.20230400	3.95553500
C	-0.44490300	0.64716400	3.54129400
C	-0.06193800	0.06089200	4.73700300
H	0.20300800	-1.78525000	5.84380600
H	-0.42576000	1.72412600	3.40916400
H	0.26524200	0.69238400	5.55830200
C	-4.69500200	0.99524200	-1.92295200
C	-5.68724000	1.51571200	-2.78360200
C	-3.88143500	1.88531300	-1.15494600
C	-5.88488200	2.87550300	-2.92152800
H	-6.30275300	0.81470300	-3.34219700
C	-4.09586700	3.27808000	-1.32616500
C	-5.06918800	3.75403500	-2.18477200
H	-6.65178000	3.25964300	-3.58490600
H	-3.49477700	3.95334400	-0.72774100
H	-5.21188100	4.82695200	-2.28178400
O	-1.18786600	0.46505000	1.32128300
O	-2.94634500	1.49728000	-0.33171900
H	-1.55416700	-2.89200900	-1.37394600
C	-2.30459400	-3.01196500	-0.58428800
C	-2.40526200	-4.48642900	-0.17027000
C	-3.65991400	-2.53989400	-1.12332700
C	-3.25995100	-5.29422000	-1.18073100
H	-1.40030900	-4.90938200	-0.10390700
H	-2.86368900	-4.55010500	0.82279800
C	-3.95678000	-3.22263800	-2.47414000
H	-4.42657700	-2.80010400	-0.38387400
C	-3.30193400	-4.61912000	-2.55614000
H	-2.86541600	-6.31099900	-1.26806600
H	-4.28349600	-5.38983600	-0.80010700
H	-3.57807800	-2.59143400	-3.28633500
H	-5.03988800	-3.30938000	-2.60806200
H	-2.27996300	-4.52514500	-2.93746800
H	-3.84831300	-5.24142800	-3.27176400
Co	-2.45670800	-0.29076100	0.07019500
S	-5.16956500	-0.47708100	1.73235800
O	-5.45702300	-0.84005300	3.12432300
O	-3.62871000	-0.43582800	1.57801200
O	-5.83471600	-1.26862600	0.67558100
C	-5.65155400	1.22534200	1.48250900
C	-6.76902600	1.52139000	0.70638100
C	-4.91253000	2.24006800	2.09026700
C	-7.14710900	2.85081900	0.53361700

H	-7.31752000	0.71317500	0.23730800
C	-5.30129800	3.56325300	1.90721800
H	-4.03249100	1.98840400	2.67062500
C	-6.41775400	3.88846600	1.12432300
H	-8.00979000	3.08689100	-0.08303100
H	-4.72463800	4.36010100	2.36987600
C	-6.79128900	5.32698400	0.87384800
H	-6.33697100	5.68631100	-0.05849400
H	-7.87383500	5.44971700	0.77438000
H	-6.44548600	5.97974900	1.68038700
S	5.52765600	-1.39408500	-0.75636300
O	4.11984600	-1.11302200	-1.33564500
O	5.47528000	-2.04142000	0.57438800
O	6.31621500	-2.05799100	-1.79664500
C	6.18892300	0.25241100	-0.50377700
C	6.06637700	1.18799900	-1.53394800
C	6.78158400	0.60122300	0.70602600
C	6.50623400	2.48948400	-1.32762900
H	5.58232700	0.90285100	-2.46039600
C	7.21168800	1.91548900	0.90206000
H	6.88620200	-0.14695500	1.48374300
C	7.07106000	2.87810600	-0.10365600
H	6.37345800	3.22859300	-2.11256000
H	7.66208200	2.19617900	1.85071700
C	7.49021700	4.30981900	0.11473200
H	7.86769000	4.46835900	1.12849000
H	8.27833700	4.60490100	-0.58706800
H	6.64422900	4.98723100	-0.04657300

IV-m (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.191770

Thermal correction to Gibbs Free Energy (a.u.): 1.015944

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6895.1180819 a.u.

N	-2.48927600	1.71286300	0.63224900
N	-3.48469300	-0.66169700	0.87499500
C	-2.18417800	2.91483500	0.28064700
H	-2.18775800	3.69107900	1.04638700
C	-3.63578500	-1.94397700	0.91038500
H	-3.98032100	-2.39442500	1.84061200
C	-1.81844300	3.33971700	-1.04203700
C	-1.61250700	4.72006200	-1.26526800
C	-1.60204000	2.40907800	-2.10710300
C	-1.21752900	5.20395600	-2.49860500
H	-1.77901400	5.40689700	-0.43879600
C	-1.19755000	2.93202800	-3.36297400
C	-1.01677100	4.29045600	-3.55135400
H	-1.07448300	6.26719500	-2.65560900
H	-1.05487800	2.22338200	-4.17186700
H	-0.71915400	4.65660300	-4.53021500
C	-3.40812200	-2.84985500	-0.17328500
C	-3.56449200	-4.23217400	0.07692100
C	-3.10674800	-2.39042700	-1.49666400
C	-3.42684900	-5.17224800	-0.92483600
H	-3.80448300	-4.54621200	1.09022700
C	-2.98487500	-3.38204100	-2.51223200
C	-3.13887300	-4.72596500	-2.23119400
H	-3.54429400	-6.22972000	-0.71516100
H	-2.77712400	-3.03425500	-3.51907000
H	-3.03813200	-5.45109000	-3.03466500
O	-1.70472400	1.11599200	-1.97521000
O	-2.96038500	-1.14699900	-1.83158100
H	-1.83982100	0.98306100	2.44702200
C	-2.78180600	1.35447900	2.02681000
C	-3.32671700	2.49620800	2.90280200
C	-3.78107000	0.19181400	2.02721700
C	-4.15471300	1.93885400	4.08496800

H	-2.49173000	3.09545100	3.27817900
H	-3.96740100	3.13249400	2.28680100
C	-3.77983800	-0.49108900	3.40049000
H	-4.76224600	0.62756700	1.83218000
C	-3.65021800	0.56077500	4.53118700
H	-4.12337200	2.64370500	4.92162800
H	-5.20543600	1.86291500	3.78330800
H	-2.94407700	-1.19871100	3.46107100
H	-4.70490300	-1.06548300	3.51928100
H	-2.59859100	0.64900300	4.82214600
H	-4.19371400	0.22147500	5.41848900
Co	-2.72263100	0.27957700	-0.59679100
H	-0.49373200	-0.17813900	-0.93006200
O	1.28209900	-1.19116600	-1.40826400
C	1.77264800	-2.18437700	-2.34745400
C	0.51104900	-2.44200100	-1.64240000
H	2.66929800	-2.69756600	-2.01809400
H	1.76882500	-1.83549700	-3.37681200
H	-0.40770900	-2.19830900	-2.16819700
C	0.37645000	-3.43140500	-0.52616100
H	1.31422000	-3.54755500	0.01655000
H	0.06177700	-4.38802700	-0.95718000
H	-0.40488500	-3.10449900	0.16064700
O	-1.01950400	-0.56610900	-0.21172000
H	-0.39782500	-0.65052200	0.56283300
N	1.64921000	1.27552100	-0.14888700
N	3.64888100	0.01786000	-1.20893300
C	1.08802700	1.97850000	0.77145100
H	0.84473900	3.01792500	0.55970400
C	4.69533700	-0.67346800	-1.52782100
H	5.35960400	-0.26865100	-2.29301000
C	0.76382600	1.48220300	2.08446100
C	0.42774700	2.40027300	3.09623100
C	0.75975900	0.08476800	2.36154600
C	0.10772300	1.96780500	4.37345800
H	0.44328300	3.46182300	2.86402400
C	0.40993600	-0.33707100	3.65679700
C	0.10178100	0.59069000	4.64442000
H	-0.12807600	2.68258700	5.15389100
H	0.41200000	-1.40238900	3.85933100
H	-0.14067400	0.24173800	5.64403900
C	5.07763500	-1.92994900	-0.96574200
C	6.28463900	-2.51849300	-1.41156300
C	4.28000500	-2.59540000	0.02245500
C	6.72921700	-3.72288500	-0.90870700
H	6.87019600	-1.98680500	-2.15684500
C	4.77350200	-3.82596700	0.53541400
C	5.95896900	-4.36868000	0.08045700
H	7.65420900	-4.16463800	-1.26267000
H	4.17700500	-4.32121300	1.29400700
H	6.30231000	-5.31311100	0.49401000
O	0.98561800	-0.82258800	1.41519600
O	3.12373800	-2.17174800	0.44347300
H	1.27213500	1.30915300	-2.15870600
C	1.97819400	1.79518300	-1.47422500
C	1.91209900	3.31368400	-1.65477400
C	3.39772900	1.33073100	-1.82845100
C	2.61576200	3.72541400	-2.97660400
H	0.87451800	3.64590500	-1.66130400
H	2.41940800	3.78338400	-0.80652400
C	3.57219500	1.38609000	-3.35792500
H	4.08292700	2.02839500	-1.34061500
C	2.74350600	2.55000700	-3.95759800
H	2.05832100	4.54109700	-3.44530700
H	3.61619800	4.11528100	-2.75550700
H	3.25224800	0.43314400	-3.79579200
H	4.63149000	1.51399600	-3.60481100
H	1.73908900	2.19495500	-4.21294200
H	3.20008900	2.88337500	-4.89458000

Co	2.40137700	-0.45566500	0.14902300
S	4.41737600	1.33079800	1.76261400
O	4.52101600	1.62946200	3.19250700
O	3.40115000	0.15968000	1.61623700
O	4.14299600	2.45201800	0.84099400
C	5.95035500	0.58028700	1.23500900
C	6.72880500	1.18609000	0.25499200
C	6.34670200	-0.62346000	1.82385600
C	7.91404000	0.56886800	-0.15159900
H	6.40460800	2.12657200	-0.17620300
C	7.53145800	-1.22031300	1.41495300
H	5.71868700	-1.08752100	2.57559800
C	8.33058900	-0.63776200	0.41869200
H	8.52530100	1.03554700	-0.91959300
H	7.83207600	-2.16703900	1.85356700
C	9.59386400	-1.32319000	-0.03402400
H	9.36624500	-2.30974000	-0.45338000
H	10.11676600	-0.74095200	-0.79722500
H	10.28338800	-1.47962700	0.80255100
S	-5.65785200	1.41534000	-0.76493100
O	-4.24440900	1.14674800	-1.33785800
O	-5.61549600	2.08698600	0.55402500
O	-6.45615000	2.04943300	-1.81675500
C	-6.28694400	-0.23817900	-0.48021100
C	-6.11021900	-1.20150600	-1.47606000
C	-6.89629200	-0.56652800	0.72705800
C	-6.50686700	-2.51060300	-1.23406700
H	-5.61006000	-0.93171000	-2.39825200
C	-7.28389700	-1.88808900	0.95871000
H	-7.04167000	0.20228600	1.47765300
C	-7.08260100	-2.87866700	-0.00890600
H	-6.32741900	-3.27063900	-1.98922100
H	-7.74452400	-2.15344100	1.90691100
C	-7.44169900	-4.31926600	0.25364300
H	-7.85201300	-4.45534200	1.25791300
H	-8.18444000	-4.68238700	-0.46549300
H	-6.55738300	-4.95905000	0.15450100

IV-m (PO-Co^{III}-OTs + H_2O-Co^{III}-OTs)

PO-Co^{III}-OTs + H_2O-Co^{III}-OTs = PG + 2Co^{III}(salen)-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4417.244182

Thermal correction to Gibbs Free Energy (a.u.): 1.020760

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6895.1710249 a.u.

N	2.11847600	-1.20720200	1.36468500
N	3.42918600	1.00701900	1.05739100
C	1.84002200	-2.45626800	1.24637500
H	1.83995200	-3.08105700	2.13783200
C	4.05001200	2.09028400	0.72576500
H	4.63664400	2.59733600	1.49281700
C	1.53013700	-3.10909100	-0.00203600
C	1.50810600	-4.51551300	-0.03613100
C	1.21767400	-2.36742800	-1.17686300
C	1.22506000	-5.20179400	-1.20674500
H	1.73492000	-5.06021700	0.87639500
C	0.95423100	-3.08086400	-2.36207000
C	0.96262300	-4.46934100	-2.37504100
H	1.23153200	-6.28594500	-1.22589600
H	0.76984600	-2.50875400	-3.26498300
H	0.77218600	-4.99362300	-3.30739800
C	4.06586300	2.69313800	-0.57059500
C	4.85998100	3.84823500	-0.75495700
C	3.33178100	2.14761200	-1.67255500
C	4.96005200	4.46911800	-1.98276800
H	5.41165500	4.23329300	0.09881300
C	3.46332800	2.80114400	-2.92858500
C	4.25308000	3.92470400	-3.07436200
H	5.57059100	5.35666800	-2.10811600

H	2.91818400	2.37906500	-3.76622100
H	4.32797000	4.39717200	-4.05018800
O	1.12752100	-1.04829800	-1.17922600
O	2.53384200	1.12394500	-1.59234200
H	1.50387300	0.00473500	2.89206500
C	2.41196400	-0.55571700	2.63972700
C	2.79138800	-1.47362200	3.80667000
C	3.54374300	0.45579200	2.41496900
C	3.48186300	-0.65630700	4.93035300
H	1.89443500	-1.96892100	4.18700500
H	3.47640600	-2.24264700	3.43743800
C	3.52629300	1.49008300	3.55464800
H	4.47669500	-0.11285000	2.42865200
C	3.08781200	0.82750800	4.88432200
H	3.23455300	-1.08345500	5.90689700
H	4.56987400	-0.73785800	4.82551600
H	2.84006100	2.30425200	3.29475600
H	4.52294600	1.92893900	3.67012500
H	2.00048200	0.91265200	4.99710100
H	3.52617900	1.36637200	5.72983000
Co	2.33901000	-0.02583200	-0.10656300
H	-0.20748300	-0.22364900	-1.31278100
O	-0.98567900	0.41803100	-1.33587300
C	-0.46630000	1.76004300	-1.37556000
C	0.29506000	2.18788900	-0.09297900
H	-1.30615900	2.42520600	-1.57109800
H	0.22893800	1.78448400	-2.21648500
H	1.17255500	2.74942100	-0.41287400
C	-0.48453600	3.02236100	0.91360200
H	-1.31981600	2.45877900	1.32738200
H	-0.88386500	3.91520700	0.42210900
H	0.18784900	3.34132900	1.71599800
O	0.81018800	1.02298000	0.58689000
H	0.01417400	0.47276700	0.88042800
N	-2.03770400	-2.04024600	-0.64654400
N	-3.54349500	-0.29489200	-1.84230200
C	-1.62557400	-2.88655100	0.23113500
H	-1.48640800	-3.92484300	-0.06646400
C	-4.22789500	0.68454300	-2.32869500
H	-4.79428700	0.50601200	-3.24288900
C	-1.33546700	-2.58125600	1.60989900
C	-1.10695400	-3.65184200	2.49518600
C	-1.23958000	-1.24311600	2.08162700
C	-0.81406300	-3.43159700	3.83156600
H	-1.16870800	-4.66575300	2.10893800
C	-0.94756700	-1.03646900	3.44521500
C	-0.74423300	-2.11010300	4.30128300
H	-0.65707500	-4.26543700	4.50680800
H	-0.90347200	-0.01241700	3.80097800
H	-0.53467700	-1.92217600	5.35066300
C	-4.33296200	2.00190300	-1.77909500
C	-5.10069800	2.96034400	-2.47992500
C	-3.71413000	2.35177300	-0.53969800
C	-5.25648500	4.24646100	-2.00520200
H	-5.57364600	2.65978800	-3.41193000
C	-3.88669400	3.68335200	-0.07604100
C	-4.63062000	4.59936800	-0.79348200
H	-5.84536800	4.97299300	-2.55413700
H	-3.43232600	3.94490600	0.87160500
H	-4.74017500	5.60994100	-0.40896300
O	-1.35452000	-0.19417300	1.28477300
O	-3.00323300	1.53276300	0.18067800
H	-1.51236200	-2.07168200	-2.63399400
C	-2.35696200	-2.41777300	-2.02517600
C	-2.59705000	-3.91453700	-2.27277000
C	-3.60713100	-1.63485900	-2.43858200
C	-3.38606800	-4.14406400	-3.58672700
H	-1.63739200	-4.43537100	-2.30436800
H	-3.16741100	-4.32469600	-1.43243500

C	-3.75732900	-1.66244500	-3.97227200
H	-4.47016000	-2.11282200	-1.96272000
C	-3.20324000	-2.97825500	-4.56491900
H	-3.07143700	-5.08511200	-4.04789700
H	-4.45316400	-4.25118000	-3.36067000
H	-3.22419700	-0.80847800	-4.40550200
H	-4.81449900	-1.55437600	-4.23538700
H	-2.13653800	-2.86250900	-4.79208200
H	-3.69805100	-3.19268100	-5.51704400
Co	-2.52054400	-0.22885900	-0.24906500
S	-5.39745300	-1.00402800	0.82737300
O	-5.83665800	-1.86759400	1.92818200
O	-3.84390800	-0.96709700	0.88844800
O	-5.91014100	-1.30591300	-0.52457600
C	-5.88683700	0.67152900	1.20040000
C	-6.81463700	1.31699400	0.38786200
C	-5.35186200	1.30520700	2.32177800
C	-7.20885200	2.61609000	0.70144100
H	-7.20899500	0.80037700	-0.47887200
C	-5.75205100	2.60316600	2.61983600
H	-4.61943000	0.79026500	2.93271900
C	-6.68043000	3.27828100	1.81407800
H	-7.92252800	3.12841700	0.06269100
H	-5.33333900	3.10744500	3.48686000
C	-7.05688600	4.70775700	2.10602000
H	-6.41260800	5.39547600	1.54376000
H	-8.08969400	4.91906400	1.81385200
H	-6.94532800	4.94571600	3.16770800
S	5.06216500	-1.58832800	-0.26572400
O	3.70388600	-1.11346500	-0.84499700
O	5.01357300	-1.83012300	1.19229900
O	5.54694600	-2.67690000	-1.11801000
C	6.11410900	-0.16556500	-0.52723200
C	6.16140800	0.40808200	-1.80062200
C	6.86416200	0.36086600	0.51870200
C	6.96271500	1.52155600	-2.01547600
H	5.55577000	-0.00541900	-2.59878600
C	7.65745500	1.48747700	0.28997900
H	6.81995000	-0.11007700	1.49437000
C	7.71764900	2.08249200	-0.97408000
H	6.98149500	1.98493100	-2.99731700
H	8.24134400	1.90657800	1.10540200
C	8.55170900	3.31306100	-1.22206200
H	9.07577000	3.63308300	-0.31755400
H	9.30164300	3.13513600	-2.00062700
H	7.92128000	4.14151500	-1.56359100

five-coordinated Co^{III}(salen)-Cl counterion addition in the terminal carbon and subsequent hydrolysis

Co^{III}(salen)-Cl counterion addition in the terminal carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.353456

Thermal correction to Gibbs Free Energy (a.u.): 0.394718

Imaginary frequencies: -388.14

Calculation of single point energy based on the optimized structure, Et = -3070.9923053 a.u.

C	4.26190100	-3.15968200	-1.17145900
C	5.05362400	-2.04496000	-0.83079400
C	2.88537300	-3.06171100	-1.25552100
H	4.73893200	-4.11644000	-1.36514500
C	4.43639800	-0.83381000	-0.59197800
H	6.13148400	-2.13910400	-0.75760900
C	2.22754800	-1.83529600	-0.98737300
H	2.26752500	-3.91643600	-1.50838000
C	3.03171800	-0.69876000	-0.67598200
H	5.02291500	0.04080900	-0.32511500
O	0.91852400	-1.81152100	-1.03011200
C	2.45389100	0.59182400	-0.46388000
Co	-0.20633000	-0.38818000	-0.63757800

N	1.19384600	0.88050500	-0.57221200
H	3.14566000	1.39198100	-0.22030900
N	-1.36949600	1.13221000	-0.75635200
C	0.67926600	2.19373100	-0.15234500
C	-2.64820500	1.08781500	-0.55657400
C	-0.62748500	2.39495100	-0.92458700
C	1.62671600	3.38051600	-0.31263100
H	-3.20104900	2.02627400	-0.51281100
C	-3.41883400	-0.10454400	-0.39721600
C	-1.34168500	3.67356400	-0.48962000
C	0.91281300	4.67223100	0.11143000
H	1.96175700	3.45307300	-1.35673000
H	2.50464600	3.23389900	0.32126500
C	-4.79586800	0.01308900	-0.09235300
C	-2.84522700	-1.39875700	-0.60485200
C	-0.40034000	4.87730400	-0.65178800
H	-2.24944200	3.83330100	-1.08185500
H	-1.64475100	3.57508600	0.56079900
H	1.57728000	5.52897400	-0.04133600
H	0.70566800	4.62134000	1.18771200
C	-5.60216200	-1.09954000	0.02396200
H	-5.20952100	1.00757500	0.05586100
C	-3.70254700	-2.52494600	-0.50186800
O	-1.58975900	-1.60371200	-0.90062900
H	-0.18480400	5.02331700	-1.71896600
H	-0.90560100	5.78568500	-0.30731500
C	-5.03927500	-2.37519200	-0.18760700
H	-6.65338100	-0.99741700	0.26978900
H	-3.26228200	-3.50195400	-0.66811100
H	-5.66688400	-3.25778800	-0.10144100
Cl	2.26474800	1.03037000	2.56698000
C	-0.26964500	-1.65101900	1.95895800
C	1.05835300	-1.30115900	2.48750600
O	-0.31809800	-0.38383200	1.32388400
H	-0.24199400	-2.47534000	1.23451400
H	1.94511200	-1.51955100	1.90906300
H	1.19683500	-0.99903000	3.51526900
C	-1.39920100	-1.83515800	2.95481000
H	-2.35172500	-1.86869400	2.41748300
H	-1.28270300	-2.77067700	3.51376000
H	-1.42413600	-0.99843200	3.65904500
H	-0.37875100	2.47180700	-1.99374700
H	0.45086600	2.07287700	0.91563400

Co^{III}(salen)-Cl counterion addition in the terminal carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.394230

Thermal correction to Gibbs Free Energy (a.u.): 0.395350

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3071.0390873 a.u.

C	3.91808200	-3.57767200	-1.01810500
C	4.81992700	-2.53219000	-0.73858000
C	2.55623000	-3.34711200	-1.08210500
H	4.29516600	-4.58396300	-1.17730600
C	4.33203900	-1.25605900	-0.54001000
H	5.88405800	-2.73053300	-0.67244000
C	2.03530200	-2.04924700	-0.86398000
H	1.85091000	-4.14550400	-1.28541600
C	2.94790300	-0.98591900	-0.61568200
H	5.00095100	-0.43700100	-0.29548400
O	0.72889600	-1.89741100	-0.89240700
C	2.50172300	0.36013000	-0.42738800
Co	-0.24669900	-0.34986700	-0.66912800
N	1.25801600	0.75936600	-0.54079000
H	3.26768200	1.10603600	-0.26732700
N	-1.26027300	1.26758400	-0.66809200
C	0.90253400	2.13023200	-0.12964500
C	-2.53032100	1.33123100	-0.42278300

C	-0.41059500	2.45919100	-0.84033900
C	1.95232200	3.21397700	-0.37264900
H	-2.98817400	2.31322100	-0.30492200
C	-3.40478600	0.20488500	-0.32110200
C	-0.98371700	3.79392500	-0.36974400
C	1.39395500	4.57147600	0.07951600
H	2.22065000	3.24141200	-1.43799300
H	2.84174500	2.98334100	0.21761700
C	-4.75161000	0.41553400	0.05507500
C	-2.96464600	-1.10854600	-0.67736200
C	0.05678100	4.90403100	-0.59218700
H	-1.90435500	4.03735800	-0.91193000
H	-1.23521100	3.72265100	0.69649300
H	2.12591600	5.35835700	-0.12928200
H	1.26264900	4.54666800	1.16855600
C	-5.65272400	-0.62837600	0.10058200
H	-5.06599300	1.42308400	0.31512100
C	-3.91831100	-2.15768200	-0.65370200
O	-1.73896000	-1.39116100	-1.03636200
H	0.21144600	5.03477800	-1.67180000
H	-0.33710500	5.85374900	-0.21527700
C	-5.22273500	-1.92102900	-0.26288100
H	-6.67988300	-0.45778000	0.40333300
H	-3.57872300	-3.14748000	-0.93819700
H	-5.92821600	-2.74655800	-0.23676400
Cl	2.98091500	1.07204700	2.25617200
C	-0.68600600	-1.89427700	1.94507900
C	0.40871200	-1.01191700	2.36442700
O	-0.60347400	-0.52829900	1.42270400
H	-0.45881100	-2.62828200	1.17519900
H	1.40817500	-1.09593900	1.95266000
H	0.36460700	-0.49944100	3.32019500
C	-1.89634800	-2.16022100	2.79318000
H	-2.78736800	-2.25800600	2.16513700
H	-1.76492900	-3.09514800	3.34820900
H	-2.05615800	-1.34895600	3.50825000
H	-0.19750400	2.52578200	-1.91769500
H	0.73564100	2.06989700	0.95559700

Co^{III}(salen)-Cl counterion addition in the terminal carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.420730

Thermal correction to Gibbs Free Energy (a.u.): 0.396829

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3071.0579565 a.u.

C	4.69996700	-1.51150100	-2.01789800
C	5.26291400	-0.31351200	-1.53535100
C	3.34167100	-1.75219800	-1.93080900
H	5.34439800	-2.26260200	-2.46646300
C	4.43112900	0.63152000	-0.97033800
H	6.33047800	-0.13786500	-1.61006200
C	2.46888000	-0.80994500	-1.33232300
H	2.90352000	-2.67357900	-2.29844900
C	3.04016000	0.40951300	-0.85387100
H	4.83920200	1.56806700	-0.59731300
O	1.19389000	-1.09588200	-1.26355700
C	2.22459200	1.44671000	-0.30299000
Co	-0.13033900	-0.18969400	-0.27925800
N	0.95414500	1.36255500	-0.08529000
H	2.72905600	2.38574900	-0.07273400
N	-1.56929500	1.11217100	-0.57612900
C	0.13582900	2.45995900	0.43250100
C	-2.82322400	0.80218000	-0.68943500
C	-1.10206700	2.50542900	-0.48597500
C	0.80103800	3.82907900	0.55022600
H	-3.55950700	1.60581100	-0.75253100
C	-3.35409800	-0.52211400	-0.73395900
C	-2.11778100	3.53586900	0.01144000

C	-0.21763700	4.86103500	1.05569200
H	1.18699700	4.13901300	-0.43047700
H	1.65356500	3.77805900	1.23563800
C	-4.76060900	-0.66887800	-0.84207600
C	-2.52024900	-1.68913100	-0.68332200
C	-1.45593800	4.91493900	0.15363300
H	-2.96579400	3.60919900	-0.67723700
H	-2.51308500	3.20511300	0.98081500
H	0.25234200	5.84819700	1.11458100
H	-0.52189200	4.59523500	2.07642600
C	-5.35636300	-1.90891000	-0.89956500
H	-5.36918200	0.23183100	-0.87822200
C	-3.16570600	-2.95565900	-0.74919500
O	-1.22346000	-1.67471900	-0.59694300
H	-1.16395200	5.27814500	-0.84092700
H	-2.18288500	5.63281600	0.54750000
C	-4.53698200	-3.05780300	-0.85268500
H	-6.43367000	-2.00407200	-0.97879300
H	-2.53093800	-3.83439200	-0.71535800
H	-4.99391400	-4.04268800	-0.89737100
Cl	2.58333400	-1.98595500	2.10646500
C	-0.19407000	-1.62553200	2.16313500
C	0.90835000	-2.58906500	1.71288300
O	-0.06844800	-0.37011200	1.55728100
H	-1.12504200	-2.12641400	1.84227300
H	0.88559500	-2.71032900	0.63079500
H	0.80705500	-3.55892800	2.20410600
C	-0.23808300	-1.43147800	3.67896500
H	-1.07257700	-0.77448700	3.93910300
H	-0.37249700	-2.38839900	4.19572400
H	0.68988500	-0.97054500	4.02617800
H	-0.75218300	2.80015100	-1.48718800
H	-0.20265500	2.12948800	1.42363400

subsequent hydrolysis (H_2O molecule is opposite the counterion Cl^-)

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.820217

Thermal correction to Gibbs Free Energy (a.u.): 0.417955

Imaginary frequencies: -629.24

Calculation of single point energy based on the optimized structure, Et = -3147.5089379 a.u.

C	2.04318000	-4.75478500	-0.85510300
C	2.73998600	-4.15922700	-1.92579600
C	1.23459100	-4.00775500	-0.02050100
H	2.14258500	-5.82257700	-0.68000500
C	2.60531400	-2.80220400	-2.13122200
H	3.37314100	-4.75746700	-2.57162400
C	1.06713200	-2.61112700	-0.20993300
H	0.70248600	-4.46231400	0.80800900
C	1.77293000	-2.00773100	-1.30783100
H	3.14119200	-2.31557900	-2.94264300
O	0.33954300	-1.95272600	0.65307000
C	1.73443900	-0.59229700	-1.53813800
Co	-0.51629600	-0.32859300	0.23019900
N	0.89664000	0.21153300	-0.97370900
H	2.48717100	-0.17884600	-2.21231100
N	-1.33423300	1.29871600	-0.36106600
C	0.98402100	1.67198600	-0.97186600
C	-2.61682300	1.48217800	-0.38128200
C	-0.44347100	2.20423000	-1.11575900
C	1.92074800	2.36145600	-1.95497000
H	-2.98952700	2.45049500	-0.72639000
C	-3.59699700	0.48172900	-0.09840400
C	-0.47083600	3.68028300	-0.71498000
C	1.90698100	3.86954900	-1.64183700
H	1.59968500	2.17667800	-2.98948100
H	2.93874900	1.97681700	-1.84360400
C	-4.94877000	0.85941900	0.06338200
C	-3.24388000	-0.90784300	-0.16468100

C	0.48697800	4.45908600	-1.63478600
H	-1.48229700	4.09308400	-0.79381400
H	-0.16257100	3.76309100	0.33356100
H	2.53007100	4.40715900	-2.36423800
H	2.36521500	4.01723200	-0.65619000
C	-5.94471200	-0.08716700	0.19349400
H	-5.19216700	1.91875700	0.09151500
C	-4.29469400	-1.85597000	-0.06370000
O	-2.02449600	-1.33379900	-0.34949000
H	0.08417600	4.44322100	-2.65684100
H	0.52093500	5.51020800	-1.32955300
C	-5.60312000	-1.45341700	0.12274900
H	-6.97701600	0.21314200	0.33664000
H	-4.02548800	-2.90484300	-0.12532200
H	-6.38326400	-2.20430000	0.21320500
H	-0.73487500	2.11952900	-2.17343900
H	1.30868700	1.90415000	0.04846800
O	-1.40792600	-0.20274400	2.09661100
H	-1.29542100	-1.08921900	2.46695200
H	-0.43179600	0.36708000	2.23933000
Cl	3.78991600	1.26053900	1.02510100
C	1.70406300	0.18339400	2.58690600
C	2.94061800	-0.18217800	1.76915000
O	0.70078500	0.79095500	1.82563700
H	1.36441600	-0.80790900	2.95303900
H	2.67843500	-0.82854400	0.93739600
H	3.69091100	-0.67035500	2.39315000
C	2.04033600	1.05360800	3.80088000
H	1.13894100	1.21347500	4.39884300
H	2.80186900	0.58617200	4.43582800
H	2.40899800	2.02796200	3.46958900

subsequent hydrolysis (H_2O molecule is opposite the counterion Cl^-)

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.848419

Thermal correction to Gibbs Free Energy (a.u.): 0.418909

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.544214 a.u.

C	4.82442400	-2.48836200	-1.26193200
C	5.46489800	-1.27287800	-0.93945600
C	3.44857300	-2.57837400	-1.32770200
H	5.42442600	-3.37206100	-1.46096400
C	4.69234900	-0.15923400	-0.69064100
H	6.54679200	-1.21861700	-0.88937900
C	2.62660400	-1.45074300	-1.06047600
H	2.94958800	-3.50913800	-1.57435700
C	3.27791100	-0.21588500	-0.74562700
H	5.16179800	0.78985000	-0.44329500
O	1.33356900	-1.60126300	-1.11833900
C	2.53772200	0.97877000	-0.49581600
Co	0.00131300	-0.32298900	-0.79940300
N	1.24708200	1.09646200	-0.52450000
H	3.12874500	1.86281400	-0.25668400
N	-1.30124200	1.08362800	-0.94613700
C	0.55929600	2.33363500	-0.11713700
C	-2.56838400	0.87751100	-0.79235700
C	-0.70100800	2.42540900	-0.99013200
C	1.36877400	3.62795000	-0.16878200
H	-3.23096500	1.73551800	-0.68732100
C	-3.18676100	-0.41225000	-0.76543500
C	-1.59018400	3.58367400	-0.53886700
C	0.48229700	4.80666800	0.26363900
H	1.74808300	3.79040800	-1.18733500
H	2.23591000	3.56747400	0.49705200
C	-4.56627600	-0.49677400	-0.46832900
C	-2.46236600	-1.59331800	-1.12157200
C	-0.79402300	4.89648900	-0.58003300
H	-2.47000600	3.66845300	-1.18622000

H	-1.93041900	3.37334200	0.48180200
H	1.05103500	5.74007700	0.19588700
H	0.20802000	4.67504400	1.31765300
C	-5.23475300	-1.70366100	-0.50307200
H	-5.09355300	0.41500500	-0.19952600
C	-3.18077500	-2.81359400	-1.18493200
O	-1.18598500	-1.61036600	-1.40984300
H	-0.52774400	5.13008600	-1.62012200
H	-1.42369200	5.71924600	-0.22569800
C	-4.52630600	-2.86448700	-0.87213500
H	-6.28933600	-1.75879600	-0.25636100
H	-2.62785700	-3.70299700	-1.46646200
H	-5.04410300	-3.81898800	-0.90823500
H	-0.37885200	2.59221100	-2.02949300
H	0.20636900	2.16109200	0.90814000
O	-1.48997800	1.62744600	2.25729300
H	-1.01753800	1.64660700	3.09889900
H	-1.15691900	0.79130000	1.84318600
Cl	1.18434100	-0.41198600	3.71618000
C	-0.24559900	-1.72747800	1.70295700
C	1.07755200	-1.74754200	2.47127800
O	-0.39866100	-0.49859100	1.06050600
H	-0.13945200	-2.53907300	0.96152100
H	1.91011400	-1.57683300	1.78931600
H	1.22440200	-2.68209800	3.01605600
C	-1.46903900	-2.02050400	2.57318000
H	-2.35662100	-2.07408400	1.93758300
H	-1.36257500	-2.97044300	3.10863800
H	-1.61690300	-1.21952400	3.30232400

subsequent hydrolysis (H_2O molecule is opposite the counterion Cl^-)

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.847407

Thermal correction to Gibbs Free Energy (a.u.): 0.420649

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5417245 a.u.

C	-5.16105400	2.91209200	0.42646800
C	-5.70908000	1.63534000	0.19646200
C	-3.79644300	3.12912100	0.36472400
H	-5.82081100	3.74424000	0.65647100
C	-4.85824300	0.58918100	-0.10116000
H	-6.78114000	1.47944000	0.24672000
C	-2.90056300	2.06762700	0.08511000
H	-3.36820800	4.11014600	0.53885900
C	-3.45891700	0.77575000	-0.15704400
H	-5.25675400	-0.40361700	-0.29609900
O	-1.61783900	2.32737100	0.04626500
C	-2.63065300	-0.32571700	-0.54710700
Co	-0.21120300	1.09831700	0.02213000
N	-1.34025500	-0.31727100	-0.57897400
H	-3.14768700	-1.23030000	-0.86676000
N	1.06655700	0.33524700	-1.22638600
C	-0.53694200	-1.44439300	-1.06821300
C	2.31469100	0.68548700	-1.28861900
C	0.53792800	-0.82258700	-1.97440600
C	-1.27960200	-2.57468700	-1.77321800
H	2.98313600	0.10782600	-1.92733100
C	2.91843300	1.77400100	-0.59275600
C	1.55679300	-1.88623100	-2.38730500
C	-0.26908500	-3.64698600	-2.20753600
H	-1.82100500	-2.18521900	-2.64691700
H	-2.01351600	-3.02078000	-1.09542900
C	4.30354200	2.00393800	-0.79200900
C	2.17200200	2.64109100	0.27087300
C	0.84243900	-3.05595100	-3.08206800
H	2.30602200	-1.46788600	-3.06797200
H	2.07248800	-2.23131300	-1.48325900
H	-0.78764600	-4.44864300	-2.74401700

H	0.17037300	-4.09514400	-1.30881500
C	4.95633900	3.05028800	-0.17973000
H	4.84704000	1.32795300	-1.44767000
C	2.87101500	3.71875100	0.88101500
O	0.90186600	2.51617300	0.52743000
H	0.41243800	-2.70385300	-4.02995700
H	1.57355000	-3.82967100	-3.33926100
C	4.21893400	3.91204900	0.66096300
H	6.01645500	3.21265200	-0.33988100
H	2.29957500	4.37738200	1.52588700
H	4.72164700	4.74354300	1.14740900
H	0.03700300	-0.42255400	-2.86937500
H	-0.01517100	-1.85598800	-0.19905200
O	0.09443800	0.21281700	1.65682900
H	0.51325000	0.88932700	2.20964300
H	1.19809400	-0.98786000	1.33364900
Cl	-0.79542200	-3.83709200	1.59580900
C	1.65785900	-2.63363700	2.28152300
C	0.21519200	-2.84148800	2.74977000
O	1.73816700	-1.80338000	1.14399000
H	2.13859800	-2.14023300	3.14871500
H	-0.29223600	-1.87932200	2.82598900
H	0.18356800	-3.37249400	3.70257800
C	2.40919600	-3.92372400	1.98693600
H	3.44464400	-3.69217800	1.72479300
H	2.40556900	-4.59049800	2.85477500
H	1.94552800	-4.44451900	1.14540800

subsequent hydrolysis (H_2O molecule is at the same side with the ion Cl^-)

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.817329

Thermal correction to Gibbs Free Energy (a.u.): 0.417627

Imaginary frequencies: -854.88

Calculation of single point energy based on the optimized structure, Et = -3147.5063782 a.u.

C	2.66868100	-4.32589900	-1.53571500
C	3.82764100	-3.60030900	-1.87719600
C	1.60440000	-3.71959300	-0.89714900
H	2.60866000	-5.38363200	-1.77728100
C	3.88794100	-2.26006000	-1.55687400
H	4.65639000	-4.08895300	-2.37761300
C	1.63085800	-2.34007100	-0.56181000
H	0.71625900	-4.27919500	-0.62485800
C	2.81123900	-1.60209500	-0.91776700
H	4.77517000	-1.67925000	-1.79866500
O	0.61417300	-1.84751800	0.09506200
C	2.96825600	-0.22326000	-0.55634400
Co	0.11520000	-0.02179500	0.02610200
N	2.00241300	0.52725500	-0.14667200
H	3.97788900	0.19212900	-0.61866100
N	-0.19786200	1.85823700	-0.21247900
C	2.14287100	1.84745800	0.46148900
C	-1.28609400	2.33419000	-0.72442100
C	1.00076500	2.71201300	-0.08839300
C	3.47278200	2.58481000	0.33994400
H	-1.37943800	3.41947300	-0.81978600
C	-2.34219300	1.54920000	-1.28664100
C	0.85270400	3.96917300	0.77073300
C	3.38066000	3.89471900	1.14512100
H	3.69495100	2.79688000	-0.71481000
H	4.29236500	1.97142600	0.72958200
C	-3.57015100	2.16624600	-1.60922800
C	-2.09654800	0.19490800	-1.68398900
C	2.17515100	4.75515800	0.73370200
H	0.03422900	4.59980000	0.40805200
H	0.60301400	3.66838900	1.79486400
H	4.30607800	4.46893700	1.03130800
H	3.29512900	3.64268600	2.20977400
C	-4.56330000	1.47818100	-2.27884700

H	-3.72567300	3.20023700	-1.31117700
C	-3.11921700	-0.47445800	-2.40183300
O	-0.97801200	-0.44036700	-1.44512400
H	2.33277800	5.13310900	-0.28564300
H	2.10437400	5.63306100	1.38426500
C	-4.32189300	0.14973500	-2.67960700
H	-5.51053300	1.95592400	-2.50412200
H	-2.92463600	-1.49625600	-2.70918800
H	-5.09258100	-0.39579200	-3.21705900
Cl	-1.21761200	-2.65099700	3.16294400
C	-2.67388800	-1.10267600	1.32257400
C	-2.05804600	-2.48445500	1.54469100
O	-1.73175700	-0.06994800	1.23051800
H	-3.16881600	-1.20001800	0.34035800
H	-1.28727900	-2.68209900	0.80287300
H	-2.82548100	-3.26044100	1.53043400
C	-3.74081300	-0.74131400	2.35721400
H	-4.18958500	0.21932300	2.09206600
H	-4.53040700	-1.50024000	2.39798800
H	-3.29167400	-0.65336200	3.35011700
H	1.27701700	3.01464100	-1.10963800
H	1.92281200	1.67050300	1.52179000
O	0.40210400	0.12987700	2.10200700
H	0.71369900	-0.74878200	2.36345300
H	-0.79045500	-0.00747700	1.97321300

subsequent hydrolysis (H_2O molecule is at the same side with the ion Cl^-)

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.848416

Thermal correction to Gibbs Free Energy (a.u.): 0.418912

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5442162 a.u.

C	4.82480100	-2.48743300	-1.26229900
C	5.46515700	-1.27205000	-0.93924800
C	3.44896500	-2.57744600	-1.32845100
H	5.42487500	-3.37105300	-1.46146300
C	4.69251700	-0.15851100	-0.69022500
H	6.54703700	-1.21777800	-0.88889700
C	2.62691900	-1.44992400	-1.06107100
H	2.95006200	-3.50813100	-1.57556100
C	3.27809600	-0.21517500	-0.74557100
H	5.16188500	0.79049000	-0.44241600
O	1.33388300	-1.60043100	-1.11947200
C	2.53782200	0.97936000	-0.49539400
Co	0.00165100	-0.32250300	-0.79965600
N	1.24718200	1.09699700	-0.52418600
H	3.12877100	1.86333100	-0.25582600
N	-1.30106900	1.08406700	-0.94583700
C	0.55929200	2.33397600	-0.11636100
C	-2.56822500	0.87788800	-0.79215200
C	-0.70098100	2.42593600	-0.98935700
C	1.36867600	3.62836300	-0.16751700
H	-3.23079500	1.73586800	-0.68684700
C	-3.18662700	-0.41184900	-0.76564600
C	-1.59027600	3.58395000	-0.53770000
C	0.48207900	4.80685400	0.26528500
H	1.74800500	3.79120500	-1.18599900
H	2.23579200	3.56772700	0.49832800
C	-4.56617500	-0.49642500	-0.46867000
C	-2.46221400	-1.59281800	-1.12208700
C	-0.79422600	4.89685300	-0.57839300
H	-2.47009300	3.66888700	-1.18503600
H	-1.93049900	3.37324900	0.48289600
H	1.05073500	5.74033700	0.19787500
H	0.20778100	4.67484000	1.31924300
C	-5.23467700	-1.70327500	-0.50384400
H	-5.09344200	0.41528900	-0.19962400
C	-3.18067800	-2.81306500	-1.18589900

O	-1.18584300	-1.60982100	-1.41019800
H	-0.52794500	5.13082900	-1.61839300
H	-1.42398500	5.71942300	-0.22378800
C	-4.52622200	-2.86401100	-0.87322400
H	-6.28927800	-1.75847600	-0.25722700
H	-2.62775800	-3.70239100	-1.46766900
H	-5.04405400	-3.81848000	-0.90967900
Cl	1.18328600	-0.41539700	3.71711500
C	-0.24581000	-1.72842900	1.70173500
C	1.07682700	-1.74973200	2.47088700
O	-0.39787600	-0.49886700	1.06031000
H	-0.13958100	-2.53939400	0.95964000
H	1.90989900	-1.57868700	1.78963700
H	1.22294700	-2.68486600	3.01486400
C	-1.46988300	-2.02167100	2.57100400
H	-2.35713000	-2.07446300	1.93487700
H	-1.36407200	-2.97205600	3.10580500
H	-1.61785900	-1.22119600	3.30067700
H	-0.37881500	2.59313600	-2.02864900
H	0.20637900	2.16101900	0.90884900
O	-1.48996500	1.62653700	2.25771700
H	-1.01775100	1.64502400	3.09946500
H	-1.15688800	0.79065600	1.84315700

The product complex cannot be located.

five-coordinated Co^{III}(salen)-Cl counterion addition in the middle carbon and subsequent hydrolysis

Co^{III}(salen)-Cl counterion addition in the middle carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.355559

Thermal correction to Gibbs Free Energy (a.u.): 0.393854

Imaginary frequencies: -340.70

Calculation of single point energy based on the optimized structure, Et = -3070.9952069 a.u.

C	4.20220400	-2.95903600	-1.59654700
C	4.96355300	-1.79511600	-1.38534000
C	2.82406500	-2.94719900	-1.46232600
H	4.70177400	-3.88639300	-1.86274900
C	4.31391200	-0.62063400	-1.05429300
H	6.04326500	-1.81920900	-1.48420300
C	2.14362500	-1.76347600	-1.09278200
H	2.23012700	-3.84248700	-1.61066600
C	2.91082200	-0.57741200	-0.91397200
H	4.87768100	0.29326100	-0.88889300
O	0.84339100	-1.82716100	-0.90293700
C	2.28310800	0.68073500	-0.63538300
Co	-0.31556400	-0.47312500	-0.39112600
N	1.00772000	0.87364300	-0.56355700
H	2.94198900	1.53602800	-0.52090300
N	-1.56372800	0.96195200	-0.71416600
C	0.43321300	2.17474100	-0.19863200
C	-2.84962900	0.85777300	-0.58958400
C	-0.89281500	2.25441800	-0.96415800
C	1.30961500	3.40121900	-0.43393700
H	-3.45473500	1.75883600	-0.69461500
C	-3.56983300	-0.34588200	-0.32525300
C	-1.67500000	3.51249400	-0.58713200
C	0.52595200	4.66798200	-0.06136100
H	1.62273700	3.44425600	-1.48674300
H	2.20154300	3.32812600	0.19338400
C	-4.97818400	-0.26909900	-0.18832100
C	-2.91634200	-1.61693700	-0.23519400
C	-0.80493100	4.75867200	-0.81614500
H	-2.59341300	3.59539900	-1.17836600
H	-1.96704700	3.44671000	0.46895300
H	1.13668700	5.55393300	-0.26380600
H	0.33455100	4.65735300	1.01899100
C	-5.74167300	-1.39434300	0.03317500
H	-5.45050800	0.70758800	-0.26098200

C	-3.73042200	-2.76149800	-0.02121600
O	-1.63036300	-1.79397900	-0.35382100
H	-0.60811500	4.86523000	-1.89165300
H	-1.35941700	5.65200200	-0.50977600
C	-5.09920400	-2.64836400	0.11279700
H	-6.81811600	-1.32071000	0.14162500
H	-3.23031700	-3.72212500	0.03592200
H	-5.69184500	-3.54287800	0.28342900
Cl	2.45285800	1.33565900	2.41538400
C	1.02366000	-0.96533300	2.91105100
C	-0.37532800	-1.16864500	2.47166300
O	-0.30220900	-0.13449900	1.52342600
H	1.23473500	-0.30256600	3.73834000
H	-1.12676100	-0.96286800	3.24562200
H	-0.55866700	-2.15923700	2.03155800
C	2.09435200	-1.83066000	2.38757800
H	3.07724500	-1.37084300	2.45747700
H	2.06478500	-2.74161800	3.01485100
H	1.88401800	-2.15307400	1.36752900
H	-0.65779400	2.28739800	-2.03872800
H	0.22439800	2.09562200	0.87584900

Co^{III}(salen)-Cl counterion addition in the middle carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.391361

Thermal correction to Gibbs Free Energy (a.u.): 0.396725

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3071.0370714 a.u.

C	4.13720200	-3.24884900	-1.18048100
C	4.94053100	-2.13129000	-0.88307400
C	2.75815600	-3.14596300	-1.22237200
H	4.60461100	-4.21121800	-1.36875000
C	4.33824900	-0.91020500	-0.64855000
H	6.01944400	-2.23019100	-0.83485000
C	2.12239800	-1.91092800	-0.95700200
H	2.12772300	-4.00298000	-1.43227200
C	2.93473500	-0.77222900	-0.69769100
H	4.93091900	-0.03620000	-0.39723200
O	0.80650600	-1.88447700	-0.94581400
C	2.36373400	0.52498500	-0.50121500
Co	-0.30085800	-0.46514400	-0.58841900
N	1.08786200	0.79628300	-0.59366000
H	3.05480000	1.34324400	-0.35086800
N	-1.47595200	1.04316100	-0.68936700
C	0.60138600	2.13922800	-0.23042200
C	-2.74905900	1.00623500	-0.45701000
C	-0.74483500	2.30112900	-0.93823700
C	1.53702800	3.30835400	-0.53414200
H	-3.29860300	1.94703000	-0.42939500
C	-3.51938000	-0.18057000	-0.24953500
C	-1.44071500	3.59705800	-0.52737100
C	0.85121200	4.62377100	-0.13811600
H	1.79453200	3.31352700	-1.60250900
H	2.44890700	3.19258000	0.05572100
C	-4.89455000	-0.05415300	0.05836400
C	-2.94646400	-1.48031400	-0.41311500
C	-0.51500500	4.79124100	-0.81254900
H	-2.38328700	3.72580000	-1.07111900
H	-1.67854100	3.55332200	0.54348200
H	1.50112700	5.46825700	-0.38916300
H	0.72752300	4.63646300	0.95202500
C	-5.69780800	-1.16489600	0.21396000
H	-5.31039900	0.94369300	0.17295500
C	-3.79883200	-2.60446400	-0.27112400
O	-1.68627900	-1.69176400	-0.69460400
H	-0.37856600	4.88395900	-1.89855700
H	-0.99888800	5.71493400	-0.47806400
C	-5.13519200	-2.44629300	0.04189700

H	-6.74869300	-1.05607400	0.45820100
H	-3.35726800	-3.58542100	-0.40815800
H	-5.76218900	-3.32578900	0.15690700
Cl	2.81719800	1.39272700	2.18015200
C	0.31063000	-0.83005900	2.65926400
C	-1.12222600	-1.11405100	2.48817500
O	-0.44938100	-0.23079200	1.55678800
H	0.61782200	-0.05899500	3.36004600
H	-1.87023900	-0.61301100	3.09801900
H	-1.42256900	-2.06639800	2.05740300
C	1.36372300	-1.83981800	2.31588400
H	2.26538700	-1.31491000	1.99342300
H	1.60787000	-2.41337800	3.21701500
H	1.01977300	-2.52813800	1.54087000
H	-0.54991500	2.33015600	-2.02065400
H	0.44987100	2.10491700	0.85724900

Co^{III}(salen)-Cl counterion addition in the middle carbon

Co^{III}(salen)-Cl + PO = Co^{III}(salen)-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1832.419001

Thermal correction to Gibbs Free Energy (a.u.): 0.396654

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3071.0561361 a.u.

C	4.40642700	-1.84497600	-2.49367900
C	5.06919400	-0.67091300	-2.08485100
C	3.05214700	-2.01802900	-2.27550400
H	4.96868800	-2.63134900	-2.98983900
C	4.34028000	0.32031900	-1.45925900
H	6.13183900	-0.54808100	-2.26295700
C	2.28341500	-1.02573600	-1.61606500
H	2.53701900	-2.91977800	-2.58807200
C	2.95731800	0.16835900	-1.20964600
H	4.82574800	1.24033400	-1.14205300
O	1.01032800	-1.24942500	-1.42105300
C	2.24324700	1.25496000	-0.60824300
Co	-0.17738900	-0.27586600	-0.33191000
N	0.99927000	1.22753800	-0.26707000
H	2.80589600	2.17601000	-0.45153000
N	-1.55562900	1.10090800	-0.61428600
C	0.27100200	2.37384700	0.27834000
C	-2.82738600	0.85596100	-0.66953000
C	-1.01376400	2.46942200	-0.57035000
C	1.01114600	3.70726600	0.33501400
H	-3.52229900	1.69628700	-0.72523300
C	-3.42995100	-0.43823500	-0.65641300
C	-1.94587000	3.55515700	-0.02799000
C	0.07687600	4.79373000	0.88740800
H	1.35030200	3.98868600	-0.67141700
H	1.90035100	3.61908600	0.96817700
C	-4.84494100	-0.50918100	-0.72451200
C	-2.66164900	-1.64817300	-0.58040700
C	-1.20872500	4.90038200	0.05903100
H	-2.82777900	3.66545400	-0.66734900
H	-2.29974400	3.25306700	0.96629700
H	0.59739200	5.75680400	0.90570400
H	-0.17814100	4.55283600	1.92744600
C	-5.51044000	-1.71448200	-0.72276700
H	-5.40296300	0.42278100	-0.77855300
C	-3.37846400	-2.87736400	-0.58440100
O	-1.36400000	-1.70662900	-0.52032400
H	-0.95881400	5.23982600	-0.95525200
H	-1.87487200	5.65704200	0.48638400
C	-4.75540800	-2.90536300	-0.65279900
H	-6.59303700	-1.75105300	-0.77321500
H	-2.79345600	-3.78912800	-0.53257300
H	-5.26724200	-3.86390700	-0.65078100
Cl	1.78018500	-0.96984200	4.05114400
C	1.07829700	-2.08390100	2.76046600

C	-0.23780700	-1.50847400	2.23150100
O	-0.04870500	-0.33411300	1.50627200
H	0.86382300	-3.01075300	3.29953500
H	-0.90640800	-1.31375700	3.08349400
H	-0.69716200	-2.30059000	1.61917800
C	2.12256700	-2.30607800	1.67975300
H	3.01194100	-2.79436800	2.08422700
H	1.69938900	-2.93226000	0.88684600
H	2.41567700	-1.35424200	1.23535000
H	-0.70797700	2.73588900	-1.59379600
H	-0.02335400	2.07207100	1.29186700

subsequent hydrolysis

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.819440

Thermal correction to Gibbs Free Energy (a.u.): 0.416788

Imaginary frequencies: -644.94

Calculation of single point energy based on the optimized structure, Et = -3147.5088795 a.u.

C	1.97237900	-4.79285400	-1.05256800
C	2.71650200	-4.14462100	-2.05966500
C	1.11386000	-4.09089300	-0.22954100
H	2.07544400	-5.86628100	-0.91850100
C	2.57578100	-2.78168200	-2.21382700
H	3.38848900	-4.70845700	-2.69720000
C	0.94261200	-2.68777400	-0.36685300
H	0.54493500	-4.58577000	0.54997000
C	1.69394500	-2.03175000	-1.39969000
H	3.14522500	-2.25528900	-2.97617600
O	0.16040900	-2.07556900	0.47835900
C	1.64132900	-0.61194100	-1.57926100
Co	-0.63152500	-0.39657100	0.16430200
N	0.76924400	0.17183000	-1.03404900
H	2.41040100	-0.17114500	-2.21615400
N	-1.42347000	1.28584700	-0.30582800
C	0.86930300	1.63515600	-1.00874800
C	-2.69097700	1.52944500	-0.19778800
C	-0.55594400	2.17885900	-1.10218100
C	1.78373600	2.32450700	-2.01420800
H	-3.04745500	2.52567400	-0.47178400
C	-3.68859600	0.56498800	0.14533900
C	-0.56143200	3.65942800	-0.71554500
C	1.78618200	3.83317100	-1.70667100
H	1.43906200	2.13742100	-3.04070400
H	2.80436800	1.93939000	-1.92821300
C	-5.00003000	0.99603900	0.44451500
C	-3.40842200	-0.83432000	0.00399800
C	0.36981100	4.42714200	-1.67012400
H	-1.57157300	4.07924100	-0.76599300
H	-0.21852400	3.75198100	0.32152200
H	2.39528600	4.36352200	-2.44624100
H	2.26699700	3.98244000	-0.73236500
C	-6.02363600	0.08995100	0.63647500
H	-5.18956300	2.06344900	0.52833400
C	-4.48811900	-1.73883400	0.17160900
O	-2.23055700	-1.30639100	-0.30309800
H	-0.06100200	4.40134300	-2.68049100
H	0.41339400	5.48119900	-1.37636300
C	-5.75422200	-1.28611500	0.49077300
H	-7.02329400	0.42989700	0.88437000
H	-4.27516500	-2.79564300	0.05249200
H	-6.55705000	-2.00512700	0.62918900
Cl	3.68919000	1.77805400	1.12256400
C	3.08015200	0.74400400	2.53219700
C	1.93558000	-0.14653800	2.05414500
O	0.79997000	0.58025400	1.71301400
H	2.69990900	1.47885900	3.24416400
H	1.73451000	-0.85253600	2.88226800
H	2.30910900	-0.75509000	1.21576900

C	4.25422300	-0.03889300	3.09602400
H	5.07426000	0.62209100	3.38415900
H	3.92740600	-0.59248900	3.98334700
H	4.62953200	-0.75729100	2.36116000
H	-0.89049900	2.08524000	-2.14662400
H	1.23023300	1.85115800	0.00170100
O	-1.30759400	-0.34873100	2.12025000
H	-1.23229400	-1.27531500	2.38894800
H	-0.26955800	0.12892200	2.21019000

subsequent hydrolysis

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.843340

Thermal correction to Gibbs Free Energy (a.u.): 0.418528

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5408425 a.u.

C	4.52360200	-2.85138900	-1.35353600
C	5.15262700	-1.60831800	-1.58626200
C	3.18472000	-2.92941300	-1.03117900
H	5.10594400	-3.76588300	-1.42646300
C	4.40491800	-0.45624800	-1.48778500
H	6.20757700	-1.56498400	-1.83370000
C	2.38866000	-1.75688000	-0.91918400
H	2.69709900	-3.88033500	-0.84675400
C	3.02533000	-0.49884500	-1.16682200
H	4.86603200	0.51414200	-1.65502100
O	1.13716100	-1.89203600	-0.58835300
C	2.31021900	0.72628600	-1.05348900
Co	-0.19878200	-0.57718900	-0.57326500
N	1.03362500	0.84422400	-0.84897800
H	2.90190000	1.63768800	-1.13500800
N	-1.54044200	0.77610800	-0.90103600
C	0.39666900	2.13237000	-0.53943100
C	-2.80114200	0.58859500	-0.70081200
C	-0.97210900	2.09400400	-1.23017100
C	1.16936200	3.40075900	-0.89013100
H	-3.47181500	1.44644900	-0.74469400
C	-3.41205900	-0.68426800	-0.45825200
C	-1.81682800	3.31126600	-0.85185500
C	0.32829500	4.62806000	-0.50576700
H	1.39762200	3.41817600	-1.96503600
H	2.12045100	3.42676500	-0.34875100
C	-4.79523000	-0.73033500	-0.17283200
C	-2.67687800	-1.90018400	-0.61289000
C	-1.04923000	4.60166100	-1.17766800
H	-2.76548600	3.30761900	-1.40019600
H	-2.03523400	3.24621500	0.22046500
H	0.86582500	5.54340600	-0.77517500
H	0.19916000	4.64051100	0.58339100
C	-5.45838700	-1.93257900	-0.02607000
H	-5.33359600	0.20881700	-0.06931800
C	-3.38750200	-3.12000900	-0.49026900
O	-1.39610700	-1.95393800	-0.88006600
H	-0.92385300	4.68759500	-2.26607400
H	-1.64014600	5.46779500	-0.86172400
C	-4.73808900	-3.13130500	-0.19411400
H	-6.51789500	-1.95536400	0.20459200
H	-2.82622100	-4.03863000	-0.62127300
H	-5.25073000	-4.08350200	-0.08892700
Cl	2.32972700	0.77811200	2.35213800
C	0.95612000	-0.06668900	3.25183200
C	0.20315400	-0.98375600	2.28702800
O	-0.46092400	-0.25445900	1.30583100
H	0.30054700	0.75668400	3.54314100
H	-0.52008900	-1.54952900	2.90448700
H	0.89944200	-1.71582200	1.85512300
C	1.53337800	-0.79623000	4.45253700
H	2.08433300	-0.11501600	5.10443000

H	0.71859400	-1.24584200	5.03144300
H	2.21048000	-1.59409800	4.13355400
H	-0.79069600	2.09457300	-2.31627900
H	0.22238300	2.11523700	0.54230400
O	-1.60817800	1.97119300	2.18221200
H	-2.37448800	1.71327600	2.70753400
H	-1.23088200	1.11254100	1.85158000

subsequent hydrolysis

Co^{III}(salen)-PO~Cl + H_2O = Co^{III}(salen)-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.844399

Thermal correction to Gibbs Free Energy (a.u.): 0.420106

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5406492 a.u.

C	-2.53956900	4.02049100	-1.81935600
C	-3.54072000	3.03705400	-1.93705000
C	-1.25440200	3.69407400	-1.42410000
H	-2.77896200	5.05726900	-2.03987400
C	-3.21937700	1.72181900	-1.66198400
H	-4.54498000	3.30794900	-2.24433700
C	-0.90433600	2.35792600	-1.10789300
H	-0.48052500	4.44798700	-1.32951400
C	-1.91778600	1.36055800	-1.24705800
H	-3.97002200	0.94033000	-1.74134200
O	0.32139600	2.10726000	-0.71727700
C	-1.62890200	-0.02582200	-1.02219800
Co	0.93633400	0.54566600	0.11961800
N	-0.52501500	-0.47503000	-0.53153900
H	-2.40729600	-0.73777500	-1.28513400
N	1.98935300	-0.96614900	-0.53699200
C	-0.21465800	-1.89649100	-0.37714900
C	3.28341100	-1.04194800	-0.47097800
C	1.15802600	-2.07276400	-1.04988000
C	-1.24252800	-2.89746600	-0.88967600
H	3.77069100	-1.94897900	-0.83496000
C	4.15625600	-0.04221700	0.05075500
C	1.69001600	-3.48881500	-0.82024800
C	-0.71270100	-4.32138500	-0.66443500
H	-1.42571500	-2.73511700	-1.96089900
H	-2.18618900	-2.75104900	-0.35742400
C	5.55218000	-0.29438000	0.00674200
C	3.67278000	1.17887300	0.63285700
C	0.66422200	-4.52442700	-1.31019400
H	2.63982800	-3.64204700	-1.34306100
H	1.88291100	-3.62298500	0.25204900
H	-1.42695300	-5.05002200	-1.06137000
H	-0.64080000	-4.50788300	0.41479300
C	6.46584900	0.60671300	0.50377200
H	5.89058700	-1.22840700	-0.43574600
C	4.64326400	2.08687600	1.14257100
O	2.42057000	1.51266600	0.73250300
H	0.56792400	-4.44275300	-2.40141900
H	1.03670200	-5.53348500	-1.10452900
C	5.99160100	1.80796000	1.07578800
H	7.52950100	0.40039100	0.46011900
H	4.27439000	3.00843200	1.57941300
H	6.70223400	2.52814700	1.47213500
Cl	-4.57538200	-1.29684300	0.41972100
C	-4.33497500	-0.36003500	1.99560800
C	-2.90375400	0.13443600	2.11348200
O	-2.00182300	-0.93596400	2.14734100
H	-4.52620300	-1.11069900	2.76461800
H	-2.87470400	0.72562300	3.04792900
H	-2.69716800	0.83391000	1.29032900
C	-5.34915400	0.77144300	2.03889800
H	-6.36840800	0.39410400	1.93552200
H	-5.26964300	1.29654500	2.99718200
H	-5.15919200	1.48898500	1.23517400

H	1.02002300	-1.90811200	-2.12940700
H	-0.08202200	-2.05507500	0.69920400
O	0.36754700	0.21194000	1.84949500
H	0.91936100	0.74083600	2.44157500
H	-1.09524800	-0.53657900	2.14762100

five-coordinated Co^{III}(salen)-OAc counterion addition in the terminal carbon and subsequent hydrolysis

Co^{III}(salen)-OAc counterion addition in the terminal carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.578263

Thermal correction to Gibbs Free Energy (a.u.): 0.439796

Imaginary frequencies: -405.25

Calculation of single point energy based on the optimized structure, Et = -2839.3258081 a.u.

C	3.47499500	-4.12794700	-1.08590700
C	4.45246900	-3.11229700	-1.10170900
C	2.12826900	-3.82529500	-1.01814000
H	3.78416900	-5.16882000	-1.12213900
C	4.04735700	-1.79424000	-1.05810900
H	5.50593100	-3.36537400	-1.14792600
C	1.68870900	-2.47917100	-0.94864300
H	1.37016000	-4.60050900	-0.99822100
C	2.67714200	-1.45013200	-0.99155700
H	4.78100800	-0.99254500	-1.07107900
O	0.40470500	-2.25173900	-0.84065600
C	2.31588400	-0.06845500	-0.98352200
Co	-0.46405400	-0.61652200	-0.69987000
N	1.10728800	0.39543900	-0.99713700
H	3.13829600	0.64146600	-0.97580500
N	-1.39755100	1.02049500	-1.06467400
C	0.83172800	1.82619300	-0.79943700
C	-2.64533200	1.22171800	-0.78177000
C	-0.49560400	2.09447600	-1.51676400
C	1.92377400	2.79967200	-1.23604100
H	-3.04897800	2.22820300	-0.89258100
C	-3.56389500	0.22175600	-0.33935800
C	-0.97146200	3.52909400	-1.29271000
C	1.44791900	4.24467900	-1.02719100
H	2.17417400	2.63176900	-2.29267200
H	2.82530600	2.62906500	-0.64271700
C	-4.87630200	0.61561200	0.01548500
C	-3.20637500	-1.16338300	-0.31327000
C	0.11805600	4.51635100	-1.73850600
H	-1.89461900	3.72418700	-1.84910500
H	-1.19168400	3.67121200	-0.22675200
H	2.21617600	4.94144100	-1.37794800
H	1.32636000	4.42620000	0.04836600
C	-5.82273500	-0.31000800	0.40093700
H	-5.12512600	1.67350800	-0.01581800
C	-4.20646200	-2.09654200	0.06392400
O	-2.02564000	-1.62018400	-0.63441100
H	0.25975000	4.43000900	-2.82427100
H	-0.21529900	5.54148300	-1.54666600
C	-5.47345500	-1.67634300	0.41877800
H	-6.82141100	0.00479600	0.68277900
H	-3.93024100	-3.14512300	0.07395300
H	-6.21305100	-2.41349400	0.71850600
C	-0.47363600	-1.28020700	2.11479300
C	0.93784200	-0.98908400	2.40852700
O	-0.42000500	-0.18260800	1.21252700
H	-0.64128300	-2.23289600	1.59728200
H	1.71075600	-1.48644600	1.83876000
H	1.22559200	-0.41268200	3.28651700
C	-1.48672100	-1.05766600	3.22015100
H	-2.49386200	-1.04402000	2.79145900
H	-1.43646600	-1.86013500	3.96473200
H	-1.29763900	-0.10145200	3.71567100
H	-0.33273100	1.93742600	-2.59365600

H	0.68146400	1.92324500	0.28309900
C	3.23921100	2.77412400	2.39632200
H	2.60127000	3.52706500	1.91856700
H	4.05720600	2.54605500	1.70660700
H	3.63463900	3.19274300	3.32337600
C	2.40532900	1.51650700	2.69080700
O	2.16853100	0.78248500	1.65935300
O	2.01131100	1.31101000	3.84997700

Co^{III}(salen)-OAc counterion addition in the terminal carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.624810

Thermal correction to Gibbs Free Energy (a.u.): 0.439721

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2839.3717294 a.u.

C	2.81253500	-4.65549700	-0.78514400
C	3.92610600	-3.79180200	-0.79895300
C	1.52267600	-4.15818400	-0.77699100
H	2.96805300	-5.73058500	-0.77342600
C	3.71977100	-2.42699800	-0.81739400
H	4.93224300	-4.19652400	-0.79220600
C	1.28989200	-2.76148300	-0.77806900
H	0.65823000	-4.81279300	-0.75641700
C	2.41367600	-1.88725000	-0.82253900
H	4.55997700	-1.73914900	-0.81662700
O	0.04754300	-2.34129900	-0.72044500
C	2.25834900	-0.46837300	-0.86878500
Co	-0.58211100	-0.60766500	-0.73646500
N	1.12137000	0.16438700	-0.93226000
H	3.16725200	0.11869300	-0.85012500
N	-1.25205700	1.15709200	-0.99066300
C	1.08253600	1.62866600	-0.78287800
C	-2.44541000	1.53162100	-0.65564000
C	-0.21082700	2.09892900	-1.44540000
C	2.28650100	2.40921300	-1.30772600
H	-2.68478000	2.59372800	-0.69487500
C	-3.50225700	0.65509000	-0.25679100
C	-0.45808000	3.58053200	-1.16541400
C	2.05827600	3.90257400	-1.02679100
H	2.42305300	2.22699300	-2.38391800
H	3.18453200	2.08430100	-0.77966400
C	-4.72888100	1.21223300	0.17118200
C	-3.36776800	-0.76441300	-0.36313500
C	0.74861500	4.40452800	-1.64490400
H	-1.36588700	3.92908900	-1.67133100
H	-0.59668700	3.71891000	-0.08611600
H	2.90202500	4.48642000	-1.41001000
H	2.03161000	4.03429500	0.06084600
C	-5.80105900	0.40917300	0.50358400
H	-4.81158900	2.29386700	0.23952100
C	-4.49286000	-1.56590600	-0.04508200
O	-2.27134600	-1.36087800	-0.75515900
H	0.80981800	4.34426700	-2.74051900
H	0.58712100	5.45913300	-1.39772500
C	-5.67228600	-0.98983400	0.38743500
H	-6.73333800	0.84692200	0.84295400
H	-4.38423900	-2.64054000	-0.14169400
H	-6.51409900	-1.62754400	0.64159300
C	-0.62518000	-1.40134900	2.26704600
C	0.36528900	-0.31753000	2.31462700
O	-0.73686700	-0.27142700	1.35047800
H	-0.34322100	-2.31463100	1.74735000
H	1.35345000	-0.41523800	1.87052000
H	0.28420800	0.46433000	3.06217300
C	-1.76327400	-1.51435600	3.24083500
H	-2.66447600	-1.86945500	2.73064500
H	-1.51271000	-2.22832100	4.03247700
H	-1.97932700	-0.54522900	3.69803500

H	-0.12106100	1.94797900	-2.53239800
H	1.03959700	1.82046800	0.30884600
C	4.01706200	2.31003400	2.91205500
H	4.66179300	2.95820600	2.30615000
H	4.64380300	1.51179200	3.31793500
H	3.59313500	2.91245300	3.71868200
C	2.91071800	1.72907900	2.01640200
O	3.21868500	0.70267500	1.33747200
O	1.80180900	2.33500300	2.00829900

Co^{III}(salen)-OAc counterion addition in the terminal carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.660799

Thermal correction to Gibbs Free Energy (a.u.): 0.443593

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2839.4080301 a.u.

C	3.14224200	-4.44078900	-0.89773000
C	4.01830200	-3.56177100	-1.57366400
C	1.92819300	-4.00902400	-0.40709600
H	3.43194300	-5.47869400	-0.75770600
C	3.64089100	-2.24874200	-1.74237700
H	4.97157100	-3.91765100	-1.94864600
C	1.50946900	-2.65733900	-0.56194500
H	1.25540900	-4.67779500	0.11839800
C	2.39593200	-1.77051200	-1.26102000
H	4.29781500	-1.55008100	-2.25534400
O	0.37301900	-2.30077900	-0.04344700
C	2.07085500	-0.39595800	-1.44883500
Co	-0.57455900	-0.69500200	-0.33861200
N	0.93214500	0.15165500	-1.15445000
H	2.85791100	0.23504500	-1.86295500
N	-1.55812400	0.82774000	-1.01377800
C	0.70677600	1.60038600	-1.17186100
C	-2.81201200	1.03600200	-0.78649000
C	-0.70971000	1.79429000	-1.72939800
C	1.73071000	2.46118800	-1.90501900
H	-3.25279900	1.98304300	-1.10140800
C	-3.70727800	0.10105600	-0.17583600
C	-1.13206000	3.26262100	-1.64586900
C	1.31277300	3.93699700	-1.82528100
H	1.80442900	2.14858100	-2.95577200
H	2.72051400	2.33409500	-1.45447300
C	-5.03846900	0.50506800	0.07711100
C	-3.30954100	-1.24638700	0.08979000
C	-0.10594400	4.15183200	-2.36484000
H	-2.11862300	3.41192900	-2.09614800
H	-1.20833700	3.54693100	-0.58868400
H	2.02707400	4.55724500	-2.37671300
H	1.35560500	4.26250700	-0.77765700
C	-5.97130500	-0.37382400	0.58875100
H	-5.31663100	1.53390100	-0.13945600
C	-4.29465500	-2.13573000	0.58942000
O	-2.10598000	-1.71278300	-0.11852600
H	-0.12267700	3.92364500	-3.43911600
H	-0.39571100	5.20301300	-2.26442100
C	-5.58399800	-1.70534100	0.83923700
H	-6.98652500	-0.04910700	0.78894300
H	-3.98969600	-3.15889900	0.77971700
H	-6.31072000	-2.40846200	1.23690600
C	0.26524400	-0.26309000	2.39998900
C	1.78698000	-0.27711200	2.17946900
O	-0.39219900	0.25604100	1.28346700
H	-0.00737800	-1.31993100	2.57266600
H	2.04313600	-0.98818300	1.39675000
H	2.32233500	-0.52077200	3.09935000
C	-0.14150800	0.55630700	3.62822800
H	-1.22411200	0.48829800	3.76528200
H	0.35884900	0.20241300	4.53512700

H	0.11595000	1.60928300	3.48137400
H	-0.69283700	1.48642500	-2.78654600
H	0.68165200	1.88016700	-0.11071500
C	3.16738600	3.15746200	1.88242900
H	2.24043300	3.67573300	1.61617800
H	3.72219000	2.97726700	0.95764300
H	3.75154500	3.78211300	2.55723800
C	2.83076500	1.84936500	2.56303500
O	2.25580500	1.00335400	1.68441300
O	3.03965300	1.60110400	3.73023300

subsequent hydrolysis (H_2O molecule is opposite the counterion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.063964

Thermal correction to Gibbs Free Energy (a.u.): 0.465454

Imaginary frequencies: -645.48

Calculation of single point energy based on the optimized structure, Et = -2915.8640066 a.u.

C	-0.46642600	5.19974900	-0.81213800
C	-1.16028700	4.82521100	-1.98070800
C	0.04388000	4.25315000	0.05467800
H	-0.32918600	6.25369100	-0.58616900
C	-1.32944500	3.48341600	-2.24954300
H	-1.55691400	5.57943600	-2.65132500
C	-0.10291000	2.86401000	-0.19792700
H	0.57220600	4.53877700	0.95767300
C	-0.80640400	2.48504300	-1.39400700
H	-1.87120000	3.16733400	-3.13793800
O	0.34927600	2.02222600	0.69305500
C	-1.08323700	1.11092800	-1.69665300
Co	0.85620000	0.26113200	0.25183400
N	-0.52584500	0.11269600	-1.09735200
H	-1.83723100	0.91337600	-2.46198000
N	1.33366300	-1.48445400	-0.37393900
C	-0.94966500	-1.28370700	-1.17631500
C	2.54134800	-1.95223700	-0.32204600
C	0.32573200	-2.12941800	-1.24012000
C	-1.93240700	-1.70067400	-2.26182800
H	2.71451500	-2.96516000	-0.69623500
C	3.69467500	-1.21071900	0.07874600
C	-0.01983100	-3.58504200	-0.92343500
C	-2.28434800	-3.18438600	-2.04312300
H	-1.49717800	-1.55034600	-3.25934600
H	-2.84144900	-1.09398500	-2.20013100
C	4.91184100	-1.89000800	0.31076200
C	3.66607800	0.22483400	0.06162700
C	-1.04021500	-4.08413700	-1.96227800
H	0.87391200	-4.21766900	-0.94409100
H	-0.43328900	-3.63335300	0.09050500
H	-2.94798800	-3.53434500	-2.84095100
H	-2.84620400	-3.26849300	-1.10514800
C	6.08050400	-1.19876700	0.55696700
H	4.90988800	-2.97728900	0.29978100
C	4.89149200	0.90582700	0.28287900
O	2.59134500	0.92175400	-0.18336900
H	-0.55385900	-4.11743400	-2.94670200
H	-1.33876300	-5.11122600	-1.72745700
C	6.05849300	0.21123400	0.53540400
H	7.00565900	-1.72968800	0.75330900
H	4.86859400	1.98994200	0.25900600
H	6.97704600	0.76232500	0.71769300
H	0.71649900	-2.07618100	-2.26746500
H	-1.40562800	-1.46642100	-0.19735900
O	1.55957600	-0.10055000	2.17102000
H	1.59498100	0.78039500	2.56906700
H	0.47472900	-0.46587800	2.20652900
C	-1.63618100	0.09189700	2.35963500
C	-2.65494400	0.73784300	1.42202200
O	-0.66050400	-0.64579800	1.66758100

H	-1.17252100	0.95159800	2.88145900
H	-2.15021800	1.38252300	0.70760300
H	-3.39065300	1.31127400	1.98854500
C	-2.30402200	-0.80821300	3.40374400
H	-1.55284000	-1.17931400	4.10648300
H	-3.08499200	-0.27954900	3.95904400
H	-2.75532900	-1.67446900	2.91015300
C	-5.17042300	-1.66545700	0.11403800
H	-6.23934900	-1.77352700	0.29460400
H	-4.66612700	-2.60551400	0.35956200
H	-4.98262900	-1.45598400	-0.94194200
C	-4.62110100	-0.56200600	0.98803200
O	-3.35577100	-0.25402100	0.62534000
O	-5.22639500	-0.03527700	1.89540500

subsequent hydrolysis (H_2O molecule is opposite the counterion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.090804

Thermal correction to Gibbs Free Energy (a.u.): 0.469169

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8966966 a.u.

C	-4.13790900	3.85219300	-0.45399600
C	-4.92152000	2.80303600	-0.98486600
C	-2.79514600	3.68290500	-0.18935800
H	-4.60252700	4.81225900	-0.24666100
C	-4.32279500	1.59031000	-1.24146600
H	-5.97706800	2.95299200	-1.18293300
C	-2.14885300	2.44070600	-0.43944600
H	-2.18960100	4.48268400	0.22250700
C	-2.94331300	1.38097900	-0.98841200
H	-4.90384800	0.76538800	-1.64675500
O	-0.88764400	2.33075100	-0.14345600
C	-2.38465200	0.09907800	-1.25953300
Co	0.27699200	0.90889300	-0.53650400
N	-1.13211800	-0.22248900	-1.14322300
H	-3.08511900	-0.67223500	-1.57923700
N	1.43389900	-0.44054500	-1.28486100
C	-0.65384700	-1.60760700	-1.26948500
C	2.70249000	-0.48844700	-1.05323000
C	0.70380100	-1.51401400	-1.97793000
C	-1.58066800	-2.60813800	-1.95406700
H	3.25807700	-1.37525100	-1.35598500
C	3.46256200	0.56591000	-0.45152100
C	1.39309000	-2.87762300	-2.03803300
C	-0.89436800	-3.98167300	-2.01218500
H	-1.82462900	-2.26402100	-2.96880800
H	-2.52169700	-2.69319700	-1.40033700
C	4.83084100	0.34564300	-0.17709000
C	2.89269200	1.85814100	-0.23286700
C	0.46762600	-3.90247600	-2.71104500
H	2.32938000	-2.80927600	-2.60298600
H	1.63046400	-3.18164000	-1.01238600
H	-1.54483800	-4.69816100	-2.52490400
H	-0.75507300	-4.35155600	-0.98896200
C	5.63599600	1.35501500	0.31255400
H	5.24182400	-0.64455800	-0.35836800
C	3.74740900	2.88512500	0.23738100
O	1.63668000	2.15440600	-0.46029700
H	0.31884300	-3.62577500	-3.76403100
H	0.94947100	-4.88577900	-2.71135900
C	5.07909100	2.63311600	0.51209900
H	6.68203500	1.17074300	0.53182700
H	3.31108600	3.86619000	0.38948400
H	5.70460100	3.43699400	0.89021200
H	0.51481700	-1.15376000	-3.00122200
H	-0.47193100	-1.93933000	-0.24290400
O	1.36046100	-2.48007000	1.23124600
H	1.96274300	-2.53978500	1.98157200

H	1.05283900	-1.53095900	1.23189300
C	-0.13844100	0.49016400	2.32114800
C	-1.60953900	0.02732100	2.31965200
O	0.51020900	0.03779000	1.16339600
H	-0.17714400	1.59174300	2.33674800
H	-2.17885600	0.61084600	1.59673700
H	-2.06157700	0.11746000	3.31009700
C	0.64841600	0.01910100	3.54814000
H	1.66245400	0.42712200	3.50086100
H	0.17505000	0.35008600	4.47752900
H	0.70934500	-1.07137600	3.57566600
C	-1.60540400	-3.66804900	2.10567800
H	-1.82581700	-4.45877900	2.82242600
H	-0.57677000	-3.76240500	1.73797700
H	-2.28274600	-3.72610300	1.24969300
C	-1.69779900	-2.32374700	2.78022700
O	-1.73217500	-1.33653500	1.85625400
O	-1.69923200	-2.13650200	3.97794600

subsequent hydrolysis (H_2O molecule is opposite the counterion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.091716

Thermal correction to Gibbs Free Energy (a.u.): 0.468406

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.8967308 a.u.

C	1.33877500	5.84783500	0.46509700
C	-0.01581700	5.93898600	0.09008000
C	1.99698700	4.63174100	0.48805800
H	1.87936400	6.74903400	0.74117300
C	-0.68742100	4.78572200	-0.26413100
H	-0.51914400	6.89948000	0.07465900
C	1.32445400	3.43066800	0.15124000
H	3.04042300	4.55530300	0.77351800
C	-0.04714900	3.52649300	-0.23630500
H	-1.72991100	4.83044600	-0.57060200
O	1.99396700	2.30689300	0.19443800
C	-0.76837800	2.37451100	-0.68765300
Co	1.30792100	0.56781400	0.11919600
N	-0.33474700	1.15924200	-0.65274400
H	-1.75254400	2.55819400	-1.11929400
N	1.16495800	-0.86444800	-1.18978400
C	-1.06679500	0.02098200	-1.21695700
C	1.94960300	-1.89800900	-1.22186800
C	-0.03417500	-0.76330100	-2.04472900
C	-2.32205500	0.32649700	-2.02538400
H	1.71698600	-2.70383200	-1.91877800
C	3.11177200	-2.09731700	-0.42021500
C	-0.63836800	-2.08673800	-2.51891200
C	-2.93265300	-0.99645000	-2.51048000
H	-2.08107300	0.97055400	-2.88267100
H	-3.04555000	0.85658500	-1.39964500
C	3.84980300	-3.29417600	-0.60713400
C	3.55461700	-1.13410900	0.54522500
C	-1.92471600	-1.82315800	-3.31664600
H	0.06771600	-2.63730900	-3.14936600
H	-0.85374300	-2.69688200	-1.63371800
H	-3.82726100	-0.79769800	-3.11077900
H	-3.25004300	-1.57236700	-1.63321800
C	4.99331500	-3.55662000	0.11306900
H	3.48893800	-4.01025400	-1.34149200
C	4.74261200	-1.43010800	1.26884100
O	2.95226000	-0.00880300	0.80021200
H	-1.67443900	-1.28886000	-4.24341100
H	-2.37141900	-2.77700500	-3.61627000
C	5.43517000	-2.60378100	1.05669700
H	5.54632900	-4.47675800	-0.03967900
H	5.07727800	-0.69485600	1.99240500
H	6.33745700	-2.79795900	1.63016000

H	0.24154000	-0.14762400	-2.91488600
H	-1.34430800	-0.62212700	-0.37671100
O	0.41224900	-0.03216600	1.65342600
H	1.12415000	-0.21715200	2.28406500
H	-0.37655000	-1.47651700	1.26998000
C	-2.01650400	-2.29436200	1.96211700
C	-2.67768900	-0.93482500	2.21166200
O	-0.97883900	-2.21823600	0.99829200
H	-1.59888800	-2.58783900	2.94208700
H	-1.90554000	-0.17185500	2.32777900
H	-3.31467700	-0.98113900	3.09651800
C	-2.99751400	-3.36748200	1.51048900
H	-2.48071800	-4.32584700	1.41613100
H	-3.82557700	-3.46833000	2.21618400
H	-3.40826600	-3.10674700	0.53012700
C	-5.54274500	-0.09877900	-0.00598100
H	-6.61820000	-0.13643000	0.16299800
H	-5.28867500	-0.69919200	-0.88372400
H	-5.23075000	0.92961900	-0.20740600
C	-4.82900400	-0.63517800	1.21242800
O	-3.48810700	-0.49692000	1.08797600
O	-5.38215900	-1.12119700	2.17460900

subsequent hydrolysis (H_2O molecule is at the same side with the ion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.065275

Thermal correction to Gibbs Free Energy (a.u.): 0.466537

Imaginary frequencies: -750.48

Calculation of single point energy based on the optimized structure, Et = -2915.8642924 a.u.

C	4.13047700	2.22445600	-2.00414500
C	3.47346000	3.42320300	-2.34948200
C	3.49804500	1.23875700	-1.27071500
H	5.15880800	2.06869400	-2.31905300
C	2.17212300	3.60965600	-1.93303700
H	3.98509700	4.18561100	-2.92679500
C	2.15427700	1.39751700	-0.83915900
H	4.00766100	0.32543200	-0.98530900
C	1.48578100	2.61862500	-1.19213300
H	1.64570200	4.53046900	-2.17400000
O	1.63458200	0.45806400	-0.09037900
C	0.16077400	2.90284200	-0.72620100
Co	-0.22628000	0.10573200	-0.00384100
N	-0.62461900	2.02137500	-0.20520700
H	-0.18076800	3.93842000	-0.80606600
N	-2.14131100	-0.04557200	-0.10499600
C	-1.87898300	2.29575100	0.48948800
C	-2.74204000	-1.10704200	-0.53530200
C	-2.87762800	1.22661900	0.02823700
C	-2.49800600	3.68587100	0.38183400
H	-3.83526000	-1.10679300	-0.55979300
C	-2.09075800	-2.25498100	-1.08824600
C	-4.08693000	1.21580700	0.96536700
C	-3.75544900	3.73184300	1.26992800
H	-2.75814600	3.90600600	-0.66253200
H	-1.78699700	4.45177700	0.70997700
C	-2.83320900	-3.43570600	-1.30629400
C	-0.74567700	-2.15875800	-1.57105300
C	-4.74796600	2.60511600	0.94172500
H	-4.81210500	0.45284000	0.66372200
H	-3.74733600	0.96042900	1.97602200
H	-4.24768800	4.70486800	1.17003800
H	-3.44426200	3.64235700	2.31853500
C	-2.27667500	-4.52264200	-1.95216100
H	-3.85775800	-3.47908200	-0.94487400
C	-0.21193900	-3.27570200	-2.26041900
O	-0.00025100	-1.09172600	-1.43377800
H	-5.17224500	2.77756800	-0.05674800
H	-5.58660100	2.62994100	1.64532700

C	-0.95652900	-4.42834600	-2.43407600
H	-2.84983900	-5.43202700	-2.09635000
H	0.80478100	-3.19406500	-2.62904800
H	-0.51367700	-5.27466000	-2.95176200
C	0.53524400	-2.75323100	1.41036000
C	1.97035600	-2.40293100	1.03515000
O	-0.33960000	-1.65864900	1.30152600
H	0.22625000	-3.51704400	0.67769100
H	2.01597800	-1.99049200	0.02643500
H	2.62467200	-3.27866900	1.09827000
C	0.43322900	-3.35721200	2.81437100
H	-0.60930700	-3.59945500	3.03640200
H	1.03191100	-4.27128400	2.89864700
H	0.78954300	-2.64033300	3.55982400
H	-3.21685900	1.50391300	-0.98119400
H	-1.64727700	2.08518400	1.54138400
O	-0.10622600	0.50998200	2.08850100
H	0.84127000	0.68464400	2.17464300
H	-0.16817100	-0.66734000	1.99605600
C	3.89108200	0.38925100	2.48804600
H	3.41453100	0.31585300	3.46751700
H	3.47085200	1.25157000	1.95892900
H	4.96596700	0.53994000	2.59241500
C	3.62490700	-0.83471000	1.64720600
O	2.44120100	-1.39108600	1.95559800
O	4.36461600	-1.25083000	0.77866600

subsequent hydrolysis (H_2O molecule is at the same side with the ion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.094813

Thermal correction to Gibbs Free Energy (a.u.): 0.468725

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.9033149 a.u.

C	-4.47647700	0.26256600	-2.33958700
C	-4.74163500	-1.05422700	-1.91406100
C	-3.22572200	0.83011000	-2.18032400
H	-5.26958400	0.84913600	-2.79434800
C	-3.72646800	-1.77999300	-1.32168900
H	-5.72710200	-1.48737000	-2.04588400
C	-2.16833700	0.10778700	-1.57281300
H	-3.02143700	1.84863700	-2.48873400
C	-2.44070200	-1.22346600	-1.13409500
H	-3.90445600	-2.79701200	-0.98111500
O	-1.00473400	0.69518500	-1.44868500
C	-1.41998600	-2.03942100	-0.54903900
Co	0.46438100	0.11208800	-0.44371600
N	-0.20825700	-1.66025000	-0.31910500
H	-1.69808600	-3.06327700	-0.30792100
N	2.19682100	-0.77256800	-0.54946100
C	0.80296400	-2.51875900	0.30058600
C	3.33825900	-0.15435800	-0.53768800
C	2.09422400	-2.24290200	-0.48771100
C	0.48541100	-4.00797500	0.39235900
H	4.25222000	-0.74962600	-0.50484100
C	3.52421200	1.25897000	-0.55810900
C	3.28190700	-2.98743700	0.12386300
C	1.67990200	-4.75430000	1.00436700
H	0.27030100	-4.40478200	-0.60929600
H	-0.40541400	-4.15565600	1.01037400
C	4.85100500	1.75876500	-0.51027900
C	2.42302300	2.17419900	-0.64254900
C	2.97204000	-4.48948500	0.22273900
H	4.18558300	-2.84100200	-0.47689000
H	3.48330300	-2.57755800	1.12229300
H	1.46909000	-5.82818500	1.03583900
H	1.81030100	-4.42876400	2.04451400
C	5.11362000	3.10973000	-0.54047600
H	5.66788900	1.04366800	-0.44669600

C	2.72681900	3.56343400	-0.67911500
O	1.17286700	1.82375200	-0.70297400
H	2.87538900	-4.90372800	-0.78991000
H	3.81456600	-5.00711000	0.69296000
C	4.02991200	4.01142400	-0.62730300
H	6.13275000	3.47780400	-0.49869600
H	1.89038000	4.25022400	-0.74834600
H	4.22480600	5.08005700	-0.65257900
C	-0.05784600	1.54612100	1.99771200
C	-1.26239000	2.25381600	1.38171000
O	0.16733000	0.28615500	1.40258300
H	0.79483900	2.21590800	1.80299700
H	-1.11172800	2.41341600	0.31390200
H	-1.43628200	3.22097900	1.86438600
C	-0.19931400	1.34520200	3.50916700
H	0.71408300	0.89533800	3.90806400
H	-0.36815900	2.30034500	4.01841100
H	-1.03281900	0.67262200	3.72502600
H	1.93505900	-2.60281900	-1.51542500
H	0.94800600	-2.12216700	1.31451500
O	-1.78287500	-1.46587800	2.28970900
H	-2.49785900	-0.83525400	2.13631800
H	-1.00969400	-0.91392500	2.03929900
C	-4.71004700	0.91636000	1.23503000
H	-4.78644200	0.64394800	2.29167800
H	-4.51660800	0.00552400	0.66163000
H	-5.64368900	1.36242500	0.89465400
C	-3.58043400	1.89453500	1.02523300
O	-2.43498600	1.42243200	1.56501800
O	-3.66523500	2.95802500	0.45141700

subsequent hydrolysis (H_2O molecule is at the same side with the ion OAc^-)

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.083433

Thermal correction to Gibbs Free Energy (a.u.): 0.469000

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.8919409 a.u.

C	3.94843600	-3.20873200	-1.57443200
C	4.97279500	-2.23540500	-1.53567800
C	2.64862300	-2.90304100	-1.22960300
H	4.18915600	-4.22349800	-1.87949700
C	4.65996100	-0.95643400	-1.13475600
H	5.98890700	-2.49700400	-1.80998200
C	2.29282500	-1.58581800	-0.82601400
H	1.86132900	-3.64869300	-1.23500200
C	3.33356500	-0.59814300	-0.78166200
H	5.43211300	-0.19233100	-1.08270900
O	1.05662900	-1.36660400	-0.48070100
C	3.08094700	0.72089900	-0.30314400
Co	0.22626900	0.30550200	-0.29371500
N	1.90378800	1.21042900	-0.06059300
H	3.95523900	1.34522800	-0.10934100
N	-0.51101600	2.08668300	-0.31702800
C	1.66416900	2.46397400	0.65920600
C	-1.73156100	2.37847000	-0.63601000
C	0.48166400	3.14118700	-0.04206200
C	2.83638300	3.42804700	0.82317400
H	-2.05080300	3.41937500	-0.56154100
C	-2.70179100	1.45956300	-1.13605600
C	-0.00525500	4.33798700	0.77952300
C	2.37617000	4.65568400	1.62623300
H	3.20511700	3.73760400	-0.16427300
H	3.66690900	2.93907900	1.34324500
C	-4.03136400	1.89980300	-1.32063000
C	-2.32839100	0.13979500	-1.52795600
C	1.15158700	5.32763100	0.99202200
H	-0.83182500	4.85047600	0.27815900
H	-0.38483800	3.97236800	1.74150400

H	3.19893800	5.37287600	1.71316700
H	2.12631000	4.33721400	2.64648200
C	-4.98899800	1.07098500	-1.86799400
H	-4.29072800	2.91002900	-1.01333600
C	-3.31778400	-0.67831200	-2.12376500
O	-1.11883400	-0.34718600	-1.39338100
H	1.43638800	5.75723900	0.02203000
H	0.81377100	6.16177100	1.61565400
C	-4.61543600	-0.22542900	-2.27340100
H	-6.01076800	1.41241500	-1.99239500
H	-3.02356700	-1.67368400	-2.43806000
H	-5.35925100	-0.88283700	-2.71524200
C	-3.10500500	-1.80398500	1.54422800
C	-2.08570500	-2.69062800	0.82661000
O	-2.87934900	-0.41938000	1.38534200
H	-4.05657600	-2.00482700	1.03111100
H	-1.85855300	-2.30797600	-0.16947300
H	-2.45707100	-3.71569300	0.74286100
C	-3.25772400	-2.18338100	3.02152300
H	-4.03783500	-1.56822400	3.47670400
H	-3.52634500	-3.23943300	3.14171400
H	-2.32096000	-2.00672300	3.55722200
H	0.84277700	3.50297000	-1.01770300
H	1.30838200	2.14953400	1.65052000
O	-0.23561900	0.10109900	1.52990200
H	-0.06337900	-0.83167000	1.73445700
H	-1.93120600	-0.19937800	1.55776900
C	1.34117200	-3.47868700	2.00129100
H	1.10540000	-3.61563100	3.06046200
H	1.76263500	-2.47811500	1.87652500
H	2.06779800	-4.22254500	1.67779200
C	0.08813300	-3.60224800	1.16908700
O	-0.84933300	-2.72300500	1.58762000
O	-0.08107200	-4.38628900	0.26077300

five-coordinated Co^{III}(salen)-OAc counterion addition in the middle carbon and subsequent hydrolysis

Co^{III}(salen)-OAc counterion addition in the middle carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.580947

Thermal correction to Gibbs Free Energy (a.u.): 0.439188

Imaginary frequencies: -328.79

Calculation of single point energy based on the optimized structure, Et = -2839.3288504 a.u.

C	3.15844500	-4.26170300	-1.34277700
C	4.13964000	-3.27078000	-1.53410100
C	1.84606200	-3.92529400	-1.06023800
H	3.43455100	-5.31012600	-1.41252300
C	3.77341100	-1.94141400	-1.44729300
H	5.16570600	-3.54791500	-1.74964900
C	1.45494600	-2.57035300	-0.94045400
H	1.08593500	-4.68242200	-0.90179600
C	2.44260700	-1.56702200	-1.16109000
H	4.51064200	-1.15703300	-1.59763800
O	0.21135400	-2.30904300	-0.60873500
C	2.10629000	-0.17553800	-1.13369400
Co	-0.61538300	-0.65982800	-0.39545800
N	0.91950600	0.30041400	-0.96179600
H	2.92275300	0.52308500	-1.29624400
N	-1.58776000	0.90256900	-0.97761600
C	0.65142000	1.73978300	-0.86758100
C	-2.84804300	1.10453500	-0.75259500
C	-0.70789400	1.94164000	-1.54933100
C	1.71754800	2.67489800	-1.42727000
H	-3.27441800	2.07128800	-1.02203800
C	-3.75504600	0.16513500	-0.17686400
C	-1.18294100	3.38835300	-1.40953300
C	1.24505400	4.12894600	-1.28879000
H	1.91093900	2.44020100	-2.48348900

H	2.64565700	2.53576200	-0.86870200
C	-5.09862100	0.56660600	0.02691400
C	-3.35488600	-1.16858100	0.15630500
C	-0.11610400	4.34897600	-1.95857600
H	-2.12442400	3.54544200	-1.94666400
H	-1.36914400	3.59938900	-0.34863100
H	1.99229600	4.80512200	-1.71685100
H	1.16960400	4.37678000	-0.22228400
C	-6.03716300	-0.29983000	0.54325000
H	-5.37767700	1.58471400	-0.23344300
C	-4.34708800	-2.04471000	0.67138100
O	-2.14786000	-1.63626100	-0.00063400
H	-0.01775800	4.19516100	-3.04176900
H	-0.44884600	5.38271600	-1.81834300
C	-5.64543100	-1.61755500	0.86210000
H	-7.06067900	0.02205800	0.70036200
H	-4.03903600	-3.05612900	0.91258400
H	-6.37822200	-2.31005600	1.26690700
C	0.98644100	-0.52021500	2.78277600
C	-0.46321700	-0.68338300	2.53812600
O	-0.38067200	0.10463300	1.37434100
H	1.34881800	0.32889100	3.37030200
H	-1.10908100	-0.22525900	3.29829600
H	-0.78254500	-1.71794400	2.34903600
C	1.91349100	-1.60640500	2.42252600
H	1.55996600	-2.17624900	1.56229900
H	2.92858100	-1.25081500	2.26373000
H	1.89714200	-2.29760400	3.28499400
H	-0.58616400	1.70515300	-2.61724300
H	0.54644600	1.92572100	0.20754100
C	3.65940800	2.98491500	1.82345400
H	3.05484200	3.76125300	1.33943600
H	4.35502800	2.58894900	1.07784000
H	4.21019800	3.44556000	2.64573600
C	2.73259600	1.87910000	2.35508100
O	2.35380900	1.01447300	1.48661000
O	2.40042500	1.90971900	3.55606100

Co^{III}(salen)-OAc counterion addition in the middle carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.622238

Thermal correction to Gibbs Free Energy (a.u.): 0.441197

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2839.3700868 a.u.

C	3.15683200	-4.39552800	-0.86350500
C	4.17162200	-3.43125900	-1.02519400
C	1.83271000	-4.02260300	-0.72630300
H	3.41796300	-5.44967200	-0.83806600
C	3.83131600	-2.09351100	-1.05840600
H	5.20756400	-3.73813400	-1.11928100
C	1.46488500	-2.65547400	-0.74095500
H	1.04452900	-4.75455100	-0.58832300
C	2.48611400	-1.68067400	-0.93335300
H	4.59516800	-1.32987500	-1.17047800
O	0.20137900	-2.35413500	-0.55167700
C	2.18750100	-0.28512200	-0.99552600
Co	-0.60362300	-0.69991600	-0.59943200
N	0.99180200	0.22747400	-0.95498700
H	3.02780100	0.39155400	-1.07945900
N	-1.47579700	0.96188600	-0.96121700
C	0.80609600	1.68452700	-0.85986200
C	-2.69790800	1.22869200	-0.63042400
C	-0.55210600	1.98412900	-1.49251400
C	1.90058700	2.56241500	-1.46302100
H	-3.05307400	2.25238400	-0.74356200
C	-3.65093400	0.27903700	-0.14441300
C	-0.94850200	3.44315300	-1.26927700
C	1.52277000	4.03274700	-1.22987200

H	2.01556400	2.35308100	-2.53704200
H	2.84176800	2.35269300	-0.95213500
C	-4.93348700	0.73429000	0.23882600
C	-3.35871700	-1.11980200	-0.11649700
C	0.14886700	4.36906900	-1.81987700
H	-1.90084300	3.67168900	-1.76154700
H	-1.07491600	3.61399400	-0.19299400
H	2.28745400	4.68713900	-1.66170500
H	1.51623800	4.20752600	-0.14770100
C	-5.91219000	-0.14814800	0.64919600
H	-5.13597200	1.80174400	0.20611400
C	-4.38964800	-2.00781600	0.28077000
O	-2.19922600	-1.62549900	-0.45178200
H	0.18399400	4.26979200	-2.91372800
H	-0.11747000	5.41019600	-1.60836100
C	-5.62851400	-1.52897500	0.66210200
H	-6.88924100	0.21321700	0.95043800
H	-4.16158400	-3.06798500	0.28520100
H	-6.39604100	-2.23006500	0.97718200
C	0.20227900	-0.26877900	2.60166300
C	-1.16526800	-0.81293000	2.58141600
O	-0.67302800	-0.06529200	1.44492000
H	0.38614000	0.68407400	3.08961400
H	-1.97603700	-0.31503700	3.10773900
H	-1.30668800	-1.87372000	2.38598000
C	1.40117200	-1.15242900	2.41751300
H	1.13568400	-2.07284800	1.89320300
H	2.18318700	-0.61727900	1.87148600
H	1.79666800	-1.41707200	3.40477400
H	-0.47865300	1.79303400	-2.57442200
H	0.79011100	1.90613300	0.22755400
C	3.71370800	2.40389000	3.02945700
H	4.74722600	2.47606800	2.68169800
H	3.68651200	1.65191800	3.82775000
H	3.38332300	3.35595100	3.45144000
C	2.78555200	1.95246100	1.88952800
O	3.28877700	1.16471200	1.03460600
O	1.59222500	2.36997700	1.92867100

Co^{III}(salen)-OAc counterion addition in the middle carbon

Co^{III}(salen)-OAc + PO = Co^{III}(salen)-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1600.664101

Thermal correction to Gibbs Free Energy (a.u.): 0.445555

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2839.4105013 a.u.

C	4.23844800	-1.43890400	-2.63287500
C	4.84818000	-0.24224800	-2.20504100
C	2.89114800	-1.67052900	-2.42979900
H	4.83763100	-2.19481700	-3.13315000
C	4.07260200	0.70922200	-1.57377300
H	5.90563200	-0.07166000	-2.37485000
C	2.07628400	-0.72164600	-1.76136100
H	2.41729600	-2.58881300	-2.75869000
C	2.69714500	0.49240900	-1.33163200
H	4.51639400	1.64443100	-1.23984700
O	0.80968200	-0.99405700	-1.59149700
C	1.94130800	1.52555500	-0.69142900
Co	-0.36504300	-0.15961800	-0.36761200
N	0.71464900	1.41701100	-0.30487000
H	2.45500900	2.47547600	-0.53568700
N	-1.84740100	1.13176800	-0.50965600
C	-0.05605900	2.50477600	0.29810000
C	-3.10126400	0.80537300	-0.46293000
C	-1.39046000	2.53019700	-0.47662400
C	0.59972100	3.88271000	0.33906600
H	-3.85117400	1.59856700	-0.43808900
C	-3.61539100	-0.52617900	-0.42968000
C	-2.35606000	3.55092900	0.12933200

C	-0.36908200	4.90273400	0.95458900
H	0.86873600	4.19602300	-0.67893800
H	1.52496600	3.84431900	0.92410500
C	-5.02222000	-0.69154600	-0.36027700
C	-2.76635500	-1.68252200	-0.46870600
C	-1.70019300	4.93843500	0.19503500
H	-3.27629900	3.61156100	-0.46079900
H	-2.63687100	3.21848900	1.13727400
H	0.09193000	5.89582500	0.96008700
H	-0.55454600	4.63508300	2.00289500
C	-5.60353900	-1.93941400	-0.32854000
H	-5.64292900	0.20110300	-0.33074900
C	-3.39714500	-2.95760600	-0.43739000
O	-1.46933700	-1.65320800	-0.54719400
H	-1.52487000	5.30272900	-0.82619400
H	-2.38801800	5.64820500	0.66619800
C	-4.76918300	-3.07766400	-0.36911800
H	-6.68095600	-2.04851400	-0.27196300
H	-2.75033400	-3.82744800	-0.47045300
H	-5.21466800	-4.06847200	-0.34382200
C	1.05693500	-2.45587100	1.89081300
C	-0.16364100	-1.52740900	2.13627500
O	-0.08464500	-0.31828400	1.43689700
H	1.26004600	-2.99824200	2.82084300
H	-0.19004100	-1.27646600	3.20346100
H	-1.07149100	-2.09793700	1.89060700
C	0.89787700	-3.43057100	0.73509900
H	0.70291800	-2.90886400	-0.20210100
H	1.80390700	-4.03492400	0.62804800
H	0.05640300	-4.10055400	0.93689100
H	-1.15828800	2.82540100	-1.51140200
H	-0.27743200	2.17153700	1.32084700
C	3.83997400	-0.01185000	2.06022500
H	3.38741000	0.93924000	1.76132200
H	4.33515200	-0.43587700	1.18593900
H	4.55283700	0.18269700	2.86260300
C	2.74007200	-0.91286700	2.57147400
O	2.23024600	-1.66220400	1.57846100
O	2.35811600	-0.94762000	3.72306000

subsequent hydrolysis

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.065362

Thermal correction to Gibbs Free Energy (a.u.): 0.465599

Imaginary frequencies: -668.03

Calculation of single point energy based on the optimized structure, Et = -2915.8632676 a.u.

C	-1.76912900	4.69548300	-0.93909600
C	-2.38251200	4.08767700	-2.05383000
C	-0.99227700	3.96606900	-0.06111800
H	-1.90804900	5.75920500	-0.76591800
C	-2.19951600	2.73546700	-2.25342700
H	-2.98847100	4.67261600	-2.73693100
C	-0.77234000	2.57468200	-0.24538000
H	-0.52085100	4.43134700	0.79767100
C	-1.40206200	1.95751100	-1.38015400
H	-2.67239300	2.23800100	-3.09710700
O	-0.05678700	1.94273900	0.64358800
C	-1.34887300	0.54063600	-1.58689100
Co	0.81500000	0.31251700	0.28517800
N	-0.55627400	-0.25681700	-0.95385400
H	-2.05414700	0.11694700	-2.30531000
N	1.64161000	-1.33302900	-0.22270700
C	-0.66147900	-1.71532900	-0.91996700
C	2.92567700	-1.50933800	-0.22978300
C	0.76517000	-2.27299000	-0.94986200
C	-1.52086100	-2.43624800	-1.95276400
H	3.30396300	-2.49133900	-0.52791300
C	3.89931500	-0.49038600	0.00445000

C	0.74234700	-3.71967600	-0.45438800
C	-1.56370600	-3.92519700	-1.55944300
H	-1.09930800	-2.30595300	-2.95897700
H	-2.54067000	-2.04624800	-1.95200200
C	5.25269800	-0.85247500	0.18772100
C	3.53936200	0.89293300	-0.13491000
C	-0.16401200	-4.54105700	-1.39071500
H	1.75052700	-4.14786500	-0.43798800
H	0.36381000	-3.73044000	0.57400300
H	-2.12939800	-4.49143500	-2.30679900
H	-2.11996300	-4.00218300	-0.61815700
C	6.24417100	0.10394200	0.27021400
H	5.50084300	-1.90783700	0.27116300
C	4.58676800	1.84938200	-0.08149000
O	2.31950900	1.30325500	-0.34442500
H	0.32111200	-4.60833100	-2.37426500
H	-0.25107300	-5.56655600	-1.01628900
C	5.89641000	1.46323000	0.12807500
H	7.27758400	-0.18380600	0.43038200
H	4.31298200	2.89244300	-0.19781200
H	6.67302300	2.22141300	0.18073600
H	1.10448700	-2.26645300	-1.99624900
H	-1.06556900	-1.91859000	0.07818100
O	1.73162000	0.27080500	2.15051000
H	1.60617000	1.16849100	2.48860600
H	0.74821000	-0.30280000	2.29955600
C	-2.76203800	-0.62553200	2.36598200
C	-1.36153900	-0.09415100	2.65145400
O	-0.37112900	-0.74097100	1.89873100
H	-2.70386600	-1.68711300	2.11995600
H	-1.17504600	-0.25208500	3.72819700
H	-1.36867300	0.99438200	2.47799700
C	-3.74173700	-0.37795600	3.50601000
H	-3.79097800	0.68835500	3.74928200
H	-4.74544000	-0.71639500	3.23382600
H	-3.42698400	-0.92335100	4.40057500
C	-4.60038400	0.26396100	-0.74274900
H	-5.61090900	0.43381900	-0.35532200
H	-4.68774200	-0.22751800	-1.71287100
H	-4.10854800	1.23248300	-0.83703500
C	-3.86797600	-0.63771300	0.22412000
O	-3.29338100	0.07843400	1.20050700
O	-3.83556400	-1.85173500	0.13741100

subsequent hydrolysis

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.093602

Thermal correction to Gibbs Free Energy (a.u.): 0.466630

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8992303 a.u.

C	-4.39880100	2.50676000	-1.94128900
C	-4.98759800	1.23064600	-2.07766400
C	-3.07348700	2.65112800	-1.58413400
H	-4.99966600	3.39409300	-2.12076300
C	-4.21637000	0.11451100	-1.83678000
H	-6.02989700	1.13389500	-2.36095400
C	-2.25209700	1.51800500	-1.33304000
H	-2.61532500	3.62841700	-1.47933400
C	-2.85558800	0.22604700	-1.46162200
H	-4.64871500	-0.87986100	-1.91848100
O	-1.01045100	1.71965300	-0.99743600
C	-2.13183200	-0.96290400	-1.14628000
Co	0.33726300	0.44103300	-0.73814100
N	-0.87678300	-1.01391700	-0.83578800
H	-2.70069300	-1.89215500	-1.14142800
N	1.69025900	-0.92843400	-0.94319400
C	-0.22047000	-2.22496900	-0.33190400
C	2.94676300	-0.71680400	-0.73575600

C	1.13003700	-2.28833500	-1.05861000
C	-0.99504100	-3.53359100	-0.42742800
H	3.62014200	-1.57067100	-0.68194500
C	3.54999100	0.57259300	-0.57791600
C	1.99482000	-3.42376700	-0.50841200
C	-0.12808200	-4.67074500	0.13418200
H	-1.26030100	-3.74525700	-1.47306400
H	-1.92032700	-3.45063500	0.15078100
C	4.93133500	0.63744400	-0.28068800
C	2.81110300	1.77846000	-0.79045000
C	1.22642200	-4.75260600	-0.57967600
H	2.92270400	-3.51359800	-1.08465600
H	2.26265700	-3.17558500	0.52557700
H	-0.66250200	-5.62254700	0.04569700
H	0.03447800	-4.49486700	1.20463000
C	5.58949000	1.84675900	-0.18240500
H	5.47106200	-0.29444800	-0.12906700
C	3.51888800	3.00520000	-0.71672500
O	1.53399700	1.81727600	-1.06810800
H	1.06468100	-5.02380900	-1.63239300
H	1.83691900	-5.54954600	-0.14223100
C	4.86648700	3.03443000	-0.41117000
H	6.64651800	1.88366400	0.05736900
H	2.95589000	3.91520200	-0.89299800
H	5.37515200	3.99220100	-0.34432000
H	0.92373300	-2.46262000	-2.12565100
H	-0.02949500	-2.00809800	0.72571100
O	2.41667200	-1.34792100	2.14415000
H	3.17565400	-0.75275900	2.12279400
H	1.67578600	-0.77800700	1.81970800
C	-0.80650100	0.91808300	3.06668200
C	0.22639900	1.34477500	2.02146700
O	0.51830200	0.28897400	1.16077500
H	-0.57472200	-0.09956300	3.39067400
H	1.13597700	1.66297800	2.56150000
H	-0.16025400	2.22186300	1.48168800
C	-0.89761500	1.88033000	4.24156000
H	-1.12020800	2.89478900	3.89515100
H	-1.68687800	1.57327000	4.93284200
H	0.05073000	1.90094800	4.78637900
C	-4.11046500	-0.03332500	1.64309300
H	-4.72215500	0.12796100	2.53719200
H	-4.47942800	-0.91070900	1.11329800
H	-4.19646800	0.85251400	1.01247100
C	-2.67769300	-0.25817800	2.07060600
O	-2.12806200	0.90580000	2.45522200
O	-2.12871500	-1.34230300	2.10197800

subsequent hydrolysis

Co^{III}(salen)-PO~OAc + H_2O = Co^{III}(salen)-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.100904

Thermal correction to Gibbs Free Energy (a.u.): 0.469560

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9018356 a.u.

C	-3.02537000	4.84955400	0.03136500
C	-4.03858700	3.98002300	-0.41572900
C	-1.71032400	4.43048800	0.12676500
H	-3.27855600	5.86935300	0.30818900
C	-3.69882900	2.68923500	-0.77221600
H	-5.06562100	4.32135700	-0.48596900
C	-1.34096300	3.10329600	-0.20449100
H	-0.92558500	5.09553700	0.47047000
C	-2.36760500	2.22809900	-0.67193000
H	-4.45831600	2.00012900	-1.13346600
O	-0.08512600	2.75354800	-0.07591500
C	-2.06506900	0.89887700	-1.11356000
Co	0.60142500	1.01360100	-0.07679200
N	-0.91552400	0.32405800	-1.00277500

H	-2.87475700	0.34466700	-1.58279700
N	1.59562600	-0.20501300	-1.21200800
C	-0.64167500	-1.02661200	-1.50626300
C	2.85855300	-0.46636100	-1.06588100
C	0.74492200	-0.94896600	-2.16258500
C	-1.67561000	-1.64559100	-2.44158700
H	3.29722300	-1.25537500	-1.67741100
C	3.75563200	0.18494400	-0.16914100
C	1.22339800	-2.35004000	-2.54753500
C	-1.20306000	-3.04886600	-2.85022200
H	-1.80559600	-1.01533200	-3.33278700
H	-2.63582200	-1.71795600	-1.92668300
C	5.10817300	-0.24129900	-0.15432500
C	3.33851600	1.25402300	0.69011200
C	0.19662900	-3.01962900	-3.47457000
H	2.19298400	-2.30973500	-3.05530000
H	1.34736900	-2.93276500	-1.62660800
H	-1.92033900	-3.49417000	-3.54778700
H	-1.18892100	-3.68861700	-1.95862500
C	6.04223600	0.35179600	0.66511600
H	5.39667100	-1.05723700	-0.81265500
C	4.32748600	1.85237700	1.51894200
O	2.12472000	1.71799000	0.75683300
H	0.15809100	-2.47001800	-4.42512300
H	0.52829000	-4.03551200	-3.71457900
C	5.63430700	1.41163400	1.50416600
H	7.07267700	0.01404500	0.66729000
H	4.00860100	2.66608700	2.16113700
H	6.36253500	1.88979600	2.15364200
H	0.65831400	-0.32753900	-3.06716700
H	-0.53807900	-1.66720100	-0.62428300
O	0.13113900	0.05840600	1.47634200
H	0.72672500	0.40333000	2.15763200
H	0.34868300	-1.58630600	1.31229300
C	-1.65994600	-3.35376700	1.86652000
C	-0.13454100	-3.40376300	1.94440500
O	0.50367900	-2.53318300	1.04215300
H	-1.97823400	-3.42341700	0.82377600
H	0.18545900	-4.42422800	1.69918400
H	0.16561200	-3.20804100	2.98654000
C	-2.33767000	-4.41862400	2.71638500
H	-2.04288200	-4.32338000	3.76623000
H	-3.42470400	-4.32128300	2.65484000
H	-2.06163700	-5.41895000	2.36828000
C	-2.95604600	0.10975500	2.22318700
H	-3.24673400	-0.01615200	3.26857300
H	-3.70206400	0.68705200	1.67844700
H	-1.98949700	0.62337200	2.19081600
C	-2.74769000	-1.22362700	1.56219600
O	-2.06887600	-2.05735600	2.37392700
O	-3.11456800	-1.51487800	0.43741200

five-coordinated Co^{III}(salen)-OTs counterion addition in the terminal carbon and subsequent hydrolysis

Co^{III}(salen)-OTs counterion addition in the terminal carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2266.846013

Thermal correction to Gibbs Free Energy (a.u.): 0.512912

Imaginary frequencies: -430.65

Calculation of single point energy based on the optimized structure, Et = -3505.8507742 a.u.

C	-0.01299300	5.62227900	0.59759700
C	1.20114100	5.20287000	1.17757300
C	-1.02741100	4.72228300	0.33017500
H	-0.15465100	6.67086400	0.35117300
C	1.36774400	3.86889500	1.48890400
H	1.99083700	5.91913900	1.37596800
C	-0.87199400	3.34355700	0.62206600
H	-1.96246900	5.03524600	-0.12139700

C	0.34845000	2.92305800	1.23171600
H	2.29396800	3.52053000	1.93832800
O	-1.84726700	2.52916000	0.30674800
C	0.56628800	1.55931700	1.60196900
Co	-1.94297400	0.68972000	0.56479300
N	-0.29167300	0.59867100	1.48470800
H	1.54321800	1.32539200	2.01882700
N	-2.24879800	-1.06900100	1.27027900
C	0.07201400	-0.80494500	1.72591400
C	-3.15101100	-1.87843200	0.81597700
C	-1.20332300	-1.49035900	2.22349500
C	1.26798700	-1.05928500	2.63846600
H	-3.14836200	-2.91007500	1.16701200
C	-4.17978900	-1.53238700	-0.11366500
C	-0.98894900	-2.99623000	2.37280200
C	1.47370900	-2.57300800	2.79690700
H	1.10859800	-0.58531400	3.61769600
H	2.16743400	-0.62283100	2.19424900
C	-5.04335300	-2.55178400	-0.57939100
C	-4.39358800	-0.17941100	-0.52399400
C	0.20392600	-3.26569900	3.30307200
H	-1.88688800	-3.47951400	2.77375600
H	-0.78811700	-3.42377800	1.38275300
H	2.30733400	-2.76350400	3.48156900
H	1.74713400	-2.98199400	1.81810800
C	-6.08858800	-2.27049200	-1.43428900
H	-4.86188500	-3.57255400	-0.25250500
C	-5.49007400	0.08619500	-1.38298800
O	-3.65298200	0.82748200	-0.13902000
H	-0.03651600	-2.90797000	4.31391400
H	0.36549700	-4.34576200	3.38258900
C	-6.30625500	-0.93500000	-1.83004100
H	-6.73611500	-3.06218900	-1.79461600
H	-5.65065400	1.11616800	-1.68198100
H	-7.12894900	-0.70282600	-2.50049500
C	-1.29726600	0.59903800	-2.26342700
C	0.06817800	1.13886600	-2.15417700
O	-1.12926900	-0.09142000	-1.03990800
H	-2.07060300	1.37809500	-2.19664300
H	0.24045200	2.01305400	-1.54127200
H	0.85366600	0.80769600	-2.82020300
C	-1.55951700	-0.35667900	-3.41279500
H	-2.51639100	-0.86090700	-3.24806500
H	-1.60999600	0.18387000	-4.36508100
H	-0.76140400	-1.10157000	-3.46356300
H	-1.47383100	-1.06183000	3.20039200
H	0.30672400	-1.21622400	0.73800300
O	1.66790900	-2.21667500	-0.54676700
O	1.60122000	0.27357900	-0.80955800
S	2.11656800	-1.05978000	-1.35677000
O	1.90028400	-1.15262100	-2.81942300
C	3.88645500	-0.92831600	-1.08943800
C	4.67036200	-0.22784800	-2.00665500
C	4.45838400	-1.47807600	0.05587900
C	6.03281600	-0.07609100	-1.76697300
H	4.21063100	0.17574400	-2.90208900
C	5.82430000	-1.31701100	0.28532000
H	3.83578200	-2.03888400	0.74361300
C	6.63081900	-0.61559700	-0.61870600
H	6.64600300	0.46614700	-2.48227200
H	6.27304300	-1.74765500	1.17682300
C	8.11423800	-0.47074600	-0.38495000
H	8.36830100	-0.60855600	0.66976900
H	8.67791400	-1.21657900	-0.95877300
H	8.47343500	0.51509500	-0.69621600

Co^{III}(salen)-OTs counterion addition in the terminal carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2266.896494
Thermal correction to Gibbs Free Energy (a.u.): 0.512919
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -3505.9044884 a.u.

C	-1.82045600	5.64806400	-0.72088800
C	-0.48153300	5.69432200	-0.28437800
C	-2.56902000	4.49081300	-0.60999600
H	-2.27189500	6.53323200	-1.15960300
C	0.08364800	4.56625200	0.27611300
H	0.09606200	6.60635600	-0.38683500
C	-2.00075300	3.31559800	-0.06255700
H	-3.59613900	4.43984400	-0.95393300
C	-0.65616600	3.36966600	0.40992600
H	1.11300500	4.57835900	0.62256900
O	-2.73504100	2.22774300	-0.03521700
C	-0.04340700	2.25104700	1.05458700
Co	-2.24960000	0.54747800	0.53402600
N	-0.62085400	1.11621600	1.30464000
H	0.99102600	2.37137600	1.36012300
N	-1.92643700	-1.09892200	1.42722000
C	0.14788100	-0.01220900	1.86182300
C	-2.44133600	-2.23181700	1.06862600
C	-0.86883900	-0.98504500	2.45226200
C	1.24870800	0.33799700	2.85986900
H	-2.06400200	-3.14141800	1.53355200
C	-3.49740900	-2.38980900	0.11826300
C	-0.18030600	-2.28192200	2.87311400
C	1.93384400	-0.95667200	3.32558100
H	0.82739800	0.89130700	3.71183900
H	1.99370000	0.96773900	2.36923700
C	-3.90223500	-3.69520900	-0.24574700
C	-4.19961800	-1.25876600	-0.40233500
C	0.92645300	-1.96344300	3.89195900
H	-0.89990600	-2.98190000	3.31340900
H	0.26266200	-2.74865200	1.98529400
H	2.69512900	-0.72087800	4.07684000
H	2.44030000	-1.39753100	2.46058100
C	-4.96386600	-3.89939800	-1.10326200
H	-3.35455800	-4.54062400	0.16210600
C	-5.30707400	-1.49619100	-1.25367600
O	-3.87899600	-0.01718400	-0.13324500
H	0.46976100	-1.56250900	4.80790700
H	1.43475900	-2.89119700	4.17428700
C	-5.66884500	-2.78419200	-1.60011800
H	-5.25815500	-4.90381500	-1.38655000
H	-5.84152500	-0.63191400	-1.63220800
H	-6.51007700	-2.93812200	-2.26969800
C	-1.59054200	-0.43814100	-2.44633700
C	-0.71585900	0.72273900	-2.22824900
O	-1.10337400	-0.12816300	-1.10432200
H	-2.65694600	-0.24238400	-2.54578200
H	-1.15957300	1.71345500	-2.19312000
H	0.34431800	0.63927900	-2.44800400
C	-1.07228900	-1.73541200	-2.99616600
H	-1.60018000	-2.57755600	-2.53618200
H	-1.24884500	-1.77386300	-4.07678600
H	0.00009600	-1.81692200	-2.80223800
H	-1.34621600	-0.52118200	3.32898600
H	0.62046700	-0.51260800	1.00920100
O	2.00557500	-1.60663500	0.03239000
O	2.06051100	0.86243300	-0.31522200
S	2.43322800	-0.48199000	-0.85870600
O	2.05019000	-0.68134900	-2.28432300
C	4.22962800	-0.52188500	-0.83227900
C	4.90746800	-1.44634200	-1.62892900
C	4.93772100	0.33078800	0.01046900
C	6.29593200	-1.51681100	-1.57003500
H	4.34233100	-2.08488100	-2.29900200
C	6.32961500	0.25104500	0.06171100

H	4.39274200	1.05975100	0.59946800
C	7.02875800	-0.67443000	-0.72084700
H	6.82409800	-2.23183700	-2.19628900
H	6.88274500	0.92214700	0.71431200
C	8.53265500	-0.77721900	-0.64868000
H	8.97088400	0.10308200	-0.17004900
H	8.84271100	-1.65607800	-0.06985800
H	8.97493400	-0.87645100	-1.64540200

Co^{III}(salen)-OTs counterion addition in the terminal carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2266.909973

Thermal correction to Gibbs Free Energy (a.u.): 0.517823

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3505.9104881 a.u.

C	3.01625700	-2.16823700	-2.86078300
C	3.64108600	-0.90953200	-2.78018000
C	1.71915700	-2.35474700	-2.41732500
H	3.56001900	-3.01083200	-3.27983500
C	2.93729000	0.14898900	-2.24095900
H	4.65824400	-0.77490100	-3.13128500
C	0.97699900	-1.28610900	-1.85459900
H	1.23062000	-3.32102700	-2.48230100
C	1.61680100	-0.01279900	-1.77030500
H	3.40266800	1.12655600	-2.15242600
O	-0.24673500	-1.51714600	-1.45484200
C	0.93411100	1.12563600	-1.23381900
Co	-1.42817300	-0.37157600	-0.54438300
N	-0.26761700	1.12325600	-0.76734500
H	1.48719100	2.06429600	-1.23311500
N	-2.84246100	0.97250800	-0.81088000
C	-0.93736800	2.31140100	-0.24017500
C	-4.10136700	0.72522300	-0.64412000
C	-2.30853400	2.33899400	-0.94643000
C	-0.19806800	3.63863100	-0.36376000
H	-4.81031600	1.55522300	-0.67261500
C	-4.67395400	-0.56402000	-0.40524000
C	-3.18059200	3.46907900	-0.39640600
C	-1.07565400	4.76727200	0.19617600
H	0.03935500	3.84441600	-1.41703100
H	0.74469500	3.58170300	0.18935900
C	-6.08030200	-0.63950500	-0.24741500
C	-3.88755900	-1.76127100	-0.32507800
C	-2.44203100	4.81270600	-0.49875400
H	-4.12819800	3.53137900	-0.94199000
H	-3.42059500	3.25087100	0.65225500
H	-0.56249000	5.72834600	0.08561900
H	-1.21893700	4.60748100	1.27245600
C	-6.72220800	-1.83745300	-0.02065100
H	-6.65301100	0.28307700	-0.30875900
C	-4.57913300	-2.98245800	-0.09630300
O	-2.59341900	-1.81901300	-0.46321200
H	-2.30134400	5.06610200	-1.55839600
H	-3.06239300	5.60564900	-0.06780600
C	-5.95042300	-3.01597700	0.05169500
H	-7.79913900	-1.87549100	0.10116000
H	-3.97985600	-3.88484000	-0.04216800
H	-6.44215800	-3.96843900	0.23017200
C	-1.09690400	-1.17628600	2.16644000
C	0.21067200	-1.91734600	1.80480500
O	-1.30892800	-0.11145400	1.29536000
H	-1.88694200	-1.94346000	2.06896900
H	0.02730900	-2.62339800	0.99407700
H	0.64811100	-2.43000400	2.66586400
C	-1.12102700	-0.64179400	3.60153000
H	-2.10346000	-0.20500200	3.80221400
H	-0.93970500	-1.44367500	4.32554000
H	-0.36535300	0.13300800	3.74361400

H	-2.12257800	2.51485000	-2.01705200
H	-1.10556300	2.08685900	0.82005000
O	1.51430800	1.36057200	1.95949300
O	1.21782100	-1.05080700	1.20501300
S	2.05051700	0.00552100	2.10798200
O	2.21805900	-0.55761100	3.44990400
C	3.57528200	-0.07674700	1.19084200
C	4.11855400	-1.31422100	0.84373000
C	4.22982300	1.11185000	0.88007300
C	5.32826100	-1.34998700	0.16241600
H	3.58583800	-2.22768800	1.07887000
C	5.44705500	1.05604700	0.20224400
H	3.78157000	2.05831500	1.15940000
C	6.00935200	-0.16949600	-0.17035300
H	5.74776000	-2.30849600	-0.12918200
H	5.96406700	1.97885200	-0.04547300
C	7.29989400	-0.22956300	-0.94660800
H	7.81961100	0.73184600	-0.93736500
H	7.97583800	-0.98769900	-0.53888100
H	7.11041600	-0.49601700	-1.99359900

subsequent hydrolysis (H_2O molecule is opposite the counterion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.313991

Thermal correction to Gibbs Free Energy (a.u.): 0.537418

Imaginary frequencies: -645.37

Calculation of single point energy based on the optimized structure, Et = -3582.3697239 a.u.

C	-0.14537400	4.84709900	-1.42093600
C	-0.61334300	4.24269600	-2.60439600
C	0.44277000	4.10036100	-0.41774400
H	-0.24837500	5.92115700	-1.29087000
C	-0.47555500	2.87759700	-2.75078900
H	-1.07747600	4.83952700	-3.38191400
C	0.60600000	2.69606000	-0.54146000
H	0.79778400	4.56189300	0.49736700
C	0.13938300	2.08464100	-1.75467500
H	-0.84473100	2.38164400	-3.64475400
O	1.11015000	2.04108500	0.47200500
C	0.16889700	0.66219200	-1.94163100
Co	1.96327100	0.37108300	0.28598200
N	0.81749500	-0.15329300	-1.17821800
H	-0.43917200	0.25710200	-2.74911300
N	2.79152600	-1.31622600	-0.04660900
C	0.63892400	-1.60675300	-1.14887100
C	4.04454400	-1.54977300	0.18647200
C	2.01858500	-2.22808200	-0.91450100
C	-0.05194000	-2.30557800	-2.31533500
H	4.42491500	-2.55246900	-0.02856100
C	5.00463100	-0.57150100	0.59138900
C	1.83657700	-3.66354600	-0.41926100
C	-0.23795600	-3.78431800	-1.92549300
H	0.55631000	-2.21374100	-3.22588200
H	-1.02794000	-1.86129500	-2.52041900
C	6.28097400	-0.99139000	1.02818100
C	4.74292000	0.82448000	0.37748300
C	1.07748700	-4.45856400	-1.49884300
H	2.80322200	-4.13714000	-0.21504300
H	1.27630600	-3.63880300	0.52223400
H	-0.68276800	-4.33441300	-2.76114400
H	-0.96311700	-3.82686000	-1.10518500
C	7.28374300	-0.07979100	1.28936900
H	6.45886700	-2.05555500	1.16341800
C	5.80611000	1.73314400	0.62122900
O	3.60493200	1.28625900	-0.05991600
H	1.73025900	-4.56358100	-2.37654100
H	0.87642400	-5.47292700	-1.13798300
C	7.03352400	1.29149300	1.07558700
H	8.25406200	-0.41170800	1.64258400

H	5.60868700	2.78563100	0.44850600
H	7.82153100	2.01450800	1.26824800
H	2.54412600	-2.25379600	-1.88052100
H	0.05319000	-1.77427800	-0.23817500
O	2.48605500	0.35496000	2.28792300
H	2.32977400	1.26889800	2.56362200
H	1.47915700	-0.19512100	2.27275700
C	-0.67554100	0.03018600	2.16576300
C	-1.70391900	0.28279800	1.06944600
O	0.45290200	-0.63463800	1.67562600
H	-0.41263400	1.04746800	2.51634700
H	-1.27238700	0.85925000	0.25483700
H	-2.57780500	0.80686900	1.47312700
C	-1.27941400	-0.75162300	3.33793000
H	-0.52969700	-0.87179000	4.12447300
H	-2.14997900	-0.23717200	3.76213400
H	-1.58671900	-1.74519200	3.00154700
O	-2.72035300	-0.04171400	-1.69795000
O	-2.13877900	-1.01319500	0.55355300
S	-3.17154000	-1.01163700	-0.69485800
O	-3.32476600	-2.42124600	-1.03694600
C	-4.67437400	-0.40184600	0.03111200
C	-5.46539000	-1.27281900	0.78303500
C	-5.01487100	0.94136200	-0.12255900
C	-6.61696100	-0.78020500	1.38650400
H	-5.18088100	-2.31455000	0.87928400
C	-6.17273800	1.41520900	0.49135100
H	-4.38517800	1.59129900	-0.71933700
C	-6.98778900	0.56674700	1.25099000
H	-7.24091700	-1.44899400	1.97251200
H	-6.44756400	2.45980300	0.37791500
C	-8.25385700	1.07837600	1.88961800
H	-8.41039200	0.63234300	2.87618200
H	-8.23359800	2.16521500	2.00358200
H	-9.12751000	0.82635200	1.27659200

subsequent hydrolysis (H_2O molecule is opposite the counterion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.337794

Thermal correction to Gibbs Free Energy (a.u.): 0.538632

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.4014118 a.u.

C	-0.81552100	5.42005200	-0.12607100
C	-1.48064000	5.06730300	-1.32065100
C	0.08007300	4.56128900	0.47762700
H	-1.01474400	6.38569000	0.33091100
C	-1.21945600	3.84042900	-1.89012900
H	-2.18795000	5.75084700	-1.77744300
C	0.36603100	3.28696400	-0.08425300
H	0.58952100	4.82356700	1.39844400
C	-0.29593400	2.93936900	-1.30570200
H	-1.72674000	3.53650700	-2.80192000
O	1.19231300	2.50452600	0.54944000
C	-0.09810700	1.67009900	-1.92414200
Co	1.92576700	0.88164700	-0.04537100
N	0.74584900	0.76526800	-1.53044200
H	-0.73723300	1.44177800	-2.77317700
N	2.83375100	-0.59946300	-0.89162300
C	0.75501000	-0.60099000	-2.07724300
C	3.72865400	-1.30788700	-0.29204000
C	2.23154300	-1.00126700	-2.17492700
C	0.01626000	-0.83703400	-3.39095400
H	4.05266600	-2.24127900	-0.74865200
C	4.36852100	-0.94493700	0.93904000
C	2.37372900	-2.47598600	-2.55659800
C	0.13839300	-2.32043700	-3.76806200
H	0.44621800	-0.20448600	-4.18054300
H	-1.03941600	-0.57640600	-3.28432400

C	5.27020400	-1.85853200	1.52795300
C	4.18798100	0.34880600	1.51723600
C	1.60412800	-2.76149400	-3.85606900
H	3.42940200	-2.73370900	-2.69964400
H	1.99001200	-3.08063100	-1.72665900
H	-0.36944100	-2.50078400	-4.72140200
H	-0.38820700	-2.91301300	-3.01109800
C	5.98204600	-1.53266400	2.66639700
H	5.39442500	-2.83401900	1.06367100
C	4.95562000	0.67154300	2.66303400
O	3.37030600	1.25670800	1.04290000
H	2.09073200	-2.23416400	-4.68873100
H	1.66534300	-3.83060300	-4.08559700
C	5.81942000	-0.25091200	3.22562700
H	6.66251000	-2.24723500	3.11663500
H	4.82381000	1.66019800	3.08890800
H	6.37989500	0.02050000	4.11601300
H	2.69184300	-0.37117400	-2.95153700
H	0.29925000	-1.22064700	-1.29556100
O	1.47831200	-3.06328200	0.62723500
H	2.06736600	-3.23225400	1.37214100
H	1.23492900	-2.11262100	0.75039000
C	0.02264100	-0.08880000	1.95509600
C	-1.29543200	0.20338100	1.22846000
O	1.00966200	-0.43584300	1.03352500
H	0.27341600	0.85070800	2.47701400
H	-1.19249100	1.06983100	0.57642300
H	-2.12079900	0.36512200	1.93198300
C	-0.12591900	-1.21115200	2.98805700
H	0.82147400	-1.33935500	3.51902900
H	-0.90690900	-0.98206900	3.72187700
H	-0.36891500	-2.15121800	2.48592200
O	-2.68458400	0.48645000	-1.34618200
O	-1.60072200	-0.96398300	0.40910100
S	-2.76272300	-0.83278500	-0.70914500
O	-2.64075900	-2.04805300	-1.50610300
C	-4.25030100	-0.89615200	0.26031400
C	-4.72679900	-2.13624200	0.69002200
C	-4.88661800	0.29170900	0.61762800
C	-5.86344700	-2.17645200	1.48976800
H	-4.21505900	-3.04427200	0.39162200
C	-6.02365700	0.22926000	1.42097700
H	-4.49915800	1.23896000	0.26037500
C	-6.52766100	-0.99891500	1.86682200
H	-6.24426500	-3.13571900	1.82862000
H	-6.52806100	1.14843600	1.70449900
C	-7.77445600	-1.06227500	2.71196900
H	-7.69508900	-1.83634700	3.48093900
H	-7.97228900	-0.10733000	3.20556400
H	-8.64943400	-1.30399600	2.09666000

subsequent hydrolysis (H_2O molecule is opposite the counterion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.340564

Thermal correction to Gibbs Free Energy (a.u.): 0.540226

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4031763 a.u.

C	1.01115400	5.56545800	-0.17757100
C	-0.25385600	5.24066400	-0.70216300
C	1.97399200	4.59350200	0.03478100
H	1.23869100	6.59887400	0.07023000
C	-0.52738900	3.92465300	-1.02218600
H	-1.00076400	6.01202300	-0.85481500
C	1.70886000	3.23335500	-0.25371600
H	2.94941000	4.83853700	0.44074800
C	0.43233400	2.91095000	-0.80589100
H	-1.49306100	3.64185600	-1.43118700
O	2.64697000	2.34656600	-0.01774900

C	0.12665900	1.57794000	-1.22910000
Co	2.40548100	0.49941400	0.11720500
N	0.85230000	0.53857400	-0.98211700
H	-0.78458800	1.44992700	-1.80851400
N	2.84219600	-1.09051500	-0.91372800
C	0.51932400	-0.80502500	-1.47053900
C	3.86560000	-1.85668300	-0.68513400
C	1.84623100	-1.40467100	-1.95723500
C	-0.55544900	-0.90801100	-2.55018400
H	3.97700200	-2.76240400	-1.28333600
C	4.88428200	-1.63597200	0.28678200
C	1.66670300	-2.88345300	-2.30772200
C	-0.75619000	-2.38731800	-2.91067300
H	-0.24921300	-0.34054900	-3.44028200
H	-1.49449400	-0.48031600	-2.19592000
C	5.92535800	-2.59455800	0.38911400
C	4.89188400	-0.48344800	1.14177000
C	0.55483300	-3.04531000	-3.35705200
H	2.59497300	-3.31242600	-2.69958300
H	1.40918100	-3.43243300	-1.39305800
H	-1.51103000	-2.47923000	-3.69913800
H	-1.14756900	-2.91499000	-2.03112200
C	6.95417900	-2.44871000	1.29163700
H	5.89373500	-3.45904100	-0.26994400
C	5.97162200	-0.35935100	2.06122500
O	3.99015700	0.45134700	1.13060900
H	0.88480400	-2.58812800	-4.29979700
H	0.39899500	-4.10964200	-3.56337200
C	6.96581000	-1.31188700	2.13020900
H	7.74270400	-3.19003500	1.35927800
H	5.97705400	0.51629900	2.70111600
H	7.77397800	-1.18402900	2.84531600
H	2.14881300	-0.85340800	-2.86100700
H	0.18444500	-1.37161500	-0.59202000
O	1.40079600	0.02738600	1.63087500
H	2.03567300	0.05778800	2.36098100
H	0.41844200	-1.28301400	1.55827700
C	-1.47112900	-1.47944900	2.03070500
C	-1.74931600	-0.01250900	1.70522200
O	-0.29978100	-1.95837900	1.40741500
H	-1.35724200	-1.49641500	3.13158100
H	-0.86028600	0.59596100	1.87774500
H	-2.58057800	0.36026100	2.30913100
C	-2.62377200	-2.39968500	1.64641300
H	-2.38915500	-3.42452700	1.94421800
H	-3.55809300	-2.09477500	2.12809000
H	-2.77049100	-2.37909800	0.56395300
O	-3.29586200	2.28943800	0.73719100
O	-2.07972900	0.11895100	0.28439400
S	-3.29122200	1.11561200	-0.13145100
O	-3.14616900	1.24766700	-1.58186200
C	-4.72421800	0.12783300	0.22582400
C	-5.06349400	-0.91309700	-0.64112600
C	-5.43387500	0.35246100	1.40348400
C	-6.12874000	-1.74158800	-0.31043200
H	-4.49969200	-1.06109000	-1.55522800
C	-6.49831400	-0.49117200	1.71859300
H	-5.15740200	1.17784200	2.04944200
C	-6.85842900	-1.54758500	0.87341800
H	-6.40032200	-2.55520700	-0.97696800
H	-7.05770000	-0.32528700	2.63459000
C	-8.02209300	-2.44547900	1.20773100
H	-7.79490500	-3.49124100	0.97989900
H	-8.29074000	-2.37555200	2.26472100
H	-8.90691700	-2.17023200	0.62149700

subsequent hydrolysis (H_2O molecule is at the same side with the ion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.312024
Thermal correction to Gibbs Free Energy (a.u.): 0.540446
Imaginary frequencies: -856.77
Calculation of single point energy based on the optimized structure, Et = -3582.3721146 a.u.

C	-2.71311700	0.57046600	4.11985000
C	-2.77901600	1.97762800	4.04118700
C	-1.92581900	-0.15862700	3.25121300
H	-3.29375300	0.04849000	4.87544900
C	-2.02676400	2.62278200	3.08110000
H	-3.40209800	2.53946700	4.72812100
C	-1.15533400	0.47560600	2.23800400
H	-1.88152900	-1.24114500	3.30062500
C	-1.20024800	1.90938100	2.18095000
H	-2.05743900	3.70708500	3.00116100
O	-0.51719800	-0.28380800	1.39472200
C	-0.51521900	2.64256000	1.15749300
Co	0.97270700	0.25869100	0.36389600
N	0.36651700	2.13430300	0.36400700
H	-0.79128700	3.69386100	1.04240000
N	2.50714700	0.99275900	-0.52260700
C	0.88307300	2.78173900	-0.84182100
C	3.66792200	0.42136500	-0.51718400
C	2.36384600	2.39835600	-0.95353200
C	0.70562300	4.28832900	-1.00365900
H	4.48297200	0.90104200	-1.06509500
C	4.00114200	-0.74606900	0.23953600
C	2.87301100	2.73190700	-2.35751000
C	1.24628500	4.70128500	-2.38516000
H	1.23936200	4.82259700	-0.20588000
H	-0.35210200	4.56439100	-0.92906400
C	5.20902200	-1.42726100	-0.02141000
C	3.19170100	-1.12505000	1.35862600
C	2.69418600	4.23879100	-2.60974600
H	3.92769400	2.46071800	-2.46980800
H	2.30515900	2.14164000	-3.08610100
H	1.17684700	5.78760900	-2.50394400
H	0.60419100	4.25779700	-3.15695300
C	5.61561700	-2.48685700	0.76658600
H	5.81304500	-1.11009600	-0.86796300
C	3.65144400	-2.19071800	2.17060400
O	2.07221700	-0.52617300	1.67721900
H	3.35898500	4.79241500	-1.93287600
H	3.01086400	4.48524900	-3.62848300
C	4.82541300	-2.85868800	1.87155600
H	6.53426500	-3.01903500	0.54516800
H	3.03923400	-2.47014300	3.02114600
H	5.14226000	-3.68491300	2.50187600
C	0.82127900	-2.87365500	-0.22351700
C	-0.69381000	-3.00877600	-0.09689700
O	1.22097900	-1.61719700	-0.71540400
H	1.19540100	-2.97611600	0.80748000
H	-1.07968500	-2.19621500	0.51970200
H	-0.96639200	-3.97338400	0.33851700
C	1.44381400	-3.97543400	-1.08295000
H	2.52977300	-3.85231400	-1.09382900
H	1.20497900	-4.96906900	-0.68742500
H	1.07157000	-3.90955900	-2.10842500
H	2.92004100	3.00581000	-0.22343000
H	0.36393200	2.26357100	-1.65713400
O	-0.08520500	0.12876700	-1.47253300
H	-1.01665500	0.01852700	-1.24221200
H	0.45365600	-0.95520000	-1.33097300
O	-3.19403400	-3.13228900	-2.93217600
O	-1.27332000	-2.92396400	-1.43374200
S	-2.89939000	-2.89324300	-1.52612600
O	-3.45343000	-3.73318800	-0.46469400
C	-3.27375900	-1.19145800	-1.14622700
C	-3.59623000	-0.82538700	0.15918700
C	-3.17842600	-0.23634400	-2.16245200

C	-3.80918600	0.52042900	0.45298600
H	-3.67159300	-1.58344300	0.92935800
C	-3.38348500	1.10353600	-1.84786500
H	-2.93278800	-0.54739900	-3.17102300
C	-3.69176000	1.50125200	-0.53769200
H	-4.04142100	0.81338700	1.47128500
H	-3.29389300	1.85355000	-2.62873000
C	-3.89809000	2.95773900	-0.20743000
H	-3.12716000	3.58048000	-0.67425400
H	-4.86667900	3.31393800	-0.57740200
H	-3.86700000	3.12406900	0.87168000

subsequent hydrolysis (H_2O molecule is at the same side with the ion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.341761

Thermal correction to Gibbs Free Energy (a.u.): 0.542012

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.4079568 a.u.

C	-2.23287800	-3.05967500	3.75912000
C	-3.22412200	-2.05783800	3.66600900
C	-0.96147400	-2.85914100	3.26249400
H	-2.47449300	-4.00749400	4.23219200
C	-2.90461000	-0.86182700	3.06239900
H	-4.21736300	-2.22971900	4.06623100
C	-0.60652300	-1.63908900	2.62358200
H	-0.19448800	-3.62235600	3.33577400
C	-1.61281200	-0.62566100	2.52955000
H	-3.64599800	-0.07171100	2.98144600
O	0.60610000	-1.51021300	2.17034300
C	-1.35597600	0.63018000	1.90754900
Co	1.33284800	-0.07617900	1.20393100
N	-0.23520500	1.00572200	1.37174200
H	-2.19615100	1.32061600	1.87283300
N	2.15393000	1.52066300	0.53258400
C	-0.13753100	2.25013900	0.58798300
C	3.27469000	1.51096900	-0.11130700
C	1.31853100	2.71983700	0.67532700
C	-1.07381300	3.39519000	0.97365200
H	3.58986900	2.41721600	-0.62736300
C	4.17544600	0.40128300	-0.16418300
C	1.56611700	3.85331400	-0.32159900
C	-0.85844900	4.56452000	0.00029000
H	-0.86937600	3.70909300	2.00628500
H	-2.11814100	3.07945500	0.93034500
C	5.31345200	0.48501800	-0.99844000
C	4.00755900	-0.72624300	0.70015100
C	0.60643400	5.01788800	-0.02869700
H	2.59783300	4.21425900	-0.25334800
H	1.40645400	3.45946700	-1.33240700
H	-1.50843900	5.40256100	0.27388600
H	-1.15630800	4.24314900	-1.00601200
C	6.27088800	-0.50888100	-1.00615400
H	5.41812100	1.35263400	-1.64509500
C	5.02798000	-1.71034800	0.70550000
O	2.97846900	-0.89344200	1.49002500
H	0.86502100	5.46146900	0.94244100
H	0.74332400	5.80420700	-0.77817300
C	6.11979800	-1.60718200	-0.13617900
H	7.13108200	-0.44293800	-1.66318400
H	4.90194700	-2.55573800	1.37288600
H	6.87235100	-2.39075800	-0.12783600
C	1.02740400	-2.01515800	-0.90119400
C	-0.36964600	-2.37301500	-1.40155000
O	1.03524300	-0.65017400	-0.58594600
H	1.19413200	-2.62379800	0.00085800
H	-1.10446600	-2.11100400	-0.63406900
H	-0.47251500	-3.42664400	-1.67604700
C	2.11501100	-2.33414200	-1.93158200

H	3.09664000	-2.09880300	-1.51603200
H	2.09859100	-3.39425100	-2.20868200
H	1.96615100	-1.73551400	-2.83379200
H	1.48723600	3.09108300	1.69838500
H	-0.32389700	1.96207000	-0.45494000
O	0.46315400	1.28279900	-2.40869100
H	0.16867300	0.84857700	-3.21971500
H	0.68651900	0.52785800	-1.80937400
O	-1.93850300	-0.54176100	-4.31455600
O	-0.59135300	-1.55596300	-2.58251700
S	-2.10195200	-1.39289700	-3.14111600
O	-2.73467800	-2.70811800	-3.21671400
C	-2.92841500	-0.45681800	-1.86839000
C	-3.75548500	-1.11483000	-0.96078300
C	-2.77315200	0.93112800	-1.83610200
C	-4.44140700	-0.36733600	-0.00415100
H	-3.87151300	-2.19062400	-1.02142000
C	-3.48928000	1.66064200	-0.89426500
H	-2.09871200	1.41909900	-2.52789000
C	-4.32922400	1.02642500	0.03553900
H	-5.07834200	-0.87564200	0.71276800
H	-3.40537100	2.74344200	-0.88831500
C	-5.09249300	1.83951500	1.05106600
H	-4.41807100	2.43127800	1.68208900
H	-5.76930300	2.54785400	0.56121200
H	-5.69128900	1.20187500	1.70613900

subsequent hydrolysis (H_2O molecule is at the same side with the ion OTs^-)

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.326529

Thermal correction to Gibbs Free Energy (a.u.): 0.541886

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.3918966 a.u.

C	-3.52018800	-0.62860800	3.26736000
C	-3.97333900	0.70902500	3.21902300
C	-2.37550200	-1.02417000	2.60840500
H	-4.09006800	-1.36524200	3.82700500
C	-3.25067400	1.63003500	2.49316400
H	-4.87653100	1.00201200	3.74316500
C	-1.59873800	-0.09201100	1.86537600
H	-2.04364000	-2.05584000	2.60640100
C	-2.05953600	1.26621600	1.81767000
H	-3.58342100	2.66373600	2.43193800
O	-0.54551900	-0.53240700	1.24340900
C	-1.39976500	2.23942200	1.01208700
Co	0.86864300	0.51715400	0.58866100
N	-0.23599000	2.07714000	0.46281000
H	-1.93330000	3.17573200	0.83922900
N	2.29302300	1.71667200	0.10822800
C	0.33961300	2.97259100	-0.54147400
C	3.54358400	1.38609600	0.07972000
C	1.83312000	3.08068300	-0.20440900
C	-0.29648000	4.34843200	-0.71555200
H	4.26542500	2.11497900	-0.29260600
C	4.08338400	0.14739500	0.54375300
C	2.57854500	3.81329200	-1.32252000
C	0.44516500	5.11377400	-1.82340400
H	-0.24519000	4.90659700	0.22923900
H	-1.35535500	4.24905000	-0.97865600
C	5.45731800	-0.11708200	0.34094400
C	3.28434100	-0.77725600	1.28154900
C	1.95177400	5.19900400	-1.54662600
H	3.63832900	3.93152700	-1.07683600
H	2.52110300	3.21013600	-2.23697800
H	0.02247000	6.11822600	-1.92949200
H	0.28135300	4.59994200	-2.77953700
C	6.04676000	-1.26028600	0.83893100
H	6.04578000	0.60177700	-0.22420300

C	3.92036700	-1.92273100	1.81589900
O	2.00587500	-0.61009800	1.51923000
H	2.12073400	5.81624800	-0.65391600
H	2.45935300	5.70340000	-2.37528300
C	5.26169700	-2.16113800	1.58582700
H	7.09836300	-1.46090700	0.66598300
H	3.30939000	-2.61373000	2.38619500
H	5.71815300	-3.06083300	1.98923600
C	1.82811300	-3.34965600	-1.05009100
C	0.52525500	-3.20854600	-0.26303300
O	2.51733200	-2.13414400	-1.25267500
H	2.47370000	-3.95784500	-0.39705300
H	0.64323300	-2.57351200	0.61565800
H	0.14972800	-4.18986800	0.03210100
C	1.61780400	-4.09917000	-2.36849200
H	2.57885500	-4.22006100	-2.87413200
H	1.17853200	-5.08950300	-2.20265900
H	0.94704300	-3.53639400	-3.02251000
H	1.91630400	3.66795200	0.72367900
H	0.26694000	2.41281300	-1.48448800
O	0.76654700	-0.04616300	-1.21537300
H	0.04766600	-0.69607900	-1.21310700
H	1.89054600	-1.38289700	-1.37547600
O	-2.34703100	-3.74244900	-2.27399100
O	-0.47205900	-2.56527400	-1.12868600
S	-2.03745300	-3.01975000	-1.04329300
O	-2.29833700	-3.64201200	0.25630300
C	-2.80209000	-1.40994000	-1.08566900
C	-3.87566800	-1.17284400	-0.22762900
C	-2.35355000	-0.43055900	-1.97007000
C	-4.49127800	0.07427300	-0.24394500
H	-4.19842500	-1.94741000	0.45601900
C	-2.96198000	0.82282800	-1.94815300
H	-1.53006800	-0.62660900	-2.64582400
C	-4.03027700	1.09482200	-1.08536800
H	-5.31227600	0.27024600	0.43782900
H	-2.59783400	1.60021100	-2.61396300
C	-4.65948900	2.46345900	-1.03287700
H	-4.20909000	3.14180500	-1.76260700
H	-5.73500500	2.41765900	-1.23443200
H	-4.54029500	2.90510800	-0.03645800

five-coordinated Co^{III}(salen)-OTs counterion addition in the middle carbon and subsequent hydrolysis

Co^{III}(salen)-OTs counterion addition in the middle carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2266.850109

Thermal correction to Gibbs Free Energy (a.u.): 0.512973

Imaginary frequencies: -305.86

Calculation of single point energy based on the optimized structure, Et = -3505.8587696 a.u.

C	2.19049400	-4.05794100	-1.45900800
C	3.12973400	-3.02601700	-1.64868500
C	0.85721000	-3.77892800	-1.21396600
H	2.51667900	-5.09378600	-1.49554700
C	2.70204500	-1.71419100	-1.60399300
H	4.17531700	-3.25723200	-1.82000500
C	0.39972400	-2.44002400	-1.13441400
H	0.13055600	-4.56801300	-1.05383700
C	1.34638700	-1.39865700	-1.36368800
H	3.40942300	-0.90059500	-1.72902300
O	-0.85763100	-2.23034200	-0.82821300
C	0.96658500	-0.02419200	-1.30723500
Co	-1.73614900	-0.60597700	-0.61898300
N	-0.23396700	0.42372600	-1.12310600
H	1.77134100	0.69602700	-1.42876600
N	-2.72413600	1.02949700	-0.86993500
C	-0.47737500	1.84200900	-0.81913000
C	-3.95891400	1.19287700	-0.51824200

C	-1.88164000	2.14674300	-1.34288200
C	0.55331200	2.84667600	-1.32373000
H	-4.38691000	2.19366000	-0.57867400
C	-4.84030900	0.16260300	-0.06694400
C	-2.32341500	3.55221000	-0.93235300
C	0.12034300	4.26036900	-0.91325300
H	0.65210300	2.77037900	-2.41587300
H	1.52162700	2.63871500	-0.86695500
C	-6.14950400	0.51994900	0.33452300
C	-4.45403300	-1.21399600	-0.08361600
C	-1.29261400	4.58927600	-1.40765600
H	-3.30486800	3.79442400	-1.35434700
H	-2.41492300	3.58735700	0.16073300
H	0.83561400	4.99263900	-1.30183600
H	0.16709500	4.32520900	0.18001900
C	-7.06733600	-0.43477300	0.71933500
H	-6.42064700	1.57283700	0.33596400
C	-5.42527200	-2.17734700	0.29242900
O	-3.27206700	-1.63770500	-0.44466800
H	-1.29760400	4.61944700	-2.50598300
H	-1.59625600	5.58465100	-1.06664500
C	-6.69123000	-1.79346400	0.68984000
H	-8.06468200	-0.14788400	1.03394500
H	-5.12891200	-3.22019000	0.26428700
H	-7.40891800	-2.55375700	0.98519400
C	-0.12686100	-0.95192900	2.63695400
C	-1.53420000	-1.16929400	2.23627100
O	-1.53490700	-0.14339600	1.28143900
H	0.10749300	-0.10001800	3.26273600
H	-2.25102600	-0.99002700	3.05329500
H	-1.71175500	-2.16680900	1.81140900
C	0.89808600	-1.97958000	2.41342700
H	0.87328000	-2.34469700	1.38387000
H	1.89256000	-1.63533500	2.68086400
H	0.60348900	-2.83725700	3.04502700
H	-1.85584900	2.08163300	-2.44111300
H	-0.49100100	1.88215600	0.27725100
O	2.12536900	2.71751700	1.67102800
O	1.17138500	0.46080400	1.28651000
S	2.27331600	1.27145600	1.94548400
O	2.46481900	0.85446800	3.35328000
C	3.73819300	0.74761400	1.03527800
C	4.36084500	-0.46110800	1.34905800
C	4.19150800	1.50479600	-0.04419500
C	5.41699900	-0.91921100	0.56685200
H	4.02635600	-1.02706600	2.21080100
C	5.25020200	1.03642800	-0.82387500
H	3.72626700	2.46292500	-0.24715400
C	5.87480300	-0.18352900	-0.53565300
H	5.89500900	-1.86398100	0.81240500
H	5.60190900	1.63029800	-1.66371100
C	7.03229200	-0.68049900	-1.36596000
H	6.99951000	-1.76790400	-1.48641200
H	7.03416000	-0.22760200	-2.36131600
H	7.99112400	-0.43667600	-0.89246800

Co^{III}(salen)-OTs counterion addition in the middle carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2266.868235

Thermal correction to Gibbs Free Energy (a.u.): 0.518527

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3505.9046634 a.u.

C	2.27948800	-3.99699500	-1.51061700
C	3.21960500	-2.94859800	-1.54066400
C	0.92870000	-3.74402800	-1.35012300
H	2.61891300	-5.02471700	-1.60444700
C	2.78269400	-1.64429200	-1.42366700
H	4.27735300	-3.16074400	-1.64834200

C	0.46191600	-2.41728600	-1.20152000
H	0.19810400	-4.54427500	-1.31010700
C	1.40907100	-1.35427600	-1.26698900
H	3.49150300	-0.82372600	-1.43351000
O	-0.82026200	-2.23201700	-0.98554100
C	1.00018100	0.00911500	-1.18730800
Co	-1.72090600	-0.65307100	-0.71968200
N	-0.22946500	0.42591600	-1.10797500
H	1.78771100	0.75399300	-1.23244000
N	-2.72967100	0.96548900	-0.80599800
C	-0.50199700	1.86393400	-0.90287900
C	-3.93154400	1.10608000	-0.34581600
C	-1.94515300	2.09113200	-1.35037000
C	0.43447800	2.84085900	-1.61343400
H	-4.36442700	2.10575500	-0.32655100
C	-4.76829500	0.04363000	0.11879700
C	-2.41283000	3.50068900	-0.99198900
C	-0.00259400	4.27455400	-1.28223400
H	0.40308900	2.65819400	-2.69709400
H	1.45330100	2.71882700	-1.24549000
C	-6.03548400	0.35897700	0.66231700
C	-4.38453600	-1.32461900	-0.03601800
C	-1.47131600	4.53310600	-1.63647900
H	-3.43749600	3.67564400	-1.33873200
H	-2.40626300	3.61229500	0.09987900
H	0.64092600	4.98416500	-1.81189000
H	0.17131200	4.43711800	-0.21258800
C	-6.90988500	-0.63277500	1.05705700
H	-6.30976900	1.40561300	0.76599300
C	-5.31222000	-2.32431100	0.34953400
O	-3.22948800	-1.70507800	-0.52107000
H	-1.59818000	4.49125400	-2.72698700
H	-1.77143600	5.53934200	-1.32567800
C	-6.53701200	-1.98220600	0.89031800
H	-7.87488100	-0.37984800	1.48200500
H	-5.01663500	-3.35900600	0.21541200
H	-7.22341800	-2.76807900	1.19187500
C	-0.73069400	-0.78392300	2.46653300
C	-2.19036500	-0.96201400	2.47830300
O	-1.56043700	-0.23483800	1.39319000
H	-0.29341900	0.02106700	3.04821200
H	-2.82586500	-0.34094400	3.10467700
H	-2.60648500	-1.92342800	2.18685200
C	0.19755100	-1.91058400	2.12282200
H	-0.29497000	-2.65861100	1.49815700
H	1.07056000	-1.50627000	1.60891200
H	0.53278700	-2.38842400	3.05001300
H	-1.97624900	1.97361300	-2.44408500
H	-0.41087200	2.01607200	0.17992700
O	2.41365400	2.99927600	0.72908700
O	1.27876200	0.87895500	1.35105200
S	2.44735400	1.79269900	1.60277300
O	2.69729300	2.03348000	3.03636300
C	3.84178400	0.82173000	0.99479600
C	4.11400300	-0.42227400	1.57019200
C	4.61886400	1.28116500	-0.06593600
C	5.15129000	-1.20390300	1.07323500
H	3.50759600	-0.77069400	2.39948600
C	5.66000300	0.48903900	-0.55876400
H	4.39721100	2.25480500	-0.48892200
C	5.94081900	-0.76286100	-0.00020100
H	5.35170900	-2.17614500	1.51662000
H	6.26339000	0.85005900	-1.38817600
C	7.07568200	-1.61153200	-0.51907900
H	6.81022200	-2.67395400	-0.52638800
H	7.35811700	-1.32408600	-1.53589000
H	7.96793200	-1.50837200	0.11059300

Co^{III}(salen)-OTs counterion addition in the middle carbon

Co^{III}(salen)-OTs + PO = Co^{III}(salen)-PO~OTs

Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2266.911777
Thermal correction to Gibbs Free Energy (a.u.): 0.521667
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -3505.9161161 a.u.

C	2.88415000	-2.66680700	-2.36470600
C	3.46374600	-1.41096300	-2.64627900
C	1.63039600	-2.76717600	-1.79815700
H	3.43532100	-3.57417200	-2.59784400
C	2.75885800	-0.26977000	-2.33418900
H	4.45081600	-1.34734200	-3.09053700
C	0.87163100	-1.60636400	-1.47855200
H	1.17769100	-3.72922100	-1.58390200
C	1.46844100	-0.33500700	-1.75604600
H	3.19268500	0.70915300	-2.51714100
O	-0.30906500	-1.76631000	-0.96096100
C	0.80421300	0.88300500	-1.42890100
Co	-1.60258500	-0.44813900	-0.59717300
N	-0.40815600	0.98189600	-0.98190600
H	1.38324600	1.79631700	-1.55245100
N	-2.96374000	0.92301700	-0.63695300
C	-0.96971700	2.24392300	-0.48686500
C	-4.19639000	0.72110000	-0.30817100
C	-2.43115700	2.25755500	-0.95285500
C	-0.24329100	3.53044700	-0.86952900
H	-4.86490800	1.57923500	-0.22638700
C	-4.78838700	-0.56028300	-0.07170300
C	-3.18506500	3.45193900	-0.36584900
C	-0.99289800	4.73561300	-0.28309200
H	-0.18990900	3.61760400	-1.96396800
H	0.77561900	3.50620300	-0.47721400
C	-6.13231600	-0.61528600	0.36436400
C	-4.08569300	-1.77051200	-0.36871500
C	-2.46150200	4.76007000	-0.72153900
H	-4.21191800	3.48984100	-0.74440400
H	-3.24109200	3.33392400	0.72386000
H	-0.49366900	5.66396000	-0.58014300
H	-0.93887200	4.68562300	0.81189900
C	-6.78799100	-1.81909500	0.52325700
H	-6.64549700	0.31981100	0.57670100
C	-4.79364800	-2.99197400	-0.22661200
O	-2.84847300	-1.81688100	-0.78416100
H	-2.51341400	4.91402700	-1.80799800
H	-2.98408100	5.60514900	-0.26091600
C	-6.10223400	-3.01165200	0.21667200
H	-7.81524800	-1.84861100	0.86991000
H	-4.26037400	-3.90566200	-0.46550100
H	-6.61007600	-3.96553200	0.33089500
C	0.30376100	-0.82254400	2.73473900
C	-0.95388200	-1.29709100	2.01207200
O	-1.52854000	-0.26424800	1.28695700
H	0.06941300	0.07712400	3.30871300
H	-1.64518100	-1.66336400	2.79286500
H	-0.68685900	-2.15951400	1.38213500
C	0.95452900	-1.88181700	3.60582900
H	1.20592100	-2.76337900	3.00703000
H	1.86098400	-1.49131900	4.07203500
H	0.26330900	-2.19128200	4.39609300
H	-2.42338400	2.34507900	-2.05039700
H	-0.96381900	2.13914100	0.60580500
O	1.65113800	2.02250600	1.26767500
O	1.25512600	-0.44666000	1.66529900
S	2.20828200	0.83183400	1.92107800
O	2.53261400	0.91676000	3.34743300
C	3.62011800	0.29633800	0.98134700
C	4.00524100	-1.04448800	0.97700600
C	4.37328300	1.26669000	0.32328500
C	5.15599900	-1.40970700	0.28910800

H	3.39565500	-1.78602100	1.47761600
C	5.53033600	0.88205000	-0.35092500
H	4.04876300	2.30102600	0.33555400
C	5.93529200	-0.45695400	-0.38217700
H	5.44997000	-2.45490500	0.26179200
H	6.12275900	1.63230900	-0.86685400
C	7.15692800	-0.88165300	-1.15550400
H	6.86867000	-1.37269800	-2.09302100
H	7.78972100	-0.02735800	-1.40904800
H	7.75940900	-1.59802100	-0.58856400

subsequent hydrolysis

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.312013

Thermal correction to Gibbs Free Energy (a.u.): 0.538020

Imaginary frequencies: -656.00

Calculation of single point energy based on the optimized structure, Et = -3582.3665589 a.u.

C	-1.28406600	4.55505800	0.27862000
C	-2.01031700	4.07972300	-0.83132300
C	-0.33592300	3.76915000	0.90588400
H	-1.46592700	5.56109200	0.64729700
C	-1.77225400	2.79546000	-1.27696300
H	-2.74362600	4.71121600	-1.32179800
C	-0.04959700	2.45374900	0.45424600
H	0.22803900	4.13500100	1.75705700
C	-0.80747300	1.96648100	-0.66312200
H	-2.33535000	2.39137900	-2.11316200
O	0.84242700	1.75601100	1.10506300
C	-0.68124500	0.61352400	-1.12098500
Co	1.78014700	0.31863400	0.32595900
N	0.28319400	-0.17708600	-0.79078700
H	-1.47234300	0.23791100	-1.77179700
N	2.65754200	-1.11051900	-0.58343500
C	0.31596100	-1.61866100	-1.04331700
C	3.93830500	-1.14639700	-0.77794900
C	1.76680500	-1.98548400	-1.37057300
C	-0.60120000	-2.20735900	-2.11016200
H	4.35063400	-2.01384100	-1.30089400
C	4.84861000	-0.08747000	-0.47492200
C	1.95020800	-3.49479100	-1.20741700
C	-0.45254200	-3.73980600	-2.06659700
H	-0.33014900	-1.81242200	-3.09917500
H	-1.64116900	-1.94822700	-1.91112400
C	6.23926000	-0.32992100	-0.53095700
C	4.36052600	1.25213300	-0.30467800
C	1.00775500	-4.20513000	-2.19730800
H	2.98707100	-3.79141500	-1.39956500
H	1.71657600	-3.76766600	-0.17210500
H	-1.05703300	-4.19429300	-2.85896400
H	-0.86954400	-4.08505100	-1.11483900
C	7.15068200	0.69719700	-0.39189700
H	6.58248000	-1.35090100	-0.67964400
C	5.32252000	2.29041100	-0.20129700
O	3.09342500	1.56044300	-0.27894500
H	1.36210000	-4.00578300	-3.21810000
H	1.06723600	-5.28916300	-2.05334000
C	6.67604100	2.01524300	-0.23118200
H	8.21644100	0.49740300	-0.41724500
H	4.95028600	3.30241200	-0.08390600
H	7.38736100	2.83071500	-0.13230300
H	1.94198700	-1.72741600	-2.42558900
H	0.06800200	-2.06059500	-0.07185000
O	2.96304100	0.01989400	2.00809700
H	2.82473400	0.81777400	2.53719100
H	2.06822400	-0.67089300	2.17350200
C	-1.31021200	-1.33161800	2.85952500
C	0.05301200	-0.65622600	2.85747900
O	0.92063400	-1.13727700	1.87467400

H	-1.18430900	-2.41186600	2.73643400
H	0.47183500	-0.82869400	3.86577600
H	-0.11793600	0.42852800	2.76180100
C	-2.11776700	-0.98594000	4.10265300
H	-2.20731200	0.10108400	4.20007100
H	-3.11534800	-1.42138800	4.06060000
H	-1.60294300	-1.36747000	4.98968200
O	-2.62192800	-2.77133800	0.17376400
O	-2.00212200	-0.81842700	1.65629400
S	-3.19066600	-1.71610600	1.01844400
O	-4.14793900	-2.09838800	2.05789500
C	-3.87694000	-0.44423000	-0.01830500
C	-4.15702800	0.81171600	0.52477000
C	-4.18072700	-0.74388400	-1.34366800
C	-4.73226900	1.78083500	-0.28582600
H	-3.90017500	1.02846600	1.55448400
C	-4.75692200	0.24407800	-2.14350500
H	-3.96686300	-1.73170000	-1.73539000
C	-5.03694100	1.51542400	-1.63015300
H	-4.92649500	2.76823400	0.12100600
H	-4.99203900	0.02185900	-3.18031200
C	-5.62441300	2.59732200	-2.49922000
H	-5.88171100	2.22116400	-3.49228500
H	-6.52922600	3.01902700	-2.04940400
H	-4.91338600	3.42246500	-2.62439600

subsequent hydrolysis

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.339792

Thermal correction to Gibbs Free Energy (a.u.): 0.540208

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.403759 a.u.

C	3.18730300	-2.55414600	-2.33957700
C	3.73132400	-1.27405500	-2.57644500
C	1.90668300	-2.70916300	-1.84944300
H	3.78727400	-3.43662300	-2.54564800
C	2.96426700	-0.16394600	-2.29963500
H	4.73994600	-1.16707800	-2.95944700
C	1.08752100	-1.58202000	-1.56762100
H	1.48058500	-3.69009500	-1.66915800
C	1.64583500	-0.28602300	-1.79987100
H	3.36853100	0.83280300	-2.45041200
O	-0.11715700	-1.79248200	-1.12134500
C	0.91338000	0.90138900	-1.50479700
Co	-1.46790600	-0.53109200	-0.80763100
N	-0.32266000	0.94753100	-1.11930800
H	1.45667700	1.83958300	-1.59565300
N	-2.88199900	0.77882800	-0.90877500
C	-0.96546600	2.18531000	-0.65730500
C	-4.08701800	0.54472500	-0.51054500
C	-2.39701200	2.13716400	-1.20763900
C	-0.27346300	3.50242100	-0.99353000
H	-4.77788400	1.37992800	-0.41017700
C	-4.61228700	-0.75244300	-0.20438200
C	-3.23633800	3.29131100	-0.65778900
C	-1.10812900	4.66595800	-0.43751400
H	-0.16623800	3.60205800	-2.08308200
H	0.72339500	3.51809700	-0.54703900
C	-5.92905500	-0.84603400	0.30122000
C	-3.87298200	-1.94286900	-0.48824600
C	-2.54868400	4.63153900	-0.96049500
H	-4.23491200	3.28864900	-1.10949400
H	-3.35362900	3.14045700	0.42192700
H	-0.63297700	5.61835800	-0.69574600
H	-1.11593900	4.60185700	0.65760700
C	-6.52206700	-2.07006500	0.53928200
H	-6.47242600	0.07460300	0.50116200
C	-4.51829000	-3.18609800	-0.26920500

O	-2.65119500	-1.95201000	-0.95566200
H	-2.54327100	4.79996100	-2.04652600
H	-3.13155200	5.44770900	-0.52066200
C	-5.80196200	-3.24355500	0.24087900
H	-7.52853400	-2.12888800	0.93904600
H	-3.95787900	-4.08524500	-0.50092800
H	-6.26115300	-4.21266800	0.41566400
H	-2.33027100	2.21753100	-2.30341700
H	-1.02040300	2.08257200	0.43309200
O	-3.19044200	1.44259700	2.19466900
H	-3.94813100	0.87933300	2.39235000
H	-2.51952700	0.80419300	1.84611200
C	0.29548600	-0.82574700	2.64708000
C	-0.91999200	-1.33865700	1.88157600
O	-1.48304100	-0.32955200	1.10946700
H	0.01709400	0.07762400	3.19526300
H	-1.63738800	-1.71015500	2.63518200
H	-0.61310300	-2.19927700	1.26978700
C	0.92732100	-1.85689200	3.56467200
H	1.22061900	-2.74446300	2.99436400
H	1.80538800	-1.43994700	4.06111700
H	0.20954100	-2.16453300	4.33160000
O	1.65568600	2.01571200	1.17342300
O	1.28123000	-0.44934900	1.61200500
S	2.19828500	0.85452100	1.88765900
O	2.44087800	0.97728600	3.32692600
C	3.67043100	0.32541300	1.04107900
C	4.06960500	-1.01075000	1.06888400
C	4.45320000	1.30082500	0.42570900
C	5.26536100	-1.36669600	0.45631700
H	3.43876300	-1.75613500	1.53623600
C	5.65439000	0.92586900	-0.17171600
H	4.11741600	2.33155100	0.41078900
C	6.07492900	-0.40889700	-0.17011200
H	5.57244200	-2.40851900	0.45486300
H	6.27006800	1.68020700	-0.65327400
C	7.34765000	-0.82305000	-0.86268900
H	7.99342700	0.03535900	-1.06425100
H	7.91240400	-1.54348000	-0.26316000
H	7.12584800	-1.30518000	-1.82272500

subsequent hydrolysis

Co^{III}(salen)-PO~OTs + H_2O = Co^{III}(salen)-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.335991

Thermal correction to Gibbs Free Energy (a.u.): 0.540939

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4000431 a.u.

C	-1.19525700	4.48641100	-0.23110500
C	-2.27768500	3.58900100	-0.31313300
C	0.11026200	4.03208100	-0.16382500
H	-1.38495000	5.55641100	-0.21687300
C	-2.01789500	2.23222600	-0.33680700
H	-3.29855800	3.95382300	-0.35691900
C	0.40411400	2.64487900	-0.16135300
H	0.94713600	4.71881200	-0.09788800
C	-0.69655200	1.74023300	-0.26340500
H	-2.83001800	1.51989800	-0.40402200
O	1.65602200	2.26784500	-0.08037600
C	-0.48700800	0.32505200	-0.36381400
Co	2.29161700	0.54134000	0.30295300
N	0.64767600	-0.26301800	-0.19957800
H	-1.35522900	-0.28179300	-0.60069900
N	3.05832600	-0.84576400	-0.84644200
C	0.86042800	-1.69713000	-0.40364400
C	4.32847800	-0.99644700	-1.06527900
C	2.04751900	-1.78106800	-1.37821900
C	-0.33221800	-2.51845900	-0.87239300
H	4.65332900	-1.83252400	-1.68819600

C	5.37159400	-0.16781100	-0.55543300
C	2.48828600	-3.23467400	-1.56233800
C	0.10287500	-3.97780700	-1.06348900
H	-0.71257500	-2.11949800	-1.82393700
H	-1.13397800	-2.46101000	-0.13521300
C	6.70436900	-0.47447900	-0.93396700
C	5.12057400	0.93362200	0.33172900
C	1.29725600	-4.09464500	-2.01901500
H	3.29594100	-3.31069500	-2.29800900
H	2.88096700	-3.60732700	-0.60735300
H	-0.74230700	-4.56697500	-1.43255700
H	0.37340200	-4.39785300	-0.08637600
C	7.77365800	0.26224200	-0.47784900
H	6.86621800	-1.31621500	-1.60330400
C	6.24813000	1.67224100	0.78896600
O	3.94599000	1.30234000	0.74905100
H	0.99068700	-3.77315300	-3.02393100
H	1.61486100	-5.13884200	-2.10920900
C	7.52791600	1.34624200	0.39349700
H	8.78609400	0.01630600	-0.77842100
H	6.05422600	2.50434200	1.45695500
H	8.36300900	1.93620900	0.76139300
H	1.70799400	-1.38087700	-2.34588700
H	1.19108400	-2.08884400	0.56453700
O	2.07099000	-0.11208100	2.01802400
H	2.78668100	0.25156400	2.55701200
H	0.70873300	-0.96328700	2.50464800
C	-2.48691100	-0.60714400	2.81799900
C	-1.01544900	-0.25461700	2.97279100
O	-0.19711600	-1.33957200	2.63375300
H	-2.71239500	-1.51838900	3.37761700
H	-0.88591000	0.05269600	4.02617900
H	-0.80412100	0.63035200	2.35462600
C	-3.38880100	0.54774800	3.22835900
H	-3.19894700	1.41569100	2.58897600
H	-4.43969800	0.26636900	3.15618100
H	-3.18136400	0.82977500	4.26495900
O	-3.48842900	-2.93439700	0.19661700
O	-2.66895500	-0.90283600	1.38687800
S	-3.97214900	-1.72477400	0.85821900
O	-4.97355800	-1.80363900	1.92073000
C	-4.49070500	-0.56854500	-0.39274400
C	-5.30800800	0.50395300	-0.03705400
C	-3.97273700	-0.68836900	-1.68211800
C	-5.58040600	1.48573200	-0.98569500
H	-5.71396600	0.56582300	0.96593500
C	-4.25224400	0.30644100	-2.61591200
H	-3.36134000	-1.54662900	-1.93690100
C	-5.03974100	1.41539200	-2.27796400
H	-6.21200900	2.32743500	-0.71672400
H	-3.84358900	0.22815800	-3.61909800
C	-5.26113200	2.53174300	-3.26486700
H	-5.23585700	2.16843100	-4.29568000
H	-6.21905600	3.03178800	-3.09821400
H	-4.47158300	3.28615000	-3.16162400

six-coordinated H_2O-Co^{III}-Cl counterion addition in the terminal carbon and subsequent hydrolysis

H_2O-Co^{III}-Cl counterion addition in the terminal carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.786572

Thermal correction to Gibbs Free Energy (a.u.): 0.423809

Imaginary frequencies: -356.02

Calculation of single point energy based on the optimized structure, Et = -3147.4833119 a.u.

C	4.31582200	-3.15752400	-0.73479900
C	5.08187300	-2.02485900	-0.40826900
C	2.94594200	-3.06637700	-0.91639300
H	4.80148900	-4.12400200	-0.83858200

C	4.44362700	-0.80605900	-0.27641000
H	6.15210100	-2.10791800	-0.25482800
C	2.27153000	-1.82907300	-0.78192500
H	2.34745500	-3.93887500	-1.15700100
C	3.05029100	-0.67728900	-0.46671600
H	5.00837900	0.08240700	-0.00777300
O	0.96583600	-1.81144000	-0.95099800
C	2.46566800	0.62573600	-0.29519800
Co	-0.18431900	-0.32500800	-0.70876700
N	1.22341200	0.92773000	-0.47263700
H	3.15113100	1.41270100	0.00455300
N	-1.35703200	1.17875800	-0.63891000
C	0.69886800	2.23287400	-0.04611400
C	-2.60273200	1.11659300	-0.31446100
C	-0.61695800	2.43625600	-0.80630300
C	1.63970500	3.42493900	-0.21459000
H	-3.14752100	2.04755900	-0.15493400
C	-3.35942100	-0.09414100	-0.15547200
C	-1.32678400	3.71390000	-0.36363800
C	0.92878100	4.71779900	0.20976200
H	1.96753300	3.49323600	-1.26120300
H	2.52366500	3.28413100	0.41222500
C	-4.67669800	-0.00186900	0.34441100
C	-2.83177100	-1.36520500	-0.53989000
C	-0.39091300	4.91863300	-0.54348500
H	-2.24596100	3.86487100	-0.94102700
H	-1.61084600	3.62163900	0.69271800
H	1.59151600	5.57441700	0.04815700
H	0.72981000	4.67131600	1.28783200
C	-5.47484800	-1.12132900	0.48517200
H	-5.05521900	0.97770700	0.62674800
C	-3.67615800	-2.49401100	-0.40527800
O	-1.62548400	-1.53556600	-1.02750400
H	-0.18529400	5.05806100	-1.61349500
H	-0.89361300	5.82868500	-0.19946200
C	-4.96027800	-2.37216700	0.09809800
H	-6.48086500	-1.03761300	0.88112600
H	-3.27249500	-3.45698900	-0.69957800
H	-5.57759200	-3.26064600	0.19872000
Cl	2.10969200	1.04204700	2.72744200
C	-0.32521400	-1.72993900	1.73993400
C	0.96696300	-1.36473900	2.33404000
O	-0.35915100	-0.43348500	1.14154600
H	-0.25659000	-2.52296500	0.98920000
H	1.88336900	-1.50398600	1.77919300
H	1.05439700	-1.07594100	3.37121900
C	-1.48873700	-1.93591300	2.69018000
H	-2.42555400	-1.99478900	2.13198100
H	-1.35880900	-2.86852100	3.25127700
H	-1.55013200	-1.10369600	3.39728300
H	-0.37872800	2.50959800	-1.87734500
H	0.48150000	2.10970100	1.02450200
O	-0.13733000	-0.26663200	-2.74958400
H	0.54561300	-0.95967300	-2.82076800
H	-0.97385800	-0.76582800	-2.82331700

H_2O-Co^{III}-Cl counterion addition in the terminal carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.818223

Thermal correction to Gibbs Free Energy (a.u.): 0.425097

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5231599 a.u.

C	3.97478900	-3.57690100	-0.63524000
C	4.83198300	-2.52522700	-0.27154000
C	2.62611600	-3.35323100	-0.86468900
H	4.36799500	-4.58556700	-0.72788400
C	4.31218200	-1.24911700	-0.15694600
H	5.88148900	-2.71290600	-0.07367600

C	2.07501600	-2.05854500	-0.74392600
H	1.95528300	-4.16345400	-1.13103500
C	2.94712500	-0.98708100	-0.40288900
H	4.94220200	-0.42040100	0.15135600
O	0.77399800	-1.91681400	-0.95380400
C	2.49125100	0.37263200	-0.26786200
Co	-0.23126500	-0.34123000	-0.71056800
N	1.27913400	0.78242800	-0.48119900
H	3.23899100	1.10249700	0.01876900
N	-1.26978000	1.25657300	-0.59544100
C	0.89243300	2.14799000	-0.09292700
C	-2.50717200	1.29745000	-0.23774200
C	-0.43150200	2.44563700	-0.80147300
C	1.92481100	3.24162000	-0.36681000
H	-2.96406300	2.27044900	-0.05486700
C	-3.36112000	0.15202700	-0.07620400
C	-1.01386100	3.78476800	-0.35632500
C	1.35405700	4.60240400	0.05666300
H	2.18851000	3.24466300	-1.43364800
H	2.82042800	3.03836700	0.22372100
C	-4.64901300	0.34339000	0.47017500
C	-2.96181800	-1.14660400	-0.51775100
C	0.00960200	4.90172500	-0.61654100
H	-1.94590200	3.99988000	-0.89169800
H	-1.24888000	3.73926000	0.71507000
H	2.07519700	5.39323700	-0.17446400
H	1.22881600	4.59928100	1.14654100
C	-5.53994600	-0.70537000	0.59934200
H	-4.92996300	1.34211600	0.79554000
C	-3.90102000	-2.19910100	-0.39884900
O	-1.78459500	-1.40796800	-1.03983200
H	0.15634600	5.00508400	-1.70030200
H	-0.39370000	5.85635600	-0.26243600
C	-5.15402400	-1.98127000	0.14988100
H	-6.52206100	-0.54683400	1.03058400
H	-3.59652700	-3.18210600	-0.74216900
H	-5.84725800	-2.81325000	0.23693000
Cl	2.72675700	1.29487600	2.52212200
C	-0.63870800	-1.85223700	1.80033700
C	0.56660800	-1.07497200	2.11193000
O	-0.44005200	-0.52112600	1.18800500
H	-0.53354100	-2.63645300	1.05544000
H	1.51293300	-1.32316700	1.65167000
H	0.65318100	-0.47367700	3.00976300
C	-1.81613100	-1.92766500	2.72633000
H	-2.75046000	-2.00382500	2.16508400
H	-1.71982600	-2.81847100	3.35651400
H	-1.85593400	-1.04788900	3.37326700
H	-0.23049000	2.48344000	-1.88188200
H	0.74129700	2.10594300	0.99698000
O	-0.17530600	-0.25064500	-2.69895100
H	0.46277200	-0.98384300	-2.79985400
H	-1.04533600	-0.68291800	-2.81258300

H_2O-Co^{III}-Cl counterion addition in the terminal carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.853941

Thermal correction to Gibbs Free Energy (a.u.): 0.425243

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5477466 a.u.

C	4.59269800	-2.78067100	-0.93318400
C	5.27824800	-1.55435800	-0.82784700
C	3.21317700	-2.83756500	-0.87618800
H	5.15684900	-3.70119500	-1.05677900
C	4.54382100	-0.39791900	-0.66232200
H	6.36142300	-1.52245800	-0.86801900
C	2.43066600	-1.66281400	-0.71438700
H	2.68133500	-3.78058900	-0.94680500

C	3.13035400	-0.41722600	-0.60940300
H	5.04852900	0.56059100	-0.56559800
O	1.13032700	-1.78611500	-0.66362200
C	2.44538100	0.82588100	-0.39150800
Co	-0.14334500	-0.36858900	-0.65020200
N	1.16599100	0.98439600	-0.37932400
H	3.08115100	1.69112200	-0.20310000
N	-1.39683300	1.06564600	-0.80771000
C	0.51897800	2.24650100	-0.00670800
C	-2.65997700	0.93585500	-0.58124400
C	-0.72004100	2.36187600	-0.91643200
C	1.38587000	3.50244500	-0.06465300
H	-3.27620800	1.83349200	-0.51685400
C	-3.34743500	-0.31004800	-0.39827700
C	-1.54912100	3.59910400	-0.57404100
C	0.54702600	4.74437900	0.26865700
H	1.81999500	3.60391600	-1.06896100
H	2.21493900	3.42014900	0.64541000
C	-4.70636000	-0.27213700	-0.01638800
C	-2.70526300	-1.56797200	-0.62327900
C	-0.67661600	4.86020700	-0.64689300
H	-2.39903300	3.69153500	-1.25912300
H	-1.95553200	3.49096300	0.44000300
H	1.16856600	5.64244400	0.18966400
H	0.21403100	4.68183100	1.31276800
C	-5.43684600	-1.43068500	0.16696800
H	-5.17224700	0.69782500	0.14261000
C	-3.47797800	-2.73949200	-0.43548400
O	-1.46536300	-1.68650600	-1.02953400
H	-0.34461900	5.01243500	-1.68272000
H	-1.27330500	5.73769000	-0.37661300
C	-4.80529000	-2.66939700	-0.04911700
H	-6.47694700	-1.38744000	0.47119600
H	-2.98614500	-3.69217600	-0.60076500
H	-5.36644400	-3.58911700	0.09300200
Cl	1.50308000	0.61533300	3.25839500
C	-0.09849300	-1.31078400	1.99273100
C	1.32146000	-1.04422500	2.50940100
O	-0.55667700	-0.31575800	1.13638100
H	-0.02194400	-2.28266900	1.47494800
H	2.04871700	-1.07024600	1.70304200
H	1.61077300	-1.75773200	3.28352000
C	-1.11979200	-1.44264000	3.12660400
H	-2.09333900	-1.69971800	2.70213600
H	-0.82519300	-2.22066300	3.83993400
H	-1.21215100	-0.49272000	3.66034200
H	-0.35930100	2.44531300	-1.95185300
H	0.15965900	2.08629900	1.01815300
O	0.07320800	-0.45729000	-2.73370100
H	0.78743400	-1.11639200	-2.74099800
H	-0.73589100	-1.00606300	-2.76478000

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.241361

Thermal correction to Gibbs Free Energy (a.u.): 0.438424

Imaginary frequencies: -570.97

Calculation of single point energy based on the optimized structure, Et = -3223.9907987 a.u.

C	2.19498400	-4.68321400	-0.60410100
C	2.91301500	-4.09414500	-1.66326900
C	1.35000000	-3.93510800	0.19422000
H	2.30356700	-5.74664500	-0.40972200
C	2.76591900	-2.74127700	-1.89342600
H	3.57243500	-4.69246300	-2.28201400
C	1.16905800	-2.54475300	-0.02298900
H	0.79921300	-4.38502300	1.01301900
C	1.89908700	-1.94750200	-1.10657200
H	3.31622900	-2.25937300	-2.69767800

O	0.38903000	-1.88485100	0.79321900
C	1.83424100	-0.53648000	-1.36927600
Co	-0.47065200	-0.28358800	0.30611800
N	0.97618800	0.26293700	-0.83756100
H	2.58280400	-0.12599900	-2.04818700
N	-1.31410900	1.30528600	-0.36738500
C	1.00640100	1.72229700	-0.93045700
C	-2.59403900	1.48940600	-0.36533200
C	-0.43400000	2.17198300	-1.17949100
C	1.95752100	2.36825100	-1.92958600
H	-2.97602900	2.43297400	-0.76278500
C	-3.57363600	0.51795100	0.02007400
C	-0.54502300	3.67798700	-0.93368600
C	1.86382800	3.89536600	-1.76001200
H	1.69172500	2.07655500	-2.95482500
H	2.98422500	2.04201100	-1.73983400
C	-4.91282400	0.92274900	0.20567200
C	-3.23851500	-0.87175800	0.04938800
C	0.42124100	4.41031600	-1.88169700
H	-1.56703300	4.03384600	-1.10096900
H	-0.29349600	3.88161000	0.11385200
H	2.50166800	4.39282900	-2.49803700
H	2.26033500	4.15686400	-0.77100100
C	-5.91121200	-0.00054400	0.45019600
H	-5.14650500	1.98355400	0.16024500
C	-4.28404100	-1.79824400	0.26765200
O	-2.02082000	-1.32317300	-0.15444000
H	0.07397500	4.27223900	-2.91461000
H	0.38925100	5.48664300	-1.68255700
C	-5.58365300	-1.36925400	0.47362600
H	-6.93432100	0.32190200	0.60977000
H	-4.02599100	-2.85171900	0.27853000
H	-6.36392400	-2.10356000	0.65340300
H	-0.67854600	1.95868900	-2.22991800
H	1.27838600	2.03902500	0.08250800
O	-1.38941500	-0.06060700	2.16643800
H	-1.27948200	-0.92891900	2.57826000
H	-0.42544800	0.51156400	2.29567600
O	-0.93036400	-1.60491600	-2.71821700
H	-0.29970400	-2.32243300	-2.57927400
H	-1.46919000	-1.61866200	-1.90721100
Cl	3.80387400	1.38921400	1.11703800
C	1.70984800	0.34936800	2.68672300
C	2.97167600	-0.03177500	1.91585300
O	0.72146500	0.91732300	1.87812200
H	1.37065500	-0.62995000	3.08475200
H	2.74206000	-0.72601100	1.11353700
H	3.71716900	-0.47162900	2.58032100
C	2.00519300	1.27221900	3.87265800
H	1.08662200	1.44676000	4.43958000
H	2.75381200	0.83874500	4.54581200
H	2.37313500	2.23601100	3.51114900

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.272580

Thermal correction to Gibbs Free Energy (a.u.): 0.441331

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3224.0227652 a.u.

C	-4.84939100	2.36793200	-1.05040300
C	-5.45232800	1.17783000	-0.59682800
C	-3.48340400	2.44995500	-1.24192100
H	-5.46694500	3.23918700	-1.25051200
C	-4.65316200	0.08211300	-0.34533900
H	-6.52510100	1.12644200	-0.44733600
C	-2.63652600	1.34140900	-0.98059700
H	-3.01250000	3.36420100	-1.58707500
C	-3.25014000	0.13156400	-0.52654000

H	-5.09483400	-0.84749900	0.00526700
O	-1.35180700	1.48315700	-1.17859600
C	-2.49312000	-1.05207200	-0.24773300
Co	0.01071500	0.22164400	-0.79495500
N	-1.21089200	-1.18230600	-0.34441300
H	-3.07355200	-1.91118200	0.08951600
N	1.34813400	-1.15503300	-0.74900600
C	-0.50511800	-2.39400400	0.10894700
C	2.59561100	-0.90942900	-0.53354600
C	0.76261300	-2.50008100	-0.75277300
C	-1.29896700	-3.69966200	0.08659300
H	3.26755000	-1.74088100	-0.32500500
C	3.18383400	0.39971200	-0.55757600
C	1.66070300	-3.63275300	-0.25892100
C	-0.40465500	-4.85885500	0.55430000
H	-1.66821900	-3.88862800	-0.93074600
H	-2.17198100	-3.63418900	0.74407000
C	4.52137100	0.54618700	-0.13060000
C	2.47576100	1.52820200	-1.07535200
C	0.88124100	-4.95591800	-0.27411600
H	2.55033800	-3.72067000	-0.89251100
H	1.98700400	-3.39283500	0.75998100
H	-0.96351300	-5.79927300	0.50242500
H	-0.14277500	-4.70147600	1.60816200
C	5.16384600	1.76829700	-0.18677700
H	5.03729300	-0.32672200	0.26090100
C	3.16583500	2.76051600	-1.15314300
O	1.23220500	1.47764600	-1.49898400
H	0.62838800	-5.21751800	-1.31064000
H	1.51611400	-5.76253500	0.10719100
C	4.47251300	2.87604200	-0.71058600
H	6.18537600	1.87193000	0.16218500
H	2.62446500	3.61205300	-1.55085700
H	4.96794000	3.84152000	-0.76403700
H	0.45079400	-2.69356500	-1.78911300
H	-0.16135600	-2.18062300	1.13028200
O	1.47605300	-1.40638600	2.41419500
H	1.02516600	-1.36417000	3.26660800
H	1.12169300	-0.60912300	1.94251200
O	-0.22171700	-0.09097500	-3.24748700
H	-0.95155400	0.54195300	-3.16323500
H	0.55881000	0.48730100	-3.21044300
Cl	-1.19872500	0.70882200	3.70911300
C	0.20815700	1.88252700	1.59275900
C	-1.11270600	1.94646000	2.36468200
O	0.37687800	0.61081700	1.05057900
H	0.08689100	2.63173600	0.78985100
H	-1.94821600	1.71444000	1.70538300
H	-1.26687900	2.91829200	2.83762400
C	1.42654600	2.26360900	2.43702700
H	2.31506400	2.28363800	1.80139100
H	1.30295300	3.24995200	2.89805000
H	1.58594000	1.52369000	3.22591100

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2Cl$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.269707

Thermal correction to Gibbs Free Energy (a.u.): 0.442583

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3224.0197965 a.u.

C	-4.21716400	3.81055700	0.64129000
C	-5.00656300	2.65172300	0.52024600
C	-2.85459900	3.77660000	0.40319000
H	-4.68269000	4.74922300	0.92901800
C	-4.39923700	1.46845000	0.14809900
H	-6.07350300	2.68964100	0.71073700
C	-2.20486300	2.57054200	0.04599900
H	-2.24029100	4.66561200	0.49755000

C	-3.00813400	1.39818500	-0.09080000
H	-4.98851800	0.56165500	0.03675800
O	-0.90877300	2.59572400	-0.16130700
C	-2.46060500	0.15062600	-0.53828300
Co	0.21804300	1.07553300	-0.28831800
N	-1.21183400	-0.10061400	-0.74744900
H	-3.18133900	-0.64452200	-0.72324200
N	1.34784100	-0.26452900	-1.10666800
C	-0.73549600	-1.43213100	-1.16425200
C	2.60540300	-0.39582700	-0.84728400
C	0.57726800	-1.20710100	-1.92585700
C	-1.70837400	-2.27923000	-1.98155400
H	3.13098300	-1.27286700	-1.22524200
C	3.39346700	0.54063000	-0.10010100
C	1.24845500	-2.54293000	-2.24056000
C	-1.04778300	-3.62186100	-2.32896400
H	-1.99141900	-1.74010100	-2.89597500
H	-2.62113000	-2.47067100	-1.41127300
C	4.72914300	0.19654000	0.20968900
C	2.88990400	1.83060800	0.26117200
C	0.29035800	-3.42866200	-3.05141500
H	2.17381800	-2.38703000	-2.80617400
H	1.50894900	-3.03365900	-1.29444100
H	-1.72782200	-4.22086500	-2.94385200
H	-0.88322500	-4.18110600	-1.39936200
C	5.56580600	1.07594200	0.86712600
H	5.08778900	-0.78846700	-0.07862600
C	3.77603100	2.72125500	0.91658100
O	1.67458600	2.24725000	-0.00681300
H	0.11221000	-2.96354200	-4.03036200
H	0.76064500	-4.39839400	-3.24573900
C	5.07460900	2.34928300	1.21346600
H	6.58477500	0.79442100	1.10886500
H	3.39205300	3.70075300	1.18076500
H	5.72404300	3.05316800	1.72664900
H	0.34791600	-0.67429900	-2.85933800
H	-0.47570500	-1.96291600	-0.24156800
O	0.24835300	0.40049800	1.50342900
H	0.73075800	1.04569800	2.03799700
H	0.76194900	-1.14230000	1.48084400
O	0.40806900	2.24439300	-2.55406400
H	-0.26794700	2.77184100	-2.09622000
H	1.22363800	2.54834500	-2.12557200
Cl	-2.33333600	-2.85097900	1.58585300
C	0.28815700	-2.65425300	2.61737500
C	-1.15022200	-2.16128400	2.80355200
O	0.88946600	-2.13425200	1.45382600
H	0.80340500	-2.26729800	3.51856600
H	-1.18887400	-1.07992200	2.66953700
H	-1.54171100	-2.44830600	3.78081000
C	0.42941200	-4.16942000	2.59785700
H	1.48724800	-4.43732400	2.53672000
H	0.00258400	-4.61914900	3.49977900
H	-0.08453600	-4.58271500	1.72628900

six-coordinated H_2O-Co^{III}-Cl counterion addition in the middle carbon and subsequent hydrolysis

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.787046

Thermal correction to Gibbs Free Energy (a.u.): 0.422668

Imaginary frequencies: -237.07

Calculation of single point energy based on the optimized structure, Et = -3147.4853475 a.u.

C	4.45531600	-2.73935100	-0.98577300
C	5.11791200	-1.53987800	-0.67328500
C	3.07614000	-2.78307600	-1.10740000
H	5.02942400	-3.65129900	-1.12547800
C	4.36713400	-0.39221600	-0.49722500

H	6.19677800	-1.51662000	-0.56662000
C	2.28684300	-1.62220800	-0.91931800
H	2.55713100	-3.70917400	-1.33187200
C	2.96132600	-0.40121100	-0.62436700
H	4.85171900	0.54549600	-0.23970900
O	0.97954900	-1.74118500	-1.00874000
C	2.25991100	0.83678400	-0.40977200
Co	-0.29783000	-0.37192100	-0.71436700
N	0.98964900	1.01575500	-0.54238400
H	2.87506800	1.68373100	-0.12133400
N	-1.60646400	1.01415200	-0.60347500
C	0.35762700	2.26781800	-0.10289300
C	-2.81515200	0.83676900	-0.19411800
C	-0.99895200	2.33343200	-0.81601400
C	1.17244800	3.54271400	-0.31572800
H	-3.43987000	1.71222300	-0.01410300
C	-3.43062400	-0.43982000	0.04315200
C	-1.81177800	3.54391800	-0.36250100
C	0.35416300	4.76750800	0.11718800
H	1.45882500	3.62721200	-1.37331200
H	2.08383700	3.49515200	0.28515900
C	-4.71326000	-0.46722600	0.63231300
C	-2.80200900	-1.66132000	-0.35122600
C	-1.00312600	4.82931200	-0.59226000
H	-2.76241200	3.59556000	-0.90556700
H	-2.04564400	3.44282600	0.70529600
H	0.92557600	5.68121200	-0.07733400
H	0.19706000	4.71817300	1.20200100
C	-5.37837000	-1.65798000	0.85683100
H	-5.17256200	0.47688800	0.91585700
C	-3.50817100	-2.86634500	-0.11988100
O	-1.62946000	-1.71895500	-0.93887600
H	-0.84803000	4.96949200	-1.67068500
H	-1.57900500	5.69297700	-0.24321500
C	-4.76095500	-2.86110600	0.46987400
H	-6.35930200	-1.66529200	1.31916500
H	-3.02831500	-3.79160900	-0.42100200
H	-5.27272400	-3.80483300	0.63789500
Cl	2.01928700	1.37614900	2.65575700
C	0.83748500	-1.21102600	2.62691800
C	-0.25495500	-1.71784100	1.76752100
O	-0.38229100	-0.45930800	1.13846800
H	0.57742700	-0.53116500	3.42792600
H	-1.17316100	-2.01598800	2.29260800
H	0.06015500	-2.51259200	1.08419700
C	2.20532800	-1.74085500	2.54285700
H	2.90758300	-1.16681400	3.14170200
H	2.14418000	-2.79282900	2.87879200
H	2.55909800	-1.78883200	1.51019900
H	-0.80742800	2.41256100	-1.89587000
H	0.19484900	2.13576700	0.97632000
O	-0.36267100	-0.33864600	-2.75451100
H	-1.15728000	-0.90643500	-2.77756400
H	0.37152200	-0.97381800	-2.85247600

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.810782

Thermal correction to Gibbs Free Energy (a.u.): 0.425377

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5165932 a.u.

C	4.26804000	-3.15042500	-0.85323800
C	5.02175900	-2.00460000	-0.54983600
C	2.88842900	-3.08817600	-0.97279500
H	4.76867900	-4.10581800	-0.98454800
C	4.36500100	-0.79875000	-0.38631600
H	6.09877900	-2.06600600	-0.43978200
C	2.19949200	-1.86884500	-0.79136000

H	2.29854900	-3.97406000	-1.18399900
C	2.96328200	-0.70191300	-0.51801100
H	4.91707900	0.10080500	-0.13098800
O	0.87735800	-1.88968500	-0.86786400
C	2.36128300	0.59334100	-0.35198200
Co	-0.28217900	-0.42145600	-0.63841700
N	1.10531700	0.86531500	-0.52329700
H	3.03309000	1.40552800	-0.10056200
N	-1.48358700	1.07226400	-0.60059500
C	0.58350300	2.18882700	-0.15153700
C	-2.72453300	1.01237600	-0.25865900
C	-0.76718200	2.33049100	-0.85893400
C	1.49838600	3.37557100	-0.45382700
H	-3.27704300	1.94525900	-0.14305200
C	-3.46638800	-0.19621500	-0.02207400
C	-1.47906100	3.61998200	-0.45663600
C	0.79230200	4.68263100	-0.06855200
H	1.76396700	3.37788900	-1.52020200
H	2.40849400	3.27881400	0.14176100
C	-4.78066500	-0.08887700	0.48494200
C	-2.92772800	-1.48165400	-0.33655500
C	-0.57213000	4.82503200	-0.75228200
H	-2.42671800	3.72589300	-0.99723800
H	-1.71085500	3.58500200	0.61594500
H	1.43118600	5.53538000	-0.32061700
H	0.66225200	4.69817400	1.02072800
C	-5.56288800	-1.20742200	0.70028800
H	-5.16924900	0.90154300	0.70963900
C	-3.75399900	-2.61056300	-0.12008000
O	-1.72175500	-1.66788200	-0.82425400
H	-0.43186200	4.90827400	-1.83861400
H	-1.07087600	5.74498400	-0.42926200
C	-5.03511400	-2.47332200	0.38678500
H	-6.56702500	-1.11203600	1.09817300
H	-3.34216700	-3.58466600	-0.36192000
H	-5.63999700	-3.36135600	0.54750900
Cl	2.53630500	1.53654700	2.45544600
C	0.33637000	-0.92133100	2.47701200
C	-1.04682900	-1.33024900	2.17768700
O	-0.38558400	-0.38925000	1.29306600
H	0.52206100	-0.09120200	3.15313200
H	-1.89759800	-0.89631800	2.69553500
H	-1.20891800	-2.30818300	1.73327300
C	1.48698600	-1.85860100	2.30219200
H	2.38421200	-1.28682200	2.06294300
H	1.65173400	-2.35298300	3.26676100
H	1.28777200	-2.61643900	1.54446700
H	-0.57529600	2.34857300	-1.94157000
H	0.44064400	2.15064200	0.93854900
O	-0.31235000	-0.45657000	-2.62173200
H	-1.13996700	-0.97499700	-2.67519200
H	0.38735500	-1.13768000	-2.69008400

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1908.850972

Thermal correction to Gibbs Free Energy (a.u.): 0.424394

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5461455 a.u.

C	4.61073700	-2.69730500	-1.08124500
C	5.25841100	-1.45777000	-0.91071000
C	3.23201100	-2.79014900	-1.08701700
H	5.20396600	-3.59940100	-1.20495700
C	4.48717300	-0.32514900	-0.74789800
H	6.34115400	-1.39741100	-0.90235900
C	2.41347900	-1.64093200	-0.92645400
H	2.72848100	-3.74347800	-1.20817000
C	3.07371400	-0.38226200	-0.75558300

H	4.96192300	0.64311400	-0.60633300
O	1.11592300	-1.79549800	-0.94686800
C	2.35067200	0.84193000	-0.55788100
Co	-0.20287500	-0.43228600	-0.75556100
N	1.06744700	0.97556900	-0.57563200
H	2.96246300	1.72337700	-0.36383300
N	-1.52654300	0.93955100	-0.77584100
C	0.39950500	2.23154900	-0.20513100
C	-2.75637100	0.76109200	-0.42933900
C	-0.92179500	2.25615600	-0.99344400
C	1.20223300	3.51534400	-0.41242300
H	-3.39910400	1.63416000	-0.30908900
C	-3.37315800	-0.51189300	-0.19428700
C	-1.76927500	3.47188700	-0.62174200
C	0.34824000	4.74106400	-0.05685500
H	1.53230600	3.57547200	-1.45854700
H	2.09965500	3.50862600	0.21406100
C	-4.69416300	-0.53514300	0.30514900
C	-2.70644900	-1.73846000	-0.50826200
C	-0.96729200	4.76199400	-0.84297900
H	-2.68768900	3.49433000	-1.21860300
H	-2.06491700	3.39775400	0.43291400
H	0.91921800	5.65635700	-0.24506700
H	0.12735000	4.72211800	1.01825600
C	-5.36380200	-1.72467600	0.51684000
H	-5.17955200	0.41237300	0.52858000
C	-3.42017800	-2.94313000	-0.29137400
O	-1.50578000	-1.79915000	-1.02431400
H	-0.75115400	4.87483100	-1.91386800
H	-1.57142500	5.62763200	-0.55176300
C	-4.70991900	-2.93287600	0.20889400
H	-6.37468300	-1.72927900	0.90983000
H	-2.91197900	-3.87183800	-0.52820600
H	-5.22488000	-3.87638400	0.36941800
Cl	1.14581500	1.19227400	3.24830700
C	0.53292000	-0.55481000	3.25724800
C	0.54343300	-1.09981800	1.83186700
O	-0.39862900	-0.42851200	1.06824600
H	-0.49695300	-0.46475000	3.60718400
H	0.33033900	-2.18348300	1.90134400
H	1.57137700	-1.00283400	1.45356700
C	1.38813300	-1.36571700	4.21606600
H	1.39043000	-0.92674100	5.21603500
H	0.98817200	-2.38338400	4.28416500
H	2.42084600	-1.42434400	3.85992400
H	-0.66693100	2.30961300	-2.06189400
H	0.14449400	2.11962000	0.85612400
O	-0.17534300	-0.49843700	-2.84940100
H	-0.97122400	-1.06533600	-2.82982800
H	0.55182600	-1.14627200	-2.87157000

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.778588

Thermal correction to Gibbs Free Energy (a.u.): 0.416606

Imaginary frequencies: -295.27

Calculation of single point energy based on the optimized structure, Et = -3147.4736933 a.u.

C	4.40372600	-2.74754300	-1.15903900
C	5.08332500	-1.55719400	-0.84169600
C	3.02230400	-2.78210200	-1.23964600
H	4.96878900	-3.65877700	-1.33479300
C	4.34923800	-0.40752800	-0.62204800
H	6.16518700	-1.54383700	-0.76874400
C	2.24853200	-1.62134300	-0.99402300
H	2.49014900	-3.69958400	-1.46758500
C	2.93922500	-0.40838200	-0.70225800
H	4.84807800	0.52265600	-0.36550700
O	0.93994800	-1.72736500	-1.03229100

C	2.24834500	0.82793200	-0.47357400
Co	-0.31320100	-0.39090300	-0.59529600
N	0.96913700	1.00599300	-0.54906900
H	2.87392100	1.68326800	-0.23908100
N	-1.62098800	1.01686500	-0.53619700
C	0.35749000	2.27149700	-0.11197200
C	-2.84838000	0.85204900	-0.17502100
C	-1.01333200	2.33001300	-0.79320300
C	1.17483000	3.53681200	-0.36662600
H	-3.47751200	1.73323300	-0.04533600
C	-3.47950900	-0.41372500	0.06350000
C	-1.81176200	3.55291900	-0.34700300
C	0.37196500	4.77237000	0.06572000
H	1.43361800	3.60230400	-1.43248900
H	2.10130300	3.49454700	0.21124800
C	-4.79672600	-0.42177700	0.57575300
C	-2.83993700	-1.64840000	-0.26831600
C	-1.00033500	4.82970000	-0.61420200
H	-2.77021600	3.60286700	-0.87580000
H	-2.02913000	3.46995800	0.72594600
H	0.94333000	5.67975300	-0.15623500
H	0.23893100	4.74149000	1.15449000
C	-5.48243900	-1.60260300	0.78056400
H	-5.26432800	0.53045500	0.81409300
C	-3.57200200	-2.84411500	-0.06711200
O	-1.63167000	-1.73505300	-0.77375900
H	-0.86812100	4.95148600	-1.69776300
H	-1.56383000	5.70207900	-0.26672800
C	-4.85506700	-2.81850200	0.44888800
H	-6.48850100	-1.59475900	1.18525800
H	-3.08306300	-3.77731600	-0.32533000
H	-5.38502300	-3.75456900	0.60180600
Cl	2.20638300	1.35154800	2.55143200
C	1.04209400	-1.15472700	2.80394400
C	-0.13386200	-1.64804900	2.05322400
O	-0.30194800	-0.43597000	1.36963000
H	0.86794600	-0.49065300	3.63948900
H	-0.99479400	-1.90522700	2.68997200
H	0.09618300	-2.49652700	1.39397200
C	2.38100200	-1.72864300	2.58769700
H	3.16442500	-1.17009900	3.09316300
H	2.32725700	-2.76955400	2.95785700
H	2.61585000	-1.80702300	1.52359200
H	-0.84809600	2.38018000	-1.87882300
H	0.22063200	2.15405600	0.97204100
O	-0.59089000	-0.47991200	-3.01963600
H	-1.31131600	-1.08349400	-2.77349100
H	0.18333100	-1.06439400	-3.01257200

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.818206

Thermal correction to Gibbs Free Energy (a.u.): 0.418383

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3147.5181825 a.u.

C	4.20489200	-3.21739300	-0.90259000
C	4.98710900	-2.08138700	-0.62056900
C	2.82716700	-3.13041000	-0.99362900
H	4.68681300	-4.18153100	-1.03834700
C	4.36355500	-0.86094200	-0.44807100
H	6.06462800	-2.16610600	-0.53226400
C	2.16829400	-1.89296900	-0.80115300
H	2.21350300	-4.00376500	-1.18700300
C	2.96093600	-0.73761600	-0.55089500
H	4.93842800	0.02662900	-0.20300100
O	0.85307200	-1.87866100	-0.84745800
C	2.37769000	0.55938300	-0.38381600
Co	-0.28402900	-0.42184400	-0.62456900

N	1.10725600	0.83382100	-0.51665800
H	3.06266400	1.37558300	-0.19641600
N	-1.46262000	1.08481000	-0.59434100
C	0.61564200	2.17539000	-0.15176600
C	-2.71426400	1.04272700	-0.27925100
C	-0.73345100	2.33620900	-0.85575500
C	1.54985000	3.34435700	-0.46286900
H	-3.25737400	1.98322400	-0.18552000
C	-3.47569600	-0.15002800	-0.04817700
C	-1.42590100	3.63570600	-0.45231700
C	0.86504200	4.66309700	-0.07653800
H	1.80676300	3.34096700	-1.53133000
H	2.46220000	3.23506700	0.12723000
C	-4.81564200	-0.02073800	0.38437800
C	-2.93272800	-1.44949700	-0.29301900
C	-0.50101200	4.82637700	-0.75220100
H	-2.37228000	3.75658800	-0.99166700
H	-1.65657000	3.60405300	0.62065500
H	1.51600200	5.50504200	-0.33368900
H	0.74131600	4.68347100	1.01350300
C	-5.61472300	-1.12775500	0.58860400
H	-5.20883900	0.97764200	0.55907400
C	-3.77868400	-2.56822000	-0.09234700
O	-1.70426800	-1.66269000	-0.70095200
H	-0.36541900	4.90728000	-1.83921000
H	-0.98310700	5.75420100	-0.42651200
C	-5.08171600	-2.40791700	0.34177500
H	-6.63811200	-1.01496600	0.92883400
H	-3.36013600	-3.55069500	-0.28245800
H	-5.70238800	-3.28593100	0.49631900
Cl	2.75996000	1.46288100	2.31387100
C	0.28751300	-0.84481600	2.71089700
C	-1.12736700	-1.18632900	2.49830900
O	-0.45476200	-0.30210000	1.57317200
H	0.54155500	-0.05135400	3.40834000
H	-1.91503900	-0.70334400	3.07228200
H	-1.37739700	-2.15919300	2.08112700
C	1.38692600	-1.82380300	2.42781500
H	2.28176300	-1.27605900	2.12520600
H	1.61866800	-2.37071600	3.34868200
H	1.09325200	-2.53797400	1.65576400
H	-0.54530800	2.34883700	-1.93884200
H	0.47023600	2.14064400	0.93690400
O	-0.48290700	-0.57983100	-2.93720200
H	-1.21604600	-1.19905900	-2.78452000
H	0.28757400	-1.16244400	-3.01995700

H_2O-Co^{III}-Cl counterion addition in the middle carbon

H_2O-Co^{III}-Cl + PO = H_2O-Co^{III}-PO~Cl

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1908.840118

Thermal correction to Gibbs Free Energy (a.u.): 0.417499

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3147.5338766 a.u.

C	4.83866200	-1.13597900	-1.78530100
C	5.29846900	0.03228400	-1.14595900
C	3.48968500	-1.42433200	-1.86626900
H	5.55644200	-1.82617100	-2.22016600
C	4.37390100	0.89692100	-0.59792200
H	6.35996300	0.24623500	-1.08685900
C	2.52067800	-0.56433000	-1.29181600
H	3.13034900	-2.32565100	-2.35099700
C	2.98667200	0.62612600	-0.65381300
H	4.70318100	1.80646700	-0.10108400
O	1.25716100	-0.88861100	-1.39608500
C	2.09151800	1.57840700	-0.07407100
Co	-0.21512500	-0.04470400	-0.52439100
N	0.80500900	1.47318400	0.00325300
H	2.55985400	2.47376900	0.33474200

N	-1.75476600	1.11687900	-0.25984800
C	-0.03471100	2.47136200	0.68145700
C	-2.96007900	0.68786700	-0.09551000
C	-1.35425600	2.51719200	-0.11091300
C	0.56558500	3.86811900	0.84769500
H	-3.74335300	1.39587100	0.18130500
C	-3.37292000	-0.67631200	-0.26048400
C	-2.36954200	3.45811000	0.53613100
C	-0.45676300	4.81736500	1.48985300
H	0.86640700	4.25073700	-0.13675200
H	1.46476200	3.82769900	1.47062000
C	-4.69455500	-1.02536600	0.09952900
C	-2.51137400	-1.65995600	-0.84315000
C	-1.76593700	4.86074700	0.69466700
H	-3.28052600	3.51079900	-0.06969700
H	-2.65373700	3.06274300	1.52053300
H	-0.02645400	5.82096400	1.57080900
H	-0.66563500	4.48120600	2.51409300
C	-5.17638200	-2.30672700	-0.07892800
H	-5.33194000	-0.25722400	0.53143100
C	-3.03778100	-2.96235200	-1.03196700
O	-1.28812100	-1.41964700	-1.24709700
H	-1.57468900	5.28605300	-0.29944200
H	-2.48811200	5.52150600	1.18540200
C	-4.33080300	-3.27467700	-0.65438100
H	-6.18852200	-2.56351700	0.21394600
H	-2.38191300	-3.70300100	-1.47659200
H	-4.69774800	-4.28656300	-0.80316500
Cl	2.66545700	-1.54266800	2.16628200
C	1.03719700	-2.29557700	2.57168500
C	0.06481700	-2.05529800	1.41794200
O	-0.17822600	-0.70058100	1.23336200
H	0.69901000	-1.73856000	3.44815500
H	-0.86779600	-2.58952800	1.68185000
H	0.46532600	-2.53505900	0.51168800
C	1.23553200	-3.76936600	2.88740500
H	1.94727300	-3.90911200	3.70397100
H	0.27716200	-4.21219100	3.18225100
H	1.60749900	-4.30540800	2.00933200
H	-1.11468600	2.87778000	-1.12114600
H	-0.26332700	2.04743600	1.66948000
O	-0.43451300	0.62383500	-3.02007400
H	-1.08946800	-0.08564100	-2.92398800
H	0.39849300	0.12495700	-2.98792800

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1985.209025

Thermal correction to Gibbs Free Energy (a.u.): 0.445935

Imaginary frequencies: -245.97

Calculation of single point energy based on the optimized structure, Et = -3223.9634969 a.u.

C	3.18393200	-4.20448400	-0.98975800
C	4.07814000	-3.24206800	-1.49167500
C	1.92240600	-3.84673000	-0.54657200
H	3.48480400	-5.24767500	-0.94727200
C	3.67773000	-1.91978300	-1.52900500
H	5.06530600	-3.53112200	-1.83507300
C	1.48513600	-2.49975900	-0.58364800
H	1.22988900	-4.58418000	-0.15468100
C	2.39595400	-1.52157200	-1.08988200
H	4.35672500	-1.15360100	-1.89545400
O	0.27380200	-2.22802700	-0.15407400
C	2.08240800	-0.11397900	-1.10483400
Co	-0.61636100	-0.59499500	-0.38226400
N	0.94234100	0.40433600	-0.80912100
H	2.89893200	0.55306900	-1.37711700
N	-1.55683700	1.04585600	-0.56959900
C	0.70590800	1.85546100	-0.75889000

C	-2.76960600	1.24940800	-0.17165500
C	-0.73736700	2.07299300	-1.22831500
C	1.67303900	2.73753200	-1.54331200
H	-3.15851000	2.26752500	-0.21015200
C	-3.68714800	0.24325000	0.27517500
C	-1.15630300	3.52889800	-1.02494100
C	1.27256000	4.20901300	-1.35940700
H	1.65353800	2.46621500	-2.60830300
H	2.69382200	2.59674200	-1.17922700
C	-4.92725100	0.65245500	0.81101400
C	-3.41232900	-1.14623700	0.09729000
C	-0.18385700	4.45851500	-1.76839500
H	-2.17370500	3.69696700	-1.39411800
H	-1.15191700	3.75548300	0.04875600
H	1.94279600	4.85250900	-1.93900200
H	1.40853400	4.47748100	-0.30434700
C	-5.88778400	-0.26957700	1.18097700
H	-5.11452600	1.71672300	0.93309100
C	-4.41687400	-2.06852300	0.46327500
O	-2.29650700	-1.59500900	-0.43391500
H	-0.29062500	4.29405900	-2.84923300
H	-0.45874100	5.50206200	-1.58225600
C	-5.62059400	-1.63808000	0.99559400
H	-6.83310700	0.05487500	1.60200500
H	-4.20355100	-3.12322800	0.32646300
H	-6.36907200	-2.37305900	1.27904600
Cl	3.25094200	2.12510500	1.65761400
C	2.59714000	0.89674500	2.88376400
C	1.66695900	-0.09119600	2.17251300
O	0.52095500	0.49297100	1.69054000
H	2.01542300	1.51259300	3.57199300
H	1.45482100	-0.88146700	2.92629700
H	2.27154700	-0.58474900	1.38811100
C	3.77725200	0.23154700	3.57141400
H	4.44221400	0.96668500	4.02993000
H	3.40710000	-0.43769600	4.35600700
H	4.35569500	-0.36269100	2.85758300
H	-0.77848300	1.83967200	-2.30318100
H	0.75750700	2.09563700	0.30715200
O	-1.39192800	-0.98142800	1.94348000
H	-0.99380500	-1.85888300	1.86771800
H	-0.59950500	-0.32769700	2.04549600
O	-0.85594400	-1.01849800	-2.31973900
H	-0.23838800	-1.75280200	-2.47226000
H	-1.71723600	-1.44577000	-2.06994300

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1985.272883

Thermal correction to Gibbs Free Energy (a.u.): 0.446663

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3224.0302949 a.u.

C	4.64260400	-2.63203300	-0.91616500
C	5.29763400	-1.38952000	-0.81676300
C	3.26262900	-2.71418900	-0.93882800
H	5.22886400	-3.54511700	-0.97089100
C	4.53459900	-0.24283200	-0.72993500
H	6.38058800	-1.33693800	-0.79732100
C	2.45713900	-1.55054200	-0.86952200
H	2.75405600	-3.67014700	-1.00423000
C	3.12068800	-0.28901800	-0.75172000
H	5.01625900	0.72747600	-0.63401700
O	1.15388500	-1.69016400	-0.93223900
C	2.40824900	0.94839400	-0.58755100
Co	-0.14842900	-0.30592700	-0.79593200
N	1.12577300	1.08797500	-0.57855700
H	3.02889500	1.83038400	-0.42601700
N	-1.46178700	1.07485400	-0.83996100

C	0.46217100	2.35064100	-0.22348500
C	-2.70365200	0.89992100	-0.53834900
C	-0.84388800	2.38912100	-1.03638900
C	1.27948900	3.62773200	-0.40963800
H	-3.34591400	1.77488700	-0.43126300
C	-3.33080500	-0.37480500	-0.33111800
C	-1.68932800	3.60758300	-0.66908500
C	0.42852100	4.85688500	-0.05780400
H	1.62649700	3.69341200	-1.45002600
H	2.16659200	3.60839800	0.23143400
C	-4.65502000	-0.40667600	0.15604500
C	-2.66043900	-1.59663100	-0.64545000
C	-0.87391800	4.89362800	-0.86494800
H	-2.59604500	3.64266700	-1.28288300
H	-2.00433800	3.52515300	0.37921800
H	1.00895200	5.76934800	-0.22956700
H	0.19054000	4.83055700	1.01337200
C	-5.31604300	-1.60346200	0.36263100
H	-5.14939100	0.53624800	0.37845300
C	-3.35582400	-2.80902000	-0.42616600
O	-1.45353100	-1.64302400	-1.15864400
H	-0.63979800	5.01481000	-1.93114200
H	-1.47662200	5.76070700	-0.57546900
C	-4.64974400	-2.80698900	0.06854400
H	-6.32973000	-1.61523900	0.74809900
H	-2.82569000	-3.73097500	-0.63929400
H	-5.15547000	-3.75418400	0.23514300
Cl	0.59584100	1.46421800	3.35894100
C	0.40089600	-0.37674800	3.26184800
C	0.62322400	-0.84145500	1.82844600
O	-0.41021300	-0.37445400	1.01851800
H	-0.64171700	-0.53780500	3.54134300
H	0.66332400	-1.94310100	1.84622900
H	1.61784100	-0.48668800	1.51916800
C	1.35741900	-1.02133300	4.25055400
H	1.19819800	-0.64307500	5.26258400
H	1.19542400	-2.10459100	4.25243500
H	2.39649700	-0.82934500	3.96722600
H	-0.56983300	2.44830500	-2.09973000
H	0.18296900	2.24124900	0.83203400
O	-0.23264300	-3.75625500	0.58248700
H	0.19020500	-3.18853700	-0.08456600
H	-0.97787700	-3.20494800	0.85170200
O	-0.04763200	-0.31775900	-2.88799600
H	0.68233400	-0.95778300	-2.94444500
H	-0.84374900	-0.88526100	-2.90770700

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1985.277818

Thermal correction to Gibbs Free Energy (a.u.): 0.446973

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3224.0319789 a.u.

C	2.90156900	-4.25652400	-0.90312100
C	3.89590100	-3.26252000	-0.98132700
C	1.55890300	-3.92624700	-0.86922800
H	3.19141600	-5.30309000	-0.86250900
C	3.50672200	-1.93859500	-1.03226400
H	4.94603700	-3.53272900	-1.00072100
C	1.13166000	-2.57435600	-0.90916500
H	0.79014500	-4.68902600	-0.80312100
C	2.14181500	-1.56759100	-1.00062600
H	4.25138900	-1.14819800	-1.08473400
O	-0.15475900	-2.32575400	-0.88106800
C	1.83362900	-0.16617400	-1.03047200
Co	-0.95397400	-0.62148300	-0.62314800
N	0.65632800	0.35395800	-0.94284800
H	2.69020100	0.50174400	-1.09331200

N	-1.78843300	1.08012300	-0.49250200
C	0.48196100	1.80846200	-0.77687500
C	-2.87098400	1.30612100	0.17100300
C	-0.97826800	2.11977300	-1.13081400
C	1.42388100	2.70411700	-1.58392100
H	-3.19112600	2.33894100	0.31526800
C	-3.72553200	0.29060600	0.71584400
C	-1.32003700	3.57280400	-0.80692900
C	1.10106500	4.17815700	-1.29606800
H	1.30606400	2.48576700	-2.65398700
H	2.46438300	2.50856500	-1.31634300
C	-4.79880900	0.68516800	1.54359500
C	-3.56184900	-1.08680500	0.36616700
C	-0.37097600	4.50827400	-1.57286600
H	-2.35806800	3.79494200	-1.07812700
H	-1.21883700	3.73730000	0.27364100
H	1.75142100	4.82419400	-1.89518000
H	1.33118100	4.38781600	-0.24372000
C	-5.69774800	-0.23651700	2.04561800
H	-4.90433600	1.74004700	1.78659100
C	-4.50557900	-2.00766700	0.88115300
O	-2.62034200	-1.52718400	-0.43405100
H	-0.56871800	4.41215300	-2.64893400
H	-0.58426000	5.54898200	-1.30700000
C	-5.54084100	-1.59145600	1.70037500
H	-6.51179400	0.07779900	2.68964700
H	-4.38090700	-3.05164700	0.61368700
H	-6.24209800	-2.32713500	2.08508000
Cl	3.96815500	1.77035500	1.04040000
C	3.58128800	0.81494800	2.57440900
C	2.28954600	0.03384700	2.40263100
O	1.20325700	0.88862100	2.19648000
H	3.43825000	1.59406500	3.32544900
H	2.17923600	-0.55346500	3.33486500
H	2.41600700	-0.69180300	1.58551300
C	4.76838800	-0.07662000	2.90017600
H	5.68748900	0.50481800	2.99547400
H	4.58593900	-0.59426300	3.84837900
H	4.91070800	-0.82921600	2.11885700
H	-1.09240100	1.96178900	-2.21327900
H	0.63728000	1.99837600	0.29359900
O	-0.66387800	-0.62602200	1.19142100
H	-0.58776200	-1.56666600	1.40363000
H	0.45281800	0.32259500	1.85185200
O	-1.43834300	-0.79262800	-2.62812600
H	-0.92050400	-1.60938000	-2.74803600
H	-2.32746800	-1.12135400	-2.38788900

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.240869

Thermal correction to Gibbs Free Energy (a.u.): 0.437686

No imaginary frequency

Calculation of single point energy based on the optimized structure, Et = -3223.9899937 a.u.

C	2.35037800	-4.59880100	-0.91130000
C	3.14949300	-3.87274000	-1.81553600
C	1.37572400	-3.97511500	-0.15432000
H	2.49961200	-5.66971500	-0.80444900
C	2.94592000	-2.51282900	-1.93790700
H	3.91091200	-4.37358400	-2.40306000
C	1.14462200	-2.57913900	-0.25925900
H	0.76245400	-4.52947900	0.54777600
C	1.94958800	-1.84475500	-1.19008300
H	3.55254200	-1.92815500	-2.62500300
O	0.23809600	-2.04038400	0.51269600
C	1.81256200	-0.42491400	-1.34917100
Co	-0.59716200	-0.39552700	0.17929800
N	0.85386200	0.29033700	-0.86804300

H	2.59243600	0.07466900	-1.92390000
N	-1.46281500	1.25247200	-0.31636800
C	0.82793400	1.75650700	-0.90020200
C	-2.72479600	1.47563800	-0.15139600
C	-0.62784800	2.15453500	-1.13582700
C	1.75448500	2.46373900	-1.88284500
H	-3.11364400	2.45761300	-0.42872800
C	-3.69286600	0.51015900	0.27788100
C	-0.80144900	3.65569900	-0.89327800
C	1.59853900	3.98188000	-1.69415000
H	1.50735400	2.17510100	-2.91365800
H	2.79441500	2.18236400	-1.69462800
C	-4.99040800	0.94216600	0.62526200
C	-3.40466600	-0.88642400	0.19564100
C	0.13801600	4.43378700	-1.83052300
H	-1.83466400	3.97118500	-1.07052000
H	-0.56700800	3.87163200	0.15612100
H	2.22519100	4.51381900	-2.41766400
H	1.97110700	4.24608300	-0.69667000
C	-5.99187300	0.03584700	0.91776500
H	-5.18931100	2.01035000	0.66519500
C	-4.45484800	-1.79357600	0.46526700
O	-2.22788000	-1.35974900	-0.14887300
H	-0.19254700	4.28345900	-2.86717700
H	0.05413000	5.50672000	-1.62798300
C	-5.71181800	-1.34011900	0.82743800
H	-6.98139300	0.37797400	1.20055500
H	-4.23439700	-2.85305300	0.39070400
H	-6.49492700	-2.06151000	1.04380900
Cl	3.68066800	1.85927500	1.15761900
C	3.08411200	0.89672500	2.62141700
C	1.94372700	-0.02560500	2.19380000
O	0.81145700	0.67264000	1.80130200
H	2.69982400	1.66556800	3.29427300
H	1.74334500	-0.67972700	3.06513400
H	2.32872900	-0.68414700	1.39865500
C	4.26500600	0.15341900	3.22304600
H	5.07982100	0.83492600	3.47611400
H	3.94362400	-0.35688500	4.13791100
H	4.64558400	-0.59836900	2.52519500
H	-0.87547300	1.92733100	-2.18317200
H	1.09463500	2.04612100	0.12140200
O	-1.30277600	-0.27779000	2.15067900
H	-1.22553700	-1.19593400	2.44576600
H	-0.29294400	0.20157300	2.26000700
O	-1.03332900	-1.59135200	-2.61451200
H	-0.43916700	-2.34039700	-2.47983600
H	-1.67177000	-1.66707800	-1.88250300

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.266958

Thermal correction to Gibbs Free Energy (a.u.): 0.440740

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3224.0202296 a.u.

C	4.63704100	-2.71551900	-1.07461000
C	5.24177000	-1.46375600	-1.31230800
C	3.29239300	-2.81676900	-0.77792700
H	5.23944800	-3.61861900	-1.12210600
C	4.46498800	-0.32714400	-1.24099800
H	6.30005700	-1.39832900	-1.53966100
C	2.46604400	-1.66279100	-0.70245300
H	2.82341600	-3.77590500	-0.58604900
C	3.08116000	-0.39355200	-0.95035700
H	4.90937400	0.65101900	-1.40835900
O	1.20546400	-1.82685700	-0.41019500
C	2.34804800	0.82935100	-0.84927300
Co	-0.15368200	-0.52656700	-0.54368300

N	1.07001600	0.93065200	-0.68464000
H	2.93682700	1.74530500	-0.90028200
N	-1.50329800	0.81016100	-0.86868100
C	0.38936100	2.20204400	-0.41545000
C	-2.75696700	0.61519800	-0.64799200
C	-0.93692600	2.12935100	-1.18748800
C	1.15684000	3.48228600	-0.73359900
H	-3.43306100	1.46877800	-0.67987200
C	-3.35998500	-0.66142100	-0.38316500
C	-1.82194100	3.33750900	-0.88086100
C	0.27211400	4.69882600	-0.42176400
H	1.44976300	3.48891600	-1.79272900
H	2.07287900	3.53210100	-0.13597500
C	-4.72959300	-0.69975500	-0.04257000
C	-2.63745500	-1.88125300	-0.55417100
C	-1.05843600	4.63646100	-1.18038900
H	-2.73624600	3.30623900	-1.48421900
H	-2.10390100	3.28804700	0.17740200
H	0.80952800	5.62015200	-0.67032400
H	0.07307400	4.72500300	0.65670000
C	-5.39137600	-1.89826800	0.14663500
H	-5.26035500	0.24239900	0.07212300
C	-3.34345900	-3.09511300	-0.38378100
O	-1.36567200	-1.93627800	-0.88254300
H	-0.86470500	4.70595700	-2.25976300
H	-1.68346400	5.49671700	-0.91850900
C	-4.68272000	-3.10001200	-0.03367200
H	-6.44077900	-1.91336800	0.42017300
H	-2.79041600	-4.01799200	-0.52149800
H	-5.19191700	-4.04961800	0.10599100
Cl	2.18840500	0.77807000	2.56864300
C	0.77061200	-0.09171600	3.37145400
C	0.08598500	-1.00128300	2.34988100
O	-0.52191000	-0.26577800	1.34048800
H	0.09149000	0.72229200	3.63394000
H	-0.66863700	-1.58051600	2.91621600
H	0.81349300	-1.72219500	1.95217400
C	1.28112600	-0.83257200	4.59524200
H	1.78588000	-0.15610900	5.28825900
H	0.43709000	-1.29705000	5.11784100
H	1.98325300	-1.62041400	4.30683200
H	-0.69035000	2.10675700	-2.25904800
H	0.15201400	2.18581800	0.65450400
O	-1.77495100	1.92181400	2.15860600
H	-2.53564200	1.63355100	2.67623600
H	-1.34719300	1.07630000	1.85312800
O	0.07408100	-0.97865700	-2.98079100
H	0.90023500	-1.47886500	-2.93043900
H	-0.59949300	-1.61652500	-2.68379300

subsequent hydrolysis

H_2O-Co^{III}-PO~Cl + PO = H_2O-Co^{III}-OH + $CH_3CHClCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1985.265285

Thermal correction to Gibbs Free Energy (a.u.): 0.441305

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3224.0188319 a.u.

C	-3.03372300	3.97034800	-1.38978400
C	-3.97131100	2.92100500	-1.42144000
C	-1.68407500	3.72084200	-1.21182800
H	-3.37295400	4.99640800	-1.50309000
C	-3.52255300	1.62172000	-1.28275800
H	-5.02685100	3.12936900	-1.55810200
C	-1.20192200	2.40098800	-1.03858700
H	-0.95790000	4.52612300	-1.18336100
C	-2.15124600	1.33731600	-1.08911100
H	-4.22272700	0.79113600	-1.29869400
O	0.08670500	2.21984600	-0.85961300
C	-1.75778500	-0.03835600	-0.97994700

Co	0.91723300	0.62024800	-0.23263500
N	-0.57393900	-0.46701000	-0.70106000
H	-2.54658400	-0.76964700	-1.13386300
N	1.94768700	-1.01541700	-0.47856100
C	-0.26883700	-1.89774800	-0.54586100
C	3.15253400	-1.18480000	-0.04659600
C	1.15116900	-2.07829100	-1.10373900
C	-1.25707300	-2.87506700	-1.17962400
H	3.60698000	-2.17325600	-0.13130900
C	3.97429000	-0.16951300	0.54335900
C	1.64824700	-3.51096000	-0.91603100
C	-0.75575200	-4.31515800	-0.99925500
H	-1.36646400	-2.64530300	-2.24837000
H	-2.23702800	-2.76892100	-0.70775000
C	5.23667900	-0.54979300	1.05700200
C	3.57994800	1.20656000	0.57631700
C	0.66066000	-4.49895400	-1.55492500
H	2.63954700	-3.63646500	-1.36492800
H	1.74416900	-3.72153400	0.15747700
H	-1.44834500	-5.00913100	-1.48660900
H	-0.76285600	-4.56347900	0.06996700
C	6.10242900	0.37477300	1.60363800
H	5.51431500	-1.60037200	1.01543200
C	4.49438600	2.13699100	1.13339900
O	2.45252000	1.66513200	0.09218100
H	0.64930300	-4.34320400	-2.64195900
H	1.00686700	-5.52442900	-1.38843200
C	5.71668200	1.72940900	1.63328500
H	7.06316400	0.06672100	2.00113700
H	4.19310100	3.17886800	1.15121500
H	6.38941100	2.46913000	2.05852300
Cl	-4.37978000	-1.57537100	0.81041200
C	-4.04950300	-0.64197300	2.37285300
C	-2.68672800	0.02649200	2.32082000
O	-1.66328500	-0.92081700	2.21128300
H	-4.04332000	-1.42410000	3.13418500
H	-2.61173300	0.60592500	3.26079600
H	-2.67639200	0.75652800	1.49826500
C	-5.18119800	0.35047400	2.58445800
H	-6.15120900	-0.15037600	2.59666800
H	-5.04319500	0.86186300	3.54350500
H	-5.18641100	1.10268700	1.79003000
H	1.11671700	-1.84183200	-2.17656400
H	-0.24484200	-2.07786000	0.53588000
O	0.47156100	0.46649200	1.58667400
H	0.89645400	1.18497500	2.07322800
H	-0.81999900	-0.41051400	2.07480800
O	1.79159200	1.07459900	-2.67256300
H	1.13609800	1.76708400	-2.47964000
H	2.55277200	1.37535900	-2.15453200

six-coordinated H_2O-Co^{III}-OAc counterion addition in the terminal carbon and subsequent hydrolysis

H_2O-Co^{III}-OAc counterion addition in the terminal carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.012502

Thermal correction to Gibbs Free Energy (a.u.): 0.468060

Imaginary frequencies: -368.72

Calculation of single point energy based on the optimized structure, Et = -2915.816743 a.u.

C	3.75307500	-3.93985700	-0.55338900
C	4.67642800	-2.87947300	-0.59121500
C	2.39001100	-3.70393700	-0.60035300
H	4.11198400	-4.96274400	-0.47906600
C	4.19830500	-1.58628100	-0.67830100
H	5.74221200	-3.07381800	-0.54491600
C	1.87707300	-2.38666600	-0.69083200
H	1.67306500	-4.51737300	-0.56180200
C	2.81373100	-1.31124500	-0.73635500

H	4.88954000	-0.74754800	-0.69577000
O	0.57256600	-2.23004100	-0.72768100
C	2.40178200	0.06376100	-0.79524200
Co	-0.37210300	-0.58748000	-0.79136400
N	1.18979900	0.48717700	-0.90066000
H	3.20121000	0.79734000	-0.73015400
N	-1.34574400	1.03947200	-1.01519000
C	0.85469800	1.90612600	-0.72327100
C	-2.56492100	1.21355500	-0.63337600
C	-0.46865800	2.12675800	-1.46775200
C	1.92387500	2.91137400	-1.14669700
H	-2.98076700	2.22121700	-0.65751900
C	-3.44888600	0.17704500	-0.18028500
C	-0.98734500	3.55050300	-1.27697300
C	1.39983300	4.34521400	-0.98349000
H	2.21165400	2.72895400	-2.19128300
H	2.81283100	2.78226700	-0.52392000
C	-4.70778000	0.54877700	0.34055600
C	-3.10457300	-1.20525800	-0.29037300
C	0.07848600	4.55920300	-1.72972000
H	-1.91233100	3.70334200	-1.84412800
H	-1.22016200	3.71110900	-0.21618400
H	2.15469800	5.05663800	-1.33428900
H	1.24915100	4.54867300	0.08437700
C	-5.62109200	-0.39835300	0.76258300
H	-4.94611300	1.60736300	0.41197800
C	-4.06436400	-2.15658900	0.13122400
O	-1.96550000	-1.63412400	-0.78149800
H	0.24501900	4.44828800	-2.80971000
H	-0.28868400	5.57864000	-1.57182700
C	-5.28648500	-1.76005100	0.64709100
H	-6.57962300	-0.09911000	1.17183300
H	-3.79908400	-3.20498300	0.04608200
H	-5.99587300	-2.51603600	0.97232700
C	-0.50820300	-1.38939800	1.92001500
C	0.85759200	-1.02538200	2.31716100
O	-0.44639700	-0.26264800	1.03792600
H	-0.59389100	-2.33172500	1.37219000
H	1.70023000	-1.42943700	1.77486000
H	1.03831400	-0.45050800	3.22511100
C	-1.59613800	-1.21281100	2.96004700
H	-2.58092300	-1.25377600	2.48825300
H	-1.53497300	-2.01089200	3.70883400
H	-1.47530500	-0.25013100	3.46400200
H	-0.28584300	1.95060200	-2.53767300
H	0.67872700	2.00803200	0.35453400
C	2.64777300	3.02628800	2.75539700
H	2.87974300	3.42680300	3.74399200
H	1.94898100	3.71277800	2.26176200
H	3.55317100	2.97681100	2.14396900
C	1.98839000	1.64259400	2.87674400
O	2.02946500	0.93345600	1.80607400
O	1.45157900	1.32459600	3.95290800
O	-0.45906300	-0.98188100	-2.79793200
H	0.12047400	-1.76423100	-2.75068700
H	-1.35588700	-1.36138000	-2.71494100

H_2O-Co^{III}-OAc counterion addition in the terminal carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.050234

Thermal correction to Gibbs Free Energy (a.u.): 0.467831

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8546316 a.u.

C	2.98355600	-4.52535300	-0.36380000
C	4.06062800	-3.62387000	-0.37655400
C	1.67664700	-4.07905100	-0.48367700
H	3.17222000	-5.58931700	-0.24959500
C	3.79871800	-2.27353800	-0.52050900

H	5.07899000	-3.97991900	-0.26618000
C	1.38949700	-2.70319100	-0.62611600
H	0.83916300	-4.76888100	-0.46605100
C	2.47978900	-1.79047900	-0.65813900
H	4.60843300	-1.54991800	-0.50861400
O	0.11993700	-2.34206500	-0.72899900
C	2.29680000	-0.36766400	-0.78153100
Co	-0.54649700	-0.57584000	-0.77375900
N	1.16072700	0.23965600	-0.89087300
H	3.19757300	0.23206200	-0.75102700
N	-1.25368400	1.19114300	-0.92903600
C	1.07203700	1.69890000	-0.73862000
C	-2.41225100	1.54377300	-0.48792600
C	-0.23316700	2.13860700	-1.40545000
C	2.26160700	2.51142100	-1.24650300
H	-2.65894600	2.60531500	-0.46930200
C	-3.43276400	0.64552500	-0.01972800
C	-0.50802700	3.61825700	-1.14130200
C	1.99384500	3.99896100	-0.97533400
H	2.41905200	2.33016500	-2.31987300
H	3.15831100	2.20781100	-0.70308600
C	-4.59004100	1.19301500	0.57469600
C	-3.32498600	-0.76735400	-0.19604900
C	0.68279100	4.46442600	-1.61883800
H	-1.42371300	3.94034500	-1.65115100
H	-0.65187300	3.76579900	-0.06371700
H	2.83009400	4.60248000	-1.34424000
H	1.94280900	4.13748500	0.11108900
C	-5.62780300	0.38791100	1.00628300
H	-4.64956000	2.27211700	0.69390700
C	-4.40803000	-1.56931500	0.23547100
O	-2.28980000	-1.35203700	-0.75704700
H	0.76191300	4.39030100	-2.71236200
H	0.49398400	5.51841100	-1.38854700
C	-5.52698200	-1.00274100	0.82418600
H	-6.50683900	0.82059600	1.47089500
H	-4.32470700	-2.64163700	0.09323500
H	-6.33769800	-1.64722300	1.15261000
C	-0.64335500	-1.45772800	2.06623000
C	0.46845100	-0.49770700	2.09395300
O	-0.62647500	-0.32716000	1.12159400
H	-0.47232500	-2.39758400	1.54922200
H	1.43374800	-0.72636300	1.65729300
H	0.48442000	0.33212700	2.79204400
C	-1.78495400	-1.40782300	3.03824800
H	-2.71924900	-1.69624600	2.54906300
H	-1.59358800	-2.10572000	3.86037500
H	-1.89809100	-0.40262100	3.45161900
H	-0.14660200	1.97016000	-2.48918000
H	1.00836800	1.87894900	0.35370600
C	3.82832800	2.39236300	3.12393900
H	3.32991100	2.95984200	3.91295900
H	4.48145300	3.07561500	2.56788000
H	4.46538700	1.61548600	3.55546300
C	2.80820700	1.77438700	2.15214600
O	3.23054100	0.82778900	1.42507100
O	1.64720400	2.27849400	2.14361300
O	-0.69266700	-0.90059800	-2.73071100
H	-0.23700300	-1.76473100	-2.71113600
H	-1.64068000	-1.13861300	-2.68508700

H_2O-Co^{III}-OAc counterion addition in the terminal carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.096521

Thermal correction to Gibbs Free Energy (a.u.): 0.471962

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9012378 a.u.

C	4.04143300	-3.73848300	-0.38994500

C	4.83430000	-2.69204900	-0.90284000
C	2.69862700	-3.55565400	-0.12219100
H	4.49342400	-4.70769700	-0.19697700
C	4.24437300	-1.46592600	-1.13063100
H	5.88847100	-2.84669300	-1.10469100
C	2.05918600	-2.30803900	-0.35929700
H	2.08668300	-4.35555700	0.28119600
C	2.86987300	-1.24489900	-0.87851800
H	4.83676000	-0.63699000	-1.51162500
O	0.78706200	-2.20171800	-0.08656600
C	2.34593000	0.07567500	-1.08390300
Co	-0.34395300	-0.75775700	-0.59260800
N	1.10581600	0.40929200	-0.97058200
H	3.07624900	0.84706600	-1.33039400
N	-1.46590500	0.65377100	-1.23863300
C	0.62737400	1.79029000	-1.03877500
C	-2.71519800	0.76489300	-0.93646400
C	-0.68342800	1.73487400	-1.84850200
C	1.59952700	2.82897500	-1.59010000
H	-3.23675600	1.68743900	-1.19479300
C	-3.50536300	-0.23106100	-0.27244600
C	-1.35008100	3.10912500	-1.91410800
C	0.92164000	4.20460800	-1.65491500
H	1.93269000	2.53182000	-2.59410900
H	2.48867000	2.88329000	-0.95295100
C	-4.82756400	0.10534000	0.09394400
C	-3.00493100	-1.54408000	-0.00574000
C	-0.37283700	4.15257300	-2.47415800
H	-2.25007900	3.07002900	-2.53728000
H	-1.66438600	3.40286500	-0.90400700
H	1.61255400	4.94036100	-2.07966300
H	0.69234500	4.53963500	-0.63458900
C	-5.65523900	-0.80324100	0.72461700
H	-5.18529300	1.10906100	-0.12481600
C	-3.87576300	-2.45793200	0.63620000
O	-1.81164800	-1.95176600	-0.35947200
H	-0.13320300	3.90270900	-3.51644100
H	-0.85352400	5.13632400	-2.49053000
C	-5.16277000	-2.09443200	0.99136400
H	-6.66501300	-0.52827300	1.00925300
H	-3.49046700	-3.45072000	0.84284100
H	-5.80138600	-2.81934000	1.48901700
C	-0.00362700	-0.48896000	2.19586300
C	1.47872700	-0.10291700	2.33003900
O	-0.58623300	0.03698000	1.04182500
H	-0.02451200	-1.59120600	2.19505500
H	2.07979600	-0.62972000	1.59223600
H	1.85762900	-0.31207500	3.33271500
C	-0.84853900	0.01223500	3.37302600
H	-1.87287600	-0.35098200	3.25733600
H	-0.44509700	-0.33245300	4.33013600
H	-0.87311100	1.10559000	3.38581500
H	-0.42643500	1.40917500	-2.86700400
H	0.36136300	2.03786800	-0.00382000
C	1.89076400	3.58148400	2.54691500
H	2.13599700	4.25362900	3.36852900
H	0.93073400	3.87636300	2.11037400
H	2.64676800	3.65152600	1.76019000
C	1.78841400	2.16260000	3.06221000
O	1.68317200	1.30231200	2.03126400
O	1.79117800	1.84865200	4.23268000
O	-0.35203000	-1.67299700	-2.48555600
H	0.32861400	-2.34898100	-2.33864600
H	-1.18022500	-2.11777300	-2.21070800

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.485774

Thermal correction to Gibbs Free Energy (a.u.): 0.485394
Imaginary frequencies: -612.42
Calculation of single point energy based on the optimized structure, Et = -2992.3459953 a.u.

C	-0.43354900	5.19910100	-0.51293800
C	-1.12890500	4.88395600	-1.69717900
C	0.04562300	4.20904400	0.32392500
H	-0.26703700	6.24032200	-0.25106500
C	-1.33687200	3.55635500	-2.01112000
H	-1.49863000	5.67081400	-2.34514600
C	-0.13783200	2.83477100	0.02225400
H	0.57742800	4.44914600	1.23807800
C	-0.84783600	2.51630000	-1.18621600
H	-1.88135100	3.28535800	-2.91244900
O	0.30437500	1.94681800	0.87398400
C	-1.15219600	1.15782300	-1.54030700
Co	0.77532400	0.20045600	0.34815100
N	-0.62917300	0.12938500	-0.96943300
H	-1.89118000	1.00494700	-2.32874700
N	1.24259500	-1.51311200	-0.37809900
C	-1.03996300	-1.25899300	-1.16134000
C	2.43206900	-2.01684200	-0.30801100
C	0.24748900	-2.07252000	-1.31716700
C	-2.02460200	-1.57857500	-2.27773000
H	2.59747000	-3.00396900	-0.74732500
C	3.58758500	-1.34505600	0.20632600
C	-0.07123500	-3.56098300	-1.16871700
C	-2.35239500	-3.08147300	-2.21578100
H	-1.59636300	-1.31938200	-3.25537000
H	-2.94069600	-0.99387300	-2.14769600
C	4.76198900	-2.08458600	0.46338100
C	3.61016600	0.08310500	0.29307000
C	-1.09159600	-3.95947600	-2.24980900
H	0.83150500	-4.17258300	-1.26873100
H	-0.47579900	-3.73470300	-0.16459500
H	-3.02123500	-3.35371800	-3.03905100
H	-2.89986400	-3.27834000	-1.28573200
C	5.93491200	-1.45629700	0.83465600
H	4.72534900	-3.16730700	0.37180000
C	4.83256600	0.70273900	0.64222000
O	2.56776700	0.83679100	0.02424400
H	-0.61520600	-3.86937500	-3.23528800
H	-1.36649900	-5.01274600	-2.13072500
C	5.96006500	-0.05099400	0.91644500
H	6.82711700	-2.03454000	1.04871800
H	4.84692500	1.78590200	0.69720200
H	6.88126700	0.45235600	1.19644200
H	0.64175800	-1.88713700	-2.32642000
H	-1.48639800	-1.53220600	-0.19941500
O	1.46608800	-0.28237300	2.25258200
H	1.51214700	0.57590800	2.69655800
H	0.38217200	-0.63083400	2.26390700
O	1.86747200	1.35179200	-2.65271500
H	1.43591900	2.21058800	-2.56167600
H	2.27939600	1.21878700	-1.78024800
C	-1.72084200	-0.04594500	2.43906000
C	-2.73277000	0.66123600	1.53912200
O	-0.75545300	-0.75895600	1.70719900
H	-1.24577900	0.77788600	3.00657600
H	-2.22244800	1.35043400	0.87167900
H	-3.47078200	1.19827100	2.13755800
C	-2.39599900	-0.99541500	3.43370200
H	-1.64695300	-1.41200400	4.11286300
H	-3.16991500	-0.48964000	4.01918600
H	-2.85756800	-1.82852200	2.89489200
C	-5.23660500	-1.65273600	0.06271300
H	-6.29254400	-1.81995100	0.27169800
H	-4.68593800	-2.58939100	0.19378500
H	-5.10263100	-1.33464000	-0.97451800
C	-4.69291900	-0.61314100	1.01477400

O	-3.42826200	-0.27539500	0.67573000
O	-5.30066600	-0.15248400	1.95571400

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.515029

Thermal correction to Gibbs Free Energy (a.u.): 0.490883

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2992.3758712 a.u.

C	-4.36649800	3.55724600	0.12237900
C	-5.10325700	2.53772300	-0.51651100
C	-3.01305700	3.42320300	0.35866900
H	-4.87269500	4.46530600	0.43828300
C	-4.44776700	1.38933900	-0.90500600
H	-6.16680100	2.65522700	-0.69220800
C	-2.30781500	2.25255900	-0.03460400
H	-2.44330800	4.20021000	0.85693000
C	-3.05823000	1.21986900	-0.68853800
H	-4.99444000	0.58495600	-1.39136500
O	-1.03364000	2.18276300	0.22938600
C	-2.45501400	-0.01498900	-1.08614800
Co	0.18664200	0.89781400	-0.43220200
N	-1.19280500	-0.28861300	-1.03016500
H	-3.13704200	-0.78496200	-1.44789300
N	1.38046400	-0.33927300	-1.29327000
C	-0.64097400	-1.62048600	-1.30465300
C	2.64838000	-0.36514900	-1.06826800
C	0.67331600	-1.37426900	-2.06171200
C	-1.54283900	-2.60642400	-2.04166600
H	3.23015800	-1.20595800	-1.44311900
C	3.38111700	0.65571600	-0.37250500
C	1.43099200	-2.68170900	-2.29379500
C	-0.78446200	-3.92231700	-2.27170300
H	-1.85771700	-2.17953200	-3.00395900
H	-2.44769800	-2.80106900	-1.45587200
C	4.74527300	0.43015000	-0.08912500
C	2.79007100	1.91604200	-0.05589900
C	0.53010400	-3.68844700	-3.02472300
H	2.33237400	-2.50015300	-2.88981800
H	1.73780500	-3.07454100	-1.31784000
H	-1.41988900	-4.62406800	-2.82230400
H	-0.56816700	-4.38226500	-1.29943000
C	5.52640800	1.40223300	0.50710100
H	5.17415300	-0.53518400	-0.34673000
C	3.61586600	2.90470000	0.52653900
O	1.53073500	2.21283700	-0.29685300
H	0.30808400	-3.31550800	-4.03407900
H	1.06632800	-4.63476700	-3.15158900
C	4.94701200	2.64791400	0.80810800
H	6.57007400	1.21156400	0.73214200
H	3.16188300	3.86181600	0.75953200
H	5.55080400	3.42277100	1.27230100
H	0.41411800	-0.91593800	-3.02724800
H	-0.38790800	-2.03295000	-0.32311100
O	1.58348800	-2.50991800	1.01960500
H	2.19186400	-2.59613900	1.76248000
H	1.20202500	-1.59231100	1.11536500
O	-0.02518700	2.23226900	-2.53220200
H	-0.77618600	2.76998600	-2.24569300
H	0.73095100	2.62987700	-2.06400400
C	-0.05981700	0.24537900	2.42294600
C	-1.48897900	-0.33372600	2.46260200
O	0.54932000	-0.06641200	1.20103300
H	-0.18362700	1.33563900	2.52532500
H	-2.14260700	0.25683100	1.82139300
H	-1.88617200	-0.35822600	3.48009600
C	0.83158700	-0.24733200	3.56727600
H	1.80934700	0.23794000	3.49179000

H	0.39429800	-0.01551900	4.54334400
H	0.97125800	-1.32970400	3.51503600
C	-1.22925000	-3.98957000	1.93710100
H	-1.34567700	-4.84961700	2.59616100
H	-0.22322900	-3.97634200	1.50131000
H	-1.95600600	-4.02938400	1.12154700
C	-1.37067300	-2.71421000	2.72756400
O	-1.53755300	-1.66260700	1.89464100
O	-1.30444800	-2.62448900	3.93490900

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OAc$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.513556

Thermal correction to Gibbs Free Energy (a.u.): 0.490498

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2992.3751607 a.u.

C	-1.23399300	5.52056600	0.57361900
C	-2.50813900	4.95776400	0.36991700
C	-0.08373700	4.77469000	0.38857900
H	-1.14968500	6.55834600	0.88417000
C	-2.59616200	3.63927600	-0.03043500
H	-3.40304600	5.55184300	0.51902900
C	-0.14808100	3.41278900	0.00569700
H	0.90049900	5.20220700	0.54695100
C	-1.44081400	2.84617700	-0.21529000
H	-3.56810200	3.18511400	-0.20796900
O	0.97429200	2.75092700	-0.14588100
C	-1.60936200	1.50818200	-0.70115000
Co	1.12259200	0.85815600	-0.25684500
N	-0.67308300	0.63519900	-0.86762500
H	-2.62843100	1.22166700	-0.95823400
N	1.41891700	-0.88348100	-1.04682900
C	-0.95149100	-0.73475500	-1.33473300
C	2.37842100	-1.67278700	-0.69740700
C	0.34355300	-1.25633900	-1.97092000
C	-2.12685300	-0.89921000	-2.29515700
H	2.38049600	-2.69669200	-1.07194800
C	3.47684500	-1.30562000	0.14806100
C	0.21031500	-2.74220800	-2.30176000
C	-2.27911500	-2.38355100	-2.65951900
H	-1.95566300	-0.29703100	-3.19768300
H	-3.05200500	-0.54710000	-1.83481800
C	4.38301100	-2.31450700	0.54731700
C	3.71934300	0.05505900	0.51976800
C	-0.98416600	-2.96149000	-3.24299100
H	1.12394900	-3.11725700	-2.77590100
H	0.06357100	-3.29571600	-1.36587400
H	-3.10461300	-2.51156400	-3.36806400
H	-2.54574500	-2.94234600	-1.75266900
C	5.50061900	-2.02121700	1.30261100
H	4.17746900	-3.33959800	0.24909400
C	4.88445400	0.33093500	1.27735300
O	2.95021800	1.06084500	0.17342200
H	-0.77525800	-2.47961700	-4.20744400
H	-1.10318000	-4.03102300	-3.44555200
C	5.74562500	-0.68149600	1.65983900
H	6.18095500	-2.80685200	1.61225200
H	5.06791500	1.36474200	1.54975700
H	6.62420700	-0.43601900	2.25006300
H	0.52975600	-0.68391900	-2.89055700
H	-1.12368500	-1.33344400	-0.43325700
O	0.63501500	0.28838000	1.49623800
H	1.33368200	0.57453800	2.10005900
H	0.16029500	-1.28819700	1.45828500
O	2.08003500	1.73599200	-2.44973600
H	1.75706900	2.54597000	-2.01996200
H	2.89806100	1.55971800	-1.95884200
C	-1.33993200	-2.16421700	2.34963100

C	-2.24621600	-0.93131400	2.24329800
O	-0.31320600	-2.16170000	1.37398600
H	-0.90041900	-2.09948400	3.36156500
H	-1.62868300	-0.03889700	2.13007200
H	-2.88798600	-0.85311300	3.12240300
C	-2.09671900	-3.48045200	2.23065700
H	-1.40947000	-4.31633800	2.38372400
H	-2.90976400	-3.53943000	2.95821800
H	-2.52253300	-3.57436200	1.22650000
C	-5.12953500	-1.36363600	-0.06775500
H	-6.16517700	-1.64923200	0.11205300
H	-4.66548000	-2.07155100	-0.76023300
H	-5.09450600	-0.37390900	-0.53251600
C	-4.37931500	-1.35400000	1.24384800
O	-3.09459700	-0.97130800	1.06194800
O	-4.86508800	-1.64632700	2.31438000

six-coordinated H_2O-Co^{III}-OAc counterion addition in the middle carbon and subsequent hydrolysis

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.013526

Thermal correction to Gibbs Free Energy (a.u.): 0.466680

Imaginary frequencies: -253.07

Calculation of single point energy based on the optimized structure, Et = -2915.8191341 a.u.

C	3.84038000	-3.79947100	-0.68123800
C	4.69615700	-2.69347800	-0.82881700
C	2.46751700	-3.63682600	-0.60870300
H	4.26015100	-4.79955800	-0.61580300
C	4.14041400	-1.43039100	-0.90370600
H	5.77091900	-2.82932600	-0.87653800
C	1.87526800	-2.35121000	-0.67982900
H	1.80342000	-4.48521400	-0.48029300
C	2.74388800	-1.23038100	-0.84181800
H	4.77967600	-0.55716400	-1.00620600
O	0.56825700	-2.26559000	-0.57464400
C	2.25315800	0.11973500	-0.90020300
Co	-0.47455700	-0.68653300	-0.70513800
N	1.01506500	0.46839200	-0.93827400
H	3.01089900	0.89921100	-0.90699400
N	-1.54986600	0.86530600	-1.00304700
C	0.60005900	1.87236800	-0.82594600
C	-2.75577300	1.00103400	-0.56828200
C	-0.75044900	1.96808100	-1.55078300
C	1.59890700	2.91258200	-1.32748900
H	-3.23020800	1.98009300	-0.64063600
C	-3.55182900	-0.04472700	0.01042900
C	-1.34841400	3.36886400	-1.44034600
C	0.98945500	4.31927900	-1.24572600
H	1.88505600	2.68435500	-2.36364400
H	2.49875100	2.87369800	-0.70854600
C	-4.80279000	0.29640600	0.56950600
C	-3.13076300	-1.40999900	-0.01131600
C	-0.35237400	4.40506100	-1.98090400
H	-2.29214300	3.42929900	-1.99406600
H	-1.56879600	3.58633100	-0.38710900
H	1.69477000	5.05137500	-1.65265400
H	0.83950200	4.58063200	-0.19064700
C	-5.63320900	-0.66334600	1.11651800
H	-5.10214400	1.34184300	0.56902600
C	-4.00293200	-2.37488000	0.54628900
O	-2.00165000	-1.81388300	-0.54716400
H	-0.19563400	4.23121900	-3.05409400
H	-0.77747200	5.40955400	-1.88426900
C	-5.21956500	-2.00761400	1.09598500
H	-6.58685600	-0.38654300	1.55227700
H	-3.67927100	-3.41018300	0.52845200
H	-5.86254600	-2.77310200	1.52174300

C	0.69516700	-0.64259200	2.67091300
C	-0.51612400	-1.23924300	2.07082500
O	-0.50884400	-0.21864400	1.08928100
H	0.60663800	0.27030900	3.27056500
H	-1.42452800	-1.20996200	2.68615200
H	-0.36970400	-2.24016900	1.65325000
C	1.98751900	-1.34418300	2.64159700
H	2.18529100	-1.81625100	1.67832900
H	2.81360100	-0.69481800	2.91816100
H	1.88515400	-2.17314900	3.36614000
H	-0.58047600	1.73187800	-2.61108400
H	0.44046200	2.02320500	0.24804100
C	2.59552800	3.49321800	2.39732400
H	2.86395000	3.96938500	3.34281400
H	1.91285200	4.16744800	1.86587600
H	3.48451500	3.35434800	1.77616400
C	1.88049600	2.15576600	2.65518900
O	1.98441500	1.28450100	1.72316100
O	1.23749200	2.02753800	3.71761400
O	-0.62865900	-1.22207400	-2.67369100
H	-1.50210600	-1.63248800	-2.51745900
H	-0.01329000	-1.97486000	-2.61224300

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.044167

Thermal correction to Gibbs Free Energy (a.u.): 0.468696

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8510919 a.u.

C	3.13617500	-4.47125100	-0.42825400
C	4.15912300	-3.53948200	-0.67074800
C	1.81614900	-4.06785600	-0.30518900
H	3.37977000	-5.52543300	-0.32835100
C	3.82719200	-2.20216500	-0.78895900
H	5.19086500	-3.86229000	-0.75580300
C	1.45673000	-2.70477700	-0.41910300
H	1.02351100	-4.78058800	-0.10238900
C	2.49110800	-1.76092800	-0.68086200
H	4.59957400	-1.45746200	-0.96000400
O	0.18502900	-2.38620200	-0.25560300
C	2.23583100	-0.34938900	-0.80278800
Co	-0.58066600	-0.69932300	-0.57448300
N	1.06764600	0.19813400	-0.83032800
H	3.10396100	0.29857700	-0.85574500
N	-1.40126900	0.98712600	-0.96766100
C	0.89290400	1.65662600	-0.82054100
C	-2.58919100	1.31736500	-0.59506300
C	-0.43289300	1.93713000	-1.53651300
C	2.02755700	2.48025300	-1.42787100
H	-2.90306000	2.35348400	-0.72079100
C	-3.56294700	0.42715500	-0.02168700
C	-0.80362300	3.41661100	-1.44249700
C	1.66748500	3.96867600	-1.32098500
H	2.18600800	2.19390300	-2.47846400
H	2.93986100	2.29234500	-0.85981700
C	-4.76805700	0.97574200	0.46758900
C	-3.35872000	-0.98467900	0.01706300
C	0.33404600	4.28024600	-2.00902900
H	-1.73221800	3.62001400	-1.98885400
H	-0.96935600	3.67378600	-0.38879300
H	2.46761200	4.57830400	-1.75419200
H	1.60207400	4.22596100	-0.25698300
C	-5.76008500	0.17351000	1.00071500
H	-4.90208700	2.05377800	0.42237100
C	-4.39135500	-1.78606300	0.55624000
O	-2.27315400	-1.57423200	-0.43875100
H	0.42452800	4.09362200	-3.08810800
H	0.07724300	5.33882800	-1.89401000

C	-5.56029700	-1.21769700	1.03602700
H	-6.67755800	0.60846600	1.38136500
H	-4.23109200	-2.85869400	0.58234800
H	-6.33229900	-1.86059600	1.44965000
C	0.15730100	-0.26947400	2.49710000
C	-1.11904500	-0.99283500	2.35741500
O	-0.66853100	-0.14911600	1.26525400
H	0.17136100	0.70868000	2.96826800
H	-2.03833000	-0.63206400	2.80999700
H	-1.08127200	-2.05275200	2.12081400
C	1.47567000	-0.97360300	2.45838200
H	1.40190400	-1.95959800	2.00130600
H	2.22008800	-0.35428600	1.94849700
H	1.80304600	-1.09695600	3.49772400
H	-0.31901500	1.65640700	-2.59424700
H	0.81515300	1.93762600	0.24888900
C	3.53591600	3.06514600	2.91695100
H	2.95330900	3.50835800	3.72777800
H	3.99295700	3.87619200	2.33733400
H	4.35087000	2.45725600	3.31960000
C	2.64736000	2.22316700	1.98509300
O	3.24481700	1.39821200	1.23375200
O	1.40092800	2.44387500	2.02866700
O	-0.73460000	-1.27823100	-2.46540400
H	-1.64565400	-1.61478400	-2.33081000
H	-0.18032700	-2.07819500	-2.43983100

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1677.101102

Thermal correction to Gibbs Free Energy (a.u.): 0.472630

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.9031151 a.u.

C	4.26112200	-2.57704700	-1.80099800
C	4.93606400	-1.34081700	-1.74357800
C	2.89988900	-2.65999800	-1.58227000
H	4.82015800	-3.48324500	-2.01839400
C	4.20924000	-0.20470600	-1.45146600
H	6.00526300	-1.28670800	-1.91670500
C	2.12335300	-1.50444100	-1.29460500
H	2.37652900	-3.60949500	-1.62239300
C	2.81421000	-0.25313700	-1.22135200
H	4.70792600	0.75931000	-1.37998300
O	0.83656500	-1.65070100	-1.12985000
C	2.15280700	0.95770100	-0.82625500
Co	-0.43515000	-0.26458900	-0.82340400
N	0.88798400	1.08615600	-0.61755400
H	2.79883400	1.81989800	-0.65817800
N	-1.70684500	1.15853500	-0.67098100
C	0.29398700	2.28014600	-0.01121700
C	-2.92981500	0.98551600	-0.30149200
C	-1.05799000	2.47487300	-0.72195800
C	1.14411500	3.54732100	-0.01944800
H	-3.53607800	1.86162600	-0.06798800
C	-3.58803700	-0.28268000	-0.16382600
C	-1.83649600	3.64605900	-0.12394100
C	0.34979400	4.71986800	0.57228400
H	1.45297300	3.78486800	-1.04714200
H	2.04785800	3.38352000	0.57539100
C	-4.89596600	-0.29972700	0.36898700
C	-2.97498600	-1.50427000	-0.58388100
C	-0.98358000	4.92245900	-0.15596600
H	-2.77117200	3.80645900	-0.67273700
H	-2.10157800	3.40795300	0.91436900
H	0.95057700	5.63444700	0.52810900
H	0.15775700	4.51821300	1.63377400
C	-5.60238700	-1.47856500	0.51227300
H	-5.34161400	0.64419200	0.67503300

C	-3.72309000	-2.69768400	-0.43271300
O	-1.78588700	-1.57046100	-1.12909800
H	-0.79110000	5.20419100	-1.20010600
H	-1.54249400	5.74979400	0.29400800
C	-4.99947900	-2.68195400	0.10162000
H	-6.60268100	-1.47751700	0.93147100
H	-3.25257000	-3.62289700	-0.74813500
H	-5.54218100	-3.61739500	0.20877000
C	0.56617400	-1.33705900	2.87662100
C	-0.29228300	-1.58373400	1.63578200
O	-0.52464400	-0.36760100	1.00037000
H	0.18965600	-0.45398500	3.39865800
H	-1.23899200	-2.05501300	1.96023700
H	0.22661000	-2.30558900	0.99147900
C	0.65072600	-2.54512200	3.79675200
H	1.04380800	-3.41349100	3.25835900
H	1.30733100	-2.34177600	4.64711800
H	-0.34291100	-2.79724900	4.17869300
H	-0.84774300	2.68440400	-1.78085300
H	0.09140100	1.98693300	1.02695800
C	3.84134400	0.24772300	2.07669000
H	4.41252800	0.00542500	2.97937100
H	4.12032000	1.24918200	1.74736600
H	4.08776700	-0.48916700	1.31190500
C	2.36663100	0.21659900	2.41393300
O	1.93146200	-1.05201800	2.45318900
O	1.70378800	1.20515500	2.66358400
O	-0.49661900	-0.17115600	-2.91579000
H	-1.29507900	-0.73487000	-2.89225900
H	0.22059700	-0.81065200	-3.06364800

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.004728

Thermal correction to Gibbs Free Energy (a.u.): 0.460579

Imaginary frequencies: -314.32

Calculation of single point energy based on the optimized structure, Et = -2915.8077437 a.u.

C	3.56172600	-4.00953200	-0.88763300
C	4.47543200	-2.95178900	-1.05373000
C	2.20761500	-3.76811600	-0.73913800
H	3.92377100	-5.03368600	-0.86794500
C	3.99854800	-1.65591700	-1.07535700
H	5.53562400	-3.15245300	-1.16155800
C	1.69758800	-2.44591700	-0.73987100
H	1.49961900	-4.57721600	-0.59456500
C	2.62126700	-1.37546800	-0.93267000
H	4.68375200	-0.82161400	-1.20026000
O	0.41106200	-2.27686000	-0.54446500
C	2.19736100	-0.00772600	-0.97867200
Co	-0.54231400	-0.65478700	-0.54227000
N	0.97537300	0.40654400	-0.94805500
H	2.98894300	0.73268400	-1.05488200
N	-1.56059900	0.93824400	-0.91964100
C	0.64397500	1.83576200	-0.85113500
C	-2.77566800	1.12728200	-0.52937700
C	-0.72683000	1.98677500	-1.52352500
C	1.67219800	2.80706700	-1.42603900
H	-3.22023400	2.11397300	-0.66273000
C	-3.61972800	0.13440400	0.06906700
C	-1.24919800	3.41847900	-1.41987100
C	1.14401900	4.24583000	-1.33569700
H	1.88412400	2.54741900	-2.47248900
H	2.60386300	2.72900300	-0.86068200
C	-4.88881200	0.53292600	0.54723600
C	-3.23866000	-1.24141700	0.13334000
C	-0.22241800	4.39466900	-2.01304600
H	-2.20516500	3.51968600	-1.94543300
H	-1.42471900	3.66196900	-0.36383800

H	1.86846600	4.93392100	-1.78357100
H	1.05551900	4.52649800	-0.27837800
C	-5.77158600	-0.37840700	1.09164600
H	-5.15835100	1.58429700	0.48365900
C	-4.16916900	-2.15899600	0.67810300
O	-2.09343200	-1.70612000	-0.31087400
H	-0.12064900	4.20176300	-3.08946800
H	-0.58986500	5.42110800	-1.91120000
C	-5.39857500	-1.73464800	1.14904300
H	-6.73730600	-0.05697400	1.46579600
H	-3.87494500	-3.20216400	0.71975500
H	-6.08511400	-2.46225600	1.57283500
C	0.86159700	-0.53594900	2.82511600
C	-0.48699700	-0.96372600	2.39792200
O	-0.45669300	-0.05460400	1.32699300
H	0.97861100	0.37355200	3.41987800
H	-1.28776300	-0.74247900	3.11784300
H	-0.55071700	-2.01437700	2.08186500
C	2.01669400	-1.43381100	2.65107200
H	1.97979500	-1.96627400	1.69964200
H	2.96720600	-0.91813400	2.75874700
H	1.91031800	-2.20479200	3.43603200
H	-0.61261300	1.71706600	-2.58304700
H	0.54016700	2.01645100	0.22551700
C	3.20783700	3.23821500	2.03712200
H	3.64512500	3.75278100	2.89504800
H	2.56458500	3.95038000	1.50644000
H	3.99384900	2.91731700	1.34754100
C	2.35949000	2.04348100	2.50587200
O	2.17535800	1.12565900	1.62910300
O	1.89993100	2.06154200	3.66388800
O	-1.00850500	-1.40389900	-2.83595300
H	-1.78821300	-1.75744500	-2.37511100
H	-0.35663800	-2.11084400	-2.71847600

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.048902

Thermal correction to Gibbs Free Energy (a.u.): 0.463314

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2915.8521332 a.u.

C	3.20680700	-4.37997100	-0.47713700
C	4.21385600	-3.43170600	-0.73805700
C	1.88475400	-3.99631200	-0.33966000
H	3.47006900	-5.42875000	-0.37270900
C	3.86763800	-2.10004100	-0.86365200
H	5.24861700	-3.74266400	-0.83137700
C	1.50949800	-2.63662300	-0.46221100
H	1.10345100	-4.71586900	-0.11923900
C	2.52524000	-1.67791800	-0.74657500
H	4.62838500	-1.34693600	-1.04671600
O	0.24601800	-2.32386900	-0.27790800
C	2.23479300	-0.28058200	-0.87745700
Co	-0.57020800	-0.68838300	-0.58632700
N	1.04594800	0.23947900	-0.88435900
H	3.08337000	0.38681400	-0.96091900
N	-1.42233400	0.98883400	-0.93262000
C	0.85932700	1.69774500	-0.85552900
C	-2.61773100	1.28711900	-0.54654900
C	-0.49228200	1.96940800	-1.51797100
C	1.96450600	2.54118200	-1.48826000
H	-2.95478700	2.31764600	-0.65480600
C	-3.56819500	0.36688500	0.00689200
C	-0.88222700	3.44047200	-1.38383400
C	1.58733600	4.02303400	-1.34655900
H	2.09614700	2.27074100	-2.54667800
H	2.89598500	2.35906900	-0.94961100
C	-4.80020000	0.87064300	0.48115800

C	-3.32534600	-1.04071100	0.02544900
C	0.22427300	4.32721300	-1.97758100
H	-1.83136500	3.64102400	-1.89466800
H	-1.01357500	3.67700000	-0.32053400
H	2.36150000	4.64975100	-1.80211100
H	1.56233000	4.26042600	-0.27656200
C	-5.77675700	0.02899200	0.97662100
H	-4.96536800	1.94469000	0.45355500
C	-4.35046300	-1.88481200	0.51587700
O	-2.21272500	-1.58990000	-0.40404200
H	0.27456400	4.15915200	-3.06236500
H	-0.04046400	5.38051400	-1.83527300
C	-5.54074100	-1.35906000	0.98535700
H	-6.71369800	0.42914500	1.34800800
H	-4.15972600	-2.95256000	0.52161500
H	-6.30376500	-2.03027400	1.36922200
C	0.15152500	-0.12402500	2.67866500
C	-1.19301400	-0.72401300	2.65458000
O	-0.69713600	-0.02560100	1.49323300
H	0.28535300	0.85988800	3.11956800
H	-2.03837500	-0.23242800	3.13067200
H	-1.28510000	-1.79971300	2.51911000
C	1.38873700	-0.96933700	2.58399800
H	1.17124700	-1.93621800	2.12634100
H	2.16269500	-0.44724800	2.01445100
H	1.77286800	-1.14192800	3.59595900
H	-0.41533900	1.70783000	-2.58373900
H	0.82872000	1.97036100	0.22076600
C	3.61909400	2.58704800	3.09743800
H	3.55948500	1.85339500	3.91092800
H	3.27080900	3.54789900	3.48374800
H	4.66604700	2.65327300	2.79100700
C	2.73903700	2.10732500	1.93081000
O	3.27849300	1.30382000	1.11404400
O	1.54338400	2.52042200	1.91500100
O	-0.84035000	-1.40855600	-2.76938700
H	-1.63894900	-1.86336100	-2.45102600
H	-0.16904800	-2.10478300	-2.80933700

H_2O-Co^{III}-OAc counterion addition in the middle carbon

H_2O-Co^{III}-OAc + PO = H_2O-Co^{III}-PO~OAc

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1677.089994

Thermal correction to Gibbs Free Energy (a.u.): 0.466240

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2915.8912017 a.u.

C	4.51848200	-1.26735700	-2.40362800
C	5.04369700	-0.05943400	-1.90568000
C	3.17759700	-1.57688700	-2.26300900
H	5.17584100	-1.97094100	-2.90717100
C	4.19347100	0.81861200	-1.26345700
H	6.09617400	0.17403200	-2.02277900
C	2.28331700	-0.69364100	-1.60393100
H	2.76726200	-2.50564200	-2.64475000
C	2.82080700	0.52824100	-1.09382900
H	4.57513900	1.75528700	-0.86417500
O	1.02320600	-1.03224200	-1.51428900
C	2.00773200	1.49171800	-0.41065400
Co	-0.37436000	-0.08760500	-0.60514700
N	0.74243300	1.39296300	-0.18448100
H	2.52775100	2.38129900	-0.05792800
N	-1.84365000	1.20064200	-0.38295700
C	-0.01454000	2.39337900	0.57715300
C	-3.07527200	0.85778600	-0.21827200
C	-1.34618800	2.56509600	-0.18151100
C	0.67876000	3.73192300	0.82254200
H	-3.80863100	1.62060500	0.05019400
C	-3.58738300	-0.47728700	-0.35273000
C	-2.28255600	3.53309100	0.54197600

C	-0.26963900	4.69466000	1.55090900
H	0.98387700	4.16972000	-0.13783800
H	1.58346700	3.58098900	1.42003600
C	-4.94577000	-0.70117600	-0.03072700
C	-2.78536300	-1.56103500	-0.83347400
C	-1.58229700	4.87812900	0.78167800
H	-3.19668500	3.68893600	-0.04106500
H	-2.57874900	3.09364500	1.50375100
H	0.22526000	5.66055600	1.69626200
H	-0.48640000	4.29777300	2.55124700
C	-5.52347900	-1.94882500	-0.15563900
H	-5.53537400	0.13955900	0.32765100
C	-3.40662100	-2.82862200	-0.96321600
O	-1.53110900	-1.44959700	-1.19772300
H	-1.37423700	5.35555700	-0.18522000
H	-2.25299100	5.55120600	1.32600300
C	-4.73564600	-3.01471000	-0.63038000
H	-6.56449400	-2.10572200	0.10475500
H	-2.79366300	-3.64515200	-1.32932500
H	-5.17601700	-4.00259800	-0.73462500
C	0.69526500	-2.08452100	2.69766300
C	-0.37770900	-1.87441300	1.62742900
O	-0.36596500	-0.55374800	1.19344600
H	0.66421200	-1.24122700	3.39236600
H	-1.35501200	-2.12541100	2.07748300
H	-0.20289900	-2.58949500	0.80824700
C	0.56238700	-3.41835600	3.41749100
H	0.59721000	-4.24792700	2.70390000
H	1.37441600	-3.55181300	4.13724600
H	-0.38917100	-3.46557200	3.95548200
H	-1.10596400	2.96424400	-1.17725700
H	-0.23699500	1.90960700	1.53728400
C	4.10853500	-1.26290800	1.47559300
H	4.63827300	-1.97602000	2.11532200
H	4.68094100	-0.34056300	1.39876500
H	4.00266600	-1.71755100	0.48875900
C	2.75168000	-0.97314100	2.07401900
O	2.00319400	-2.09446900	2.06606900
O	2.40669600	0.09809000	2.52896800
O	-0.68531300	0.43132800	-3.15514900
H	-1.38595900	-0.21300400	-2.97002200
H	0.10569700	-0.13110800	-3.12002700

subsequent hydrolysis

H_2O-Co^{III}-PO~OAc + PO = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1753.453263

Thermal correction to Gibbs Free Energy (a.u.): 0.494254

Imaginary frequencies: -266.50

Calculation of single point energy based on the optimized structure, Et = -2992.3174753 a.u.

C	2.92693000	-3.87173900	-1.64274800
C	3.62563000	-2.86595800	-2.33816200
C	1.79744100	-3.57753400	-0.90257700
H	3.27697400	-4.89924100	-1.69055500
C	3.17302100	-1.56410200	-2.25097800
H	4.50610800	-3.10853500	-2.92285500
C	1.29555000	-2.25180100	-0.81316400
H	1.25395800	-4.34874400	-0.36728100
C	2.02441000	-1.22581300	-1.49915000
H	3.70508400	-0.76595500	-2.76293800
O	0.20529600	-2.04761900	-0.12007300
C	1.68625300	0.16848800	-1.35576200
Co	-0.83443200	-0.49220100	-0.28390800
N	0.61316300	0.60761900	-0.80434600
H	2.41855500	0.89011600	-1.71639800
N	-1.89107900	1.09196100	-0.46573900
C	0.33489900	2.01633500	-0.52856400
C	-3.15553600	1.16462300	-0.21979400
C	-1.11815700	2.24268200	-0.96720700

C	1.27167300	3.04857600	-1.14805500
H	-3.64011600	2.13728400	-0.31389500
C	-4.02010600	0.08156200	0.14907200
C	-1.59490900	3.63016100	-0.53314200
C	0.80845900	4.45247100	-0.73108800
H	1.26267200	2.95820900	-2.24391700
H	2.29018600	2.88552400	-0.78854900
C	-5.35990000	0.39286300	0.46955100
C	-3.58752800	-1.27882000	0.16579900
C	-0.65730500	4.70698400	-1.10354100
H	-2.61609700	3.82246700	-0.87802000
H	-1.60474700	3.67165600	0.56317000
H	1.45180600	5.20840800	-1.19346700
H	0.93573100	4.55178400	0.35392900
C	-6.26993500	-0.58927500	0.81124600
H	-5.66626700	1.43611600	0.44975300
C	-4.53764400	-2.26682800	0.51287000
O	-2.37178200	-1.66849400	-0.15342600
H	-0.75626900	4.72084600	-2.19769200
H	-0.97515200	5.69328500	-0.74909100
C	-5.84302900	-1.92869100	0.82761900
H	-7.29329600	-0.33279700	1.06233500
H	-4.20153300	-3.29829900	0.52842900
H	-6.54551000	-2.71347900	1.09484700
C	2.78707200	-0.02235300	2.78787000
C	1.41506200	-0.60358900	2.43370600
O	0.64473000	0.28239200	1.70825000
H	2.66412400	1.02560500	3.06939400
H	0.93209200	-0.88129600	3.39537100
H	1.58785200	-1.55549800	1.89783200
C	3.51956300	-0.81875200	3.85746200
H	4.52041700	-0.41322500	4.03038700
H	2.96458600	-0.78275200	4.79938700
H	3.62083500	-1.86678800	3.55677900
H	-1.14467400	2.18226800	-2.06613300
H	0.39737800	2.08200100	0.56450000
O	-1.69265800	-0.22405300	2.00308100
H	-1.68816200	-1.16883300	2.20349100
H	-0.68165700	0.07039000	2.05219500
C	4.91372000	0.80377300	-0.15907300
H	5.91314300	0.89693000	0.27936700
H	4.81791800	1.55493800	-0.94488700
H	4.81626500	-0.20313900	-0.56626400
C	3.88667900	1.05894100	0.92420700
O	3.64236000	-0.06680700	1.60375400
O	3.40008200	2.14968500	1.15555100
O	-1.16610600	-0.96995100	-2.20310500
H	-1.86562800	-1.59601400	-1.89352400
H	-0.41074900	-1.51530400	-2.48020800

subsequent hydrolysis

H_2O-Co^{III}-PO~OAc + PO = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1753.527157

Thermal correction to Gibbs Free Energy (a.u.): 0.495053

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2992.3902261 a.u.

C	4.58860300	-2.29377900	-1.61112200
C	5.17667100	-1.01487400	-1.54310800
C	3.22476000	-2.46331800	-1.46722500
H	5.21684500	-3.16465800	-1.77774900
C	4.36205600	0.07487900	-1.31144600
H	6.24801700	-0.89274600	-1.65829000
C	2.36004400	-1.35701600	-1.24961800
H	2.76796700	-3.44608100	-1.51724000
C	2.96322400	-0.06280600	-1.15608300
H	4.79217100	1.07018700	-1.22670500
O	1.07623700	-1.58521800	-1.16082400
C	2.20516200	1.10391500	-0.80187300

Co	-0.29255800	-0.27880700	-0.95273300
N	0.92589000	1.15214900	-0.66634000
H	2.78384600	2.00379300	-0.59310900
N	-1.65734200	1.06152300	-0.87633800
C	0.22646500	2.29902100	-0.08062000
C	-2.88142800	0.81090600	-0.56170700
C	-1.09705100	2.42252600	-0.85620200
C	0.98966600	3.61890900	-0.02687200
H	-3.54847800	1.64398700	-0.34905600
C	-3.45866500	-0.50054200	-0.44444200
C	-1.98512400	3.50831600	-0.24820900
C	0.09196000	4.71090600	0.57274300
H	1.31386200	3.90794200	-1.03661800
H	1.88259800	3.49928700	0.59434700
C	-4.77515300	-0.60388400	0.05665000
C	-2.75093700	-1.67880200	-0.83458500
C	-1.22692900	4.84277100	-0.19691500
H	-2.90105100	3.62881300	-0.83813100
H	-2.27138600	3.19059300	0.76177100
H	0.62652800	5.66680700	0.57994200
H	-0.12226600	4.45735400	1.61828500
C	-5.40038800	-1.82913600	0.19532800
H	-5.29299400	0.30979000	0.33997100
C	-3.41795000	-2.92013700	-0.69415800
O	-1.54027300	-1.66404700	-1.33737100
H	-1.01952700	5.18467600	-1.22047300
H	-1.86109100	5.60630900	0.26585700
C	-4.70577700	-2.98994700	-0.19107000
H	-6.40834400	-1.89488500	0.59020700
H	-2.87638000	-3.81259200	-0.98927700
H	-5.18432800	-3.96020800	-0.08906100
C	0.51446300	-1.39398100	2.80858500
C	-0.26774800	-1.64074800	1.51876000
O	-0.46057100	-0.41636800	0.87242400
H	0.13143900	-0.48694100	3.28371300
H	-1.23465900	-2.10891300	1.77774600
H	0.28698900	-2.35038300	0.89435100
C	0.48826200	-2.58264400	3.75700600
H	1.10239700	-2.38610000	4.63974300
H	-0.53627800	-2.78060800	4.08525600
H	0.87311100	-3.48071400	3.26308700
H	-0.84921400	2.68106000	-1.89590400
H	-0.00614300	1.98856400	0.94448100
O	-2.21739800	1.08089000	2.28238600
H	-2.97491200	0.48412600	2.31572000
H	-1.54611200	0.56176900	1.77705200
C	3.88560400	0.03923400	2.14229800
H	4.38554600	-0.21354100	3.08346500
H	4.22975900	1.01917900	1.81196700
H	4.14582400	-0.72207100	1.40607000
C	2.39231600	0.07832700	2.37893300
O	1.91350300	-1.17455300	2.47323500
O	1.74310200	1.09657100	2.50947800
O	-0.22640500	-0.17418600	-3.01893800
H	-0.99041500	-0.78225800	-3.07009000
H	0.53772200	-0.76272800	-3.14221600

subsequent hydrolysis

H_2O-Co^{III}-PO~OAc + PO = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1753.525719

Thermal correction to Gibbs Free Energy (a.u.): 0.496304

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2992.3880783 a.u.

C	2.22068000	-4.76771900	-0.19589600
C	3.28609900	-3.92492600	-0.56575100
C	0.92332000	-4.29311100	-0.12130200
H	2.41808500	-5.80982900	0.04128900
C	3.01384200	-2.60285500	-0.85933700

H	4.29975000	-4.30761100	-0.61780600
C	0.61762000	-2.93966000	-0.41320400
H	0.10103500	-4.93851300	0.16955600
C	1.69851900	-2.08866100	-0.79407500
H	3.81167500	-1.92021800	-1.13828100
O	-0.63439600	-2.55390100	-0.33745700
C	1.52325800	-0.69506700	-1.07705500
Co	-1.26471600	-0.76865800	-0.47598800
N	0.39891300	-0.05867700	-1.06418300
H	2.43484100	-0.14095300	-1.28353800
N	-1.95540900	0.98514700	-0.76195200
C	0.36567600	1.40743200	-1.13572700
C	-3.01138100	1.45566900	-0.18994000
C	-1.04971400	1.78713800	-1.59064900
C	1.43274600	2.07388700	-2.00603400
H	-3.24368300	2.51492700	-0.30897700
C	-3.94301100	0.68958100	0.58619900
C	-1.25282100	3.30121600	-1.57276000
C	1.22970100	3.59589300	-2.00721200
H	1.35792000	1.68115900	-3.02896200
H	2.43174700	1.83913300	-1.63179500
C	-4.98105300	1.37458100	1.25588800
C	-3.88383700	-0.73898600	0.63374200
C	-0.18754700	3.98470200	-2.44330000
H	-2.25344400	3.56022900	-1.93590100
H	-1.17653100	3.66408100	-0.53893500
H	1.97139900	4.06747200	-2.66018700
H	1.41507400	3.98159300	-0.99509400
C	-5.94446700	0.69679200	1.97737700
H	-5.00663400	2.46039700	1.19591400
C	-4.89179100	-1.40964600	1.36996400
O	-2.98181800	-1.45210700	0.00615300
H	-0.33797200	3.69129400	-3.49079900
H	-0.31794600	5.07127500	-2.40035500
C	-5.88952200	-0.70898100	2.02405500
H	-6.73074100	1.23554700	2.49481700
H	-4.84566000	-2.49303500	1.40403100
H	-6.64190900	-1.25621300	2.58569400
C	3.06737200	2.13053200	1.78916900
C	1.84454700	1.39475200	2.33466600
O	1.68565200	0.19585900	1.63033100
H	2.91625000	2.36175900	0.73214500
H	0.97118400	2.06031100	2.23358900
H	1.99723400	1.22127900	3.41436800
C	3.43489100	3.37524900	2.57724800
H	4.32415100	3.85162900	2.15640900
H	2.61155100	4.09614200	2.54907100
H	3.63853100	3.12581800	3.62295400
H	-1.17053100	1.42106300	-2.62039300
H	0.48166200	1.75755400	-0.10105000
O	-0.84860400	-0.34144200	1.27053200
H	-1.04368500	-1.16832300	1.73535300
H	0.71395800	-0.02959000	1.53801800
C	5.40883100	-0.65804200	1.15174700
H	5.98035200	-0.46531500	2.06083700
H	6.07046400	-0.89890200	0.31882800
H	4.74887300	-1.51339000	1.33340000
C	4.53685200	0.51586500	0.78988700
O	4.18013600	1.20427100	1.88585300
O	4.20170600	0.79062300	-0.34907200
O	-1.86612000	-1.38921600	-2.35815800
H	-2.76826400	-1.56680300	-2.02823900
H	-1.42123600	-2.25199600	-2.26299300

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.486600

Thermal correction to Gibbs Free Energy (a.u.): 0.485804

Imaginary frequencies: -620.64
Calculation of single point energy based on the optimized structure, Et = -2992.3453535 a.u.

C	1.83625800	-4.66426100	-0.76040900
C	2.47010000	-4.06825600	-1.86906200
C	1.04628300	-3.92414600	0.09809200
H	1.96625100	-5.72727400	-0.57698800
C	2.29807400	-2.71552000	-2.08168600
H	3.08389000	-4.66096500	-2.53818100
C	0.83696100	-2.53400400	-0.10176000
H	0.55671000	-4.38083000	0.95133900
C	1.49014300	-1.92803900	-1.22740600
H	2.78514200	-2.22687800	-2.92216700
O	0.09205700	-1.89237400	0.75738600
C	1.43158900	-0.51243900	-1.45589000
Co	-0.75932800	-0.26251900	0.36115600
N	0.63989600	0.29288900	-0.83828800
H	2.12879800	-0.10091000	-2.18751600
N	-1.59443400	1.36642700	-0.20395000
C	0.71030200	1.75305400	-0.88525600
C	-2.87299700	1.56040000	-0.17145300
C	-0.72834000	2.26329300	-0.99684900
C	1.58144800	2.41932800	-1.94487900
H	-3.25119400	2.52844300	-0.51028200
C	-3.85534000	0.57525600	0.16803500
C	-0.76354500	3.74926900	-0.63513200
C	1.56939200	3.93509500	-1.67534700
H	1.19526700	2.19580900	-2.94855500
H	2.61091000	2.06166600	-1.88101100
C	-5.18803500	0.97823600	0.39921300
C	-3.53270100	-0.81689200	0.09999700
C	0.14712900	4.51537700	-1.61229400
H	-1.78262900	4.14700300	-0.68787500
H	-0.41848900	3.86667700	0.39871400
H	2.14826300	4.45428400	-2.44631900
H	2.08455300	4.10937100	-0.72336500
C	-6.19156400	0.04951400	0.59689300
H	-5.41218900	2.04172000	0.42718600
C	-4.58484500	-1.74637500	0.27121300
O	-2.32309000	-1.26398000	-0.15134700
H	-0.30335800	4.47600100	-2.61341300
H	0.18624100	5.57261200	-1.32924100
C	-5.87690500	-1.32074900	0.52462600
H	-7.20923400	0.36947200	0.79242200
H	-4.33687700	-2.80043900	0.20806800
H	-6.66177900	-2.05846100	0.66664900
C	2.83071400	0.69345300	2.46126900
C	1.42233700	0.16527400	2.71201700
O	0.45100800	0.81948600	1.94043600
H	2.78138100	1.75710500	2.22258300
H	1.21092800	0.31756200	3.78501200
H	1.42883500	-0.92210000	2.53333100
C	3.78353400	0.43023200	3.62029400
H	4.79501900	0.76435100	3.37295300
H	3.45248400	0.97000900	4.51237600
H	3.82130300	-0.63835500	3.85565100
H	-1.04295700	2.14291800	-2.04317100
H	1.08253800	2.02695800	0.10840000
O	-1.67135200	-0.12920500	2.23683200
H	-1.56115100	-1.01659700	2.60610300
H	-0.68415000	0.42419800	2.36131700
C	4.68228100	-0.16403400	-0.64971500
H	5.70376600	-0.29091900	-0.27484600
H	4.73848000	0.31652000	-1.62760100
H	4.22567400	-1.15144300	-0.72386700
C	3.92999900	0.72345300	0.31547400
O	3.38614800	-0.00240300	1.30250600
O	3.85952300	1.93475000	0.21864100
O	-1.34650400	-1.45802700	-2.77971700
H	-1.83676700	-1.47556600	-1.93845700

H	-0.71796900	-2.18421900	-2.68258300

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.517272

Thermal correction to Gibbs Free Energy (a.u.): 0.488685

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2992.3782426 a.u.

C	4.44975500	-2.56158200	-1.61624100
C	5.03171400	-1.29383500	-1.82681400
C	3.12133100	-2.69001800	-1.26203700
H	5.05653100	-3.45530200	-1.73337800
C	4.25086900	-0.16992100	-1.65932100
H	6.07606300	-1.20698400	-2.10556000
C	2.28766000	-1.54995800	-1.09470100
H	2.66941400	-3.66196900	-1.09583600
C	2.88633500	-0.26343800	-1.29536500
H	4.68031800	0.81998700	-1.79346400
O	1.03987700	-1.74185600	-0.77097200
C	2.16828700	0.94714800	-1.03292400
Co	-0.31658700	-0.42786700	-0.70629400
N	0.91236000	1.02221700	-0.74675100
H	2.75278400	1.86704300	-1.04157100
N	-1.66118000	0.94847600	-0.87897000
C	0.25264300	2.24900600	-0.29148500
C	-2.90525900	0.74893800	-0.61391800
C	-1.08688300	2.29428000	-1.04243200
C	1.03727100	3.54887600	-0.42242000
H	-3.57007700	1.60756800	-0.53933800
C	-3.51178600	-0.53840300	-0.41140600
C	-1.94907300	3.45881000	-0.55367000
C	0.16943900	4.71528900	0.07325500
H	1.32522800	3.71435800	-1.47028400
H	1.95000100	3.48318600	0.17772000
C	-4.86277200	-0.58264900	-0.00254400
C	-2.81316900	-1.75391700	-0.68321300
C	-1.16916900	4.77719400	-0.67179800
H	-2.86982100	3.52736300	-1.14431900
H	-2.22772200	3.26126000	0.48836800
H	0.71427000	5.65810800	-0.04391200
H	-0.01696400	4.58559600	1.14642100
C	-5.52895600	-1.78337000	0.15584700
H	-5.37507100	0.35711000	0.19010700
C	-3.52516000	-2.96839900	-0.54269400
O	-1.55982500	-1.80312500	-1.07672000
H	-0.98419000	4.99798700	-1.73232200
H	-1.78072100	5.59840800	-0.28332600
C	-4.84513400	-2.97994600	-0.12573200
H	-6.56293100	-1.80329000	0.48256800
H	-2.99102000	-3.88768800	-0.75762400
H	-5.35789900	-3.93099700	-0.01134200
C	0.70612300	-0.84518400	3.16087800
C	-0.26798700	-1.33717300	2.08716900
O	-0.57893200	-0.31382900	1.19804200
H	0.42517700	0.17130300	3.44753200
H	-1.18012800	-1.68991300	2.60207900
H	0.17861300	-2.20375100	1.57789700
C	0.78668900	-1.77224700	4.36440500
H	1.53779300	-1.41922500	5.07605800
H	-0.18043900	-1.81295000	4.87401500
H	1.05743600	-2.78683000	4.05439200
H	-0.86319600	2.41399300	-2.11231000
H	0.04467100	2.07010600	0.76989000
O	-2.30018700	1.47978800	2.19961800
H	-3.08054700	0.92950500	2.33648800
H	-1.62548000	0.83760900	1.85964600
C	4.03163800	0.18234000	1.83893200
H	4.62355200	0.07265900	2.75398600

H	4.38593100	1.05517000	1.29143100
H	4.16523800	-0.71994100	1.24094500
C	2.58070300	0.37238600	2.22116100
O	2.04978500	-0.80131100	2.59901600
O	2.00480400	1.44303100	2.22622000
O	-0.23279900	-0.68523200	-3.18386400
H	-0.91446200	-1.32009800	-2.89915000
H	0.57481400	-1.21690800	-3.20413400

subsequent hydrolysis

H_2O-Co^{III}-PO-OAc + H_2O = H_2O-Co^{III}-OH + $CH_3CHOAcCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -1753.522526

Thermal correction to Gibbs Free Energy (a.u.): 0.492289

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2992.3796104 a.u.

C	-4.46489900	3.47109200	0.75280600
C	-5.16515100	2.34905600	0.27179600
C	-3.08393900	3.53213300	0.69321700
H	-5.01538800	4.30421200	1.18110400
C	-4.44878300	1.30080300	-0.27256400
H	-6.24773900	2.31122100	0.32378100
C	-2.32633200	2.46065300	0.16047100
H	-2.53811600	4.39275800	1.06485100
C	-3.03744700	1.32823900	-0.33722600
H	-4.96521600	0.42476500	-0.65701600
O	-1.01828000	2.57090300	0.13717400
C	-2.36786500	0.20796100	-0.93304000
Co	0.22348500	1.18793600	-0.24587600
N	-1.09116800	0.04447400	-1.01682200
H	-3.01117600	-0.57185500	-1.33376600
N	1.48740500	0.11698800	-1.24859900
C	-0.48954300	-1.17730800	-1.57634200
C	2.73690500	0.01980800	-0.94192400
C	0.82375300	-0.73964100	-2.23987300
C	-1.36285300	-1.99621700	-2.52271200
H	3.34057300	-0.74130600	-1.43514500
C	3.42298400	0.85165900	0.00376800
C	1.61426900	-1.95308600	-2.72593400
C	-0.56844500	-3.20555800	-3.03815500
H	-1.69125900	-1.36991000	-3.36380100
H	-2.24906700	-2.34995500	-1.99064900
C	4.77016400	0.55013600	0.30597500
C	2.80669600	2.00452800	0.58371900
C	0.75451400	-2.78574800	-3.68830100
H	2.53419700	-1.63717700	-3.23065300
H	1.89532700	-2.55319600	-1.85209500
H	-1.17895500	-3.77281000	-3.74876500
H	-0.36087300	-3.87556300	-2.19397200
C	5.51255200	1.34217800	1.15917900
H	5.21480800	-0.33198800	-0.14795500
C	3.59619700	2.81184400	1.43944700
O	1.56971400	2.37463400	0.34622700
H	0.54611400	-2.19540300	-4.59093100
H	1.31571000	-3.66824100	-4.01377900
C	4.91044100	2.48432500	1.72021900
H	6.54227300	1.09263700	1.39044100
H	3.12595900	3.68964300	1.86961500
H	5.48426800	3.11931600	2.38965900
C	-0.22918500	-3.68299300	1.89831900
C	1.20854400	-3.17490700	1.78709000
O	1.37633400	-2.17573200	0.81339300
H	-0.61780600	-3.90510900	0.90173800
H	1.84654300	-4.02307200	1.50686500
H	1.53324300	-2.83696100	2.78458600
C	-0.36801000	-4.88361000	2.82267400
H	-1.41500300	-5.18807900	2.90015500
H	0.20927300	-5.73047000	2.43859200
H	-0.00498000	-4.64432300	3.82727100

H	0.57779200	-0.08764400	-3.08977300
H	-0.21674100	-1.79786600	-0.71700700
O	0.25010100	0.13840100	1.36122900
H	0.65395200	0.68636000	2.04797300
H	0.96396800	-1.31831600	1.12510200
C	-2.58845700	-0.86134300	2.41505800
H	-2.70014200	-1.05949000	3.48309300
H	-3.54399200	-0.59536300	1.96495000
H	-1.87600200	-0.03994800	2.28404900
C	-1.99017500	-2.04516900	1.70853800
O	-1.02381800	-2.60695000	2.45991200
O	-2.30810300	-2.43542000	0.59866100
O	0.42181100	2.82658300	-2.20847200
H	1.20121600	3.06338400	-1.68142300
H	-0.29819800	3.21285100	-1.68270700

six-coordinated H_2O-Co^{III}-OTs counterion addition in the terminal carbon and subsequent hydrolysis

H_2O-Co^{III}-OTs counterion addition in the terminal carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.280589

Thermal correction to Gibbs Free Energy (a.u.): 0.541819

Imaginary frequencies: -383.18

Calculation of single point energy based on the optimized structure, Et = -3582.3422174 a.u.

C	-0.41800400	5.63122400	-0.43659100
C	0.76421300	5.45188600	0.30363800
C	-1.33894400	4.60670400	-0.57254500
H	-0.61271000	6.58668000	-0.91599100
C	0.99475300	4.22660000	0.89954000
H	1.48359100	6.25766900	0.39885700
C	-1.12535600	3.34277300	0.03113500
H	-2.24910700	4.73661300	-1.14877400
C	0.07232700	3.16262100	0.78665700
H	1.90614100	4.05795900	1.46766200
O	-2.03584700	2.41055100	-0.14128100
C	0.40559200	1.91062400	1.41275700
Co	-1.98865300	0.63610000	0.53321500
N	-0.33255500	0.85691000	1.43820800
H	1.38478900	1.86609400	1.88573100
N	-2.03348700	-1.10202200	1.31904200
C	0.17269800	-0.43865500	1.90733800
C	-2.67531100	-2.09888400	0.81348800
C	-1.04311500	-1.23363900	2.39863900
C	1.30214100	-0.40344200	2.93334200
H	-2.49895000	-3.09366900	1.22203300
C	-3.62941200	-2.01480000	-0.25744900
C	-0.64023800	-2.65905700	2.77399400
C	1.68776800	-1.83794500	3.32340000
H	0.99336700	0.16951200	3.81941700
H	2.17571600	0.09393500	2.50084000
C	-4.13489100	-3.21505100	-0.80124200
C	-4.10227900	-0.75893100	-0.74545500
C	0.47603300	-2.62891400	3.82810900
H	-1.50329100	-3.21595500	3.15649900
H	-0.27556000	-3.17067800	1.87498000
H	2.47328200	-1.81656600	4.08664300
H	2.09742400	-2.33597200	2.43726800
C	-5.07812700	-3.20686400	-1.81200800
H	-3.75747700	-4.15812000	-0.41357400
C	-5.08158100	-0.77595800	-1.76601200
O	-3.69325300	0.40076700	-0.28125400
H	0.09408000	-2.17425300	4.75276800
H	0.76855900	-3.65390500	4.07887600
C	-5.55188900	-1.97065100	-2.28606700
H	-5.44857700	-4.13627400	-2.23010800
H	-5.43827400	0.18055000	-2.13308700
H	-6.29540600	-1.94885100	-3.07808200
C	-1.26285000	0.39257500	-2.18818500

C	0.08724900	0.97135200	-2.13360000
O	-1.08667800	-0.14918800	-0.88373200
H	-2.05547100	1.14905600	-2.21227000
H	0.24748000	1.90307600	-1.61010100
H	0.88710000	0.57257900	-2.74269500
C	-1.47755100	-0.71070200	-3.20792100
H	-2.43226200	-1.20762500	-3.02164100
H	-1.49620000	-0.28776100	-4.21930700
H	-0.66453000	-1.43761500	-3.14124300
H	-1.46815300	-0.72479400	3.27601800
H	0.54264600	-0.94616000	1.01140500
O	1.80437300	-2.16199800	-0.12098600
O	1.68862400	0.26443500	-0.70724500
S	2.19448000	-1.12102500	-1.10336800
O	1.89828000	-1.41390600	-2.52623600
C	3.97589800	-0.95748300	-0.96267500
C	4.73020000	-0.61545300	-2.08326300
C	4.58756500	-1.12154900	0.28005700
C	6.10573400	-0.43419400	-1.95323100
H	4.23543300	-0.50959500	-3.04220700
C	5.96252000	-0.93477800	0.39702800
H	3.98840200	-1.40745200	1.13738200
C	6.74234900	-0.58934400	-0.71517400
H	6.69654500	-0.17122900	-2.82692100
H	6.44157200	-1.06380600	1.36434200
C	8.23668800	-0.42446200	-0.58839800
H	8.51609700	-0.06008700	0.40465800
H	8.75279700	-1.38037100	-0.74158900
H	8.62572900	0.27789500	-1.33131000
O	-3.12790700	1.41276100	2.04256900
H	-3.95065900	1.09043300	1.62443200
H	-3.06569100	2.33519000	1.73490400

H_2O-Co^{III}-OTs counterion addition in the terminal carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.326522

Thermal correction to Gibbs Free Energy (a.u.): 0.542683

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.3903107 a.u.

C	-6.07181000	1.65301400	-2.47050200
C	-5.63122000	2.97061600	-2.24530700
C	-5.40409000	0.57175800	-1.92401500
H	-6.95039300	1.47820500	-3.08520400
C	-4.50883700	3.17065800	-1.46693600
H	-6.16051800	3.81118300	-2.67994600
C	-4.25321300	0.75045400	-1.11676800
H	-5.73878700	-0.44586100	-2.09579500
C	-3.80310100	2.08807400	-0.89142200
H	-4.14260500	4.17814000	-1.28502900
O	-3.67443400	-0.31981400	-0.61891500
C	-2.62137700	2.38517500	-0.12818000
Co	-2.17206200	-0.35885100	0.54387600
N	-1.86419900	1.52502500	0.46349100
H	-2.33982200	3.43728200	-0.07811400
N	-0.71233800	-0.40064900	1.75335400
C	-0.58589900	1.88481800	1.10240000
C	0.10374300	-1.39775000	1.82220000
C	-0.42502900	0.93327100	2.29804500
C	-0.40610300	3.34425100	1.51006700
H	1.04944200	-1.26746200	2.33528000
C	-0.16462900	-2.69986000	1.26906300
C	0.93654800	1.10873600	2.96899900
C	0.96944700	3.51282700	2.17541500
H	-1.20884600	3.64653200	2.19849400
H	-0.46072200	3.99564700	0.63112600
C	0.88357200	-3.63960300	1.22519700
C	-1.46787000	-3.06374800	0.82671300
C	1.12706600	2.57605700	3.37869100

H	1.00323300	0.45889700	3.84947100
H	1.72053200	0.80886100	2.26694200
H	1.10507300	4.55573900	2.48137400
H	1.73976100	3.27799800	1.43254600
C	0.65856600	-4.93494200	0.79084000
H	1.87806500	-3.30676600	1.50469200
C	-1.68520700	-4.39821800	0.42629700
O	-2.48183400	-2.21037400	0.78419200
H	0.39449600	2.84475600	4.15322000
H	2.11821000	2.70155300	3.82688800
C	-0.63998200	-5.31191200	0.41207000
H	1.47343400	-5.64902500	0.74470700
H	-2.68486600	-4.67590800	0.10901600
H	-0.83055700	-6.32988400	0.08327300
C	-1.24393400	-1.38626500	-2.09732900
C	-0.82874800	0.02565300	-2.12361200
O	-0.90272400	-0.67943200	-0.84364800
H	-2.31375000	-1.57160200	-2.14546000
H	-1.58832700	0.79081800	-2.24707500
H	0.20400400	0.27322700	-2.35372000
C	-0.30852600	-2.50462000	-2.44507700
H	-0.56187000	-3.40454300	-1.88025200
H	-0.41356200	-2.72738400	-3.51336900
H	0.72126200	-2.20777600	-2.23658900
H	-1.22528600	1.15349100	3.01968300
H	0.20909800	1.62450000	0.38799600
O	2.52522000	-0.74665500	0.65235600
O	1.99058200	1.43622000	-0.42089000
S	2.62040800	0.08740600	-0.58401600
O	2.19137600	-0.61666900	-1.82446700
C	4.37291400	0.41573200	-0.80115700
C	5.12988900	-0.39217400	-1.64705300
C	4.97875300	1.44946000	-0.08672000
C	6.49977500	-0.16482600	-1.77122000
H	4.63385600	-1.17427500	-2.21071800
C	6.34762600	1.66705200	-0.21853100
H	4.37074000	2.08531000	0.54739200
C	7.13030800	0.86121900	-1.05710400
H	7.08897500	-0.78996400	-2.43761300
H	6.81827800	2.47850700	0.33136200
C	8.61859100	1.08363200	-1.17058100
H	8.87251900	2.14469300	-1.08478100
H	9.15925900	0.55539700	-0.37514000
H	9.00578800	0.71763300	-2.12595800
O	-3.48714100	-0.24310400	2.03358100
H	-3.42242000	-1.20770000	2.20306500
H	-4.30048800	-0.15300200	1.50537000

H_2O-Co^{III}-OTs counterion addition in the terminal carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.342483

Thermal correction to Gibbs Free Energy (a.u.): 0.545307

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4009875 a.u.

C	-2.30822700	4.12222500	-1.76414600
C	-3.27485600	3.13783500	-2.04437500
C	-1.01743400	3.77644200	-1.40769400
H	-2.57772900	5.17319200	-1.82704600
C	-2.91198700	1.80843800	-1.94554800
H	-4.28413600	3.41862600	-2.32575900
C	-0.61440700	2.41757600	-1.31132100
H	-0.26927000	4.53183000	-1.19051800
C	-1.60370800	1.42082400	-1.58279600
H	-3.64409000	1.02702400	-2.13056700
O	0.62555300	2.16306300	-0.98135500
C	-1.34066700	0.02035200	-1.40817300
Co	1.44394300	0.44729600	-0.89824400
N	-0.19520000	-0.49551500	-1.12507200

H	-2.20578000	-0.63748000	-1.49367100
N	2.27944000	-1.27507100	-0.96755200
C	-0.01898900	-1.91140700	-0.78931300
C	3.43033800	-1.52629900	-0.44423700
C	1.33953300	-2.31889800	-1.39045300
C	-1.13229500	-2.86019800	-1.22891300
H	3.75250100	-2.56451700	-0.35663700
C	4.35066700	-0.54222500	0.05177900
C	1.69902700	-3.75653800	-1.01542700
C	-0.77101700	-4.30300400	-0.85128900
H	-1.27697800	-2.78135200	-2.31553300
H	-2.07620400	-2.58189300	-0.75202100
C	5.50541000	-0.99046600	0.72903400
C	4.14260500	0.85758200	-0.15053200
C	0.58025000	-4.71631400	-1.44553400
H	2.64377200	-4.05147800	-1.48540300
H	1.83899600	-3.81839500	0.07149300
H	-1.55902000	-4.98480700	-1.18889100
H	-0.72750700	-4.38390200	0.24264100
C	6.44290600	-0.10277300	1.22293800
H	5.64208400	-2.06083100	0.86587300
C	5.12231200	1.74505500	0.35594400
O	3.11793700	1.35169500	-0.80211300
H	0.50891500	-4.72191900	-2.54160600
H	0.83467500	-5.73744400	-1.14250200
C	6.23894700	1.27498300	1.02583700
H	7.31959000	-0.46068800	1.75168500
H	4.95833000	2.80669400	0.20436500
H	6.96655300	1.98511900	1.40955700
C	1.36086000	1.20435300	1.81097600
C	-0.02836500	1.87911500	1.96178600
O	1.34974600	0.15024200	0.90651400
H	2.05166800	2.00359000	1.49458000
H	-0.11667500	2.74443900	1.30824500
H	-0.24274200	2.17466100	2.99299600
C	1.86543800	0.63202800	3.14194300
H	2.87566000	0.23837100	3.00346000
H	1.88934900	1.40290300	3.92060000
H	1.21799800	-0.18561800	3.47103700
H	1.25140900	-2.24103600	-2.48391000
H	0.07637800	-1.93342000	0.30395200
O	-0.98780900	-1.37577500	2.38033900
O	-1.10657300	1.02224900	1.48952600
S	-1.72866800	-0.11367700	2.45633200
O	-1.98232100	0.47759300	3.77211500
C	-3.23727700	-0.32356100	1.52843200
C	-3.96941800	0.78703700	1.10877200
C	-3.66896200	-1.61910100	1.24903000
C	-5.14295400	0.58768000	0.38886500
H	-3.60366900	1.78704300	1.30641500
C	-4.84728000	-1.80008500	0.52674700
H	-3.07499900	-2.46236100	1.58209500
C	-5.60047900	-0.70335300	0.08732700
H	-5.70361200	1.44984600	0.03976900
H	-5.18526700	-2.80699300	0.29842600
C	-6.88608300	-0.90315000	-0.67477000
H	-6.90520900	-1.87188400	-1.18129000
H	-7.74863700	-0.86878400	0.00160000
H	-7.03125100	-0.12032400	-1.42500200
O	1.77225100	0.74609900	-2.95171800
H	2.67788600	1.04200800	-2.73126100
H	1.27594400	1.57948500	-3.01332600

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.734724

Thermal correction to Gibbs Free Energy (a.u.): 0.558001

Imaginary frequencies: -617.79

Calculation of single point energy based on the optimized structure, Et = -3658.8520453 a.u.

C	0.10392800	4.89476900	1.11326300
C	0.57093100	4.35980200	2.32929300
C	-0.44526200	4.08461600	0.13643400
H	0.17308500	5.96474500	0.93663200
C	0.47689200	2.99764100	2.53485800
H	1.00174400	5.00547200	3.08654200
C	-0.56549000	2.68341300	0.32228200
H	-0.80168300	4.49323200	-0.80296600
C	-0.09618500	2.14212800	1.56631100
H	0.84565100	2.55427200	3.45595000
O	-1.05271300	1.96675700	-0.65836400
C	-0.09709200	0.72779700	1.82115800
Co	-1.86517600	0.28913000	-0.38800000
N	-0.70458300	-0.13756900	1.08462300
H	0.49293100	0.37841900	2.66611200
N	-2.67808700	-1.38813100	0.04244300
C	-0.53056900	-1.58842200	1.17139400
C	-3.91129000	-1.67175300	-0.22525700
C	-1.91565900	-2.21571500	1.00097600
C	0.15958400	-2.18091400	2.39566400
H	-4.27977500	-2.66184600	0.05624200
C	-4.87574100	-0.76005100	-0.76440600
C	-1.75161100	-3.69628300	0.65330700
C	0.33246900	-3.69055500	2.14799000
H	-0.44596800	-1.99820300	3.29378900
H	1.13943900	-1.72727700	2.55584500
C	-6.10906200	-1.25815900	-1.23676000
C	-4.66838400	0.65263800	-0.66400400
C	-0.99327700	-4.38879800	1.80168000
H	-2.72334300	-4.17950100	0.50406200
H	-1.19705000	-3.77411400	-0.28899100
H	0.78121100	-4.16120100	3.02875300
H	1.04865700	-3.81872200	1.32835600
C	-7.11766200	-0.40488300	-1.64054900
H	-6.25029300	-2.33509800	-1.28498100
C	-5.73040100	1.50320800	-1.05187800
O	-3.56357400	1.18676800	-0.19691500
H	-1.63936600	-4.39683300	2.69021700
H	-0.80785000	-5.43650400	1.54188500
C	-6.91758900	0.98499300	-1.53763900
H	-8.05481300	-0.79803500	-2.01935500
H	-5.57204700	2.57266900	-0.96383000
H	-7.70978200	1.66379800	-1.84118400
H	-2.44233200	-2.13006900	1.96193500
H	0.05155500	-1.83379800	0.27630500
O	-2.35893800	0.12958700	-2.39800500
H	-2.21717200	1.02742800	-2.72900100
H	-1.34648200	-0.39468000	-2.33366900
O	-3.14723100	1.54338100	2.56417100
H	-2.53169200	2.28692500	2.55849900
H	-3.44810700	1.49734600	1.63933400
C	0.80109100	-0.11374700	-2.21195200
C	1.81740200	0.22135400	-1.12668500
O	-0.31949000	-0.76894000	-1.69029700
H	0.52297100	0.87498900	-2.62653500
H	1.37521400	0.84967400	-0.35741100
H	2.69107500	0.72332200	-1.55817900
C	1.42480900	-0.95721800	-3.32967500
H	0.68250100	-1.13811800	-4.11160800
H	2.29004500	-0.45606400	-3.77965900
H	1.74495000	-1.92277100	-2.92976800
O	2.81482800	0.10064600	1.65900600
O	2.25443600	-1.03270000	-0.52056000
S	3.27576500	-0.94018700	0.73454100
O	3.42409000	-2.32119100	1.17935100
C	4.78589000	-0.38587600	-0.01987100
C	5.58067900	-1.30930700	-0.70212900
C	5.12928900	0.96385900	0.04265100

C	6.73891600	-0.86293500	-1.32826300
H	5.29401600	-2.35457500	-0.72769000
C	6.29401900	1.39076000	-0.59242600
H	4.49688500	1.65532100	0.58759900
C	7.11292600	0.48926400	-1.28369900
H	7.36589700	-1.57261300	-1.86046600
H	6.57143900	2.43992300	-0.54934700
C	8.38629400	0.95155600	-1.94496900
H	8.54720000	0.44124600	-2.89915500
H	8.37307900	2.02871700	-2.12968900
H	9.25411300	0.73533800	-1.31039100

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.761493

Thermal correction to Gibbs Free Energy (a.u.): 0.560826

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3658.8808156 a.u.

C	0.64568600	5.36801700	-0.72773100
C	1.25312600	5.26633700	0.54043800
C	-0.14797800	4.35291500	-1.22552700
H	0.80606400	6.25914200	-1.32868100
C	1.04241400	4.12693400	1.28858200
H	1.87995000	6.06756000	0.91620600
C	-0.38587600	3.16894000	-0.47584400
H	-0.61009200	4.42095800	-2.20466600
C	0.22189300	3.07465800	0.81839500
H	1.51200000	4.01497100	2.26233800
O	-1.12563300	2.23663900	-1.01203600
C	0.09253800	1.90184500	1.62997300
Co	-1.87458400	0.75486700	-0.10889000
N	-0.67805400	0.89689000	1.37032800
H	0.72615900	1.85557800	2.51256000
N	-2.70611000	-0.63880800	0.92981000
C	-0.65372600	-0.35799100	2.13197500
C	-3.52143600	-1.49669100	0.42439500
C	-2.12170500	-0.78521200	2.27311000
C	0.06389600	-0.34192400	3.47803800
H	-3.79721100	-2.36878400	1.01380500
C	-4.13038200	-1.39011500	-0.87425600
C	-2.22543700	-2.17461800	2.90477600
C	-0.02291700	-1.74021500	4.10537200
H	-0.40176700	0.40293500	4.13880500
H	1.11298600	-0.06787100	3.34248100
C	-4.90442500	-2.47323600	-1.34180700
C	-4.03944400	-0.19645300	-1.65067800
C	-1.47759800	-2.20322100	4.24708800
H	-3.27571500	-2.44113900	3.07021100
H	-1.80021800	-2.90099000	2.20228400
H	0.47090500	-1.73696300	5.08286700
H	0.53399700	-2.43880100	3.47020300
C	-5.57278700	-2.41206600	-2.55100100
H	-4.96369000	-3.36876100	-0.72779800
C	-4.75572000	-0.14554400	-2.86858800
O	-3.34379800	0.85990800	-1.28664600
H	-1.99618000	-1.55209800	4.96472500
H	-1.51484500	-3.21653800	4.66101700
C	-5.49518000	-1.23051400	-3.30912100
H	-6.15412800	-3.25667200	-2.90463300
H	-4.68794100	0.76735300	-3.45054200
H	-6.02010500	-1.16569100	-4.25823400
H	-2.62026700	-0.04195200	2.91204900
H	-0.16269400	-1.08385400	1.47298400
O	-1.20040200	-3.21852600	-0.15525600
H	-1.72617200	-3.56098200	-0.88784000
H	-1.01607400	-2.28667100	-0.43395600
O	-3.35768800	2.49063200	0.88970200
H	-2.86511600	3.26735500	0.59106100

H	-3.83244300	2.19619800	0.09167500
C	0.08911700	-0.43999000	-1.95225600
C	1.39042700	0.00442500	-1.27345600
O	-0.89429500	-0.67114400	-0.99321000
H	-0.18524300	0.39972900	-2.61331200
H	1.25479500	0.96018000	-0.76963800
H	2.21935000	0.07531200	-1.98788100
C	0.28461400	-1.70212800	-2.79984900
H	-0.65564400	-1.94609800	-3.30252500
H	1.05913300	-1.56048100	-3.56218900
H	0.56134800	-2.54368000	-2.15914600
O	2.73119300	0.74593500	1.23178400
O	1.72027700	-1.00650800	-0.27447400
S	2.85502100	-0.65780700	0.82363400
O	2.75074700	-1.72712900	1.81006000
C	4.36269500	-0.83901400	-0.09938400
C	4.87520600	-2.11977000	-0.31521300
C	4.97927900	0.29103100	-0.63417900
C	6.02799800	-2.25994600	-1.07978200
H	4.37792100	-2.98031500	0.11795200
C	6.13322100	0.12851300	-1.39859600
H	4.56358600	1.27331900	-0.44108400
C	6.67316000	-1.14235000	-1.63179900
H	6.43664600	-3.25145900	-1.25295100
H	6.62255900	1.00230600	-1.81902900
C	7.93740000	-1.31005000	-2.43584100
H	7.88821900	-2.19708800	-3.07428800
H	8.12620200	-0.44056200	-3.07070600
H	8.80473900	-1.43239500	-1.77601400

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOHCH_2OTs$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.762640

Thermal correction to Gibbs Free Energy (a.u.): 0.562976

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3658.8799405 a.u.

C	1.82402400	5.57898000	0.47012300
C	0.46338400	5.50164900	0.12088800
C	2.65302500	4.47347800	0.37918500
H	2.23433100	6.52114300	0.82356600
C	-0.04211900	4.29869300	-0.33404700
H	-0.17678300	6.37307800	0.20449000
C	2.15303200	3.22277800	-0.05288300
H	3.70133500	4.52704000	0.65295400
C	0.77835600	3.15177300	-0.42873700
H	-1.08787900	4.20653800	-0.61491100
O	2.97717600	2.19957400	-0.10741800
C	0.19860700	1.95665500	-0.96656700
Co	2.44869400	0.38496500	-0.22738800
N	0.77236600	0.80097600	-1.02975100
H	-0.81768600	2.05185000	-1.34021700
N	2.17299000	-1.37480900	-0.98660700
C	0.05861400	-0.39407900	-1.51248600
C	2.75488400	-2.44169100	-0.55221100
C	1.12600900	-1.37265300	-2.01473800
C	-1.01667100	-0.16457900	-2.57317100
H	2.42924000	-3.41012200	-0.93347000
C	3.82970100	-2.46632400	0.39694000
C	0.49407000	-2.72328900	-2.34952800
C	-1.66017500	-1.51107600	-2.93777800
H	-0.56518400	0.29526600	-3.46282600
H	-1.78285400	0.51978700	-2.20363200
C	4.27560700	-3.72083600	0.87226000
C	4.50753400	-1.27144700	0.79997100
C	-0.61576800	-2.53598100	-3.39591100
H	1.24665700	-3.42057900	-2.73399100
H	0.07731300	-3.15147000	-1.42901800
H	-2.41337600	-1.36431000	-3.72022300

H	-2.18726900	-1.90129000	-2.05692700
C	5.35006100	-3.82568500	1.73250200
H	3.74617000	-4.61309100	0.54689700
C	5.62072300	-1.41014500	1.66674300
O	4.18285800	-0.06851700	0.39141900
H	-0.16642000	-2.19679800	-4.33879100
H	-1.09208900	-3.50009600	-3.60418200
C	6.02403200	-2.65209400	2.12177400
H	5.67376000	-4.79385400	2.09849900
H	6.13616600	-0.50274400	1.96280100
H	6.87473000	-2.72037900	2.79433700
H	1.59123800	-0.94440300	-2.91374200
H	-0.39399600	-0.84938100	-0.62428000
O	1.62471700	0.07416400	1.47678600
H	2.32354200	0.11123900	2.14339500
H	0.58038800	-1.15507600	1.43596700
O	3.88843800	0.79283200	-2.29563500
H	3.81371200	1.68050800	-1.90634200
H	4.52669600	0.36679400	-1.70163400
C	-1.23533400	-1.33037700	2.15784000
C	-1.46919300	0.17621300	2.04185500
O	-0.19494200	-1.77947100	1.31792200
H	-0.96546500	-1.47729200	3.22156000
H	-0.52562700	0.71178400	2.15939000
H	-2.19470900	0.52393800	2.78041200
C	-2.47768500	-2.15901600	1.85460100
H	-2.25015000	-3.21926500	1.99021100
H	-3.31048100	-1.89040600	2.51142400
H	-2.79173600	-2.00413400	0.81942000
O	-3.44463500	2.28117100	1.71455000
O	-1.95014400	0.51324700	0.69728000
S	-3.24987600	1.46774500	0.51707800
O	-3.05833300	2.08489000	-0.79688200
C	-4.56935800	0.28365700	0.40164700
C	-4.71969700	-0.45561200	-0.77357400
C	-5.38026600	0.05597300	1.51062400
C	-5.69404700	-1.44538100	-0.82409300
H	-4.08610500	-0.25200200	-1.62862200
C	-6.35481200	-0.93817300	1.43867600
H	-5.24687700	0.65188000	2.40610300
C	-6.52308400	-1.70413600	0.27903700
H	-5.81635300	-2.02843600	-1.73249500
H	-6.99273800	-1.12312200	2.29794600
C	-7.58876400	-2.76720500	0.19988600
H	-7.22285400	-3.65848400	-0.31862700
H	-7.93091000	-3.06545900	1.19401700
H	-8.46119300	-2.40333800	-0.35586700

six-coordinated H_2O-Co^{III}-OTs counterion addition in the middle carbon and subsequent hydrolysis

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.281025

Thermal correction to Gibbs Free Energy (a.u.): 0.542634

Imaginary frequencies: -248.34

Calculation of single point energy based on the optimized structure, Et = -3582.3486832 a.u.

C	2.23087900	-4.09649200	-1.18429800
C	3.18740000	-3.07560700	-1.31426900
C	0.87853000	-3.80403700	-1.09420300
H	2.55190400	-5.13389400	-1.14255400
C	2.75729900	-1.76227700	-1.36263800
H	4.24511400	-3.30941800	-1.36314200
C	0.41573700	-2.46633400	-1.12867700
H	0.13704500	-4.58790500	-0.97925700
C	1.38711400	-1.43458300	-1.28129200
H	3.47798900	-0.95407100	-1.43728200
O	-0.87716900	-2.25065000	-1.00712500
C	1.03615500	-0.04174900	-1.26793400

Co	-1.72810000	-0.56268200	-0.83871400
N	-0.15431500	0.44160900	-1.17778100
H	1.87455400	0.64803500	-1.31776400
N	-2.63226400	1.12354700	-0.81727300
C	-0.36592000	1.86441900	-0.87507100
C	-3.75114400	1.32895200	-0.21144300
C	-1.78490000	2.20308800	-1.34564300
C	0.66507300	2.84153900	-1.43468700
H	-4.10863300	2.35400000	-0.11060500
C	-4.59369500	0.31072100	0.35229200
C	-2.16877600	3.62759600	-0.94630600
C	0.28505400	4.27323700	-1.03598800
H	0.71830400	2.74148900	-2.52787000
H	1.64946100	2.61584200	-1.02201500
C	-5.71714600	0.71439500	1.10630900
C	-4.35026600	-1.07925600	0.12756500
C	-1.13583600	4.62733400	-1.48918300
H	-3.16638100	3.87997300	-1.32344100
H	-2.20217100	3.69373600	0.14885000
H	1.00436500	4.97953700	-1.46369500
H	0.36925500	4.35719200	0.05402400
C	-6.58866400	-0.20886700	1.65274700
H	-5.88382300	1.77840600	1.25701300
C	-5.26227300	-2.00450900	0.68967100
O	-3.35102900	-1.53489400	-0.59176900
H	-1.18035500	4.62944400	-2.58694200
H	-1.40167900	5.63837100	-1.16304400
C	-6.34992800	-1.57738600	1.43263700
H	-7.44248300	0.11492500	2.23766500
H	-5.07435600	-3.05886700	0.51618900
H	-7.02761900	-2.31475400	1.85423300
C	-0.20039100	-1.11843400	2.41582000
C	-1.51411900	-1.46016400	1.82766900
O	-1.49988000	-0.32514700	0.99179600
H	-0.15065000	-0.25741300	3.07043400
H	-2.35531900	-1.44951100	2.53686700
H	-1.50712700	-2.40488200	1.27520900
C	0.96072700	-2.00938100	2.32204100
H	1.15253900	-2.31171700	1.28891900
H	1.84543000	-1.56495100	2.76948800
H	0.67329200	-2.93472900	2.85313700
H	-1.81025400	2.11086400	-2.44102300
H	-0.33501600	1.91843400	0.22027700
O	2.09289300	2.74181500	1.84122700
O	1.14079800	0.51880500	1.30902300
S	2.21869200	1.28354000	2.05282000
O	2.35041600	0.79631000	3.44540300
C	3.72089900	0.78994400	1.18693300
C	4.36674300	-0.39956100	1.52358800
C	4.18172900	1.55216400	0.11334200
C	5.45381000	-0.83509600	0.76977300
H	4.02516700	-0.96785600	2.38080000
C	5.26833400	1.10577500	-0.63903700
H	3.69975300	2.49891300	-0.10399500
C	5.91751800	-0.09633700	-0.32742400
H	5.95121100	-1.76462800	1.03447600
H	5.62409000	1.70269900	-1.47507000
C	7.10855600	-0.56479900	-1.12636300
H	7.07844200	-0.18258700	-2.15073900
H	8.04680000	-0.21858000	-0.67573500
H	7.15488300	-1.65711900	-1.17136900
O	-2.16929400	-0.85353200	-2.80554600
H	-1.63152500	-1.66401600	-2.88063100
H	-3.06140400	-1.19268000	-2.59553100

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.309880

Thermal correction to Gibbs Free Energy (a.u.): 0.544124
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -3582.3848742 a.u.

C	2.26821000	-4.14585500	-1.22947300
C	3.22429400	-3.12021000	-1.30940400
C	0.91729200	-3.85934100	-1.10130000
H	2.58760300	-5.18412500	-1.25759300
C	2.79795100	-1.80588700	-1.27181700
H	4.28022000	-3.35143300	-1.39290000
C	0.46216000	-2.52379700	-1.04318200
H	0.17710100	-4.64851600	-1.02041900
C	1.42858000	-1.48424900	-1.15088900
H	3.51748700	-0.99555000	-1.31676600
O	-0.83324200	-2.31696500	-0.87318700
C	1.06932500	-0.09511700	-1.12674700
Co	-1.69219600	-0.64530800	-0.72196800
N	-0.12992800	0.37731300	-1.06576000
H	1.89399000	0.61074500	-1.17818300
N	-2.61656300	1.03044800	-0.72298900
C	-0.35907900	1.82893800	-0.93665200
C	-3.74571300	1.24543200	-0.14161400
C	-1.80874700	2.08067200	-1.35896700
C	0.58371300	2.72498800	-1.74136000
H	-4.11239100	2.27041500	-0.08275100
C	-4.59186000	0.23113600	0.42731600
C	-2.21376500	3.52739800	-1.08490800
C	0.20633800	4.19324400	-1.50389100
H	0.51332900	2.46403200	-2.80706300
H	1.60875800	2.59114100	-1.39708700
C	-5.72514400	0.63479300	1.16666400
C	-4.34640300	-1.15761400	0.20347300
C	-1.26348400	4.47665300	-1.83432500
H	-3.24647000	3.71003200	-1.40401000
H	-2.15908900	3.71789400	-0.00533400
H	0.85590000	4.83924500	-2.10348200
H	0.42009500	4.42342400	-0.45455100
C	-6.60501900	-0.29055500	1.69635500
H	-5.89334300	1.69829200	1.31751900
C	-5.27022200	-2.08420600	0.74007800
O	-3.31891100	-1.61510900	-0.48122100
H	-1.42793400	4.35850600	-2.91427700
H	-1.51971100	5.51308200	-1.59054300
C	-6.36823900	-1.65801500	1.46929900
H	-7.46638500	0.03159400	2.27071800
H	-5.08191100	-3.13808300	0.56455800
H	-7.05446000	-2.39598300	1.87509200
C	-0.61270000	-0.84724800	2.30570400
C	-2.04162400	-1.19229900	2.24426700
O	-1.46504200	-0.38074900	1.18499700
H	-0.29945500	0.02500900	2.86836100
H	-2.78552500	-0.65743700	2.82732700
H	-2.31526800	-2.19339800	1.92384400
C	0.45510400	-1.86659800	2.07133700
H	0.09332800	-2.72039000	1.49931000
H	1.30279000	-1.39864700	1.57267800
H	0.79203000	-2.21634400	3.05407400
H	-1.87732000	1.88811200	-2.43955500
H	-0.22895800	2.04953200	0.13052500
O	2.39447100	3.10657900	0.68470200
O	1.25808600	1.06171700	1.52109200
S	2.45064100	1.97005000	1.64584500
O	2.77874100	2.31533400	3.04173500
C	3.80576800	0.93349300	1.05225500
C	4.08616600	-0.27115400	1.70336400
C	4.55994900	1.31378200	-0.05536600
C	5.10518200	-1.09319900	1.23473700
H	3.50272600	-0.55546800	2.57258800
C	5.58531800	0.48321900	-0.51760200
H	4.33692000	2.26045100	-0.53518300

C	5.87236200	-0.73036500	0.11669900
H	5.31069700	-2.03482000	1.73783700
H	6.17154100	0.78411500	-1.38257700
C	6.98794300	-1.62186600	-0.37096500
H	7.26488800	-1.38830400	-1.40292500
H	7.88786500	-1.50478000	0.24518100
H	6.70390400	-2.67857500	-0.32528100
O	-2.10019400	-0.92909600	-2.63854800
H	-1.54673500	-1.72894900	-2.73566700
H	-2.99494800	-1.28735100	-2.46768100

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2343.347832

Thermal correction to Gibbs Free Energy (a.u.): 0.545932

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.4073616 a.u.

C	3.04050700	-2.37279100	-2.50462800
C	3.63814500	-1.09961700	-2.56555800
C	1.73761200	-2.53154800	-2.07088500
H	3.61101100	-3.24878400	-2.80256500
C	2.90257000	-0.00387100	-2.16156800
H	4.66109200	-0.98424500	-2.90591300
C	0.94757400	-1.41725300	-1.68078300
H	1.27089100	-3.51009200	-2.02601900
C	1.56830300	-0.13005500	-1.71512100
H	3.35260200	0.98479300	-2.16398100
O	-0.29546500	-1.62958300	-1.33689600
C	0.89957800	1.04887800	-1.24344400
Co	-1.58982100	-0.30917500	-0.86798200
N	-0.33066400	1.11398400	-0.86740300
H	1.51210700	1.94637200	-1.17596600
N	-2.90727400	1.04076800	-0.55948800
C	-0.90409900	2.30499700	-0.23535100
C	-4.05519600	0.80841300	-0.02085300
C	-2.35522300	2.38734400	-0.74427100
C	-0.15406000	3.61892900	-0.44142900
H	-4.67402500	1.65469800	0.28023600
C	-4.61294300	-0.49200300	0.22154400
C	-3.11374600	3.53682400	-0.08225300
C	-0.92242900	4.77449700	0.21463000
H	-0.03609900	3.81135100	-1.51712600
H	0.84155300	3.54273000	0.00225200
C	-5.82775300	-0.57332400	0.93677900
C	-4.00010100	-1.68335700	-0.27883300
C	-2.36447200	4.85967300	-0.29781300
H	-4.12872400	3.61167600	-0.48819400
H	-3.20456800	3.33559600	0.99320400
H	-0.39805700	5.71863200	0.03265400
H	-0.93074700	4.62358100	1.30180000
C	-6.44050900	-1.78699700	1.18442200
H	-6.27626100	0.34863400	1.30025700
C	-4.65298500	-2.91315600	-0.01871400
O	-2.90015600	-1.69046800	-0.99017600
H	-2.35740200	5.10043600	-1.36953400
H	-2.90115700	5.67270900	0.20260500
C	-5.83821100	-2.96038800	0.69431200
H	-7.36866200	-1.83513200	1.74349500
H	-4.18364200	-3.81524100	-0.39683300
H	-6.30819500	-3.92240700	0.88075700
C	0.20578700	-1.29140400	2.42857900
C	-0.97278900	-1.59643400	1.51095300
O	-1.47486300	-0.42292900	0.96178300
H	-0.08386600	-0.51082000	3.13647900
H	-1.74023700	-2.10131500	2.12669600
H	-0.64826300	-2.31433500	0.74779400
C	0.76628700	-2.50472200	3.14818100
H	1.08968500	-3.25882300	2.42314300

H	1.61368200	-2.22030200	3.77511900
H	-0.00380500	-2.95082300	3.78540700
H	-2.31103100	2.56268100	-1.82902600
H	-0.93526700	2.06867000	0.83550900
O	1.57838800	1.77172300	1.65724900
O	1.26350100	-0.74342200	1.55210400
S	2.13608800	0.49313600	2.11464100
O	2.35864600	0.31138600	3.55165600
C	3.62825300	0.18069200	1.19873800
C	4.10378100	-1.12214800	1.04779300
C	4.34279700	1.27198100	0.71002700
C	5.30635300	-1.32480600	0.38226600
H	3.52404400	-1.95803100	1.41901100
C	5.55175900	1.04905000	0.05351700
H	3.94828400	2.27364500	0.83720300
C	6.04744600	-0.24732300	-0.12407900
H	5.67287500	-2.33753900	0.24169100
H	6.11465100	1.89440700	-0.33200200
C	7.32921400	-0.49283600	-0.87792900
H	7.91010100	0.42576900	-0.99318000
H	7.95558100	-1.23255700	-0.36981300
H	7.11959100	-0.88228700	-1.88170000
O	-1.93207200	-0.24690400	-2.92951500
H	-1.20223700	-0.84410900	-3.16657900
H	-2.68471200	-0.85714800	-2.79638100

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.273699

Thermal correction to Gibbs Free Energy (a.u.): 0.535502

Imaginary frequencies: -304.98

Calculation of single point energy based on the optimized structure, Et = -3582.3372415 a.u.

C	2.23043200	-4.09826000	-1.19071000
C	3.18283700	-3.07675900	-1.36115000
C	0.88454700	-3.80633000	-1.04439200
H	2.55350000	-5.13535800	-1.16209000
C	2.75606000	-1.76353300	-1.39418700
H	4.23684000	-3.31443200	-1.45382900
C	0.42523300	-2.46597300	-1.05241300
H	0.14733300	-4.58851300	-0.89719400
C	1.38968100	-1.43493000	-1.25364000
H	3.47327600	-0.95628900	-1.50310300
O	-0.85461200	-2.24441200	-0.86010600
C	1.03017700	-0.04985400	-1.24739400
Co	-1.70791300	-0.57510100	-0.69037400
N	-0.16302600	0.43113800	-1.12565300
H	1.85851300	0.64725000	-1.34185600
N	-2.63455600	1.11034400	-0.77734800
C	-0.37242100	1.86080800	-0.84447100
C	-3.79886300	1.31646900	-0.26107600
C	-1.78954800	2.18521800	-1.32300700
C	0.65687600	2.82866000	-1.42213100
H	-4.18002600	2.33734200	-0.22831300
C	-4.66599700	0.30635800	0.27282700
C	-2.18284400	3.61445500	-0.95024600
C	0.27070000	4.26527900	-1.04690600
H	0.70936300	2.70998800	-2.51345000
H	1.64010100	2.61583600	-1.00105200
C	-5.86293800	0.71481400	0.90349100
C	-4.38562900	-1.08614600	0.12009800
C	-1.15067600	4.60853600	-1.50582400
H	-3.17757800	3.85795200	-1.33999200
H	-2.22522800	3.69740500	0.14347700
H	0.98832900	4.96648300	-1.48557400
H	0.35541700	4.36578500	0.04142600
C	-6.76934600	-0.20536600	1.39205800
H	-6.05749200	1.77983000	1.00313400
C	-5.34016400	-2.00959300	0.61055200

O	-3.31103900	-1.55421400	-0.47187000
H	-1.19475700	4.59437400	-2.60345400
H	-1.41969500	5.62346400	-1.19468700
C	-6.49653900	-1.57731000	1.23487600
H	-7.67857800	0.12205900	1.88404500
H	-5.12343200	-3.06512400	0.48602200
H	-7.20345300	-2.31138000	1.61142800
C	-0.08338900	-0.99518400	2.64336500
C	-1.43844800	-1.31194800	2.14448200
O	-1.47384200	-0.23954900	1.24865700
H	0.03561700	-0.11890300	3.26809400
H	-2.21319200	-1.25158800	2.92751700
H	-1.49630400	-2.29544700	1.65783700
C	1.03148200	-1.94419100	2.51643700
H	1.13713500	-2.29887400	1.48776200
H	1.96572600	-1.52575200	2.88019000
H	0.74291900	-2.82776400	3.11401000
H	-1.81299500	2.07003300	-2.41602800
H	-0.34026100	1.92952900	0.25022700
O	2.10189000	2.75120400	1.66407000
O	1.20454800	0.46476000	1.32931700
S	2.27880200	1.31676000	1.98056900
O	2.46503100	0.94317800	3.40085200
C	3.76606900	0.80118900	1.10133800
C	4.40851500	-0.38754600	1.45059900
C	4.22100300	1.54342600	0.01249600
C	5.48307500	-0.84273800	0.69230300
H	4.07757600	-0.93783500	2.32356000
C	5.29681100	1.07676400	-0.74499200
H	3.74683600	2.49251600	-0.21105700
C	5.93634600	-0.12734100	-0.42566800
H	5.98070600	-1.76829100	0.97024600
H	5.65152500	1.66126200	-1.59001400
C	7.07389900	-0.65302700	-1.26589900
H	7.86655600	-1.07919000	-0.64314200
H	6.73204700	-1.44673600	-1.94192700
H	7.51331400	0.13560800	-1.88265500
O	-2.31902800	-1.05819200	-2.98594700
H	-1.69892500	-1.80276600	-2.98944800
H	-3.10007500	-1.43117400	-2.54279800

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.318518

Thermal correction to Gibbs Free Energy (a.u.): 0.537665

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3582.3881429 a.u.

C	2.70849700	-3.02222300	-2.13021200
C	3.44241000	-1.82100300	-2.13532900
C	1.34880800	-3.03278300	-1.86896200
H	3.21813500	-3.96267600	-2.32062500
C	2.78661200	-0.63083200	-1.88952600
H	4.51247400	-1.82877700	-2.30671900
C	0.66410300	-1.82855700	-1.58350800
H	0.78169800	-3.95700000	-1.84072600
C	1.40007900	-0.60937500	-1.61909900
H	3.32564200	0.30896100	-1.85979200
O	-0.61067200	-1.89572700	-1.26559800
C	0.80120200	0.64854600	-1.30414900
Co	-1.74744700	-0.51146500	-0.78300300
N	-0.45377000	0.83454700	-1.02260900
H	1.47767400	1.50330100	-1.27488300
N	-2.95890300	0.91654900	-0.40116500
C	-0.90570700	2.14475400	-0.50916300
C	-4.07479300	0.78954500	0.23793500
C	-2.40479500	2.21738800	-0.81173500
C	-0.17726300	3.37429400	-1.05285300
H	-4.62556700	1.69240200	0.50145400

C	-4.67491400	-0.45112900	0.63070000
C	-3.04035100	3.46294000	-0.19828200
C	-0.80426100	4.64124000	-0.45325500
H	-0.26254100	3.38929100	-2.14870400
H	0.88262100	3.33415400	-0.79112800
C	-5.85350500	-0.41262900	1.41157600
C	-4.14527800	-1.71054600	0.20944600
C	-2.31365500	4.71820200	-0.70859900
H	-4.10476200	3.52242800	-0.45255900
H	-2.96315500	3.40561800	0.89561700
H	-0.30584200	5.52459300	-0.86448600
H	-0.61307200	4.65183500	0.62745200
C	-6.50272300	-1.57060400	1.78910200
H	-6.24136300	0.55633500	1.71562600
C	-4.84075700	-2.88338700	0.59498900
O	-3.06264700	-1.83857400	-0.51932600
H	-2.49738100	4.82124200	-1.78655100
H	-2.74211400	5.60576800	-0.23115800
C	-5.98453800	-2.81127900	1.36846100
H	-7.40074100	-1.52765600	2.39527500
H	-4.43468300	-3.83476700	0.26862100
H	-6.48973600	-3.72855600	1.65711900
C	-0.29439000	-0.91820900	2.26721500
C	-1.71632400	-1.21210900	2.50403100
O	-1.32730900	-0.37473700	1.39244400
H	0.18147900	-0.12174000	2.83182900
H	-2.27684000	-0.68726700	3.27419900
H	-2.10836400	-2.18450700	2.21464400
C	0.63014100	-1.94684900	1.68729400
H	0.08441000	-2.67557300	1.08478000
H	1.38560500	-1.45577100	1.07332400
H	1.14233700	-2.46972900	2.50271400
H	-2.51805400	2.25546000	-1.90449100
H	-0.75400700	2.09555000	0.57651600
O	2.88943200	2.57422300	-0.28638500
O	1.56277700	1.17922300	1.28553600
S	2.84523800	1.93153000	1.07123600
O	3.22026500	2.81791500	2.18695900
C	4.09935600	0.64076300	0.95895800
C	3.98641700	-0.51730000	1.72787400
C	5.17704700	0.79371900	0.08755900
C	4.92948500	-1.53311100	1.59613000
H	3.14803300	-0.62203800	2.40594900
C	6.11986900	-0.22638500	-0.03456500
H	5.24513300	1.69693000	-0.50870100
C	6.00808900	-1.40703200	0.71004500
H	4.82590800	-2.44228500	2.18374100
H	6.95242400	-0.10824900	-0.72402000
C	7.03268400	-2.50756000	0.58305500
H	7.75106500	-2.47838600	1.41159100
H	6.56190200	-3.49592100	0.59958300
H	7.60241200	-2.41813900	-0.34639400
O	-2.51580500	-0.65080000	-2.95416900
H	-1.75449000	-1.10942900	-3.33903700
H	-3.09788000	-1.37112200	-2.65882600

H_2O-Co^{III}-OTs counterion addition in the middle carbon

H_2O-Co^{III}-OTs + PO = H_2O-Co^{III}-PO-OTs

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2343.337448

Thermal correction to Gibbs Free Energy (a.u.): 0.539598

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3582.3955124 a.u.

C	2.88302300	-2.80968400	-2.24852900
C	3.48248200	-1.57784000	-2.58015500
C	1.64039600	-2.86223200	-1.64870200
H	3.40601300	-3.73688700	-2.46795400
C	2.81139100	-0.41157900	-2.27962500
H	4.45834200	-1.54859000	-3.05205700

C	0.91296900	-1.67677800	-1.34962800
H	1.17253900	-3.80722000	-1.39372800
C	1.53457500	-0.42747900	-1.67215700
H	3.26560500	0.55100300	-2.49636500
O	-0.26851200	-1.79909300	-0.81633500
C	0.91933900	0.82492200	-1.35358600
Co	-1.53617100	-0.42246800	-0.54926100
N	-0.27941400	0.97472200	-0.89871200
H	1.53658800	1.71114200	-1.49431900
N	-2.84204700	0.99079900	-0.54578100
C	-0.81432500	2.26315400	-0.44989900
C	-4.05704500	0.83850000	-0.14472200
C	-2.27323800	2.29006000	-0.92909900
C	-0.05449900	3.51493400	-0.87975500
H	-4.68967400	1.72105100	-0.04100100
C	-4.68204100	-0.41993800	0.15194900
C	-3.00288900	3.53228100	-0.41721000
C	-0.78265600	4.76427500	-0.36399300
H	0.01557600	3.54774300	-1.97606500
H	0.95851800	3.48461200	-0.47197400
C	-5.97876700	-0.41054100	0.71117500
C	-4.06986500	-1.66182700	-0.20113500
C	-2.24225500	4.80153800	-0.83056900
H	-4.02375600	3.57231400	-0.81196600
H	-3.07528600	3.47717100	0.67679300
H	-0.25555700	5.66496200	-0.69609500
H	-0.74881200	4.76589400	0.73302200
C	-6.67179200	-1.58289900	0.94402700
H	-6.42673300	0.54806000	0.96244900
C	-4.81203900	-2.84668700	0.02070500
O	-2.87711000	-1.75949900	-0.74103500
H	-2.27171400	4.89716100	-1.92440000
H	-2.75111300	5.68261800	-0.42536300
C	-6.07415000	-2.80560800	0.58663300
H	-7.66179100	-1.56187300	1.38646600
H	-4.34559700	-3.78612700	-0.25604400
H	-6.61008200	-3.73515700	0.75834800
C	0.30926200	-0.81488500	2.83138900
C	-0.92930200	-1.30491400	2.08584200
O	-1.49690700	-0.28361700	1.34196100
H	0.05657700	0.09057700	3.38879500
H	-1.63396200	-1.66845000	2.85604200
H	-0.64225000	-2.17025400	1.46938500
C	0.94462300	-1.86167500	3.72875500
H	1.21190100	-2.74872000	3.14514100
H	1.83954700	-1.46302800	4.20972300
H	0.23675400	-2.16478500	4.50666500
H	-2.25523400	2.30575800	-2.02853700
H	-0.81587700	2.20145100	0.64562700
O	1.65068900	2.03717600	1.43101300
O	1.28301500	-0.44637400	1.77902300
S	2.22753000	0.83600800	2.04683800
O	2.57857500	0.89137600	3.46830500
C	3.62358500	0.32993300	1.06809200
C	4.03725100	-1.00274700	1.05748600
C	4.33628700	1.31335800	0.38563200
C	5.17540900	-1.34604900	0.33875800
H	3.45798600	-1.75497700	1.57799000
C	5.48172400	0.95050700	-0.32072800
H	3.99070000	2.34071400	0.40553700
C	5.91477300	-0.37927600	-0.35790900
H	5.49077200	-2.38479200	0.30621200
H	6.04308400	1.71110600	-0.85591200
C	7.12453200	-0.78159300	-1.16111600
H	7.77839300	-1.44863500	-0.59062500
H	6.82387700	-1.32178400	-2.06702100
H	7.70966600	0.08805100	-1.47051300
O	-1.88191200	-0.74067300	-3.07077700
H	-1.08794600	-1.28083700	-3.18291700

H	-2.49394800	-1.33714600	-2.60204600

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2419.701127

Thermal correction to Gibbs Free Energy (a.u.): 0.566876

Imaginary frequencies: -256.98

Calculation of single point energy based on the optimized structure, Et = -3658.8234576 a.u.

C	-1.91222000	4.12156700	-0.79482500
C	-2.76472500	3.17970100	-1.39811000
C	-0.68413600	3.74666000	-0.27823600
H	-2.21836700	5.16236800	-0.73151300
C	-2.36158200	1.85914500	-1.45774000
H	-3.72812200	3.47987300	-1.79572300
C	-0.23934700	2.40124200	-0.33912200
H	-0.02362400	4.46704300	0.19252700
C	-1.11432800	1.44451100	-0.94499000
H	-3.01475600	1.10865000	-1.89171300
O	0.93430300	2.10971200	0.16823300
C	-0.80635000	0.03564800	-0.96429800
Co	1.87706600	0.54517300	-0.25486900
N	0.33271500	-0.47167100	-0.65765400
H	-1.61820700	-0.63308300	-1.24400700
N	2.85170200	-1.04014200	-0.68228000
C	0.60086000	-1.90904800	-0.58241200
C	4.13243900	-1.16904100	-0.58546200
C	1.98756800	-2.11091300	-1.20746200
C	-0.42383700	-2.83909300	-1.22551300
H	4.56624100	-2.14472300	-0.80786600
C	5.07274300	-0.14290700	-0.24159200
C	2.46478200	-3.54855600	-0.99249300
C	0.02930900	-4.29362300	-1.03145400
H	-0.51457000	-2.60959100	-2.29710900
H	-1.39763800	-2.70290700	-0.75362700
C	6.42628900	-0.51517800	-0.08974000
C	4.69542100	1.22630500	-0.09894400
C	1.44059100	-4.53260800	-1.58106000
H	3.43740500	-3.71635300	-1.46638400
H	2.58920300	-3.72167400	0.08379400
H	-0.68300000	-4.97201200	-1.51278800
H	0.00651100	-4.52453200	0.04073700
C	7.40384800	0.41599100	0.20558700
H	6.68946900	-1.56418400	-0.20362800
C	5.71354600	2.16195900	0.19496100
O	3.46655700	1.66844300	-0.25872700
H	1.42768600	-4.41916100	-2.67378400
H	1.76129100	-5.55986300	-1.37765700
C	7.03177600	1.76462100	0.34432400
H	8.43807800	0.11332700	0.32758300
H	5.42023100	3.20060600	0.30602800
H	7.78820500	2.50948700	0.57629300
H	1.89033000	-1.92534200	-2.28826300
H	0.65944300	-2.11002000	0.49373900
O	3.03372800	0.15954700	1.90656400
H	3.03108600	1.09291900	2.15435700
H	2.05279800	-0.16972200	2.06433000
C	-1.40762400	-0.09987600	3.03773700
C	-0.03710000	0.44682800	2.64362900
O	0.68797200	-0.42561600	1.86466400
H	-1.29088200	-1.12747500	3.39352100
H	0.47358600	0.68008600	3.60333100
H	-0.20360800	1.42223400	2.15216000
C	-2.14261200	0.77161400	4.04230200
H	-2.24713900	1.78842700	3.64957800
H	-3.13262100	0.36749300	4.25809200
H	-1.57361000	0.82126300	4.97574300
O	-2.63653500	-2.53690600	1.09768300
O	-2.20368800	-0.14105600	1.78479200

S	-3.28334700	-1.33146400	1.62682200
O	-4.08494200	-1.44068900	2.84693900
C	-4.24491700	-0.58650800	0.32668600
C	-4.86110600	0.64563400	0.55125300
C	-4.40279500	-1.26400400	-0.87920200
C	-5.63268100	1.20656600	-0.45875400
H	-4.72232400	1.15823200	1.49595400
C	-5.17991600	-0.68500600	-1.88326200
H	-3.92615900	-2.22753000	-1.01886300
C	-5.80004800	0.55546600	-1.69115600
H	-6.10682100	2.16997300	-0.29528300
H	-5.30808000	-1.20608400	-2.82761400
C	-6.61147400	1.19742500	-2.78776400
H	-7.55871500	1.58862900	-2.40380700
H	-6.06916500	2.04095600	-3.23135500
H	-6.83454500	0.48845900	-3.58889200
O	1.96751300	1.16193600	-2.15428800
H	1.21175600	1.76147100	-2.27335300
H	2.73697800	1.72906500	-1.89689900

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2419.773734

Thermal correction to Gibbs Free Energy (a.u.): 0.567932

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3658.8946132 a.u.

C	3.23812000	-2.50917300	-2.32367500
C	3.81315500	-1.23138000	-2.45483100
C	1.92342400	-2.66442300	-1.92446900
H	3.83518300	-3.39178600	-2.53810000
C	3.04288900	-0.12549200	-2.15617100
H	4.84515500	-1.11834700	-2.76718700
C	1.10034700	-1.54251100	-1.64263000
H	1.47407800	-3.64711300	-1.82541800
C	1.69619600	-0.24833800	-1.74829300
H	3.47383500	0.86985900	-2.21397600
O	-0.15111800	-1.75772600	-1.32458200
C	0.98954000	0.94701100	-1.38319100
Co	-1.48256900	-0.43427600	-1.00177800
N	-0.25375800	1.01378700	-1.05514500
H	1.58226200	1.85956000	-1.35490500
N	-2.83545200	0.90448100	-0.82607400
C	-0.86870600	2.23153200	-0.51640900
C	-3.97857100	0.68771700	-0.27253200
C	-2.30714200	2.25574200	-1.06368000
C	-0.14115300	3.54685700	-0.78209400
H	-4.61221400	1.53865200	-0.02969200
C	-4.50076200	-0.60608900	0.07308000
C	-3.10247800	3.40897800	-0.45219200
C	-0.94220300	4.71090900	-0.18150700
H	-0.01743700	3.69091300	-1.86483600
H	0.85114100	3.51400200	-0.32576300
C	-5.70102700	-0.66234400	0.81442000
C	-3.85923200	-1.81553800	-0.33755800
C	-2.38123200	4.74029400	-0.70844800
H	-4.11076500	3.44841600	-0.88049800
H	-3.19750100	3.22485800	0.62478700
H	-0.43769000	5.65840000	-0.39939500
H	-0.95691400	4.60230500	0.91003800
C	-6.27231800	-1.86963900	1.17227600
H	-6.17220400	0.27365700	1.10647200
C	-4.47164500	-3.03807400	0.03009500
O	-2.76390700	-1.84592100	-1.05747800
H	-2.36993800	4.94654200	-1.78776500
H	-2.94107400	5.55640400	-0.23939000
C	-5.64402700	-3.06097100	0.76639000
H	-7.18968800	-1.89862200	1.75011000
H	-3.98196400	-3.95435900	-0.28236800

H	-6.08211500	-4.01765800	1.03799000
H	-2.24310200	2.38281100	-2.15406900
H	-0.92412700	2.07333700	0.56629600
O	-2.76813500	1.32808900	2.35015000
H	-3.52224100	0.80926700	2.65486100
H	-2.25257400	0.68357300	1.80742300
C	0.22227400	-1.10952900	2.45479600
C	-0.89335300	-1.54344500	1.51289800
O	-1.40441600	-0.43335700	0.84163900
H	-0.12701900	-0.26084400	3.04922800
H	-1.67763300	-2.02515500	2.12375500
H	-0.50778400	-2.29808400	0.81900200
C	0.75747300	-2.22233000	3.33768700
H	1.12373300	-3.05131800	2.72314800
H	1.57022900	-1.85228100	3.96525200
H	-0.03811700	-2.60165000	3.98666000
O	1.59127100	1.87596000	1.45952300
O	1.31291200	-0.64253600	1.57590800
S	2.15333300	0.65611800	2.04962100
O	2.33401500	0.60547100	3.50236900
C	3.67478400	0.28334500	1.20696900
C	4.16433200	-1.02255300	1.17255000
C	4.39550200	1.34025600	0.65540100
C	5.38776500	-1.26461500	0.56013300
H	3.58013600	-1.83234800	1.59141100
C	5.62568800	1.07884400	0.05513100
H	3.98972100	2.34485700	0.69128700
C	6.13610000	-0.22256100	-0.00611900
H	5.76611600	-2.28153900	0.51026700
H	6.19379900	1.89720900	-0.37796100
C	7.44227600	-0.51322700	-0.69960500
H	8.05718600	-1.20688400	-0.11791400
H	7.26669100	-0.97926700	-1.67695300
H	8.02052100	0.39908900	-0.86635800
O	-1.75299100	-0.51440600	-3.04649500
H	-1.01284400	-1.11805400	-3.23116400
H	-2.51148800	-1.11881700	-2.92049700

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2419.767535

Thermal correction to Gibbs Free Energy (a.u.): 0.569535

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3658.8912656 a.u.

C	1.52261800	-4.46743200	0.12388500
C	2.56079500	-3.53095300	-0.04526200
C	0.19544700	-4.09201300	0.01749000
H	1.76388400	-5.50346800	0.34662500
C	2.23094900	-2.21905600	-0.32352800
H	3.59954000	-3.83025500	0.04636900
C	-0.17227900	-2.74999900	-0.26298700
H	-0.60733100	-4.80973400	0.15049300
C	0.88423400	-1.80380300	-0.43673000
H	3.00934800	-1.47658300	-0.45088200
O	-1.44603800	-2.46073700	-0.36711500
C	0.63984100	-0.40874600	-0.67201900
Co	-2.19697000	-0.71867700	-0.51594700
N	-0.51654800	0.15790200	-0.73161000
H	1.52577700	0.21213500	-0.76509500
N	-2.96603100	1.00034700	-0.77586000
C	-0.64777400	1.62480000	-0.76234600
C	-4.13210000	1.34199300	-0.34335900
C	-2.01353500	1.92867900	-1.39157800
C	0.45819400	2.39468000	-1.48276700
H	-4.42408400	2.39138200	-0.40023500
C	-5.11101300	0.43718900	0.18733100
C	-2.33511900	3.41969500	-1.30529600
C	0.15848000	3.89938600	-1.43072900

H	0.52396500	2.04847000	-2.52393300
H	1.42030800	2.22546500	-1.00046400
C	-6.28876400	0.97417400	0.75062900
C	-4.95260600	-0.98001600	0.08041000
C	-1.22722400	4.23008200	-1.99735400
H	-3.30083300	3.63420600	-1.77637500
H	-2.41049500	3.71276900	-0.25009500
H	0.93366000	4.44795000	-1.97539000
H	0.22157000	4.22956500	-0.38671600
C	-7.29899300	0.15748300	1.22208500
H	-6.38639200	2.05562900	0.81263700
C	-6.00830300	-1.79335600	0.55726200
O	-3.91050900	-1.55504700	-0.47132100
H	-1.24386400	4.00786200	-3.07305700
H	-1.43631200	5.30027300	-1.89568500
C	-7.14667000	-1.23705000	1.11491700
H	-8.19438700	0.58225500	1.66262700
H	-5.88654900	-2.86819900	0.47425800
H	-7.93405100	-1.89171300	1.47884100
H	-1.95515900	1.63827000	-2.45094700
H	-0.66299900	1.93303100	0.29145400
O	-2.20642100	-0.43543500	1.29858600
H	-2.20355500	-1.33237900	1.66121200
H	-1.13471600	0.55313600	2.01098200
C	1.96413900	0.56706900	2.87297100
C	0.53348000	0.05326500	2.81667000
O	-0.36342100	1.04644500	2.40966400
H	2.01447800	1.46435000	3.49447300
H	0.30933200	-0.31546700	3.83473700
H	0.50617000	-0.81978800	2.14810300
C	2.92262200	-0.51056000	3.35930700
H	2.93793700	-1.34580800	2.65209900
H	3.93096200	-0.11384700	3.47961800
H	2.58936400	-0.88699400	4.33107900
O	3.13015900	3.03454900	0.40240700
O	2.29354100	0.96542000	1.49307000
S	3.59581300	1.88907400	1.18178600
O	4.37320800	2.08151100	2.40467500
C	4.45815600	0.78414400	0.07932700
C	5.26535800	-0.22273800	0.60859200
C	4.24412200	0.88841300	-1.29484400
C	5.83402600	-1.15547000	-0.25370600
H	5.44054200	-0.27300000	1.67640300
C	4.81994500	-0.05529200	-2.14270500
H	3.63917000	1.69840000	-1.68523600
C	5.60591600	-1.09899200	-1.63657700
H	6.46056200	-1.94451500	0.15204300
H	4.65130700	0.01571300	-3.21324500
C	6.16404500	-2.15811300	-2.55150300
H	7.11079000	-2.55495500	-2.17498000
H	5.46377000	-2.99834400	-2.63257300
H	6.32957100	-1.77035500	-3.56016000
O	-2.37189400	-1.19627100	-2.52584900
H	-1.89120100	-2.03876800	-2.43768500
H	-3.30376700	-1.45361300	-2.37546900

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.733242

Thermal correction to Gibbs Free Energy (a.u.): 0.558612

Imaginary frequencies: -437.48

Calculation of single point energy based on the optimized structure, Et = -3658.8492566 a.u.

C	-1.50996500	4.43221200	0.18328700
C	-2.35260400	3.78991300	-0.74418100
C	-0.41304600	3.78576800	0.72369200
H	-1.72010100	5.45612500	0.48040200
C	-2.06945300	2.48838900	-1.10741700
H	-3.20916000	4.30776300	-1.16225900

C	-0.09562800	2.44985200	0.36494000
H	0.23767500	4.27710400	1.43892200
C	-0.95420100	1.80125100	-0.58020500
H	-2.71055600	1.96152500	-1.80741400
O	0.93832900	1.88500000	0.93160800
C	-0.75755500	0.43490300	-0.96622300
Co	1.81605600	0.36495400	0.26773000
N	0.28298200	-0.27343500	-0.69224100
H	-1.56980800	-0.02907300	-1.52452800
N	2.69459900	-1.14022100	-0.54118900
C	0.36302700	-1.72005100	-0.91599700
C	3.97869800	-1.25241600	-0.63742700
C	1.80520000	-2.02832000	-1.31502900
C	-0.58640300	-2.34725000	-1.93290700
H	4.37898100	-2.16036400	-1.09444400
C	4.93488100	-0.24284900	-0.29307000
C	2.05431600	-3.53360100	-1.19524700
C	-0.38051700	-3.87136200	-1.90270100
H	-0.38179000	-1.94171200	-2.93314200
H	-1.62278900	-2.13101400	-1.67684900
C	6.30469400	-0.57789000	-0.24567000
C	4.53012400	1.12155800	-0.16706600
C	1.08416900	-4.27256200	-2.13483200
H	3.08581600	-3.79097300	-1.45728100
H	1.89557800	-3.83443100	-0.15297800
H	-1.01954000	-4.34768700	-2.65395900
H	-0.71795400	-4.23585600	-0.92587900
C	7.27164800	0.38985200	-0.04984200
H	6.58886100	-1.62105300	-0.36051900
C	5.54048200	2.09696900	-0.00363800
O	3.27612300	1.50903000	-0.22876200
H	1.36192200	-4.04435900	-3.17287800
H	1.20248600	-5.35422600	-2.01061900
C	6.87500200	1.73514300	0.06426300
H	8.32073800	0.11989700	0.00260000
H	5.22903000	3.13267000	0.07979900
H	7.62796400	2.50545900	0.20621700
H	1.92733900	-1.73087900	-2.36678200
H	0.17695900	-2.15050300	0.07463200
O	2.94305400	0.03286600	2.02151900
H	2.85716100	0.86746100	2.50282000
H	2.01938100	-0.55950400	2.21376800
C	-1.40720000	-1.02005200	2.94898900
C	-0.03916900	-0.35948500	2.84682600
O	0.81384400	-0.97541900	1.93471100
H	-1.28427800	-2.10627700	2.99425600
H	0.38177400	-0.39175400	3.86988300
H	-0.20384300	0.70457400	2.61082700
C	-2.22130400	-0.48677700	4.11844300
H	-2.30981200	0.60240800	4.04643400
H	-3.21843400	-0.92605700	4.13526700
H	-1.71592600	-0.72746100	5.05869400
O	-2.63318300	-2.77994400	0.35816900
O	-2.10180100	-0.69291200	1.68292400
S	-3.24468300	-1.71404500	1.15752500
O	-4.12745900	-2.08668500	2.26391400
C	-4.06696600	-0.57023100	0.06939900
C	-4.52482900	0.64734300	0.57689700
C	-4.29007100	-0.93008700	-1.25708400
C	-5.20086700	1.51728400	-0.26878800
H	-4.33428100	0.91202000	1.61017300
C	-4.96783800	-0.04166400	-2.09296000
H	-3.94157700	-1.89010900	-1.61994400
C	-5.42847500	1.19087800	-1.61496900
H	-5.54474300	2.47324100	0.11458000
H	-5.14306900	-0.31264600	-3.12996300
C	-6.12603100	2.16778900	-2.52670000
H	-6.42917500	1.69576000	-3.46441900
H	-7.01728600	2.58828700	-2.05087500

H	-5.46557000	3.00731800	-2.77510600
O	1.72592400	2.06315700	-2.46278600
H	1.09692700	2.70092000	-2.10302200
H	2.43009600	2.03219800	-1.79061300

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.766105

Thermal correction to Gibbs Free Energy (a.u.): 0.565026

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -3658.8857235 a.u.

C	2.81657800	-3.82950100	-1.37317600
C	3.50004000	-2.82879800	-2.09329800
C	1.60347500	-3.57214100	-0.76476700
H	3.24499700	-4.82565900	-1.30150600
C	2.95122800	-1.56441900	-2.15546200
H	4.44325800	-3.04932800	-2.58155900
C	0.99176300	-2.29064700	-0.84881300
H	1.06717600	-4.34190400	-0.22018000
C	1.71216200	-1.26520900	-1.54468700
H	3.47353400	-0.76526100	-2.67391800
O	-0.17926500	-2.12828500	-0.30319600
C	1.23685500	0.08501800	-1.59075600
Co	-1.33429100	-0.66036300	-0.58255900
N	0.07641700	0.48084200	-1.18641900
H	1.93289700	0.82535600	-1.98373000
N	-2.47774600	0.81536500	-1.04628900
C	-0.33793200	1.88450700	-1.14670500
C	-3.71021900	0.88559400	-0.67697000
C	-1.76693000	1.92242000	-1.70592600
C	0.56911200	2.90106300	-1.82883200
H	-4.24557000	1.82395500	-0.82016200
C	-4.46804500	-0.19610900	-0.11247500
C	-2.36956400	3.31578500	-1.51791300
C	-0.03075100	4.30408100	-1.65281000
H	0.67170000	2.66283800	-2.89708100
H	1.56759200	2.86764700	-1.38216300
C	-5.76816300	0.07320900	0.36687400
C	-3.98296000	-1.53913600	-0.12971900
C	-1.46906800	4.37015400	-2.18057000
H	-3.37192100	3.36837400	-1.95689400
H	-2.44953700	3.50151900	-0.43998200
H	0.59573700	5.04373800	-2.16286800
H	-0.02269700	4.55725500	-0.58580400
C	-6.58545000	-0.93736700	0.83711900
H	-6.11677200	1.10295300	0.36548300
C	-4.84903500	-2.55948200	0.32628000
O	-2.78881900	-1.87613200	-0.56724200
H	-1.46402000	4.21411600	-3.26838300
H	-1.88813800	5.36721700	-2.00913000
C	-6.11342500	-2.26177000	0.80570200
H	-7.57675100	-0.71476200	1.21654100
H	-4.47775100	-3.57845000	0.30249700
H	-6.74811300	-3.06668400	1.16612700
H	-1.72145100	1.66783000	-2.77492200
H	-0.41444100	2.13718400	-0.08666600
O	-1.68815700	2.59591600	1.76203900
H	-0.74963700	2.77004000	1.92126800
H	-1.70696800	1.62263500	1.60136700
C	-0.02863800	-0.27070900	3.11222400
C	-1.15275500	-0.89657800	2.29246800
O	-1.50216300	-0.06613300	1.23590000
H	-0.32588500	0.74291800	3.39764900
H	-2.00623500	-1.04796800	2.97676000
H	-0.82421100	-1.88690300	1.94682000
C	0.40484700	-1.08655700	4.31522700
H	0.72495300	-2.08466800	4.00002500
H	1.22907600	-0.59532000	4.83540000

H	-0.43367600	-1.19691000	5.00998700
O	1.29305000	2.29743100	1.60192300
O	1.11284300	-0.16789900	2.17486100
S	1.99700700	1.17747900	2.24831500
O	2.47931100	1.37250900	3.61678600
C	3.30491300	0.64556400	1.17123300
C	3.83598500	-0.64020900	1.29604400
C	3.82727400	1.56086900	0.26150400
C	4.89838400	-1.00746500	0.48140700
H	3.40320400	-1.34138400	1.99873200
C	4.89717700	1.17362200	-0.54533500
H	3.39822400	2.55373200	0.19057100
C	5.44487700	-0.11006000	-0.44885400
H	5.29940200	-2.01369200	0.55089700
H	5.31092000	1.87986300	-1.25947600
C	6.57428500	-0.54609000	-1.34485800
H	6.95546600	0.28273900	-1.94635100
H	7.40642400	-0.95665600	-0.76378100
H	6.23841900	-1.33517900	-2.02754300
O	-1.49808500	-1.57444300	-2.92838300
H	-0.77170100	-2.21174100	-2.89939100
H	-2.21031400	-2.00432500	-2.42009100

subsequent hydrolysis

H_2O-Co^{III}-PO-OTs + H_2O = H_2O-Co^{III}-OH + $CH_3CHOTsCH_2OH$

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2419.756289

Thermal correction to Gibbs Free Energy (a.u.): 0.562744

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -3658.8783436 a.u.

C	-1.53176100	4.46465200	0.01445000
C	-2.56054100	3.50696800	-0.06225900
C	-0.20028400	4.09188500	-0.05306900
H	-1.78266200	5.51543000	0.13197500
C	-2.22160000	2.17632400	-0.21556600
H	-3.60200800	3.80489700	-0.00252400
C	0.17359100	2.73196500	-0.18657600
H	0.59659400	4.82533500	0.00793600
C	-0.87141600	1.76599400	-0.27870800
H	-2.99316100	1.42014600	-0.28025400
O	1.45073200	2.43115300	-0.24077000
C	-0.60232300	0.36966700	-0.47469300
Co	2.20989200	0.68482000	-0.07383300
N	0.55993700	-0.18764500	-0.45329300
H	-1.47023800	-0.25947900	-0.64297700
N	3.01605800	-0.93273600	-0.80695400
C	0.74120100	-1.63854600	-0.62137800
C	4.25344200	-1.26219300	-0.64305500
C	2.02287700	-1.80069100	-1.45188500
C	-0.42955900	-2.40091400	-1.23486600
H	4.58560600	-2.24336600	-0.98609000
C	5.26094300	-0.43718800	-0.04365600
C	2.39776100	-3.27325600	-1.61552600
C	-0.05719600	-3.87953100	-1.40742900
H	-0.68267600	-1.95986900	-2.20981500
H	-1.30418900	-2.33382900	-0.58767700
C	6.54813100	-0.99183300	0.14886900
C	5.01699500	0.92883100	0.30859700
C	1.22402700	-4.05190500	-2.23007000
H	3.28365600	-3.37671000	-2.25166600
H	2.64826600	-3.69194600	-0.63175200
H	-0.89026000	-4.41326000	-1.87545600
H	0.07982800	-4.32726400	-0.41504000
C	7.58230600	-0.24964500	0.68107000
H	6.70859600	-2.03025500	-0.13117400
C	6.10084400	1.67158900	0.84273600
O	3.87408800	1.54511100	0.13362100
H	1.05243400	-3.69184300	-3.25351400
H	1.48921300	-5.11136600	-2.31076500

C	7.34409000	1.09557800	1.02440100
H	8.56125300	-0.69143100	0.83076300
H	5.91208300	2.70754100	1.10311200
H	8.14971500	1.69292300	1.44240700
H	1.83186700	-1.36083400	-2.44100700
H	0.92130600	-2.02958300	0.38728300
O	2.09250600	0.19696300	1.73317800
H	2.68290800	0.76366600	2.24690600
H	0.90290900	-0.77517500	2.33259700
C	-2.27968800	-0.68386400	2.87573500
C	-0.83252400	-0.21850800	2.92984000
O	0.05120300	-1.23608600	2.55134800
H	-2.40220400	-1.59552700	3.46562700
H	-0.66399700	0.11321100	3.97079900
H	-0.73051000	0.67197000	2.29278900
C	-3.23292500	0.41392700	3.32653200
H	-3.15714800	1.27513600	2.65528900
H	-4.26244900	0.05613700	3.34621000
H	-2.96724600	0.73963800	4.33666700
O	-3.35484400	-3.06114300	0.29065300
O	-2.52861500	-1.03169000	1.46544200
S	-3.83749200	-1.89947000	1.03443000
O	-4.72865500	-2.06238800	2.18165500
C	-4.53847700	-0.74551600	-0.12811200
C	-5.38087200	0.26619700	0.33176100
C	-4.14257700	-0.80524600	-1.46440700
C	-5.80137800	1.24963700	-0.55945400
H	-5.69357200	0.28095000	1.36912300
C	-4.57016300	0.18966900	-2.34019700
H	-3.50971400	-1.61801800	-1.80178500
C	-5.38607100	1.24034100	-1.89902700
H	-6.45408600	2.04382500	-0.20872500
H	-4.25714300	0.15703300	-3.37962800
C	-5.77173800	2.35917100	-2.83118500
H	-5.82989300	2.01673100	-3.86778400
H	-6.73570600	2.79635500	-2.55723800
H	-5.02223400	3.15896400	-2.79020400
O	2.69781900	1.56649400	-2.52793100
H	2.17384700	2.24518900	-2.06807500
H	3.56727000	1.68003500	-2.11680000

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon and subsequent hydration

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3163.779196

Thermal correction to Gibbs Free Energy (a.u.): 0.785100

Imaginary frequencies: -451.69

Calculation of single point energy based on the optimized structure, Et = -5640.9813907 a.u.

C	5.64560300	-3.20559600	-3.11866600
C	4.91201200	-4.18528800	-2.42404700
C	5.61383900	-1.87712600	-2.73196500
H	6.24356600	-3.49332000	-3.97925200
C	4.16072700	-3.80003900	-1.33102100
H	4.93948300	-5.22240500	-2.73981000
C	4.83857700	-1.45144100	-1.62616800
H	6.17203500	-1.11855100	-3.27051100
C	4.10547100	-2.45158200	-0.91100500
H	3.58922500	-4.53705400	-0.77177900
O	4.85696400	-0.18090700	-1.30078400
C	3.34422500	-2.14616400	0.26400300
Co	3.51121200	0.63844300	-0.23179200
N	3.15401900	-0.96434400	0.75047100
H	2.88740500	-2.99501500	0.77847700
N	2.34807300	1.46841700	1.02352500
C	2.27701100	-0.76098400	1.91835900
C	1.66900100	2.54455800	0.82562400
C	2.35925000	0.72240600	2.28473400

C	2.61614200	-1.60018900	3.15444000
H	0.96378900	2.87610000	1.58656200
C	1.78352900	3.36182800	-0.35123500
C	1.30566900	1.06139600	3.33376100
C	1.61819400	-1.27923500	4.28053400
H	3.64164000	-1.36740300	3.46946900
H	2.59050700	-2.66903900	2.92136000
C	0.83113900	4.38505100	-0.55061300
C	2.85969800	3.18598600	-1.27738400
C	1.57120400	0.22197300	4.59442200
H	1.34777400	2.12578800	3.59021400
H	0.31019500	0.84423900	2.92954200
H	1.88011200	-1.84661800	5.17980900
H	0.61552500	-1.60461400	3.97951300
C	0.90230000	5.22199200	-1.64922200
H	0.02367100	4.49030600	0.16852100
C	2.91063700	4.06369800	-2.38668400
O	3.80954300	2.28303700	-1.14131900
H	2.52620700	0.53374400	5.03917900
H	0.79430700	0.42262900	5.33879800
C	1.95469100	5.05185000	-2.56556900
H	0.15644700	5.99440300	-1.80148600
H	3.72549700	3.93205900	-3.09091400
H	2.02186000	5.70216300	-3.43359400
O	2.21084800	0.15147300	-1.44485000
H	2.39518100	0.69803300	-2.22181900
O	5.15643500	1.19961400	0.86564600
H	5.20070700	2.08084900	0.44936100
H	5.74197800	0.64739600	0.31014900
C	-0.54560800	1.02682900	-1.28578300
C	0.21202600	-0.21698800	-1.30553200
O	-1.56389000	0.02873100	-1.22632100
H	-0.45489600	1.59781300	-0.36669100
H	0.38149800	-0.73149400	-0.37641400
H	0.29548300	-0.76492600	-2.23191400
C	-0.61882500	1.89139000	-2.52165200
H	-1.44411800	2.60344500	-2.42989700
H	0.30627300	2.46002600	-2.64785600
H	-0.78437700	1.27199900	-3.40855500
C	-1.73104200	4.47397300	2.28374300
C	-2.63544200	5.01716200	1.35089300
C	-1.48801000	3.11404900	2.33936500
H	-1.21852200	5.13208100	2.98088300
C	-3.32892700	4.14657600	0.53242400
H	-2.81517100	6.08560300	1.30841100
C	-2.11634700	2.19824300	1.44333000
H	-0.81820100	2.70266600	3.08273500
C	-3.11155100	2.75099900	0.56927000
H	-4.08134300	4.52909400	-0.15401900
O	-1.75121000	0.95421500	1.45644500
C	-3.99854400	1.91704900	-0.18908000
Co	-2.51985500	-0.45279100	0.40357500
N	-3.94490500	0.63336100	-0.25940500
H	-4.81245900	2.43464000	-0.69810100
N	-3.26423800	-1.82662500	-0.69860900
C	-4.98196100	-0.17357500	-0.90883500
C	-2.93899000	-3.07174100	-0.66405800
C	-4.23478800	-1.28695000	-1.65688300
C	-5.95702100	0.56207200	-1.82652700
H	-3.46090000	-3.76476100	-1.32476800
C	-1.92817300	-3.64992500	0.16830500
C	-5.20816900	-2.28506900	-2.28505100
C	-6.93763800	-0.43607400	-2.45880500
H	-5.39682000	1.08493000	-2.61375400
H	-6.51515900	1.31841100	-1.26486100
C	-1.77074000	-5.05396900	0.12758300
C	-1.06232800	-2.85102400	0.98311900
C	-6.19919700	-1.55395400	-3.20248500
H	-4.66640400	-3.04019700	-2.86395900

H	-5.75008600	-2.81034600	-1.48779200
H	-7.61602100	0.09036000	-3.13853300
H	-7.56073100	-0.87549200	-1.66888600
C	-0.80426100	-5.70300700	0.86947900
H	-2.44043300	-5.62556700	-0.51134800
C	-0.09021200	-3.55344200	1.74865500
O	-1.08323500	-1.55071100	1.03754100
H	-5.65234700	-1.12398100	-4.05248300
H	-6.91414400	-2.27083400	-3.61986800
C	0.03558900	-4.92841400	1.69109700
H	-0.70115500	-6.78172800	0.82889200
H	0.53665600	-2.97187200	2.40740700
H	0.79002700	-5.41752400	2.30271500
H	-5.53592500	-0.64815800	-0.08795300
H	-3.64340000	-0.80506300	-2.44777000
H	3.35833800	0.89894400	2.70768900
H	1.24363100	-0.96875800	1.60939000
Cl	-3.84293400	-1.10345600	2.12973000

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3163.794042

Thermal correction to Gibbs Free Energy (a.u.): 0.781950

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5640.9951122 a.u.

C	5.57961900	-3.53147700	-3.08882700
C	4.78088900	-4.46533300	-2.40225000
C	5.61414500	-2.20191100	-2.70867100
H	6.17644300	-3.85675900	-3.93686900
C	4.03234700	-4.03132600	-1.32581600
H	4.75700800	-5.50462200	-2.71141700
C	4.84438900	-1.72568300	-1.61722100
H	6.22286400	-1.47782300	-3.24017400
C	4.04403300	-2.68000900	-0.91125400
H	3.41149900	-4.73296100	-0.77327800
O	4.92421400	-0.45643600	-1.30432200
C	3.26935400	-2.32663800	0.24253900
Co	3.68249900	0.44973600	-0.18221100
N	3.15121800	-1.14065400	0.73727700
H	2.73471300	-3.14658600	0.72840500
N	2.58699100	1.35678100	1.07856000
C	2.23857700	-0.88657500	1.86580800
C	2.01351000	2.49346900	0.88192700
C	2.45832900	0.56623000	2.30209700
C	2.42364300	-1.79906200	3.08389700
H	1.30980800	2.86922000	1.62344600
C	2.24618600	3.32388400	-0.26680500
C	1.39562700	0.97270400	3.31870700
C	1.41223700	-1.41685000	4.17796000
H	3.45090700	-1.68517300	3.45372500
H	2.30343700	-2.85189000	2.81126700
C	1.40103100	4.43555900	-0.47177500
C	3.33847000	3.07228100	-1.15844000
C	1.51198000	0.06691200	4.55502500
H	1.52615700	2.01918700	3.61672200
H	0.40301000	0.86474800	2.86663700
H	1.56777800	-2.04456800	5.06184400
H	0.39590900	-1.61799000	3.81923900
C	1.58634100	5.28816000	-1.54468800
H	0.57965400	4.59601200	0.22118900
C	3.50850800	3.96956000	-2.24107100
O	4.19745700	2.09163300	-1.00606500
H	2.47345000	0.25676600	5.05129400
H	0.72739800	0.32269200	5.27418900
C	2.65266200	5.04310600	-2.42818800
H	0.92080900	6.13010700	-1.70194300
H	4.33341000	3.78028600	-2.92006400
H	2.81000700	5.70461000	-3.27611900

O	2.30688900	0.22469300	-1.35954500
H	2.75060300	0.37982200	-2.20592400
O	5.39917600	0.80133400	0.96116000
H	5.49880900	1.68475400	0.55828400
H	5.92599300	0.22247800	0.37849700
C	-0.38706200	0.90521800	-1.28787900
C	-0.43615700	-0.48585400	-1.70149400
O	-1.68144300	0.17942200	-1.29308400
H	-0.04025200	1.08372900	-0.27903500
H	-0.09493800	-1.24317200	-1.00979400
H	-0.42898800	-0.73724800	-2.75859300
C	-0.31455500	2.04326300	-2.25740000
H	-0.82384100	2.92531200	-1.86022700
H	0.73604900	2.29531300	-2.41485600
H	-0.76850000	1.76693800	-3.21375200
C	-1.41920100	4.55545800	2.09672100
C	-2.32994600	5.14992500	1.20102300
C	-1.27855200	3.18297300	2.17208700
H	-0.81999200	5.18522300	2.74949800
C	-3.12861600	4.32242100	0.43807000
H	-2.42799400	6.22816200	1.14332100
C	-2.02614100	2.30281900	1.33591800
H	-0.60137700	2.73432900	2.88618500
C	-3.01638500	2.91356000	0.49649200
H	-3.88228100	4.74897800	-0.22025800
O	-1.77175100	1.03077500	1.38031700
C	-3.99207400	2.13746200	-0.20743900
Co	-2.66890400	-0.32359300	0.37622600
N	-4.03374200	0.85072600	-0.26005700
H	-4.78478500	2.70451500	-0.69651400
N	-3.51961800	-1.64227700	-0.71743100
C	-5.14322100	0.11103000	-0.86834900
C	-3.29879900	-2.91194700	-0.65986600
C	-4.49295200	-1.04651400	-1.64081800
C	-6.10323100	0.90428100	-1.75328300
H	-3.89708400	-3.57327100	-1.28707000
C	-2.31389500	-3.54926900	0.15640500
C	-5.54652700	-1.98514700	-2.22923400
C	-7.16509500	-0.03331000	-2.34608300
H	-5.54130200	1.39092200	-2.56211600
H	-6.59251300	1.69413500	-1.17394200
C	-2.27106400	-4.96321500	0.15431300
C	-1.35522900	-2.80074100	0.91238300
C	-6.52434900	-1.19581900	-3.11212800
H	-5.07282600	-2.77292600	-2.82426700
H	-6.08980900	-2.47472300	-1.41058200
H	-7.83384300	0.53255300	-3.00304700
H	-7.78516400	-0.43226100	-1.53273200
C	-1.32650600	-5.66283800	0.87625900
H	-3.01110600	-5.49788100	-0.43699600
C	-0.39895500	-3.55240500	1.64660400
O	-1.27663800	-1.49954000	0.92952700
H	-5.98468000	-0.80216500	-3.98398500
H	-7.29666900	-1.86850900	-3.49936900
C	-0.38566300	-4.93356700	1.62852400
H	-1.31016000	-6.74702800	0.86858100
H	0.31170100	-3.00020600	2.24156200
H	0.36114800	-5.46381300	2.21427400
H	-5.69772400	-0.32929300	-0.02903800
H	-3.91031700	-0.59966900	-2.45930200
H	3.44843000	0.61498200	2.77762100
H	1.20982700	-0.97132700	1.48790500
Cl	-3.95771300	-0.88856200	2.12553800

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3163.803624

Thermal correction to Gibbs Free Energy (a.u.): 0.789915

No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -5641.0130897 a.u.

C	4.94802000	-3.57391000	-3.08786000
C	4.13174300	-4.43970500	-2.33776600
C	5.11096900	-2.24569300	-2.72821500
H	5.45429100	-3.94798000	-3.97344500
C	3.49949900	-3.94987700	-1.21126700
H	4.00334800	-5.47357800	-2.63835100
C	4.45726200	-1.71359300	-1.59450500
H	5.73135000	-1.57414400	-3.31207000
C	3.64903200	-2.60040200	-0.81795900
H	2.86102500	-4.59369200	-0.61130200
O	4.64536100	-0.44405700	-1.29466100
C	3.00677700	-2.17959400	0.39149600
Co	3.42135500	0.54964100	-0.23355700
N	2.96182000	-0.96418700	0.83253000
H	2.49274600	-2.95179600	0.96652300
N	2.35033500	1.53225600	0.98936500
C	2.16715600	-0.62985200	2.03110600
C	1.72818500	2.62902900	0.72278900
C	2.34066800	0.86527400	2.29562600
C	2.53300400	-1.39569000	3.30552800
H	1.03991600	3.03975700	1.45943600
C	1.88845100	3.36779400	-0.50035600
C	1.31779800	1.31757700	3.33267000
C	1.56142300	-0.97667000	4.42231700
H	3.56878000	-1.15849900	3.58215500
H	2.48619500	-2.47594200	3.14383300
C	0.98683200	4.41893400	-0.77242600
C	2.95412800	3.08244800	-1.40696100
C	1.56460800	0.54344000	4.63970100
H	1.41032200	2.39235600	3.52442900
H	0.31018900	1.11868600	2.95046900
H	1.81978200	-1.49122600	5.35360600
H	0.54691400	-1.29291400	4.15165100
C	1.11501300	5.18611200	-1.91638300
H	0.17216400	4.59760600	-0.07685300
C	3.07197200	3.89174200	-2.55759600
O	3.83817600	2.11071800	-1.22493100
H	2.53211500	0.84967400	5.06098100
H	0.79924000	0.81597800	5.37272400
C	2.16998000	4.91759900	-2.80326700
H	0.40702900	5.98023100	-2.12574300
H	3.88517400	3.67734200	-3.24299600
H	2.28116000	5.51478400	-3.70398800
O	2.04637600	0.14419500	-1.50587200
H	2.10664900	0.78970600	-2.22494700
O	5.07187600	0.98624000	0.77408000
H	5.21669100	1.84803500	0.33537000
H	5.62415000	0.35764100	0.26401600
C	-0.38768000	0.79043800	-1.27401600
C	0.65865700	-0.32231100	-1.34157000
O	-1.61769400	0.16727800	-1.19913500
H	-0.17875800	1.40761300	-0.38983000
H	0.63748500	-0.90174400	-0.42609200
H	0.45559600	-0.97855900	-2.19315500
C	-0.37018900	1.68444800	-2.52032700
H	-1.12092800	2.46949500	-2.40313900
H	0.59309400	2.18029200	-2.69372300
H	-0.62965900	1.08803000	-3.40194800
C	-1.61232500	4.68932300	1.92237700
C	-2.53635300	5.14765100	0.96578500
C	-1.37596700	3.33758800	2.10023200
H	-1.08070600	5.40606800	2.54402700
C	-3.26370800	4.20377600	0.26222600
H	-2.71296300	6.20822500	0.82426800
C	-2.02887600	2.34050000	1.31099400
H	-0.70029600	2.99754000	2.87368700
C	-3.05506200	2.81862600	0.42628200

H	-4.03996700	4.52425000	-0.42975300
O	-1.67873400	1.10173300	1.43989500
C	-3.98659700	1.92405800	-0.20317800
Co	-2.42086700	-0.36387700	0.43157400
N	-3.93002300	0.64241900	-0.16342400
H	-4.83084900	2.39904800	-0.70462300
N	-3.14834000	-1.78226000	-0.63553600
C	-4.96121900	-0.22370500	-0.73326300
C	-2.72291800	-2.99332700	-0.67484200
C	-4.19716900	-1.28984300	-1.53502600
C	-6.04023600	0.44961600	-1.57885600
H	-3.20279700	-3.69701200	-1.35638300
C	-1.66523600	-3.53445300	0.13044200
C	-5.14759100	-2.33997400	-2.11285100
C	-7.00051000	-0.60632500	-2.14313500
H	-5.57100400	1.00023100	-2.40573600
H	-6.59695700	1.17564200	-0.97663700
C	-1.41893000	-4.92066900	0.04002400
C	-0.88386300	-2.71968500	1.01313300
C	-6.24593200	-1.66836100	-2.94982500
H	-4.60155100	-3.05338900	-2.73893300
H	-5.59791300	-2.90744200	-1.28794300
H	-7.76092600	-0.12345000	-2.76641600
H	-7.53239600	-1.08965700	-1.31314400
C	-0.46549200	-5.55165100	0.81879400
H	-2.01503900	-5.50056400	-0.66155200
C	0.02713600	-3.41377700	1.86006200
O	-0.92968000	-1.42184000	1.06154800
H	-5.78950800	-1.19614000	-3.83040100
H	-6.94035700	-2.42766400	-3.32541800
C	0.23897700	-4.77759000	1.75759100
H	-0.29614500	-6.61972500	0.73703600
H	0.52700700	-2.83789900	2.62411400
H	0.94656200	-5.25720300	2.43033400
H	-5.42411700	-0.72842500	0.12464300
H	-3.67361100	-0.76891300	-2.34801600
H	3.35283800	1.01904500	2.69578200
H	1.11020200	-0.80426400	1.78369700
Cl	-3.66466800	-1.08286600	2.24464800

subsequent hydration

Cl-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-Cl + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3240.190375

Thermal correction to Gibbs Free Energy (a.u.): 0.810455

Imaginary frequencies: -470.02

Calculation of single point energy based on the optimized structure, Et = -5717.4517929 a.u.

C	5.26769800	-3.62601200	-3.00508800
C	4.44402200	-4.51529600	-2.28937900
C	5.38198700	-2.29779300	-2.63435800
H	5.82057000	-3.98476600	-3.86896400
C	3.75228000	-4.04113900	-1.19273000
H	4.35717000	-5.55256000	-2.59327900
C	4.66976800	-1.77993100	-1.52455200
H	6.01126100	-1.60863900	-3.18770900
C	3.84512700	-2.68901000	-0.78851900
H	3.11230800	-4.70676500	-0.61826300
O	4.81863900	-0.51108100	-1.22307600
C	3.12032600	-2.28925400	0.38236700
Co	3.63214300	0.46680100	-0.10139200
N	3.03956800	-1.08575200	0.84404200
H	2.58008800	-3.08110500	0.90564500
N	2.54337100	1.42906200	1.11186800
C	2.16617800	-0.77503700	1.99120700
C	1.95205400	2.53954500	0.83051500
C	2.40272900	0.69161700	2.36663600
C	2.37497700	-1.63469400	3.24258900
H	1.21953900	2.94182200	1.52702300
C	2.20849100	3.30289700	-0.35919800

C	1.33369900	1.14080000	3.35787000
C	1.34316800	-1.22324600	4.30602700
H	3.39696000	-1.47890600	3.61185100
H	2.28399600	-2.70153700	3.01820700
C	1.33581800	4.36301300	-0.68194100
C	3.35232200	3.03690000	-1.17498300
C	1.42799400	0.27585300	4.62623800
H	1.47340100	2.19520000	3.62147300
H	0.34712100	1.02704200	2.89531000
H	1.49166200	-1.81313000	5.21653800
H	0.33653700	-1.45253400	3.93620300
C	1.55938600	5.15490300	-1.79450000
H	0.46987600	4.53497400	-0.05000100
C	3.56708800	3.87432700	-2.29138000
O	4.22167400	2.07728600	-0.91957000
H	2.37782700	0.48676100	5.13655800
H	0.62709600	0.55461700	5.31797200
C	2.68764700	4.90409600	-2.59280300
H	0.87318000	5.95655600	-2.04497200
H	4.43703600	3.67567100	-2.90860000
H	2.87506400	5.52138300	-3.46735100
O	2.26758900	0.35348700	-1.34393100
H	2.75062400	0.33905800	-2.18240200
O	5.30013600	0.75271900	1.03670200
H	5.44928800	1.63928100	0.65152600
H	5.85461900	0.16200300	0.49307200
C	-0.31464400	0.52323300	-1.37997500
C	0.58645300	-0.70116000	-1.68601400
O	-1.66958200	0.13501900	-1.30719300
H	0.01671800	0.90280400	-0.41170600
H	0.85706000	-1.37155500	-0.88820200
H	1.00623400	-0.87444800	-2.66308700
C	-0.18483500	1.60594000	-2.44952800
H	-0.80626800	2.45774300	-2.16316900
H	0.84663100	1.94516900	-2.55220700
H	-0.54527900	1.22530300	-3.41181500
C	-1.30080000	4.73237400	1.95330300
C	-2.17462200	5.29501600	1.00411000
C	-1.15644600	3.36223800	2.07244300
H	-0.73422300	5.38303400	2.61482500
C	-2.95319600	4.43692000	0.25126500
H	-2.27427000	6.37036600	0.90738000
C	-1.85430900	2.45033400	1.22465500
H	-0.51845600	2.94380200	2.83821800
C	-2.84118300	3.03310800	0.36100300
H	-3.69918200	4.83790300	-0.43161800
O	-1.57646600	1.18550500	1.28781000
C	-3.85199800	2.23551000	-0.26673200
Co	-2.53303600	-0.20777500	0.37653300
N	-3.92914900	0.95271700	-0.21869300
H	-4.65234900	2.78981900	-0.75775800
N	-3.51296900	-1.57539500	-0.55502900
C	-5.09296900	0.21135200	-0.70899100
C	-3.33156400	-2.84329600	-0.43546800
C	-4.52433700	-1.00497900	-1.45130200
C	-6.08963500	0.97854100	-1.57680900
H	-3.99806600	-3.52214900	-0.96771200
C	-2.28652300	-3.46478300	0.32462400
C	-5.63189400	-1.94515200	-1.92600000
C	-7.20797300	0.03878500	-2.04970700
H	-5.56901400	1.40401300	-2.44548700
H	-6.52260500	1.81220500	-1.01420300
C	-2.27579800	-4.87848400	0.38304200
C	-1.24815200	-2.70650000	0.96517600
C	-6.64250300	-1.17768900	-2.79054800
H	-5.21153300	-2.77399500	-2.50532100
H	-6.13766300	-2.37736400	-1.05259800
H	-7.90478900	0.58614800	-2.69325700
H	-7.78353100	-0.30147100	-1.17885700

C	-1.29552400	-5.57645000	1.05806300
H	-3.07462100	-5.41573900	-0.12324700
C	-0.26436400	-3.46221200	1.66420500
O	-1.12684600	-1.41382000	0.91076300
H	-6.14683900	-0.84331300	-3.71178700
H	-7.45209200	-1.84903000	-3.09566800
C	-0.28582000	-4.84250300	1.70844800
H	-1.30750700	-6.65998300	1.09507000
H	0.49316800	-2.90832700	2.19441600
H	0.48621800	-5.36679300	2.26657900
Cl	-3.73094900	-0.65971800	2.27015100
O	-0.87393500	-1.89896800	-2.26368700
H	-0.91562000	-2.58617100	-1.58187200
H	-1.48411600	-1.10648800	-1.89365800
H	-3.97485500	-0.62190400	-2.32301900
H	-5.60059200	-0.16322500	0.18993500
H	1.12626400	-0.86379200	1.64517500
H	3.39001500	0.75280800	2.84590400

subsequent hydration

$Cl\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}Cl + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3240.230225

Thermal correction to Gibbs Free Energy (a.u.): 0.811920

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5717.5017539 a.u.

C	4.83521100	-3.74141200	-3.03356100
C	4.04165400	-4.57472800	-2.22481400
C	5.01827800	-2.40315200	-2.72555600
H	5.30757500	-4.14893100	-3.92289800
C	3.45218600	-4.04060300	-1.09597200
H	3.89608100	-5.61733800	-2.48402000
C	4.40789100	-1.82655600	-1.58857600
H	5.62183800	-1.75629000	-3.35342600
C	3.62202300	-2.67896300	-0.75314100
H	2.83261500	-4.65939500	-0.45173900
O	4.60335600	-0.54133900	-1.35719900
C	3.01244900	-2.21475300	0.45860700
Co	3.51626700	0.50293700	-0.20563500
N	3.00340100	-0.99071300	0.87410200
H	2.49178600	-2.96455500	1.05651500
N	2.49470000	1.52749400	1.01714200
C	2.23295200	-0.61462200	2.07678400
C	1.86681300	2.61145100	0.70824200
C	2.46559400	0.87644100	2.32852900
C	2.57178900	-1.38418700	3.35650900
H	1.17184400	3.04346700	1.42614700
C	2.03185900	3.30263600	-0.54047500
C	1.46114400	1.37353500	3.36298200
C	1.61643500	-0.92052600	4.46964900
H	3.61593000	-1.18348500	3.62997500
H	2.48557500	-2.46393800	3.20613100
C	1.12007900	4.32818300	-0.86945600
C	3.11999100	2.99891000	-1.41433400
C	1.67755100	0.60022700	4.67581500
H	1.59140900	2.44632800	3.54337400
H	0.44736700	1.20640800	2.98252200
H	1.85555400	-1.43738000	5.40471700
H	0.59141300	-1.20263300	4.20035000
C	1.25955700	5.05002900	-2.04148400
H	0.29251900	4.52674400	-0.19523400
C	3.24995600	3.76340400	-2.59187000
O	4.01922800	2.05880400	-1.16156600
H	2.65567400	0.87218900	5.09589700
H	0.92266300	0.90679300	5.40620700
C	2.33664200	4.76362900	-2.89576300
H	0.54427400	5.82406900	-2.29641800
H	4.07946700	3.53582700	-3.25296200
H	2.45593700	5.32620800	-3.81753700

O	2.06476700	0.30836100	-1.42485900
H	2.45019400	0.10277500	-2.28714000
O	5.20596800	0.85270700	0.77040000
H	5.35158400	1.71830200	0.33513200
H	5.75143300	0.22632100	0.25616500
C	-0.36535000	0.75336000	-1.33124900
C	0.73740300	-0.30479000	-1.25659400
O	-1.57777900	0.07867800	-1.19404700
H	-0.20717400	1.46191900	-0.51037100
H	0.71002600	-0.78687000	-0.28546000
H	0.61008400	-1.05025100	-2.04393800
C	-0.34865700	1.51595900	-2.65684600
H	-1.14146900	2.26849400	-2.64929700
H	0.60558400	2.02715400	-2.81958600
H	-0.53574200	0.82564300	-3.48688900
C	-1.35050500	4.80162800	1.91326400
C	-2.24186900	5.29573200	0.94362700
C	-1.16777300	3.44165700	2.09202400
H	-0.80121500	5.49686100	2.54358100
C	-2.99729100	4.38135900	0.23128200
H	-2.37453700	6.36235400	0.80019200
C	-1.84321400	2.47211500	1.28869100
H	-0.51713900	3.07595600	2.87482500
C	-2.84530000	2.98899300	0.39955100
H	-3.75436200	4.73127300	-0.46747400
O	-1.52684800	1.22167200	1.40142700
C	-3.82308600	2.13322100	-0.21181300
Co	-2.40953500	-0.23746700	0.49853100
N	-3.84699900	0.85173300	-0.13288200
H	-4.64044000	2.64295700	-0.72315800
N	-3.30558700	-1.66041700	-0.41897900
C	-4.96454500	0.04591400	-0.63032900
C	-2.99793400	-2.90597800	-0.36520500
C	-4.32256300	-1.15023800	-1.34351200
C	-5.98282300	0.75064800	-1.52454300
H	-3.57972300	-3.61448600	-0.95425400
C	-1.92539400	-3.47008000	0.40372500
C	-5.37106300	-2.15133200	-1.82769500
C	-7.04572400	-0.25112400	-1.99773500
H	-5.46988700	1.18535100	-2.39326400
H	-6.46443200	1.57185600	-0.98300700
C	-1.78594300	-4.87590200	0.39442500
C	-1.00751700	-2.65955000	1.15124000
C	-6.40770600	-1.44610300	-2.71418700
H	-4.89371600	-2.95363000	-2.39884300
H	-5.86503400	-2.60795800	-0.95980600
H	-7.76153800	0.25110200	-2.65742200
H	-7.61404800	-0.60857200	-1.12887500
C	-0.80341600	-5.52321400	1.11963900
H	-2.48825900	-5.45369500	-0.20256000
C	-0.05178900	-3.36428100	1.93909500
O	-0.97445400	-1.36219500	1.13433200
H	-5.91577200	-1.09755100	-3.63204900
H	-7.17777400	-2.16126200	-3.02275900
C	0.05378000	-4.74294200	1.91634100
H	-0.71664700	-6.60393400	1.10041600
H	0.57161800	-2.77778400	2.59668800
H	0.79969800	-5.22880500	2.54150500
Cl	-3.63065200	-0.70314500	2.39191900
O	-1.36281600	-2.07756700	-2.83260600
H	-1.13009100	-2.76261700	-2.19327900
H	-1.51850900	-1.28728600	-2.25580700
H	-3.76873600	-0.76305300	-2.20885800
H	-5.46622500	-0.33780700	0.26794300
H	1.16791800	-0.74829700	1.83823300
H	3.48349000	0.99359200	2.72637100

subsequent hydration

Cl-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-Cl + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3240.256182
Thermal correction to Gibbs Free Energy (a.u.): 0.813705
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = - 5717.515657 a.u.

C	7.14078900	-2.74876000	-1.53179200
C	6.69433600	-3.67197800	-0.56749800
C	6.57988000	-1.48848600	-1.62956900
H	7.93692300	-3.02979400	-2.21591900
C	5.67855500	-3.29503700	0.28855500
H	7.13768200	-4.65943300	-0.50108600
C	5.53400600	-1.07640300	-0.76453500
H	6.91705000	-0.77556900	-2.37472500
C	5.08324300	-2.01401600	0.21611800
H	5.31218900	-3.98924500	1.04140000
O	5.05917700	0.13827300	-0.90158400
C	4.00970200	-1.72518500	1.12516500
Co	3.56011500	0.86994000	0.01497100
N	3.33832800	-0.62639300	1.18077900
H	3.72980900	-2.53543700	1.79805000
N	2.17890500	1.67058900	1.04254900
C	2.12089700	-0.49465600	1.99818600
C	1.39638100	2.59551000	0.60832700
C	2.00243300	0.99333300	2.33753500
C	2.01684900	-1.39235500	3.22806200
H	0.54843500	2.88956300	1.21740200
C	1.55453900	3.29072700	-0.63842300
C	0.70766500	1.27976100	3.09175200
C	0.71608700	-1.08472700	3.98493300
H	2.88984700	-1.23455000	3.87708100
H	2.01339700	-2.44369600	2.92286800
C	0.52278000	4.16082700	-1.05174800
C	2.74596400	3.16268600	-1.41852400
C	0.61813100	0.40056300	4.34718900
H	0.66393900	2.33797300	3.37606800
H	-0.14464300	1.06177600	2.43922500
H	0.66348700	-1.70195000	4.88822800
H	-0.14212300	-1.35640500	3.35908100
C	0.61726900	4.87252900	-2.23437100
H	-0.36112600	4.24983100	-0.42453400
C	2.81556200	3.90411900	-2.62359600
O	3.77583200	2.43784300	-1.05416400
H	1.42229200	0.66801800	5.04757800
H	-0.32982600	0.59957800	4.85679900
C	1.77711700	4.73132200	-3.01881600
H	-0.18445200	5.53230300	-2.54846300
H	3.71350200	3.79912700	-3.22322600
H	1.86294100	5.28102800	-3.95231300
O	2.37658900	0.13231400	-1.18836900
H	2.96344900	-0.05942600	-1.93464700
O	5.00687000	1.80171300	1.16284200
H	4.90975300	2.62147300	0.63988500
H	5.74194700	1.33911800	0.72069200
C	-1.46144000	1.42249200	-1.91932900
C	-0.36860400	1.14888900	-2.96564100
O	-2.11498100	0.13535700	-1.70074600
H	-0.99229700	1.70801000	-0.97756000
H	0.36271100	1.96416600	-2.95321900
H	-0.81673200	1.09682600	-3.96569400
C	-2.48427500	2.44945800	-2.35516500
H	-3.22676300	2.62580100	-1.57444400
H	-1.97878400	3.39695100	-2.56487100
H	-2.99594600	2.11868300	-3.26492900
C	-2.74181800	4.41710000	2.09602100
C	-4.10004900	4.53340400	1.74675700
C	-2.03590500	3.25248800	1.86184000
H	-2.23498900	5.25313500	2.57075900
C	-4.72309300	3.43531900	1.19224100
H	-4.64589400	5.45142900	1.93305800

C	-2.62932700	2.11871900	1.23454000
H	-1.00868300	3.17320500	2.18367500
C	-4.02652100	2.23090200	0.93609800
H	-5.78118800	3.47619700	0.94330000
O	-1.89068700	1.08343900	0.95970500
C	-4.78308200	1.12854800	0.43440200
Co	-2.47436300	-0.56589700	0.16480700
N	-4.31785700	-0.03012800	0.11601500
H	-5.85651300	1.29743200	0.34818900
N	-3.10469100	-2.17077000	-0.66676400
C	-5.21437900	-1.14869300	-0.21297700
C	-2.49933300	-3.31289100	-0.62437900
C	-4.44879900	-2.00662800	-1.22387000
C	-6.60686700	-0.78487500	-0.73157400
H	-3.04040500	-4.20120300	-0.94980300
C	-1.12878200	-3.50291000	-0.28767900
C	-5.21644100	-3.28062000	-1.57419500
C	-7.38385700	-2.05652000	-1.10354400
H	-6.50724100	-0.13367200	-1.61041700
H	-7.16981200	-0.22860700	0.02449300
C	-0.59793000	-4.81507500	-0.35209800
C	-0.25641200	-2.38029800	-0.12887100
C	-6.61103200	-2.92076800	-2.10543600
H	-4.67018600	-3.86157400	-2.32475000
H	-5.31205200	-3.90838600	-0.67844500
H	-8.36325000	-1.78377200	-1.51034400
H	-7.57293300	-2.63991700	-0.19275600
C	0.76107000	-5.04252900	-0.32952800
H	-1.29320800	-5.64601500	-0.44873000
C	1.13722200	-2.63540900	-0.26078700
O	-0.65676300	-1.15172500	0.06333700
H	-6.50653700	-2.37554500	-3.05295900
H	-7.16967700	-3.83543100	-2.32955300
C	1.62381000	-3.92612800	-0.33402000
H	1.15794200	-6.05093500	-0.37512800
H	1.78958800	-1.77931600	-0.37630200
H	2.69684900	-4.07585500	-0.42819700
Cl	-2.80098900	-1.45780500	2.20629900
O	0.22296800	-0.10967500	-2.70052900
H	0.91819400	0.00834500	-1.99682300
H	-1.36776300	-0.47800900	-1.93046400
H	-4.32744800	-1.40377900	-2.13565800
H	-5.30769000	-1.73809000	0.70958200
H	1.27691800	-0.71382800	1.33395900
H	2.86796500	1.27710000	2.95295100

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon and subsequent hydration

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3163.775756

Thermal correction to Gibbs Free Energy (a.u.): 0.782596

Imaginary frequencies: -357.98

Calculation of single point energy based on the optimized structure, Et = -5640.9778283 a.u.

C	-7.07662000	1.88270500	3.11512700
C	-6.76968500	0.84797000	4.02066700
C	-6.48991900	1.93783900	1.86499900
H	-7.78453800	2.65497100	3.40370000
C	-5.86647700	-0.12121900	3.63581500
H	-7.23426500	0.81596100	4.99999300
C	-5.55420700	0.95732700	1.44438100
H	-6.72121600	2.73456100	1.16588000
C	-5.24450100	-0.09449500	2.36467100
H	-5.61314900	-0.93159600	4.31567900
O	-5.05280200	1.05479500	0.24045100
C	-4.32462100	-1.14625100	2.04922600
Co	-3.59235300	0.03833200	-0.44348500
N	-3.65245100	-1.26954700	0.95365400

H	-4.18937700	-1.90060700	2.82697400
N	-2.25986400	-1.05327000	-1.21738900
C	-2.62990200	-2.31628800	0.78734600
C	-1.33466500	-0.62884700	-2.01327600
C	-2.36168100	-2.42846600	-0.72063100
C	-2.95157900	-3.69238200	1.37583500
H	-0.53304700	-1.30527000	-2.29261100
C	-1.30652000	0.68458900	-2.59589600
C	-1.19489600	-3.36817200	-1.00757600
C	-1.79509400	-4.66473700	1.08977700
H	-3.88298300	-4.06302000	0.92841300
H	-3.11491100	-3.62912000	2.45634100
C	-0.14991900	1.08705200	-3.30208500
C	-2.45420100	1.53638700	-2.55441800
C	-1.47740800	-4.75199100	-0.40804200
H	-1.02167900	-3.45476600	-2.08252900
H	-0.27241500	-2.96456300	-0.57695900
H	-2.03947900	-5.65530300	1.48767800
H	-0.90092500	-4.32168400	1.62783800
C	-0.12376300	2.28175800	-3.99826600
H	0.73730700	0.46809900	-3.23476200
C	-2.39985500	2.74848200	-3.27865100
O	-3.56526800	1.23332200	-1.91396800
H	-2.32663000	-5.21034700	-0.93254100
H	-0.61105300	-5.39841000	-0.57886300
C	-1.26403100	3.10370100	-3.98975700
H	0.77443000	2.58708900	-4.52325100
H	-3.27718300	3.38642500	-3.25610700
H	-1.25258100	4.04430900	-4.53423900
O	-2.36364000	1.01726300	0.52394600
H	-2.70155000	1.91769500	0.41308900
O	-5.06761200	-0.85546100	-1.57850000
H	-4.85419600	-0.26809100	-2.33102600
H	-5.78596900	-0.38150600	-1.12006900
C	-0.19520300	1.25821900	0.66643300
C	0.20629500	-0.07118700	1.11334600
O	1.47952700	0.54148000	1.14220900
H	-0.06027800	1.45147300	-0.38904100
H	0.11354600	-0.86594400	0.37390000
H	-0.14217200	-0.37999400	2.10579800
C	-0.34814000	2.41751500	1.59561800
H	-1.01393600	3.16459700	1.15806200
H	-0.73992800	2.10375900	2.56569900
H	0.62347800	2.89975200	1.72916000
C	1.45380800	5.28721700	-0.78842500
C	2.25304000	5.68255600	0.30437900
C	1.46435200	3.98825600	-1.25466400
H	0.81318100	6.01825600	-1.27548100
C	3.05580100	4.73642200	0.90701700
H	2.23885400	6.70745000	0.65897100
C	2.27555400	2.98583400	-0.64813300
H	0.84803700	3.68366300	-2.09156300
C	3.08142900	3.39103500	0.46745400
H	3.68610100	5.01274500	1.74986900
O	2.22448000	1.78144300	-1.12677700
C	3.93240100	2.47484900	1.16518100
Co	2.83914300	0.24373900	-0.21168300
N	3.97712600	1.20144100	0.97532400
H	4.58498500	2.91287700	1.92165700
N	3.35884700	-1.31233900	0.78460600
Cl	4.60674000	-0.03696800	-1.61611600
C	4.87177200	0.30092700	1.70264500
C	3.18937600	-2.53380500	0.41169700
C	4.01827800	-0.93816400	2.04023300
C	5.54983000	0.86593900	2.94992000
H	3.55855400	-3.33613500	1.05236100
C	2.58408700	-2.94467300	-0.82331900
C	4.85101700	-2.02145400	2.72491500
C	6.38893300	-0.22155800	3.63542700

H	4.78588400	1.24036800	3.64488900
H	6.19045600	1.71283000	2.68281100
C	2.63094800	-4.31307900	-1.16627600
C	1.96463900	-2.00411300	-1.70929500
C	5.54194400	-1.45343600	3.97306500
H	4.21986900	-2.87038000	3.00986000
H	5.60341400	-2.39677100	2.01902400
H	6.85104700	0.18240000	4.54243700
H	7.20910200	-0.51710400	2.96814100
C	2.14062200	-4.77651000	-2.37365300
H	3.08574200	-5.00607700	-0.46151400
C	1.53810800	-2.49855400	-2.97316700
O	1.72007600	-0.76521600	-1.39452700
H	4.77890500	-1.17681700	4.71324300
H	6.16235400	-2.22787900	4.43647500
C	1.61620900	-3.84352300	-3.28769200
H	2.19412500	-5.82961000	-2.62718100
H	1.15517400	-1.78231600	-3.69183200
H	1.27328100	-4.18155300	-4.26210100
H	5.63389100	-0.01779700	0.97971800
H	3.22244700	-0.60076000	2.71873600
H	-3.27285300	-2.84290600	-1.17532600
H	-1.71279400	-1.93747200	1.25635100

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3163.796505

Thermal correction to Gibbs Free Energy (a.u.): 0.780116

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5640.9985203 a.u.

C	7.49822600	-1.64135300	3.35024800
C	7.54601300	-0.29131900	3.75122000
C	6.64760300	-2.05998400	2.34531100
H	8.13858700	-2.36932400	3.84118100
C	6.72005700	0.61506400	3.11913800
H	8.21543000	0.02601600	4.54320800
C	5.78953100	-1.14842100	1.67364000
H	6.60478700	-3.09907800	2.03605800
C	5.83827700	0.22246000	2.08412000
H	6.73292200	1.66220300	3.41358600
O	5.02829100	-1.60733200	0.71605600
C	4.99823200	1.22844900	1.50340500
Co	3.75785400	-0.61492100	-0.29542600
N	4.15578500	1.05153900	0.54237200
H	5.08583900	2.22367100	1.94226600
N	2.60982300	0.38807400	-1.43560800
C	3.21034400	2.09445200	0.12089600
C	1.61686400	-0.09779800	-2.10394700
C	2.91593900	1.82021600	-1.36279400
C	3.63928500	3.54506800	0.34772400
H	0.94532500	0.58616300	-2.62284100
C	1.32068300	-1.49676800	-2.22640500
C	1.86843800	2.77878700	-1.91967700
C	2.58460400	4.50784900	-0.21878900
H	4.60628000	3.71506600	-0.14423700
H	3.77936300	3.74421700	1.41520000
C	0.10628900	-1.87226400	-2.84410900
C	2.23036400	-2.49969100	-1.76542500
C	2.30645400	4.23146100	-1.69961500
H	1.70571900	2.59506800	-2.98469500
H	0.90602700	2.61017600	-1.42331200
H	2.91502300	5.54207900	-0.07520700
H	1.65090600	4.39325600	0.34860700
C	-0.23638600	-3.20227700	-3.00087100
H	-0.59227700	-1.09505200	-3.13486500
C	1.85230400	-3.85370500	-1.94016900
O	3.39801500	-2.23541400	-1.22947000
H	3.21358200	4.43534300	-2.28462200

H	1.52588000	4.89963700	-2.07402100
C	0.65140700	-4.19197600	-2.54180400
H	-1.17842400	-3.47335900	-3.46373600
H	2.54062900	-4.61308500	-1.58419100
H	0.39019200	-5.24102000	-2.65294100
O	2.40609500	-0.86444400	0.90538900
H	2.63892100	-1.71862000	1.29690200
O	5.30786900	-0.51695800	-1.70406100
H	4.90472300	-1.27361600	-2.17379000
H	5.95344800	-0.94438600	-1.11408600
C	-0.73799800	-1.58296600	0.41108800
C	-0.29711900	-0.25479800	0.80831500
O	-1.70603400	-0.63021500	1.00005200
H	-0.94609900	-1.73488300	-0.63944100
H	-0.14932400	0.49473100	0.04166100
H	0.24250800	-0.12328400	1.73762700
C	-0.46415400	-2.81201100	1.21999600
H	0.44738900	-3.27766600	0.83264000
H	-0.31799600	-2.57030400	2.27634500
H	-1.28631100	-3.52629700	1.12084300
C	-3.96057700	-5.11167300	-0.39938900
C	-4.66529200	-5.10608000	0.82306900
C	-3.51997600	-3.93945200	-0.97874800
H	-3.75987500	-6.05708600	-0.89675300
C	-4.90841200	-3.89634300	1.43809900
H	-5.00982200	-6.03410100	1.26593700
C	-3.74873100	-2.67515300	-0.36409400
H	-2.97350200	-3.93883500	-1.91469300
C	-4.45995800	-2.67445000	0.88105600
H	-5.45292600	-3.86240100	2.37935600
O	-3.29526200	-1.61602400	-0.95973000
C	-4.75275400	-1.46577100	1.58747300
Co	-3.16000000	0.09172800	-0.17809700
N	-4.33204700	-0.28775300	1.26981800
H	-5.38626600	-1.57099100	2.46906300
N	-2.90165900	1.79078600	0.66503800
Cl	-4.89821700	0.90267100	-1.35215600
C	-4.69844800	0.92998900	1.99629300
C	-2.41230900	2.83658500	0.08968400
C	-3.41794700	1.78732600	2.03817500
C	-5.28751000	0.74530400	3.39414000
H	-2.38681300	3.77650900	0.64286000
C	-1.90947900	2.88224900	-1.25273500
C	-3.67788700	3.15009000	2.67879800
C	-5.54767100	2.11216300	4.04374100
H	-4.58954800	0.16377300	4.01156400
H	-6.22374400	0.18029000	3.34082400
C	-1.57926400	4.14256500	-1.79956300
C	-1.74327100	1.69325900	-2.03817400
C	-4.27777700	2.96960400	4.08093300
H	-2.74891400	3.72670700	2.74713400
H	-4.37060700	3.71955100	2.04554300
H	-5.94127200	1.97240900	5.05598200
H	-6.32408800	2.63878600	3.47354500
C	-1.12660300	4.27251100	-3.09869100
H	-1.70707100	5.02510500	-1.17646400
C	-1.29264100	1.86195700	-3.37691700
O	-1.93325800	0.49116000	-1.58322400
H	-3.53449100	2.48983700	4.73181500
H	-4.49243900	3.94973700	4.51953900
C	-0.99702100	3.11224800	-3.88719000
H	-0.89574700	5.24874600	-3.51077500
H	-1.21726000	0.97329100	-3.99399800
H	-0.66698700	3.20016700	-4.91892800
H	-5.41983400	1.45810900	1.35894000
H	-2.68470300	1.23674000	2.64519300
H	3.86045100	1.96163800	-1.90806200
H	2.28062200	1.89800700	0.67380900

PO-Co^{III}-Cl + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3163.800229
Thermal correction to Gibbs Free Energy (a.u.): 0.787884
No imaginary frequency
Calculation of single point energy based on the optimized structure, Ep = -5641.0118886 a.u.

C	7.53664700	-1.49345400	2.61930700
C	7.56051900	-0.23832700	3.25726500
C	6.56341500	-1.80553400	1.68768000
H	8.29480200	-2.23282900	2.86152300
C	6.58465400	0.68452600	2.94179700
H	8.32781500	-0.00548300	3.98702300
C	5.55452300	-0.87292300	1.33969300
H	6.53893000	-2.77222600	1.19608600
C	5.57615600	0.40025100	1.99004600
H	6.57433800	1.65683800	3.42843800
O	4.66514900	-1.23072400	0.44087900
C	4.57314100	1.39983600	1.75498200
Co	3.36560900	-0.09781000	-0.36140800
N	3.62350700	1.33039900	0.88482100
H	4.62954900	2.28637700	2.38753600
N	2.09037600	1.02330400	-1.18482700
C	2.56095700	2.34102700	0.76852600
C	1.16907300	0.62003000	-2.00144200
C	2.21554400	2.41688300	-0.72555200
C	2.85481900	3.72634600	1.34270600
H	0.40561300	1.32566900	-2.30340400
C	1.08703600	-0.69074700	-2.57775700
C	1.01325000	3.32594500	-0.96436900
C	1.65155600	4.65277800	1.09990500
H	3.75344400	4.13813000	0.86341200
H	3.05574000	3.66441500	2.41755400
C	-0.04946000	-1.01460900	-3.35471900
C	2.15588600	-1.62412300	-2.45876200
C	1.27874400	4.72087800	-0.38512100
H	0.78960600	3.40575000	-2.02998400
H	0.12784000	2.88955000	-0.49226700
H	1.87525500	5.65213600	1.48733500
H	0.79269100	4.27696800	1.67099600
C	-0.09887400	-2.19193100	-4.07653200
H	-0.90059900	-0.34527600	-3.32439300
C	2.08335800	-2.81959300	-3.20142500
O	3.23334600	-1.40952100	-1.71395500
H	2.09308900	5.20278500	-0.94336000
H	0.38687200	5.33845300	-0.52825600
C	0.98510700	-3.08239000	-4.00892000
H	-0.98005200	-2.43895400	-4.65706500
H	2.90845200	-3.51903300	-3.11985000
H	0.95277600	-4.01211900	-4.57019700
O	2.14170500	-0.92146800	0.87076100
H	2.64356500	-1.73212800	1.06050800
O	4.78926100	0.56204300	-1.59356200
H	4.56584200	-0.16096400	-2.22493200
H	5.61051300	0.26773000	-1.16636100
C	0.68536300	-1.26418900	0.79069600
C	-0.12143500	-0.00710500	1.16451200
O	-1.45381300	-0.29123400	1.35369300
H	0.46562300	-1.56635300	-0.23085200
H	0.03643800	0.75563900	0.39086900
H	0.31881500	0.37871100	2.10815500
C	0.46933100	-2.40371800	1.76519600
H	0.96012000	-3.32407600	1.43146000
H	0.83448200	-2.12633300	2.76100900
H	-0.60168800	-2.59296800	1.83195500
C	-1.00180300	-5.21902700	-0.65344400
C	-1.89767000	-5.68337500	0.33064700
C	-1.00191000	-3.89986300	-1.05954700
H	-0.29378000	-5.91067300	-1.10429800

C	-2.78266800	-4.78190300	0.88717100
H	-1.89309000	-6.72302100	0.64014900
C	-1.90103100	-2.94285400	-0.50197800
H	-0.31112800	-3.54848700	-1.81359000
C	-2.80424100	-3.42050100	0.50574900
H	-3.48554700	-5.11037100	1.65039200
O	-1.82761300	-1.71787800	-0.91232800
C	-3.73702100	-2.55809700	1.17001500
Co	-2.68776700	-0.23470200	-0.09505000
N	-3.82142400	-1.28360700	1.01990600
H	-4.42301400	-3.04983800	1.86141300
N	-3.46360600	1.27856600	0.79177400
Cl	-4.40468100	-0.22549200	-1.65612800
C	-4.82183200	-0.46001800	1.70167100
C	-3.43215500	2.49773300	0.38702100
C	-4.10349500	0.86076800	2.03978900
C	-5.47701700	-1.07058400	2.94089300
H	-3.92227100	3.26787800	0.98514400
C	-2.83199500	2.94270200	-0.84182700
C	-5.04872500	1.86566400	2.69628700
C	-6.42588300	-0.05926000	3.59883000
H	-4.69613400	-1.36885000	3.65343700
H	-6.03495100	-1.97363500	2.67251100
C	-3.04737100	4.27653600	-1.24219600
C	-2.05669700	2.06060200	-1.66304400
C	-5.70322900	1.24826500	3.93992300
H	-4.50615800	2.77482700	2.97842700
H	-5.82397300	2.15937300	1.97602700
H	-6.86801700	-0.49699100	4.50049900
H	-7.25604900	0.15474600	2.91264300
C	-2.57857900	4.76144200	-2.45159600
H	-3.61768000	4.92610500	-0.58106500
C	-1.66306500	2.56361800	-2.93607900
O	-1.65085300	0.88437500	-1.28316700
H	-4.92932300	1.04866800	4.69346300
H	-6.40080900	1.96478300	4.38725300
C	-1.90565600	3.87450600	-3.30973900
H	-2.76259400	5.78844700	-2.74799000
H	-1.17349600	1.88188800	-3.62338800
H	-1.57930200	4.21673200	-4.28869700
H	-5.58918500	-0.23040400	0.95016100
H	-3.28087100	0.61278700	2.72311100
H	3.09393300	2.83239500	-1.24107300
H	1.68839300	1.92179600	1.28325000

subsequent hydration

$Cl\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}Cl + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3240.186174

Thermal correction to Gibbs Free Energy (a.u.): 0.807091

Imaginary frequencies: -421.20

Calculation of single point energy based on the optimized structure, Et = -5717.4519243 a.u.

C	-5.71198700	3.32268400	-2.66941500
C	-4.76476100	4.27895100	-2.25587200
C	-5.69765300	2.03629500	-2.16258200
H	-6.46928100	3.59690100	-3.39881700
C	-3.80485100	3.90784300	-1.33660400
C	-4.72798100	1.63286600	-1.20970200
C	-3.75611000	2.59794400	-0.80313400
H	-3.05649900	4.61931200	-1.00470100
O	-4.79028700	0.40461800	-0.75059700
C	-2.71453900	2.29790000	0.13696900
Co	-3.62273900	-0.39198000	0.50130200
N	-2.56062900	1.17578700	0.76138000
H	-1.99618000	3.09857500	0.31474700
N	-2.52913200	-1.18437100	1.84639800
C	-1.41068300	0.93563300	1.65072600
C	-2.33442300	-2.45613200	1.96806200
C	-1.83337500	-0.16542600	2.63780000

C	-0.88001600	2.14771100	2.41680800
H	-1.58634300	-2.80703400	2.67976500
C	-3.02029400	-3.46002900	1.20818200
C	-0.63597100	-0.63374100	3.46424100
C	0.31982100	1.70800500	3.26688300
H	-1.67645400	2.56615700	3.04714800
H	-0.55700300	2.92681200	1.72385400
C	-2.53229500	-4.78566000	1.24297100
C	-4.20105300	-3.14756300	0.46155200
C	-0.03127400	0.56010700	4.21916600
H	-0.93659900	-1.40805700	4.17843500
H	0.11395900	-1.07185600	2.79308600
H	0.71205900	2.56196600	3.83007000
H	1.10989600	1.37928900	2.58438000
C	-3.16539400	-5.79863800	0.54924100
H	-1.63259200	-4.99262300	1.81736100
C	-4.84126200	-4.20978100	-0.22018500
O	-4.72950000	-1.94938900	0.41922300
H	-0.75036200	0.91155800	4.97094800
H	0.86056000	0.23504000	4.76633500
C	-4.33194800	-5.49597100	-0.17943700
H	-4.84061900	-6.28560900	-0.72566400
O	-2.53288800	-1.03762100	-0.83815700
H	-2.84883200	-0.62683100	-1.65542700
O	-5.02945200	0.14036400	1.90189200
H	-5.42314700	-0.75472700	1.85227500
H	-5.58753800	0.66872500	1.30500000
H	-0.58827400	0.54503500	1.03828500
H	-2.59042600	0.26542000	3.30864300
C	-0.51984600	-1.71692000	-0.80297900
C	0.17382400	-0.40371300	-1.12984200
O	1.14792400	-0.10941200	-0.14840500
H	-0.84726100	-1.89354600	0.20030900
H	-0.59966200	0.36959900	-1.16458600
H	0.62122700	-0.47602600	-2.12463000
C	-0.78982600	-2.72987800	-1.87000500
H	0.15543800	-3.04993000	-2.31770500
H	-1.33436900	-3.59082800	-1.48268900
H	-1.37669400	-2.27051800	-2.66973800
O	1.18547300	-2.54654000	0.01707900
H	1.41672900	-1.54089400	0.12369000
H	1.80036000	-2.86677600	-0.66180600
H	-5.73688800	-3.97297500	-0.78426500
H	-2.77508200	-6.81018000	0.56830800
H	-6.42588100	1.29542700	-2.47530000
H	-4.78797700	5.28682000	-2.65557200
C	-0.53163700	4.35883100	-2.21532000
C	-0.34192600	5.02063300	-0.98127300
C	0.19011600	3.23070000	-2.54047700
H	-1.26208000	4.74232300	-2.92213300
C	0.58894300	4.51103800	-0.09714900
H	-0.89454600	5.92439700	-0.74629300
C	1.16723200	2.68245600	-1.65367700
H	0.05662100	2.72855400	-3.49263400
C	1.33737100	3.34706200	-0.39015700
H	0.77034000	5.01261300	0.85174700
O	1.83393100	1.65020200	-2.04280800
C	2.30655000	2.90782700	0.56943300
Co	2.83656700	0.52011700	-0.89665300
N	2.99070600	1.81943600	0.49153100
H	2.46608600	3.56667200	1.42484300
N	3.78202900	-0.64075500	0.30471700
C	4.04169000	1.45175100	1.44368400
C	4.31740000	-1.77013800	-0.01657300
C	3.88402300	-0.06519700	1.65050800
C	4.08447200	2.21294900	2.76785700
H	4.90201800	-2.30478100	0.73288400
C	4.18707200	-2.42713000	-1.28337100
C	4.98276000	-0.62377000	2.55476400

C	5.19509400	1.64673400	3.66378600
H	3.11988000	2.12909400	3.28261100
H	4.26352800	3.27771300	2.58487300
C	4.84003900	-3.67276700	-1.45531000
C	3.37865200	-1.89139500	-2.34392800
C	5.01841200	0.14071400	3.88568700
H	4.81829500	-1.68929100	2.74738300
H	5.94924500	-0.52905600	2.04327900
H	5.20388900	2.17507400	4.62314000
H	6.16892800	1.83153300	3.19225500
C	4.71793000	-4.40239800	-2.61832100
H	5.44742500	-4.05043600	-0.63555700
C	3.26485600	-2.67664600	-3.52926000
O	2.71836500	-0.78231200	-2.27764600
H	4.08067800	-0.03799800	4.43043400
H	5.82502500	-0.25018900	4.51483300
C	3.91429000	-3.88696600	-3.65791700
H	5.22608100	-5.35346900	-2.73350200
H	2.65779900	-2.26910000	-4.33065100
H	3.80714100	-4.45103800	-4.58078300
Cl	4.83303100	1.25616600	-1.73066700
H	4.98674400	1.60237300	0.90662400
H	2.90776900	-0.22835500	2.13290100

subsequent hydration

$Cl\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}Cl + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3240.230941

Thermal correction to Gibbs Free Energy (a.u.): 0.811598

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5717.5018756 a.u.

C	5.81861800	-2.87784000	-2.59057100
C	4.93310000	-3.91810900	-2.25623900
C	5.69552600	-1.62228500	-2.02016800
H	6.61376400	-3.05770900	-3.30865700
C	3.92523100	-3.66765000	-1.34659400
C	4.67186900	-1.34306600	-1.08479700
C	3.76880500	-2.39478900	-0.74935600
H	3.21917200	-4.44544600	-1.07643500
O	4.61915600	-0.12475300	-0.57640900
C	2.69158200	-2.22629700	0.18527900
Co	3.35251200	0.52128300	0.66634900
N	2.42439300	-1.14721700	0.84449900
H	2.04510200	-3.09363100	0.32256700
N	2.13132900	1.16338500	1.96844100
C	1.25169700	-1.05023000	1.73975200
C	1.74373400	2.39050300	2.05851500
C	1.58054800	0.05505500	2.75361800
C	0.86738100	-2.33348400	2.47405400
H	0.91232600	2.63094500	2.71489300
C	2.33188900	3.46568400	1.30595300
C	0.38974300	0.37163800	3.65539600
C	-0.33614400	-2.04216200	3.38075000
H	1.72207800	-2.69213000	3.06437900
H	0.59949600	-3.11639100	1.76247700
C	1.65513400	4.70137500	1.24777800
C	3.59373600	3.30707300	0.65651100
C	-0.05560000	-0.91053000	4.37533000
H	0.67047700	1.13322700	4.39232400
H	-0.42737300	0.78344000	3.05411700
H	-0.63350700	-2.95331500	3.91128700
H	-1.17597800	-1.75379000	2.74142600
C	2.19272200	5.77570100	0.56218200
H	0.68823300	4.78294100	1.73642100
C	4.13190400	4.42390400	-0.01684500
O	4.28313700	2.18008200	0.68682000
H	0.72679000	-1.22666500	5.07853400
H	-0.94958900	-0.70263300	4.97309500
C	3.44318100	5.62680800	-0.06262300

H	3.87624500	6.46514100	-0.60097300
O	2.35228700	1.14068700	-0.84717200
H	2.75780300	0.73709500	-1.62930500
O	4.68955600	0.09083200	2.06862200
H	5.00297100	1.02038400	2.10726400
H	5.34563000	-0.35724400	1.50400700
H	0.39814100	-0.72126700	1.12501700
H	2.41174700	-0.30926300	3.37428700
C	0.91525200	1.41691100	-1.05033500
C	0.11033400	0.12184200	-1.25908100
O	-0.91774900	-0.00738300	-0.30359700
H	0.61318800	1.89088600	-0.12253300
H	0.80674600	-0.72910500	-1.20090800
H	-0.30310800	0.12045800	-2.27054500
C	0.81755200	2.41371100	-2.19029400
H	-0.22934800	2.69727900	-2.32708000
H	1.40919700	3.30882500	-1.97982400
H	1.15712300	1.96969400	-3.13409200
O	-1.12639100	2.08478400	1.29978300
H	-1.09405600	1.28017600	0.69913300
H	-1.64841000	2.71530600	0.78768900
H	5.09248000	4.30282700	-0.50574100
H	1.65932200	6.71817300	0.50685900
H	6.37503300	-0.81564000	-2.27413500
H	5.03831200	-4.89810500	-2.70828100
C	0.70199400	-4.48747800	-2.24820500
C	0.50413900	-5.10814600	-0.99444200
C	-0.02157600	-3.37401300	-2.61832000
H	1.43739600	-4.89411600	-2.93743100
C	-0.44582200	-4.57698700	-0.14128000
H	1.05691900	-6.00195800	-0.72395500
C	-1.00770000	-2.79610200	-1.75885300
H	0.11939800	-2.90338500	-3.58547200
C	-1.19238100	-3.42550100	-0.47838100
H	-0.64397900	-5.05501600	0.81662100
O	-1.66784700	-1.77522100	-2.18140400
C	-2.19247200	-2.96781200	0.44376200
Co	-2.61531400	-0.56645600	-1.04990600
N	-2.85781800	-1.87239900	0.32849600
H	-2.39764600	-3.62116800	1.29418600
N	-3.53999600	0.61281600	0.14309500
C	-3.94976900	-1.48636400	1.22529500
C	-3.92291100	1.80983700	-0.14613500
C	-3.75434200	0.01861300	1.46708600
C	-4.10920900	-2.26886200	2.52722600
H	-4.48497100	2.37214400	0.60101800
C	-3.65020800	2.50653800	-1.36553500
C	-4.89711400	0.60103200	2.29984200
C	-5.26789600	-1.68163300	3.34570800
H	-3.18674000	-2.22186700	3.11852400
H	-4.30324000	-3.32512600	2.31174500
C	-4.12384400	3.83613100	-1.48729900
C	-2.90200800	1.91210300	-2.43914100
C	-5.05987800	-0.18601000	3.60810100
H	-4.70516100	1.65376200	2.53126300
H	-5.82484200	0.55614200	1.71522500
H	-5.36839900	-2.22471900	4.29170900
H	-6.20698300	-1.82637400	2.79620400
C	-3.88127700	4.59617800	-2.61146200
H	-4.69372800	4.25413900	-0.65960300
C	-2.67530600	2.72437800	-3.59161000
O	-2.40427900	0.72234300	-2.42549000
H	-4.16054500	-0.04885900	4.22489900
H	-5.89872400	0.22098100	4.18284100
C	-3.14628000	4.01818100	-3.66916100
H	-4.25134700	5.61291400	-2.68659000
H	-2.12170200	2.27179100	-4.40743400
H	-2.95162700	4.60077000	-4.56611000
Cl	-4.64214500	-1.19522200	-1.93502800

H	-4.86175000	-1.59649000	0.62536100
H	-2.81211700	0.15627300	2.01786600

subsequent hydration

$Cl\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}Cl + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3240.241600

Thermal correction to Gibbs Free Energy (a.u.): 0.808943

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5717.5075315 a.u.

C	6.36289500	-2.60140100	-3.01516700
C	5.53078900	-3.69689000	-2.71125100
C	6.21590500	-1.38968300	-2.36685500
H	7.13331800	-2.70731900	-3.77422200
C	4.55394500	-3.53857300	-1.74934200
C	5.22024500	-1.20022900	-1.37271500
C	4.37225100	-2.31071400	-1.06996200
H	3.89553000	-4.36470100	-1.49584000
O	5.14977400	-0.03470300	-0.78155500
C	3.31792300	-2.23344800	-0.10220500
Co	3.81883100	0.52358300	0.44875200
N	3.02720100	-1.20438900	0.62165800
H	2.70579100	-3.12898800	-0.00264000
N	2.58243700	1.07106300	1.78934600
C	1.82711900	-1.19062200	1.47199900
C	2.21955700	2.29105200	2.00018100
C	2.03023500	-0.07734000	2.51116900
C	1.47527700	-2.50319600	2.17559200
H	1.42616500	2.48410200	2.72366200
C	2.78460500	3.44204800	1.35843300
C	0.74887000	0.15239000	3.31313600
C	0.20649600	-2.30633000	3.01699700
H	2.31804200	-2.81120400	2.80836300
H	1.30009600	-3.29641300	1.44558600
C	2.15698900	4.69345700	1.54896700
C	3.98059100	3.35166700	0.57769500
C	0.34262100	-1.15214500	4.01572800
H	0.89366100	0.94048100	4.05972300
H	-0.04833600	0.47626200	2.63147800
H	-0.04457400	-3.23637900	3.53918800
H	-0.62295300	-2.08552700	2.33828000
C	2.65489200	5.84394700	0.96939500
H	1.25466100	4.73374600	2.15502900
C	4.47497600	4.54993200	0.00476800
O	4.65337600	2.24258100	0.40710100
H	1.09792100	-1.40514500	4.77147400
H	-0.60070400	-1.00370800	4.55359200
C	3.82629500	5.75719900	0.19275500
H	4.22881800	6.65403100	-0.27040300
O	2.62116200	0.96454500	-0.85441600
H	3.18309500	1.05881900	-1.63689900
O	5.31788000	0.18678700	1.87674600
H	5.54705800	1.13624200	1.83378800
H	5.92383900	-0.21629600	1.23011600
H	0.98642100	-0.90261600	0.82830000
H	2.82491700	-0.41488100	3.19255100
C	-0.42175200	2.70573200	-0.25791500
C	-0.41430500	1.20607100	-0.53729600
O	-1.46524900	0.60465000	0.28650300
H	-0.01642000	2.90005800	0.73926700
H	0.54457600	0.75314800	-0.30125200
H	-0.64854500	1.00650800	-1.58218900
C	0.38605200	3.46593500	-1.29476400
H	-0.06051100	3.34350600	-2.28823900
H	0.42689200	4.52992300	-1.05097600
H	1.40183400	3.06041800	-1.31566300
O	-1.79519300	3.13541300	-0.16302000
H	-2.02232600	1.38934400	0.49339000
H	-2.21537300	2.90886100	-1.01038300

H	5.37863500	4.48021000	-0.59132900
H	2.15580100	6.79625200	1.11100000
H	6.85297500	-0.54259300	-2.59868400
H	5.65554700	-4.64389100	-3.22490000
C	1.13076700	-3.46483800	-2.52596600
C	0.90659700	-4.44293200	-1.52875700
C	0.34099400	-2.33988400	-2.61413800
H	1.94413200	-3.59906100	-3.23275500
C	-0.11158700	-4.24093600	-0.62181800
H	1.51624500	-5.33945500	-1.48822600
C	-0.74097800	-2.11672200	-1.71090600
H	0.50414100	-1.59184100	-3.38166300
C	-0.93436500	-3.08732700	-0.67170600
H	-0.30693600	-4.97743500	0.15496600
O	-1.47123700	-1.06428500	-1.88195100
C	-1.95426000	-2.94642900	0.31715400
Co	-2.85899300	-0.46327100	-0.75863600
N	-2.74629700	-1.93393900	0.45375500
H	-2.05139100	-3.77750900	1.01712700
N	-4.17683600	0.23332500	0.44280800
C	-3.85154900	-1.92544100	1.42328600
C	-5.09997100	1.07954600	0.11578200
C	-4.12009300	-0.44465200	1.74159900
C	-3.64382900	-2.73321900	2.70637900
H	-5.88109100	1.30654100	0.84184200
C	-5.18829100	1.76050500	-1.13737000
C	-5.32813200	-0.27844200	2.66174800
C	-4.85095200	-2.56684500	3.64082400
H	-2.73180100	-2.38870400	3.20968600
H	-3.50591400	-3.79442200	2.47752200
C	-6.32894900	2.55678800	-1.39211400
C	-4.13126900	1.69753600	-2.10108600
C	-5.12583800	-1.09086700	3.94866200
H	-5.47900400	0.77823600	2.90758500
H	-6.23021100	-0.62543600	2.14128500
H	-4.67984300	-3.12371300	4.56806400
H	-5.73671500	-3.00919400	3.16651900
C	-6.45877900	3.27208900	-2.56455700
H	-7.11416800	2.59099800	-0.64025700
C	-4.28675600	2.45080900	-3.29248500
O	-3.01203900	1.05034000	-1.91030900
H	-4.27942700	-0.67274500	4.51035800
H	-6.00716600	-0.99253900	4.59079800
C	-5.41938300	3.21126400	-3.51441600
H	-7.34239300	3.87179600	-2.75318400
H	-3.48737900	2.39510900	-4.02348300
H	-5.51008300	3.76902600	-4.44257200
Cl	-4.42126800	-1.61599600	-1.88568200
H	-4.73244200	-2.30435600	0.88749400
H	-3.22690800	-0.06223000	2.25869400

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon and subsequent hydration

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.017906

Thermal correction to Gibbs Free Energy (a.u.): 0.830352

Imaginary frequencies: -449.05

Calculation of single point energy based on the optimized structure, Et = -5409.3212641 a.u.

C	5.91839600	-3.16431000	-3.23937600
C	5.13055700	-4.18738300	-2.67949900
C	5.88982100	-1.87781200	-2.73079400
H	6.55711000	-3.38428900	-4.09057700
C	4.32699800	-3.88794600	-1.59715000
H	5.15687700	-5.19110300	-3.08921500
C	5.06380500	-1.53942800	-1.63123200
H	6.49082600	-1.08537400	-3.16420300
C	4.27195300	-2.58338000	-1.05516600

H	3.71340000	-4.66139100	-1.14126100
O	5.09243100	-0.30708400	-1.18433100
C	3.44685900	-2.37068300	0.09720900
Co	3.72651600	0.44569000	-0.09236900
N	3.24835100	-1.23765200	0.68498400
H	2.94760100	-3.25486600	0.50063600
N	2.54187900	1.18834600	1.19511000
C	2.30562700	-1.12054900	1.81432500
C	1.93056500	2.31769600	1.09655000
C	2.45067500	0.30255100	2.35888000
C	2.51400900	-2.12200900	2.95549400
H	1.20746600	2.60002900	1.86017100
C	2.14481200	3.25764400	0.03047400
C	1.37084000	0.58693100	3.39674600
C	1.49239800	-1.85820200	4.07567400
H	3.53805100	-2.01445400	3.33613800
H	2.41443100	-3.15102900	2.59570500
C	1.25736300	4.34976400	-0.08740500
C	3.25342900	3.12796800	-0.86381900
C	1.53021800	-0.40384200	4.56085000
H	1.46517900	1.61078400	3.77494200
H	0.38405200	0.48306600	2.93063100
H	1.67808400	-2.54251800	4.91037800
H	0.48434900	-2.07578700	3.70528000
C	1.42515400	5.30129700	-1.07677400
H	0.42384100	4.41963900	0.60556300
C	3.40416500	4.12249000	-1.85953300
O	4.14784200	2.16271400	-0.79368200
H	2.48420900	-0.21031600	5.07021800
H	0.73837700	-0.23634300	5.29788200
C	2.51052300	5.17764800	-1.96155000
H	0.72874000	6.12755600	-1.16829900
H	4.24437300	4.02600000	-2.53923000
H	2.65334100	5.91831000	-2.74378300
O	2.47085200	0.16029800	-1.41248100
H	2.72587300	0.77542900	-2.11479000
O	5.33617200	0.80101100	1.13907000
H	5.43443500	1.72128900	0.83009900
H	5.92577100	0.29189800	0.54776300
C	-0.22407500	1.22326100	-1.31562600
C	0.45102200	-0.06532200	-1.40981800
O	-1.31270000	0.30693800	-1.40059000
H	-0.14954900	1.70368800	-0.34511400
H	0.52153100	-0.67784600	-0.52834300
H	0.54526600	-0.53307800	-2.37840200
C	-0.16009300	2.19722700	-2.46838900
H	-0.94367100	2.95292800	-2.36150900
H	0.80499600	2.71088000	-2.48493500
H	-0.30499200	1.67252300	-3.41784900
C	-1.35044800	4.34483700	2.70811200
C	-2.15135200	5.07566000	1.81059000
C	-1.19523600	2.97648300	2.57898900
H	-0.84777600	4.86036100	3.52254100
C	-2.83682600	4.37983600	0.83240800
H	-2.26102300	6.14969400	1.91125700
C	-1.81402100	2.24328900	1.52269500
H	-0.60347400	2.41870400	3.29277700
C	-2.71211100	2.98108100	0.68175300
H	-3.51170200	4.90828700	0.16241900
O	-1.52376700	0.98884700	1.36858500
C	-3.58536400	2.33186500	-0.25504400
Co	-2.38382300	-0.22786600	0.14757300
N	-3.64844200	1.06677600	-0.48238100
H	-4.28425400	2.98836800	-0.77483200
N	-3.21448100	-1.41464000	-1.08006300
C	-4.67067900	0.47457400	-1.35685100
C	-3.16068300	-2.69641400	-1.01471100
C	-3.98760000	-0.68922100	-2.09088400
C	-5.36780700	1.40918100	-2.34329500

H	-3.77267700	-3.28128400	-1.70069200
C	-2.33495600	-3.44407400	-0.11010000
C	-5.00786900	-1.49936100	-2.88757000
C	-6.38652700	0.61405100	-3.17487600
H	-4.62323200	1.87831000	-3.00168300
H	-5.88881300	2.21414600	-1.81406400
C	-2.48988200	-4.84684200	-0.08149700
C	-1.30987500	-2.81430900	0.66819500
C	-5.73661200	-0.58160700	-3.88046200
H	-4.51445100	-2.30967200	-3.43545100
H	-5.72267900	-1.95332000	-2.19050400
H	-6.86389800	1.27403600	-3.90732500
H	-7.18051600	0.25187600	-2.50929600
C	-1.67612200	-5.65546500	0.68895600
H	-3.27650800	-5.28740000	-0.68996200
C	-0.47482300	-3.67743200	1.42853500
O	-1.07782700	-1.53178700	0.68324300
H	-5.01694600	-0.21551500	-4.62538400
H	-6.49228800	-1.15389900	-4.42914500
C	-0.65559600	-5.04849400	1.44197700
H	-1.81544400	-6.73079000	0.70655500
H	0.30600000	-3.22138400	2.01897300
H	0.00201700	-5.66344400	2.05165000
C	-4.88652900	-1.90124200	3.06831100
H	-4.26695700	-2.78893300	3.23420200
H	-5.93961700	-2.17544000	3.14526600
H	-4.62409300	-1.17046600	3.83728800
C	-4.58582700	-1.34701100	1.67791500
O	-3.41395600	-0.78656400	1.63185900
O	-5.40205700	-1.47812900	0.76022600
H	-5.39890700	0.01775400	-0.67749400
H	-3.24399000	-0.25791100	-2.77417100
H	3.43673700	0.36619800	2.84059100
H	1.28507900	-1.22287700	1.42005300

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.032844

Thermal correction to Gibbs Free Energy (a.u.): 0.827638

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5409.3351704 a.u.

C	5.95654100	-3.42763500	-3.16282300
C	5.14191000	-4.41579800	-2.57823800
C	5.94704000	-2.12512000	-2.69803300
H	6.60145100	-3.68881500	-3.99769400
C	4.33105700	-4.06259300	-1.51781100
H	5.15335600	-5.43358900	-2.95266400
C	5.11514400	-1.73175000	-1.61882000
H	6.56860800	-1.35910800	-3.14990700
C	4.29578700	-2.74036300	-1.01844200
H	3.69616500	-4.80804600	-1.04424600
O	5.15970600	-0.48522800	-1.22075600
C	3.44961800	-2.47288500	0.10821300
Co	3.87918500	0.33121600	-0.07405200
N	3.28312500	-1.32563400	0.67444300
H	2.90257500	-3.33125000	0.50528400
N	2.74629700	1.14270600	1.21708900
C	2.30062000	-1.15239300	1.76006200
C	2.20650500	2.30742500	1.10632600
C	2.53980700	0.24211300	2.35057000
C	2.36946500	-2.19075100	2.88627500
H	1.47908100	2.62944100	1.84986500
C	2.50541400	3.23659000	0.05288400
C	1.44471000	0.58835500	3.35439600
C	1.32670800	-1.86750800	3.97021300
H	3.38095600	-2.17718700	3.31273600
H	2.20370600	-3.20177400	2.50116700
C	1.69481600	4.38489200	-0.07693800

C	3.62723200	3.04136400	-0.81560000
C	1.47302100	-0.43573600	4.49900500
H	1.59869500	1.59534900	3.75820800
H	0.47129900	0.56506500	2.85065200
H	1.41359400	-2.58792400	4.79070900
H	0.32030600	-1.98196700	3.55178900
C	1.94331600	5.32934600	-1.05609700
H	0.85103700	4.50254300	0.59725600
C	3.86057900	4.03063000	-1.80196500
O	4.45838900	2.02997100	-0.72168100
H	2.42009300	-0.33895300	5.04710700
H	0.67075700	-0.21671800	5.21103500
C	3.03775400	5.13949900	-1.91851200
H	1.30453600	6.20014400	-1.15715100
H	4.70749100	3.88398900	-2.46419100
H	3.24398200	5.87305000	-2.69357200
O	2.55242200	0.23880500	-1.32251900
H	3.03953900	0.43687000	-2.13548900
O	5.54853400	0.54874500	1.17200200
H	5.67066000	1.46545900	0.85958500
H	6.09534900	0.02398500	0.55749700
C	-0.10705500	1.05047500	-1.34457300
C	-0.22562000	-0.29836500	-1.87111800
O	-1.44193000	0.41251600	-1.45301400
H	0.20874400	1.12773900	-0.31326000
H	0.03525200	-1.12981800	-1.23111600
H	-0.19292100	-0.46416800	-2.94466100
C	0.07194000	2.25375900	-2.21694500
H	-0.40643700	3.13020700	-1.77219800
H	1.14060400	2.45799300	-2.30940000
H	-0.35144900	2.07882600	-3.21053900
C	-1.12803500	4.43297700	2.47450700
C	-1.94979900	5.17449600	1.60371000
C	-1.04724400	3.05590900	2.38566000
H	-0.54940200	4.94896100	3.23651100
C	-2.72689900	4.48462600	0.69437800
H	-1.99970400	6.25535700	1.67312500
C	-1.77014800	2.32136200	1.40025900
H	-0.43758800	2.49219800	3.07888000
C	-2.67933700	3.07551400	0.58713700
H	-3.41493100	5.02417400	0.04718600
O	-1.56797300	1.04393800	1.29306300
C	-3.63414800	2.44143300	-0.27316100
Co	-2.52443500	-0.15624800	0.14247200
N	-3.76649400	1.17285300	-0.45763900
H	-4.33094200	3.11298200	-0.77578500
N	-3.42206200	-1.31812900	-1.06437100
C	-4.85160800	0.60300000	-1.26851900
C	-3.40889900	-2.60280000	-0.98708500
C	-4.23599300	-0.57823500	-2.03444900
C	-5.58244000	1.54910100	-2.21872100
H	-4.07029800	-3.17248700	-1.63869000
C	-2.57054900	-3.36621200	-0.11130500
C	-5.31657400	-1.36883200	-2.76915700
C	-6.66459700	0.77330100	-2.98605900
H	-4.86774100	1.99903800	-2.92202900
H	-6.05289200	2.36752800	-1.66351400
C	-2.76445600	-4.76465100	-0.05838000
C	-1.49517900	-2.75868300	0.61387700
C	-6.08210400	-0.43867000	-3.72221500
H	-4.87273700	-2.19123700	-3.34094000
H	-5.99876800	-1.80475500	-2.02948600
H	-7.16848800	1.44078500	-3.69324900
H	-7.42688300	0.43121900	-2.27449500
C	-1.93839300	-5.58447700	0.68488700
H	-3.59023400	-5.18985500	-0.62415800
C	-0.64583900	-3.63360400	1.34104100
O	-1.22715400	-1.48123500	0.60114100
H	-5.40001700	-0.09116400	-4.51014600

H	-6.88006200	-0.99728000	-4.22269500
C	-0.86475900	-4.99808900	1.37996300
H	-2.10579100	-6.65516800	0.72386500
H	0.17811200	-3.19039300	1.87947600
H	-0.19479800	-5.62546200	1.96258600
C	-4.93731800	-1.71645800	3.16897000
H	-4.33091000	-2.61212700	3.33974900
H	-5.99242500	-1.96515700	3.28992800
H	-4.63235300	-0.96863900	3.90479900
C	-4.67756900	-1.21271200	1.75265100
O	-3.49732100	-0.66877000	1.65593500
O	-5.52006700	-1.36044300	0.86422800
H	-5.55354600	0.16497400	-0.55093200
H	-3.52892300	-0.16241100	-2.76619300
H	3.50763900	0.21014200	2.87145100
H	1.29894900	-1.15674400	1.30662400

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.041119

Thermal correction to Gibbs Free Energy (a.u.): 0.835274

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5409.3521946 a.u.

C	4.87103200	-3.75517800	-3.25183700
C	3.93566100	-4.59029300	-2.61447300
C	5.14536500	-2.48441700	-2.77281700
H	5.38355700	-4.10674000	-4.14299500
C	3.29606500	-4.12932800	-1.48015600
H	3.72283400	-5.57866600	-3.00624500
C	4.48937800	-1.98061800	-1.62741800
H	5.85929200	-1.83551700	-3.26874500
C	3.55513000	-2.83788500	-0.96712700
H	2.57002700	-4.75255700	-0.96406000
O	4.79015600	-0.76693800	-1.21155700
C	2.89313300	-2.45104100	0.24325000
Co	3.62298000	0.26105500	-0.11994200
N	2.95292900	-1.27895500	0.78745100
H	2.27183800	-3.20847000	0.72583300
N	2.59999500	1.24727700	1.14020500
C	2.14179100	-0.96169500	1.97915400
C	2.10886900	2.42325500	0.94807300
C	2.46002900	0.47808500	2.38038900
C	2.37110900	-1.86591800	3.19391300
H	1.43063900	2.84205900	1.68958600
C	2.40773200	3.24167800	-0.19534700
C	1.44592000	0.95002800	3.41682100
C	1.40827100	-1.43750400	4.31477800
H	3.41465200	-1.76835300	3.52101500
H	2.21529500	-2.91764800	2.93856000
C	1.63660200	4.40441800	-0.40811400
C	3.48311400	2.92073900	-1.07819600
C	1.55954400	0.05095200	4.66047700
H	1.63879800	1.99009600	3.70198400
H	0.44069400	0.88943400	2.98461100
H	1.57776600	-2.05100600	5.20577800
H	0.37738000	-1.62210900	3.99000400
C	1.90380000	5.24854700	-1.47093400
H	0.81040900	4.61060100	0.26605900
C	3.74473300	3.80822000	-2.14419700
O	4.25041400	1.84645400	-0.94788700
H	2.53616800	0.21749700	5.13546600
H	0.79886400	0.34269500	5.39121800
C	2.96925200	4.94371000	-2.33319000
H	1.29494600	6.13025300	-1.63697500
H	4.56520800	3.56613800	-2.81145900
H	3.18897000	5.60044000	-3.17026100
O	2.28502300	0.11341600	-1.48369600
H	2.45326400	0.80718800	-2.13778400

O	5.25729900	0.43063700	0.99159300
H	5.51135400	1.30635300	0.63840000
H	5.76596700	-0.20752700	0.44903000
C	-0.07524600	1.00431800	-1.29832200
C	0.84715900	-0.20837000	-1.42776800
O	-1.36715700	0.52018200	-1.33127700
H	0.15578100	1.51348300	-0.35253400
H	0.71154700	-0.86571000	-0.57645800
H	0.62329200	-0.75451700	-2.34911200
C	0.10248900	1.99733500	-2.45408900
H	-0.56355600	2.84859700	-2.29452800
H	1.12128700	2.39470500	-2.54278600
H	-0.17649100	1.51378700	-3.39676900
C	-1.04685000	4.71896600	2.21766200
C	-1.86336000	5.35778800	1.26742600
C	-0.96136700	3.33869600	2.27588900
H	-0.47894700	5.31532200	2.92808200
C	-2.64212600	4.56453000	0.44250500
H	-1.92117400	6.43963500	1.21877300
C	-1.66894000	2.49318600	1.36606300
H	-0.36693700	2.86013400	3.04279800
C	-2.58834700	3.15610600	0.48426500
H	-3.33867700	5.02784900	-0.25334900
O	-1.46004900	1.21646800	1.39138400
C	-3.56045700	2.42860700	-0.28537600
Co	-2.29912100	-0.06960900	0.21434200
N	-3.65631800	1.15043000	-0.36074100
H	-4.29705300	3.04073600	-0.80723600
N	-3.11367100	-1.30456000	-0.98911100
C	-4.71359100	0.47773000	-1.11882200
C	-2.91135000	-2.56952000	-1.02235000
C	-4.00488300	-0.62019700	-1.93070700
C	-5.58813600	1.35213400	-2.01374500
H	-3.46517200	-3.17196800	-1.74193300
C	-2.02014200	-3.29290800	-0.15551100
C	-5.02103800	-1.49771900	-2.66034200
C	-6.61217800	0.47757500	-2.75154000
H	-4.96212500	1.88742000	-2.74172900
H	-6.11263700	2.10669900	-1.41692700
C	-2.04651200	-4.70056000	-0.21817100
C	-1.11742800	-2.62638400	0.73463400
C	-5.92445000	-0.63381800	-3.55187800
H	-4.51328300	-2.24566900	-3.27933300
H	-5.61991500	-2.03186900	-1.91286000
H	-7.22584800	1.09922600	-3.41292200
H	-7.29177800	0.02697500	-2.01696900
C	-1.24526400	-5.48909500	0.58989600
H	-2.73206200	-5.16736900	-0.92208200
C	-0.34960100	-3.46629100	1.58921300
O	-0.94026900	-1.33681800	0.77832500
H	-5.31845800	-0.18249900	-4.34961700
H	-6.67165500	-1.26562400	-4.04450700
C	-0.40364700	-4.84849800	1.51322300
H	-1.28695800	-6.57115900	0.52997500
H	0.26063700	-2.98614000	2.33841900
H	0.20281500	-5.44159700	2.19408400
C	-4.53127800	-2.00596400	3.23010200
H	-3.77627600	-2.78752000	3.36864100
H	-5.52639400	-2.44196300	3.33176900
H	-4.36514000	-1.25088400	4.00300200
C	-4.35318500	-1.39539600	1.83991500
O	-3.28108600	-0.67468700	1.75916900
O	-5.17939700	-1.63347700	0.94801600
H	-5.32437600	-0.04691600	-0.37492200
H	-3.34202400	-0.12232900	-2.65058400
H	3.46363400	0.48598300	2.82870400
H	1.08501300	-0.99930100	1.67661800

subsequent hydration

$OAc\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OAc + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3008.428921
Thermal correction to Gibbs Free Energy (a.u.): 0.855462
Imaginary frequencies: -467.48
Calculation of single point energy based on the optimized structure, Et = -5485.7914541 a.u.

C	5.58982400	-3.50823900	-3.12337500
C	4.72248100	-4.44729000	-2.53378900
C	5.68218500	-2.21531600	-2.63990200
H	6.19512900	-3.79962300	-3.97736900
C	3.96369100	-4.05821100	-1.44832700
H	4.65421700	-5.45653200	-2.92434400
C	4.90343200	-1.78413100	-1.53747600
H	6.34565700	-1.48754300	-3.09513500
C	4.03144800	-2.74347900	-0.93079000
H	3.29038500	-4.76552600	-0.96988000
O	5.03839800	-0.54534600	-1.12562400
C	3.23434300	-2.43506000	0.22066000
Co	3.80941100	0.34634600	0.02110500
N	3.13419100	-1.27558500	0.78044200
H	2.65826900	-3.26314200	0.64043300
N	2.67778000	1.21363900	1.26501800
C	2.19782900	-1.05168300	1.89856700
C	2.12218000	2.35962400	1.06425600
C	2.45727300	0.36128100	2.43203800
C	2.30494900	-2.04142900	3.06378000
H	1.36424200	2.71215600	1.76042700
C	2.45147400	3.22501500	-0.03381800
C	1.35789700	0.74882500	3.41516200
C	1.24552000	-1.69314100	4.12290200
H	3.31458600	-1.97583900	3.48970100
H	2.17426300	-3.07419400	2.72662200
C	1.61392300	4.32892800	-0.29770700
C	3.63070600	3.01079000	-0.81353900
C	1.36916600	-0.23783900	4.59441000
H	1.51955200	1.76679900	3.78675000
H	0.39085900	0.71788500	2.90079700
H	1.33497900	-2.37607200	4.97433700
H	0.24811300	-1.84582000	3.69429200
C	1.90676200	5.21438800	-1.32006300
H	0.72177600	4.46248100	0.30636200
C	3.91525400	3.94198300	-1.83585100
O	4.47085500	2.01435900	-0.60393500
H	2.30357100	-0.11461800	5.15893900
H	0.55083700	0.00236600	5.28053000
C	3.06911700	5.01349700	-2.08273500
H	1.24809600	6.05066300	-1.52752900
H	4.81163000	3.78250900	-2.42600700
H	3.31039900	5.70419300	-2.88629800
O	2.51586900	0.38289400	-1.29792200
H	3.04243100	0.40411200	-2.10960400
O	5.41838900	0.48725600	1.26832200
H	5.59729600	1.40452800	0.97928100
H	5.99408900	-0.05641000	0.69843500
C	-0.04624300	0.69247100	-1.46218600
C	0.80803100	-0.56286100	-1.77973500
O	-1.42066100	0.37589400	-1.48449000
H	0.24816800	1.00596800	-0.45910700
H	0.99952600	-1.27999900	-1.00048000
H	1.26641000	-0.71689900	-2.74287700
C	0.20176200	1.81753100	-2.46497600
H	-0.39263400	2.68581000	-2.17103800
H	1.25287700	2.10773700	-2.48970900
H	-0.11811800	1.50439800	-3.46522700
C	-1.04490800	4.60627000	2.35669300
C	-1.83060300	5.31786700	1.43196400
C	-0.95483100	3.22647200	2.30886600
H	-0.50300400	5.14512900	3.12990000
C	-2.58173300	4.59298800	0.52535000

H	-1.88677200	6.40019500	1.46498800
C	-1.62096300	2.45802800	1.30732100
H	-0.38311900	2.69024000	3.05347700
C	-2.52665500	3.18347000	0.46446600
H	-3.26199400	5.10716800	-0.15024900
O	-1.38661800	1.18554800	1.21790700
C	-3.50683400	2.51598300	-0.34172400
Co	-2.37946500	-0.05886900	0.13194800
N	-3.66365900	1.24335800	-0.44062900
H	-4.21368900	3.16875600	-0.85464700
N	-3.38920900	-1.27613000	-0.93785900
C	-4.79631800	0.65032300	-1.16307100
C	-3.41584100	-2.54943400	-0.77517500
C	-4.23627000	-0.57220900	-1.90356700
C	-5.56772200	1.56002700	-2.11719600
H	-4.13995000	-3.13767200	-1.33729800
C	-2.52858700	-3.28650900	0.08193000
C	-5.35669200	-1.38096700	-2.55224900
C	-6.69197500	0.76317900	-2.79702500
H	-4.88515000	1.97189000	-2.87360000
H	-6.00416500	2.40612800	-1.57570500
C	-2.75925800	-4.67162000	0.23056500
C	-1.37935900	-2.67522500	0.68670500
C	-6.15501600	-0.48355700	-3.50920600
H	-4.94611600	-2.23319800	-3.10519300
H	-6.01177600	-1.77446100	-1.76535700
H	-7.22529500	1.40546000	-3.50619200
H	-7.42089200	0.45761100	-2.03546400
C	-1.90613800	-5.48149100	0.95568300
H	-3.63965200	-5.09661800	-0.24586700
C	-0.50931700	-3.54483200	1.39902300
O	-1.06661400	-1.41416200	0.57242700
H	-5.50495900	-0.17617200	-4.33958900
H	-6.97986000	-1.05323600	-3.95041200
C	-0.76631300	-4.89704100	1.53439900
H	-2.10541600	-6.54146800	1.06747500
H	0.36294700	-3.10480700	1.85587900
H	-0.07472000	-5.51331000	2.10372100
O	-0.68094200	-1.66678200	-2.47360800
H	-0.79315500	-2.34366300	-1.79052200
H	-1.26419900	-0.84885400	-2.11907200
H	-3.55423900	-0.20194000	-2.68129400
H	-5.45975600	0.25510400	-0.38569900
H	1.17894000	-1.06633500	1.48442900
H	3.42198300	0.34075100	2.95850300
C	-4.62622300	-1.50946200	3.38829500
H	-5.66998700	-1.76048900	3.58232900
H	-4.28152500	-0.74481400	4.08923200
H	-4.00362400	-2.39753900	3.54044700
C	-4.45562900	-1.02776700	1.94893800
O	-3.27568100	-0.52671100	1.74707300
O	-5.37482100	-1.15957500	1.13251100

subsequent hydration

$OAc\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OAc + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3008.467971

Thermal correction to Gibbs Free Energy (a.u.): 0.856558

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5485.8411187 a.u.

C	5.03910000	-3.70139400	-3.18884600
C	4.16584400	-4.57023900	-2.50986300
C	5.24701200	-2.40437400	-2.74982100
H	5.55549000	-4.04786100	-4.07955900
C	3.52036000	-4.11310400	-1.37832300
H	4.00315300	-5.57993900	-2.86951800
C	4.58277100	-1.90540300	-1.60600900
H	5.91330500	-1.72944500	-3.27652400
C	3.71128800	-2.79436700	-0.90345800

H	2.84214500	-4.76343000	-0.83184200
O	4.81111900	-0.65574400	-1.24787100
C	3.03752600	-2.41404000	0.30355300
Co	3.71109000	0.32656200	-0.05643600
N	3.05625000	-1.23634700	0.83607700
H	2.44625200	-3.19044500	0.79324500
N	2.67097400	1.28061500	1.20572000
C	2.23120100	-0.93571600	2.02361800
C	2.11169300	2.41942200	0.97137700
C	2.53255300	0.50567900	2.43988900
C	2.44559900	-1.85034000	3.23317800
H	1.39676200	2.81713000	1.68937800
C	2.38062800	3.21564300	-0.19402400
C	1.50202300	0.95913100	3.46808800
C	1.46228600	-1.43700400	4.34178400
H	3.48358600	-1.75211300	3.57682800
H	2.29753100	-2.90133700	2.96847300
C	1.53495700	4.31019400	-0.47344700
C	3.50511500	2.94192700	-1.03093000
C	1.60194200	0.04869500	4.70437900
H	1.68283600	1.99888300	3.76200300
H	0.50387200	0.89428700	3.02084000
H	1.62069500	-2.05849200	5.22919200
H	0.43862200	-1.62611200	3.99717800
C	1.77463800	5.12880900	-1.56288500
H	0.67977100	4.48782500	0.17131600
C	3.73807200	3.80451400	-2.12141100
O	4.34628000	1.93974900	-0.81813800
H	2.57056000	0.21475600	5.19550800
H	0.82927700	0.32952700	5.42675600
C	2.88756600	4.87095700	-2.37945800
H	1.10983100	5.95690200	-1.78206400
H	4.59525200	3.59950600	-2.75397400
H	3.08538900	5.50968900	-3.23577700
O	2.32651200	0.33918300	-1.36147200
H	2.74477700	0.19265900	-2.22056400
O	5.35625300	0.48540400	1.04205000
H	5.56539800	1.38249300	0.70811900
H	5.90154900	-0.11156800	0.49393400
C	-0.07746600	0.91354900	-1.42376800
C	0.96011200	-0.20690500	-1.31651800
O	-1.33056600	0.30385500	-1.40244300
H	0.05854100	1.57921500	-0.56375000
H	0.83615000	-0.72120100	-0.37009400
H	0.85166100	-0.92062900	-2.13557700
C	0.08052000	1.73002800	-2.70733300
H	-0.68099000	2.51404300	-2.73085300
H	1.06400600	2.20823800	-2.76601300
H	-0.06254200	1.08668300	-3.58294600
C	-0.98984200	4.71423300	2.29192500
C	-1.77245000	5.37951100	1.33180200
C	-0.89570300	3.33311200	2.30655700
H	-0.45454800	5.28953800	3.04343100
C	-2.51670300	4.60974200	0.45455700
H	-1.83440400	6.46199300	1.31553900
C	-1.55545100	2.51592500	1.33779100
H	-0.32778900	2.83343300	3.07971500
C	-2.45709600	3.20067500	0.45578400
H	-3.19390700	5.09113100	-0.24791900
O	-1.31223400	1.24442600	1.30125500
C	-3.42229800	2.49393500	-0.34059900
Co	-2.27447200	-0.05432300	0.22983200
N	-3.56128000	1.21847500	-0.40223200
H	-4.12918500	3.12245800	-0.88333900
N	-3.24668200	-1.31371100	-0.81219100
C	-4.67216800	0.58630700	-1.12564900
C	-3.17681300	-2.58870900	-0.70345100
C	-4.07986500	-0.64856800	-1.81601900
C	-5.43950100	1.45574900	-2.11909500

H	-3.83454600	-3.20363500	-1.31587600
C	-2.27046100	-3.30020400	0.15728000
C	-5.17083700	-1.49364400	-2.46820700
C	-6.53954700	0.62087100	-2.79249600
H	-4.74964300	1.85265900	-2.87697100
H	-5.89700900	2.31229100	-1.61195500
C	-2.40604600	-4.70279200	0.23293200
C	-1.21189500	-2.63779400	0.86341600
C	-5.96813900	-0.63473200	-3.46056300
H	-4.72693800	-2.34199100	-2.99944400
H	-5.83150500	-1.88845500	-1.68646200
H	-7.07335300	1.23355800	-3.52737500
H	-7.27425900	0.32373500	-2.03301700
C	-1.55597700	-5.48442100	0.99399300
H	-3.21277900	-5.16760300	-0.32934100
C	-0.36659900	-3.47185700	1.64858300
O	-0.96518300	-1.36221000	0.80224900
H	-5.30802700	-0.33746700	-4.28655400
H	-6.77500200	-1.22995700	-3.90180000
C	-0.53075900	-4.84443700	1.71036400
H	-1.68295800	-6.56023300	1.04340900
H	0.40117400	-2.98790000	2.23255300
H	0.13896600	-5.43138300	2.33483600
O	-1.08740600	-1.92109800	-2.95707400
H	-1.01732600	-2.60251300	-2.27675000
H	-1.25124800	-1.10278800	-2.42461500
H	-3.37985100	-0.30045200	-2.58589300
H	-5.34267700	0.20655700	-0.34626800
H	1.17733100	-0.97706900	1.71175200
H	3.53160500	0.51866300	2.89795300
C	-4.58473800	-1.42167700	3.48928300
H	-5.62577700	-1.69979100	3.66038100
H	-4.28882400	-0.61894100	4.17002800
H	-3.93908700	-2.28146500	3.69767900
C	-4.38105200	-0.98940300	2.03708000
O	-3.21089600	-0.46377500	1.85073500
O	-5.27428600	-1.17506700	1.20183600

subsequent hydration

$OAc\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OAc + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3008.478688

Thermal correction to Gibbs Free Energy (a.u.): 0.855276

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5485.8430819 a.u.

C	6.36006700	-3.49186200	-2.89779400
C	5.44063400	-4.45611000	-2.44194400
C	6.36148800	-2.20662600	-2.38809300
H	7.07900900	-3.75838600	-3.66796500
C	4.53627200	-4.09687600	-1.46299100
H	5.44458800	-5.46010500	-2.85192400
C	5.43559800	-1.80591300	-1.39084400
H	7.06408400	-1.45903500	-2.74120500
C	4.50844400	-2.79086600	-0.92084700
H	3.81850600	-4.82398900	-1.08996300
O	5.49595100	-0.57789200	-0.94307800
C	3.55644300	-2.51701200	0.11510800
Co	4.13659900	0.26898500	0.08702800
N	3.37673700	-1.37987900	0.69868900
H	2.93449000	-3.36151800	0.42226700
N	2.89156300	1.09358600	1.25200100
C	2.28875100	-1.19181500	1.67562300
C	2.39202200	2.26799900	1.07485400
C	2.51638600	0.17793400	2.32733400
C	2.18847100	-2.25788500	2.77333700
H	1.57234200	2.59749400	1.70967600
C	2.86456700	3.20511300	0.09454300
C	1.33335200	0.54862900	3.21497500
C	1.04840800	-1.91252300	3.74733800

H	3.14762400	-2.30058800	3.30544600
H	2.02334300	-3.25200400	2.34507400
C	2.11289900	4.37864500	-0.12963300
C	4.10295000	3.00033400	-0.59291500
C	1.19484300	-0.50106400	4.32814000
H	1.48608600	1.53881100	3.65906600
H	0.41781700	0.57855500	2.61284800
H	1.01664500	-2.65466700	4.55237200
H	0.08976000	-1.97502500	3.22097100
C	2.54113400	5.34314100	-1.02315700
H	1.17551300	4.50249800	0.40598100
C	4.52537100	4.01416900	-1.48571200
O	4.87421400	1.95206300	-0.41197700
H	2.07895600	-0.45739300	4.97862700
H	0.32815200	-0.26371100	4.95335700
C	3.76095500	5.15016700	-1.69607600
H	1.94854700	6.23438200	-1.19951600
H	5.46576700	3.86185500	-2.00508800
H	4.11120100	5.90221400	-2.39826400
O	2.95035400	0.30510700	-1.29930000
H	3.52141800	0.52702100	-2.04911500
O	5.65417100	0.34894700	1.52127800
H	5.85453400	1.26977700	1.26518100
H	6.24682400	-0.17960800	0.95451700
C	-0.24603200	0.60048600	-1.60195000
C	0.33204300	-0.48367500	-2.52114700
O	-1.70540300	0.42268200	-1.66266000
H	0.05330500	0.40905100	-0.57101200
H	1.37787000	-0.64935400	-2.25050200
H	0.26236400	-0.17802700	-3.57058600
C	0.12242300	2.01027300	-2.00110500
H	-0.32687800	2.73682300	-1.31990700
H	1.20915900	2.10703500	-1.94391600
H	-0.21304800	2.22935300	-3.02037600
C	-0.98429700	4.52516800	2.21309200
C	-1.88366900	5.28135400	1.43743500
C	-0.92576100	3.14836700	2.10532100
H	-0.32842100	5.02826100	2.91903200
C	-2.75602200	4.60533900	0.60881700
H	-1.91659100	6.36185300	1.52036600
C	-1.74478600	2.42833500	1.18857500
H	-0.26152200	2.57480100	2.73518100
C	-2.72929900	3.19665300	0.48515200
H	-3.50407600	5.15442200	0.04135400
O	-1.56053800	1.15025900	1.04507800
C	-3.77663000	2.57863600	-0.26807900
Co	-2.67563800	-0.03074000	0.04215900
N	-3.94993800	1.31199700	-0.43273700
H	-4.51307600	3.25995400	-0.69454600
N	-3.76917900	-1.20021200	-1.00052900
C	-5.13759800	0.76684900	-1.10833700
C	-3.87797400	-2.46466300	-0.77958300
C	-4.65766400	-0.45852600	-1.90095600
C	-5.92548100	1.71825000	-2.00738800
H	-4.67599500	-3.01703300	-1.27343300
C	-3.00146600	-3.22670700	0.06136900
C	-5.83928000	-1.22311700	-2.49184900
C	-7.10883900	0.96947200	-2.64135300
H	-5.26798900	2.12282800	-2.78936200
H	-6.30805000	2.56731000	-1.43146800
C	-3.32717900	-4.57615100	0.31800700
C	-1.76045500	-2.68580100	0.52333300
C	-6.65548600	-0.28645100	-3.39489600
H	-5.48899400	-2.08495600	-3.07072700
H	-6.46490100	-1.59979700	-1.67354400
H	-7.65229800	1.64032400	-3.31508900
H	-7.81048200	0.68036600	-1.84846600
C	-2.46668500	-5.40898600	1.00776800
H	-4.27989400	-4.95387500	-0.04517400

C	-0.87351800	-3.58106600	1.16904400
O	-1.37631300	-1.44898000	0.30686600
H	-6.04139100	0.00736400	-4.25685400
H	-7.52276100	-0.82140400	-3.79567100
C	-1.22197700	-4.89782100	1.41483700
H	-2.73458400	-6.44013000	1.20958100
H	0.09079700	-3.19668600	1.46869100
H	-0.51736200	-5.54498500	1.93060600
O	-0.46799100	-1.67315100	-2.40893800
H	-0.47327900	-1.90823300	-1.46367800
H	-1.77079400	-0.46164700	-2.09651800
H	-4.02683300	-0.09078600	-2.72344400
H	-5.77540700	0.37849800	-0.30735800
H	1.34250200	-1.14366400	1.11723800
H	3.41644100	0.08744300	2.95231400
C	-4.70610600	-1.47041700	3.39490500
H	-5.74469200	-1.64281300	3.67997200
H	-4.23247600	-0.76258100	4.07907000
H	-4.15097700	-2.41238000	3.45836300
C	-4.63499200	-0.96105500	1.95941100
O	-3.44828800	-0.49963800	1.68116500
O	-5.61104200	-1.04050900	1.21000000

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon and subsequent hydration

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.015019

Thermal correction to Gibbs Free Energy (a.u.): 0.828307

Imaginary frequencies: -350.91

Calculation of single point energy based on the optimized structure, Et = -5409.3181441 a.u.

C	-7.47122700	1.64001300	2.85894800
C	-7.15765400	0.62450500	3.78372900
C	-6.83090100	1.71821900	1.63665700
H	-8.22743900	2.37882100	3.11016500
C	-6.19267100	-0.30195900	3.44654200
H	-7.66467600	0.57420000	4.74097500
C	-5.83167300	0.78155200	1.26518200
H	-7.06725200	2.50034900	0.92290200
C	-5.51500600	-0.25065900	2.20495100
H	-5.93247200	-1.09648000	4.14231000
O	-5.28075300	0.89816500	0.08463200
C	-4.53138600	-1.25758400	1.93912600
Co	-3.75062100	-0.05673300	-0.53126700
N	-3.80525300	-1.35396100	0.87580400
H	-4.39414500	-1.99950600	2.72831200
N	-2.33888100	-1.09089700	-1.24051700
C	-2.72420000	-2.34808600	0.76511900
C	-1.40742700	-0.63179900	-2.00856400
C	-2.38678200	-2.46356300	-0.72867200
C	-2.99631100	-3.73273000	1.35838100
H	-0.56434600	-1.27027400	-2.24835200
C	-1.42005500	0.67535700	-2.60636900
C	-1.15561000	-3.33749300	-0.94961900
C	-1.77574400	-4.64191000	1.13763300
H	-3.88493000	-4.16008200	0.87585300
H	-3.21055600	-3.66630400	2.42972800
C	-0.25720500	1.12546300	-3.27156500
C	-2.60676700	1.47218300	-2.61766700
C	-1.38506200	-4.72805100	-0.34301600
H	-0.92743000	-3.42748600	-2.01442000
H	-0.28083500	-2.87271400	-0.48340500
H	-1.98258700	-5.64019000	1.53746700
H	-0.92778000	-4.24319500	1.71087900
C	-0.26035600	2.31319000	-3.98029800
H	0.65466400	0.55012200	-3.16075400
C	-2.58157800	2.67867900	-3.35314200
O	-3.72526400	1.12281100	-2.01555500

H	-2.18128100	-5.24127200	-0.89884100
H	-0.47662500	-5.32628900	-0.46461400
C	-1.43727000	3.08061100	-4.02433400
H	0.64153200	2.65572800	-4.47536300
H	-3.48791200	3.27484900	-3.37079700
H	-1.44890900	4.01550500	-4.57852700
O	-2.60527300	0.98874600	0.46985200
H	-2.99277200	1.86851200	0.35557700
O	-5.13614000	-1.03128700	-1.71136800
H	-4.92178400	-0.44025500	-2.46088700
H	-5.89513900	-0.59006900	-1.28729600
C	-0.46254000	1.33798900	0.67023200
C	-0.03662700	0.05454200	1.21758300
O	1.21841500	0.70197800	1.25901900
H	-0.28499700	1.47256400	-0.38809400
H	-0.07737200	-0.78652200	0.52609900
H	-0.41939000	-0.20213700	2.21225400
C	-0.68703700	2.54859500	1.51509400
H	-1.35913500	3.24229500	1.00470900
H	-1.10370300	2.28542900	2.48993100
H	0.26329100	3.07118500	1.65064300
C	1.26843200	5.39204500	-0.83104000
C	2.02329900	5.81952100	0.28059200
C	1.29152700	4.07793100	-1.25289500
H	0.65154600	6.10890600	-1.36741400
C	2.79410800	4.88989800	0.94805100
H	1.99901700	6.85526600	0.60163700
C	2.07339000	3.09369000	-0.58170200
H	0.70650400	3.74715100	-2.10227700
C	2.83378200	3.53141300	0.55275100
H	3.38737100	5.19097300	1.80911000
O	2.04198400	1.87440600	-1.02294200
C	3.64157000	2.63421900	1.32493900
Co	2.62860100	0.36141200	-0.03877700
N	3.71090700	1.35642900	1.17304300
H	4.23268300	3.09486100	2.11765800
N	3.11183500	-1.16378700	1.00362600
C	4.52840100	0.48601400	2.02309400
C	3.06326900	-2.38290600	0.59935300
C	3.66211100	-0.76051400	2.30130600
C	5.05203000	1.08919600	3.32472700
H	3.44653100	-3.17064300	1.24801800
C	2.58906900	-2.79848000	-0.69455100
C	4.46029400	-1.81830500	3.05992000
C	5.84629400	0.03236000	4.10661800
H	4.21141600	1.45438600	3.93139300
H	5.69896100	1.94786100	3.11520700
C	2.80511400	-4.13378600	-1.08986400
C	1.91959300	-1.88787800	-1.57434800
C	5.00988100	-1.22583500	4.36573500
H	3.83184000	-2.68672200	3.28867300
H	5.28324400	-2.16043800	2.42089600
H	6.19747000	0.45630900	5.05366300
H	6.73944700	-0.24045400	3.53017800
C	2.43287000	-4.58918600	-2.34360500
H	3.29737700	-4.80583100	-0.39044000
C	1.60787400	-2.36539100	-2.87592500
O	1.53530800	-0.69438800	-1.21471400
H	4.17079700	-0.97305900	5.02849600
H	5.60837800	-1.97825900	4.89052600
C	1.84939300	-3.67973400	-3.24240100
H	2.61695200	-5.61680800	-2.63730700
H	1.17613800	-1.66511200	-3.58277600
H	1.59007800	-4.00722500	-4.24584100
H	5.35828600	0.13903600	1.39778000
H	2.80519900	-0.43241500	2.90571800
H	-3.25251100	-2.93481500	-1.21576600
H	-1.84891300	-1.91575600	1.26621700
C	5.69739700	-0.74548200	-2.67203000

H	5.06246800	-1.44778400	-3.22274600
H	6.70819300	-1.14928600	-2.59885200
H	5.70005300	0.19617500	-3.22651500
C	5.10453200	-0.54453800	-1.28009300
O	4.00546100	0.14648700	-1.32484000
O	5.65387100	-1.03464400	-0.28678100

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.036384

Thermal correction to Gibbs Free Energy (a.u.): 0.825512

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5409.3391276 a.u.

C	-7.78812000	1.44805300	3.14731300
C	-7.75707500	0.11403600	3.59996400
C	-6.95347500	1.87990500	2.13453200
H	-8.47760700	2.15314500	3.60391800
C	-6.86999300	-0.76295100	3.01059900
H	-8.41453300	-0.21376600	4.39769300
C	-6.03281300	0.99862500	1.50710500
H	-6.97130000	2.90709900	1.78560900
C	-6.00188900	-0.35604900	1.96960200
H	-6.82222000	-1.79705800	3.34480500
O	-5.29062700	1.46662700	0.53900000
C	-5.09871300	-1.33124800	1.43295300
Co	-3.92592400	0.52481700	-0.39645100
N	-4.25386800	-1.13924900	0.47686800
H	-5.13748600	-2.31524200	1.90316800
N	-2.68611800	-0.44010000	-1.47077400
C	-3.24716400	-2.14305000	0.10327800
C	-1.69395500	0.08244000	-2.11175300
C	-2.92463600	-1.88385500	-1.37709900
C	-3.61331000	-3.60821600	0.34721500
H	-0.96860100	-0.57583500	-2.58849200
C	-1.46874000	1.49291200	-2.25699700
C	-1.81810700	-2.80170400	-1.88595400
C	-2.49885800	-4.53023900	-0.17088500
H	-4.55705800	-3.83259200	-0.16751700
H	-3.77405000	-3.79432500	1.41409200
C	-0.25322200	1.92116800	-2.83682500
C	-2.45013800	2.45403600	-1.85839600
C	-2.19251300	-4.26950800	-1.64910900
H	-1.63327000	-2.62930000	-2.94938700
H	-0.88053500	-2.57889600	-1.36532000
H	-2.78397500	-5.57608600	-0.01493400
H	-1.58781400	-4.36036900	0.41902700
C	0.02084900	3.26435000	-3.01618500
H	0.49910200	1.17700000	-3.07531400
C	-2.14142800	3.82266300	-2.05527700
O	-3.62187100	2.13838800	-1.36014000
H	-3.07185300	-4.52847900	-2.25443700
H	-1.37026300	-4.90609400	-1.98803600
C	-0.93819700	4.21348700	-2.61923100
H	0.96437900	3.57748600	-3.44856800
H	-2.88494500	4.55028200	-1.74710400
H	-0.73164000	5.27256800	-2.74888400
O	-2.63752100	0.88613300	0.84470000
H	-2.89730000	1.76559100	1.15486500
O	-5.42117100	0.30057700	-1.84909800
H	-5.04734000	1.06232300	-2.33376400
H	-6.10035900	0.71179800	-1.28509500
C	0.51002800	1.79946300	0.45235200
C	0.06354100	0.49910900	0.92909600
O	1.47533200	0.88529800	1.10034900
H	0.71773200	1.88657900	-0.60535300
H	-0.08213400	-0.29472100	0.20899700
H	-0.47224700	0.42022400	1.86637900
C	0.24244500	3.07921600	1.18148700

H	-0.66237300	3.53015700	0.76133900
H	0.09115100	2.90717800	2.25076000
H	1.07173800	3.77834200	1.04061400
C	3.85248100	5.26694200	-0.53614900
C	4.55368800	5.31071700	0.68712200
C	3.37622200	4.07659100	-1.04686900
H	3.68185200	6.18742100	-1.08855200
C	4.75577800	4.13196700	1.37395300
H	4.92527900	6.25192700	1.07719400
C	3.56665100	2.84373300	-0.35946400
H	2.83127200	4.03761600	-1.98316100
C	4.27396200	2.89340900	0.88649600
H	5.29345600	4.13733700	2.31973500
O	3.08606000	1.76424100	-0.89348500
C	4.51359000	1.72270800	1.67505400
Co	2.93182800	0.09119400	-0.02988300
N	4.08416000	0.53230300	1.42052200
H	5.10851900	1.87500000	2.57649600
N	2.64744100	-1.55889600	0.87687200
C	4.36227900	-0.62505500	2.27997200
C	2.25778100	-2.64570500	0.30862000
C	3.07470300	-1.47456500	2.27663400
C	4.81361400	-0.33034300	3.70916800
H	2.24374800	-3.56843300	0.88853400
C	1.86885600	-2.75149800	-1.07196300
C	3.29531900	-2.79751300	3.00607900
C	5.02222600	-1.64857800	4.47049500
H	4.06023200	0.28707000	4.21797200
H	5.75064100	0.23636900	3.70691600
C	1.68953400	-4.03752800	-1.62340000
C	1.65100100	-1.58632800	-1.87924300
C	3.76606700	-2.52706500	4.44281800
H	2.37074100	-3.38565100	3.02742900
H	4.04879900	-3.37792800	2.46019600
H	5.31424800	-1.43759600	5.50480500
H	5.85517200	-2.19598100	4.01114200
C	1.34131400	-4.21378000	-2.95106000
H	1.85100700	-4.90150700	-0.98280200
C	1.31660700	-1.79970900	-3.24378700
O	1.69382100	-0.37174600	-1.41341500
H	2.96054300	-2.02637400	4.99716100
H	3.95597000	-3.47629100	4.95497700
C	1.16637300	-3.07544900	-3.75968600
H	1.22526400	-5.20911400	-3.36583200
H	1.20025400	-0.92432300	-3.87370100
H	0.91658000	-3.19752400	-4.81034900
H	5.11599500	-1.22085600	1.75440800
H	2.29972000	-0.89469700	2.79834900
H	-3.84602200	-2.08020000	-1.94434300
H	-2.34335100	-1.89239800	0.67714000
C	5.79818400	-1.87758600	-2.33661400
H	5.07124400	-2.28396000	-3.04774900
H	6.59139300	-2.60746000	-2.16957600
H	6.20402500	-0.96146400	-2.77209700
C	5.07890300	-1.57477100	-1.02620000
O	4.29832100	-0.53922200	-1.14699200
O	5.25010500	-2.28506300	-0.03158500

PO-Co^{III}-OAc + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OAc + H_2O-Co^{III}-OH = OAc-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2932.038962

Thermal correction to Gibbs Free Energy (a.u.): 0.833329

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5409.3519046 a.u.

C	-7.87525400	1.28522300	2.33997800
C	-7.87246400	0.04163000	3.00058500
C	-6.88163200	1.62007700	1.43829100
H	-8.67065600	1.99742400	2.54060500

C	-6.84963400	-0.84622900	2.73813100
H	-8.65608600	-0.20920500	3.70664000
C	-5.82412200	0.72324900	1.14489200
H	-6.87779000	2.57814100	0.92950900
C	-5.81875700	-0.53796900	1.81827500
H	-6.81838700	-1.80860000	3.24326700
O	-4.91815400	1.10061100	0.27106500
C	-4.76960800	-1.50065500	1.63815900
Co	-3.53352000	0.01456500	-0.44806400
N	-3.78942000	-1.40773300	0.80469400
H	-4.81684700	-2.37929200	2.28235000
N	-2.17628900	-1.06275700	-1.19503800
C	-2.68335500	-2.37681000	0.75198100
C	-1.24200700	-0.63699000	-1.98354600
C	-2.26083600	-2.45476400	-0.72187400
C	-2.94908000	-3.76706900	1.32750700
H	-0.43775900	-1.31381000	-2.23802800
C	-1.18871900	0.66574500	-2.58076800
C	-1.00617900	-3.30959700	-0.88762600
C	-1.69562400	-4.64196400	1.15894100
H	-3.80326800	-4.22209500	0.80778500
H	-3.20750800	-3.70336100	2.38981500
C	-0.03744100	1.01723000	-3.32215300
C	-2.29473800	1.55970700	-2.51796000
C	-1.24155800	-4.70826800	-0.30356500
H	-0.72698000	-3.39284000	-1.94063800
H	-0.16785300	-2.82263900	-0.38046200
H	-1.89584700	-5.64666000	1.54535500
H	-0.88566000	-4.22338700	1.77020100
C	-0.00408600	2.18226200	-4.06446400
H	0.83344100	0.37699600	-3.25214000
C	-2.23722700	2.74532500	-3.27859400
O	-3.39114400	1.31652200	-1.81146700
H	-2.00371700	-5.23102100	-0.89760100
H	-0.31930500	-5.29097300	-0.38974300
C	-1.12074900	3.03440400	-4.05077600
H	0.88679000	2.45140500	-4.61999500
H	-3.08942100	3.41533000	-3.23984400
H	-1.10139600	3.95494000	-4.62753900
O	-2.40549300	0.90973700	0.82403800
H	-2.93778900	1.71090300	0.96381500
O	-4.86911800	-0.72061100	-1.73585500
H	-4.64870700	0.00365600	-2.36640400
H	-5.71962800	-0.45528800	-1.34867500
C	-0.95547100	1.28946600	0.80467300
C	-0.14009300	0.06857100	1.26840300
O	1.17686400	0.38896800	1.49935500
H	-0.69037400	1.55729100	-0.21562500
H	-0.25068900	-0.72842900	0.52165900
H	-0.61465100	-0.28576200	2.20793200
C	-0.81602000	2.47203200	1.74063200
H	-1.31308400	3.36517500	1.34736000
H	-1.22015600	2.22489300	2.72933900
H	0.24597000	2.69180100	1.84862700
C	0.75504100	5.25965000	-0.70531300
C	1.61668700	5.76718400	0.28728700
C	0.77259800	3.92450700	-1.05622400
H	0.05891600	5.92876200	-1.20600900
C	2.48323800	4.89190100	0.91155300
H	1.59845200	6.81832300	0.55470700
C	1.65838400	2.99608600	-0.43339000
H	0.10618600	3.53928700	-1.81553900
C	2.52342200	3.51677900	0.58569100
H	3.15557000	5.25339900	1.68722900
O	1.60946900	1.75525400	-0.79911600
C	3.42161100	2.68319500	1.33249600
Co	2.46638700	0.30877500	0.09491900
N	3.53228100	1.40574600	1.23292800
H	4.04894100	3.20416300	2.05759400

N	3.24345700	-1.16204500	1.03014700
C	4.46731300	0.62139100	2.04819300
C	3.38113100	-2.35261500	0.57472200
C	3.75942300	-0.72040700	2.32467100
C	4.94336900	1.26558500	3.34946200
H	3.91719000	-3.09188800	1.17060600
C	2.92338100	-2.78684100	-0.72201100
C	4.68440200	-1.68663100	3.05981000
C	5.85875900	0.29707800	4.11310300
H	4.07482600	1.53238500	3.96753700
H	5.49248400	2.19062000	3.14388000
C	3.37091100	-4.03075300	-1.20391400
C	2.04971900	-1.97501800	-1.51595200
C	5.17226700	-1.04946400	4.36861600
H	4.16393800	-2.62658400	3.27781900
H	5.54041200	-1.92280600	2.41522000
H	6.17209600	0.75003400	5.06036000
H	6.77022300	0.12992700	3.52462700
C	3.02891300	-4.49138400	-2.46565800
H	4.02046500	-4.62596800	-0.56570100
C	1.76147700	-2.45050500	-2.82528100
O	1.47873800	-0.88772000	-1.07519000
H	4.31389200	-0.89778900	5.03738200
H	5.85617100	-1.73291400	4.88400700
C	2.22949000	-3.67428900	-3.27972400
H	3.39342500	-5.44737400	-2.82568900
H	1.17352500	-1.81830100	-3.48223400
H	1.98152900	-3.99584000	-4.28824700
H	5.31434800	0.38747800	1.39254800
H	2.87030700	-0.50453900	2.93039800
H	-3.09241000	-2.91703500	-1.27406800
H	-1.85513600	-1.91814800	1.30426700
C	5.46476200	-0.35655900	-2.80517400
H	4.89296000	-1.16113600	-3.28051600
H	6.52633100	-0.60899400	-2.81768100
H	5.28349900	0.55640800	-3.37854800
C	4.96810700	-0.19354100	-1.36883200
O	3.78016600	0.31872000	-1.32162300
O	5.67530700	-0.56378300	-0.42186100

subsequent hydration

OAc-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-OAc + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3008.425129

Thermal correction to Gibbs Free Energy (a.u.): 0.856182

Imaginary frequencies: -385.98

Calculation of single point energy based on the optimized structure, Et = -5485.7921028 a.u.

C	5.87353400	-2.54883600	-3.38167400
C	4.87455800	-3.51916200	-3.18389500
C	5.96072600	-1.43385900	-2.56547100
H	6.58752100	-2.67028400	-4.19177100
C	3.97611800	-3.34703500	-2.14901300
C	5.04550000	-1.22773400	-1.50666400
C	4.03512900	-2.21787300	-1.30110200
H	3.19543500	-4.07905500	-1.96884500
O	5.19353700	-0.15978200	-0.75377300
C	3.09095700	-2.13921100	-0.22499600
Co	3.82009900	0.54417400	0.34294500
N	2.98338200	-1.15188600	0.60351000
H	2.41263800	-2.98796400	-0.11305300
N	2.57178900	1.18184300	1.63471200
C	1.92505800	-1.14325800	1.62991100
C	2.17798700	2.40225700	1.75834700
C	2.16794400	0.08488100	2.51571400
C	1.88230800	-2.39017300	2.51746000
H	1.40436400	2.63631300	2.49109500
C	2.69123400	3.49488800	0.97731600
C	0.97944500	0.29893500	3.44775500
C	0.76530000	-2.24137900	3.56045200

H	2.85884500	-2.50889900	3.00503800
H	1.70133900	-3.28452100	1.91646400
C	1.99938800	4.72613300	0.99769400
C	3.90243500	3.36428000	0.22408500
C	0.85860200	-0.93444500	4.36075000
H	1.11392400	1.19550800	4.06274200
H	0.07266600	0.43251200	2.84499000
H	0.77252300	-3.09952700	4.24120600
H	-0.19214400	-2.26276200	3.03514200
C	2.45772700	5.81846800	0.28690000
H	1.07987700	4.79401900	1.57346100
C	4.35728300	4.50538300	-0.47899900
O	4.62128200	2.26405900	0.17727700
H	1.73566900	-0.96945200	5.02029500
H	-0.01592700	-0.83080000	5.01216100
C	3.64999800	5.69584400	-0.44966000
H	4.02318200	6.54813500	-1.01072500
O	2.76265600	0.85184700	-1.14151800
H	3.33101600	1.43068800	-1.67099700
O	5.24370800	0.27169500	1.80035200
H	5.54824600	1.19748100	1.75381400
H	5.83025400	-0.19860900	1.17520000
H	0.95817900	-1.00856500	1.12489000
H	3.05888600	-0.12589500	3.12396000
C	0.79871900	1.61993700	-1.24535200
C	0.13335800	0.26412600	-1.11473500
O	-0.76641100	0.22670200	-0.02808400
H	1.09963200	2.15690700	-0.36854200
H	0.93013500	-0.47643800	-1.00581600
H	-0.36806200	0.04626200	-2.06243600
C	1.06017000	2.20438200	-2.60003700
H	0.11337700	2.42450800	-3.09757700
H	1.65268000	3.11951300	-2.53977600
H	1.58196100	1.46541600	-3.21535900
O	-0.99179700	2.58215400	-0.83011000
H	-1.08898400	1.80666600	-0.19160700
H	-1.57617200	2.22307100	-1.53307700
H	5.27755100	4.40817200	-1.04527700
H	1.90877900	6.75339600	0.29571700
H	6.72708900	-0.68101300	-2.71699700
H	4.81233600	-4.38636800	-3.83215000
C	0.54527400	-4.65369100	-1.59629100
C	0.46089500	-5.10834400	-0.26193900
C	-0.14670700	-3.53745100	-2.01944400
H	1.15815300	-5.19916200	-2.30964500
C	-0.35460300	-4.41915100	0.61591300
H	1.00150100	-5.99263000	0.05765700
C	-0.99350300	-2.80139100	-1.13516800
H	-0.08731500	-3.18922900	-3.04500700
C	-1.07666300	-3.26984600	0.22037400
H	-0.45633700	-4.75986600	1.64444700
O	-1.63701400	-1.78652400	-1.60134800
C	-1.89966700	-2.62157300	1.20193000
Co	-2.51110100	-0.46861800	-0.54762700
N	-2.52320000	-1.50582700	1.05010700
H	-1.98041400	-3.13539100	2.16094300
N	-3.38967300	0.87193000	0.48956700
C	-3.33635600	-0.88949700	2.10668400
C	-4.25784400	1.69517600	0.01358700
C	-3.18576700	0.63533700	1.91645600
C	-3.01425200	-1.29429000	3.54412200
H	-4.85316000	2.29375100	0.70229600
C	-4.53785700	1.86410000	-1.38802800
C	-4.09533300	1.39581300	2.87781700
C	-3.90368100	-0.51723500	4.52585900
H	-1.95864000	-1.08540700	3.75824200
H	-3.16825900	-2.36882000	3.68896100
C	-5.68866900	2.58480400	-1.76501300
C	-3.67517400	1.31848500	-2.38882300

C	-3.77526300	0.99717500	4.32503000
H	-3.97033200	2.47688800	2.74738900
H	-5.13924400	1.15077700	2.64749800
H	-3.64437000	-0.78853800	5.55520400
H	-4.94906300	-0.81377900	4.37320900
C	-6.02134600	2.76073100	-3.09687100
H	-6.32812600	2.98769300	-0.98309300
C	-4.02937500	1.52265100	-3.74164600
O	-2.54659300	0.70966800	-2.09566000
H	-2.75054200	1.31087400	4.56949000
H	-4.43913300	1.52988000	5.01420300
C	-5.17619700	2.22196500	-4.08300500
H	-6.91833100	3.30308400	-3.37570600
H	-3.37628700	1.09986000	-4.49762900
H	-5.42756600	2.35066500	-5.13253900
H	-4.37954700	-1.11707000	1.85596200
H	-2.13726000	0.89330700	2.12309400
C	-6.38128100	-1.47845400	-1.84871400
H	-6.45277800	-0.61158800	-2.51506100
H	-7.36161600	-1.68049300	-1.41407400
H	-6.04238900	-2.32659100	-2.44801200
C	-5.36999700	-1.15247000	-0.75425300
O	-4.15020500	-1.21472500	-1.19006200
O	-5.75734400	-0.83826800	0.37929400

subsequent hydration

$OAc\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OAc + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3008.469243

Thermal correction to Gibbs Free Energy (a.u.): 0.857620

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5485.8404768 a.u.

C	5.94312800	-2.57004100	-2.95917100
C	5.01802100	-3.60750300	-2.74814200
C	5.89943500	-1.40777400	-2.20693000
H	6.70465600	-2.67600100	-3.72678100
C	4.05429800	-3.45184400	-1.77120700
C	4.92062900	-1.22509800	-1.20441900
C	3.97905100	-2.27522400	-0.99094600
H	3.32290500	-4.23129200	-1.58718000
O	4.95390400	-0.10706400	-0.50359000
C	2.95555400	-2.20702700	0.01222600
Co	3.56391800	0.50730600	0.61858400
N	2.73022300	-1.20242500	0.79445600
H	2.30974300	-3.08296500	0.09509100
N	2.30026600	1.08718300	1.91423600
C	1.58176500	-1.19237700	1.72612500
C	1.87729500	2.29530900	2.06050900
C	1.84007100	-0.05183600	2.71759300
C	1.34627600	-2.49439400	2.49118200
H	1.07696200	2.49195100	2.76624300
C	2.38396900	3.41352300	1.30622900
C	0.63385600	0.17760200	3.62468300
C	0.14241800	-2.30959300	3.42523000
H	2.24888700	-2.74941400	3.06319200
H	1.14574400	-3.31631200	1.80100900
C	1.64834500	4.61588200	1.31180400
C	3.60715900	3.32705000	0.57838200
C	0.31872500	-1.12334300	4.38063900
H	0.84447200	0.97783600	4.34311400
H	-0.22122700	0.49935400	3.02144200
H	-0.03830700	-3.23004300	3.99090600
H	-0.74159300	-2.13574900	2.80568600
C	2.09048200	5.72703500	0.61597400
H	0.70819600	4.63777400	1.85457900
C	4.04706500	4.47844100	-0.11022900
O	4.35339900	2.23253800	0.52883200
H	1.13389600	-1.33868800	5.08458300
H	-0.58662800	-0.98646200	4.98176900

C	3.30224200	5.64896300	-0.09021200
H	3.66164500	6.51516100	-0.63844600
O	2.56701100	0.91151400	-0.97649900
H	3.13440200	1.57952800	-1.39345700
O	4.91242800	0.19378500	2.04737500
H	5.19617500	1.12839800	2.09505800
H	5.55812700	-0.21742700	1.43684100
H	0.68321700	-0.93875800	1.14079800
H	2.70140600	-0.34317300	3.33538400
C	1.14109200	1.33170400	-1.07832100
C	0.28998800	0.05690500	-1.19664200
O	-0.70223200	-0.01062700	-0.19738400
H	0.89317100	1.86219200	-0.16440200
H	0.96748200	-0.80530300	-1.13735300
H	-0.15922000	0.03007500	-2.19184300
C	1.03190500	2.27317300	-2.26197000
H	-0.00755000	2.59649900	-2.36007900
H	1.65524800	3.16539400	-2.12445600
H	1.31166000	1.76877300	-3.19291800
O	-0.83618500	2.14737900	1.31955300
H	-0.81859100	1.31471800	0.75586200
H	-1.36652600	2.75382500	0.78748500
H	4.98229200	4.41255700	-0.65627800
H	1.50982900	6.64278200	0.61231600
H	6.61085700	-0.60432600	-2.36571100
H	5.05945600	-4.51253000	-3.34405000
C	0.73024400	-4.54144100	-2.18543300
C	0.60240900	-5.12483300	-0.90523700
C	0.00499000	-3.42324000	-2.53990800
H	1.40913000	-4.98315900	-2.91056100
C	-0.29140000	-4.55989100	-0.01287300
H	1.16195000	-6.01670300	-0.64316600
C	-0.91644300	-2.80754100	-1.63697700
H	0.09759800	-2.97696500	-3.52425200
C	-1.04249400	-3.40829100	-0.33680400
H	-0.44120200	-5.01225100	0.96595400
O	-1.58331100	-1.78213400	-2.03848300
C	-1.99291700	-2.91985500	0.62278900
Co	-2.44582700	-0.53057000	-0.87354300
N	-2.65285400	-1.81946800	0.52291200
H	-2.16409900	-3.55613400	1.49314900
N	-3.28710100	0.68126900	0.33260100
C	-3.67301800	-1.39487600	1.48363000
C	-3.67955100	1.87133000	0.03944700
C	-3.45140600	0.11350600	1.67593500
C	-3.74133700	-2.13327100	2.81799100
H	-4.21346200	2.44407800	0.79739100
C	-3.45583700	2.54877300	-1.20411200
C	-4.56178800	0.71837700	2.53499700
C	-4.86198000	-1.53043300	3.67779100
H	-2.78568000	-2.05094600	3.35241000
H	-3.93227500	-3.20002300	2.65661500
C	-3.93713100	3.87337200	-1.33295300
C	-2.74022100	1.93911400	-2.28980900
C	-4.66052300	-0.02397500	3.87531400
H	-4.36519300	1.77835200	2.72788000
H	-5.50115400	0.64112400	1.97676600
H	-4.90417100	-2.04039900	4.64668000
H	-5.82528200	-1.70488500	3.18252200
C	-3.73229600	4.61595000	-2.47788700
H	-4.48287100	4.30292800	-0.49521800
C	-2.54726100	2.73291800	-3.46045000
O	-2.24812400	0.74562300	-2.27083700
H	-3.73869300	0.14359900	4.45087400
H	-5.48034900	0.39374200	4.46975400
C	-3.02579700	4.02476600	-3.54591600
H	-4.10933700	5.62975400	-2.55811000
H	-2.01492100	2.26920300	-4.28444500
H	-2.85868200	4.59334500	-4.45737800

H	-4.63434500	-1.48151700	0.96494000
H	-2.48473600	0.25730200	2.18092900
C	-6.23223600	-1.02722800	-2.64934000
H	-6.04930200	-0.23364900	-3.38162100
H	-7.28100000	-1.00806900	-2.34847900
H	-5.98901200	-1.97666000	-3.13310100
C	-5.32703300	-0.79782300	-1.44057200
O	-4.08817600	-1.06635800	-1.70543300
O	-5.80800900	-0.39813800	-0.37047500

subsequent hydration

$OAc\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OAc + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3008.481987

Thermal correction to Gibbs Free Energy (a.u.): 0.855364

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5485.8489332 a.u.

C	6.21821500	-3.00312400	-3.15969300
C	5.41471600	-4.06086200	-2.69016000
C	6.12745200	-1.73760300	-2.61162100
H	6.92149300	-3.18206100	-3.96861300
C	4.52261100	-3.80951800	-1.66746300
C	5.22072200	-1.45254300	-1.55670900
C	4.39978000	-2.52487300	-1.08762700
H	3.88744700	-4.60507800	-1.28658200
O	5.20470800	-0.23998600	-1.06491400
C	3.42604700	-2.35192700	-0.05001000
Co	4.00209000	0.43047800	0.24046100
N	3.19821700	-1.26089400	0.60089900
H	2.82161800	-3.22906100	0.17739300
N	2.90859400	1.09575800	1.65274400
C	2.06984600	-1.15639800	1.53772700
C	2.59329000	2.33634900	1.81749600
C	2.39073100	0.00858900	2.48741800
C	1.74016400	-2.41421000	2.34498300
H	1.86782100	2.59478400	2.59022600
C	3.12307800	3.42924000	1.05619700
C	1.19252400	0.32402800	3.38328000
C	0.56335700	-2.13037400	3.28815900
H	2.62884100	-2.71792800	2.91407200
H	1.47169000	-3.23878000	1.68094100
C	2.54902900	4.70888600	1.22937900
C	4.23330700	3.25691600	0.16914100
C	0.82055100	-0.92457900	4.19766400
H	1.42484900	1.14932800	4.06485500
H	0.34370800	0.63441300	2.75967000
H	0.34187100	-3.02034900	3.88758300
H	-0.32286200	-1.92775000	2.68003200
C	3.01068000	5.80636300	0.52992000
H	1.71768900	4.81401600	1.92282300
C	4.69268300	4.40277800	-0.52739300
O	4.86154700	2.12157300	0.00435600
H	1.63669000	-1.15572400	4.89499000
H	-0.06414600	-0.71680100	4.81000400
C	4.09355500	5.63745200	-0.35430000
H	4.46615000	6.49159100	-0.91326600
O	2.69858200	0.81450300	-0.97511200
H	3.19955900	0.89027800	-1.79999500
O	5.62449500	0.14934800	1.54750100
H	5.86385500	1.08842400	1.42001000
H	6.15863200	-0.30736300	0.87389900
H	1.19292400	-0.87751500	0.93902200
H	3.23301100	-0.31433700	3.11664300
C	-0.22929400	2.96029500	-0.36890900
C	-0.17578600	1.43329000	-0.28953200
O	-1.31454000	0.99073600	0.51904100
H	0.13370300	3.39808200	0.56679000
H	0.74254100	1.07465700	0.16066600
H	-0.26475700	0.98506900	-1.27637500

C	0.60341500	3.47099500	-1.53344900
H	0.15872700	3.14311500	-2.47963800
H	0.65896100	4.56200500	-1.52469800
H	1.61217700	3.05342700	-1.46727300
O	-1.61147200	3.35402300	-0.43413700
H	-1.86105700	1.81104900	0.54875600
H	-2.00546100	2.85805100	-1.18099300
H	5.52899200	4.26994800	-1.20542800
H	2.55107600	6.77986900	0.66029000
H	6.74333600	-0.91973800	-2.97076500
H	5.49538500	-5.05076800	-3.12581100
C	1.01578200	-3.73685000	-1.98838900
C	0.66029200	-4.62530700	-0.94718000
C	0.40507500	-2.50894000	-2.12102000
H	1.79226300	-4.01937100	-2.69279900
C	-0.31333900	-4.23750000	-0.05003900
H	1.13867800	-5.59534100	-0.86206700
C	-0.62872700	-2.09417500	-1.23073000
H	0.67928900	-1.82135600	-2.91284800
C	-0.96580700	-2.98380000	-0.15635100
H	-0.60103200	-4.89866900	0.76475600
O	-1.18911300	-0.94793300	-1.43539300
C	-1.92286100	-2.63226500	0.84607200
Co	-2.63226000	-0.21560100	-0.46650900
N	-2.57756900	-1.52012700	0.92295100
H	-2.08756500	-3.37976400	1.62513400
N	-4.02159900	0.59649400	0.55028200
C	-3.58992600	-1.29730500	1.97192200
C	-5.01723800	1.22822700	0.02889000
C	-3.92939600	0.20283400	1.95544100
C	-3.20595600	-1.71737000	3.39220400
H	-5.86241800	1.49565900	0.66292400
C	-5.10114100	1.59832100	-1.35604200
C	-5.13498100	0.48708600	2.84705300
C	-4.38202700	-1.43359600	4.34067200
H	-2.31689500	-1.15870000	3.71240800
H	-2.95045700	-2.78073100	3.43583900
C	-6.33263300	2.06847800	-1.85991900
C	-3.95300300	1.54409100	-2.20828700
C	-4.82266800	0.03555900	4.28312600
H	-5.37760300	1.55560300	2.83844200
H	-6.00497000	-0.05547000	2.45758900
H	-4.10834500	-1.70451000	5.36606300
H	-5.22643700	-2.07537900	4.05828200
C	-6.46384500	2.46382400	-3.17803200
H	-7.18823600	2.10271300	-1.18965200
C	-4.10960900	1.97298400	-3.54640100
O	-2.76215100	1.18079300	-1.78605600
H	-4.02206000	0.66888200	4.68885200
H	-5.69891300	0.19251900	4.92073100
C	-5.33491200	2.41499400	-4.01644700
H	-7.41846500	2.80962100	-3.55926800
H	-3.23744100	1.92923100	-4.18981500
H	-5.42474500	2.72542200	-5.05393800
H	-4.48963400	-1.82506500	1.64093400
H	-3.05763600	0.73588700	2.36250700
C	-5.62676500	-2.22412400	-2.55094300
H	-5.94291800	-1.35833900	-3.14272300
H	-6.49947900	-2.82765000	-2.29792600
H	-4.92300700	-2.79781000	-3.15803000
C	-4.95534700	-1.71564300	-1.28092600
O	-3.76391800	-1.24943000	-1.53399000
O	-5.54128700	-1.74171000	-0.19685700

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon and subsequent hydration

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.276329
Thermal correction to Gibbs Free Energy (a.u.): 0.906373
Imaginary frequencies: -450.04
Calculation of single point energy based on the optimized structure, Et = -6075.8446775 a.u.

C	-7.13097700	2.88980700	-1.40628400
C	-6.32853100	3.83609100	-0.74299800
C	-6.88059700	1.53280400	-1.29486300
H	-7.95932400	3.22737100	-2.02347000
C	-5.28292100	3.38653700	0.04034500
H	-6.53022000	4.89707400	-0.84203100
C	-5.80516700	1.04553500	-0.51387100
H	-7.49338900	0.80125100	-1.81106900
C	-4.99980100	2.00870200	0.17288500
H	-4.65067300	4.09492200	0.57051000
O	-5.62407600	-0.25215500	-0.43600500
C	-3.93110200	1.62420700	1.04812400
Co	-3.96581300	-1.03428900	0.07486900
N	-3.50876800	0.41739000	1.23082900
H	-3.43791500	2.43103400	1.59545500
N	-2.42646100	-1.88101100	0.81082600
C	-2.34503300	0.15129400	2.09776800
C	-1.74150200	-2.81320100	0.24672500
C	-2.16213300	-1.36556700	2.15861000
C	-2.44690500	0.68886300	3.52950400
H	-0.83379200	-3.16947600	0.73043000
C	-2.10026100	-3.43868800	-0.99736300
C	-0.82635500	-1.69319400	2.82085500
C	-1.14996900	0.35904600	4.29013800
H	-3.31413700	0.22553400	4.01848500
H	-2.62378000	1.76855700	3.53205300
C	-1.15327100	-4.27923400	-1.62149700
C	-3.40036400	-3.26653200	-1.56954400
C	-0.83754400	-1.14298000	4.25718400
H	-0.66502400	-2.77702000	2.84892300
H	-0.01331200	-1.23176900	2.24960900
H	-1.23420300	0.70251200	5.32673500
H	-0.30489900	0.89219000	3.84176300
C	-1.44631800	-4.93238400	-2.80481000
H	-0.17386200	-4.38465100	-1.16295400
C	-3.67325000	-3.95380200	-2.77699600
O	-4.35355600	-2.53925800	-1.02629600
H	-1.58377500	-1.69321000	4.84722100
H	0.13550900	-1.32633600	4.72393600
C	-2.71931700	-4.76131100	-3.37649500
H	-0.70579200	-5.56288000	-3.28472500
H	-4.65798600	-3.82365900	-3.21364100
H	-2.96293900	-5.26746500	-4.30674500
O	-3.10842500	-0.19161400	-1.32428000
H	-3.49074400	-0.60676600	-2.11016800
O	-5.18450100	-1.98938300	1.43059300
H	-5.26689500	-2.78711800	0.87527000
H	-5.94598900	-1.43695700	1.16345100
C	-0.30934600	-0.63377200	-1.97682800
C	-1.17991700	0.48636100	-1.66178700
O	0.56599600	0.50376500	-1.99386300
H	-0.11792000	-1.30795100	-1.14873900
H	-1.20256600	0.86362900	-0.65581700
H	-1.57050600	1.09456700	-2.46431600
C	-0.41234200	-1.32767000	-3.31239100
H	0.48445500	-1.92717400	-3.49399500
H	-1.27701700	-1.99586900	-3.32693000
H	-0.51385500	-0.59088400	-4.11512700
C	2.17521700	-4.27631700	0.31246100
C	2.96360800	-4.43760200	-0.84269200
C	1.73904100	-3.02837800	0.71503900
H	1.91419300	-5.14533800	0.91099800
C	3.33706900	-3.30556000	-1.53979700
H	3.29594400	-5.42106600	-1.15617600
C	2.04167100	-1.84935100	-0.02387800

H	1.18100000	-2.91010700	1.63182900
C	2.90741500	-2.01645100	-1.15281000
H	3.99210200	-3.38941800	-2.40416300
O	1.53182500	-0.71634500	0.36331500
C	3.48226100	-0.89260500	-1.82924800
Co	1.74366800	0.97135700	-0.51846100
N	3.19518300	0.34119800	-1.60251100
H	4.26055100	-1.12490500	-2.55702700
N	1.97932100	2.62228700	-1.46554200
C	3.91069800	1.45510600	-2.22806200
C	1.51700000	3.76565200	-1.09241600
C	2.81993600	2.45250400	-2.65275900
C	4.84647000	1.10915800	-3.38491100
H	1.77311500	4.64829200	-1.67905300
C	0.68945300	3.99335200	0.04926000
C	3.42535100	3.72318600	-3.25008700
C	5.45443500	2.38863300	-3.97609100
H	4.28359600	0.57471700	-4.16227800
H	5.64522000	0.44188700	-3.04340300
C	0.37696600	5.33193400	0.38205200
C	0.17484000	2.91525200	0.83530700
C	4.36438600	3.37295100	-4.41300400
H	2.63508300	4.39363300	-3.60389900
H	3.98338900	4.25808500	-2.47037800
H	6.10063800	2.13391300	-4.82259100
H	6.09484300	2.86572400	-3.22266800
C	-0.39962900	5.64355000	1.47871400
H	0.77453900	6.12409000	-0.24849700
C	-0.58234500	3.27179500	1.98171200
O	0.32108500	1.65201500	0.54223300
H	3.77967200	2.92842300	-5.22959500
H	4.81471700	4.28798400	-4.81148600
C	-0.86537300	4.58921700	2.28722200
H	-0.62546300	6.67475200	1.72666800
H	-0.89260000	2.47516000	2.63667900
H	-1.44116800	4.81222400	3.18198500
H	4.48304300	1.93088500	-1.41940000
H	2.19828600	1.95110900	-3.40739200
H	-2.97742300	-1.77036700	2.77476800
H	-1.45712100	0.57279000	1.60840000
S	3.15514600	1.28951200	2.24703000
O	4.16575600	2.19843400	2.80466000
O	1.86670000	1.18293500	2.94887300
O	3.02367900	1.64311300	0.73697100
C	3.86263400	-0.35669700	2.23109500
C	4.88628500	-0.66802200	1.33713000
C	3.40476100	-1.30640200	3.13951800
C	5.42537500	-1.95104000	1.33329600
H	5.23539300	0.08616200	0.64107200
C	3.96169900	-2.58369600	3.13348200
H	2.60521900	-1.03941100	3.82091000
C	4.96642600	-2.93095400	2.22301100
H	6.20835100	-2.20282600	0.62250400
H	3.59722500	-3.33086500	3.83391600
C	5.50145300	-4.33869800	2.15963100
H	5.38333200	-4.85690600	3.11563000
H	4.96222500	-4.91622600	1.39897700
H	6.56235200	-4.35455200	1.89173500

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.290481

Thermal correction to Gibbs Free Energy (a.u.): 0.903680

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6075.8587168 a.u.

C	-6.73539200	3.54559100	-1.48873900
C	-5.85150500	4.37487000	-0.77361600
C	-6.64824400	2.16674100	-1.40837100

H	-7.49739300	3.99309500	-2.12148900
C	-4.89301000	3.78581900	0.02853000
H	-5.92468500	5.45441800	-0.84852500
C	-5.66354000	1.53598700	-0.60764800
H	-7.32333600	1.52464300	-1.96458800
C	-4.77738300	2.38150900	0.13212800
H	-4.19979300	4.40152300	0.59726600
O	-5.63155300	0.22620600	-0.56890300
C	-3.78433900	1.85437400	1.02245200
Co	-4.13254100	-0.77830900	0.03579000
N	-3.51922300	0.60387000	1.19845800
H	-3.20571200	2.59057300	1.58444200
N	-2.73759900	-1.82521400	0.79834100
C	-2.39547900	0.19931800	2.06041700
C	-2.17855300	-2.83637300	0.23026900
C	-2.39236800	-1.33065800	2.13281400
C	-2.43028200	0.74640200	3.49274000
H	-1.32596100	-3.30875900	0.71462500
C	-2.61373100	-3.41292900	-1.01171500
C	-1.08990600	-1.79888400	2.78076800
C	-1.17560400	0.27991900	4.25021900
H	-3.34224000	0.38062800	3.98280800
H	-2.49060100	1.83870900	3.49889200
C	-1.78533200	-4.37267100	-1.63163400
C	-3.87977000	-3.07355600	-1.58868700
C	-1.02480400	-1.24768900	4.21591100
H	-1.03401500	-2.89345600	2.80657700
H	-0.24092600	-1.42036800	2.20044400
H	-1.22064200	0.62725000	5.28805900
H	-0.28268200	0.72698500	3.80117500
C	-2.15453500	-4.98372400	-2.81560500
H	-0.82821300	-4.60225000	-1.17107800
C	-4.23588300	-3.72526300	-2.79560300
O	-4.72826100	-2.23296400	-1.04797600
H	-1.82007200	-1.71480300	4.81310100
H	-0.07395200	-1.53532300	4.67664200
C	-3.39375600	-4.64949000	-3.39132500
H	-1.50145300	-5.70694400	-3.29201400
H	-5.19359000	-3.46792000	-3.23592300
H	-3.69793000	-5.12161100	-4.32184300
O	-3.05529100	-0.15096300	-1.29814900
H	-3.66155100	-0.16030700	-2.05287200
O	-5.54290700	-1.55090100	1.37201300
H	-5.69463000	-2.31794000	0.78799100
H	-6.20579800	-0.89996800	1.07344200
C	-0.40326600	-0.36647700	-1.96015500
C	-0.50536200	1.04949800	-2.27135600
O	0.83069800	0.46180000	-2.09074000
H	-0.58827400	-0.63499800	-0.92968600
H	-0.80023400	1.72587100	-1.48072700
H	-0.67456000	1.37049700	-3.29598500
C	-0.52615800	-1.44084900	-2.99400300
H	0.10671600	-2.29584100	-2.74256200
H	-1.56438300	-1.77758400	-3.01530700
H	-0.24307400	-1.06620000	-3.98217500
C	1.74804200	-4.38532300	-0.05174600
C	2.67242300	-4.55543500	-1.10088200
C	1.39611400	-3.12730100	0.39599900
H	1.31313900	-5.25858500	0.42798400
C	3.25160700	-3.42973600	-1.64997500
H	2.93883300	-5.54668500	-1.45060700
C	1.92928000	-1.94450300	-0.18755200
H	0.72458600	-3.00405800	1.23245000
C	2.90784400	-2.12855500	-1.21663900
H	4.00006600	-3.52843600	-2.43294400
O	1.51992500	-0.79189900	0.25833600
C	3.64813400	-1.02934100	-1.75524100
Co	1.94169100	0.90025300	-0.50782700
N	3.42954200	0.21398400	-1.49837400

H	4.48152000	-1.29026300	-2.40852400
N	2.34317500	2.55953700	-1.38152700
C	4.27623000	1.30055500	-1.99219200
C	1.92440700	3.71633400	-0.98973200
C	3.29912100	2.38563500	-2.47962400
C	5.30366400	0.94176700	-3.06394900
H	2.28671200	4.60485500	-1.50735000
C	1.02600100	3.94576600	0.09531600
C	4.04189800	3.63843500	-2.94449400
C	6.04973800	2.20201800	-3.52439000
H	4.79342300	0.48026200	-3.92033200
H	6.01776400	0.20756500	-2.67569700
C	0.78099700	5.28496500	0.48228500
C	0.38729400	2.86810800	0.78643100
C	5.07664500	3.27747400	-4.01979100
H	3.33755900	4.37598500	-3.34362600
H	4.54459300	4.09833400	-2.08372700
H	6.76371500	1.94178500	-4.31260400
H	6.63629500	2.60042500	-2.68626700
C	-0.04215500	5.58979100	1.54562400
H	1.27137300	6.07980100	-0.07514700
C	-0.41254700	3.21337400	1.90479400
O	0.46171200	1.61544600	0.42439300
H	4.55628000	2.91209800	-4.91534800
H	5.62380600	4.17688200	-4.32029400
C	-0.62624200	4.52927500	2.26607300
H	-0.21571900	6.61951700	1.83765700
H	-0.81576600	2.40369600	2.48908900
H	-1.24022600	4.74589800	3.13657100
H	4.78935900	1.70483400	-1.10875200
H	2.74166900	1.95925300	-3.32627000
H	-3.23716400	-1.63018900	2.76948400
H	-1.46956000	0.51254400	1.55896200
S	3.16295400	1.00515700	2.34205900
O	4.22779800	1.78645300	2.98342100
O	1.83089400	1.00737200	2.96198800
O	3.15002600	1.44522700	0.84275600
C	3.70259700	-0.70033000	2.27894200
C	4.79815500	-1.05331100	1.49233300
C	3.03659900	-1.65778700	3.03796600
C	5.20266600	-2.38425800	1.44262700
H	5.31243100	-0.29231000	0.91612100
C	3.45813600	-2.98431900	2.98599900
H	2.18565400	-1.35541000	3.63672300
C	4.53444300	-3.37121200	2.17862100
H	6.04474000	-2.66695100	0.81612000
H	2.93163700	-3.73694300	3.56710800
C	4.92811900	-4.82122000	2.05943100
H	4.68284300	-5.37999600	2.96727800
H	4.39381800	-5.29130100	1.22517100
H	5.99964000	-4.93296700	1.86855200

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.305871

Thermal correction to Gibbs Free Energy (a.u.): 0.911266

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6075.8796332 a.u.

C	-6.71144900	2.96469600	-1.42441500
C	-5.87461500	3.86024100	-0.73526700
C	-6.55177300	1.59302300	-1.30504200
H	-7.49383600	3.35187800	-2.07130900
C	-4.88817700	3.35139700	0.08831000
H	-6.00377900	4.93111400	-0.84637500
C	-5.53712300	1.04766200	-0.48806000
H	-7.19075500	0.90086100	-1.84301600
C	-4.70226400	1.95795000	0.22989600
H	-4.22617600	4.01795500	0.63568100

O	-5.42899400	-0.26431300	-0.40403100
C	-3.69378800	1.50384500	1.14249500
Co	-3.80630300	-1.11940600	0.09110200
N	-3.32296300	0.27495600	1.29620200
H	-3.18523200	2.26842800	1.73235900
N	-2.28369000	-2.02116600	0.78857500
C	-2.19792200	-0.06359200	2.19234600
C	-1.60193800	-2.91913200	0.16669300
C	-2.02359100	-1.58048400	2.16529200
C	-2.35910000	0.37724400	3.65032400
H	-0.68687100	-3.29243600	0.62045500
C	-1.97508100	-3.48145000	-1.10397000
C	-0.69083900	-1.93815000	2.81845200
C	-1.07876500	0.01077300	4.42153100
H	-3.23580500	-0.12724000	4.07884200
H	-2.54707700	1.45244500	3.71673900
C	-1.02919100	-4.26948000	-1.79327100
C	-3.28279200	-3.29301300	-1.64506400
C	-0.73569000	-1.48036000	4.28808400
H	-0.51620100	-3.01960600	2.78067000
H	0.12134400	-1.42941800	2.28796800
H	-1.19864300	0.27268600	5.47819200
H	-0.23544100	0.59134700	4.03436500
C	-1.34462400	-4.86561900	-3.00122400
H	-0.03590200	-4.37611300	-1.36711400
C	-3.58396600	-3.92607900	-2.87071000
O	-4.22619800	-2.56868300	-1.05955200
H	-1.47801100	-2.08505900	4.82808900
H	0.23415700	-1.67589800	4.75597200
C	-2.63340700	-4.69203800	-3.53080800
H	-0.60535500	-5.45487300	-3.53228200
H	-4.57984400	-3.78635100	-3.27789400
H	-2.89334500	-5.15679400	-4.47774400
O	-2.95503000	-0.25280400	-1.39713300
H	-3.12857900	-0.78721100	-2.18522400
O	-5.00362500	-2.04014400	1.37217400
H	-5.13096700	-2.83695900	0.82015800
H	-5.77158100	-1.46981000	1.15831100
C	-0.48873200	-0.36068300	-1.90581500
C	-1.69839000	0.49683500	-1.52994400
O	0.60428000	0.48520000	-2.00913600
H	-0.35236500	-1.11672400	-1.12188600
H	-1.52682200	0.97051700	-0.57071800
H	-1.87632500	1.26240400	-2.29183700
C	-0.67395600	-1.06875400	-3.25271100
H	0.20150500	-1.69078900	-3.45346500
H	-1.55254700	-1.72460700	-3.28202800
H	-0.75773200	-0.32294400	-4.05091500
C	2.31038400	-4.26726800	0.02436300
C	3.10526300	-4.31388800	-1.13566300
C	1.81286400	-3.06961300	0.50352500
H	2.09641300	-5.18441300	0.56793600
C	3.43097200	-3.11798200	-1.74849600
H	3.48616300	-5.25671700	-1.51282800
C	2.05452800	-1.82838700	-0.15601200
H	1.26400900	-3.03799300	1.43331800
C	2.94241600	-1.87976200	-1.28069400
H	4.09802900	-3.11262500	-2.60796300
O	1.49703500	-0.75114100	0.30451700
C	3.48753900	-0.68796700	-1.86247400
Co	1.61653900	0.98569600	-0.50573900
N	3.15122100	0.51160400	-1.54921900
H	4.28746700	-0.83971600	-2.58833700
N	1.76036000	2.69117700	-1.38058400
C	3.79763600	1.69727400	-2.10906400
C	1.15635500	3.77222400	-1.03447600
C	2.64134200	2.61496400	-2.54712400
C	4.79912600	1.46664500	-3.23920200
H	1.31786700	4.67684700	-1.62215900

C	0.30207000	3.91228100	0.10679200
C	3.15615900	3.94504900	-3.09894900
C	5.31992700	2.80896100	-3.76993100
H	4.30954900	0.91634700	-4.05411700
H	5.63507100	0.85223000	-2.88697700
C	-0.14193500	5.20872200	0.44645500
C	-0.06146200	2.79024600	0.91651900
C	4.16630100	3.70665000	-4.22972700
H	2.32464100	4.55211600	-3.47246200
H	3.63395500	4.51033700	-2.28781500
H	6.02077700	2.63559600	-4.59348300
H	5.88378700	3.31803100	-2.97716200
C	-0.88098500	5.44940400	1.58940000
H	0.12912600	6.03261700	-0.21034900
C	-0.72977600	3.08542200	2.13612000
O	0.14487200	1.54724000	0.58567100
H	3.65497700	3.23291100	-5.07862100
H	4.55011300	4.66690800	-4.59027900
C	-1.13965300	4.36850900	2.45237500
H	-1.20771400	6.45251800	1.84074600
H	-0.85509800	2.27660100	2.83725600
H	-1.64600200	4.54463700	3.39846700
H	4.29952500	2.19107500	-1.26522200
H	2.07882200	2.07734000	-3.32211100
H	-2.84014700	-2.02322700	2.75305800
H	-1.29263700	0.38371300	1.75914300
S	2.98367500	1.25512600	2.32811700
O	3.91995900	2.17202100	2.99560700
O	1.69852600	0.99845200	3.00692700
O	2.83512700	1.70670300	0.86111300
C	3.79941200	-0.33794500	2.19974800
C	4.83657900	-0.51823000	1.28563400
C	3.40931200	-1.38061700	3.03498400
C	5.45529400	-1.76080900	1.18528500
H	5.13151600	0.30521500	0.64556400
C	4.04358300	-2.61726300	2.93244000
H	2.59952400	-1.21559200	3.73636800
C	5.06243000	-2.83232300	1.99754800
H	6.24805200	-1.90916400	0.45620400
H	3.72969400	-3.43662900	3.57449100
C	5.68171700	-4.19589900	1.82466900
H	5.58034700	-4.80090600	2.73046100
H	5.18970400	-4.73556000	1.00648500
H	6.74600000	-4.12673700	1.57864400

subsequent hydration

OTs-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-OTs + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.690516

Thermal correction to Gibbs Free Energy (a.u.): 0.932603

Imaginary frequencies: -450.96

Calculation of single point energy based on the optimized structure, Et = -6152.3185253 a.u.

C	7.18956300	-2.78008200	-2.13110800
C	6.46108400	-3.80331700	-1.49548600
C	6.95536200	-1.44754100	-1.84217000
H	7.94681800	-3.03819200	-2.86630100
C	5.50511300	-3.45497700	-0.56268600
H	6.64970900	-4.84428800	-1.73323500
C	5.96969000	-1.06087400	-0.90067900
H	7.51171600	-0.65622900	-2.33346200
C	5.23794600	-2.10227800	-0.24634800
H	4.93265300	-4.22578100	-0.05212600
O	5.79791600	0.21952500	-0.66844300
C	4.25048000	-1.83177700	0.75764800
Co	4.28043800	0.96087900	0.20571200
N	3.84398700	-0.66118500	1.12154000
H	3.80477700	-2.70594800	1.23765900
N	2.84946800	1.71534000	1.18859200
C	2.73866500	-0.50735900	2.08711500

C	2.11570300	2.68881300	0.76911300
C	2.64361100	0.98157100	2.43691100
C	2.86837800	-1.30938700	3.38648800
H	1.22238700	2.95861500	1.32774000
C	2.40893400	3.46404600	-0.40393500
C	1.36449900	1.24312400	3.22558000
C	1.61915500	-1.07281300	4.25140700
H	3.77390000	-0.98195600	3.91372500
H	2.99092100	-2.37858600	3.18928400
C	1.41497900	4.32910700	-0.90764900
C	3.69689600	3.40691600	-1.02236100
C	1.39349000	0.42040200	4.52450000
H	1.27679500	2.30839500	3.46739000
H	0.50303100	0.95517100	2.61286400
H	1.71334800	-1.61930900	5.19547300
H	0.74257000	-1.48026300	3.73419900
C	1.65848000	5.12411600	-2.01368900
H	0.44480100	4.34710000	-0.42080900
C	3.92364800	4.24483500	-2.13621000
O	4.67953600	2.64191400	-0.58666700
H	2.19548400	0.79901600	5.17289500
H	0.45379900	0.56139300	5.06762700
C	2.92512700	5.07775200	-2.61961200
H	0.88297400	5.77352800	-2.40498700
H	4.90164300	4.20497500	-2.60429200
H	3.12861300	5.69988000	-3.48707000
O	3.18757700	0.56082600	-1.23011500
H	3.80406500	0.59173600	-1.97553000
O	5.65312300	1.58829200	1.57857700
H	5.68949900	2.48092100	1.18050300
H	6.39445600	1.11247700	1.15943500
C	0.65521600	0.31562900	-1.70902000
C	1.75780500	-0.77465700	-1.75545600
O	-0.62845600	-0.26324700	-1.83123700
H	0.75535100	0.79899200	-0.73632300
H	1.98398700	-1.33304400	-0.86390300
H	2.36539500	-0.93536900	-2.63098700
C	0.81808800	1.33735200	-2.83220400
H	0.04499100	2.10193300	-2.72738900
H	1.79425000	1.82178100	-2.79016400
H	0.68988200	0.84895500	-3.80469900
C	-1.59417600	4.36495200	1.38220600
C	-2.38095500	4.77743500	0.29112400
C	-1.21102500	3.04380100	1.53007400
H	-1.28547500	5.09195900	2.12907300
C	-2.82807900	3.80970000	-0.58961900
H	-2.66523400	5.81687300	0.17065900
C	-1.56809700	2.04089300	0.58005400
H	-0.64750000	2.73262200	2.39879000
C	-2.47099700	2.45135100	-0.45373800
H	-3.50570900	4.08092200	-1.39589000
O	-1.09143800	0.84076800	0.71367700
C	-3.19651000	1.50003400	-1.24096900
Co	-1.65385300	-0.70619000	-0.28617200
N	-3.09548100	0.22019500	-1.15770100
H	-3.94855400	1.92026300	-1.90728700
N	-2.28936900	-2.22456700	-1.25180300
C	-3.99189600	-0.67667100	-1.89582300
C	-2.13220000	-3.44086200	-0.86513800
C	-3.12552100	-1.84056200	-2.39134500
C	-4.81301000	-0.06652500	-3.02834500
H	-2.68876300	-4.22897200	-1.37013100
C	-1.22069400	-3.86332600	0.15861600
C	-3.99058500	-2.93522300	-3.01087000
C	-5.67247400	-1.15787700	-3.68509300
H	-4.14563800	0.39080600	-3.77170400
H	-5.46559200	0.72257300	-2.63979800
C	-1.21708100	-5.23086000	0.51038800
C	-0.26088100	-2.96663800	0.73370400

C	-4.82449700	-2.34480700	-4.15763900
H	-3.36513300	-3.75126700	-3.38959900
H	-4.65054200	-3.34790200	-2.23800900
H	-6.23321100	-0.73305100	-4.52452800
H	-6.41316700	-1.51240600	-2.95655200
C	-0.30014600	-5.75191400	1.40236500
H	-1.96561500	-5.87675400	0.05811000
C	0.68913800	-3.54410900	1.61557900
O	-0.17205900	-1.69238100	0.45081100
H	-4.15079000	-2.01419800	-4.95972600
H	-5.46634500	-3.12146100	-4.58661200
C	0.66516300	-4.88733100	1.94552200
H	-0.31983300	-6.80209700	1.67103500
H	1.42635200	-2.88691000	2.04847600
H	1.40358500	-5.27434500	2.64328900
O	0.61331300	-2.22275700	-2.42976300
H	0.53734300	-2.81539500	-1.66726400
H	-0.15805700	-1.52010500	-2.27420900
H	-2.43647300	-1.44445800	-3.14976100
H	-4.67058500	-1.10396600	-1.15174600
H	1.80896700	-0.78205400	1.56792200
H	3.51270600	1.22823500	3.06290700
S	-4.08904300	-1.53867100	1.61375700
O	-2.60198300	-1.27246700	1.31995300
O	-4.74358700	-2.35896900	0.56640200
O	-4.21818300	-1.99826400	3.00062200
C	-4.81639300	0.09716400	1.49755900
C	-4.19861000	1.15577300	2.16666400
C	-5.95646700	0.31568300	0.72983300
C	-4.70684100	2.44143200	2.03008200
H	-3.30390000	0.96976500	2.74901600
C	-6.44947000	1.61458800	0.58968500
H	-6.43440300	-0.52424600	0.23848400
C	-5.82766100	2.69454700	1.22631600
H	-4.20117900	3.26960600	2.51715400
H	-7.32945200	1.79109000	-0.02385200
C	-6.32788200	4.10597200	1.04891600
H	-5.52459300	4.75616300	0.68527200
H	-7.15608200	4.15261100	0.33653100
H	-6.67875200	4.52658100	1.99826200

subsequent hydration

$OTs\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OTs + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.730424

Thermal correction to Gibbs Free Energy (a.u.): 0.933474

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6152.3699301 a.u.

C	6.86841100	-2.82836700	-2.19667200
C	6.14739100	-3.81478600	-1.49984700
C	6.68313600	-1.48165400	-1.93166200
H	7.57903700	-3.12413300	-2.96317700
C	5.25045200	-3.42003200	-0.52755500
H	6.29388500	-4.86545700	-1.72314900
C	5.75698900	-1.05084700	-0.95453500
H	7.23221000	-0.71836300	-2.47274300
C	5.03785700	-2.05280100	-0.23254100
H	4.68227800	-4.16104000	0.02876200
O	5.61678200	0.24721900	-0.75867700
C	4.11996800	-1.73045200	0.82054700
Co	4.16227400	1.03813700	0.16281000
N	3.76986500	-0.53817900	1.17671600
H	3.67284300	-2.57592600	1.34676900
N	2.76178800	1.82966100	1.16214500
C	2.72971000	-0.33382800	2.20602300
C	1.99892500	2.77154400	0.72026500
C	2.62762000	1.17111900	2.46358300
C	2.96010700	-1.04702900	3.54173100
H	1.12195400	3.05711000	1.29773500

C	2.23719700	3.48559600	-0.50364700
C	1.38052900	1.45847300	3.29299100
C	1.75118300	-0.78151300	4.45515900
H	3.88402800	-0.66578000	3.99590100
H	3.09706400	-2.12317300	3.40133200
C	1.21082800	4.30608100	-1.01842200
C	3.49917000	3.40914300	-1.16774300
C	1.49540800	0.72127400	4.63868700
H	1.27687500	2.53457100	3.47109600
H	0.50073600	1.11233300	2.73935700
H	1.90974900	-1.25802600	5.42787300
H	0.86195200	-1.24681600	4.01362000
C	1.40482800	5.03933000	-2.17552800
H	0.25739700	4.33719900	-0.50053500
C	3.67709000	4.18333100	-2.33261400
O	4.50939000	2.67184000	-0.72999100
H	2.31536600	1.16307100	5.22134000
H	0.57874200	0.87418400	5.21647100
C	2.64920300	4.97659600	-2.82354700
H	0.60534000	5.65318500	-2.57522200
H	4.63768100	4.12895800	-2.83377500
H	2.81199700	5.55103700	-3.73120400
O	3.01597200	0.57390300	-1.28609200
H	3.58639000	0.42905100	-2.05316600
O	5.54930300	1.70963200	1.41111500
H	5.59146800	2.59276900	0.98896900
H	6.29382600	1.21582300	1.01643400
C	0.58490700	0.53588600	-1.70162900
C	1.82147400	-0.28407200	-1.32269500
O	-0.49940500	-0.34409000	-1.74437900
H	0.44459300	1.30407100	-0.93381900
H	1.68309400	-0.71061900	-0.33571200
H	1.99796300	-1.08785300	-2.04001900
C	0.73704400	1.22229300	-3.05934500
H	-0.16606100	1.79871900	-3.27600700
H	1.59023000	1.90847600	-3.07007200
H	0.86412100	0.47365900	-3.84948700
C	-1.70876200	4.37907000	1.37416700
C	-2.47098600	4.74148000	0.24935800
C	-1.28732500	3.07390500	1.56228500
H	-1.45054200	5.13117200	2.11554500
C	-2.85727700	3.73918900	-0.62391000
H	-2.78717800	5.76750600	0.09698100
C	-1.58003600	2.03831700	0.62346000
H	-0.74511400	2.79985900	2.45726100
C	-2.46147600	2.39784800	-0.44855500
H	-3.51711900	3.97131400	-1.45679800
O	-1.06015900	0.86211000	0.78906200
C	-3.12330100	1.40679200	-1.24836800
Co	-1.53753700	-0.73218900	-0.20544200
N	-2.97688900	0.13455500	-1.14302800
H	-3.86508300	1.79049300	-1.94775100
N	-2.09806900	-2.28648800	-1.14234200
C	-3.81001300	-0.80684000	-1.90115600
C	-1.84994200	-3.49189800	-0.77979100
C	-2.88522800	-1.95128900	-2.32896000
C	-4.59650900	-0.24668300	-3.08266400
H	-2.32065100	-4.30914800	-1.32390300
C	-0.94487100	-3.86874000	0.26891200
C	-3.67953400	-3.08619400	-2.96922300
C	-5.38840100	-1.37951000	-3.75393300
H	-3.90876000	0.21553200	-3.80416500
H	-5.29168000	0.52911200	-2.74373600
C	-0.84998700	-5.24004600	0.58918200
C	-0.09064900	-2.91556900	0.91415300
C	-4.47945500	-2.54454200	-4.16315200
H	-3.00292600	-3.87728300	-3.30902600
H	-4.35787000	-3.51620900	-2.22177600
H	-5.92531000	-0.99053000	-4.62597400

H	-6.14847100	-1.74519100	-3.05113900
C	0.04707400	-5.71343200	1.52802300
H	-1.51285300	-5.93095400	0.07381700
C	0.82226400	-3.43832700	1.86968600
O	-0.07256000	-1.63728500	0.65485600
H	-3.77986100	-2.20428400	-4.93846000
H	-5.07397700	-3.34992500	-4.60752600
C	0.88716400	-4.78764600	2.16854600
H	0.09713800	-6.76971400	1.76762000
H	1.44963800	-2.73395700	2.39339500
H	1.59312200	-5.13061800	2.92127900
O	0.47840600	-2.68883800	-2.78040500
H	0.55503900	-3.21156700	-1.97219900
H	0.05250900	-1.85927200	-2.45671800
H	-2.16491000	-1.55411100	-3.05494400
H	-4.50777700	-1.23758000	-1.17641000
H	1.77235100	-0.66027700	1.77453300
H	3.51889800	1.47411100	3.03076700
S	-4.03034900	-1.58273800	1.63302300
O	-2.54416500	-1.28180000	1.39071800
O	-4.62728700	-2.43991700	0.58124800
O	-4.20807100	-2.01261100	3.02513700
C	-4.79829300	0.03072500	1.45540900
C	-4.24562800	1.11758700	2.13620900
C	-5.90602900	0.20475700	0.63120400
C	-4.78568300	2.38506900	1.95756600
H	-3.37475400	0.96669900	2.76330900
C	-6.43115000	1.48575500	0.44856600
H	-6.33365100	-0.65632100	0.13020300
C	-5.87429200	2.59271400	1.09845700
H	-4.32981500	3.23512900	2.45625400
H	-7.28538300	1.62674700	-0.20911400
C	-6.40957200	3.98521500	0.87784200
H	-5.61131500	4.65633500	0.54197600
H	-7.20469200	3.99589600	0.12722900
H	-6.81775600	4.40712600	1.80350900

subsequent hydration

$OTs\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OTs + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.737324

Thermal correction to Gibbs Free Energy (a.u.): 0.932011

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6152.366488 a.u.

C	7.81195600	-2.86620600	-1.82508500
C	7.04275700	-3.90878400	-1.27338300
C	7.51286100	-1.54136400	-1.56622600
H	8.65331600	-3.10425300	-2.47044100
C	5.97844200	-3.58464900	-0.45647700
H	7.28312900	-4.94461800	-1.48632800
C	6.41850700	-1.17885200	-0.73962500
H	8.09961700	-0.73512600	-1.99390500
C	5.64309300	-2.24028600	-0.17232900
H	5.37081200	-4.37091100	-0.01420700
O	6.19601400	0.09246400	-0.52357600
C	4.53837700	-1.99834000	0.70823100
Co	4.60061900	0.80660100	0.23036900
N	4.08048900	-0.84166800	1.05223800
H	4.05106200	-2.88930300	1.11137400
N	3.10608100	1.54836400	1.12838900
C	2.86062900	-0.72091300	1.87133400
C	2.44174500	2.57289400	0.71744400
C	2.76223200	0.74763900	2.30274600
C	2.79762000	-1.61470400	3.11577900
H	1.51375100	2.83792900	1.21878700
C	2.85485500	3.42547300	-0.36192100
C	1.42574800	1.01178500	2.98923100
C	1.48809900	-1.36135300	3.88162000
H	3.66480800	-1.38974200	3.75020500

H	2.87153900	-2.67376200	2.84880800
C	1.94634700	4.39600100	-0.83659700
C	4.17645900	3.34982100	-0.90527600
C	1.31030300	0.11986400	4.23492800
H	1.35220800	2.06514500	3.28355200
H	0.60800400	0.79028100	2.29366700
H	1.46905800	-1.97323500	4.78958700
H	0.63966900	-1.68247100	3.26739900
C	2.29953100	5.27653100	-1.84244700
H	0.95014100	4.42693300	-0.40380300
C	4.51547700	4.27645000	-1.92054700
O	5.08861700	2.50150300	-0.48963100
H	2.07308800	0.42027500	4.96615900
H	0.33620100	0.27456300	4.70969500
C	3.59872500	5.20898600	-2.37721600
H	1.58871100	6.00862600	-2.21038100
H	5.51804200	4.22143200	-2.33176200
H	3.89071300	5.89719700	-3.16612900
O	3.59003600	0.40242200	-1.23585800
H	4.19921600	0.60875700	-1.95976300
O	5.90372200	1.39495500	1.75269700
H	5.96988100	2.28694200	1.36092000
H	6.64358100	0.91025300	1.34126900
C	0.47883300	0.11924400	-1.92712400
C	1.31604500	-0.95738200	-2.63287800
O	-0.91908600	-0.32974600	-2.06522500
H	0.70678100	0.12433700	-0.86162900
H	2.33719500	-0.90967700	-2.24688700
H	1.31518200	-0.80108600	-3.71655900
C	0.63794800	1.50402300	-2.50851200
H	0.00926200	2.22373700	-1.97943600
H	1.68142200	1.80441700	-2.38806300
H	0.37161900	1.51700200	-3.57066000
C	-1.38302500	4.34798000	1.16881400
C	-2.29250000	4.80215900	0.19426000
C	-1.05594100	3.00926500	1.27577800
H	-0.93367500	5.05843300	1.85783600
C	-2.90048800	3.86429300	-0.61593800
H	-2.53321000	5.85575600	0.10695300
C	-1.59870500	2.02853300	0.39669200
H	-0.39153100	2.66556200	2.05530000
C	-2.59787600	2.48722200	-0.52101500
H	-3.65765500	4.17266800	-1.33282200
O	-1.17998100	0.80113600	0.48598600
C	-3.43472500	1.58026600	-1.24057500
Co	-1.94281800	-0.70739500	-0.40298500
N	-3.37970800	0.29314400	-1.18628900
H	-4.22454200	2.03894600	-1.83347000
N	-2.73143800	-2.19769200	-1.29818000
C	-4.38335900	-0.55401400	-1.84507400
C	-2.66719200	-3.40407100	-0.84448400
C	-3.63519700	-1.78349500	-2.37588700
C	-5.23562600	0.09126500	-2.93509500
H	-3.33380400	-4.15592100	-1.26364100
C	-1.73725500	-3.85740600	0.14415300
C	-4.61632700	-2.82962400	-2.89873500
C	-6.21138000	-0.95006800	-3.50634700
H	-4.59013300	0.48785700	-3.73073800
H	-5.80655900	0.93084400	-2.52499500
C	-1.84540300	-5.18770500	0.60407600
C	-0.63689700	-3.04308000	0.55476800
C	-5.48591600	-2.20709800	-4.00152100
H	-4.07757400	-3.69808300	-3.29339600
H	-5.24724400	-3.17341600	-2.07010800
H	-6.79446500	-0.50348700	-4.31852600
H	-6.92591300	-1.23279500	-2.72245600
C	-0.89453500	-5.74162900	1.43921200
H	-2.70099300	-5.77596500	0.28235100
C	0.35487100	-3.65898700	1.35249000

O	-0.45697100	-1.79935400	0.16374800
H	-4.84995300	-1.94743800	-4.85853100
H	-6.21080500	-2.94458100	-4.36110800
C	0.22210500	-4.96495200	1.79238000
H	-0.99608200	-6.75978200	1.79765200
H	1.22138000	-3.06961200	1.61499000
H	0.99719600	-5.39276600	2.42275000
O	0.70427600	-2.24193100	-2.42509500
H	0.66322100	-2.36950400	-1.46055600
H	-0.78470200	-1.26294800	-2.36623200
H	-2.99614500	-1.45084700	-3.20694200
H	-5.03698200	-0.92146100	-1.04849800
H	2.00176300	-0.93167200	1.21776600
H	3.57551400	0.92571700	3.02083800
S	-4.22744500	-1.32307900	1.69001300
O	-2.74796000	-1.17036100	1.25642800
O	-5.03177600	-2.08974700	0.71180900
O	-4.23529100	-1.78138900	3.08116500
C	-4.83241600	0.36205100	1.64692400
C	-4.09396600	1.35591200	2.29342500
C	-6.00453300	0.67839700	0.96681300
C	-4.52105400	2.67601800	2.22592700
H	-3.17816300	1.09276000	2.80962100
C	-6.41407500	2.01126100	0.89492300
H	-6.57626200	-0.11239100	0.49463500
C	-5.67690100	3.02718400	1.51361400
H	-3.92803600	3.45325000	2.69794200
H	-7.32132800	2.26469300	0.35251600
C	-6.09295600	4.47261900	1.41163100
H	-5.28636000	5.07494000	0.97960200
H	-6.98253400	4.59222600	0.78746900
H	-6.31660000	4.89238700	2.39878700

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon and subsequent hydration

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.276245

Thermal correction to Gibbs Free Energy (a.u.): 0.903285

Imaginary frequencies: -389.20

Calculation of single point energy based on the optimized structure, Et = -6075.8437945 a.u.

C	7.94890300	-2.61963500	2.60132200
C	8.13157300	-1.37305000	3.23225600
C	7.03828000	-2.77561600	1.57376800
H	8.53117000	-3.47660600	2.92913100
C	7.37964100	-0.29884700	2.80363700
H	8.84742600	-1.26265000	4.03930900
C	6.25067400	-1.68801500	1.11263200
H	6.89248000	-3.73424200	1.08708200
C	6.43709900	-0.42242400	1.75487200
H	7.50006700	0.67406500	3.27493200
O	5.42619800	-1.89719500	0.12026300
C	5.69553800	0.74541400	1.38252100
Co	4.12811000	-0.66746800	-0.54609800
N	4.79445400	0.81687800	0.46081600
H	5.92311300	1.64663900	1.95471300
N	2.94877300	0.57515900	-1.34426700
C	3.97917300	2.02634100	0.26350800
C	1.83890300	0.27500500	-1.93641700
C	3.43302700	1.94908800	-1.16862000
C	4.66823600	3.37082000	0.50910900
H	1.18253500	1.07801200	-2.25012000
C	1.41192300	-1.05614600	-2.26132200
C	2.44485500	3.07801200	-1.44979000
C	3.69024300	4.52196500	0.22254100
H	5.54789300	3.44627500	-0.14347900
H	5.02381300	3.44637900	1.54161100
C	0.12681600	-1.22789400	-2.82879100

C	2.30223500	-2.16848000	-2.14649700
C	3.10852900	4.43702800	-1.19334600
H	2.08227800	3.02994200	-2.47898100
H	1.56439000	2.97033500	-0.80743900
H	4.19670400	5.48130400	0.37234200
H	2.87007700	4.48233200	0.95228400
C	-0.26662900	-2.45540200	-3.32838800
H	-0.57463400	-0.40176800	-2.82707600
C	1.86289300	-3.41568900	-2.64862600
O	3.51986200	-2.08563700	-1.65000800
H	3.91209600	4.59409400	-1.92539700
H	2.37355000	5.23209200	-1.35419500
C	0.61600300	-3.54593400	-3.24194600
H	-1.25185800	-2.56752600	-3.76607600
H	2.54395000	-4.25664200	-2.56940200
H	0.31354900	-4.51572600	-3.62902100
O	2.95818500	-1.04748000	0.82531200
H	3.08123700	-2.00318200	0.91932600
O	5.48466900	-0.44873200	-2.09390600
H	4.98460900	-1.10472400	-2.62037900
H	6.16770500	-0.99021300	-1.65836100
C	0.81666200	-0.71901800	1.27019300
C	0.76073000	0.71900400	1.49710500
O	-0.60098600	0.37457500	1.71635100
H	0.54126000	-1.04153300	0.27738600
H	0.92089200	1.34814500	0.62369500
H	1.24956800	1.10316700	2.39822300
C	0.87561100	-1.71960700	2.37993200
H	1.24913900	-2.67420300	2.00489100
H	1.51463900	-1.37104500	3.19471600
H	-0.13340400	-1.89909100	2.75819800
C	-1.46671100	-4.54225300	0.59071900
C	-2.33998200	-4.64599100	1.69260700
C	-1.24790000	-3.33448100	-0.04166600
H	-0.95394300	-5.42895800	0.22671800
C	-2.96823000	-3.50304500	2.14464500
H	-2.50766000	-5.60119600	2.17853400
C	-1.89725800	-2.14505300	0.39124900
H	-0.58911700	-3.25899400	-0.89662800
C	-2.75023900	-2.24658400	1.53498100
H	-3.64464200	-3.55148900	2.99523100
O	-1.68607000	-1.05000500	-0.27742200
C	-3.42374500	-1.10682500	2.07824300
Co	-1.97917800	0.68957200	0.39448200
N	-3.21966700	0.11567200	1.72609900
H	-4.15409000	-1.31202500	2.86142500
N	-2.21776900	2.44143800	1.14577100
C	-3.94190600	1.25487200	2.28969300
C	-1.96763100	3.54711700	0.53122100
C	-2.88432900	2.36891200	2.44783400
C	-4.69681400	1.00418400	3.59439300
H	-2.21614800	4.48963000	1.02152500
C	-1.43163700	3.64823600	-0.79446500
C	-3.50643800	3.66301000	2.97047100
C	-5.31605700	2.30867600	4.11459800
H	-4.00314600	0.59720300	4.34257400
H	-5.48279500	0.25748300	3.43951800
C	-1.40244200	4.91908400	-1.40958600
C	-0.98881300	2.49294900	-1.51366700
C	-4.25647500	3.40288000	4.28443200
H	-2.73295300	4.42288700	3.12763500
H	-4.20351000	4.05773800	2.21959900
H	-5.82745800	2.12242000	5.06483300
H	-6.08172900	2.65238900	3.40666400
C	-1.00816900	5.07438000	-2.72514800
H	-1.72379400	5.78194900	-0.83015900
C	-0.67213700	2.67033500	-2.88599900
O	-0.80629900	1.32563600	-0.95743900
H	-3.53879900	3.09724700	5.05771700

H	-4.71976800	4.33102600	4.63512300
C	-0.67110800	3.92631000	-3.46645900
H	-1.00157300	6.05401100	-3.19033200
H	-0.45928500	1.78645000	-3.47451700
H	-0.42069100	4.02273900	-4.51947600
H	-4.64381500	1.58815400	1.51292200
H	-2.13784100	2.00177700	3.16559700
H	4.29488800	2.05442100	-1.84375900
H	3.12343600	1.93622600	0.94544400
S	-3.95571100	0.37241200	-1.99278000
O	-5.10504300	1.12247200	-2.51730700
O	-2.85745100	0.05174100	-2.91769500
O	-3.48109100	1.12225100	-0.71429500
C	-4.58982600	-1.17652900	-1.34978700
C	-5.61744400	-1.15055400	-0.40745800
C	-4.05448300	-2.38748200	-1.77815700
C	-6.08841200	-2.34881100	0.12518900
H	-6.04015600	-0.19987000	-0.10004000
C	-4.53696200	-3.57825700	-1.24216500
H	-3.24208400	-2.37719800	-2.49352400
C	-5.54977100	-3.57845400	-0.27572400
H	-6.88535400	-2.33205400	0.86466500
H	-4.09910200	-4.52131500	-1.55650500
C	-6.01790000	-4.87357500	0.33859300
H	-6.91259300	-4.72796000	0.95041900
H	-6.25017200	-5.61985100	-0.42845700
H	-5.23504100	-5.29673100	0.97823400

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.293514

Thermal correction to Gibbs Free Energy (a.u.): 0.902815

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6075.8615794 a.u.

C	7.94692600	-2.16478500	2.60738000
C	7.90629700	-1.00206800	3.40295400
C	7.15529300	-2.29044100	1.48244600
H	8.60954900	-2.98053100	2.88423600
C	7.05525100	0.01955600	3.03581500
H	8.53019000	-0.91497500	4.28575500
C	6.26824500	-1.25567700	1.08010000
H	7.18048000	-3.18538600	0.86957700
C	6.22945200	-0.07436800	1.89000900
H	7.00374100	0.92732200	3.63322400
O	5.56609600	-1.42947500	-0.00566800
C	5.37226400	1.03468200	1.59369900
Co	4.17783900	-0.28563300	-0.64391200
N	4.55522500	1.12199700	0.59803000
H	5.42342700	1.86688900	2.29871700
N	2.91402500	0.91038000	-1.39672200
C	3.59165200	2.22705600	0.47869800
C	1.84815200	0.54072700	-2.02604600
C	3.19534500	2.29039800	-1.00393300
C	4.04224200	3.59900200	0.98356700
H	1.06772600	1.27071100	-2.22475200
C	1.61167800	-0.78553600	-2.51342800
C	2.09432500	3.31547600	-1.25792300
C	2.93345100	4.63597100	0.74245800
H	4.95878900	3.89342300	0.45579200
H	4.28121800	3.56489200	2.05136300
C	0.36013200	-1.05600500	-3.10691000
C	2.62716900	-1.79227100	-2.47567900
C	2.51692000	4.69330300	-0.73232500
H	1.87526000	3.37731000	-2.32796500
H	1.16970000	2.98845500	-0.77278300
H	3.26848100	5.62155800	1.08269300
H	2.06029400	4.37436700	1.35589800
C	0.09568300	-2.28956900	-3.67487100

H	-0.41840000	-0.30203600	-3.07839800
C	2.32268200	-3.04713700	-3.05377600
O	3.82332800	-1.60763700	-1.96035900
H	3.36031300	5.06590800	-1.32889000
H	1.69556700	5.40419700	-0.86983700
C	1.08924900	-3.28282200	-3.64290600
H	-0.86744700	-2.47506600	-4.13638000
H	3.09078500	-3.81289600	-3.02127300
H	0.88949300	-4.25791500	-4.08006100
O	2.91700700	-0.92044700	0.51519200
H	3.03478100	-1.87971000	0.47151100
O	5.63984000	0.27251100	-2.03706300
H	5.23796300	-0.33777200	-2.68607400
H	6.31359500	-0.28126800	-1.60189300
C	0.57442300	0.51676400	1.75977100
C	0.16080500	1.91894400	1.91241900
O	-0.85161900	0.87859300	1.90480500
H	0.81858900	0.16937500	0.76232200
H	0.11862200	2.55918300	1.03918400
H	0.25141600	2.40866100	2.87969700
C	1.11942200	-0.30449500	2.88703100
H	2.19694500	-0.40795700	2.73899300
H	0.89539700	0.14060200	3.86134700
H	0.68838400	-1.30879000	2.84231600
C	0.24116800	-4.00844800	0.61982300
C	-0.59581600	-4.44880500	1.66782700
C	0.05214600	-2.78383000	0.01346100
H	1.05288300	-4.64391800	0.27551600
C	-1.61693600	-3.62295400	2.08728200
H	-0.43581500	-5.41503300	2.13411600
C	-0.99872000	-1.91701900	0.42014000
H	0.69426700	-2.44901300	-0.78735400
C	-1.83221900	-2.35417900	1.49747200
H	-2.28264200	-3.93735800	2.88789600
O	-1.14994500	-0.79254800	-0.22216600
C	-2.93428900	-1.57380300	1.96253000
Co	-2.15181600	0.67184500	0.39286500
N	-3.19500800	-0.36201100	1.60201100
H	-3.59671000	-2.05867500	2.67929800
N	-3.09879900	2.18299600	1.10664400
C	-4.36677000	0.38823300	2.04829800
C	-3.22459200	3.31027400	0.49001700
C	-3.86145300	1.82345800	2.30641900
C	-5.11814900	-0.17135700	3.25440300
H	-3.89282300	4.06412300	0.90846800
C	-2.57938400	3.65862400	-0.74022100
C	-5.00835200	2.75527600	2.69558000
C	-6.26581600	0.76930500	3.64789400
H	-4.42347900	-0.28597200	4.09761600
H	-5.51538400	-1.16502100	3.02187500
C	-2.95609700	4.86900200	-1.36629800
C	-1.59868800	2.81209500	-1.35004100
C	-5.76068000	2.19266000	3.91030800
H	-4.62850800	3.75698100	2.92483400
H	-5.69659200	2.85318500	1.84593800
H	-6.77852000	0.37830600	4.53285800
H	-7.00692300	0.79143300	2.83818400
C	-2.42337700	5.24910200	-2.58165100
H	-3.69661800	5.49595800	-0.87472500
C	-1.10095100	3.20895700	-2.61694200
O	-1.10837300	1.74114200	-0.78157300
H	-5.09027600	2.18598500	4.78036700
H	-6.59675600	2.85259500	4.16380500
C	-1.49735400	4.39403200	-3.20873900
H	-2.72909500	6.17486200	-3.05637600
H	-0.41763000	2.53718000	-3.12227200
H	-1.09659300	4.65980700	-4.18312000
H	-5.04326800	0.43896100	1.18452200
H	-3.14362300	1.76544100	3.13746800

H	4.09595800	2.58775900	-1.56083500
H	2.69935800	1.91522000	1.03585300
S	-3.78778500	-0.32999300	-2.07935700
O	-5.11507000	0.00631900	-2.61049800
O	-2.64096700	-0.31221700	-2.99571500
O	-3.58279000	0.59542600	-0.83784000
C	-3.90919200	-1.97530200	-1.38000900
C	-4.98277400	-2.27771200	-0.54271700
C	-2.94054400	-2.93371900	-1.66474000
C	-5.06256200	-3.54306000	0.03598500
H	-5.74698600	-1.53029400	-0.35716900
C	-3.04011800	-4.19831700	-1.09181200
H	-2.10377700	-2.67066800	-2.29749300
C	-4.09062200	-4.51876100	-0.22426300
H	-5.89417600	-3.78126700	0.69463100
H	-2.26697400	-4.93406000	-1.29229700
C	-4.14972100	-5.87603100	0.42972300
H	-5.04164500	-5.98426100	1.05302300
H	-4.16058200	-6.67847300	-0.31594400
H	-3.26933600	-6.03362000	1.06263400

PO-Co^{III}-OTs + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OTs + H_2O-Co^{III}-OH = OTs-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3598.303453

Thermal correction to Gibbs Free Energy (a.u.): 0.910132

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6075.8816318 a.u.

C	8.18029800	-2.50142500	2.17142800
C	8.60426700	-1.19808100	2.49455200
C	6.98838300	-2.72323900	1.50591300
H	8.79850400	-3.35064800	2.44851900
C	7.80184000	-0.13260800	2.14121900
H	9.54030500	-1.03682600	3.01738100
C	6.15012100	-1.64635900	1.12288200
H	6.65590600	-3.72558500	1.25788000
C	6.57895600	-0.32270200	1.45457000
H	8.10061900	0.88277000	2.39037300
O	5.03352300	-1.92455200	0.48892600
C	5.77761800	0.83508000	1.17148800
Co	3.92225800	-0.66374500	-0.40379500
N	4.68291900	0.84588000	0.48995600
H	6.13708100	1.77662600	1.58813300
N	2.81810400	0.58189700	-1.29408500
C	3.84756900	2.04237000	0.31442300
C	1.73884400	0.28281200	-1.94646500
C	3.30081100	1.96274300	-1.11830400
C	4.50448100	3.39417700	0.58819000
H	1.11540600	1.09079800	-2.30666300
C	1.30136600	-1.04278600	-2.27204400
C	2.29119600	3.07722600	-1.37978700
C	3.49549400	4.52327900	0.32027600
H	5.38399800	3.51215300	-0.05945300
H	4.85105400	3.45118900	1.62571300
C	0.04782300	-1.19376300	-2.90871300
C	2.13478100	-2.17800100	-2.05984800
C	2.92392000	4.44575400	-1.09964600
H	1.92944500	3.04338500	-2.40931300
H	1.41746600	2.93014600	-0.73829300
H	3.97675600	5.49200500	0.48998700
H	2.67480200	4.44641100	1.04533200
C	-0.34085300	-2.42142500	-3.41276400
H	-0.63852300	-0.35631000	-2.95215800
C	1.71317700	-3.42026700	-2.57378900
O	3.30656600	-2.11993100	-1.43599900
H	3.72612800	4.63634900	-1.82568000
H	2.16848900	5.22282700	-1.25118500
C	0.50830300	-3.52809900	-3.25767500
H	-1.30264900	-2.51772400	-3.90255700

H	2.35926900	-4.27847500	-2.42269400
H	0.20958600	-4.49664200	-3.64965700
O	2.74554100	-0.92039900	1.09578300
H	3.10461800	-1.76572700	1.41565200
O	5.25217000	-0.59885300	-1.88719800
H	4.79737900	-1.36392200	-2.31198200
H	6.06462000	-0.97049600	-1.50680900
C	1.25540400	-0.95012200	1.20678700
C	0.77228000	0.49286300	1.43676500
O	-0.56671500	0.53936500	1.76419800
H	0.85664500	-1.33847000	0.27221600
H	1.00335900	1.08698300	0.54399100
H	1.37553300	0.89840400	2.27474600
C	0.93325300	-1.86446200	2.37113500
H	1.19132200	-2.90613600	2.15349100
H	1.46005200	-1.53060200	3.27293400
H	-0.13852600	-1.81053200	2.56025900
C	-1.34483600	-4.53159400	0.58850900
C	-2.23411600	-4.64007500	1.67637600
C	-1.10728600	-3.31817400	-0.02500100
H	-0.83507400	-5.41870400	0.22011100
C	-2.86348600	-3.49563300	2.12541700
H	-2.41738200	-5.59837000	2.15072400
C	-1.74687900	-2.12255500	0.41172600
H	-0.43340100	-3.24197100	-0.86660000
C	-2.62978400	-2.23497500	1.53357500
H	-3.55836100	-3.54852700	2.96089500
O	-1.49628400	-1.02157900	-0.22536700
C	-3.31790100	-1.10181300	2.07615800
Co	-1.87872500	0.71969900	0.41785000
N	-3.13050800	0.12257300	1.72805900
H	-4.05159500	-1.32137400	2.85253000
N	-2.21800500	2.47584600	1.11130300
C	-3.87218600	1.24571400	2.29987600
C	-2.02405300	3.57937500	0.47980300
C	-2.84266800	2.38961700	2.42938100
C	-4.59034900	0.98080900	3.62306600
H	-2.30584700	4.51974700	0.95700100
C	-1.50786800	3.67911000	-0.85713500
C	-3.48343000	3.66696800	2.96896500
C	-5.22677400	2.27018500	4.15948600
H	-3.86815400	0.59057600	4.35280300
H	-5.36309600	0.21627900	3.48971000
C	-1.55113100	4.93494200	-1.49744100
C	-1.01185800	2.53226800	-1.55615600
C	-4.18928800	3.38899300	4.30317000
H	-2.72501300	4.44649100	3.10282100
H	-4.21261500	4.04448200	2.23963100
H	-5.71046700	2.07193100	5.12204600
H	-6.01750100	2.59658800	3.47088300
C	-1.17991300	5.08751700	-2.82154800
H	-1.91099500	5.79109000	-0.93034600
C	-0.72400900	2.70231500	-2.93777400
O	-0.75369000	1.39143000	-0.97940900
H	-3.44302400	3.09796400	5.05475400
H	-4.66472800	4.30515900	4.66968900
C	-0.79393900	3.94453500	-3.54437200
H	-1.23039700	6.05743000	-3.30437000
H	-0.47904700	1.82025200	-3.51725300
H	-0.56320000	4.03119300	-4.60298000
H	-4.60080800	1.55444000	1.53716700
H	-2.05849200	2.04040300	3.11360000
H	4.15715600	2.07979200	-1.79899300
H	2.99671000	1.91711900	0.99466000
S	-3.90808700	0.31108000	-1.99352600
O	-5.08033100	1.01444200	-2.53648200
O	-2.82203600	-0.02067700	-2.93562200
O	-3.42611400	1.07961500	-0.74831000
C	-4.50920700	-1.23791900	-1.31515000

C	-5.54071800	-1.21032500	-0.37683500
C	-3.95122500	-2.44957300	-1.71127500
C	-5.99589400	-2.40417700	0.17854300
H	-5.97957900	-0.26009100	-0.09144000
C	-4.41872500	-3.63710400	-1.15465600
H	-3.13584100	-2.44192500	-2.42296200
C	-5.43820400	-3.63367300	-0.19593000
H	-6.79595800	-2.38446800	0.91476600
H	-3.96260800	-4.57927700	-1.44495100
C	-5.89437800	-4.92403200	0.43729500
H	-6.77293500	-4.77198200	1.07074400
H	-6.14958000	-5.67390100	-0.31935100
H	-5.09680900	-5.34676700	1.05869600

subsequent hydration

OTs-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-OTs + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.686513

Thermal correction to Gibbs Free Energy (a.u.): 0.929443

Imaginary frequencies: -396.72

Calculation of single point energy based on the optimized structure, Et = -6152.317986 a.u.

C	6.24824900	-1.58659500	-4.27288400
C	5.40968200	-2.70542900	-4.11384100
C	6.29306000	-0.58530200	-3.31910900
H	6.87141900	-1.50344600	-5.15916000
C	4.62021200	-2.78832000	-2.98437500
C	5.49495200	-0.64850300	-2.15110100
C	4.63425300	-1.77755200	-1.99503100
H	3.96331300	-3.63800600	-2.83322500
O	5.61694100	0.31499000	-1.26688300
C	3.78982100	-1.95512400	-0.84990600
Co	4.45335200	0.60561900	0.19273000
N	3.69390700	-1.14298300	0.15194000
H	3.17744700	-2.85807100	-0.84879600
N	3.47734300	0.83257300	1.82286100
C	2.71400100	-1.36955200	1.23013400
C	3.14958600	1.96524000	2.34836800
C	3.12819900	-0.46854600	2.40313100
C	2.58180200	-2.81353100	1.71827400
H	2.53043700	1.97164300	3.24549900
C	3.50407400	3.24391800	1.80054700
C	2.05683600	-0.47792900	3.49242500
C	1.52880200	-2.87050500	2.83366500
H	3.55693700	-3.16498100	2.08108800
H	2.27576500	-3.46904100	0.90065800
C	2.83249300	4.39069000	2.27982000
C	4.51715400	3.37041000	0.79765500
C	1.84888800	-1.91711100	3.98989200
H	2.34794300	0.16134800	4.33285100
H	1.12175100	-0.08130300	3.07657100
H	1.42807200	-3.89683000	3.20330900
H	0.56453400	-2.58747300	2.40274900
C	3.12316400	5.64842100	1.78776400
H	2.05929300	4.26037800	3.03246000
C	4.80810400	4.67392000	0.32687300
O	5.20115700	2.35608600	0.32168000
H	2.75785100	-2.25292200	4.50629600
H	1.04169900	-1.93711200	4.73031500
C	4.12515300	5.77837000	0.80755600
H	4.36587800	6.76260000	0.41534900
O	3.10980500	1.19023000	-0.93902200
H	3.55020100	1.90466400	-1.42293500
O	6.12074100	0.06716200	1.27319400
H	6.38322700	0.99394700	1.42854800
H	6.61037600	-0.17499800	0.46318400
H	1.73201900	-1.02948500	0.87188600
H	4.06503200	-0.87268500	2.81228300
C	1.13385700	1.81203100	-0.26531500
C	0.42990800	0.56831700	-0.76708200

O	-0.26697700	-0.05821100	0.29535500
H	1.69429000	1.75885400	0.63898800
H	1.20517500	-0.08233000	-1.18402900
H	-0.24892600	0.83946100	-1.57999500
C	1.13802000	3.05930000	-1.08705500
H	0.11400000	3.43037800	-1.19122100
H	1.76946500	3.83605700	-0.65383200
H	1.48413100	2.82061300	-2.09774200
O	-0.31749500	2.25281300	1.11720600
H	-0.49920700	1.24039300	1.00822200
H	-1.09817300	2.68360500	0.73300700
H	5.57998400	4.77067200	-0.42925000
H	2.59060600	6.52071500	2.14995200
H	6.93917700	0.27841600	-3.43537700
H	5.38434800	-3.48691500	-4.86538400
C	1.25786900	-3.67537500	-3.17100800
C	1.42259500	-4.62980000	-2.14283000
C	0.39658700	-2.60861400	-3.02644000
H	1.81824500	-3.78040900	-4.09577400
C	0.69267300	-4.47725100	-0.97961400
H	2.08508300	-5.47866600	-2.27559600
C	-0.37635100	-2.42645200	-1.84065400
H	0.26063500	-1.88021200	-3.81845000
C	-0.19070100	-3.38902600	-0.79136100
H	0.77901400	-5.21262300	-0.18204600
O	-1.20065600	-1.43309400	-1.79561100
C	-0.94961600	-3.33291700	0.42386800
Co	-1.98963700	-0.75875100	-0.21207800
N	-1.69711400	-2.35108800	0.79041800
H	-0.88155300	-4.20727300	1.07326000
N	-2.70856400	-0.04549500	1.41505400
C	-2.57297000	-2.38401600	1.96477700
C	-3.27957800	1.10154700	1.54721800
C	-2.53073600	-0.96542800	2.55097300
C	-2.29041400	-3.44757100	3.02369200
H	-3.69702400	1.36647900	2.51795200
C	-3.38004400	2.11444200	0.53391500
C	-3.52627300	-0.81961300	3.70287600
C	-3.29902000	-3.30455600	4.17284100
H	-1.26903600	-3.33959400	3.41077900
H	-2.36997300	-4.44845500	2.58666300
C	-3.93894800	3.36325800	0.89562200
C	-2.88261400	1.91226900	-0.79667300
C	-3.26566100	-1.89331900	4.76926000
H	-3.44343700	0.17042400	4.16424400
H	-4.53567300	-0.91802600	3.28981500
H	-3.08926600	-4.05101100	4.94651700
H	-4.30630300	-3.51288700	3.79175400
C	-3.99350200	4.41833000	0.00807300
H	-4.32209900	3.47963600	1.90679900
C	-2.93880500	3.02617400	-1.68441100
O	-2.37209200	0.80527600	-1.22865100
H	-2.28251700	-1.71854200	5.22985200
H	-4.00663000	-1.80196000	5.57043200
C	-3.47123300	4.23720000	-1.28888200
H	-4.41879900	5.37091400	0.30395400
H	-2.56228800	2.87249700	-2.68952900
H	-3.49185500	5.06331300	-1.99481500
H	-3.58868700	-2.52602800	1.58284000
H	-1.50805100	-0.79488200	2.92473300
S	-5.12220100	-1.41656000	-0.45746900
O	-5.89861100	-2.51308400	-1.05072000
O	-5.35072200	-1.14501800	0.98281800
O	-3.63395400	-1.64426700	-0.78584600
C	-5.52970500	0.08604400	-1.33385500
C	-5.11219300	0.23476800	-2.65658200
C	-6.27229000	1.07995800	-0.70314700
C	-5.43906900	1.39977700	-3.34220700
H	-4.51377900	-0.54034200	-3.12082300

C	-6.59243400	2.24185500	-1.40258600
H	-6.57565200	0.93879900	0.32764900
C	-6.17586700	2.42107000	-2.72574400
H	-5.10610300	1.52829800	-4.36881300
H	-7.15826500	3.02725000	-0.90913800
C	-6.46153900	3.71042100	-3.45124100
H	-5.68560300	4.45409600	-3.22916300
H	-6.48003400	3.56747800	-4.53552100
H	-7.42023200	4.14026000	-3.14573200

subsequent hydration

OTs-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-OTs + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.731230

Thermal correction to Gibbs Free Energy (a.u.): 0.934697

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -6152.3681682 a.u.

C	6.09959900	-1.06711400	-4.26887100
C	5.34578200	-2.24969900	-4.16895500
C	6.08304000	-0.12028200	-3.25810000
H	6.70462300	-0.88755400	-5.15318600
C	4.57862900	-2.45711400	-3.03963200
C	5.30428100	-0.31036500	-2.09458900
C	4.53387100	-1.50657100	-1.99357000
H	3.98249600	-3.35676400	-2.93438000
O	5.35877100	0.61724800	-1.15680000
C	3.72126200	-1.81284500	-0.85139000
Co	4.17971000	0.74456400	0.31180000
N	3.55966500	-1.05727600	0.18570700
H	3.19081500	-2.76596400	-0.88583600
N	3.16093000	0.82409100	1.91419600
C	2.62437300	-1.42239900	1.27184100
C	2.67088400	1.89297900	2.44127100
C	2.97906600	-0.52449500	2.46357400
C	2.66385600	-2.88783800	1.70508600
H	2.02222300	1.80417700	3.30653200
C	2.90347400	3.21631500	1.92195300
C	1.97353700	-0.68378800	3.60100200
C	1.67164100	-3.09418500	2.85790700
H	3.68467200	-3.14638800	2.01775800
H	2.39494100	-3.54234900	0.87379500
C	2.07935000	4.26858000	2.37045600
C	3.94706400	3.47484000	0.98504100
C	1.94219200	-2.15643400	4.03990600
H	2.25739000	-0.05281900	4.45072900
H	0.98506200	-0.35249000	3.26620900
H	1.69210500	-4.13860800	3.18726600
H	0.66598400	-2.89848000	2.47684900
C	2.25929200	5.56162000	1.91271000
H	1.28028700	4.03245300	3.06685300
C	4.12296600	4.80509500	0.54529200
O	4.76407400	2.53938900	0.52315900
H	2.90375000	-2.41658100	4.50247700
H	1.17617500	-2.29216300	4.81081300
C	3.29505300	5.82144800	0.99984000
H	3.44890300	6.83309400	0.63531700
O	2.84178400	1.34606600	-0.92940600
H	3.25824300	2.14734700	-1.28497300
O	5.81415000	0.30625600	1.35519200
H	6.01166800	1.23418500	1.59208600
H	6.36259700	0.14448700	0.56062700
H	1.60859300	-1.16156900	0.93475900
H	3.97179500	-0.83364400	2.82025600
C	1.40062400	1.60633000	-0.66310200
C	0.62523800	0.31994200	-0.99709400
O	-0.12820800	-0.13140400	0.10793600
H	1.30378500	1.83240900	0.39376900
H	1.35455200	-0.43710000	-1.31554100
H	-0.02425600	0.50966400	-1.85555300

C	1.00619000	2.81830900	-1.48413000
H	-0.04761400	3.04435900	-1.30349800
H	1.59566200	3.69953800	-1.20313700
H	1.12412000	2.62290700	-2.55555400
O	-0.12314300	1.54380900	2.17523600
H	-0.15715700	0.88459100	1.42253600
H	-0.73434900	2.23137000	1.87990500
H	4.92318900	5.00081800	-0.16071900
H	1.61045200	6.36192400	2.25067500
H	6.66367900	0.79329500	-3.32936600
H	5.36521600	-2.98464000	-4.96603400
C	1.38825800	-3.83383000	-3.27015800
C	1.60519200	-4.73252200	-2.20231300
C	0.49816900	-2.78679700	-3.15633500
H	1.92818700	-3.96978800	-4.20363700
C	0.88555500	-4.55182400	-1.03526800
H	2.29047400	-5.56675500	-2.30963100
C	-0.25486100	-2.56815800	-1.96230600
H	0.32334500	-2.10095900	-3.97827400
C	-0.02626700	-3.48362900	-0.87842300
H	1.00078600	-5.25376400	-0.21140100
O	-1.09548600	-1.59090800	-1.93785800
C	-0.79128400	-3.41168900	0.33475300
Co	-1.84640400	-0.84799300	-0.35457300
N	-1.55877500	-2.43569000	0.67026600
H	-0.71753300	-4.27282300	1.00153400
N	-2.55573600	-0.12546800	1.26654400
C	-2.44998100	-2.46027200	1.83330600
C	-2.97880200	1.07985100	1.42209700
C	-2.41262600	-1.04016200	2.40984700
C	-2.19720300	-3.51944300	2.90321000
H	-3.34232800	1.37839900	2.40526300
C	-2.96875800	2.11060000	0.42549000
C	-3.43437800	-0.87891100	3.53747500
C	-3.23759700	-3.36427400	4.02255800
H	-1.18844100	-3.41243900	3.32251100
H	-2.26660300	-4.52313300	2.47028300
C	-3.36295400	3.41217000	0.81459600
C	-2.57187200	1.85713400	-0.92946500
C	-3.20848100	-1.95046700	4.61385700
H	-3.34908900	0.11126100	3.99721300
H	-4.43376000	-0.96883400	3.10089300
H	-3.05649800	-4.10962100	4.80478400
H	-4.23488000	-3.56479100	3.61238300
C	-3.35450100	4.47059000	-0.07141400
H	-3.67877300	3.56541200	1.84456900
C	-2.58822000	2.96839600	-1.82328600
O	-2.21030100	0.70435200	-1.38826400
H	-2.23542300	-1.78178900	5.09782600
H	-3.96833300	-1.85117200	5.39640800
C	-2.95335900	4.23129400	-1.40151300
H	-3.65122200	5.46417000	0.24640700
H	-2.30338600	2.77448300	-2.85140700
H	-2.93681400	5.05336300	-2.11259600
H	-3.45871500	-2.60046500	1.43367000
H	-1.40171500	-0.86025200	2.80842500
S	-4.99771000	-1.46476800	-0.56029600
O	-5.81729600	-2.46222300	-1.26169700
O	-5.21649600	-1.33658100	0.90172100
O	-3.52102500	-1.71071800	-0.91479600
C	-5.36796300	0.13429900	-1.26745100
C	-5.05532400	0.37363800	-2.60600800
C	-5.98458200	1.11260700	-0.49360600
C	-5.35825100	1.61174400	-3.16094300
H	-4.55747600	-0.39412200	-3.18665800
C	-6.28341500	2.34932400	-1.06345900
H	-6.21424200	0.89586400	0.54311900
C	-5.96994700	2.61831800	-2.39900700
H	-5.10675700	1.80950900	-4.19968800

H	-6.75303300	3.12053800	-0.45897500
C	-6.23191500	3.97902600	-2.99017600
H	-5.38619500	4.64932700	-2.79209600
H	-6.36646000	3.92822600	-4.07465000
H	-7.12318600	4.44158000	-2.55548800

subsequent hydration

OTs-Co^{III}-PO-OH-Co^{III}-H_2O + H_2O = PG + Co^{III}(salen)-OTs + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -3674.737225

Thermal correction to Gibbs Free Energy (a.u.): 0.930804

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -6152.3697757 a.u.

C	6.50354600	-2.26660100	-4.05002200
C	5.76845400	-3.40719700	-3.67101300
C	6.44891200	-1.10191100	-3.30831300
H	7.12426200	-2.29983700	-4.94138100
C	4.97913600	-3.34009500	-2.54107200
C	5.65031700	-1.00827000	-2.13787200
C	4.89512600	-2.16237200	-1.76110900
H	4.39609100	-4.20117400	-2.22854900
O	5.66639500	0.11630000	-1.46855100
C	4.02030100	-2.17417700	-0.62468600
Co	4.64970100	0.52288900	0.07719400
N	3.85894600	-1.20673400	0.21518400
H	3.43340900	-3.08248100	-0.49386300
N	3.74495100	0.91417800	1.70733900
C	2.82795500	-1.25813300	1.26272700
C	3.47794500	2.10313200	2.13154500
C	3.29024500	-0.30657100	2.37800300
C	2.50668100	-2.63736500	1.84050600
H	2.86345300	2.21517400	3.02598800
C	3.92440300	3.31889400	1.51664700
C	2.20532900	-0.14782600	3.44365900
C	1.42852700	-2.50113900	2.92526700
H	3.42175900	-3.07757800	2.25872100
H	2.14464000	-3.30581000	1.05697500
C	3.37989100	4.54013600	1.97236300
C	4.92258000	3.31572300	0.49167300
C	1.84260700	-1.52117400	4.02753800
H	2.54347800	0.51637200	4.24603300
H	1.31738400	0.30684000	2.98577600
H	1.20475300	-3.48479400	3.35302400
H	0.50799100	-2.13882600	2.45559900
C	3.77202300	5.74842000	1.42967400
H	2.62575100	4.51092000	2.75565900
C	5.31467900	4.57044000	-0.03746700
O	5.51234400	2.23069900	0.05930600
H	2.70756900	-1.92192800	4.57243500
H	1.03514700	-1.40904900	4.75954400
C	4.75088400	5.74916100	0.41728500
H	5.06907300	6.69248400	-0.01834600
O	3.21541500	1.11894300	-0.88249900
H	3.59297300	1.24162400	-1.76549100
O	6.39862000	0.01625000	1.11168600
H	6.63866400	0.96437300	1.12549500
H	6.86331400	-0.31913800	0.32566200
H	1.91388400	-0.83777000	0.82547100
H	4.18339400	-0.75526900	2.83673900
C	0.47360000	2.49810300	0.43303000
C	0.22668000	1.15769900	-0.25451900
O	-0.54732300	0.33853200	0.68388600
H	1.19950400	2.35781600	1.23602300
H	1.16638900	0.65788400	-0.48262300
H	-0.36469100	1.27621000	-1.16202400
C	0.98741800	3.54578200	-0.53579700
H	0.26315400	3.71434000	-1.34187700
H	1.17337500	4.48999100	-0.01871700
H	1.92705700	3.18745200	-0.96479200

O	-0.73213100	2.89257400	1.12483600
H	-0.97910700	1.02448000	1.24037000
H	-1.37451300	3.19948100	0.46488300
H	6.06936300	4.56813500	-0.81671000
H	3.33789100	6.67921300	1.77794700
H	7.01273400	-0.22054600	-3.59548000
H	5.82065300	-4.31769300	-4.25792700
C	1.53075900	-3.22642900	-2.92453000
C	1.52803000	-4.31942600	-2.02791400
C	0.69804700	-2.14475300	-2.73495700
H	2.20380200	-3.23688600	-3.77657100
C	0.69361900	-4.27361000	-0.93172300
H	2.16042400	-5.18204100	-2.20792000
C	-0.20363900	-2.08421400	-1.63148800
H	0.68699500	-1.31064300	-3.42766900
C	-0.15833500	-3.16661400	-0.69245500
H	0.67071900	-5.10118400	-0.22580900
O	-1.00451200	-1.07028000	-1.55293700
C	-0.98742600	-3.19433300	0.46987000
Co	-2.12238000	-0.64058200	-0.09464200
N	-1.75766900	-2.24111400	0.87699100
H	-0.95094000	-4.11258200	1.05732700
N	-3.08717500	-0.08905200	1.46708900
C	-2.72614500	-2.41774000	1.96830200
C	-3.78395100	0.99349900	1.57969600
C	-2.92241300	-1.03134300	2.58968800
C	-2.39095700	-3.46077800	3.03424400
H	-4.31946800	1.16703900	2.51216600
C	-3.88950500	2.03280800	0.60283100
C	-4.04534900	-1.05397600	3.62761900
C	-3.50988700	-3.49498800	4.08608000
H	-1.43117500	-3.21694500	3.50836500
H	-2.28950500	-4.45298900	2.58359300
C	-4.61805400	3.19526600	0.94447300
C	-3.22153700	1.95336600	-0.66210400
C	-3.74672400	-2.11147700	4.70069400
H	-4.14994500	-0.07684800	4.11068200
H	-4.98312500	-1.27604100	3.10735900
H	-3.26207700	-4.22131100	4.86739700
H	-4.43479400	-3.84271000	3.60944500
C	-4.68038000	4.28450500	0.09971600
H	-5.12499400	3.21994400	1.90613800
C	-3.28130400	3.10156400	-1.50126400
O	-2.55003100	0.92478700	-1.07672100
H	-2.85493100	-1.80978800	5.26793300
H	-4.57407000	-2.15101500	5.41681000
C	-3.98577900	4.22984000	-1.12501800
H	-5.23623300	5.17246200	0.37921700
H	-2.76756300	3.04397100	-2.45425400
H	-4.00478200	5.08850700	-1.79075600
H	-3.67805300	-2.68195500	1.49545400
H	-1.97648900	-0.75851700	3.08600800
S	-5.04018100	-1.63289700	-0.76127200
O	-5.57473900	-2.78149100	-1.50052700
O	-5.45764900	-1.48470200	0.65124500
O	-3.49515900	-1.66689200	-0.92166600
C	-5.52590600	-0.13920600	-1.60703900
C	-4.98635000	0.13608200	-2.86373300
C	-6.44662800	0.72223800	-1.01756800
C	-5.37143100	1.29801000	-3.52324500
H	-4.25382700	-0.53639900	-3.29433400
C	-6.82396600	1.88170200	-1.69183800
H	-6.84321100	0.48439000	-0.03755600
C	-6.28746700	2.18955600	-2.94640200
H	-4.94524200	1.52720000	-4.49621300
H	-7.53054800	2.56536300	-1.22987900
C	-6.64193300	3.48160000	-3.63525900
H	-5.98386300	4.28961900	-3.29147000
H	-6.52943700	3.40418700	-4.72036500

H	-7.67022200	3.78478500	-3.41727200

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon and subsequent hydration

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OH + H_2O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.357620

Thermal correction to Gibbs Free Energy (a.u.): 0.797713

Imaginary frequencies: -447.72

Calculation of single point energy based on the optimized structure, Et = -5256.5700238 a.u.

C	5.26488300	-3.45387500	-3.09977400
C	4.47624400	-4.36705900	-2.37565700
C	5.33627800	-2.12015600	-2.73585900
H	5.82323600	-3.79741600	-3.96651800
C	3.77717100	-3.91235000	-1.27443600
H	4.42168800	-5.40782500	-2.67559000
C	4.61476500	-1.62255300	-1.62424400
H	5.93584000	-1.41250600	-3.29873100
C	3.82926800	-2.55721700	-0.87689400
H	3.16282900	-4.59564600	-0.69277400
O	4.72568900	-0.35041500	-1.32186900
C	3.12166300	-2.17974000	0.31017700
Co	3.43910300	0.57388600	-0.26461400
N	3.02380200	-0.97702700	0.77349900
H	2.62098500	-2.98420300	0.85417900
N	2.33033500	1.49715500	0.97532400
C	2.19408600	-0.69595500	1.95827900
C	1.69374100	2.59317300	0.74656900
C	2.33122600	0.79751100	2.26189000
C	2.55456300	-1.48790700	3.21926300
H	1.00693700	2.97647900	1.50050100
C	1.83683500	3.36930100	-0.45443100
C	1.30459800	1.20736300	3.31272000
C	1.58596600	-1.10253800	4.35034400
H	3.58979800	-1.25550600	3.50085700
H	2.51070900	-2.56463800	3.03199000
C	0.93117600	4.42901100	-0.67814000
C	2.89769600	3.11846200	-1.38120900
C	1.57200200	0.41180400	4.60194700
H	1.37570800	2.27976400	3.52575900
H	0.29761600	0.99857400	2.93350800
H	1.85385200	-1.63607000	5.26844700
H	0.57290000	-1.42262300	4.07873700
C	1.03502700	5.23255100	-1.79862000
H	0.12959100	4.58607000	0.03812100
C	2.98361100	3.96353900	-2.51323200
O	3.80336500	2.17334600	-1.22836500
H	2.53986400	0.72148500	5.01924200
H	0.81228400	0.65887400	5.35051900
C	2.07367700	4.98991300	-2.71425800
H	0.32343600	6.03279900	-1.96994200
H	3.78679100	3.77458100	-3.21781100
H	2.16583500	5.61293100	-3.59983000
O	2.09865700	0.11153900	-1.44596700
H	2.26193800	0.65691300	-2.22836800
O	5.12545400	1.08579000	0.78959400
H	5.21042000	1.94702000	0.33886900
H	5.67202300	0.48142400	0.24853700
C	-0.62142000	1.02941700	-1.21122200
C	0.13698400	-0.21631900	-1.26521400
O	-1.66598900	0.07629000	-1.13803100
H	-0.48693000	1.59849400	-0.29235000
H	0.29306800	-0.75430800	-0.34639200
H	0.16518100	-0.76104000	-2.19721900
C	-0.69434100	1.91137700	-2.43827600
H	-1.49587900	2.64634700	-2.31849600
H	0.24291400	2.45271400	-2.59080500
H	-0.90695800	1.30277700	-3.32285600

C	-1.69344900	4.56555200	2.06647400
C	-2.58588300	5.05320900	1.09428200
C	-1.50977300	3.20680400	2.25331100
H	-1.14109300	5.26526100	2.68895800
C	-3.32687500	4.13637700	0.37073700
H	-2.72051500	6.11914300	0.94747700
C	-2.19057000	2.23589400	1.46064500
H	-0.84302900	2.84164200	3.02382200
C	-3.16744800	2.74455800	0.53954200
H	-4.07102200	4.48298300	-0.34335000
O	-1.90164300	0.97823300	1.61464700
C	-4.10247400	1.87485600	-0.12374500
Co	-2.60603600	-0.45905900	0.54114500
N	-4.05662700	0.59171300	-0.10705400
H	-4.93449200	2.36896200	-0.62807400
N	-3.31785200	-1.84790300	-0.55914000
C	-5.10552900	-0.26428500	-0.65626900
C	-2.93361100	-3.07476000	-0.55256100
C	-4.36748500	-1.35209800	-1.45469900
C	-6.18851400	0.41527100	-1.49113900
H	-3.43800200	-3.78513300	-1.20940600
C	-1.87919400	-3.62066600	0.25132200
C	-5.34178900	-2.39274700	-2.00930600
C	-7.16932200	-0.63234100	-2.03588500
H	-5.72339000	0.95473600	-2.32772700
H	-6.72782700	1.15298700	-0.88709100
C	-1.64928400	-5.01173200	0.16430900
C	-1.06060800	-2.80733800	1.10184700
C	-6.43900600	-1.71269700	-2.84087300
H	-4.81387300	-3.12270500	-2.63176800
H	-5.79159800	-2.94254300	-1.17216900
H	-7.92969400	-0.14433700	-2.65499000
H	-7.69885000	-1.10061100	-1.19572400
C	-0.66358400	-5.64146200	0.89967200
H	-2.28025200	-5.59271100	-0.50512900
C	-0.08581700	-3.49576800	1.87933400
O	-1.12843200	-1.51193700	1.18359000
H	-5.98584300	-1.25585900	-3.73111300
H	-7.14875000	-2.46487700	-3.20149500
C	0.11181800	-4.86023200	1.77560800
H	-0.50521000	-6.71127100	0.81917800
H	0.48713700	-2.91091200	2.58321000
H	0.86965000	-5.33538000	2.39437500
H	-5.55522400	-0.75340200	0.21806700
H	-3.85130600	-0.84911900	-2.28459500
H	3.34102500	0.95705600	2.66582300
H	1.14544100	-0.88902900	1.69384200
O	-3.67435100	-1.06118200	1.91657900
H	-3.30516100	-0.60645400	2.68613800

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OH + H_2O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.376556

Thermal correction to Gibbs Free Energy (a.u.): 0.794257

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5256.5872523 a.u.

C	5.26861200	-3.71159600	-3.10746000
C	4.41586700	-4.59350500	-2.41727900
C	5.39312100	-2.38818500	-2.72406800
H	5.83582600	-4.07230000	-3.96151000
C	3.70644100	-4.11547000	-1.33287900
H	4.32098700	-5.62772100	-2.72986400
C	4.66434500	-1.86612900	-1.62569500
H	6.04306700	-1.70367900	-3.25920900
C	3.81047700	-2.76934900	-0.91488200
H	3.04480200	-4.77618400	-0.77723100
O	4.82684300	-0.60513500	-1.31076300
C	3.07466900	-2.37064700	0.24911500

Co	3.63464600	0.37466400	-0.19613500
N	3.03900100	-1.17947700	0.74500900
H	2.49472900	-3.15516200	0.74190100
N	2.58220300	1.34383100	1.05558700
C	2.16139000	-0.87467500	1.88732500
C	2.05045000	2.49750800	0.84115500
C	2.43297400	0.57875900	2.29185700
C	2.35235500	-1.76510400	3.12080300
H	1.35891500	2.90925000	1.57565900
C	2.31882200	3.30315100	-0.31725500
C	1.39300200	1.03541800	3.31084300
C	1.36604800	-1.33832700	4.22096200
H	3.38754200	-1.66210700	3.47099500
H	2.20887700	-2.82070300	2.87240900
C	1.51996300	4.44544800	-0.53845400
C	3.40283800	2.99794500	-1.20254500
C	1.50161000	0.15147600	4.56422300
H	1.55259900	2.08419200	3.58563600
H	0.39277700	0.94360500	2.87226200
H	1.52021200	-1.94931900	5.11679200
H	0.34172400	-1.52720300	3.87797700
C	1.74420700	5.27932700	-1.61831600
H	0.70061300	4.64401000	0.14685300
C	3.61538000	3.87843100	-2.29147100
O	4.21841300	1.98240900	-1.04041900
H	2.47243000	0.32994600	5.04604800
H	0.73206500	0.44006800	5.28767300
C	2.80496300	4.98379900	-2.49314300
H	1.11281500	6.14481800	-1.78809400
H	4.43480000	3.64887900	-2.96465400
H	2.99322800	5.63040300	-3.34625500
O	2.24292200	0.19780000	-1.36127700
H	2.68132700	0.33900900	-2.21281100
O	5.37430100	0.66058300	0.93380000
H	5.51310900	1.53114100	0.51482000
H	5.86571000	0.04627900	0.35635000
C	-0.46645400	0.91870900	-1.20875200
C	-0.53560700	-0.46992000	-1.62927100
O	-1.76414300	0.21451500	-1.21803400
H	-0.11326300	1.09109400	-0.19985700
H	-0.20775900	-1.23901700	-0.94341100
H	-0.52158100	-0.71243400	-2.68849300
C	-0.36432200	2.05602700	-2.17798600
H	-0.85024700	2.95159500	-1.78112800
H	0.69178000	2.27861900	-2.34122100
H	-0.83029700	1.79093800	-3.13183600
C	-1.34283300	4.60180000	1.94117100
C	-2.22259600	5.17170400	1.00169800
C	-1.28101300	3.23287700	2.12716900
H	-0.70299900	5.24678900	2.53836000
C	-3.07084600	4.33052800	0.30756900
H	-2.25966700	6.24546200	0.85555400
C	-2.08329300	2.33240100	1.36869300
H	-0.62084500	2.80556500	2.87046200
C	-3.03669300	2.92838200	0.47737000
H	-3.80189400	4.74490700	-0.38331700
O	-1.91993700	1.05158900	1.53353400
C	-4.06354000	2.14984600	-0.15716600
Co	-2.77823600	-0.31140200	0.49221700
N	-4.13607600	0.86589500	-0.13874800
H	-4.85751800	2.71673400	-0.64571700
N	-3.62903500	-1.62678900	-0.59944500
C	-5.27306400	0.10990200	-0.66023700
C	-3.39625900	-2.89308500	-0.54625700
C	-4.65817400	-1.04560200	-1.46862600
C	-6.30637500	0.88271100	-1.47677300
H	-4.00429400	-3.56264100	-1.15597200
C	-2.38392200	-3.52451800	0.24394000
C	-5.73703200	-1.99709000	-1.98758100

C	-7.39232300	-0.07293900	-1.99105500
H	-5.81232300	1.37243200	-2.32718800
H	-6.76137800	1.67042200	-0.86665800
C	-2.31575000	-4.93659600	0.21183400
C	-1.43322200	-2.77494300	1.01086900
C	-6.78550700	-1.22428600	-2.80077300
H	-5.29376600	-2.77889800	-2.61327600
H	-6.21586900	-2.49425300	-1.13391600
H	-8.11654700	0.47961500	-2.59884900
H	-7.94525300	-0.48245600	-1.13550300
C	-1.35773200	-5.63810300	0.91538300
H	-3.04852100	-5.47084800	-0.38913900
C	-0.47035800	-3.53047700	1.73537400
O	-1.37163600	-1.47546500	1.05353200
H	-6.31355600	-0.82068700	-3.70677800
H	-7.57092700	-1.90984900	-3.13590200
C	-0.43167900	-4.91068000	1.68670500
H	-1.32276800	-6.72139500	0.88101300
H	0.22799300	-2.98031300	2.34696000
H	0.32239800	-5.44087900	2.26345500
H	-5.74921800	-0.33264100	0.22489800
H	-4.13071700	-0.59500200	-2.32223300
H	3.42738700	0.60285800	2.76023800
H	1.12131700	-0.94073600	1.53752100
O	-3.85276600	-0.82296300	1.88052300
H	-3.42916400	-0.40066600	2.64118300

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the terminal carbon

PO-Co^{III}-OH + H_2O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.376645

Thermal correction to Gibbs Free Energy (a.u.): 0.802116

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5256.5966207 a.u.

C	4.71319100	-3.66880600	-3.10917200
C	3.89292800	-4.50540700	-2.33082800
C	4.91978900	-2.34188100	-2.76743700
H	5.18726700	-4.06457200	-4.00316800
C	3.30187000	-3.98872000	-1.19387200
H	3.72924600	-5.53803200	-2.61842700
C	4.30793000	-1.78164600	-1.62394700
H	5.54227800	-1.69245900	-3.37367900
C	3.49737700	-2.64007000	-0.81829300
H	2.65993000	-4.60886600	-0.57290100
O	4.53436700	-0.51437000	-1.34211800
C	2.89718500	-2.19080000	0.40218200
Co	3.35326900	0.51951900	-0.27038100
N	2.89288900	-0.96930700	0.82911800
H	2.37907600	-2.94346000	0.99913500
N	2.32185400	1.53904000	0.95592900
C	2.13416200	-0.60421600	2.04109100
C	1.70543600	2.63693700	0.67920500
C	2.32686800	0.89461200	2.27212400
C	2.52931200	-1.34652900	3.32060800
H	1.02884900	3.06505700	1.41722000
C	1.86317800	3.35847700	-0.55449200
C	1.32842200	1.37534000	3.32003200
C	1.59008600	-0.89760800	4.45330200
H	3.57345500	-1.11144600	3.56562300
H	2.46969000	-2.42913700	3.18171300
C	0.97650000	4.42174700	-0.82789100
C	2.91305800	3.04562200	-1.47062900
C	1.60220000	0.62735000	4.63716300
H	1.42864500	2.45356900	3.48676600
H	0.31180700	1.17367700	2.96361600
H	1.86995800	-1.39218000	5.38930200
H	0.56853500	-1.21698000	4.21437400
C	1.10506700	5.17608700	-1.98003600
H	0.17043300	4.61873300	-0.12737500

C	3.03211000	3.84244000	-2.63000900
O	3.78070600	2.05939100	-1.29089800
H	2.58037200	0.93881400	5.02861600
H	0.85670400	0.91863700	5.38380000
C	2.14565600	4.88140000	-2.87569200
H	0.40756500	5.97931300	-2.18999400
H	3.83299000	3.60632900	-3.32273300
H	2.25690600	5.46787900	-3.78344400
O	1.93811400	0.12286000	-1.49608500
H	1.98010500	0.76454800	-2.21998200
O	5.03725100	0.94101600	0.69516900
H	5.18550100	1.79038800	0.23375400
H	5.56285500	0.29155600	0.18325300
C	-0.48899900	0.81755000	-1.21818100
C	0.54181800	-0.31092700	-1.27786700
O	-1.71476300	0.21169900	-1.10502400
H	-0.24837700	1.45717700	-0.35214100
H	0.53559200	-0.86317500	-0.34559100
H	0.30473800	-0.98766700	-2.10398100
C	-0.47009600	1.68615300	-2.48455600
H	-1.21423400	2.47928900	-2.37753500
H	0.49488300	2.17096700	-2.68151300
H	-0.74580200	1.07182400	-3.34896500
C	-1.61486200	4.69641500	1.84131900
C	-2.52579700	5.12179800	0.85908200
C	-1.42227400	3.35025500	2.10357000
H	-1.05633900	5.43337200	2.41403500
C	-3.28275600	4.15796400	0.21311800
H	-2.66929900	6.17639600	0.65049500
C	-2.11180200	2.32816000	1.38309400
H	-0.74938100	3.03698400	2.89157300
C	-3.11693400	2.78131500	0.46132700
H	-4.04783600	4.45951800	-0.49957200
O	-1.82461100	1.08423200	1.61270900
C	-4.07837700	1.87390300	-0.11192900
Co	-2.50849700	-0.39144600	0.56338800
N	-4.02506400	0.59669500	-0.02133800
H	-4.93222900	2.33849200	-0.60829600
N	-3.20206200	-1.81004800	-0.51417600
C	-5.05621100	-0.30161200	-0.52725900
C	-2.75282900	-3.01112400	-0.55842700
C	-4.29759800	-1.34506600	-1.36913100
C	-6.20321000	0.33202700	-1.31076500
H	-3.22524700	-3.72699100	-1.23342500
C	-1.67383800	-3.53232500	0.23559600
C	-5.24225700	-2.42076600	-1.90833800
C	-7.15488400	-0.75575200	-1.82609700
H	-5.79962700	0.89684700	-2.16237100
H	-6.74756200	1.04166100	-0.67781700
C	-1.39001000	-4.90892800	0.12372800
C	-0.91504500	-2.71115300	1.13487400
C	-6.40613200	-1.78400400	-2.68109800
H	-4.70502500	-3.11207200	-2.56624600
H	-5.62999100	-3.00836900	-1.06572900
H	-7.96721500	-0.29974500	-2.40250600
H	-7.61996900	-1.26343000	-0.97072700
C	-0.42588400	-5.53081600	0.89867300
H	-1.96637000	-5.49213000	-0.59172300
C	-0.00080700	-3.40120600	1.98419000
O	-0.98474000	-1.41762100	1.19637200
H	-6.01464000	-1.28876400	-3.58011300
H	-7.09165900	-2.56545000	-3.02675600
C	0.24727900	-4.75752700	1.86044500
H	-0.22885300	-6.59261500	0.79831500
H	0.47960400	-2.82567300	2.76201900
H	0.95965800	-5.23149300	2.53234600
H	-5.44161000	-0.81823600	0.36144200
H	-3.82363100	-0.80463400	-2.19988800
H	3.34726600	1.04520100	2.65240600

H	1.06945000	-0.77750200	1.82765200
O	-3.51581900	-1.04796100	1.98873200
H	-3.21960800	-0.49973800	2.72771600

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2855.767568
Thermal correction to Gibbs Free Energy (a.u.): 0.822595
Imaginary frequencies: -495.71
Calculation of single point energy based on the optimized structure, Et = -5333.0399412 a.u.

C	5.02132700	-3.72626400	-3.05810500
C	4.17327200	-4.58667000	-2.33582500
C	5.19289100	-2.40551600	-2.68214400
H	5.54724100	-4.10120500	-3.93189500
C	3.51619700	-4.09260100	-1.22663400
H	4.04052500	-5.61753400	-2.64485700
C	4.51659800	-1.86693300	-1.56018900
H	5.84034700	-1.73820900	-3.24126700
C	3.66856300	-2.74774100	-0.81662800
H	2.85742400	-4.73520500	-0.64731500
O	4.71714300	-0.60562200	-1.25475300
C	2.97877800	-2.32696900	0.36766700
Co	3.57418600	0.41009600	-0.12215300
N	2.95173400	-1.12280700	0.83454500
H	2.41625400	-3.09940600	0.89653000
N	2.52514900	1.40567100	1.09975900
C	2.11129900	-0.78720100	1.99828200
C	1.95834400	2.52935400	0.81953500
C	2.38388700	0.67728700	2.35870800
C	2.33914600	-1.63921200	3.25174100
H	1.23910500	2.95010300	1.51967600
C	2.22768900	3.28449600	-0.37241800
C	1.34001600	1.15318800	3.36403400
C	1.33784000	-1.20448400	4.33463800
H	3.37125400	-1.49352800	3.59599200
H	2.22894100	-2.70626600	3.03859300
C	1.38285400	4.36837400	-0.68992900
C	3.35816900	2.98715600	-1.19616100
C	1.44646800	0.29710200	4.63794800
H	1.50001900	2.20757900	3.61578500
H	0.34383500	1.05131100	2.91940300
H	1.49947000	-1.78663000	5.24795800
H	0.32153200	-1.42774800	3.98801900
C	1.62229300	5.15569900	-1.80218700
H	0.52350500	4.56141900	-0.05529500
C	3.59055100	3.82062900	-2.31197800
O	4.20067300	2.00166900	-0.94960300
H	2.40855100	0.50037900	5.12774100
H	0.66426500	0.59271800	5.34450400
C	2.73903600	4.87530600	-2.60680700
H	0.95628400	5.97544600	-2.04861300
H	4.45058900	3.59791300	-2.93483200
H	2.93880100	5.48845600	-3.48153300
O	2.18949200	0.33663900	-1.34652400
H	2.65667000	0.30366800	-2.19332600
O	5.26429000	0.64868900	0.99318900
H	5.43548000	1.52819300	0.60081600
H	5.79113500	0.03770100	0.44424300
C	-0.38662800	0.56060000	-1.32797000
C	0.50457800	-0.66827800	-1.64936100
O	-1.73660600	0.18091900	-1.23791100
H	-0.03454500	0.93368100	-0.36193200
H	0.75908900	-1.35670700	-0.86177600
H	0.88339800	-0.86283100	-2.63917600
C	-0.25211900	1.64658800	-2.39514300
H	-0.86427900	2.50307100	-2.10195500
H	0.78071200	1.97821200	-2.51027100
H	-0.62687200	1.27054000	-3.35384300

C	-1.24490300	4.75077100	1.90630500
C	-2.09476500	5.29625500	0.92767300
C	-1.15809100	3.38284300	2.09805300
H	-0.64844400	5.41157700	2.53060200
C	-2.90712000	4.43059400	0.21770300
H	-2.15019300	6.36801600	0.77246700
C	-1.89680100	2.45710300	1.30298500
H	-0.53077100	2.97938000	2.88149500
C	-2.85287800	3.03255200	0.40027300
H	-3.63487400	4.82557200	-0.48802200
O	-1.69422800	1.18231600	1.45607800
C	-3.90267600	2.24200100	-0.18121700
Co	-2.61598900	-0.20874400	0.48579900
N	-4.00303700	0.96523900	-0.08930900
H	-4.70284000	2.80275000	-0.66645300
N	-3.59659000	-1.56010900	-0.45391400
C	-5.18371300	0.22082400	-0.52133000
C	-3.42720900	-2.82719900	-0.32263100
C	-4.64209900	-0.98581600	-1.30396000
C	-6.23307600	0.98739700	-1.32408900
H	-4.11041900	-3.50644700	-0.83365900
C	-2.37217400	-3.45407400	0.42189900
C	-5.76625200	-1.92450200	-1.74174800
C	-7.36527300	0.04367200	-1.75311000
H	-5.76397600	1.42802600	-2.21439900
H	-6.64023900	1.81163600	-0.72848900
C	-2.36721400	-4.86711700	0.47317500
C	-1.32262700	-2.70344800	1.05513000
C	-6.82421700	-1.15298000	-2.54317800
H	-5.36787100	-2.74211300	-2.35190100
H	-6.22711900	-2.37354800	-0.85194100
H	-8.10108600	0.59307000	-2.35000700
H	-7.89057800	-0.31853600	-0.85947200
C	-1.38619100	-5.57608300	1.13749300
H	-3.17240800	-5.39770200	-0.03043600
C	-0.34337900	-3.47071200	1.75025400
O	-1.19209500	-1.41349900	1.00212300
H	-6.37707400	-0.79606000	-3.48067400
H	-7.64104300	-1.82721200	-2.82191600
C	-0.37030800	-4.85153100	1.78747700
H	-1.40382200	-6.65986100	1.16666500
H	0.41965700	-2.92426600	2.28096200
H	0.40146600	-5.38254900	2.33994800
O	-1.00791600	-1.85948100	-2.21547700
H	-1.04848400	-2.53768100	-1.52573100
H	-1.58335000	-1.03182900	-1.82343700
H	-4.12994500	-0.58957800	-2.19249500
H	-5.62811700	-0.16824300	0.40459600
H	1.06156200	-0.86362400	1.67897100
H	3.37864500	0.72053700	2.82446200
O	-3.60533000	-0.66032500	1.98360700
H	-3.19339000	-0.12609900	2.67626400

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2855.804994

Thermal correction to Gibbs Free Energy (a.u.): 0.824016

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5333.0871495 a.u.

C	4.49346100	-3.89609900	-3.06632700
C	3.67134800	-4.68111400	-2.23811500
C	4.76221500	-2.57057200	-2.76521200
H	4.91944900	-4.33075900	-3.96622800
C	3.14151500	-4.11382400	-1.09566700
H	3.45753800	-5.71293700	-2.49331500
C	4.21330300	-1.95898100	-1.61543800
H	5.38702500	-1.96042300	-3.40887200
C	3.40045200	-2.76464700	-0.75971500

H	2.49952600	-4.69366800	-0.43713900
O	4.48656300	-0.68691600	-1.38999500
C	2.84857900	-2.26449700	0.46493400
Co	3.46329400	0.41843400	-0.23672900
N	2.91304500	-1.03880300	0.87136400
H	2.30348400	-2.98230700	1.08007200
N	2.50271600	1.49936300	0.98775900
C	2.18772400	-0.61936600	2.08673500
C	1.91169000	2.60254900	0.67315700
C	2.47107000	0.86817200	2.30752500
C	2.54238900	-1.37438000	3.37084200
H	1.23904000	3.06631800	1.39309500
C	2.09406100	3.27734200	-0.58171900
C	1.50149800	1.41203100	3.35172600
C	1.62802800	-0.86636500	4.49884900
H	3.59773800	-1.19463400	3.61402500
H	2.42552100	-2.45368600	3.24185200
C	1.22688900	4.34204400	-0.90645400
C	3.15743500	2.92038800	-1.46627000
C	1.72781300	0.65681000	4.67382900
H	1.66182000	2.48433400	3.50947900
H	0.47594600	1.26472200	2.99507000
H	1.87792900	-1.37024100	5.43825700
H	0.59088300	-1.13062400	4.25896900
C	1.38739900	5.05390700	-2.08155500
H	0.41297700	4.57686100	-0.22730600
C	3.31010600	3.67510000	-2.64763600
O	4.01445200	1.94007500	-1.22211600
H	2.72118000	0.91317400	5.06672100
H	0.99843500	0.99487700	5.41661400
C	2.44144600	4.71571700	-2.94564300
H	0.70476200	5.85804100	-2.33289200
H	4.12067600	3.40654400	-3.31680700
H	2.57700400	5.26919100	-3.87069500
O	1.97880300	0.27071700	-1.41937800
H	2.33211800	0.06132200	-2.29429200
O	5.18701200	0.70979100	0.70431100
H	5.36081000	1.55915100	0.24791500
H	5.69064900	0.04920800	0.19003600
C	-0.43967800	0.80196400	-1.24305700
C	0.62919600	-0.29294100	-1.22413400
O	-1.65867300	0.15696500	-1.09299700
H	-0.23499700	1.48429000	-0.40549200
H	0.61118500	-0.79896400	-0.26470700
H	0.45178700	-1.01079600	-2.02722500
C	-0.42278800	1.60211800	-2.54782800
H	-1.18830900	2.38134200	-2.49960400
H	0.54414700	2.08291700	-2.72715500
H	-0.65888800	0.93963300	-3.38801200
C	-1.27473100	4.83357100	1.81168100
C	-2.15444400	5.29913500	0.81924100
C	-1.15456700	3.48104300	2.08403800
H	-0.68233500	5.54408500	2.38344600
C	-2.95837800	4.37255300	0.17637600
H	-2.23963700	6.35813900	0.60166500
C	-1.88947700	2.49215000	1.36293800
H	-0.50445800	3.13888900	2.87892200
C	-2.86859600	2.99086600	0.43801900
H	-3.70431100	4.70870900	-0.54090000
O	-1.65718300	1.23520200	1.58917800
C	-3.89242600	2.13637600	-0.10671400
Co	-2.49890700	-0.22834900	0.63874700
N	-3.93513300	0.86189600	0.02597500
H	-4.71620700	2.64624000	-0.60881800
N	-3.37718400	-1.64116400	-0.29974000
C	-5.06702300	0.04229400	-0.39952000
C	-3.04614700	-2.88047800	-0.27388900
C	-4.44797800	-1.13790700	-1.16364500
C	-6.15684800	0.73314600	-1.21564000

H	-3.62622000	-3.59157300	-0.86287200
C	-1.95175000	-3.44141900	0.46955900
C	-5.50837600	-2.15084500	-1.59537700
C	-7.22933800	-0.28499300	-1.62734700
H	-5.71307600	1.18299300	-2.11430000
H	-6.61222500	1.54321600	-0.63519800
C	-1.77968000	-4.84153300	0.41362100
C	-1.05733400	-2.63635700	1.25339400
C	-6.61503100	-1.45643400	-2.40172800
H	-5.05446500	-2.93666000	-2.20724100
H	-5.93548100	-2.62865400	-0.70358500
H	-7.99972600	0.20834700	-2.22994600
H	-7.72841700	-0.66587900	-0.72635900
C	-0.79430200	-5.49493900	1.13178600
H	-2.46089600	-5.41359100	-0.21297200
C	-0.11297300	-3.35217500	2.04749100
O	-1.03951900	-1.34110500	1.26749900
H	-6.19195600	-1.08440800	-3.34437400
H	-7.38891500	-2.18370900	-2.67027100
C	0.02466200	-4.72707600	1.97868600
H	-0.68341300	-6.57217200	1.07428700
H	0.48065500	-2.77615300	2.74203900
H	0.76451100	-5.21964000	2.60608300
O	-1.60314300	-1.87461000	-2.84942400
H	-1.36036000	-2.60069300	-2.26163100
H	-1.69491400	-1.10889900	-2.21922400
H	-3.94898100	-0.73566200	-2.05510900
H	-5.48928200	-0.35740700	0.53196000
H	1.11302600	-0.73014500	1.88051300
H	3.49836300	0.95869100	2.68808800
O	-3.50202800	-0.68768200	2.13328200
H	-3.11603300	-0.13180000	2.82378300

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2855.820250

Thermal correction to Gibbs Free Energy (a.u.): 0.821582

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5333.0935943 a.u.

C	6.60913300	-3.21928500	-2.34973100
C	5.92933100	-4.21506000	-1.62184700
C	6.35611300	-1.87731200	-2.13520800
H	7.34256100	-3.50838300	-3.09781400
C	5.00101000	-3.82573800	-0.67748300
H	6.13195300	-5.26533700	-1.80090100
C	5.40079200	-1.44855200	-1.17715800
H	6.87296900	-1.10720600	-2.69828100
C	4.71702000	-2.46208100	-0.43243600
H	4.46362800	-4.57442400	-0.09954700
O	5.21683400	-0.16412100	-1.01435800
C	3.75077500	-2.15221600	0.58017000
Co	3.79563600	0.63072600	-0.02558500
N	3.36362400	-0.97086000	0.92561000
H	3.30927300	-3.01221200	1.08817200
N	2.50221900	1.46362100	1.08310300
C	2.25792800	-0.77811000	1.87858300
C	1.81697600	2.50458100	0.75190100
C	2.29517600	0.69281300	2.30947800
C	2.26559200	-1.68087100	3.11638400
H	0.98819400	2.81761800	1.38416600
C	2.07965800	3.31186600	-0.40584700
C	1.07413400	1.03317000	3.15827400
C	1.05288400	-1.35572200	4.00247600
H	3.20137400	-1.51668700	3.66649600
H	2.24542800	-2.73953900	2.83945900
C	1.14479500	4.31125000	-0.75205000
C	3.28288800	3.15785800	-1.16463200
C	1.02973200	0.12558200	4.39649300

H	1.11651400	2.08223600	3.47231600
H	0.16322300	0.88996400	2.56546400
H	1.06693200	-1.98889800	4.89593800
H	0.13309700	-1.59255400	3.45426000
C	1.35634800	5.14552100	-1.83416500
H	0.23988900	4.40211100	-0.15850200
C	3.47918500	4.03642900	-2.25708200
O	4.21732400	2.28051300	-0.87983900
H	1.88932700	0.34710700	5.04386100
H	0.12920900	0.34586100	4.97903400
C	2.53784400	4.99917500	-2.58269100
H	0.62367000	5.89989100	-2.10013600
H	4.39123400	3.92020400	-2.83322700
H	2.71717300	5.64889000	-3.43540800
O	2.52994500	0.21397700	-1.27102400
H	3.02332200	0.31370300	-2.09803700
O	5.36015300	1.22183600	1.23374900
H	5.37259600	2.09714400	0.80037900
H	6.00498100	0.70511900	0.71587800
C	-0.56702800	0.36553000	-1.41345100
C	0.01210800	-0.99720300	-1.89893000
O	-2.01144200	0.21425200	-1.31172500
H	-0.20607300	0.58842200	-0.41146400
H	0.49777600	-1.52440600	-1.08007300
H	0.75443500	-0.83115500	-2.67825900
C	-0.26928500	1.50987000	-2.36514900
H	-0.74611400	2.43081400	-2.02102800
H	0.81077600	1.66426800	-2.39852700
H	-0.63555600	1.27940000	-3.37232300
C	-1.59574000	4.63228800	1.78576700
C	-2.53049100	5.15817100	0.87458500
C	-1.47057600	3.26841500	1.97841200
H	-0.96206200	5.30694400	2.35565400
C	-3.37541300	4.27766100	0.22746000
H	-2.61507900	6.22809700	0.72077100
C	-2.25219300	2.32907800	1.24683400
H	-0.77501500	2.87720700	2.70801000
C	-3.27662400	2.87986200	0.40718200
H	-4.15802400	4.65548400	-0.42682100
O	-2.02188100	1.05674400	1.40470700
C	-4.33481200	2.05949100	-0.10560000
Co	-2.90798500	-0.34074900	0.44535100
N	-4.36961400	0.77500100	-0.03555100
H	-5.19589000	2.58874100	-0.51635100
N	-3.84840100	-1.69672700	-0.54091200
C	-5.55123400	-0.02343800	-0.35199100
C	-3.55063200	-2.95123300	-0.53382500
C	-5.04337500	-1.18024400	-1.22429600
C	-6.73048200	0.69584800	-1.00179600
H	-4.22281800	-3.65148200	-1.03093300
C	-2.37225200	-3.53027100	0.03632300
C	-6.15817100	-2.18430000	-1.52081000
C	-7.85610600	-0.30769800	-1.29130700
H	-6.40663800	1.16931700	-1.93891400
H	-7.09855000	1.49128300	-0.34499800
C	-2.20528300	-4.93155800	-0.10416100
C	-1.35401300	-2.74181200	0.67808600
C	-7.36013600	-1.47059600	-2.15804800
H	-5.80396400	-2.97036700	-2.19580700
H	-6.45983000	-2.66830600	-0.58293900
H	-8.69214000	0.20159300	-1.78192700
H	-8.23944900	-0.70047400	-0.34050400
C	-1.07695300	-5.58163900	0.34567000
H	-2.99976600	-5.49358500	-0.58999900
C	-0.19518700	-3.45055400	1.11286300
O	-1.39956900	-1.45828300	0.84408800
H	-7.06894800	-1.08788800	-3.14554400
H	-8.16733400	-2.19076300	-2.32769800
C	-0.06351200	-4.81423400	0.95475000

H	-0.96648700	-6.65364800	0.22746300
H	0.58545300	-2.87243800	1.58202500
H	0.84050700	-5.30362300	1.30859900
O	-1.05111900	-1.79926100	-2.45860600
H	-1.21312800	-2.53551500	-1.85196800
H	-2.16891300	-0.56510700	-1.89415400
H	-4.70209600	-0.74015500	-2.17471600
H	-5.85848000	-0.45637100	0.60915000
H	1.32212700	-0.91928900	1.32061900
H	3.20692300	0.83540700	2.90724500
O	-3.81111400	-0.89537200	1.93890500
H	-3.37617600	-0.39430900	2.64322900

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon and subsequent hydration

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OH + H_2O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.354743

Thermal correction to Gibbs Free Energy (a.u.): 0.795676

Imaginary frequencies: -342.79

Calculation of single point energy based on the optimized structure, Et = -5256.5666315 a.u.

C	6.93448500	-1.87191900	3.16688700
C	6.56812000	-0.88906300	4.10718400
C	6.39368100	-1.88307400	1.89490800
H	7.65223800	-2.63886100	3.44519600
C	5.65339100	0.07433100	3.73463500
H	6.99674700	-0.89142500	5.10328700
C	5.44706600	-0.90824900	1.48667000
H	6.67058800	-2.64014900	1.16882800
C	5.07739300	0.09130900	2.44206400
H	5.35484300	0.84543500	4.44125100
O	4.99025200	-0.96144200	0.26198900
C	4.14349600	1.13498900	2.14051300
Co	3.51359100	0.03560800	-0.41671900
N	3.50527900	1.29091800	1.02902600
H	3.96459800	1.85217700	2.94424700
N	2.16640800	1.11597600	-1.17803800
C	2.46434200	2.32197200	0.87458400
C	1.26530300	0.69225900	-2.00061000
C	2.22058300	2.47588200	-0.63360600
C	2.74765600	3.68626400	1.50845900
H	0.44667700	1.35235000	-2.26784400
C	1.28594800	-0.60250900	-2.62579900
C	1.03292700	3.39240600	-0.90991400
C	1.57198600	4.63940100	1.23498100
H	3.67614400	4.09118000	1.08524900
H	2.89801000	3.59419900	2.58880100
C	0.15065700	-1.01722800	-3.35756700
C	2.45783000	-1.42028700	-2.59591000
C	1.27118200	4.76371700	-0.26395000
H	0.87247100	3.50835800	-1.98409700
H	0.11611500	2.95061400	-0.50585400
H	1.78743900	5.62330500	1.66495800
H	0.67972200	4.25922800	1.75055900
C	0.16903300	-2.19013500	-4.09072300
H	-0.75366600	-0.42501100	-3.27803700
C	2.44958900	-2.60988900	-3.35830100
O	3.55027200	-1.10543700	-1.92891600
H	2.11461200	5.26005200	-0.76275900
H	0.39035900	5.39237200	-0.42696900
C	1.33336700	-2.97729700	-4.09382600
H	-0.71229900	-2.50660900	-4.63756500
H	3.34548300	-3.22173600	-3.34394000
H	1.35684400	-3.90048700	-4.66694900
O	2.29753600	-1.01925700	0.49151800
H	2.64397500	-1.90859900	0.32886900
O	4.98418700	1.01005800	-1.48133800
H	4.80642100	0.44883700	-2.26243600

H	5.70397600	0.53739800	-1.02307300
C	0.19822600	-1.28950000	0.60648000
C	-0.27900300	0.00285400	1.09929400
O	-1.53886200	-0.61432000	1.09205900
H	0.05740000	-1.45397100	-0.45338200
H	-0.18569500	0.83144000	0.39440600
H	0.06682800	0.28512900	2.10348700
C	0.34144200	-2.48035100	1.49888900
H	0.98817900	-3.22845100	1.03435600
H	0.74967700	-2.19863100	2.47236600
H	-0.63706400	-2.94674400	1.63273700
C	-1.32553900	-5.24212400	-0.87558600
C	-2.07888700	-5.65991700	0.23897200
C	-1.42747800	-3.95606800	-1.37067100
H	-0.64692100	-5.94197000	-1.35713600
C	-2.93287200	-4.75108000	0.83318800
H	-1.99371500	-6.67268300	0.61792300
C	-2.28646400	-2.99222200	-0.77110800
H	-0.84266000	-3.63334600	-2.22354200
C	-3.04807000	-3.42217700	0.36606700
H	-3.53217600	-5.04739800	1.69187000
O	-2.32965100	-1.79516700	-1.27868100
C	-3.95756900	-2.54368900	1.04757300
Co	-2.91576700	-0.27199500	-0.30212300
N	-4.04946500	-1.27727000	0.84404800
H	-4.60831400	-3.00934100	1.78993600
N	-3.46956300	1.25013600	0.71619500
C	-4.99667900	-0.40107100	1.52620100
C	-3.34838100	2.47564600	0.34281200
C	-4.17696300	0.84352700	1.93279900
C	-5.74587100	-0.99365000	2.71818400
H	-3.76778000	3.26418600	0.97047600
C	-2.72739200	2.91401000	-0.87696100
C	-5.05737200	1.90075100	2.59881000
C	-6.63171800	0.07280900	3.37659100
H	-5.02227400	-1.37585300	3.45118600
H	-6.35981100	-1.84155500	2.39575800
C	-2.80368300	4.28423900	-1.20324600
C	-2.05753000	2.00226200	-1.75868500
C	-5.81160700	1.29894300	3.79280700
H	-4.45106900	2.74930600	2.93486100
H	-5.77529000	2.28538900	1.86244000
H	-7.14572300	-0.35402200	4.24450800
H	-7.41166100	0.38169600	2.66812900
C	-2.29507800	4.78193000	-2.39035400
H	-3.29554700	4.95386700	-0.50047300
C	-1.61304700	2.53151600	-3.00406700
O	-1.78437800	0.76885800	-1.45676800
H	-5.08932100	1.00589300	4.56681500
H	-6.46101100	2.05856100	4.24110000
C	-1.71929100	3.87873200	-3.30223400
H	-2.37127900	5.83731400	-2.62840900
H	-1.18479200	1.83964400	-3.72176500
H	-1.35713900	4.24092500	-4.26110100
H	-5.70718400	-0.07921900	0.75361700
H	-3.40856400	0.50058500	2.63961600
H	3.12768300	2.92965000	-1.05794000
H	1.54750200	1.91162800	1.31542800
O	-4.35005400	0.03064700	-1.42430500
H	-4.20108800	-0.61155900	-2.13196000

PO-Co^{III}-OH + H_2O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OH + H_2O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.379965

Thermal correction to Gibbs Free Energy (a.u.): 0.792769

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -5256.590821 a.u.

C	7.46998100	-1.49365100	3.36704100

C	7.46104700	-0.15099500	3.79452000
C	6.64088400	-1.92668100	2.35028200
H	8.13768000	-2.20447800	3.84660300
C	6.60099500	0.73317900	3.17642600
H	8.11387300	0.17777500	4.59567000
C	5.74854600	-1.03792700	1.69265600
H	6.64154100	-2.96040500	2.02070000
C	5.73984800	0.32550500	2.13008200
H	6.56991200	1.77398600	3.49133300
O	5.01020600	-1.50837900	0.72305400
C	4.86215400	1.30818100	1.56486200
Co	3.70069800	-0.54929000	-0.27159700
N	4.03088700	1.11625700	0.59716400
H	4.90854700	2.29753900	2.02292300
N	2.51381900	0.42725300	-1.39415000
C	3.04682900	2.12950400	0.19125600
C	1.53674200	-0.08573300	-2.06526600
C	2.76395100	1.86866400	-1.29713700
C	3.42178400	3.59130200	0.44136800
H	0.83711300	0.57960300	-2.57087300
C	1.29503700	-1.49346400	-2.20886300
C	1.68172000	2.79623100	-1.84021500
C	2.33289300	4.52364300	-0.11124100
H	4.38227300	3.80431900	-0.04665000
H	3.55374300	3.77878100	1.51200500
C	0.09143200	-1.90645600	-2.82342000
C	2.24812800	-2.46653500	-1.77300900
C	2.06549500	4.26044900	-1.59650700
H	1.52596200	2.62387700	-2.90794600
H	0.72524000	2.58521800	-1.34842100
H	2.62535400	5.56690400	0.04886900
H	1.40405300	4.36618400	0.45384700
C	-0.19692500	-3.24647200	-3.00412100
H	-0.64126800	-1.15192400	-3.09043400
C	1.92571000	-3.83137500	-1.97312400
O	3.40726100	-2.16439300	-1.23839700
H	2.96490000	4.50676900	-2.17722800
H	1.26113000	4.90477500	-1.96226900
C	0.73525400	-4.20737700	-2.57279200
H	-1.13088400	-3.54834500	-3.46470900
H	2.64749800	-4.56828300	-1.63674000
H	0.51715400	-5.26403400	-2.70355900
O	2.35870000	-0.87436800	0.92100500
H	2.62600700	-1.72346300	1.30134700
O	5.24869000	-0.36549700	-1.67766800
H	4.87247100	-1.12931900	-2.15825900
H	5.90746300	-0.77863100	-1.09209600
C	-0.80932600	-1.57736500	0.39692400
C	-0.39291400	-0.23522500	0.77502900
O	-1.78543700	-0.63877400	0.98393600
H	-1.02579300	-1.74824500	-0.64924600
H	-0.27115800	0.51235700	0.00128500
H	0.16598700	-0.09166100	1.69161700
C	-0.48642800	-2.78834500	1.21649200
H	0.43068700	-3.23431600	0.81931400
H	-0.32538700	-2.52597900	2.26573900
H	-1.29045600	-3.52618600	1.14642800
C	-3.75534900	-5.16126900	-0.28246600
C	-4.39791900	-5.15406800	0.97189700
C	-3.44860500	-3.98401600	-0.93683700
H	-3.49278900	-6.10941300	-0.74457100
C	-4.72118300	-3.93854700	1.54107000
H	-4.63621600	-6.08429600	1.47599500
C	-3.75490600	-2.71638100	-0.36886000
H	-2.94383500	-3.98446300	-1.89620200
C	-4.40731200	-2.71423500	0.90782500
H	-5.22423600	-3.90472800	2.50520700
O	-3.42875900	-1.64599400	-1.03383200
C	-4.79247100	-1.49523000	1.56002600

Co	-3.27104000	0.07108000	-0.25725500
N	-4.45209900	-0.31298400	1.17791600
H	-5.42524000	-1.60258800	2.44264400
N	-3.06602300	1.78834800	0.55233100
C	-4.90291400	0.92085300	1.81753000
C	-2.62423600	2.83321800	-0.05940200
C	-3.65212500	1.82307200	1.89528500
C	-5.57941500	0.78383500	3.18030500
H	-2.66102500	3.79749600	0.45040100
C	-2.08789200	2.85177200	-1.39098500
C	-3.99136600	3.20087100	2.46288500
C	-5.91877600	2.16926600	3.74807500
H	-4.90785100	0.25468900	3.87010200
H	-6.49195400	0.18470500	3.09197400
C	-1.77849400	4.10569700	-1.96255000
C	-1.86033600	1.64702100	-2.13784300
C	-4.67495700	3.06131100	3.83067300
H	-3.08538200	3.80896100	2.56211500
H	-4.65938200	3.72227800	1.76483700
H	-6.37700100	2.06338900	4.73706500
H	-6.66695600	2.64914200	3.10351700
C	-1.28547100	4.21806000	-3.24931000
H	-1.95238100	4.99984600	-1.36746800
C	-1.37107100	1.79812800	-3.46660400
O	-2.02795100	0.45259700	-1.66002000
H	-3.96444600	2.62783100	4.54737300
H	-4.94119000	4.05220000	4.21353400
C	-1.09391200	3.04278700	-4.00114600
H	-1.06839700	5.19040900	-3.67787000
H	-1.24089400	0.89643000	-4.05572400
H	-0.72863300	3.11321200	-5.02246100
H	-5.59072500	1.38850800	1.10063600
H	-2.93769500	1.32109500	2.56400500
H	3.70280100	2.05534600	-1.83860400
H	2.12494400	1.88976800	0.73998000
O	-4.66186600	0.75517500	-1.22988500
H	-4.82351800	0.05677900	-1.87996000

PO-Co^{III}-OH + H$_2$O-Co^{III}-OH bimetallic PO ring-opening in the middle carbon

PO-Co^{III}-OH + H$_2$O-Co^{III}-OH = OH-Co^{III}-PO-OH-Co^{III}-H$_2$O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2779.373971

Thermal correction to Gibbs Free Energy (a.u.): 0.799552

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5256.5948158 a.u.

C	6.81433000	-1.78150600	3.15588500
C	6.50377400	-0.75116300	4.06320200
C	6.21720500	-1.84240500	1.90948200
H	7.53293500	-2.54609500	3.43731500
C	5.58581500	0.20828500	3.68779400
H	6.97551100	-0.71471500	5.03873700
C	5.26969500	-0.87216800	1.50239400
H	6.45116200	-2.63621600	1.20807600
C	4.95514800	0.17510700	2.42122700
H	5.32731200	1.01370600	4.37091600
O	4.75080000	-0.98216100	0.29851300
C	4.01316800	1.21255000	2.11665300
Co	3.34197700	0.07664300	-0.42037500
N	3.33716900	1.33725200	1.02433100
H	3.86302800	1.95642400	2.90051400
N	2.03328300	1.17990300	-1.20742900
C	2.30106200	2.37490800	0.86002000
C	1.16016100	0.78440600	-2.07574800
C	2.08756800	2.53933600	-0.64981700
C	2.57248100	3.73044700	1.51497100
H	0.36822400	1.46587900	-2.36253600
C	1.18038200	-0.49898400	-2.72156200
C	0.89876000	3.45157200	-0.93258400
C	1.39716400	4.68154000	1.23057600

H	3.50791300	4.14491700	1.11609400
H	2.69808300	3.62538900	2.59734600
C	0.06518000	-0.88360800	-3.49767200
C	2.32811000	-1.34148700	-2.65552500
C	1.12098900	4.81808700	-0.27155400
H	0.74848700	3.57846500	-2.00687800
H	-0.01460700	2.99445900	-0.54101800
H	1.60294800	5.66148400	1.67379000
H	0.49892400	4.29200700	1.72723800
C	0.09668600	-2.04148000	-4.25339000
H	-0.83230600	-0.28068700	-3.43311300
C	2.33638700	-2.51712300	-3.43225700
O	3.40048600	-1.05644200	-1.92807700
H	1.96819200	5.32567800	-0.75277700
H	0.23750300	5.44057100	-0.44225100
C	1.24611000	-2.84758100	-4.22515000
H	-0.76892300	-2.33814300	-4.83473900
H	3.21803700	-3.14766000	-3.38869900
H	1.27699800	-3.76114000	-4.81258300
O	2.15967700	-1.06971600	0.56699000
H	2.65537400	-1.90321000	0.52405400
O	4.78793200	1.01181000	-1.42827400
H	4.63440600	0.44921000	-2.21840400
H	5.54235600	0.58275300	-0.98386000
C	0.69404800	-1.39484100	0.51200200
C	-0.11161300	-0.18680400	1.02019000
O	-1.42640100	-0.52400300	1.19121500
H	0.43399200	-1.60805100	-0.52410400
H	0.02200400	0.64464300	0.31185700
H	0.35758400	0.12060100	1.98277000
C	0.51789800	-2.61729000	1.38901400
H	0.99667100	-3.50409500	0.95924700
H	0.92139900	-2.42618300	2.38982300
H	-0.55071300	-2.81192900	1.47531600
C	-1.11387400	-5.24231500	-1.02720800
C	-1.89564900	-5.71730800	0.04352500
C	-1.18673900	-3.92573000	-1.43963200
H	-0.43736700	-5.92172500	-1.54085000
C	-2.74860800	-4.83234600	0.67558500
H	-1.83444100	-6.75324600	0.35965100
C	-2.04414600	-2.98470500	-0.79818700
H	-0.58181800	-3.56083100	-2.26030100
C	-2.83867400	-3.47635100	0.29164000
H	-3.36891100	-5.17268400	1.50268100
O	-2.05164400	-1.75960900	-1.22418000
C	-3.74926300	-2.63289300	1.01775600
Co	-2.74814200	-0.28475600	-0.23116900
N	-3.85283100	-1.36030000	0.87960700
H	-4.39499500	-3.14193300	1.73587600
N	-3.40521900	1.19706600	0.77634000
C	-4.81073500	-0.53728800	1.61338100
C	-3.37817900	2.42625500	0.40670900
C	-4.03069200	0.73450100	2.01363300
C	-5.48343700	-1.18610800	2.82278600
H	-3.83321000	3.18524500	1.04652900
C	-2.81718400	2.90469200	-0.83064100
C	-4.92071900	1.73556200	2.74833600
C	-6.37684500	-0.17334700	3.55164200
H	-4.71099800	-1.55882900	3.50908500
H	-6.08154300	-2.04819700	2.50830400
C	-3.00738000	4.26000700	-1.16244800
C	-2.09094100	2.04128400	-1.71801000
C	-5.58629400	1.07366600	3.96250000
H	-4.33401000	2.60243300	3.07294200
H	-5.69345100	2.10570300	2.06110900
H	-6.83202000	-0.64328400	4.43042000
H	-7.20159100	0.12314500	2.88983600
C	-2.56450800	4.79154600	-2.36352900
H	-3.53641400	4.89311100	-0.45251400

C	-1.72616200	2.59666800	-2.97937100
O	-1.69635000	0.84494500	-1.40549200
H	-4.81293900	0.78908100	4.68881800
H	-6.24171600	1.79294700	4.46589100
C	-1.94362800	3.93025500	-3.28381500
H	-2.72937000	5.83640300	-2.60374500
H	-1.26942100	1.93722500	-3.71046200
H	-1.63607200	4.31113500	-4.25472700
H	-5.56715400	-0.23380400	0.87727400
H	-3.20318300	0.41047000	2.65831900
H	3.00035000	2.99524000	-1.05958300
H	1.37815400	1.95604900	1.27747200
O	-4.19794500	-0.06410900	-1.38597100
H	-4.00428000	-0.70086700	-2.08703200

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2855.766279

Thermal correction to Gibbs Free Energy (a.u.): 0.819327

Imaginary frequencies: -429.18

Calculation of single point energy based on the optimized structure, Et = -5333.0400512 a.u.

C	5.79580300	-3.20407300	-2.56368400
C	4.83455700	-4.17376800	-2.22046500
C	5.75270800	-1.93223300	-2.02263400
H	6.58669600	-3.45568300	-3.26510200
C	3.83276100	-3.83117400	-1.33501100
C	4.73865800	-1.55812600	-1.10465700
C	3.75416300	-2.53710300	-0.76832400
H	3.07353400	-4.55390400	-1.05679300
O	4.77389600	-0.34281600	-0.60983500
C	2.67238500	-2.26799500	0.13640900
Co	3.52491700	0.42693600	0.58022600
N	2.47998500	-1.16152200	0.77697900
H	1.95640900	-3.07964600	0.26807500
N	2.35404600	1.18918700	1.87660200
C	1.28891700	-0.95288500	1.61997900
C	2.12915900	2.45583300	1.99723900
C	1.64305900	0.15141000	2.62948600
C	0.75713400	-2.18086600	2.36000000
H	1.34093800	2.78701100	2.67401500
C	2.83049600	3.47799600	1.27635400
C	0.39738400	0.59038800	3.39892100
C	-0.49095100	-1.77444600	3.15646100
H	1.53523100	-2.58109000	3.02446200
H	0.48489700	-2.96597900	1.65221900
C	2.31466300	4.79313800	1.29419700
C	4.05154100	3.19331300	0.58572000
C	-0.21300100	-0.61916600	4.12403900
H	0.64573000	1.36958900	4.12786600
H	-0.32932700	1.01157000	2.69272900
H	-0.88441500	-2.63947300	3.70200000
H	-1.25810600	-1.46595100	2.43966800
C	2.96025700	5.82290500	0.63746000
H	1.38347600	4.97798800	1.82413600
C	4.70268700	4.27227100	-0.05836900
O	4.60468800	2.00578200	0.56218500
H	0.47805300	-0.95367400	4.90927500
H	-1.13758300	-0.31662000	4.62831100
C	4.16649100	5.54800900	-0.03525400
H	4.68509700	6.35094800	-0.55204100
O	2.49122100	1.05923800	-0.81065600
H	2.83204800	0.63578700	-1.61109900
O	4.87369100	-0.08891400	2.04441100
H	5.24811200	0.81544600	2.02264800
H	5.46634200	-0.59437100	1.46050700
H	0.48105600	-0.57988200	0.97638800
H	2.37713700	-0.26574700	3.33393000
C	0.46790000	1.69333000	-0.83990500

C	-0.21197900	0.38162700	-1.19348800
O	-1.17223500	0.05436700	-0.21617200
H	0.75707000	1.86606300	0.17460300
H	0.57393800	-0.37986300	-1.25768800
H	-0.66554500	0.47413500	-2.18563400
C	0.74658200	2.72466200	-1.88549700
H	-0.19668700	3.05663600	-2.32850900
H	1.29258200	3.57647300	-1.48058000
H	1.33371200	2.27710900	-2.69233000
O	-1.27857900	2.48160000	-0.02147300
H	-1.47301300	1.45737800	0.06185100
H	-1.89972200	2.79425200	-0.69741800
H	5.62886600	4.05658500	-0.58001900
H	2.54883200	6.82624000	0.64241700
H	6.49110700	-1.18059900	-2.28119300
H	4.87965000	-5.17010500	-2.64649000
C	0.57146300	-4.30528200	-2.34375800
C	0.38976000	-4.98890400	-1.12224300
C	-0.19183700	-3.20205200	-2.66552400
H	1.32737900	-4.64999500	-3.04388000
C	-0.57041900	-4.52329000	-0.24316200
H	0.97199400	-5.87470800	-0.89008800
C	-1.20091500	-2.70327900	-1.78743500
H	-0.06333400	-2.68300000	-3.60951200
C	-1.35536300	-3.38440700	-0.53094900
H	-0.74444000	-5.04265400	0.69759500
O	-1.91871900	-1.70164800	-2.17751600
C	-2.35934500	-2.99456500	0.41938900
Co	-2.90690200	-0.58067000	-0.99569000
N	-3.05628100	-1.91615400	0.35025700
H	-2.53212000	-3.68517600	1.24731400
N	-3.86547400	0.54328200	0.22194100
C	-4.15723300	-1.59385900	1.25650400
C	-4.42109100	1.66428700	-0.08801500
C	-4.01771600	-0.08484800	1.53709400
C	-4.26445400	-2.41335900	2.54152000
H	-5.03765800	2.16957500	0.65687000
C	-4.27443900	2.35601700	-1.33637700
C	-5.15641000	0.42906800	2.41829200
C	-5.41418100	-1.88811300	3.41220200
H	-3.32366700	-2.35258900	3.10285000
H	-4.43118000	-3.46923900	2.30261900
C	-4.93328300	3.60095700	-1.48220000
C	-3.45028800	1.85378300	-2.40227600
C	-5.24785800	-0.39414600	3.71061200
H	-5.00535000	1.48573100	2.66390200
H	-6.09989200	0.35494100	1.86213600
H	-5.46616100	-2.46018100	4.34483800
H	-6.36604000	-2.04877700	2.88937000
C	-4.80507800	4.36464700	-2.62343400
H	-5.55122400	3.95254200	-0.65853700
C	-3.33217400	2.67379000	-3.56459500
O	-2.78814000	0.74577800	-2.36154600
H	-4.33415500	-0.24219700	4.30229900
H	-6.08065300	-0.03143400	4.32247700
C	-3.98733200	3.88376400	-3.66773300
H	-5.31773400	5.31582300	-2.71628400
H	-2.71023200	2.29543600	-4.36925000
H	-3.87249800	4.47441200	-4.57304600
H	-5.06428400	-1.72178500	0.65161500
H	-3.06342000	0.06112700	2.06646700
O	-4.54675000	-1.14610900	-1.64039100
H	-4.31545200	-1.50896400	-2.50629000

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2855.809526

Thermal correction to Gibbs Free Energy (a.u.): 0.824196

No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -5333.0872546 a.u.

C	5.91371500	-2.80446800	-2.33269100
C	5.00041700	-3.84600900	-2.09116700
C	5.75923100	-1.56528700	-1.73455900
H	6.75522800	-2.96972400	-2.99971700
C	3.93436000	-3.61398600	-1.24450900
C	4.67530000	-1.30505000	-0.86379700
C	3.74480100	-2.35841200	-0.62183700
H	3.20702700	-4.39364300	-1.04632100
O	4.59516000	-0.10232000	-0.32333700
C	2.60985500	-2.20977300	0.24733800
Co	3.21762300	0.53420700	0.80443400
N	2.29883300	-1.14548000	0.91014500
H	1.95720800	-3.07980900	0.32501500
N	1.89452300	1.16132900	2.00698100
C	1.06624100	-1.06540300	1.72298000
C	1.48344900	2.38229400	2.06449500
C	1.30600000	0.04605400	2.75413000
C	0.65294900	-2.35393200	2.43177900
H	0.60458000	2.61303400	2.65854200
C	2.10995500	3.46366000	1.35097700
C	0.04777400	0.34592300	3.56554200
C	-0.61467000	-2.08183800	3.25406900
H	1.47031900	-2.70043800	3.07986900
H	0.44623900	-3.14142000	1.70473500
C	1.41934800	4.68677500	1.23291200
C	3.41911900	3.32194700	0.79976000
C	-0.42392100	-0.94104500	4.25940800
H	0.26044700	1.11616700	4.31615600
H	-0.73047700	0.74021400	2.90399400
H	-0.92942000	-2.99641700	3.76887300
H	-1.41457400	-1.81227100	2.55832700
C	1.99034500	5.76649900	0.58314500
H	0.41565500	4.75244900	1.64307800
C	3.98898600	4.44377000	0.16155300
O	4.12147200	2.20582400	0.88926000
H	0.31318000	-1.23968000	5.01720500
H	-1.36118500	-0.74741700	4.79251500
C	3.28670900	5.63523600	0.05616600
H	3.74595900	6.47770000	-0.45341600
O	2.32985000	1.12560300	-0.78730700
H	2.78962600	0.70416600	-1.52848100
O	4.45201500	0.12461700	2.30520100
H	4.74372800	1.05975300	2.36826700
H	5.15048400	-0.30516600	1.77730600
H	0.25371000	-0.74675400	1.04535700
H	2.09528800	-0.30224600	3.43606500
C	0.91707400	1.41413600	-1.12249100
C	0.10095700	0.12761600	-1.34684900
O	-0.91711600	-0.03305800	-0.39175900
H	0.54672600	1.93672200	-0.24653300
H	0.80330700	-0.72369900	-1.33007300
H	-0.32128200	0.15795900	-2.35568700
C	0.94292700	2.35816200	-2.31101700
H	-0.08012600	2.67260800	-2.53563700
H	1.55138100	3.24129800	-2.09729500
H	1.33419200	1.85834500	-3.20609100
O	-1.24310400	2.09833500	1.11063400
H	-1.16097400	1.26757800	0.54236600
H	-1.74775300	2.69581700	0.54370800
H	4.98557300	4.33564100	-0.25270300
H	1.44689900	6.69927100	0.48038300
H	6.45961300	-0.75702600	-1.91664700
H	5.12967800	-4.81332100	-2.56399800
C	0.77680000	-4.41430300	-2.42342500
C	0.56719400	-5.07350100	-1.19311800
C	0.02509800	-3.31449000	-2.78279400
H	1.54342100	-4.77775000	-3.10277100

C	-0.41633000	-4.59063600	-0.34778100
H	1.13993500	-5.95752600	-0.93176800
C	-0.99877200	-2.79055900	-1.93525600
H	0.17650000	-2.81380200	-3.73334600
C	-1.18739900	-3.45354500	-0.67258200
H	-0.62130000	-5.09856900	0.59320200
O	-1.69632900	-1.78799300	-2.35271900
C	-2.23261700	-3.05462500	0.23139300
Co	-2.65563300	-0.60840900	-1.18563900
N	-2.90444400	-1.96391100	0.13183500
H	-2.46761600	-3.75229500	1.03839700
N	-3.61238800	0.51912100	0.02451900
C	-4.06617900	-1.63638800	0.95623700
C	-3.98429000	1.72624300	-0.22381800
C	-3.90332000	-0.14496400	1.29733000
C	-4.32260400	-2.49664900	2.19175400
H	-4.57631700	2.25716600	0.52350500
C	-3.64796700	2.48400100	-1.39319700
C	-5.10386100	0.38173200	2.08504900
C	-5.53873100	-1.95969800	2.95926300
H	-3.44577900	-2.48872200	2.85103300
H	-4.49569900	-3.53751000	1.89692800
C	-4.07424600	3.83343700	-1.44754700
C	-2.89055000	1.92745200	-2.48243800
C	-5.35330600	-0.48366800	3.32826800
H	-4.93721900	1.41966400	2.39099300
H	-5.98848700	0.36925100	1.43545300
H	-5.70685900	-2.56038500	3.85983100
H	-6.43530600	-2.06700400	2.33495400
C	-3.77719700	4.65218800	-2.51717800
H	-4.65164300	4.22093900	-0.61010400
C	-2.61224400	2.80042100	-3.57939100
O	-2.44251700	0.72054700	-2.53287800
H	-4.49887200	-0.38694800	4.01298100
H	-6.23064200	-0.11187700	3.86852200
C	-3.03627400	4.11297600	-3.59027700
H	-4.10983400	5.68435100	-2.53759400
H	-2.05338900	2.37927300	-4.40880200
H	-2.79842700	4.74078100	-4.44547500
H	-4.91574000	-1.71298400	0.26545400
H	-2.99859900	-0.03516800	1.91483100
O	-4.30197300	-1.10777200	-1.88656900
H	-4.06220400	-1.42855900	-2.76640300

subsequent hydration

$OH\text{-}Co^{III}\text{-}PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + Co^{III}(salen)\text{-}OH + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2855.824873

Thermal correction to Gibbs Free Energy (a.u.): 0.822440

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -5333.1009234 a.u.

C	6.41594300	-2.50435700	-2.95229700
C	5.56398700	-3.60136200	-2.71749200
C	6.25807100	-1.31615200	-2.26414100
H	7.21040200	-2.58990100	-3.68885600
C	4.55747300	-3.46883500	-1.78237800
C	5.23100800	-1.15311500	-1.29770100
C	4.36396100	-2.26560400	-1.06377800
H	3.88439500	-4.29741300	-1.58137700
O	5.15056700	-0.00963300	-0.66659800
C	3.28009300	-2.21476900	-0.12660400
Co	3.76466000	0.52430100	0.51478600
N	2.96894700	-1.20793900	0.61920700
H	2.66199900	-3.11024800	-0.07508600
N	2.47476200	1.04173800	1.81479500
C	1.73824800	-1.21341300	1.42573500
C	2.09312500	2.25565200	2.02661300
C	1.90193500	-0.12208500	2.49484100
C	1.35810400	-2.54030500	2.08592400

H	1.27001600	2.43276900	2.72015600
C	2.67432300	3.41909700	1.42217400
C	0.59323700	0.09027700	3.25642800
C	0.05536200	-2.35729500	2.87785300
H	2.17312300	-2.86391300	2.74670700
H	1.21275200	-3.31713100	1.33202100
C	2.02726900	4.66243100	1.59843700
C	3.90374700	3.34805600	0.69352100
C	0.15846600	-1.22999300	3.91082800
H	0.71354100	0.85944200	4.02686300
H	-0.17842000	0.43096400	2.55469500
H	-0.22140800	-3.29892600	3.36546300
H	-0.74406100	-2.11266900	2.17127400
C	2.54038000	5.82407000	1.05520300
H	1.09788600	4.68758000	2.16288400
C	4.41353600	4.55724400	0.15882700
O	4.59222700	2.24578900	0.53817800
H	0.88456600	-1.50591500	4.68703900
H	-0.80375600	-1.09146800	4.41695600
C	3.74649800	5.75689200	0.33199200
H	4.16167400	6.66273200	-0.10159800
O	2.62119200	0.98514400	-0.82955200
H	3.21939000	1.13305100	-1.57599200
O	5.20830200	0.16155100	1.99352500
H	5.43222400	1.11298000	1.98631500
H	5.83638700	-0.21779100	1.35305300
H	0.92197200	-0.91179100	0.75836200
H	2.67433000	-0.47159400	3.19559800
C	-0.48711400	2.64868800	-0.28602200
C	-0.45007200	1.15130000	-0.57337400
O	-1.47178300	0.51499900	0.25806000
H	-0.07541400	2.84383800	0.70873400
H	0.52591500	0.72487200	-0.35607200
H	-0.69476600	0.95341100	-1.61705400
C	0.30226400	3.43324400	-1.32005800
H	-0.13786400	3.30200300	-2.31502600
H	0.30992300	4.49752000	-1.07318600
H	1.33041700	3.05967000	-1.33696500
O	-1.86585000	3.04797300	-0.18124700
H	-2.02938000	1.28279500	0.51227100
H	-2.30396500	2.73061100	-0.99303700
H	5.34367900	4.50233900	-0.39676800
H	2.02615300	6.77006800	1.18441800
H	6.91009400	-0.46753300	-2.44276900
H	5.69681000	-4.52990900	-3.26196500
C	1.12623900	-3.30982800	-2.70173200
C	0.93371400	-4.32117000	-1.73404800
C	0.27961700	-2.22400300	-2.77680200
H	1.95830700	-3.38527100	-3.39552700
C	-0.10494300	-4.18802500	-0.83588300
H	1.58337800	-5.18957400	-1.70567500
C	-0.82430400	-2.07507100	-1.88676800
H	0.41846500	-1.45029600	-3.52377900
C	-0.97802300	-3.07350100	-0.86812700
H	-0.27521100	-4.95169100	-0.07957700
O	-1.62203600	-1.06664100	-2.05703300
C	-2.02342600	-3.01051200	0.10799600
Co	-2.95158500	-0.48361800	-0.84566800
N	-2.84160500	-2.02661900	0.27007200
H	-2.10974500	-3.87766500	0.76484100
N	-4.24759900	0.15052800	0.40973800
C	-3.96215600	-2.07611300	1.21638900
C	-5.20792200	0.95995500	0.10424900
C	-4.20151800	-0.61818900	1.65502600
C	-3.79823300	-3.00236000	2.42365600
H	-6.00607700	1.12508900	0.82916200
C	-5.32239300	1.67921100	-1.12792000
C	-5.40490200	-0.50092200	2.58816700
C	-5.00024400	-2.87314900	3.37009500

H	-2.87539000	-2.74239800	2.95749700
H	-3.70129000	-4.04332500	2.09904100
C	-6.50106000	2.42196000	-1.36240100
C	-4.26314100	1.69844900	-2.08960300
C	-5.22227800	-1.42006100	3.80364500
H	-5.53402300	0.53696600	2.91420400
H	-6.31485500	-0.78814100	2.04531900
H	-4.85115600	-3.51416700	4.24540400
H	-5.90125000	-3.23994900	2.86105500
C	-6.66940600	3.16138200	-2.51653800
H	-7.28720500	2.39558700	-0.61098100
C	-4.45813500	2.47324400	-3.25977200
O	-3.10878100	1.10685100	-1.90855100
H	-4.35872400	-1.07862900	4.39064000
H	-6.09608100	-1.34661700	4.45936400
C	-5.62921700	3.18041200	-3.46516500
H	-7.58310600	3.71962100	-2.68899100
H	-3.65372100	2.48628900	-3.98766300
H	-5.74706300	3.75913400	-4.37742500
H	-4.83921800	-2.37940700	0.62860000
H	-3.29983800	-0.29440700	2.19640400
O	-4.30493300	-1.30333100	-1.76108500
H	-3.90929300	-1.45383700	-2.63137600

PO + H_2O-Co^{III}-OH PO ring-opening in the terminal carbon and subsequent hydration

PO + H_2O-Co^{III}-OH PO ring-opening in the terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.367487

Thermal correction to Gibbs Free Energy (a.u.): 0.435066

Imaginary frequencies: -453.18

Calculation of single point energy based on the optimized structure, Et = -2763.0959824 a.u.

C	4.65984800	-2.91413000	-0.12585600
C	5.26541800	-1.71796800	0.30530000
C	3.34461300	-2.93878800	-0.55207900
H	5.23213200	-3.83771600	-0.11779600
C	4.52183500	-0.55610700	0.28966700
H	6.29521800	-1.71239600	0.64467000
C	2.55491600	-1.76231600	-0.56716300
H	2.87240300	-3.85976000	-0.87718000
C	3.17368300	-0.54527400	-0.14134400
H	4.96505100	0.38105200	0.61746000
O	1.31715500	-1.85081400	-0.98954600
C	2.48330500	0.70841400	-0.14346600
Co	-0.00587200	-0.51214500	-0.78159800
N	1.25286500	0.90024000	-0.49114200
H	3.06641800	1.56864700	0.18898500
N	-1.32436800	0.86094100	-0.75072600
C	0.60722700	2.20988700	-0.29931000
C	-2.56351700	0.68669000	-0.43407700
C	-0.72513800	2.16222800	-1.06120700
C	1.41891900	3.43569900	-0.72499500
H	-3.20965800	1.55955800	-0.33386600
C	-3.17230100	-0.59255800	-0.20857100
C	-1.56253200	3.40777900	-0.77858500
C	0.60058100	4.71166200	-0.47296700
H	1.67350100	3.34409300	-1.78889600
H	2.35994500	3.49169200	-0.16991600
C	-4.48227500	-0.63229100	0.32028600
C	-2.51028600	-1.80915300	-0.56989000
C	-0.76519100	4.66270500	-1.16977700
H	-2.50161500	3.37548600	-1.34149900
H	-1.81971100	3.44292700	0.28806800
H	1.16547500	5.58650600	-0.81089400
H	0.45207600	4.83111400	0.60807300
C	-5.14283100	-1.82942100	0.51368600
H	-4.96219700	0.30659500	0.58518500
C	-3.21802800	-3.01988300	-0.37833800

O	-1.30745900	-1.85848800	-1.09678400
H	-0.61833500	4.66693200	-2.25801100
H	-1.34587600	5.55856700	-0.92793100
C	-4.49616500	-3.02624400	0.15298100
H	-6.14194400	-1.84815700	0.93441800
H	-2.71644900	-3.94056300	-0.65699500
H	-5.00582000	-3.97486500	0.29719700
O	-0.05410300	-0.78405900	1.07756500
H	-0.17125600	-1.73672900	1.21381100
O	0.08442100	-0.46169000	-2.85081700
H	-0.68157600	-1.06141300	-2.93167100
H	0.85025300	-1.06618000	-2.87301500
C	0.10399800	0.21320100	3.60330600
C	-0.78115500	0.06229200	2.40202200
O	-0.84930400	0.94581400	4.22210700
H	0.33529500	-0.77957100	4.05943400
H	-1.67795400	-0.52490100	2.56279100
H	-0.95617000	1.00491500	1.90302100
C	1.43512100	0.92262800	3.31831500
H	1.93842800	1.15280500	4.26314900
H	2.10236100	0.30845500	2.70118700
H	1.24147300	1.87663800	2.81075300
H	-0.48374800	2.13027100	-2.13313200
H	0.37538500	2.29522900	0.77099200

PO + H_2O-Co^{III}-OH PO ring-opening in the terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.419943

Thermal correction to Gibbs Free Energy (a.u.): 0.431804

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2763.1287379 a.u.

C	5.51936900	-1.79015500	1.00752100
C	5.84939800	-0.42462200	1.11914600
C	4.25706700	-2.19199000	0.61563200
H	6.26854900	-2.54306700	1.23730900
C	4.88190500	0.51479600	0.82924100
H	6.84241100	-0.12057300	1.43136200
C	3.24212400	-1.24714600	0.30759300
H	3.99712600	-3.24210100	0.53321500
C	3.57911800	0.13967100	0.42200800
H	5.10885300	1.57530900	0.91313000
O	2.07690500	-1.69549000	-0.07806300
C	2.63316700	1.18397800	0.16218400
Co	0.54063800	-0.65298500	-0.47797600
N	1.41549600	1.02456200	-0.23575500
H	2.99495100	2.19831400	0.33768400
N	-0.96275700	0.37087700	-1.03751100
C	0.46402500	2.14243500	-0.31289700
C	-2.18407000	-0.04099400	-0.98731700
C	-0.57786200	1.74334300	-1.37180800
C	1.05128600	3.52391700	-0.60832400
H	-2.98567900	0.66561900	-1.20214300
C	-2.58695500	-1.38177300	-0.67954200
C	-1.70103600	2.77461700	-1.46424000
C	-0.07099400	4.56649400	-0.72167800
H	1.62337700	3.47916700	-1.54456700
H	1.74557300	3.82658000	0.18173300
C	-3.96166900	-1.64378300	-0.48650400
C	-1.63893200	-2.45202200	-0.62311700
C	-1.11804300	4.16244000	-1.76550000
H	-2.41695300	2.49250400	-2.24371000
H	-2.24566600	2.80028300	-0.51230800
H	0.35644500	5.54376500	-0.96905700
H	-0.55872800	4.67490800	0.25618000
C	-4.42039700	-2.91960000	-0.22258000
H	-4.66100700	-0.81262600	-0.54109800
C	-2.13910100	-3.75198100	-0.36742100
O	-0.35590700	-2.29715300	-0.83874900

H	-0.65512200	4.15190600	-2.76123300
H	-1.92397100	4.90274300	-1.80189900
C	-3.49049200	-3.97488600	-0.16918800
H	-5.47636000	-3.10585600	-0.06089500
H	-1.42003100	-4.56320700	-0.32589500
H	-3.83758700	-4.98409400	0.03555700
O	-0.04277800	-0.58196700	1.24718400
H	0.33497600	-1.38610800	1.63186000
O	1.15780500	-0.92533600	-2.46728400
H	0.52495700	-1.66703300	-2.53873300
H	1.98720900	-1.36753900	-2.21460600
C	-2.64214800	0.86294000	2.43594800
C	-3.57008600	1.73791500	1.70161600
O	-3.96041000	1.15090700	2.94247800
H	-2.50896800	-0.15334800	2.06844300
H	-4.10015400	1.36786900	0.82283800
H	-3.41796000	2.81944400	1.71966400
C	-1.48495700	1.40926900	3.22913100
H	-1.42071500	0.89645000	4.19507700
H	-0.55628600	1.20896300	2.68821800
H	-1.60229900	2.48065000	3.42217000
H	-0.05555300	1.69299200	-2.33805700
H	-0.05700900	2.16575000	0.65402900

PO + H_2O-Co^{III}-OH PO ring-opening in the terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.371697

Thermal correction to Gibbs Free Energy (a.u.): 0.435079

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2763.1072112 a.u.

C	4.72288500	-2.85020900	-0.24830200
C	5.34122900	-1.64692900	0.14360800
C	3.38546700	-2.88813700	-0.59643300
H	5.30342800	-3.76830700	-0.27229900
C	4.58652400	-0.49285600	0.17034400
H	6.38913100	-1.63047800	0.42156100
C	2.58455300	-1.71889000	-0.56819000
H	2.90355500	-3.81443800	-0.89091200
C	3.21525700	-0.49459300	-0.18241000
H	5.03915000	0.44895900	0.47083200
O	1.32227500	-1.82513300	-0.90765100
C	2.51341300	0.75255900	-0.13525300
Co	0.00931300	-0.46714700	-0.75891700
N	1.26959300	0.93993800	-0.43496000
H	3.10208600	1.61045700	0.19270200
N	-1.30518200	0.91056000	-0.74196700
C	0.61653400	2.23910700	-0.19785500
C	-2.56139700	0.73726400	-0.49488800
C	-0.69413200	2.21983900	-0.99828600
C	1.43621100	3.48571000	-0.53966700
H	-3.20731300	1.61199500	-0.41383400
C	-3.19087000	-0.53900300	-0.31760100
C	-1.54032100	3.45662500	-0.70227500
C	0.60467500	4.74858700	-0.26730100
H	1.73229200	3.44007300	-1.59584300
H	2.35428400	3.52275400	0.05393400
C	-4.53060200	-0.57123400	0.13331400
C	-2.51692900	-1.75964100	-0.64152800
C	-0.73206000	4.72494700	-1.01836600
H	-2.45853600	3.44565800	-1.29922000
H	-1.83603600	3.45327500	0.35500400
H	1.18012200	5.63700000	-0.54684200
H	0.41373000	4.82379200	0.81107000
C	-5.20867700	-1.76375300	0.28613200
H	-5.01932000	0.37044100	0.37085500
C	-3.24173200	-2.96641400	-0.49028800
O	-1.28636700	-1.81647100	-1.09738400
H	-0.54300500	4.76831900	-2.09920100

H	-1.32375000	5.61102100	-0.76735500
C	-4.54847600	-2.96489900	-0.03507100
H	-6.23104800	-1.77658400	0.64682900
H	-2.73037400	-3.89018400	-0.73936500
H	-5.07135600	-3.91035500	0.07920100
O	-0.02991100	-0.78729200	1.16156500
H	-0.00099600	-1.75021800	1.27048900
O	0.13450000	-0.43144200	-2.85006600
H	-0.62864200	-1.03696200	-2.91642600
H	0.90038800	-1.03385800	-2.86303200
C	-0.06408200	-0.10339500	3.62526100
C	-0.81683000	-0.17525400	2.25701500
O	-0.93580700	0.52492900	4.40036500
H	0.18009200	-1.16801800	3.91008000
H	-1.76282800	-0.70859800	2.36155800
H	-1.00066100	0.84694600	1.93622300
C	1.28863200	0.62150600	3.42278400
H	1.79516000	0.71204100	4.38842300
H	1.94912000	0.09232900	2.72326300
H	1.10316800	1.63914000	3.05258800
H	-0.42166100	2.21989800	-2.06340400
H	0.35435100	2.27102700	0.86928100

subsequent hydration

PO-OH-Co^{III}-H_2O + H_2O = PG + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.781865

Thermal correction to Gibbs Free Energy (a.u.): 0.461524

Imaginary frequencies: -506.04

Calculation of single point energy based on the optimized structure, Et = -2839.5668362 a.u.

C	4.98746600	-2.54258900	0.40999100
C	5.46185800	-1.24826100	0.69709200
C	3.71121000	-2.74615200	-0.08314400
H	5.63143300	-3.40008900	0.58454200
C	4.62919300	-0.17147100	0.47130300
H	6.46200300	-1.10235200	1.08959900
C	2.83350900	-1.65945000	-0.31387100
H	3.34023300	-3.74220800	-0.29963900
C	3.31747100	-0.34477900	-0.03037700
H	4.97097100	0.83850100	0.68397200
O	1.64362800	-1.91234800	-0.80443300
C	2.52498500	0.82558200	-0.25407000
Co	0.18617100	-0.70032400	-0.77692000
N	1.29742600	0.85371000	-0.65948500
H	3.01742600	1.77750800	-0.04748600
N	-1.25846500	0.53070100	-0.98877200
C	0.54483200	2.12267100	-0.69050000
C	-2.49806600	0.26804300	-0.75020500
C	-0.78619400	1.86017600	-1.40885900
C	1.23499100	3.33375100	-1.32099800
H	-3.22127500	1.08058000	-0.79307300
C	-3.00664100	-1.03105300	-0.40896900
C	-1.73525000	3.03634300	-1.17052700
C	0.32286600	4.55887200	-1.13525700
H	1.42178300	3.13911400	-2.38507100
H	2.20411800	3.52490400	-0.85000500
C	-4.34925400	-1.13694800	0.01758400
C	-2.20553600	-2.20740900	-0.53835300
C	-1.08300500	4.32374900	-1.70543000
H	-2.68269400	2.87977700	-1.69844200
H	-1.94982000	3.09682600	-0.09173200
H	0.77827500	5.43594200	-1.60696100
H	0.24534800	4.77803600	-0.06310100
C	-4.90986400	-2.36097500	0.32853400
H	-4.93666500	-0.22651900	0.10601400
C	-2.80700700	-3.44910000	-0.22753500
O	-0.95690700	-2.20046500	-0.95884800
H	-1.01912600	4.26291600	-2.80074000
H	-1.72511200	5.18015000	-1.47639300

C	-4.12360000	-3.51965000	0.19687400
H	-5.93772800	-2.42814100	0.66706600
H	-2.19696200	-4.34022700	-0.33046300
H	-4.55236400	-4.48879300	0.43595300
O	0.12122200	-0.78046000	1.10021600
H	-0.19158000	-1.67299500	1.31372600
O	0.36116400	-0.86554900	-2.79540100
H	-0.33679500	-1.54476100	-2.86481200
H	1.18540700	-1.38711200	-2.73174100
C	-0.17863900	0.60625100	3.27437100
C	-0.89237800	0.46571600	1.93393700
O	-1.03820400	1.19642100	4.20847800
H	0.06688600	-0.40920200	3.62234000
H	-1.83361600	-0.06317000	1.91193100
H	-0.71421000	1.16302300	1.15619400
C	1.12606500	1.39558500	3.11036500
H	1.61141200	1.50649900	4.08360300
H	1.81649600	0.89184000	2.42565900
H	0.89817600	2.39874100	2.73217200
O	-2.07677300	2.29092300	2.20242700
H	-1.56002500	1.83691100	3.60642600
H	-2.99286000	1.97824700	2.23640000
H	0.31838300	2.38474300	0.34928100
H	-0.56396200	1.76758900	-2.48180900

subsequent hydration

$PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.815536

Thermal correction to Gibbs Free Energy (a.u.): 0.460915

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2839.6016454 a.u.

C	4.85887700	-2.74228700	0.17709800
C	5.39521600	-1.46659200	0.42855400
C	3.54360200	-2.89922300	-0.22526200
H	5.48270800	-3.62237200	0.30604300
C	4.58508400	-0.36089700	0.26083600
H	6.42448800	-1.35457400	0.75059400
C	2.69266600	-1.78218200	-0.39473300
H	3.12357500	-3.88132400	-0.41496600
C	3.23800600	-0.48677500	-0.14951200
H	4.97456200	0.63601800	0.45089700
O	1.45595000	-1.99858400	-0.79190000
C	2.47083100	0.71547400	-0.30875200
Co	0.06138600	-0.72150300	-0.76525500
N	1.22585300	0.79109600	-0.64095600
H	3.00595600	1.64572300	-0.11551600
N	-1.33668600	0.56256600	-0.92574900
C	0.50215600	2.07827400	-0.62361700
C	-2.57313000	0.35120300	-0.62672100
C	-0.81290500	1.86026500	-1.38149000
C	1.24792700	3.28381400	-1.19889800
H	-3.26553600	1.19212800	-0.64938500
C	-3.11627400	-0.92578300	-0.25467700
C	-1.72740500	3.07311300	-1.21468000
C	0.35148700	4.52673400	-1.07514400
H	1.51092100	3.09260100	-2.24857800
H	2.18157600	3.45937500	-0.65534500
C	-4.43751800	-0.97785400	0.24151500
C	-2.37296900	-2.13347400	-0.43008400
C	-1.00730000	4.31943600	-1.75613000
H	-2.66711100	2.92824800	-1.75992400
H	-1.94324900	3.20490200	-0.14700300
H	0.86176900	5.39740700	-1.50056900
H	0.18699500	4.72556600	-0.01055500
C	-5.03100800	-2.17960600	0.57778500
H	-4.98038800	-0.04449800	0.36601700
C	-3.00797600	-3.35076800	-0.09371300
O	-1.14690800	-2.17490000	-0.91451900

H	-0.86209700	4.21625900	-2.84065600
H	-1.64037800	5.20001400	-1.60610200
C	-4.30231900	-3.36896900	0.40001300
H	-6.04109000	-2.20587500	0.97094500
H	-2.44293500	-4.26625600	-0.23362400
H	-4.75811100	-4.32090700	0.65748000
O	0.05278500	-0.82892200	1.15141900
H	-0.05015600	-1.76359100	1.38411500
O	0.18597500	-0.89785300	-2.77257800
H	-0.54778900	-1.54060900	-2.82802700
H	0.98398100	-1.46115900	-2.73345400
C	0.02546700	0.52358600	3.34235700
C	-0.72070300	0.05261400	2.07335200
O	-0.79831400	1.48828100	3.83619200
H	0.12502400	-0.34946900	4.02756100
H	-1.65464500	-0.45188200	2.32643500
H	-0.93275700	0.93234000	1.48163900
C	1.45296400	1.00826100	3.01793200
H	1.92882000	1.34067300	3.94567800
H	2.07430100	0.22687700	2.56396200
H	1.40040400	1.87138300	2.34606000
O	-0.88553900	3.15864000	1.98254500
H	-0.87994200	2.48415800	2.82480300
H	-0.58491200	3.99793700	2.35069200
H	0.23706300	2.31180200	0.42005900
H	-0.57288000	1.72056500	-2.44590800

subsequent hydration

$PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.869509

Thermal correction to Gibbs Free Energy (a.u.): 0.461115

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2839.6394141 a.u.

C	5.17079000	-2.22989300	0.88929800
C	5.58006700	-0.88516600	0.80275600
C	3.88579400	-2.60976800	0.54979600
H	5.87414600	-2.98369400	1.23303800
C	4.66972900	0.05611400	0.36604800
H	6.58947300	-0.59649700	1.07474600
C	2.92812700	-1.66241500	0.10297200
H	3.56453900	-3.64378500	0.61924900
C	3.34696300	-0.29721700	0.01132100
H	4.96057300	1.10148600	0.28937900
O	1.73578500	-2.09113600	-0.22127000
C	2.47235300	0.74923600	-0.43357400
Co	0.22462000	-0.99523700	-0.58391300
N	1.23661300	0.61420400	-0.77776500
H	2.91250600	1.74763900	-0.46265300
N	-1.26552600	0.05217300	-1.12599600
C	0.37942400	1.77969200	-1.05538600
C	-2.48627600	-0.18879900	-0.79047100
C	-0.82990300	1.25284200	-1.84261900
C	1.03642700	2.95042600	-1.78869400
H	-3.25070500	0.55512200	-1.01728100
C	-2.93053200	-1.39515900	-0.15126100
C	-1.87235500	2.34779300	-2.06088600
C	-0.00086800	4.05894300	-2.02652200
H	1.44887000	2.59802800	-2.74376800
H	1.87010900	3.35620000	-1.20648900
C	-4.26411500	-1.46438000	0.30524900
C	-2.07886300	-2.54070900	-0.04925100
C	-1.22517400	3.53613600	-2.78794900
H	-2.71017800	1.96128100	-2.65247800
H	-2.25685700	2.67355600	-1.08818800
H	0.46141100	4.88880500	-2.57191900
H	-0.32475600	4.45150900	-1.05478900
C	-4.77355500	-2.61839500	0.87039500
H	-4.89024400	-0.58039400	0.20759800

C	-2.63181500	-3.71485900	0.51716100
O	-0.84204000	-2.57107600	-0.48570300
H	-0.92070500	3.22610100	-3.79703800
H	-1.96152800	4.33687100	-2.91449500
C	-3.94072800	-3.74815300	0.96686100
H	-5.79701400	-2.65527400	1.22751700
H	-1.98645600	-4.58388000	0.59112100
H	-4.32853300	-4.66414400	1.40467300
O	-0.05672200	-0.58232400	1.17389100
H	0.13675500	-1.41913800	1.62046000
O	0.52904000	-1.67443000	-2.53824900
H	-0.15904800	-2.35522200	-2.40825000
H	1.35037700	-2.13467800	-2.28488000
C	-0.57998800	2.23628200	3.24112300
C	-1.66449100	1.97297400	2.20098100
O	-0.86089200	3.55934600	3.73535900
H	-0.70049900	1.49966900	4.05055000
H	-2.64360500	1.94722600	2.70150500
H	-1.47268000	1.01381600	1.71516100
C	0.83181600	2.13380600	2.67339800
H	1.58205900	2.30201100	3.45598900
H	0.97798200	1.13981500	2.23892500
H	0.97564300	2.88760900	1.89241900
O	-1.65259100	2.99566900	1.20006700
H	-0.07806800	3.87417900	4.20335000
H	-1.57637800	3.82249700	1.70159400
H	-0.00549500	2.13370700	-0.09263100
H	-0.46163700	0.90195800	-2.81766100

PO + H_2O-Co^{III}-OH PO ring-opening in the middle carbon and subsequent hydration

PO + H_2O-Co^{III}-OH PO ring-opening in the middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.366163

Thermal correction to Gibbs Free Energy (a.u.): 0.436482

Imaginary frequencies: -359.17

Calculation of single point energy based on the optimized structure, Et = -2763.0858754 a.u.

C	4.78214000	-2.96192800	0.27186700
C	5.43404300	-1.71680100	0.35620800
C	3.42042400	-3.04335500	0.04496600
H	5.35587800	-3.87713900	0.38931500
C	4.68651200	-0.56599700	0.20937000
C	2.63093600	-1.87625900	-0.11215800
C	3.29169400	-0.61261500	-0.02390900
H	5.16434800	0.40837900	0.27692400
O	1.34829400	-2.02511000	-0.34753700
C	2.59048400	0.63289800	-0.14488400
Co	0.06253900	-0.64993800	-0.52316200
N	1.32143000	0.78346700	-0.33001800
H	3.20480700	1.52782100	-0.04629300
N	-1.22036700	0.72873100	-0.82347000
C	0.68888800	2.11662100	-0.31538700
C	-2.49213600	0.57984500	-0.65332500
C	-0.58190300	2.00794900	-1.17314400
C	1.54129400	3.29949500	-0.77643500
H	-3.13446800	1.45818800	-0.72290800
C	-3.13983600	-0.66823400	-0.37129200
C	-1.43289600	3.26792000	-1.01474800
C	0.70817700	4.58265900	-0.62596000
H	1.86496800	3.15595600	-1.81684100
H	2.43935000	3.39103900	-0.15845700
C	-4.50042300	-0.65359000	0.00907700
C	-2.45589100	-1.91371600	-0.53412900
C	-0.60585500	4.50163800	-1.41208100
H	-2.33229200	3.21222800	-1.63790100
H	-1.74915900	3.35482200	0.03240000
H	1.29260400	5.44793800	-0.95591000
H	0.48876900	4.72215500	0.43963300

C	-5.18944900	-1.82651100	0.24955900
H	-4.99828400	0.30691400	0.11868800
C	-3.18982900	-3.09955000	-0.29886700
O	-1.21009200	-2.00525600	-0.93687300
H	-0.38776300	4.45589400	-2.48793000
H	-1.20041400	5.40664900	-1.25025500
C	-4.51853100	-3.05310200	0.08635900
H	-5.05066100	-3.98246500	0.26996400
O	-0.37467700	-0.77477900	1.28958200
H	0.32703600	-1.30464000	1.69526400
O	0.40317500	-0.81173500	-2.53768600
H	-0.36989900	-1.40796000	-2.62132000
H	1.15773400	-1.42363200	-2.48112800
C	-0.68862800	0.78141200	2.31347500
C	0.54187300	1.41429400	2.87388600
O	-0.02740800	2.65521400	2.86138600
H	-1.04382800	1.27061100	1.42863600
H	1.45287400	1.25620200	2.25463900
H	0.77793200	0.99737000	3.87903900
C	-1.75017100	0.30018500	3.25813100
H	-1.36954000	-0.49831700	3.90362300
H	-2.03565900	1.14499700	3.89078000
H	-2.62753100	-0.06506300	2.72046700
H	0.39171800	2.34187800	0.72120500
H	-0.26978500	1.90789800	-2.22281700
H	-6.22984200	-1.80427900	0.55461400
H	-2.66882700	-4.04261200	-0.42361000
H	2.91235300	-3.99978300	-0.01840800
H	6.50174800	-1.66429600	0.53794500

PO + H_2O-Co^{III}-OH PO ring-opening in the middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.427133

Thermal correction to Gibbs Free Energy (a.u.): 0.433827

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2763.1299989 a.u.

C	5.43508800	-2.02812800	0.92181300
C	5.82170700	-0.68016100	1.05335400
C	4.15180400	-2.37026100	0.53952400
H	6.15548000	-2.81538000	1.12762300
C	4.88879900	0.30318300	0.79325100
C	3.17312300	-1.37950200	0.26197900
C	3.56743600	-0.01062300	0.39771300
H	5.15991900	1.35193800	0.89291700
O	1.98572400	-1.77289000	-0.11975800
C	2.66036300	1.07782800	0.17092500
Co	0.48739000	-0.65702900	-0.47020800
N	1.43140400	0.97618700	-0.20543500
H	3.06629300	2.07335200	0.35720400
N	-0.97480600	0.44091500	-1.00445200
C	0.52075000	2.13119900	-0.24817500
C	-2.21326000	0.09209800	-0.94547700
C	-0.52815100	1.80040700	-1.32257100
C	1.16218400	3.49670600	-0.49494900
H	-2.98017700	0.84480500	-1.12805800
C	-2.67745200	-1.23577500	-0.65689400
C	-1.60660500	2.87867500	-1.41110100
C	0.07884200	4.58106400	-0.59340900
H	1.74731400	3.46085500	-1.42411300
H	1.85466300	3.75012300	0.31449800
C	-4.06207300	-1.43631100	-0.46759600
C	-1.78073400	-2.34976400	-0.61589000
C	-0.95802100	4.24567100	-1.67129400
H	-2.31298400	2.64251700	-2.21519000
H	-2.15982600	2.90400400	-0.46639300
H	0.54509700	5.55046200	-0.79973800
H	-0.42714500	4.66958800	0.37631500
C	-4.58138800	-2.69225300	-0.21592400

H	-4.72091100	-0.57250800	-0.52097800
C	-2.34162800	-3.62735200	-0.37010300
O	-0.49215500	-2.25511200	-0.83415500
H	-0.47151100	4.24098500	-2.65639300
H	-1.73161100	5.01998000	-1.70667900
C	-3.70187900	-3.78980400	-0.17193700
H	-4.09509300	-4.78409800	0.02259000
O	-0.04876900	-0.59745500	1.27435100
H	0.24170100	-1.45945600	1.60610400
O	1.06518000	-0.92548400	-2.46801400
H	0.39460700	-1.63115600	-2.55218700
H	1.87018000	-1.41560100	-2.22265800
C	-2.54580300	0.81004700	2.34262200
C	-1.62877000	1.71534300	3.04292300
O	-2.14795500	2.07142400	1.74792700
H	-2.07492500	-0.04570400	1.86213000
H	-0.56985700	1.46365800	3.05745600
H	-1.99348200	2.33080000	3.86575200
C	-3.99869200	0.69560200	2.71556700
H	-4.14600500	-0.13170300	3.41844300
H	-4.36111200	1.61911000	3.17697400
H	-4.60866000	0.48601900	1.83073600
H	-0.01734200	2.13649100	0.70737100
H	-0.00180700	1.73178900	-2.28583900
H	-5.64586200	-2.83110800	-0.06123300
H	-1.66113600	-4.47176500	-0.33878200
H	3.84818400	-3.40724900	0.44090700
H	6.83025900	-0.42187600	1.35711800

PO + H_2O-Co^{III}-OH PO ring-opening in the middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1524.396433

Thermal correction to Gibbs Free Energy (a.u.): 0.438753

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2763.1109192 a.u.

C	5.00910800	-2.69269600	0.10309400
C	5.63347400	-1.46863400	-0.18716200
C	3.63687900	-2.76626200	0.28666800
H	5.60567900	-3.59699600	0.18398200
C	4.85636000	-0.32722400	-0.27971800
C	2.82128700	-1.61476900	0.19149700
C	3.45644100	-0.36920500	-0.10487900
H	5.32050400	0.63329300	-0.49019300
O	1.52183700	-1.74859600	0.38716800
C	2.71478700	0.86911200	-0.16343700
Co	0.24383500	-0.51895300	-0.26860200
N	1.42765200	0.95976800	-0.17785200
H	3.29773900	1.78981800	-0.18654300
N	-1.03726300	0.73758300	-0.91699000
C	0.66819000	2.18272600	-0.07835400
C	-2.29129300	0.49802400	-1.08669700
C	-0.44888100	2.07965800	-1.12673500
C	1.43239300	3.49401400	-0.15920200
H	-2.93462900	1.32369900	-1.38802600
C	-2.94576300	-0.76678000	-0.88056700
C	-1.42802700	3.24688200	-0.98612800
C	0.43185800	4.64636500	0.02023500
H	1.96127100	3.58975500	-1.12200900
H	2.18815700	3.53380000	0.63404200
C	-4.35387800	-0.80987900	-0.98642000
C	-2.22267800	-1.95813500	-0.57137500
C	-0.67112300	4.58269800	-1.04297800
H	-2.18131500	3.22194400	-1.78276200
H	-1.91049100	3.13176000	-0.00744400
H	0.95322400	5.60878600	-0.02768700
H	-0.02323300	4.54774700	1.01211500
C	-5.05691100	-1.98289400	-0.78817800
H	-4.88175300	0.11109200	-1.22101000

C	-2.96399000	-3.14666100	-0.37271000
O	-0.91104600	-2.01629000	-0.48073800
H	-0.22930000	4.71938300	-2.04114500
H	-1.38194400	5.40369100	-0.90013600
C	-4.34438400	-3.15551700	-0.48025200
H	-4.88347100	-4.08492600	-0.31886600
O	-0.15944200	-0.24664300	1.58494700
H	0.27884500	-1.02367000	1.96976900
O	0.77246400	-1.00090100	-2.13383900
H	0.22822400	-1.81595000	-2.11269600
H	1.69735700	-1.29422600	-2.08386900
C	-1.45986000	0.02549600	2.24678400
C	-1.34977700	1.43919500	2.85097800
O	-1.16344600	2.40187800	1.92303400
H	-2.19893500	0.04829900	1.44746700
H	-0.54770500	1.36568400	3.63179900
H	-2.29799900	1.55553300	3.43678500
C	-1.74927300	-1.11132200	3.20972200
H	-0.99570000	-1.15324500	4.00554300
H	-2.72167800	-0.95144500	3.68334100
H	-1.78026400	-2.07628200	2.69280900
H	0.08385000	2.16348100	0.91760800
H	-0.00256800	2.06905200	-2.13425800
H	-6.13831600	-1.99923500	-0.86664600
H	-2.40888300	-4.04751100	-0.13343900
H	3.14705200	-3.70656100	0.51749400
H	6.70743800	-1.41720600	-0.32955700

subsequent hydration

$PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.784884

Thermal correction to Gibbs Free Energy (a.u.): 0.461408

Imaginary frequencies: -468.74

Calculation of single point energy based on the optimized structure, Et = -2839.563534 a.u.

C	4.86163200	-2.85248200	0.38694700
C	5.46033800	-1.57931600	0.44161400
C	3.51756700	-3.00020600	0.09660300
H	5.46284300	-3.73677600	0.57944500
C	4.67911300	-0.46828900	0.19757100
C	2.69332500	-1.87510300	-0.15535600
C	3.30076500	-0.58317900	-0.10131400
H	5.11596900	0.52653500	0.23748000
O	1.42925500	-2.08593000	-0.44138900
C	2.56339100	0.62435900	-0.33591500
Co	0.08409700	-0.77013000	-0.64240400
N	1.29891600	0.71561400	-0.58302700
H	3.14336000	1.54637100	-0.28231000
N	-1.25633000	0.54393300	-0.97113500
C	0.62828400	2.02864100	-0.67536100
C	-2.51336600	0.36556800	-0.73407700
C	-0.68418200	1.81532200	-1.44631300
C	1.41509200	3.18821400	-1.28769000
H	-3.18602300	1.21804800	-0.82833000
C	-3.10426400	-0.88395500	-0.35116000
C	-1.56353600	3.05881900	-1.30779000
C	0.55147800	4.45741600	-1.17926600
H	1.66835300	2.96691200	-2.33364900
H	2.35343600	3.35126200	-0.74882100
C	-4.44800200	-0.89165400	0.08371100
C	-2.38427600	-2.11348600	-0.47049100
C	-0.80875000	4.27695900	-1.86473900
H	-2.50786400	2.93390000	-1.84927100
H	-1.77143600	3.21010000	-0.23994500
H	1.08590700	5.30981100	-1.61177200
H	0.38515400	4.66983100	-0.11637800
C	-5.08529100	-2.07019500	0.42076300
H	-4.97493300	0.05678600	0.15656800
C	-3.06494900	-3.30658900	-0.13499400

O	-1.15296000	-2.18853300	-0.92145300
H	-0.66398000	4.15379000	-2.94725000
H	-1.41876500	5.17602700	-1.72901500
C	-4.37838700	-3.28126100	0.30222400
H	-4.86937400	-4.21515000	0.56172900
O	-0.28244000	-0.80543900	1.19194400
H	0.40649700	-1.35356200	1.59677300
O	0.36316500	-1.04271300	-2.64659500
H	-0.39385700	-1.66349900	-2.67953300
H	1.13645400	-1.62929600	-2.56608100
H	0.35901500	2.33964800	0.34087700
H	-0.43136100	1.64898000	-2.50350700
C	-0.60959700	0.84679100	2.09917700
C	0.73887800	1.02659800	2.78974100
O	0.68773300	2.04707700	3.74032600
H	-0.80840100	1.22602400	1.13118000
H	1.51460100	1.18876500	2.02388300
H	0.98554200	0.08291500	3.29864500
C	-1.77641000	0.48619900	2.96792600
H	-2.72645200	0.60459800	2.44433200
H	-1.69032100	-0.55625500	3.28881300
H	-1.75523500	1.11726900	3.85927000
O	-0.83196100	3.06746900	2.04613000
H	0.13200900	2.73254400	3.22748200
H	-1.69014100	3.27606700	2.43984700
H	-2.51655100	-4.23788700	-0.22652400
H	-6.11316700	-2.06411400	0.76632800
H	3.05044000	-3.97849200	0.05648900
H	6.51409900	-1.47492500	0.67471900

subsequent hydration

$PO\text{-}OH\text{-}Co^{III}\text{-}H_2O + H_2O = PG + H_2O\text{-}Co^{III}\text{-}OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.819542

Thermal correction to Gibbs Free Energy (a.u.): 0.462465

No imaginary frequency

Calculation of single point energy based on the optimized structure, Er = -2839.6010196 a.u.

C	4.86102800	-2.84227600	0.18087100
C	5.46095100	-1.58852700	0.38962700
C	3.51722400	-2.94610100	-0.13847400
H	5.45633300	-3.74640000	0.27216000
C	4.68449800	-0.45158200	0.27129500
C	2.70465200	-1.79581300	-0.26287300
C	3.31036600	-0.52305800	-0.05173700
H	5.12462000	0.52927800	0.43257100
O	1.43312500	-1.96867400	-0.57943100
C	2.57704500	0.71097400	-0.14585700
Co	0.12195400	-0.61685700	-0.73617100
N	1.31829600	0.83983000	-0.40226700
H	3.15479100	1.61698500	0.03534900
N	-1.19698300	0.72631000	-0.96500900
C	0.63301500	2.13908700	-0.36292300
C	-2.45169000	0.54829200	-0.73023400
C	-0.58524300	2.02323300	-1.28841400
C	1.47162000	3.36388900	-0.72519900
H	-3.10590500	1.41891200	-0.72035600
C	-3.05417700	-0.73434400	-0.48545900
C	-1.48249200	3.24971300	-1.14735300
C	0.58653700	4.61650400	-0.61827300
H	1.88605000	3.25945700	-1.73939400
H	2.31503600	3.47189900	-0.03515700
C	-4.38361100	-0.78438600	-0.01668200
C	-2.35131300	-1.94434100	-0.77087300
C	-0.66782100	4.50600300	-1.49388700
H	-2.35182000	3.17297900	-1.81146500
H	-1.80524100	3.29109700	-0.09808500
H	1.16518700	5.50632700	-0.88881300
H	0.28020700	4.71571100	0.42814100
C	-5.02341700	-1.99319600	0.19041900

H	-4.89568800	0.15125400	0.19248000
C	-3.03248900	-3.16435400	-0.57226500
O	-1.11828000	-1.96908500	-1.24069600
H	-0.37611300	4.47727800	-2.55370800
H	-1.29468700	5.39498900	-1.36576700
C	-4.33527300	-3.18424700	-0.09907500
H	-4.82876700	-4.13960200	0.05596400
O	-0.31049300	-0.95729700	1.09463100
H	0.31234600	-1.63542700	1.39855900
O	0.50494100	-0.64792200	-2.68539900
H	-0.26186400	-1.23270800	-2.86636500
H	1.26506100	-1.25773500	-2.66076600
H	0.20747000	2.31965000	0.66305300
H	-0.23314800	1.93061700	-2.32718800
C	-0.74116600	-0.05984300	2.18745400
C	0.45722400	0.47796500	2.98086600
O	0.03400300	1.52417300	3.78862900
H	-1.21041200	0.78700100	1.68943600
H	1.24427200	0.77080200	2.26131000
H	0.87982500	-0.33153300	3.60168700
C	-1.74088600	-0.80783900	3.04548100
H	-2.63275300	-1.08546100	2.47843900
H	-1.29434400	-1.71464300	3.47249000
H	-2.01787400	-0.14547900	3.86926100
O	-0.94465800	2.86820400	1.91005500
H	-0.38218400	2.20228600	3.09860100
H	-1.04164700	3.80401200	2.12865600
H	-2.49663600	-4.08124600	-0.79295500
H	-6.04033000	-2.02225600	0.56575200
H	3.04680400	-3.91040200	-0.29962200
H	6.51287200	-1.51520100	0.64235700

subsequent hydration

PO-OH-Co^{III}-H_2O + H_2O = PG + H_2O-Co^{III}-OH

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.868186

Thermal correction to Gibbs Free Energy (a.u.): 0.458598

No imaginary frequency

Calculation of single point energy based on the optimized structure, Ep = -2839.6393154 a.u.

C	5.75486700	-1.37096600	1.35298800
C	6.00622500	0.01518600	1.32553700
C	4.53015400	-1.88431100	0.97153300
H	6.53538600	-2.05080800	1.68405000
C	4.99879900	0.86116200	0.90998100
C	3.47719600	-1.03793200	0.53280900
C	3.73389400	0.37015100	0.50798500
H	5.16351200	1.93613300	0.88783700
O	2.35316700	-1.59224200	0.16148600
C	2.73555700	1.32462600	0.12495100
Co	0.79296300	-0.68984100	-0.43939000
N	1.54749300	1.05068300	-0.29701000
H	3.02220500	2.37230400	0.22669500
N	-0.71279500	0.18016300	-1.22610300
C	0.51465400	2.07998900	-0.47509400
C	-1.89711500	-0.31933600	-1.31752600
C	-0.40305300	1.56641700	-1.59666500
C	0.99582000	3.50423400	-0.75014000
H	-2.70414600	0.30896200	-1.68776600
C	-2.25644800	-1.65736100	-0.93977400
C	-1.59912600	2.49232100	-1.82010300
C	-0.20817800	4.43371100	-0.96251200
H	1.63784000	3.50627900	-1.64139900
H	1.59771100	3.87524900	0.08558400
C	-3.62677400	-2.00301300	-0.92903500
C	-1.27091000	-2.63631000	-0.60245000
C	-1.11979300	3.92654400	-2.08498000
H	-2.19314900	2.14255100	-2.67172500
H	-2.25019100	2.45955200	-0.93826500
H	0.14216100	5.44716200	-1.18449700

H	-0.78231700	4.49583100	-0.02888300
C	-4.05198100	-3.26359800	-0.55334800
H	-4.35237900	-1.25381300	-1.24183800
C	-1.73421500	-3.92395300	-0.23018300
O	0.01858200	-2.42134100	-0.66337000
H	-0.57269900	3.95648100	-3.03708900
H	-1.98491900	4.58777600	-2.19947800
C	-3.08450400	-4.22348000	-0.20024700
H	-3.40172300	-5.21889800	0.09833700
O	0.09659700	-0.47464300	1.23307800
H	0.39087000	-1.27724300	1.68758200
O	1.57108700	-1.12019700	-2.34039400
H	0.99668900	-1.90897400	-2.38428600
H	2.40553300	-1.47677100	-1.98813400
H	-0.07393100	2.06680600	0.45215200
H	0.20122500	1.52051100	-2.51435700
C	-2.81460100	0.67211100	1.89657900
C	-2.53313100	2.08270000	2.40267500
O	-3.72934200	2.77348200	2.72198400
H	-1.87745500	0.21219500	1.55962500
H	-1.95784500	2.62682900	1.63370200
H	-1.91758000	2.04072000	3.30657600
C	-3.47835900	-0.21167300	2.94597300
H	-3.74628700	-1.18400000	2.51595000
H	-2.78911600	-0.39869000	3.77553300
H	-4.37847400	0.26697600	3.34176900
O	-3.70737900	0.87518500	0.77126500
H	-4.33118100	2.55987900	1.99257600
H	-4.07562200	0.01058500	0.54958300
H	-0.98567800	-4.66383800	0.03293600
H	-5.10749100	-3.51238200	-0.54086300
H	4.33076100	-2.95051600	0.99619300
H	6.96985700	0.40768400	1.63111100

coordinates of transitant states, corresponding reactant complexes and product complexes where Co^{III}(salen)-Cl are unsimplified were listed in the following:

II-t (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
transitant state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2537.504701
Thermal correction to Gibbs Free Energy (a.u.): 0.851824
Imaginary frequencies: -473.61

C	-2.78868900	-0.60172400	2.62711500
C	-1.50992900	-1.26570700	2.35412200
O	-2.06870400	0.38458800	3.39203400
H	-3.24967800	-0.16988300	1.73933900
H	-1.02237600	-1.24247000	1.38873600
H	-1.03028200	-1.76126100	3.19304900
C	-3.79792300	-1.32780000	3.48876700
H	-4.55248600	-0.61330400	3.82837800
H	-4.29422200	-2.10691400	2.90432600
H	-3.32072600	-1.77551100	4.36482600
O	-0.29899600	0.81115000	1.72465500
H	-1.40695100	0.82310700	2.72957800
H	0.51831600	0.52896300	2.15961900
C	-4.53452100	-1.45708300	-0.60720900
C	-5.18379800	-0.21039900	-0.43789200
C	-3.16392500	-1.62436600	-0.73350900
H	-5.15986600	-2.33928200	-0.65614900
C	-4.37937900	0.91133600	-0.46394800
C	-2.32429800	-0.45692200	-0.61104000
C	-2.97112300	0.81831000	-0.55085300
H	-4.81200400	1.90444400	-0.39891100
O	-1.03766400	-0.60981600	-0.52423000
C	-2.23757300	2.05394400	-0.58953700
Co	0.24294500	0.75662400	-0.13979200

N	-0.95922100	2.17663800	-0.51412700
H	-2.84224800	2.95420000	-0.70990300
N	1.51758300	2.11279200	0.24738200
Cl	0.90967500	0.74385500	-2.31302800
C	-0.25147800	3.45101000	-0.66010500
C	2.79372200	1.92380200	0.31406200
C	0.87740800	3.42317400	0.38761000
C	-1.08829600	4.72364900	-0.54572100
H	3.43905200	2.79268800	0.44916000
C	3.46091400	0.66084100	0.22393500
C	1.78162200	4.64855100	0.25861900
C	-0.18441600	5.95920500	-0.66916000
H	-1.60750000	4.73561800	0.42244300
H	-1.85476700	4.74896000	-1.32744900
C	4.87438000	0.67762200	0.16844000
C	2.74150700	-0.57265000	0.22824400
C	0.94842900	5.93447500	0.36315800
H	2.54925800	4.64314000	1.03972500
H	2.29934200	4.61412600	-0.70877200
H	-0.78277800	6.86935500	-0.55560900
H	0.24568600	5.98859200	-1.67883200
C	5.60968600	-0.48600800	0.09349400
H	5.36543000	1.64535600	0.17708800
C	3.49779900	-1.78994100	0.13762100
O	1.44168300	-0.62771200	0.35626400
H	0.52094400	6.00523000	1.37248800
H	1.59764300	6.80712700	0.23598400
C	4.87897400	-1.69886800	0.07770100
H	5.44500500	-2.61898100	0.00458100
H	0.39656600	3.42860200	1.37632600
H	0.22503500	3.40908700	-1.64848000
C	-2.54847200	-2.99947800	-1.04171700
C	-3.62766400	-4.08119000	-1.22791300
H	-3.14491000	-5.02602800	-1.49465400
H	-4.20404600	-4.25384200	-0.31184300
H	-4.32578000	-3.82844200	-2.03207400
C	-1.74358300	-2.89794100	-2.35950600
H	-2.41107500	-2.65165400	-3.19172400
H	-0.97129100	-2.13141400	-2.29545200
H	-1.26459500	-3.85809700	-2.58075800
C	-1.61154800	-3.47375600	0.09122400
H	-0.72662000	-2.84560600	0.15438400
H	-2.13943000	-3.47475300	1.05622000
H	-1.27907200	-4.50046800	-0.09664900
C	-6.70549500	-0.16560800	-0.26603500
C	-7.22447100	1.27233100	-0.10689700
H	-6.78550100	1.76540200	0.76666900
H	-7.00523700	1.88014400	-0.99053700
H	-8.31054800	1.26260900	0.02740300
C	-7.09486000	-0.96287100	0.99845000
H	-8.18135400	-0.95829500	1.13965000
H	-6.77135400	-2.00598100	0.93238200
H	-6.63314300	-0.52401900	1.88935700
C	-7.39084100	-0.79452100	-1.49859100
H	-7.09194600	-1.83689100	-1.64112900
H	-8.48040200	-0.77267000	-1.38510900
H	-7.12913300	-0.24504600	-2.40808400
C	7.13979800	-0.52357600	0.01804000
C	7.75247400	0.88576700	0.05029300
H	7.49746800	1.41526700	0.97421100
H	8.84362800	0.81772000	-0.00329000
H	7.41517300	1.49108200	-0.79718100
C	7.57371900	-1.20922400	-1.29594900
H	8.66668100	-1.24982400	-1.36593100
H	7.19680600	-2.23397000	-1.36018000
H	7.19319000	-0.65953800	-2.16238800
C	7.69601800	-1.31985800	1.21860700
H	7.40849700	-0.84714400	2.16327100
H	7.31950600	-2.34674800	1.23128600

H	8.79014800	-1.36559800	1.17648900
C	2.77265600	-3.14194500	0.07361500
C	3.75120000	-4.32218200	-0.05570800
H	4.35311000	-4.25484100	-0.96769100
H	4.42944300	-4.39269400	0.80172400
H	3.18270100	-5.25632300	-0.10499500
C	1.84726000	-3.15969100	-1.16459700
H	1.13809800	-2.33411700	-1.14401400
H	2.44077900	-3.07186000	-2.08017200
H	1.29421900	-4.10515900	-1.20764800
C	1.95344000	-3.36252500	1.36620400
H	2.61728200	-3.40391800	2.23727300
H	1.23982500	-2.55243100	1.51183100
H	1.40707100	-4.31102300	1.31047100

II-t (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.579402

Thermal correction to Gibbs Free Energy (a.u.): 0.851717

No imaginary frequency

C	-3.62858200	-0.50201000	2.69013800
C	-2.61904700	-1.03429300	3.61391100
O	-2.41823400	0.24553200	2.97369100
H	-3.65261800	-0.92082600	1.68912700
H	-1.95000600	-1.82380300	3.27664600
H	-2.78328500	-0.97672500	4.68850800
C	-4.90092500	0.13604300	3.17064300
H	-5.20594600	0.92763200	2.48002600
H	-5.70329700	-0.60799700	3.20512200
H	-4.77318600	0.56483400	4.16845700
O	-0.03239100	0.76208800	1.90683400
H	-0.95939900	0.50948800	2.14843500
H	0.53573600	-0.00778300	2.08676500
C	-4.42186800	-1.58463500	-0.75538100
C	-5.11345800	-0.34669700	-0.73554000
C	-3.04970500	-1.72591200	-0.63358300
H	-5.01332800	-2.48244000	-0.88229300
C	-4.33915100	0.78817000	-0.62591000
C	-2.25279800	-0.53518500	-0.45489500
C	-2.92931700	0.72445700	-0.50092800
H	-4.79446200	1.77319900	-0.64457300
O	-0.97806500	-0.65393000	-0.24636100
C	-2.22264800	1.96889900	-0.49097700
Co	0.30331000	0.72962200	-0.06895300
N	-0.94636000	2.12589300	-0.37130900
H	-2.83918200	2.85777600	-0.63097400
N	1.57965600	2.10892800	0.20486800
Cl	0.78838800	0.65775400	-2.25720300
C	-0.27628200	3.41961100	-0.55327900
C	2.85917100	1.94070600	0.19283800
C	0.92954600	3.40704200	0.40038900
C	-1.12878200	4.67213400	-0.35159900
H	3.49732900	2.82191000	0.26819200
C	3.54121500	0.68464700	0.10578500
C	1.79863700	4.65039000	0.21498400
C	-0.26468000	5.93039900	-0.52488700
H	-1.57134800	4.65335300	0.65357100
H	-1.95390900	4.69669400	-1.07060000
C	4.94741600	0.72275000	-0.03971200
C	2.84990900	-0.55610900	0.23579800
C	0.95128800	5.91661900	0.40820600
H	2.62733700	4.64986700	0.93076000
H	2.23573000	4.63960600	-0.79201400
H	-0.87190300	6.82385000	-0.34524300
H	0.07857300	5.98724700	-1.56623600
C	5.70138800	-0.43091400	-0.07337500
H	5.41689600	1.69685000	-0.12986400

C	3.62535700	-1.76268300	0.21675100
O	1.55197100	-0.62137900	0.41688200
H	0.60937800	5.96424000	1.45083700
H	1.56926000	6.80485800	0.24014900
C	4.99896600	-1.65160800	0.06301500
H	5.58107500	-2.56389000	0.04014300
H	0.53069300	3.39869700	1.42530100
H	0.12069400	3.40680800	-1.57762200
C	-2.36828900	-3.09841000	-0.72530000
C	-3.38488500	-4.23979900	-0.90315700
H	-2.84698900	-5.19029100	-0.97095400
H	-4.07697100	-4.31110700	-0.05646400
H	-3.97164900	-4.12907800	-1.82082700
C	-1.43746900	-3.09907300	-1.96021500
H	-2.02963400	-2.98661900	-2.87463800
H	-0.71520500	-2.28474300	-1.91751900
H	-0.89283800	-4.04733300	-2.02248400
C	-1.56509100	-3.39464700	0.56219400
H	-0.79698700	-2.64202900	0.72836300
H	-2.23666500	-3.42400400	1.42930700
H	-1.08039200	-4.37372600	0.48391000
C	-6.63833700	-0.32895700	-0.88708700
C	-7.20790400	1.09610800	-0.80336200
H	-6.96868300	1.57010600	0.15459000
H	-6.82376100	1.73287400	-1.60651800
H	-8.29791900	1.06698500	-0.89714700
C	-7.28592300	-1.17217500	0.23254900
H	-8.37497900	-1.19408100	0.11515400
H	-6.92935300	-2.20603000	0.22060000
H	-7.05871200	-0.74991900	1.21618400
C	-7.02115800	-0.92591200	-2.25932800
H	-6.67221300	-1.95759300	-2.36076500
H	-8.10917500	-0.92574400	-2.38973600
H	-6.57682900	-0.34250000	-3.07159200
C	7.22391200	-0.44907300	-0.24647400
C	7.80560800	0.96799300	-0.37372900
H	7.60189100	1.56946100	0.51831000
H	8.89189400	0.91358200	-0.49630100
H	7.39876800	1.49386900	-1.24341500
C	7.58541800	-1.23708000	-1.52444900
H	8.67208200	-1.26687300	-1.66307600
H	7.22629700	-2.26914900	-1.47741200
H	7.13838700	-0.76867400	-2.40675000
C	7.87430800	-1.13102500	0.97693400
H	7.63797900	-0.58494100	1.89583700
H	7.52322400	-2.15957000	1.10038700
H	8.96407600	-1.16110700	0.86593100
C	2.93894400	-3.13144500	0.34029400
C	3.94585800	-4.29361300	0.28122600
H	4.49393600	-4.31179000	-0.66640000
H	4.67225800	-4.25406800	1.10035600
H	3.40426500	-5.24092800	0.36547500
C	1.94251600	-3.30687600	-0.82540200
H	1.20207600	-2.51040400	-0.82892800
H	2.46960000	-3.29099600	-1.78490200
H	1.42590000	-4.26929900	-0.73623000
C	2.19605900	-3.23326300	1.69198800
H	2.89645100	-3.11946300	2.52705100
H	1.42696500	-2.46572800	1.77166000
H	1.71545100	-4.21383300	1.78279300

II-t (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.599019

Thermal correction to Gibbs Free Energy (a.u.): 0.855412

No imaginary frequency

C	-2.08331700	1.64640900	2.67234500

C	-1.34024700	0.32446000	2.54662700
O	-1.22385700	2.63091400	3.24514700
H	-2.38242600	1.96016400	1.66506200
H	-1.92680300	-0.42634400	2.01550500
H	-1.07322800	-0.04926100	3.54154900
C	-3.32590500	1.51035000	3.53688200
H	-3.81080700	2.48385900	3.64494100
H	-4.03756400	0.81807400	3.07589000
H	-3.06677200	1.14621600	4.53595900
O	-0.11348500	0.60536700	1.83471800
H	-0.33603800	2.42780100	2.91664900
H	0.52184200	-0.14000400	1.89146200
C	-4.52492900	-1.90030000	-0.35458700
C	-5.23850200	-0.68871600	-0.54202600
C	-3.14627900	-2.01081400	-0.31375700
H	-5.10751500	-2.80580800	-0.24333000
C	-4.48423400	0.44925200	-0.71279100
C	-2.36523900	-0.80576800	-0.43604900
C	-3.06743400	0.41959400	-0.65958300
H	-4.95812900	1.41049200	-0.88307900
O	-1.07111100	-0.87630500	-0.32026900
C	-2.38762400	1.66230400	-0.83797500
Co	0.15714000	0.54984400	-0.22773500
N	-1.12155100	1.87460200	-0.68053300
H	-3.01892200	2.50797200	-1.11232300
N	1.36929500	1.99879200	-0.00094000
Cl	0.71497600	0.34569500	-2.37526300
C	-0.48879200	3.17099500	-0.95501400
C	2.65509400	1.88305400	0.02684700
C	0.66610300	3.28455800	0.05401000
C	-1.39467400	4.40071900	-0.88776500
H	3.25578600	2.79268400	0.05701700
C	3.38958200	0.65276700	0.02569900
C	1.49917200	4.54204700	-0.18625000
C	-0.57064400	5.67615200	-1.11901900
H	-1.88057500	4.43867200	0.09647500
H	-2.18569100	4.33856200	-1.64184400
C	4.79417900	0.74242200	-0.11055200
C	2.75099700	-0.60820800	0.20649300
C	0.59713000	5.78395900	-0.13186600
H	2.29046500	4.62847900	0.56596900
H	1.98596300	4.47183300	-1.16767300
H	-1.21933700	6.55437000	-1.03666300
H	-0.17931200	5.66859800	-2.14484400
C	5.59319900	-0.38149800	-0.09192600
H	5.22565600	1.72941200	-0.23992300
C	3.56869100	-1.78248000	0.23564500
O	1.45048300	-0.71262800	0.39071900
H	0.20255500	5.89686700	0.88654600
H	1.19007600	6.68041000	-0.34070400
C	4.93911100	-1.62257800	0.08596000
H	5.55653700	-2.51128900	0.10099400
H	0.20410000	3.35179400	1.05000900
H	-0.04371700	3.09099600	-1.95575200
C	-2.44879800	-3.37242300	-0.17848800
C	-3.45620700	-4.52649600	-0.03324600
H	-2.90896900	-5.47036100	0.05040300
H	-4.07494800	-4.42213800	0.86490400
H	-4.11803900	-4.60709300	-0.90170800
C	-1.61954400	-3.62726300	-1.45820800
H	-2.28080700	-3.69580200	-2.32851900
H	-0.90179300	-2.82642000	-1.63226100
H	-1.07243000	-4.57239600	-1.37163900
C	-1.53416400	-3.39802400	1.06726500
H	-0.75063500	-2.64719800	0.99330900
H	-2.11971000	-3.21754700	1.97682300
H	-1.06223500	-4.38190900	1.16318600
C	-6.77023100	-0.70745500	-0.55443500
C	-7.36046500	0.69442400	-0.77492300

H	-7.05997800	1.38786500	0.01742400
H	-7.05044000	1.11574000	-1.73665100
H	-8.45357800	0.64154400	-0.77280200
C	-7.28508200	-1.24229200	0.79985600
H	-8.38027200	-1.27340800	0.81017000
H	-6.92054100	-2.25405600	0.99972000
H	-6.95298200	-0.59902200	1.62132400
C	-7.26776400	-1.62695100	-1.69098500
H	-6.90848700	-2.65273200	-1.56859700
H	-8.36290000	-1.65693100	-1.70873900
H	-6.91809000	-1.26462700	-2.66271200
C	7.11683200	-0.34503000	-0.25278800
C	7.64251400	1.08829100	-0.43135100
H	7.40654000	1.71582000	0.43440500
H	8.73115400	1.07258700	-0.54246200
H	7.22437000	1.56277700	-1.32492900
C	7.52050300	-1.16753500	-1.49589600
H	8.60855700	-1.15817200	-1.62496500
H	7.20348100	-2.21083800	-1.41057900
H	7.06312200	-0.75287500	-2.39953300
C	7.78178300	-0.95192200	1.00191400
H	7.51502700	-0.38069800	1.89686200
H	7.47199200	-1.98849800	1.16266100
H	8.87270400	-0.94143400	0.90063400
C	2.93663800	-3.17095700	0.41605200
C	3.98680500	-4.29528400	0.37553400
H	4.52232300	-4.31982200	-0.57912200
H	4.72170600	-4.20583900	1.18299500
H	3.48268200	-5.25921300	0.49447500
C	1.92532700	-3.42867900	-0.72198900
H	1.15111000	-2.66508800	-0.74324400
H	2.43400000	-3.42889800	-1.69149800
H	1.45184400	-4.40733700	-0.58576700
C	2.22950200	-3.25083100	1.78794700
H	2.94485400	-3.08432200	2.60105400
H	1.43424500	-2.51027700	1.86352800
H	1.78465000	-4.24258500	1.92441700

II-m (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl
transition state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2537.513809
Thermal correction to Gibbs Free Energy (a.u.): 0.846725
Imaginary frequencies: -326.02

C	-4.48510800	-1.86194900	-0.46177300
C	-5.19061400	-0.64315900	-0.68671800
C	-3.11834400	-1.97199700	-0.32298800
H	-5.07331400	-2.76928900	-0.40980500
C	-4.43813200	0.50256700	-0.75652400
C	-2.31972900	-0.76110200	-0.38137400
C	-3.02651700	0.48528500	-0.56451900
H	-4.90405200	1.46708100	-0.92875400
O	-1.05087500	-0.83607500	-0.23741300
C	-2.33843700	1.74292400	-0.67568200
Co	0.21457200	0.59228200	-0.10828100
N	-1.07407600	1.93346000	-0.53142300
H	-2.97097300	2.59850300	-0.91313300
N	1.45380300	2.02135700	0.04388500
C	-0.44026900	3.23494600	-0.78294400
C	2.73847900	1.89054500	-0.01215600
C	0.77184700	3.31060500	0.16053000
C	-1.32981800	4.46914600	-0.63298300
H	3.34908500	2.79407600	-0.02678400
C	3.45533800	0.65496300	-0.03655800
C	1.60239400	4.56440900	-0.11128700
C	-0.50891400	5.74340400	-0.88151000
H	-1.75694400	4.47802100	0.37842800

H	-2.16304800	4.43605500	-1.34236200
C	4.85794200	0.72087300	-0.21582600
C	2.79985500	-0.59415100	0.19025900
C	0.72166500	5.81470500	0.02951800
H	2.44284900	4.62562900	0.58812100
H	2.02292600	4.51056200	-1.12386500
H	-1.14174100	6.62517700	-0.73486700
H	-0.18369800	5.76035200	-1.93012800
C	5.64440700	-0.40953000	-0.18568100
H	5.29637500	1.69929000	-0.38425400
C	3.61717700	-1.77615800	0.25209700
O	1.51525500	-0.69151300	0.39267300
H	0.39477000	5.90692700	1.07386500
H	1.31005100	6.71033000	-0.19626500
C	4.98110500	-1.63779900	0.05870800
H	5.59034600	-2.53216800	0.09310300
C	-2.42534100	-3.32963600	-0.15232300
C	-1.54576900	-3.58855700	-1.39752200
H	-2.17353400	-3.66656800	-2.29157200
H	-0.82551600	-2.78603500	-1.55058000
H	-0.99835900	-4.53004200	-1.28233900
C	-1.56224800	-3.34093400	1.13123100
H	-0.78427000	-2.58139400	1.09352200
H	-2.19030500	-3.16704400	2.01489200
H	-1.08799500	-4.32090300	1.25022000
C	-3.43667400	-4.48377300	-0.04019800
H	-4.10078600	-4.36705200	0.82391200
H	-4.05363700	-4.58115200	-0.93950700
H	-2.89261800	-5.42453400	0.08589100
C	2.97271800	-3.14514900	0.51294300
C	4.00908500	-4.28203200	0.53105100
H	4.53279100	-4.37320000	-0.42626600
H	4.75547300	-4.14846600	1.32184300
H	3.49676700	-5.23125500	0.71727900
C	2.26628500	-3.13705700	1.88840300
H	2.99061000	-2.95290000	2.69023100
H	1.49746400	-2.36580900	1.92481300
H	1.79539700	-4.10928200	2.07416900
C	1.95158700	-3.45175000	-0.60352000
H	1.46371200	-4.41441100	-0.41149300
H	1.19149800	-2.67564500	-0.65838200
H	2.45304300	-3.51182900	-1.57505100
C	7.16238100	-0.39851200	-0.39424900
C	7.69876700	1.02025100	-0.64333100
H	7.25479700	1.46674600	-1.53881700
H	7.49856900	1.68188200	0.20592900
H	8.78302800	0.98725000	-0.79018200
C	7.86137400	-0.96591200	0.86048000
H	7.54340300	-1.99104800	1.07112200
H	8.94888500	-0.97458700	0.72487500
H	7.63008100	-0.35727700	1.74061700
C	7.51906100	-1.27143900	-1.61723700
H	7.19089500	-2.30621000	-1.48359200
H	7.03881800	-0.88407900	-2.52112500
H	8.60292000	-1.28225300	-1.77976100
C	-6.71398100	-0.67372100	-0.83523000
C	-7.29587900	0.72682600	-1.08342500
H	-7.07840900	1.40774800	-0.25379600
H	-6.90151000	1.16945100	-2.00355700
H	-8.38370100	0.66431200	-1.18437100
C	-7.34082800	-1.23684600	0.45949000
H	-8.43193200	-1.27973700	0.37161200
H	-6.98402800	-2.24793000	0.67602100
H	-7.09246500	-0.60230000	1.31704400
C	-7.09967900	-1.57770400	-2.02655400
H	-6.74301100	-2.60255700	-1.89057500
H	-8.18851600	-1.61574100	-2.14132700
H	-6.66893700	-1.19511100	-2.95684500
H	0.37749900	3.36689500	1.18535200

H	-0.04801100	3.17475000	-1.80725700
Cl	0.68179700	0.40208000	-2.33245800
O	-0.18875900	0.74777000	1.75500100
H	0.64707900	0.50329700	2.17340500
H	-0.96171400	1.79156800	2.21716000
C	-2.48155500	0.44081000	3.25475900
C	-2.13934600	1.76801000	3.82809500
O	-1.75774400	2.39077300	2.61176100
H	-1.69925800	-0.31237500	3.21113500
H	-1.33448100	1.72401000	4.57276200
H	-3.00603000	2.28479400	4.25184100
C	-3.66830100	0.20183400	2.48887700
H	-3.35043000	0.36679600	1.41389900
H	-3.97418700	-0.84769100	2.47185700
H	-4.49275700	0.88863900	2.68769100

II-m (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.571950

Thermal correction to Gibbs Free Energy (a.u.): 0.851748

No imaginary frequency

C	-4.37292600	-2.14299900	-0.25550000
C	-5.13222600	-0.94973900	-0.38321400
C	-2.99410100	-2.21678000	-0.32178800
H	-4.92077600	-3.06360400	-0.09878100
C	-4.42401100	0.20760100	-0.60740600
C	-2.25123300	-0.99172400	-0.50489700
C	-3.00627400	0.21642300	-0.66092700
H	-4.93511100	1.15569900	-0.74230200
O	-0.95687700	-1.03411500	-0.54297700
C	-2.37606000	1.47417200	-0.90276100
Co	0.19487100	0.44464100	-0.29435700
N	-1.11129600	1.72075600	-0.80733400
H	-3.04118000	2.29364400	-1.17881600
N	1.32558700	1.95993300	0.01215700
C	-0.50858200	3.01963200	-1.11430500
C	2.61436500	1.89716100	0.10537700
C	0.58486000	3.22660600	-0.04917300
C	-1.45080000	4.22089300	-1.17261500
H	3.17585600	2.83131300	0.14158000
C	3.39885800	0.70232500	0.15340400
C	1.39628000	4.49079400	-0.33104700
C	-0.64886700	5.50136000	-1.44839400
H	-1.98460200	4.31300300	-0.21699500
H	-2.20187700	4.08193400	-1.95719400
C	4.80455400	0.85140000	0.09205700
C	2.80202800	-0.58686600	0.28464000
C	0.46119400	5.70697300	-0.41125900
H	2.14224300	4.65377700	0.45411500
H	1.93837000	4.36811600	-1.27755500
H	-1.32171300	6.36533800	-1.46058200
H	-0.20281000	5.43509500	-2.44924500
C	5.64695500	-0.23872800	0.13358000
H	5.20029700	1.85737800	-0.00215100
C	3.66827600	-1.72842100	0.32735700
O	1.50594700	-0.74518500	0.41343700
H	0.00875400	5.87707200	0.57498300
H	1.04195900	6.60430600	-0.64914400
C	5.03547300	-1.50998400	0.25114600
H	5.68755500	-2.37363900	0.27655800
C	-2.25014800	-3.55512400	-0.21532500
C	-1.47060400	-3.80640200	-1.52697800
H	-2.16519900	-3.89190700	-2.36977800
H	-0.77145200	-2.99748800	-1.73468900
H	-0.90808900	-4.74389600	-1.45454600
C	-1.28057900	-3.52651400	0.98749900
H	-0.55279500	-2.72503000	0.88365300

H	-1.83589300	-3.38303300	1.92188100
H	-0.74324800	-4.47869000	1.05711600
C	-3.21185700	-4.73840900	-0.00942500
H	-3.78664100	-4.64550400	0.91870400
H	-3.91485200	-4.84759500	-0.84210900
H	-2.63124700	-5.66384300	0.05402000
C	3.08335800	-3.14318200	0.44594400
C	4.17574800	-4.22660500	0.41271400
H	4.74653100	-4.20239400	-0.52143900
H	4.87683900	-4.13496300	1.24959500
H	3.70417300	-5.21149800	0.48514300
C	2.33539900	-3.28113300	1.79118800
H	3.02437100	-3.12929900	2.62995400
H	1.52653800	-2.55557800	1.86504400
H	1.90527500	-4.28455700	1.88245600
C	2.12284100	-3.40829900	-0.73498800
H	1.68115700	-4.40645700	-0.63841000
H	1.32194900	-2.67313200	-0.77100200
H	2.66758400	-3.36776600	-1.68391900
C	7.17394500	-0.13855300	0.05258800
C	7.64965000	1.31817600	-0.06683500
H	7.26000200	1.79648900	-0.97117400
H	7.34220400	1.91526200	0.79806200
H	8.74246500	1.34846300	-0.11959200
C	7.79884700	-0.74864500	1.32620000
H	7.52209100	-1.79970400	1.44854200
H	8.89237100	-0.69413400	1.28149500
H	7.46473900	-0.20924800	2.21835400
C	7.67419400	-0.91409300	-1.18562400
H	7.39585900	-1.97079300	-1.13989500
H	7.24640900	-0.49629000	-2.10220000
H	8.76624000	-0.85853300	-1.25816700
C	-6.65898000	-1.00807900	-0.27647200
C	-7.30026300	0.37907600	-0.44115800
H	-6.95481500	1.07684500	0.32946500
H	-7.07713900	0.81319300	-1.42102700
H	-8.38824400	0.29934500	-0.35279400
C	-7.05480400	-1.56121700	1.11006500
H	-8.14486300	-1.62149200	1.20484800
H	-6.64893500	-2.56314500	1.27589600
H	-6.67671300	-0.91254200	1.90726800
C	-7.22115200	-1.93478400	-1.37639200
H	-6.82453900	-2.95030100	-1.28986800
H	-8.31319900	-1.99531800	-1.30814700
H	-6.95885000	-1.55812400	-2.36991000
H	0.06985400	3.34926300	0.91501100
H	-0.00271200	2.89918700	-2.08103500
Cl	0.93887900	0.29929800	-2.40585300
O	-0.43037100	0.42016600	1.61307000
H	0.37038800	0.01363700	1.98423300
H	-0.60656600	1.30048500	2.02080900
C	-2.96681300	1.97802200	2.43514900
C	-2.34455800	2.04206400	3.76173500
O	-1.63881900	2.55926000	2.60782200
H	-2.93889600	1.02297100	1.91481200
H	-1.91120600	1.14376600	4.19722400
H	-2.65974400	2.80577600	4.46973400
C	-4.04799200	2.92944100	2.00897600
H	-3.95536400	3.16195600	0.94460200
H	-5.02899500	2.46914400	2.16489400
H	-3.99930700	3.86278700	2.57617100

II-m (PO + H_2O-Co^{III}-Cl)

PO + H_2O-Co^{III}-Cl = PG + Co^{III}(salen)-Cl

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.596812

Thermal correction to Gibbs Free Energy (a.u.): 0.854896

No imaginary frequency

C	-4.65401300	-1.69550100	-0.45054600
C	-5.34892000	-0.46402300	-0.56289200
C	-3.27814900	-1.82707400	-0.38675200
H	-5.24961500	-2.59895900	-0.42565200
C	-4.57830500	0.67361800	-0.62720500
C	-2.48175500	-0.62672500	-0.40059000
C	-3.16335700	0.62146700	-0.54572900
H	-5.03724400	1.65086200	-0.73638200
O	-1.19060300	-0.72336600	-0.26778900
C	-2.46508900	1.86304800	-0.62875400
Co	0.07138700	0.66761900	-0.17418800
N	-1.19316300	2.04427000	-0.47320400
H	-3.08495400	2.73656500	-0.83350300
N	1.34112200	2.06641000	0.05180600
C	-0.54160900	3.34191300	-0.69629300
C	2.62184800	1.91943100	-0.01424400
C	0.67839100	3.36016000	0.23868700
C	-1.40796500	4.58555500	-0.49324200
H	3.24791500	2.81161900	0.02201300
C	3.32184900	0.67270400	-0.11754800
C	1.52768000	4.61228800	0.02660300
C	-0.56543200	5.85440100	-0.69211900
H	-1.83460200	4.56898300	0.51874600
H	-2.24461000	4.59286700	-1.19875200
C	4.71791900	0.73240900	-0.33252600
C	2.66235300	-0.57721900	0.05881900
C	0.66535300	5.86828500	0.22130200
H	2.36856400	4.62995900	0.72801600
H	1.94748200	4.59816900	-0.98766100
H	-1.18314500	6.74016000	-0.51096800
H	-0.23985700	5.90664300	-1.73934900
C	5.48743500	-0.41087300	-0.39122700
H	5.16702500	1.71216100	-0.45684500
C	3.45044000	-1.77056000	0.02064100
O	1.36918900	-0.65669700	0.30431400
H	0.34001700	5.92196400	1.26890000
H	1.26782400	6.76316000	0.03413000
C	4.81401700	-1.63998700	-0.20363000
H	5.40917500	-2.54311100	-0.24147000
C	-2.60033200	-3.20559500	-0.36287800
C	-1.77689200	-3.36132700	-1.66237000
H	-2.44148500	-3.34891800	-2.53268100
H	-1.05170400	-2.55549400	-1.77179500
H	-1.23944100	-4.31588900	-1.65828200
C	-1.68422200	-3.35504800	0.87312200
H	-0.87772900	-2.62553200	0.85504600
H	-2.26186500	-3.22892300	1.79684400
H	-1.24266700	-4.35741300	0.89009000
C	-3.62505800	-4.35281200	-0.31441100
H	-4.24619600	-4.31164600	0.58722600
H	-4.28411100	-4.35411000	-1.18857500
H	-3.09190100	-5.30833600	-0.30567400
C	2.79471100	-3.14670700	0.21162800
C	3.81713000	-4.29312900	0.11837300
H	4.31086900	-4.32184700	-0.85840400
H	4.58746500	-4.22516300	0.89426400
H	3.29772600	-5.24696900	0.25177100
C	2.13699100	-3.22922900	1.60844200
H	2.88219900	-3.07575600	2.39687100
H	1.35213600	-2.48145700	1.71675000
H	1.68762600	-4.21766400	1.75345700
C	1.73444000	-3.36618900	-0.88858800
H	1.23938200	-4.33285300	-0.74374200
H	0.98126700	-2.58179400	-0.87070700
H	2.20480200	-3.36958600	-1.87725600
C	6.99955900	-0.40651500	-0.64083900
C	7.54971900	1.01800600	-0.81614400
H	7.09077400	1.52517000	-1.67090000
H	7.38233300	1.62849400	0.07734300

H	8.62896900	0.97919800	-0.99340800
C	7.72167600	-1.06051600	0.55730600
H	7.39636400	-2.09334500	0.71128500
H	8.80467300	-1.07294500	0.39178000
H	7.52223800	-0.50619000	1.47997900
C	7.30844300	-1.20661800	-1.92502900
H	6.97068500	-2.24387900	-1.84585800
H	6.80934500	-0.75843700	-2.78974000
H	8.38688300	-1.21993500	-2.11828900
C	-6.87973000	-0.46313900	-0.62404600
C	-7.44938300	0.95920100	-0.74569900
H	-7.16648500	1.58150800	0.10966800
H	-7.10618600	1.45431500	-1.65984700
H	-8.54252500	0.91949100	-0.78054500
C	-7.44449300	-1.10268900	0.66313100
H	-8.53965900	-1.12127400	0.63455100
H	-7.09675400	-2.13210300	0.78913900
H	-7.13410400	-0.53466100	1.54601700
C	-7.34781300	-1.27862900	-1.84918100
H	-7.00217600	-2.31524700	-1.80138900
H	-8.44201900	-1.29385800	-1.90491900
H	-6.96249500	-0.84086800	-2.77532100
H	0.29353200	3.36035800	1.26920900
H	-0.16208900	3.32227300	-1.72700800
Cl	0.49008600	0.56515200	-2.36022200
O	-0.05603000	0.63231100	1.92111000
H	0.61792800	-0.08042300	1.82243400
H	0.65881200	0.96033100	4.18861000
C	-1.18628900	0.11777100	2.68367300
C	-0.62194300	-0.46590900	3.97810800
O	0.03416100	0.50675700	4.77174400
H	-1.66143400	-0.67715600	2.10420100
H	0.04989400	-1.30516700	3.72902800
H	-1.44097100	-0.87139800	4.58048300
C	-2.14547300	1.26903800	2.91985500
H	-1.67676900	2.02570200	3.55363900
H	-2.44807500	1.71773600	1.97442000
H	-3.04179300	0.90084500	3.42737900

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl
transition state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2537.511870
Thermal correction to Gibbs Free Energy (a.u.): 0.850505
Imaginary frequencies: -379.16

C	-4.75536000	-1.60882200	-0.26942800
C	-5.41779500	-0.35962600	-0.17227500
C	-3.38555200	-1.77104700	-0.38662500
H	-5.37257400	-2.49799600	-0.26688700
C	-4.62454400	0.76479400	-0.24031400
C	-2.55745200	-0.59145800	-0.35470800
C	-3.21447200	0.67928400	-0.33579500
H	-5.06493200	1.75654100	-0.22205400
O	-1.26419400	-0.72770400	-0.34558900
C	-2.49944300	1.91053600	-0.48707400
Co	0.02687800	0.65710100	-0.17811800
N	-1.21722400	2.04968200	-0.51484000
H	-3.11845900	2.79963000	-0.61597200
N	1.30523100	2.05085200	0.05533900
C	-0.54040100	3.31462100	-0.80834000
C	2.58425000	1.87481300	0.07547500
C	0.67264900	3.37170100	0.13671600
C	-1.37658600	4.58937700	-0.71578500
H	3.22589800	2.75411400	0.13733200
C	3.26612800	0.61782300	0.01099700
C	1.55622900	4.58081700	-0.16983000
C	-0.49827700	5.81255300	-1.01810100

H	-1.80687600	4.67559900	0.29161200
H	-2.21085700	4.55199200	-1.42385100
C	4.67628000	0.65905600	-0.09739500
C	2.57207000	-0.62867100	0.07498900
C	0.72624000	5.87138900	-0.09753200
H	2.38682200	4.63982000	0.54096600
H	1.98869400	4.46480300	-1.17189400
H	-1.09068500	6.72854200	-0.92125900
H	-0.16410600	5.76233400	-2.06256400
C	5.43227100	-0.49148800	-0.16556300
H	5.14751300	1.63581400	-0.13470100
C	3.35019500	-1.83412700	-0.00415600
O	1.27948500	-0.70649500	0.25008700
H	0.39387200	6.02673600	0.93800400
H	1.35505000	6.72989400	-0.35582500
C	4.72642000	-1.71753400	-0.11736700
H	5.30839700	-2.62813300	-0.18147400
C	-0.67609200	-0.39029400	2.40688300
C	0.58564300	-0.29346900	3.13752400
O	-0.46940400	0.82582800	1.69507800
H	-0.65535800	-1.23134300	1.70404500
H	1.49380300	-0.41921100	2.56173400
H	0.66402400	-0.18266000	4.21321500
C	-1.96837100	-0.38106200	3.20197400
H	-2.81236700	-0.32005200	2.51124100
H	-2.06417600	-1.30010200	3.79004400
H	-2.00758400	0.47943000	3.87820100
C	-2.75510300	-3.15662700	-0.60138100
C	-2.02486600	-3.16128700	-1.96505700
H	-2.74105400	-3.00727000	-2.77910100
H	-1.27092900	-2.37551100	-2.01441700
H	-1.53236800	-4.12723300	-2.12401800
C	-1.75406000	-3.49642000	0.52447200
H	-0.89135400	-2.83657500	0.48452900
H	-2.23006600	-3.41242200	1.50875800
H	-1.39839800	-4.52641700	0.41052300
C	-3.81458500	-4.27261200	-0.62897100
H	-4.35244600	-4.35431900	0.32222600
H	-4.54735500	-4.12382100	-1.42857000
H	-3.31945500	-5.23117500	-0.81156000
C	2.65762000	-3.20475300	0.02338000
C	3.65769600	-4.36431700	-0.12970600
H	4.20355600	-4.30840200	-1.07699200
H	4.38619700	-4.39469500	0.68799900
H	3.11112200	-5.31246100	-0.11981200
C	1.93588500	-3.39653600	1.37678500
H	2.65351900	-3.35401800	2.20448900
H	1.18141800	-2.62508800	1.52254900
H	1.43864700	-4.37224100	1.40827700
C	1.64641300	-3.29793000	-1.14154900
H	1.12205500	-4.25968800	-1.10615300
H	0.91360100	-2.49487600	-1.09811900
H	2.16833400	-3.23023000	-2.10141900
C	6.95916200	-0.50182100	-0.29489100
C	7.54349700	0.91945400	-0.32799200
H	7.16458100	1.49096500	-1.18132800
H	7.31008800	1.47293500	0.58752300
H	8.63324700	0.87085300	-0.41816500
C	7.57328500	-1.24912800	0.90898000
H	7.21830600	-2.28216000	0.96685700
H	8.66588600	-1.27543900	0.82895700
H	7.31005500	-0.75220100	1.84832000
C	7.35994900	-1.22028300	-1.60182500
H	7.00123000	-2.25337300	-1.62114100
H	6.93869200	-0.70520800	-2.47067300
H	8.45033100	-1.24274900	-1.70939900
C	-6.94315500	-0.32088600	-0.03492400
C	-7.47696400	1.11788600	0.05161400
H	-7.06247800	1.65030100	0.91398300

H	-7.24129900	1.69049400	-0.85121700
H	-8.56596000	1.10423300	0.16055300
C	-7.36009800	-1.06966000	1.24982300
H	-8.45011600	-1.06423500	1.36242900
H	-7.03116100	-2.11273900	1.23341400
H	-6.92177800	-0.59498100	2.13373300
C	-7.59178600	-1.00457600	-1.25846900
H	-7.27827400	-2.04820100	-1.35214600
H	-8.68417300	-0.99040700	-1.17261900
H	-7.31280000	-0.48846300	-2.18238300
H	0.28242900	3.47920300	1.15998000
H	-0.14744700	3.20694600	-1.82810700
Cl	0.51347700	0.54701500	-2.38462100
O	1.04819200	1.98802200	3.37965400
H	0.49325200	2.35729900	4.08110900
H	0.43127100	1.82766600	2.61429000

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl
reactant complex
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2537.574122
Thermal correction to Gibbs Free Energy (a.u.): 0.852805
No imaginary frequency

C	-4.57375800	-1.75367200	-0.28524800
C	-5.26288400	-0.51616300	-0.22025400
C	-3.20512300	-1.89269500	-0.44438000
H	-5.16908900	-2.65528000	-0.21979000
C	-4.49939900	0.62009000	-0.37305400
C	-2.40192000	-0.69549900	-0.48633700
C	-3.08951900	0.55886400	-0.50752900
H	-4.96253300	1.60194900	-0.39623400
O	-1.10605400	-0.80069700	-0.50470500
C	-2.40353000	1.80067500	-0.70139000
Co	0.13147300	0.61386500	-0.26334400
N	-1.12511300	1.96974600	-0.69090900
H	-3.03887600	2.67208500	-0.85668900
N	1.32939700	2.04264200	0.10639600
C	-0.48021000	3.27154800	-0.88392900
C	2.61345300	1.91539400	0.19531200
C	0.63291000	3.33209800	0.17947600
C	-1.38529800	4.49949900	-0.79341600
H	3.21559400	2.81786600	0.30607600
C	3.33807900	0.68338400	0.15222000
C	1.48214500	4.59213900	0.02332100
C	-0.54831800	5.77945800	-0.93546100
H	-1.90788300	4.48457900	0.17178700
H	-2.14458100	4.47088400	-1.58234300
C	4.74988000	0.76556500	0.09628600
C	2.67614800	-0.58164100	0.19002800
C	0.58369000	5.83619900	0.09692500
H	2.24519800	4.64304600	0.80749500
H	2.00509400	4.55858900	-0.94129400
H	-1.19545600	6.65698700	-0.83483300
H	-0.11948200	5.81843500	-1.94558700
C	5.53654500	-0.36482800	0.05024100
H	5.19558900	1.75471500	0.07770800
C	3.48611700	-1.76507500	0.13367100
O	1.37695600	-0.68593200	0.31950200
H	0.15204300	5.90702900	1.10404000
H	1.18843000	6.73710200	-0.05052000
C	4.86180300	-1.60966000	0.06857100
H	5.46987600	-2.50387300	0.02026400
C	-0.79809200	-0.47369700	2.43509500
C	0.25673800	0.46621600	2.83082100
O	-0.56734600	0.75872900	1.66338400
H	-0.47235500	-1.33855300	1.87016900
H	1.28461900	0.23112700	2.57760500
H	0.08517200	1.16454200	3.64591200

C	-2.14038800	-0.55447900	3.10015400
H	-2.89499600	-0.86861600	2.37302200
H	-2.10837900	-1.30123400	3.90012400
H	-2.43129900	0.41179200	3.51960000
C	-2.55004000	-3.27311100	-0.61092900
C	-1.83224200	-3.32156900	-1.98028900
H	-2.55674700	-3.20658100	-2.79344700
H	-1.08617400	-2.53158500	-2.06531700
H	-1.33143400	-4.28798000	-2.10602200
C	-1.53190200	-3.54188100	0.51812600
H	-0.70435000	-2.83943000	0.46353700
H	-2.01139000	-3.46518700	1.50122200
H	-1.12553700	-4.55459100	0.42253200
C	-3.58680200	-4.40987400	-0.58126500
H	-4.10984800	-4.46650100	0.37986400
H	-4.33322200	-4.30597800	-1.37545000
H	-3.07468000	-5.36469300	-0.73365500
C	2.83142600	-3.15411900	0.13357500
C	3.86691200	-4.28463400	-0.00107000
H	4.43422700	-4.20899200	-0.93443600
H	4.57508600	-4.30034600	0.83454400
H	3.34626600	-5.24722500	-0.00893100
C	2.08418800	-3.37067700	1.46873200
H	2.78798300	-3.35280200	2.30854000
H	1.33741200	-2.59437300	1.62669700
H	1.57929400	-4.34286400	1.46852800
C	1.85685100	-3.26808700	-1.06071100
H	1.36479700	-4.24718000	-1.04840000
H	1.09567500	-2.49142400	-1.03352900
H	2.40347800	-3.17440000	-2.00459400
C	7.06668100	-0.33515300	-0.02707500
C	7.61473400	1.10087500	-0.03248300
H	7.25119300	1.66784000	-0.89550500
H	7.33626500	1.64262400	0.87747600
H	8.70772900	1.08059200	-0.08518500
C	7.65831400	-1.07446900	1.19283400
H	7.32889200	-2.11670700	1.23278600
H	8.75316600	-1.07180000	1.14952100
H	7.35092100	-0.59086900	2.12565800
C	7.52894800	-1.03466400	-1.32395800
H	7.19858000	-2.07663500	-1.36104900
H	7.12388500	-0.52505500	-2.20367000
H	8.62242400	-1.02793400	-1.39472100
C	-6.78157700	-0.50419900	-0.02059600
C	-7.34464300	0.92536000	0.01983200
H	-6.90808000	1.50818300	0.83769900
H	-7.16071500	1.45859000	-0.91842300
H	-8.42731800	0.89393100	0.17607600
C	-7.12466300	-1.19789100	1.31596200
H	-8.20845300	-1.21050100	1.47622300
H	-6.77208200	-2.23318900	1.33544900
H	-6.66066200	-0.67078100	2.15606900
C	-7.46432300	-1.26136100	-1.18052500
H	-7.13071700	-2.30144800	-1.23704400
H	-8.55194500	-1.26660900	-1.04796700
H	-7.23732000	-0.78546400	-2.13956300
H	0.13124000	3.36740600	1.15801600
H	0.00694600	3.23114200	-1.86680800
Cl	0.80601000	0.51592500	-2.38619100
O	-2.63397200	2.67223100	2.22388100
H	-3.40440400	2.21886000	1.85778700
H	-1.90124400	2.09075100	1.96191000

III-t (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.596742

Thermal correction to Gibbs Free Energy (a.u.): 0.856777

No imaginary frequency

C	-4.73642200	-1.56672300	-0.29720800
C	-5.39614800	-0.32507900	-0.11387400
C	-3.37454700	-1.71978100	-0.49095800
H	-5.35075200	-2.45797900	-0.29884400
C	-4.60984800	0.80346900	-0.17544400
C	-2.54678300	-0.53980700	-0.45164000
C	-3.20526800	0.72621800	-0.34519000
H	-5.04956400	1.79229800	-0.09265500
O	-1.25517100	-0.67208100	-0.52269000
C	-2.49840100	1.96187300	-0.48415700
Co	0.02355900	0.69595100	-0.25603200
N	-1.21639600	2.10067500	-0.54624700
H	-3.11949000	2.85532900	-0.56437700
N	1.27830700	2.08544700	0.11336500
C	-0.53718100	3.37272800	-0.79030300
C	2.56095900	1.91116600	0.16769500
C	0.64261400	3.40778500	0.19879200
C	-1.37810200	4.64367200	-0.69524200
H	3.19506800	2.79037900	0.28573700
C	3.24974600	0.66524000	0.06952600
C	1.53585400	4.62288000	-0.05187900
C	-0.49097700	5.87250300	-0.94477300
H	-1.83882300	4.71039000	0.30009700
H	-2.19061300	4.61767100	-1.42880300
C	4.66496700	0.71777100	0.02414800
C	2.55943400	-0.58650300	0.02913600
C	0.70306400	5.91233900	0.01628600
H	2.34280900	4.66990400	0.68677700
H	2.00205900	4.52427600	-1.04047900
H	-1.08590400	6.78672300	-0.84789500
H	-0.12358500	5.84354400	-1.97877000
C	5.42760300	-0.42318000	-0.08401600
H	5.13190100	1.69636200	0.06742200
C	3.34756100	-1.78214700	-0.10339700
O	1.26411300	-0.67866200	0.14791900
H	0.33721900	6.04953500	1.04301600
H	1.34080400	6.77437000	-0.20543000
C	4.72537200	-1.65248700	-0.14947200
H	5.31505500	-2.55445400	-0.25203100
C	-0.62225400	-0.51784900	2.42622900
C	0.63041600	-0.57062300	3.30339700
O	-0.55409100	0.72932900	1.68529900
H	-0.59003600	-1.31351900	1.68599600
H	1.50278400	-0.74972900	2.67569900
H	0.55457900	-1.37199100	4.04812600
C	-1.94053800	-0.55308700	3.18514000
H	-2.77241100	-0.42908700	2.48827300
H	-2.05661300	-1.51354900	3.69768700
H	-1.99863000	0.24917700	3.93084600
C	-2.75230900	-3.09465900	-0.78266300
C	-2.07048200	-3.05098700	-2.17040500
H	-2.81282200	-2.86109500	-2.95294000
H	-1.31185700	-2.26953700	-2.21438000
H	-1.59168200	-4.01354200	-2.38296300
C	-1.71016000	-3.46776900	0.29346000
H	-0.86587200	-2.78434100	0.26066000
H	-2.15744500	-3.44355700	1.29430900
H	-1.33532900	-4.48203700	0.11712500
C	-3.81053800	-4.21150500	-0.81156900
H	-4.31153400	-4.33006200	0.15567500
H	-4.57371400	-4.03486200	-1.57647400
H	-3.32150800	-5.16141600	-1.04798500
C	2.66464600	-3.15457200	-0.20284100
C	3.67864600	-4.29187200	-0.41931600
H	4.25252700	-4.15606800	-1.34177000
H	4.38192200	-4.38558100	0.41544000
H	3.13937400	-5.24048000	-0.50296900
C	1.90998100	-3.45363500	1.11163000

H	2.60559700	-3.47401200	1.95838600
H	1.15026000	-2.69786800	1.30025800
H	1.41651200	-4.42993400	1.05275700
C	1.68608900	-3.16532300	-1.39951500
H	1.17672300	-4.13409700	-1.45546200
H	0.93855900	-2.37949400	-1.31341900
H	2.23223100	-3.01397200	-2.33618800
C	6.95852400	-0.42310500	-0.14712900
C	7.53772400	0.99788000	-0.05861400
H	7.19550000	1.62495800	-0.88816900
H	7.26109500	1.48833300	0.88048900
H	8.63057700	0.95666500	-0.10256600
C	7.52230500	-1.24929600	1.02949100
H	7.16968500	-2.28434100	1.00202900
H	8.61741000	-1.26860400	0.99562600
H	7.21618700	-0.81737800	1.98771100
C	7.41854300	-1.05112600	-1.48086000
H	7.06527000	-2.08091900	-1.58579800
H	7.03386600	-0.47870700	-2.33060900
H	8.51260700	-1.06530400	-1.54165900
C	-6.91217300	-0.29915200	0.10571300
C	-7.44393300	1.13259300	0.27841800
H	-6.98579300	1.63145300	1.13876300
H	-7.25723700	1.74219500	-0.61159700
H	-8.52567100	1.10999200	0.44374300
C	-7.25774900	-1.10048200	1.37984700
H	-8.34013000	-1.10496900	1.55097800
H	-6.92724500	-2.14044900	1.30402700
H	-6.77364600	-0.65932800	2.25721200
C	-7.62404100	-0.93613600	-1.10773400
H	-7.31352500	-1.97368300	-1.26023600
H	-8.71026700	-0.93062300	-0.96294900
H	-7.39654300	-0.38197200	-2.02371400
H	0.20777900	3.50007100	1.20786000
H	-0.10869600	3.29315900	-1.79782000
Cl	0.59191900	0.69974700	-2.42385400
O	0.85308400	0.70710900	3.92028900
H	0.20507500	0.81771500	4.62883400
H	0.03315500	1.30184100	2.21514800

III-m (PO-Co^{III}-Cl + H_2O)
PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl
transition state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2537.518112
Thermal correction to Gibbs Free Energy (a.u.): 0.849196
Imaginary frequencies: -269.22

C	-4.77079500	-1.69983100	-0.20308400
C	-5.44853500	-0.45522600	-0.20573400
C	-3.39710800	-1.85263100	-0.27408600
H	-5.37836200	-2.59455200	-0.15822600
C	-4.66484400	0.67239900	-0.31813800
C	-2.58044100	-0.66379300	-0.30759500
C	-3.25218200	0.59916500	-0.37317600
H	-5.11631300	1.65805100	-0.37033600
O	-1.28733700	-0.78551300	-0.28833900
C	-2.55054800	1.83185200	-0.56880800
Co	-0.01823100	0.62040200	-0.18659400
N	-1.27021300	1.98815600	-0.58542700
H	-3.17981600	2.70667900	-0.73974500
N	1.24822100	2.03075000	0.00145800
C	-0.60584300	3.25676000	-0.89101300
C	2.52827200	1.87108700	-0.00982100
C	0.59697900	3.34280500	0.06754200
C	-1.46060700	4.52096400	-0.82133100
H	3.16202400	2.75851500	0.01264600
C	3.22134500	0.61731700	-0.06140900
C	1.46473000	4.56186500	-0.24399000

C	-0.59767800	5.75501500	-1.12311500
H	-1.90353500	4.60910700	0.18032900
H	-2.28586900	4.46526100	-1.53871000
C	4.62528500	0.66863100	-0.22384300
C	2.54080800	-0.63259200	0.06595500
C	0.61465300	5.83998500	-0.18854700
H	2.28971000	4.63946100	0.47204200
H	1.90635700	4.44553500	-1.24216900
H	-1.20547100	6.66230500	-1.04045800
H	-0.25045700	5.70211500	-2.16324600
C	5.38975300	-0.47709700	-0.28456300
H	5.08465100	1.64794400	-0.31096700
C	3.32876000	-1.83240200	-0.00065300
O	1.25569800	-0.70919500	0.29569700
H	0.26834500	5.99569700	0.84209400
H	1.23264400	6.70664900	-0.44588100
C	4.69858300	-1.70676500	-0.16971200
H	5.28701900	-2.61366200	-0.22572300
C	-2.74860700	-3.24192900	-0.38196800
C	-2.01732800	-3.33738600	-1.74177900
H	-2.73633600	-3.25646800	-2.56389700
H	-1.27702600	-2.54510500	-1.85121100
H	-1.50875400	-4.30409800	-1.82895100
C	-1.74835400	-3.48185600	0.76990700
H	-0.91356900	-2.78914000	0.70578000
H	-2.24133600	-3.36354700	1.74228100
H	-1.35333800	-4.50229100	0.71491200
C	-3.79201200	-4.37211800	-0.32862300
H	-4.33966200	-4.38302500	0.62043300
H	-4.51768600	-4.30122900	-1.14527300
H	-3.28132400	-5.33496500	-0.42671900
C	2.65620300	-3.20892200	0.10486200
C	3.66096000	-4.36250500	-0.06228000
H	4.15843800	-4.33084500	-1.03699300
H	4.42933700	-4.36085300	0.71867400
H	3.12612700	-5.31507000	0.00420100
C	2.00811400	-3.36154500	1.49931400
H	2.77075400	-3.30739100	2.28500100
H	1.27334000	-2.57690500	1.67128400
H	1.50378900	-4.33069900	1.58053700
C	1.58959300	-3.35101600	-1.00350900
H	1.08401500	-4.31916200	-0.91386200
H	0.84689900	-2.55866000	-0.94525700
H	2.06060100	-3.30280300	-1.99051300
C	6.91034000	-0.47811600	-0.47375800
C	7.47907100	0.94633800	-0.57414800
H	7.06154300	1.48743600	-1.42925000
H	7.27638200	1.52660600	0.33212000
H	8.56487300	0.90419800	-0.70558600
C	7.57890600	-1.18219600	0.72719800
H	7.23621700	-2.21570400	0.83147400
H	8.66763600	-1.20200100	0.60429700
H	7.34891000	-0.65801600	1.66051600
C	7.26590400	-1.23377200	-1.77279900
H	6.91648300	-2.26984300	-1.74565700
H	6.80540700	-0.74967900	-2.63950400
H	8.35131800	-1.25038200	-1.92312000
C	-6.97790400	-0.42634500	-0.11951400
C	-7.52906100	1.00836300	-0.14073500
H	-7.14969500	1.59824600	0.70017300
H	-7.26847000	1.52678400	-1.06907800
H	-8.62097800	0.98820000	-0.06754300
C	-7.43049800	-1.09882100	1.19498600
H	-8.52374100	-1.09978900	1.27073100
H	-7.09063300	-2.13675000	1.25481600
H	-7.02729000	-0.56481200	2.06158600
C	-7.57868900	-1.19250500	-1.31845700
H	-7.25152900	-2.23596100	-1.33639200
H	-8.67345500	-1.18633800	-1.26936100

H	-7.27416300	-0.73145900	-2.26317900
H	0.19980100	3.44793500	1.08739100
H	-0.20045800	3.14236400	-1.90533600
Cl	0.47503700	0.42970600	-2.38756700
O	-0.40570700	2.55177600	3.56482200
H	-1.28599400	2.79320600	3.88230100
H	-0.55562100	2.11793700	2.67933600
C	0.16614400	0.12952800	3.55987900
C	-0.70504700	-0.28077900	2.44731200
O	-0.57360700	0.86892700	1.65021600
H	-0.24190500	0.30388800	4.55272600
H	-1.74438500	-0.47589300	2.73949000
H	-0.30629400	-1.16683900	1.93362200
C	1.61431500	0.29381600	3.39712000
H	1.91499800	1.29499600	3.72628200
H	2.10020100	-0.40807800	4.09502800
H	1.93797800	0.10228900	2.37801100

III-m (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.569216

Thermal correction to Gibbs Free Energy (a.u.): 0.850765

No imaginary frequency

C	-4.65449400	-1.80168900	-0.19800100
C	-5.35282800	-0.56823800	-0.24300200
C	-3.27941600	-1.93808200	-0.27616500
H	-5.24747800	-2.70298600	-0.11023400
C	-4.58807700	0.56435700	-0.41110200
C	-2.48091400	-0.73996600	-0.35885900
C	-3.17232100	0.50679200	-0.47348400
H	-5.05326800	1.54078400	-0.50567600
O	-1.18449800	-0.83910200	-0.33059400
C	-2.48696000	1.74379500	-0.68910600
Co	0.05943400	0.57987800	-0.21510500
N	-1.20924400	1.92263300	-0.65699900
H	-3.12352200	2.60654000	-0.88137900
N	1.27320400	2.01619700	0.04537400
C	-0.57503200	3.22376500	-0.89114600
C	2.56030100	1.89247900	0.05247000
C	0.57586400	3.30247100	0.12901800
C	-1.48276900	4.44909800	-0.78260800
H	3.16706500	2.79763300	0.09669000
C	3.28055200	0.65863200	0.01095900
C	1.41168000	4.56530700	-0.06723900
C	-0.65891900	5.73340300	-0.95810300
H	-1.98038100	4.43592900	0.19583100
H	-2.26392900	4.41298600	-1.54926300
C	4.68691600	0.73733300	-0.12770100
C	2.62248500	-0.60372200	0.13998800
C	0.50837200	5.80385700	0.03336900
H	2.20459700	4.62353300	0.68646000
H	1.89730600	4.53035200	-1.05111800
H	-1.30811500	6.60721700	-0.83995300
H	-0.26515300	5.77014500	-1.98251600
C	5.47235300	-0.39377800	-0.16526600
H	5.12862200	1.72462600	-0.21475400
C	3.43291000	-1.78856000	0.09675600
O	1.33351600	-0.70247700	0.34641900
H	0.11245800	5.87659600	1.05500900
H	1.10074300	6.70837400	-0.13978300
C	4.80227100	-1.63611800	-0.05115400
H	5.40922400	-2.53149000	-0.09002300
C	-2.60945300	-3.32004300	-0.32655300
C	-1.87085700	-3.45871900	-1.67852500
H	-2.58643100	-3.41899100	-2.50662800
H	-1.13914300	-2.66269800	-1.81448600
H	-1.34991200	-4.42149400	-1.72542400

C	-1.61000300	-3.49392700	0.83789400
H	-0.79723800	-2.77687200	0.75760600
H	-2.11399100	-3.36283100	1.80301700
H	-1.18388100	-4.50289500	0.81678300
C	-3.63516200	-4.46325800	-0.23106800
H	-4.18412300	-4.44624300	0.71703000
H	-4.36028900	-4.43511300	-1.05085900
H	-3.10939900	-5.42103200	-0.29081300
C	2.78588800	-3.17758100	0.19870100
C	3.81808400	-4.31111300	0.06470600
H	4.33584200	-4.27939100	-0.89947500
H	4.56873000	-4.28530400	0.86216600
H	3.30186000	-5.27386600	0.12995300
C	2.10810100	-3.33168800	1.57832100
H	2.84863500	-3.25283300	2.38223500
H	1.35267300	-2.56168700	1.72454500
H	1.62296400	-4.31075000	1.65620900
C	1.74883700	-3.35026600	-0.93330900
H	1.26358200	-4.32907900	-0.84850600
H	0.98601300	-2.57584200	-0.89661300
H	2.24096100	-3.29788300	-1.90984400
C	6.99578800	-0.36849500	-0.32757700
C	7.53968400	1.06539000	-0.43079100
H	7.12773700	1.59135300	-1.29801500
H	7.31075100	1.64947000	0.46671700
H	8.62813500	1.04211000	-0.54281300
C	7.65477300	-1.04962000	0.89173000
H	7.33015500	-2.08862200	0.99888200
H	8.74562200	-1.04954500	0.78852400
H	7.39784800	-0.52222400	1.81606200
C	7.38776200	-1.12891500	-1.61328300
H	7.05741600	-2.17113700	-1.58302900
H	6.93449900	-0.66098200	-2.49263000
H	8.47574000	-1.12663400	-1.74384500
C	-6.88114800	-0.55836600	-0.13764200
C	-7.45304900	0.86656100	-0.20832600
H	-7.07181100	1.49532900	0.60317400
H	-7.21303300	1.35129700	-1.16010500
H	-8.54328200	0.83422100	-0.11870600
C	-7.30586000	-1.18427200	1.20870600
H	-8.39770300	-1.19801700	1.29922800
H	-6.94989600	-2.21399200	1.30548900
H	-6.90023700	-0.61014600	2.04815000
C	-7.48523900	-1.38043100	-1.29713000
H	-7.14321900	-2.41910700	-1.27775400
H	-8.57909600	-1.38787900	-1.23343400
H	-7.20004800	-0.95317200	-2.26350700
H	0.11025400	3.34391000	1.12556300
H	-0.12317300	3.17486900	-1.89076100
Cl	0.63098000	0.39227500	-2.35811100
O	-2.81496600	2.55115100	2.22240600
H	-3.62363000	2.10077500	1.94738900
H	-2.11457200	1.97104000	1.88106100
C	-0.06565900	0.81987000	3.08447100
C	-0.79116900	-0.36104600	2.59748800
O	-0.65193700	0.79774600	1.73543700
H	-0.62603500	1.51573500	3.70734300
H	-1.81758600	-0.54673100	2.90017800
H	-0.22410100	-1.21411800	2.24489000
C	1.42852500	0.86181600	3.20718600
H	1.80700000	1.86444400	2.99084900
H	1.70416700	0.61239700	4.23745000
H	1.89614500	0.15197500	2.52747400

III-m (PO-Co^{III}-Cl + H_2O)

PO-Co^{III}-Cl + H_2O = PG + Co^{III}(salen)-Cl

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2537.592768

Thermal correction to Gibbs Free Energy (a.u.): 0.856872
No imaginary frequency

C	-4.80464400	-1.62796100	-0.21139900
C	-5.47855900	-0.38244100	-0.13214100
C	-3.43594800	-1.78194400	-0.34029300
H	-5.41354200	-2.52256900	-0.18280200
C	-4.69579600	0.74585800	-0.21896900
C	-2.61555600	-0.59544400	-0.35282900
C	-3.28435200	0.67015300	-0.33001400
H	-5.14319200	1.73468500	-0.20585900
O	-1.32350400	-0.72357400	-0.40093500
C	-2.58325300	1.90313200	-0.49798500
Co	-0.05067000	0.66046000	-0.22975200
N	-1.30007400	2.05351200	-0.53761100
H	-3.20910900	2.78821500	-0.62212000
N	1.21321700	2.06441100	0.04557500
C	-0.63279100	3.32229600	-0.83103700
C	2.49786000	1.89849300	0.03133300
C	0.57589800	3.38499900	0.12086900
C	-1.47714500	4.59173400	-0.73860900
H	3.13231200	2.78364200	0.08596600
C	3.18683100	0.65205400	-0.05992400
C	1.45417500	4.59947800	-0.17980900
C	-0.60482400	5.82077300	-1.03458500
H	-1.91285800	4.67371300	0.26683600
H	-2.30807700	4.54938500	-1.45021100
C	4.59772900	0.70899300	-0.17580900
C	2.50097700	-0.60256800	-0.01399200
C	0.61611500	5.88525300	-0.10939000
H	2.28336400	4.66322000	0.53255600
H	1.88987400	4.48609600	-1.18066300
H	-1.20272100	6.73298600	-0.93715300
H	-0.26683300	5.77552000	-2.07799800
C	5.36112800	-0.43216000	-0.27291800
H	5.06009900	1.69056500	-0.19418300
C	3.28937600	-1.79891300	-0.14205400
O	1.21527100	-0.69134700	0.18288700
H	0.27977000	6.03853700	0.92508300
H	1.24160500	6.74684200	-0.36500900
C	4.66282300	-1.66517300	-0.25850900
H	5.25199400	-2.56796900	-0.35594600
C	-2.79537600	-3.16733500	-0.51770100
C	-2.10439900	-3.22031500	-1.90043200
H	-2.84567300	-3.10637100	-2.69862700
H	-1.36113000	-2.43002300	-2.00278300
H	-1.60592200	-4.18685400	-2.03522300
C	-1.76168100	-3.44144200	0.59623200
H	-0.94212600	-2.72990500	0.54126200
H	-2.23115300	-3.37375400	1.58482300
H	-1.35163900	-4.45144600	0.48612000
C	-3.83868300	-4.29750400	-0.46967300
H	-4.35761400	-4.33830900	0.49450500
H	-4.58846200	-4.19965300	-1.26155000
H	-3.33300100	-5.25726200	-0.61356200
C	2.61441100	-3.17877700	-0.16479100
C	3.62345500	-4.31483000	-0.40983200
H	4.14378000	-4.19816000	-1.36602700
H	4.37291900	-4.38446000	0.38619800
H	3.08714300	-5.26830700	-0.44002400
C	1.93828500	-3.44895200	1.19697800
H	2.68262900	-3.45632900	2.00169900
H	1.19324000	-2.68649700	1.41496500
H	1.43865300	-4.42379700	1.18767100
C	1.56878000	-3.22811900	-1.30132100
H	1.06782300	-4.20271600	-1.30424300
H	0.81925200	-2.44815200	-1.18842000
H	2.05686900	-3.09346000	-2.27195300
C	6.88745300	-0.42913000	-0.40596800
C	7.46250400	0.99624100	-0.39716100

H	7.08010100	1.59022900	-1.23347000
H	7.22552200	1.52086900	0.53431200
H	8.55249400	0.95748700	-0.48856100
C	7.50814800	-1.20848500	0.77395400
H	7.15966600	-2.24492900	0.80153900
H	8.60065800	-1.22561300	0.69109700
H	7.24371700	-0.74165200	1.72823700
C	7.28980700	-1.10541700	-1.73474900
H	6.93787300	-2.13978800	-1.78456700
H	6.86367600	-0.56708100	-2.58699000
H	8.38003600	-1.11758800	-1.84486600
C	-7.00368700	-0.35577600	0.01132200
C	-7.55053200	1.07922400	0.07587900
H	-7.13925000	1.62911200	0.92878800
H	-7.32150100	1.63931100	-0.83649500
H	-8.63918900	1.05764600	0.18723900
C	-7.41009500	-1.08707000	1.30936900
H	-8.49984100	-1.08997300	1.42509300
H	-7.07155300	-2.12719000	1.30924900
H	-6.97365000	-0.59393600	2.18401100
C	-7.65009300	-1.06538700	-1.19856600
H	-7.32589400	-2.10703000	-1.27689000
H	-8.74229000	-1.06130100	-1.10879000
H	-7.37987700	-0.56123800	-2.13168100
H	0.17369400	3.49856000	1.14178800
H	-0.23298700	3.22327200	-1.84887100
Cl	0.44363700	0.58620700	-2.41151300
O	0.12701500	1.26542700	4.19517100
H	-0.72300200	1.23728200	4.65608000
H	-0.32695900	1.50262700	2.24482300
C	0.43216300	-0.06753100	3.72955100
C	-0.53487400	-0.39869900	2.58897600
O	-0.62527500	0.74019500	1.71682400
H	0.28026200	-0.79434100	4.53939500
H	-1.54154700	-0.60499900	2.97319000
H	-0.19979500	-1.24373400	1.99302800
C	1.89429200	-0.05330600	3.31687000
H	2.51663600	0.22743500	4.17002400
H	2.20029300	-1.03664600	2.95558700
H	2.06109200	0.66280700	2.51084800

PO + H_2O-Co^{III}-OH terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

transition state

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2153.099432

Thermal correction to Gibbs Free Energy (a.u.): 0.862267

Imaginary frequencies: -482.08

C	4.70849400	-1.60823400	-0.33529400
C	5.38935300	-0.36673900	-0.30058600
C	3.33136400	-1.75911700	-0.33446800
H	5.31443100	-2.50467600	-0.35065600
C	4.60602000	0.76377200	-0.25050100
C	2.52329300	-0.57099800	-0.32607900
C	3.19029200	0.69081100	-0.26405400
H	5.05595900	1.74925500	-0.19380100
O	1.21763300	-0.68477500	-0.37828300
C	2.48241100	1.92807400	-0.14931800
Co	-0.06858000	0.70742100	-0.48690700
N	1.19917800	2.08741100	-0.19131200
H	3.10509100	2.80956900	0.00466400
N	-1.33457800	2.10837700	-0.71595100
C	0.54017900	3.37403200	0.06139300
C	-2.61397500	1.96275800	-0.62060300
C	-0.67681900	3.41037000	-0.87915300
C	1.39880900	4.63002000	-0.08502300
H	-3.24150900	2.85409500	-0.64872800
C	-3.31104600	0.71710800	-0.48276900

C	-1.53241500	4.65325400	-0.63843500
C	0.54337700	5.88444700	0.14595000
H	1.83887400	4.65362900	-1.09104300
H	2.22483700	4.61411600	0.63296400
C	-4.70223300	0.78053300	-0.23728400
C	-2.64995700	-0.53718300	-0.62429300
C	-0.67433500	5.91897200	-0.78423100
H	-2.36658100	4.68817700	-1.34725500
H	-1.96193200	4.60759400	0.37095800
H	1.15660000	6.77997600	0.00296800
H	0.20385300	5.89975200	1.18982000
C	-5.46438600	-0.36183800	-0.10722900
H	-5.15307300	1.76291700	-0.14463900
C	-3.42843600	-1.73149300	-0.49494700
O	-1.36154300	-0.62354900	-0.89661900
H	-0.33546500	6.00648900	-1.82517400
H	-1.28531500	6.80369400	-0.57815200
C	-4.78713000	-1.59540000	-0.24384600
H	-5.37456200	-2.49804200	-0.13844900
O	0.27289800	0.61538700	-2.54145400
H	1.01843200	-0.00805300	-2.51544600
H	-0.50667900	0.03800500	-2.65249800
C	-2.76851600	-3.11439600	-0.61564300
C	-3.77579100	-4.25691400	-0.39616900
H	-3.25475900	-5.21484100	-0.48512900
H	-4.22698700	-4.21886000	0.60072000
H	-4.57881100	-4.24855800	-1.14079400
C	-2.16753700	-3.28776000	-2.02861300
H	-2.95109600	-3.22039600	-2.79121700
H	-1.41566400	-2.52522700	-2.23005100
H	-1.69119800	-4.27020600	-2.11665100
C	-1.65969900	-3.25577200	0.45014200
H	-0.87674700	-2.51536500	0.30079000
H	-2.07284400	-3.13783700	1.45768500
H	-1.20346600	-4.24947900	0.38880100
C	-6.97049400	-0.35218100	0.17628600
C	-7.71386900	-1.07321900	-0.96923400
H	-7.38567400	-2.11123800	-1.07495500
H	-8.79266100	-1.08243400	-0.77895200
H	-7.53859600	-0.56798400	-1.92438500
C	-7.24545700	-1.08443800	1.50784200
H	-8.31915700	-1.09290800	1.72519100
H	-6.90362500	-2.12295700	1.47681100
H	-6.73119100	-0.58814600	2.33666400
C	-7.52547600	1.07688000	0.28760000
H	-7.05362900	1.63078000	1.10556800
H	-7.37985600	1.64042000	-0.63988600
H	-8.60057000	1.04175700	0.48840200
C	2.67556400	-3.14801100	-0.28432000
C	3.71539100	-4.28125700	-0.34322000
H	4.29688200	-4.25757500	-1.27132600
H	4.41003900	-4.24736700	0.50200500
H	3.19729200	-5.24409700	-0.30175900
C	1.91474900	-3.27933200	1.05473000
H	2.61243600	-3.22042100	1.89606800
H	1.17572800	-2.48797700	1.16912600
H	1.39787200	-4.24369200	1.10647000
C	1.71014700	-3.34745900	-1.47501300
H	0.89479000	-2.62749800	-1.44816900
H	2.24774800	-3.24497900	-2.42521400
H	1.28090500	-4.35472400	-1.44153000
C	6.92134300	-0.34381300	-0.29465500
C	7.47392600	1.08970500	-0.24891200
H	8.56794400	1.06505000	-0.25199200
H	7.15266100	1.67438000	-1.11730600
H	7.15712900	1.61535200	0.65755900
C	7.44141400	-1.10352300	0.94529800
H	7.07826700	-0.63698700	1.86604800
H	7.11323100	-2.14689000	0.94833400

H	8.53680800	-1.09861800	0.96506800
C	7.44924400	-1.02711200	-1.57483400
H	7.10132600	-0.49908500	-2.46853600
H	8.54474000	-1.03045800	-1.58326500
H	7.11269300	-2.06539400	-1.64764400
C	0.24778800	0.18895600	3.95932400
C	0.74303500	0.69007600	2.63285800
O	1.44268800	0.47522500	4.52108800
H	-0.62300600	0.79279200	4.31238200
H	0.92903900	1.75567700	2.60898500
H	1.53040800	0.07848700	2.21009600
C	-0.16135500	-1.29104600	3.96206900
H	-0.30765000	-1.62625500	4.99406700
H	-1.09917500	-1.47064000	3.41315100
H	0.63533300	-1.90035400	3.52189100
O	-0.44500400	0.61434600	1.35198100
H	-0.79931100	-0.28201700	1.46552500
H	-0.28793700	3.43617100	-1.90751900
H	0.14987300	3.32495500	1.08837300

PO + H_2O-Co^{III}-OH terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2153.151190

Thermal correction to Gibbs Free Energy (a.u.): 0.860701

No imaginary frequency

C	4.61966700	-1.50237000	-0.52447700
C	5.29342900	-0.26024000	-0.44558600
C	3.24398000	-1.66316200	-0.46649500
H	5.22834100	-2.39027200	-0.63603800
C	4.50399800	0.86153800	-0.31354900
C	2.42917100	-0.48706500	-0.31583800
C	3.09190800	0.77795600	-0.26025300
H	4.94982300	1.84850100	-0.24575000
O	1.12840100	-0.61278300	-0.22669000
C	2.37566700	2.00941600	-0.08502600
Co	-0.16605400	0.76987600	-0.40637400
N	1.09392700	2.15067200	-0.10570100
H	2.99367700	2.89189500	0.08689700
N	-1.43614700	2.15878700	-0.65795600
C	0.41183700	3.41198400	0.19577000
C	-2.71247700	1.99583300	-0.55444800
C	-0.79128700	3.47058600	-0.76535600
C	1.25305700	4.68511300	0.12243700
H	-3.35090500	2.88019000	-0.56186800
C	-3.39495800	0.74160800	-0.42758500
C	-1.66427500	4.69434700	-0.48956400
C	0.37598700	5.91661900	0.39110700
H	1.71148300	4.76287800	-0.87285900
H	2.06758000	4.64826000	0.85348900
C	-4.78418600	0.78997000	-0.17170100
C	-2.72124500	-0.50433500	-0.58933900
C	-0.82098600	5.97547600	-0.56452300
H	-2.48673400	4.74863700	-1.21081700
H	-2.11074900	4.60083500	0.50905200
H	0.97870800	6.82657500	0.30315300
H	0.01179100	5.87882000	1.42619700
C	-5.53568300	-0.35993700	-0.04367700
H	-5.24316600	1.76778500	-0.06833100
C	-3.48978500	-1.70557400	-0.45244000
O	-1.44440200	-0.57043500	-0.89464200
H	-0.45924600	6.11045500	-1.59272200
H	-1.44753100	6.84401100	-0.33633200
C	-4.84728500	-1.58613800	-0.19015500
H	-5.42467000	-2.49543200	-0.08328800
O	0.18606000	0.65606000	-2.48149900
H	0.95309000	0.06292900	-2.50431800
H	-0.58338800	0.05154700	-2.52405200

C	-2.81605000	-3.08016100	-0.57911200
C	-3.80242400	-4.23669800	-0.33911400
H	-3.26737900	-5.18746500	-0.42587000
H	-4.24363900	-4.19660500	0.66223000
H	-4.61406100	-4.24749900	-1.07447100
C	-2.23886700	-3.25148000	-2.00202000
H	-3.03920300	-3.20429600	-2.74870400
H	-1.50881900	-2.47413800	-2.22358600
H	-1.74461500	-4.22500500	-2.09483000
C	-1.68973200	-3.19864100	0.47106700
H	-0.94948300	-2.41236200	0.33922900
H	-2.10283500	-3.12352600	1.48283800
H	-1.19148300	-4.17014200	0.38014800
C	-7.04030900	-0.36596200	0.24774600
C	-7.78382000	-1.08882200	-0.89655400
H	-7.44471900	-2.12257500	-1.00930300
H	-8.86176100	-1.11030400	-0.70092600
H	-7.61834500	-0.57722900	-1.85008400
C	-7.30299500	-1.10633800	1.57727200
H	-8.37570100	-1.12695200	1.80010500
H	-6.94995400	-2.14088800	1.53994400
H	-6.78915300	-0.60821300	2.40533900
C	-7.60910400	1.05695100	0.36818900
H	-7.13796700	1.61172900	1.18598100
H	-7.47222400	1.62587600	-0.55728500
H	-8.68312500	1.01094800	0.57374800
C	2.59665000	-3.05549000	-0.53868700
C	3.63198100	-4.16305500	-0.80288400
H	4.16138700	-4.01182300	-1.74975100
H	4.37301300	-4.23560200	-0.00025000
H	3.11774200	-5.12717500	-0.86054800
C	1.91111900	-3.36512900	0.81011500
H	2.65520500	-3.40993000	1.61291800
H	1.17305600	-2.60432100	1.05744900
H	1.40396400	-4.33500800	0.76577600
C	1.56068700	-3.10832300	-1.68518800
H	0.75131000	-2.40099600	-1.51577300
H	2.04217900	-2.88569100	-2.64515600
H	1.12917000	-4.11258000	-1.75396000
C	6.82418900	-0.22377300	-0.50413800
C	7.36956200	1.20939700	-0.39877700
H	8.46291100	1.19410400	-0.44319400
H	7.01291100	1.83884100	-1.22067400
H	7.08264800	1.68161300	0.54636100
C	7.40149900	-1.04875700	0.66686000
H	7.07742400	-0.63692000	1.62768300
H	7.07691300	-2.09242900	0.62501000
H	8.49676900	-1.03850400	0.64001400
C	7.30335100	-0.82764700	-1.84214800
H	6.91299400	-0.25341300	-2.68846500
H	8.39756400	-0.81883400	-1.89707900
H	6.97241800	-1.86354000	-1.96012000
C	1.11198400	-0.33812400	3.83574200
C	2.35663600	-0.19910700	3.06372400
O	2.39024700	-0.36881700	4.48694400
H	0.54234100	0.57379600	4.02272800
H	2.66030900	0.78053300	2.69626000
H	2.72773300	-1.03994900	2.48066000
C	0.31081400	-1.61534200	3.84631400
H	-0.14194300	-1.77700800	4.83022600
H	-0.49614600	-1.56775500	3.10716600
H	0.94892000	-2.47195400	3.61475800
O	-0.59437200	0.75406400	1.36409500
H	0.00781400	0.07916300	1.70427800
H	-0.38658200	3.54154300	-1.78579600
H	0.00563100	3.28656600	1.20836000

PO + H_2O-Co^{III}-OH terminal carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

product complex

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2153.104453
Thermal correction to Gibbs Free Energy (a.u.): 0.863028
No imaginary frequency

C	4.73947900	-1.61310400	-0.27651000
C	5.42308600	-0.37291100	-0.24093500
C	3.36206400	-1.75997100	-0.29234900
H	5.34325100	-2.51116300	-0.27967100
C	4.64240200	0.76007100	-0.20550000
C	2.55771000	-0.56954800	-0.30157100
C	3.22644700	0.69132300	-0.23458900
H	5.09476200	1.74451500	-0.14913200
O	1.25298100	-0.67957500	-0.37239400
C	2.52091200	1.93118300	-0.13152100
Co	-0.02928200	0.71331600	-0.49088900
N	1.23722500	2.09328900	-0.17920800
H	3.14592900	2.81158100	0.01965700
N	-1.29761400	2.11584300	-0.69582300
C	0.58511800	3.38821600	0.05587300
C	-2.57784600	1.97122600	-0.60220000
C	-0.63978500	3.41601200	-0.87432000
C	1.44633000	4.63930800	-0.11774300
H	-3.20534800	2.86281800	-0.62616600
C	-3.27650000	0.72443500	-0.47647300
C	-1.49076600	4.66326300	-0.64001400
C	0.59717500	5.89984400	0.10406400
H	1.87598100	4.64578900	-1.12843600
H	2.27975400	4.63228700	0.59171500
C	-4.66842800	0.78844500	-0.23320800
C	-2.61970200	-0.53083300	-0.63490800
C	-0.63161300	5.92503800	-0.81182300
H	-2.33215600	4.69084100	-1.34050600
H	-1.91010000	4.63165500	0.37425000
H	1.21146900	6.79109700	-0.05949800
H	0.27025500	5.93197600	1.15159300
C	-5.43548500	-0.35258600	-0.12477300
H	-5.11578800	1.77084300	-0.12529700
C	-3.40579000	-1.72390200	-0.53875700
O	-1.32746300	-0.62069000	-0.88798300
H	-0.30508800	5.99819100	-1.85778600
H	-1.23789300	6.81391000	-0.60989100
C	-4.76408400	-1.58638300	-0.28724000
H	-5.35666100	-2.48795800	-0.20427900
O	0.31144100	0.61573800	-2.57328200
H	1.05561300	-0.00827200	-2.53432200
H	-0.46839300	0.03722900	-2.66985500
C	-2.75489100	-3.10765300	-0.69875500
C	-3.77304200	-4.24835000	-0.52432300
H	-3.25990200	-5.20714300	-0.64419400
H	-4.22899200	-4.24125900	0.47107200
H	-4.57198900	-4.20656500	-1.27213100
C	-2.14471100	-3.23965300	-2.11237700
H	-2.92102300	-3.13707200	-2.87838200
H	-1.38210900	-2.47978800	-2.28158500
H	-1.67903900	-4.22408200	-2.23016800
C	-1.65447100	-3.29515500	0.36832000
H	-0.86116800	-2.56093000	0.24471500
H	-2.07095100	-3.20326400	1.37695800
H	-1.20921600	-4.29175300	0.27859800
C	-6.94160300	-0.34166800	0.15853400
C	-7.68838200	-1.03533000	-1.00157500
H	-7.36563900	-2.07267700	-1.12857600
H	-8.76718900	-1.04297000	-0.81144300
H	-7.51055200	-0.51150900	-1.94619100
C	-7.21977100	-1.09993800	1.47477600
H	-8.29346400	-1.10781700	1.69206200
H	-6.88289900	-2.13922000	1.42221100
H	-6.70311000	-0.62337800	2.31359400

C	-7.48969600	1.08744300	0.29940700
H	-7.01463300	1.62226500	1.12811800
H	-7.34228700	1.66910500	-0.61655800
H	-8.56477400	1.05325400	0.50036300
C	2.70039600	-3.14639800	-0.24516700
C	3.73739200	-4.28330000	-0.27808700
H	4.33476900	-4.26789400	-1.19617500
H	4.41755800	-4.24543300	0.57868900
H	3.21572800	-5.24429000	-0.23893200
C	1.91430000	-3.26908700	1.08031900
H	2.59553300	-3.20636900	1.93472300
H	1.17393300	-2.47649100	1.17659000
H	1.39502700	-4.23231200	1.12758700
C	1.75684300	-3.34970500	-1.45278700
H	0.94470300	-2.62548500	-1.44721300
H	2.31319000	-3.25646900	-2.39299200
H	1.32201800	-4.35461200	-1.42042400
C	6.95506400	-0.35403000	-0.21951200
C	7.51123700	1.07816700	-0.17596800
H	8.60514300	1.05046600	-0.16795700
H	7.20032500	1.65901900	-1.05064400
H	7.18698400	1.60974200	0.72442500
C	7.46094100	-1.10861100	1.02940000
H	7.09099000	-0.63573700	1.94424300
H	7.12934800	-2.15088000	1.03519700
H	8.55608600	-1.10716500	1.05951400
C	7.49379100	-1.04557000	-1.49075700
H	7.15594500	-0.52152200	-2.39061800
H	8.58929300	-1.05167200	-1.48841200
H	7.15532100	-2.08337700	-1.56127400
C	-0.03969700	0.20351200	3.90876100
C	0.52834500	0.64070100	2.50811700
O	0.97618600	0.41211800	4.72845400
H	-0.95387600	0.84165900	4.07205100
H	0.80571500	1.69154700	2.55241600
H	1.39706000	0.02260800	2.27597100
C	-0.52407400	-1.26551600	3.82560400
H	-0.85557500	-1.58558500	4.81777500
H	-1.37352000	-1.40653100	3.13476300
H	0.30281900	-1.91796700	3.52183200
O	-0.44667000	0.52882500	1.41088700
H	-0.79551200	-0.37798700	1.44373600
H	-0.25930200	3.43075300	-1.90607500
H	0.20302100	3.36275300	1.08754900

PO + H_2O-Co^{III}-OH middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O
transition state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2153.097875
Thermal correction to Gibbs Free Energy (a.u.): 0.865434
Imaginary frequencies: -357.72

C	4.83322800	-1.73402600	0.12147000
C	5.49380000	-0.48965800	-0.00290200
C	3.45689100	-1.89948900	0.17065500
H	5.45118200	-2.62031300	0.18281500
C	4.69194200	0.62903800	-0.08004500
C	2.63271700	-0.72697900	0.08281800
C	3.27970600	0.53734500	-0.04751400
H	5.12701900	1.61866200	-0.17057500
O	1.32375000	-0.85521400	0.12400700
C	2.55213500	1.77298300	-0.12335700
Co	0.04728200	0.45354600	-0.37101300
N	1.27017100	1.91093400	-0.18640500
H	3.16443600	2.67447500	-0.12844400
N	-1.20023200	1.78298800	-0.91996500
C	0.61655800	3.22677800	-0.25925900
C	-2.47991100	1.60748800	-0.91751400

C	-0.55319700	3.06596100	-1.24609400
C	1.48505700	4.42530600	-0.63610200
H	-3.11972500	2.46413200	-1.13076000
C	-3.15292500	0.37341200	-0.63505200
C	-1.44226700	4.30980000	-1.20911400
C	0.60555500	5.68519100	-0.59500300
H	1.92898600	4.28534200	-1.63213600
H	2.30367700	4.54062500	0.08140100
C	-4.55058500	0.43378400	-0.43277600
C	-2.45719500	-0.87024100	-0.60355200
C	-0.60384500	5.55800200	-1.52923900
H	-2.26353100	4.22491800	-1.92918800
H	-1.87618500	4.40495400	-0.20586800
H	1.19972200	6.56498300	-0.86340600
H	0.25878200	5.82210500	0.43649300
C	-5.28908200	-0.70265700	-0.17393700
H	-5.02475400	1.40853200	-0.47529400
C	-3.21408600	-2.05756000	-0.35020900
O	-1.16290600	-0.94608700	-0.84458500
H	-0.25937700	5.50298100	-2.57126000
H	-1.23580600	6.44891300	-1.45390700
C	-4.58127100	-1.92598100	-0.14577700
H	-5.15081600	-2.82368100	0.05647200
O	-0.59205700	0.43277700	1.38406000
H	0.12471500	0.02371400	1.89133700
O	0.60448800	0.16065200	-2.32543000
H	-0.11564700	-0.49817800	-2.41865800
H	1.41574700	-0.36559200	-2.24180400
C	-1.08228200	2.05662000	2.25495500
C	0.07208800	2.73818500	2.90296800
O	-0.51650100	3.96257300	2.75150600
H	-1.33745600	2.46749700	1.29877900
H	1.04534300	2.56338200	2.38955100
H	0.20818500	2.39024500	3.95108800
C	-2.23619700	1.60010800	3.09683200
H	-1.91619800	0.85128500	3.82881400
H	-2.61684300	2.46963100	3.63969800
H	-3.03397600	1.17828400	2.48175400
C	2.82135400	-3.28921700	0.33034500
C	2.05442800	-3.34410400	1.67083500
H	1.28441100	-2.57534400	1.71647000
H	1.57332400	-4.32053700	1.79244600
H	2.74537400	-3.19918900	2.50813500
C	3.87546800	-4.41040200	0.35232700
H	3.36952800	-5.37453500	0.46060000
H	4.45800100	-4.44500400	-0.57452300
H	4.56913300	-4.30792500	1.19317700
C	1.86655800	-3.57667500	-0.85120600
H	1.05907500	-2.84846900	-0.89272500
H	2.41837000	-3.55798300	-1.79869200
H	1.42376700	-4.57248200	-0.74279900
C	7.02521100	-0.44437100	-0.04062000
C	7.55498600	0.99240400	-0.17308100
H	7.20792300	1.46762500	-1.09640300
H	7.24657000	1.61610300	0.67210600
H	8.64899300	0.98307800	-0.19623100
C	7.58905300	-1.05054000	1.26303900
H	7.27477200	-2.08986100	1.39537800
H	8.68438800	-1.03202200	1.25158800
H	7.24535000	-0.48390500	2.13403500
C	7.53360000	-1.26212200	-1.24790600
H	8.62838900	-1.24858000	-1.28636500
H	7.21514700	-2.30711600	-1.19202000
H	7.15285200	-0.84589500	-2.18608400
C	-6.79992200	-0.69426400	0.08215100
C	-7.08148500	-1.25483200	1.49332900
H	-6.59277600	-0.64256600	2.25764400
H	-8.15831800	-1.26156500	1.69500200
H	-6.71504800	-2.27970700	1.60177900

C	-7.50633700	-1.57555500	-0.97083700
H	-7.32519700	-1.19394300	-1.98069100
H	-7.15319100	-2.61017500	-0.93614200
H	-8.58794400	-1.58639500	-0.79711500
C	-7.38908700	0.72300500	-0.00072900
H	-7.23884400	1.16571600	-0.99083800
H	-8.46670300	0.68760500	0.18625500
H	-6.94494200	1.38944300	0.74560700
C	-2.52277900	-3.42745200	-0.28497700
C	-3.51210200	-4.56488100	0.02453200
H	-4.00540400	-4.42709300	0.99223300
H	-4.28361600	-4.66324000	-0.74666700
H	-2.96570700	-5.51207700	0.06650200
C	-1.46185400	-3.40792400	0.83670200
H	-0.93851100	-4.36949600	0.87583500
H	-0.73116700	-2.61936000	0.67143900
H	-1.93903300	-3.24178600	1.80840700
C	-1.86165800	-3.74861800	-1.64419200
H	-2.61593100	-3.79060400	-2.43760800
H	-1.12013000	-2.99566100	-1.90798800
H	-1.36232100	-4.72263300	-1.59872100
H	0.19732100	3.46478500	0.72755700
H	-0.12939000	2.94591800	-2.25376500

PO + H_2O-Co^{III}-OH middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2153.158834

Thermal correction to Gibbs Free Energy (a.u.): 0.862457

No imaginary frequency

C	5.11807500	-1.44456600	0.23917600
C	5.69934500	-0.15684200	0.16307800
C	3.75529000	-1.69876200	0.24398000
H	5.79105500	-2.29013100	0.30047600
C	4.82817500	0.90928400	0.08951300
C	2.85530200	-0.58073300	0.15264300
C	3.42523600	0.72679600	0.07183700
H	5.20061100	1.92719600	0.03705100
O	1.56188800	-0.79685300	0.14506600
C	2.61691300	1.91368000	0.01321600
Co	0.22068900	0.44243700	-0.37974100
N	1.33817700	1.95027600	-0.13929000
H	3.15657300	2.85701200	0.10977000
N	-1.08255100	1.68227400	-0.99632000
C	0.54377000	3.18266100	-0.11869300
C	-2.34982100	1.45281300	-1.01219000
C	-0.49973100	3.00651600	-1.23815000
C	1.30916100	4.49621900	-0.25798600
H	-3.02536900	2.27966300	-1.22821900
C	-2.97394600	0.18693800	-0.74645500
C	-1.47001700	4.18548500	-1.29793300
C	0.32641500	5.67514800	-0.31197100
H	1.91285100	4.47400300	-1.17588500
H	2.00000700	4.62616500	0.58232200
C	-4.38002700	0.18312900	-0.61601000
C	-2.22096500	-1.01731200	-0.63127600
C	-0.69267800	5.50135200	-1.44381700
H	-2.15810400	4.06636600	-2.14266500
H	-2.06212800	4.19911000	-0.37691100
H	0.87988000	6.61215700	-0.43565500
H	-0.20596100	5.74309600	0.64536400
C	-5.07656300	-0.97568200	-0.33658000
H	-4.89694200	1.13052100	-0.72654700
C	-2.93315600	-2.22837600	-0.35308100
O	-0.91622700	-1.04220400	-0.80565300
H	-0.16849700	5.51578300	-2.40943600
H	-1.39344900	6.34279300	-1.45475100
C	-4.31321800	-2.15836700	-0.21318700

H	-4.84683800	-3.07296400	0.01117200
O	-0.40637300	0.61801900	1.32612600
H	0.03540500	-0.11229000	1.78232800
O	0.83198300	0.07648200	-2.35259400
H	0.11257100	-0.58632700	-2.40099400
H	1.63155500	-0.45052300	-2.19790000
C	-2.96125400	1.96338400	2.31119000
C	-2.00470700	2.86014900	2.96885800
O	-2.52883300	3.18751700	1.66915100
H	-2.52844300	1.07631100	1.85431700
H	-0.95625800	2.56871100	2.97750000
H	-2.33863100	3.51513000	3.77433900
C	-4.41308100	1.90815800	2.70221000
H	-4.58079900	1.10518800	3.42881400
H	-4.74040400	2.85495600	3.14209800
H	-5.03548300	1.69563000	1.82726100
C	3.20626200	-3.12917100	0.36398000
C	2.42229700	-3.25706500	1.68945000
H	1.61279000	-2.53009600	1.73741800
H	1.99155800	-4.26023500	1.78068900
H	3.09046400	-3.09466500	2.54196600
C	4.32876100	-4.18188800	0.38297200
H	3.88381100	-5.17836700	0.46374900
H	4.92758000	-4.15981700	-0.53392000
H	5.00085500	-4.05275600	1.23759300
C	2.28680100	-3.45689400	-0.83529700
H	1.42695200	-2.79061000	-0.86545600
H	2.84347300	-3.37180400	-1.77649400
H	1.92060200	-4.48626700	-0.75688100
C	7.22503800	-0.01246500	0.17111700
C	7.66452500	1.45792300	0.08498200
H	7.31174300	1.93120300	-0.83713800
H	7.29313300	2.04046700	0.93431200
H	8.75719800	1.51966900	0.09280900
C	7.79221900	-0.61129800	1.47674000
H	7.54086200	-1.67098600	1.57803800
H	8.88425700	-0.52356400	1.49702400
H	7.38941500	-0.08782400	2.34953200
C	7.81940800	-0.76685000	-1.03818600
H	8.91188400	-0.68273000	-1.04462300
H	7.56707200	-1.83090600	-1.01451000
H	7.43818900	-0.35380100	-1.97754600
C	-6.59592600	-1.02807200	-0.14296100
C	-6.90836600	-1.49442300	1.29586000
H	-6.48427900	-0.79925700	2.02734900
H	-7.99092800	-1.54627400	1.45785800
H	-6.49156700	-2.48556700	1.49701800
C	-7.21473500	-2.02119200	-1.15040800
H	-7.01006500	-1.70734800	-2.17893100
H	-6.81348000	-3.03062900	-1.02338400
H	-8.30103900	-2.07508200	-1.01771400
C	-7.25298600	0.34485600	-0.35864900
H	-7.07029000	0.72530000	-1.36885500
H	-8.33609800	0.26228700	-0.22472100
H	-6.88808000	1.08703100	0.35864700
C	-2.17921800	-3.55817000	-0.20048700
C	-3.12125500	-4.72637900	0.14006100
H	-3.64928700	-4.56432500	1.08560000
H	-3.86445900	-4.90029400	-0.64540400
H	-2.53211000	-5.64273600	0.24473800
C	-1.14706600	-3.43847200	0.94204800
H	-0.59577100	-4.37902100	1.05101400
H	-0.43611700	-2.63966400	0.74197200
H	-1.65200400	-3.22987700	1.89162800
C	-1.46636200	-3.90879000	-1.52586400
H	-2.19625300	-4.03030900	-2.33376700
H	-0.76072200	-3.12822900	-1.80751900
H	-0.91580400	-4.85034800	-1.42079700
H	-0.01333500	3.16850900	0.82548100

H	0.05165900	2.93767000	-2.18749300

PO + H_2O-Co^{III}-OH middle carbon

PO + H_2O-Co^{III}-OH = PO-OH-Co^{III}-H_2O

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2153.185342

Thermal correction to Gibbs Free Energy (a.u.): 0.868406

No imaginary frequency

C	4.79933600	-1.73652000	-0.00585900
C	5.49166900	-0.49995900	-0.02974100
C	3.42451000	-1.87524300	-0.09595500
H	5.39223200	-2.63509100	0.10770400
C	4.72057000	0.63718800	-0.11979600
C	2.63586700	-0.68600200	-0.26893700
C	3.30850400	0.57315400	-0.22809100
H	5.17739400	1.62124200	-0.10323400
O	1.35082200	-0.79685500	-0.47931100
C	2.60443400	1.81810900	-0.24421800
Co	0.04029700	0.58569900	-0.45475900
N	1.32192800	1.98216800	-0.30193400
H	3.23038400	2.70737100	-0.16462600
N	-1.23549500	1.97641400	-0.70335800
C	0.68263300	3.29600700	-0.13702100
C	-2.51989500	1.83261600	-0.66327600
C	-0.58325100	3.25981600	-1.00209000
C	1.53676400	4.52296500	-0.45428800
H	-3.14385000	2.72030700	-0.77260800
C	-3.22102000	0.59884000	-0.47770700
C	-1.42397900	4.52166000	-0.80744200
C	0.70335600	5.80025100	-0.27255400
H	1.90999300	4.45578900	-1.48541800
H	2.40653100	4.56444000	0.20836900
C	-4.61180500	0.67316800	-0.22783400
C	-2.55740700	-0.66098800	-0.57987500
C	-0.57793700	5.76676600	-1.11287500
H	-2.30204600	4.50798700	-1.46159000
H	-1.78652500	4.55725200	0.22830600
H	1.30600200	6.67622600	-0.53438700
H	0.43958900	5.90428900	0.78785200
C	-5.37346500	-0.46225100	-0.05457400
H	-5.05969800	1.65932300	-0.16319200
C	-3.34573100	-1.85009200	-0.42519200
O	-1.27669300	-0.75489100	-0.83945900
H	-0.31404300	5.76739200	-2.17901300
H	-1.17277800	6.66912100	-0.93688900
C	-4.70000700	-1.70281000	-0.16724600
H	-5.28995500	-2.60070800	-0.03604000
O	-0.04403500	0.38400600	1.38043900
H	1.25940000	1.66487200	2.16154800
O	0.27924700	0.45167700	-2.53607100
H	-0.50106700	-0.13504400	-2.57919600
H	1.02079300	-0.17535600	-2.45261500
C	-0.96974600	0.98037500	2.25409300
C	-0.14273600	1.61008500	3.39679100
O	0.98079300	2.28937700	2.85867200
H	-1.52108000	1.79430800	1.76111400
H	0.17863900	0.81430900	4.08871700
H	-0.74202700	2.33057000	3.96452600
C	-1.96708600	-0.03958000	2.80470500
H	-1.42276500	-0.87511100	3.25627800
H	-2.60744800	0.41390100	3.57204500
H	-2.60730200	-0.43749400	2.01676100
C	2.73678500	-3.23938400	0.06511500
C	1.87877400	-3.18601100	1.35132600
H	1.16778500	-2.36020900	1.32080600
H	1.32306600	-4.12189200	1.47564500
H	2.52328600	-3.05485000	2.22721900
C	3.75375500	-4.38355600	0.22309100

H	3.21406700	-5.32701800	0.34985000
H	4.39744800	-4.48564700	-0.65762800
H	4.39085800	-4.25027200	1.10338800
C	1.85191400	-3.57462300	-1.15700000
H	1.04158900	-2.85707200	-1.26398300
H	2.45034500	-3.57754400	-2.07570600
H	1.41758200	-4.57335200	-1.03710300
C	7.02031900	-0.48707300	0.07559100
C	7.58771900	0.94077400	0.03288700
H	7.32657300	1.45058700	-0.90025900
H	7.22253100	1.54543600	0.86928500
H	8.67964500	0.90824000	0.09969400
C	7.45192100	-1.13975800	1.40706300
H	7.10836800	-2.17558600	1.48012500
H	8.54401300	-1.14332100	1.49638400
H	7.03920900	-0.59027800	2.25887900
C	7.62169000	-1.28268200	-1.10337900
H	8.71553800	-1.29452700	-1.04041800
H	7.27656400	-2.32060900	-1.10823400
H	7.33803900	-0.83184600	-2.05975100
C	-6.87493100	-0.44220300	0.25027300
C	-7.12957300	-1.13622600	1.60623700
H	-6.60018000	-0.61752600	2.41161000
H	-8.19957200	-1.13700400	1.84203100
H	-6.78873300	-2.17549000	1.59868800
C	-7.63801100	-1.19359700	-0.86222600
H	-7.47762000	-0.71496100	-1.83354200
H	-7.31201200	-2.23435900	-0.94486700
H	-8.71375400	-1.19643500	-0.65445800
C	-7.42642000	0.99022600	0.33062100
H	-7.29463300	1.52729400	-0.61442000
H	-8.49826400	0.96304200	0.54983000
H	-6.93979200	1.56586400	1.12462100
C	-2.68720900	-3.23470500	-0.51150500
C	-3.70166900	-4.37282400	-0.30463600
H	-4.17524900	-4.32488500	0.68147900
H	-4.48814800	-4.36957200	-1.06721900
H	-3.18057100	-5.33266300	-0.37182400
C	-1.60849300	-3.35375200	0.58656200
H	-1.10941100	-4.32654500	0.51679600
H	-0.86066900	-2.57011400	0.48816600
H	-2.06291900	-3.27567600	1.57990500
C	-2.04804100	-3.43014800	-1.90500800
H	-2.80778100	-3.36079600	-2.69158800
H	-1.28005600	-2.68015800	-2.09038300
H	-1.58343200	-4.42014400	-1.96814200
H	0.38003700	3.34282700	0.91824700
H	-0.26089200	3.20464400	-2.05231900

PO-Co^{III}-Cl + H$_2$O-Co^{III}-OH terminal carbon

PO-Co^{III}-Cl + H$_2$O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H$_2$O
transition state
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -4421.254940
Thermal correction to Gibbs Free Energy (a.u.): 1.644661
Imaginary frequencies: -432.09

C	-1.24633900	6.54250500	-0.85658400
C	-1.19657300	6.91032400	0.51099300
C	-0.50098500	5.52663600	-1.42973500
H	-1.91024100	7.10797800	-1.49832200
C	-0.31140500	6.21223200	1.30309200
C	0.36132900	4.74600100	-0.57564200
C	0.46737900	5.14539800	0.79478100
H	-0.19155500	6.46090900	2.35291500
O	1.00601400	3.73837800	-1.07872700
C	1.38290100	4.52335800	1.70381400
Co	1.91804500	2.40853300	-0.08760500
N	2.09905900	3.47829500	1.46706400

H	1.46974800	4.99998900	2.68141500
N	2.77479700	1.03842700	0.92042100
Cl	3.94482100	3.13194800	-0.84078000
C	3.02143500	2.87947700	2.43136000
C	3.33651500	-0.00839600	0.42544300
C	2.77392400	1.35966200	2.34667000
C	2.92065500	3.36683000	3.87649100
H	3.85778900	-0.68896100	1.09631700
C	3.34093600	-0.37141200	-0.96501000
C	3.74815800	0.57986000	3.22557500
C	3.89368100	2.58496700	4.77197800
H	1.89201300	3.22747900	4.23587000
H	3.14348900	4.43744600	3.93489900
C	4.19870200	-1.42452000	-1.35208500
C	2.51651600	0.29706500	-1.92188100
C	3.65869000	1.07260000	4.67587600
H	3.52254700	-0.48846400	3.18315100
H	4.76914500	0.72007900	2.84580700
H	3.79403600	2.92128300	5.80967900
H	4.92363900	2.80988600	4.46511100
C	4.28969200	-1.84851500	-2.66307600
H	4.81340500	-1.87295000	-0.58086400
C	2.60171000	-0.13981500	-3.29375000
O	1.68938200	1.24457000	-1.59445800
H	2.66376900	0.83352800	5.07579300
H	4.38301800	0.53388300	5.29736500
C	3.47396700	-1.17140400	-3.60429900
H	3.55008600	-1.47662100	-4.64085000
C	1.77964200	0.57640200	-4.37405000
C	2.04654700	0.01218100	-5.78050000
H	1.43208600	0.55387400	-6.50636200
H	3.09299600	0.13519900	-6.07784100
H	1.78963300	-1.05045600	-5.85906100
C	0.27068300	0.40761800	-4.08546800
H	-0.02739800	-0.63994100	-4.20721400
H	0.02575100	0.72295200	-3.07294000
H	-0.31944300	1.00526400	-4.78838800
C	2.15690900	2.07593700	-4.39123800
H	1.98771900	2.54134400	-3.42286100
H	3.21489100	2.19609000	-4.64518000
H	1.56140500	2.60064600	-5.14678100
C	5.25069700	-2.94569200	-3.13456300
C	4.47202400	-4.06353500	-3.86144800
H	3.90343900	-3.67539300	-4.71150700
H	5.16020600	-4.82639200	-4.24207000
H	3.76740700	-4.55316200	-3.18125000
C	6.28147600	-2.33107900	-4.10699500
H	6.98497400	-3.09402800	-4.45965200
H	5.79312100	-1.89348900	-4.98236800
H	6.85026000	-1.53772400	-3.61300600
C	6.01316300	-3.58521600	-1.96255100
H	6.62495900	-2.85158800	-1.42898500
H	5.32930400	-4.04989400	-1.24298200
H	6.68177300	-4.36776600	-2.33467500
C	-0.54732000	5.24935100	-2.94042400
C	-1.51806400	6.19263800	-3.67252800
H	-2.55059700	6.06940600	-3.32693800
H	-1.23781300	7.24440000	-3.55349500
H	-1.49858000	5.96604200	-4.74323300
C	0.86453500	5.47215100	-3.53116200
H	1.16498700	6.51851900	-3.41000200
H	1.60260900	4.84031100	-3.03742700
H	0.86575400	5.24031800	-4.60258700
C	-1.00739900	3.80184700	-3.21923800
H	-0.29415200	3.08871800	-2.81465000
H	-1.99157100	3.61535000	-2.77366200
H	-1.08919700	3.63644600	-4.29972700
C	-2.08782500	8.04684700	1.02198600
C	-3.56974200	7.68221400	0.78481800

H	-4.22704100	8.48721900	1.13346300
H	-3.77820900	7.51586000	-0.27604700
H	-3.83247000	6.76617800	1.32380600
C	-1.89074900	8.30200500	2.52487600
H	-2.13182700	7.41420500	3.11859000
H	-0.86105400	8.59672500	2.75167000
H	-2.54869900	9.11262100	2.85437600
C	-1.75533700	9.35037100	0.26353400
H	-1.91167800	9.24173000	-0.81352700
H	-2.39028000	10.17301300	0.61237800
H	-0.70955600	9.63219200	0.42127100
C	2.38032100	-2.79870200	3.65994900
C	3.33731600	-3.19538700	2.70169300
C	1.05209500	-2.49548200	3.37806000
H	2.70253200	-2.72106300	4.68731900
C	2.89948100	-3.26976100	1.39208900
C	0.60274700	-2.60711100	2.01978600
C	1.56551200	-2.98433200	1.03181900
H	3.58156700	-3.55432000	0.59749000
O	-0.65612000	-2.36637700	1.72911300
C	1.24287800	-3.06947600	-0.36750000
Co	-1.55473500	-2.85609100	0.11745800
N	0.05479300	-3.02103400	-0.86694000
H	2.08972600	-3.18041000	-1.04368000
N	-2.42920900	-3.47053900	-1.45834200
C	-0.22103100	-3.09470300	-2.30606800
C	-3.68148300	-3.29756100	-1.71251400
C	-1.46512200	-3.99255600	-2.43493900
C	0.92015000	-3.59549600	-3.18402800
H	-4.05327500	-3.57136000	-2.70014700
C	-4.65364300	-2.74437400	-0.81034000
C	-1.93315100	-4.08560500	-3.88632000
C	0.46037100	-3.71673500	-4.64234200
H	1.25519700	-4.57565000	-2.81760600
H	1.76702000	-2.90986800	-3.12365000
C	-5.93057200	-2.44988800	-1.33919200
C	-4.35738100	-2.50174200	0.56184100
C	-0.78800600	-4.59574500	-4.77515900
H	-2.79459900	-4.75711800	-3.97069900
H	-2.25473400	-3.09241000	-4.22605700
H	1.27761500	-4.12020300	-5.24902900
H	0.24423000	-2.71603200	-5.03531800
C	-6.92316400	-1.89193400	-0.55839500
H	-6.10378700	-2.66445900	-2.38830500
C	-5.36945900	-1.90753500	1.37894900
O	-3.18912100	-2.82521800	1.08988300
H	-0.54218000	-5.62673800	-4.48718500
H	-1.12167500	-4.63208200	-5.81727000
C	-6.59859700	-1.63322100	0.79224900
H	-7.36373100	-1.18070000	1.40928800
O	-1.48511200	-4.77846900	0.84909400
H	-0.87402700	-4.68750400	1.59819500
H	-2.37339800	-4.67274600	1.24361200
C	-5.08682600	-1.56951500	2.85084400
C	-6.28112600	-0.87105300	3.52446000
H	-6.02231100	-0.64148600	4.56242500
H	-6.53475200	0.07309800	3.03140100
H	-7.17432300	-1.50432900	3.54109100
C	-4.79985400	-2.86719300	3.63810000
H	-5.67210800	-3.52942000	3.61625500
H	-3.94666000	-3.39931900	3.21912300
H	-4.57808500	-2.63211900	4.68473000
C	-3.87603300	-0.61264600	2.93763100
H	-2.98194300	-1.07069900	2.51892500
H	-4.08403100	0.31794800	2.39815800
H	-3.67458600	-0.35623100	3.98304700
C	-8.31879000	-1.53760500	-1.08366300
C	-9.38250200	-2.31405700	-0.27725800
H	-9.33949100	-2.07204900	0.78857200

H	-10.38802800	-2.06725600	-0.63478900
H	-9.23723300	-3.39398300	-0.38146900
C	-8.55702000	-0.02043000	-0.92101300
H	-9.55305900	0.25134600	-1.28691900
H	-8.49058300	0.29031500	0.12559200
H	-7.81584600	0.55183800	-1.48760500
C	-8.48207500	-1.89592500	-2.56942900
H	-7.77158400	-1.34915200	-3.19774200
H	-8.34386600	-2.96794000	-2.74433400
H	-9.48991400	-1.63301900	-2.90453700
C	0.08771200	-2.05755300	4.49282300
C	0.76256700	-2.05339600	5.87637700
H	1.12338000	-3.04691000	6.16245000
H	1.60399300	-1.35419900	5.92227600
H	0.03323600	-1.73808300	6.62846800
C	-0.40627800	-0.62120400	4.21588000
H	0.43543900	0.07800700	4.19331800
H	-0.93106500	-0.56191500	3.26512200
H	-1.09399900	-0.29821200	5.00498800
C	-1.11720600	-3.02329500	4.56492700
H	-1.67915400	-3.01548600	3.63270900
H	-0.77692000	-4.04455300	4.77391400
H	-1.79126900	-2.72399900	5.37464500
C	4.78097400	-3.56304800	3.07581600
C	4.97437200	-5.08140400	2.86939500
H	5.99613500	-5.38094900	3.12786900
H	4.28107800	-5.65024900	3.49719300
H	4.79265700	-5.36424300	1.82789900
C	5.78053400	-2.80281900	2.17893500
H	5.65211200	-3.05066800	1.12232400
H	5.66848800	-1.72010600	2.29097200
H	6.80850100	-3.06464700	2.45058100
C	5.10478700	-3.22200900	4.54051600
H	4.48637000	-3.79218300	5.24059100
H	6.14984600	-3.46718700	4.75231600
H	4.96381500	-2.15596200	4.74763500
C	-0.85509400	1.57068600	-0.15992400
C	-0.46682800	0.23509100	0.29058300
O	0.23879700	1.87729500	0.69574400
H	-0.63780900	1.77316300	-1.20664800
H	0.36708000	-0.23268400	-0.20377900
H	-0.72340800	-0.07730000	1.28718800
C	-2.15984800	2.18285400	0.29692200
H	-2.11675500	3.26843100	0.17088500
H	-2.99608500	1.80017400	-0.30024200
H	-2.34421600	1.96052000	1.35268100
O	-1.72834800	-1.11555600	-0.49824400
H	-2.57191400	-0.80139200	-0.14102800
H	4.03232000	3.06631600	2.04532000
H	1.74736300	1.18271700	2.69559700
H	-1.17815500	-4.99423100	-2.08378500
H	-0.51021200	-2.08151000	-2.61093900

PO-Co^{III}-Cl + H_2O-Co^{III}-OH terminal carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

reactant complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4421.271076

Thermal correction to Gibbs Free Energy (a.u.): 1.641958

No imaginary frequency

C	3.69991800	5.64708000	-0.99342200
C	3.87510400	5.94364200	0.38181300
C	3.61816100	4.37118100	-1.52377500
H	3.63691800	6.48442200	-1.67680900
C	4.00622000	4.86750800	1.23122500
C	3.66492000	3.25281700	-0.61473200
C	3.91068300	3.53303700	0.76649400
H	4.18304200	5.01548300	2.29180400
O	3.48940100	2.05257000	-1.08060300

C	4.11798900	2.49420600	1.72919100
Co	3.24148900	0.48339500	-0.05588200
N	3.97566700	1.22813500	1.52631000
H	4.43426200	2.82635600	2.71896300
N	2.89508100	-1.06090400	0.99638900
Cl	5.24874600	-0.33068100	-0.65779800
C	4.22812100	0.20139300	2.53819800
C	2.60806300	-2.22624800	0.52567300
C	3.05040100	-0.78460100	2.42651600
C	4.40551500	0.67794000	3.97914600
H	2.49611600	-3.05415500	1.22230800
C	2.40727000	-2.54184400	-0.85861300
C	3.24155900	-1.99116300	3.34135300
C	4.59064000	-0.52630500	4.91543500
H	3.52107000	1.25347400	4.28456800
H	5.27110000	1.34415300	4.05770400
C	2.28608600	-3.90962300	-1.19426000
C	2.30304800	-1.52717600	-1.85777500
C	3.43165300	-1.52231100	4.78999200
H	2.37353800	-2.65089800	3.27973100
H	4.12067400	-2.56007700	3.01055400
H	4.68521000	-0.17943300	5.94995300
H	5.53179800	-1.03336000	4.66541300
C	2.06977900	-4.32459300	-2.49204700
H	2.39313100	-4.62950200	-0.39208700
C	2.06660900	-1.94860700	-3.21504300
O	2.37493000	-0.25713900	-1.57971700
H	2.50436900	-1.04572300	5.13536700
H	3.59998100	-2.38699200	5.44147700
C	1.96982900	-3.30688100	-3.47346100
H	1.81181900	-3.61736300	-4.49880900
C	1.95327300	-0.90373400	-4.33342900
C	1.73779900	-1.54928900	-5.71356600
H	1.66270900	-0.76126300	-6.46923600
H	2.57283500	-2.19842600	-5.99666700
H	0.81377000	-2.13673300	-5.75779800
C	0.74227800	0.01730900	-4.06052800
H	-0.19132000	-0.55343400	-4.10958000
H	0.81012800	0.47817600	-3.07730100
H	0.69107900	0.81020500	-4.81434600
C	3.25781000	-0.07667900	-4.39972700
H	3.47202100	0.40762700	-3.44946400
H	4.10350900	-0.72513400	-4.65080900
H	3.17367700	0.69066600	-5.17739400
C	1.97410200	-5.79648200	-2.90752100
C	0.62566300	-6.06120200	-3.61151900
H	0.49049500	-5.41803700	-4.48586500
H	0.56647600	-7.10139000	-3.95035500
H	-0.21055400	-5.87894000	-2.92885500
C	3.12898000	-6.12587300	-3.87867900
H	3.08354600	-7.17513600	-4.19171300
H	3.08552300	-5.50501500	-4.77811400
H	4.09681800	-5.94989000	-3.39964200
C	2.07224000	-6.74238400	-1.69961100
H	3.02510300	-6.63028600	-1.17337400
H	1.26170800	-6.56584800	-0.98354000
H	1.99674800	-7.78205600	-2.03297500
C	3.51327300	4.13282600	-3.03833800
C	3.50821800	5.45196500	-3.83065900
H	2.64302700	6.07737000	-3.58400200
H	4.41753000	6.03742900	-3.65955900
H	3.45786800	5.22663200	-4.90041300
C	4.73578400	3.30661900	-3.50234700
H	5.66041700	3.86850000	-3.33189700
H	4.80094500	2.36052800	-2.96507400
H	4.66020200	3.09489100	-4.57505200
C	2.21214100	3.37687900	-3.38482700
H	2.21835000	2.38217700	-2.94674700
H	1.33537500	3.92560900	-3.02146300

H	2.11692200	3.27273400	-4.47150200
C	3.93212000	7.40467700	0.83927300
C	2.60821300	8.10842600	0.46886500
H	2.63012400	9.15973200	0.77777400
H	2.42499400	8.08052400	-0.60917200
H	1.76100800	7.62285300	0.96397500
C	4.13176900	7.52455100	2.35856800
H	3.31538500	7.04772900	2.91081900
H	5.07452100	7.06895900	2.67833600
H	4.15808700	8.57986400	2.64807900
C	5.10625900	8.12323400	0.13932300
H	5.00161500	8.10268200	-0.94920300
H	5.15597000	9.17294000	0.45041900
H	6.05756300	7.64439700	0.39167500
C	-0.12578000	-3.31963500	3.72796100
C	0.30534300	-4.31566100	2.82563700
C	-0.88265700	-2.20635700	3.37717900
H	0.14861000	-3.43027900	4.76643800
C	-0.04003500	-4.13155300	1.49766800
C	-1.28631100	-2.05691300	2.00636500
C	-0.81526100	-3.03397500	1.07078600
H	0.27242200	-4.84594100	0.74249000
O	-2.05602500	-1.05514800	1.65705900
C	-1.09207200	-2.94049000	-0.34191400
Co	-3.14731300	-1.02142000	0.07737500
N	-1.97079000	-2.16214200	-0.87095700
H	-0.50033500	-3.58894900	-0.98835800
N	-4.25613800	-1.09941700	-1.46558300
C	-2.23971900	-2.08511200	-2.30775100
C	-5.18595000	-0.24686400	-1.72976800
C	-3.77764200	-2.09982800	-2.42706800
C	-1.60172900	-3.16227900	-3.17652600
H	-5.67310300	-0.29421100	-2.70425700
C	-5.63794700	0.80483300	-0.86156200
C	-4.21833800	-1.92693500	-3.88044100
C	-2.04702500	-3.00308700	-4.63567700
H	-1.90259400	-4.15193700	-2.80702900
H	-0.51317800	-3.10473500	-3.11068800
C	-6.53618500	1.74684700	-1.41014800
C	-5.19971200	0.91537600	0.48900200
C	-3.57454500	-3.00749600	-4.76311500
H	-5.30915100	-1.98629100	-3.96142900
H	-3.91670800	-0.93097500	-4.23009700
H	-1.61133900	-3.80497400	-5.24110000
H	-1.65112000	-2.06023900	-5.03338700
C	-6.99552500	2.82195600	-0.67516900
H	-6.84542600	1.60682300	-2.44060600
C	-5.64719300	2.03750500	1.25504000
O	-4.41922800	0.00856200	1.04606900
H	-3.96168000	-3.99171700	-4.46672500
H	-3.87229900	-2.85457400	-5.80568600
C	-6.52022000	2.93304400	0.65040200
H	-6.85771000	3.78242800	1.23009700
O	-4.22112000	-2.59671300	0.94452100
H	-3.65477500	-2.88745000	1.67617100
H	-4.82520400	-1.93784900	1.33990200
C	-5.16310100	2.23906500	2.69957000
C	-5.67990400	3.55571800	3.30614300
H	-5.29219900	3.65792000	4.32434300
H	-5.34516100	4.42804300	2.73511100
H	-6.77283200	3.58148700	3.36760300
C	-5.68308400	1.08316100	3.58237000
H	-6.77820700	1.08359100	3.60460800
H	-5.34283200	0.11970900	3.20493200
H	-5.32215100	1.19767100	4.61045800
C	-3.61764000	2.28755600	2.73507900
H	-3.18485000	1.35712000	2.37214600
H	-3.24824100	3.11603200	2.11970900
H	-3.27138500	2.45221300	3.76131900

C	-7.96092400	3.87769600	-1.22557000
C	-9.24108600	3.90205400	-0.36227900
H	-9.02000600	4.14059300	0.68206100
H	-9.94144900	4.65702400	-0.73623000
H	-9.74198100	2.92898300	-0.38397900
C	-7.28525900	5.26556200	-1.18023500
H	-7.96359200	6.03489200	-1.56538700
H	-7.00678700	5.54701600	-0.16060600
H	-6.37593500	5.27363400	-1.78933700
C	-8.36520400	3.58556500	-2.67951700
H	-7.49801800	3.58605200	-3.34774200
H	-8.87054300	2.61862600	-2.77161700
H	-9.05672100	4.35624100	-3.03367300
C	-1.31461500	-1.17652100	4.43358600
C	-0.79191600	-1.52766100	5.83788500
H	-1.17834900	-2.48841500	6.19360500
H	0.30203900	-1.56277000	5.87399500
H	-1.12014700	-0.75943200	6.54445600
C	-0.75924300	0.21771200	4.06801100
H	0.33552700	0.20063700	4.03652000
H	-1.13124200	0.54668600	3.09978900
H	-1.06330500	0.95408500	4.81998700
C	-2.85735700	-1.12230400	4.50895800
H	-3.28241000	-0.82742000	3.55140000
H	-3.25959400	-2.10073200	4.79735900
H	-3.17385100	-0.39518400	5.26442300
C	1.06419500	-5.57161800	3.28162000
C	0.12238200	-6.78882100	3.14742400
H	0.62615500	-7.70783400	3.46754600
H	-0.77286900	-6.65601200	3.76315800
H	-0.20121900	-6.92319100	2.11063900
C	2.31143500	-5.80723800	2.40458000
H	2.05066100	-5.95209000	1.35329100
H	3.00864300	-4.96642900	2.47106800
H	2.84098300	-6.70765900	2.73310700
C	1.52732300	-5.47133100	4.74543800
H	0.68335700	-5.39566700	5.43771200
H	2.09175800	-6.36921700	5.01476400
H	2.17993700	-4.60673100	4.90549700
C	0.59632200	1.91509700	-0.31122500
C	0.22279800	0.61914100	0.24253200
O	1.51545700	1.22761600	0.60398000
H	0.97852900	1.91575900	-1.32499400
H	0.31372900	-0.25763000	-0.38132500
H	-0.45082900	0.54539800	1.08286900
C	0.06839600	3.21994700	0.20651200
H	0.84194600	3.99169100	0.14918000
H	-0.78161300	3.53704800	-0.40708500
H	-0.26448600	3.12467200	1.24405200
O	-2.31787000	0.43817400	-0.64955600
H	-2.48822900	1.14014800	-0.00650800
H	5.13060300	-0.33195400	2.21147600
H	2.14521900	-0.24358000	2.73709800
H	-4.11825100	-3.07931100	-2.06072600
H	-1.89499400	-1.09140500	-2.62064500

PO-Co^{III}-Cl + H_2O-Co^{III}-OH terminal carbon

PO-Co^{III}-Cl + H_2O-Co^{III}-OH = Cl-Co^{III}-PO-OH-Co^{III}-H_2O

product complex

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -4421.273812

Thermal correction to Gibbs Free Energy (a.u.): 1.647098

No imaginary frequency

C	-5.77957400	3.29202100	-0.59788700
C	-5.95678000	3.67994100	0.75256200
C	-4.55251800	3.11700500	-1.21415900
H	-6.67247400	3.12847900	-1.18864200
C	-4.80906800	3.90852000	1.48147000
C	-3.35444600	3.31124500	-0.43221300

C	-3.52055800	3.72993200	0.92744700
H	-4.86574900	4.22759500	2.51769600
O	-2.19745000	3.12929400	-0.98647000
C	-2.40724100	4.00787900	1.78582900
Co	-0.57867500	2.88241800	-0.03595000
N	-1.16600700	3.80077100	1.51260900
H	-2.66090800	4.43073400	2.75943000
N	1.04597400	2.58176200	0.92225100
Cl	0.29585800	4.86207700	-0.86178400
C	-0.06652500	4.05480900	2.44141000
C	2.18643700	2.30696700	0.39612300
C	0.84137500	2.80803900	2.34964800
C	-0.44646100	4.34387500	3.89371900
H	3.06347800	2.24308000	1.03932300
C	2.41761000	2.08003300	-1.00686000
C	2.09549600	2.95206600	3.20742400
C	0.81331500	4.49033400	4.75993400
H	-1.06526000	3.52115300	4.27673600
H	-1.04657400	5.25785400	3.95577500
C	3.75900600	2.06886400	-1.44518500
C	1.33761300	1.90895100	-1.93042000
C	1.71186000	3.25126000	4.66242000
H	2.69455600	2.03805600	3.15876000
H	2.71199000	3.77126800	2.81303000
H	0.52853400	4.67358500	5.80183000
H	1.37832000	5.37140000	4.42781800
C	4.09563300	1.90017100	-2.77518200
H	4.52531000	2.24377300	-0.69915000
C	1.67987100	1.71889900	-3.32115900
O	0.09583400	1.89665900	-1.56027700
H	1.18150500	2.38510200	5.08177800
H	2.61657100	3.38695800	5.26652300
C	3.01832800	1.72866800	-3.68164100
H	3.26214900	1.62258700	-4.73202800
C	0.56111300	1.60697300	-4.36687700
C	1.10776300	1.49312300	-5.80059800
H	0.26891700	1.40727000	-6.49839200
H	1.68494400	2.37819200	-6.08661700
H	1.74369400	0.61126300	-5.94002700
C	-0.29989100	0.35288200	-4.09223100
H	0.27737000	-0.56042800	-4.28303200
H	-0.65331200	0.34211000	-3.06200800
H	-1.17068800	0.33716200	-4.75633800
C	-0.32070600	2.87591900	-4.30529800
H	-0.75800600	3.01077600	-3.31892000
H	0.27832400	3.76304200	-4.53283400
H	-1.12506000	2.80407100	-5.04606300
C	5.53365600	1.99008500	-3.30097700
C	5.89600300	0.73654900	-4.12615900
H	5.19708000	0.57766300	-4.95244600
H	6.89911500	0.83695400	-4.55516200
H	5.88760100	-0.16135900	-3.49927700
C	5.65735100	3.23916500	-4.20195000
H	6.67835400	3.34119700	-4.58783000
H	4.97751600	3.18138100	-5.05679500
H	5.40654200	4.14353400	-3.63993000
C	6.55701500	2.11480400	-2.15995900
H	6.39758500	3.02235400	-1.57020600
H	6.51236000	1.25329700	-1.48329800
H	7.57077400	2.15978900	-2.57022900
C	-4.44739500	2.76068800	-2.70464400
C	-5.82759000	2.55866100	-3.35438000
H	-6.38432000	1.73757600	-2.88877800
H	-6.44271300	3.46316700	-3.30423300
H	-5.69354300	2.31087500	-4.41242700
C	-3.74211000	3.92010500	-3.44540800
H	-4.34528100	4.83220600	-3.38005000
H	-2.76212400	4.12127200	-3.01404200
H	-3.61537400	3.67174900	-4.50591600

C	-3.64903200	1.45203800	-2.89454000
H	-2.63587400	1.56400200	-2.51659400
H	-4.13574400	0.62463300	-2.36428000
H	-3.60278700	1.19181900	-3.95876300
C	-7.37272100	3.83393000	1.31720200
C	-8.11730800	2.48457200	1.21612000
H	-9.13858500	2.57463900	1.60482600
H	-8.18243200	2.13855500	0.18043700
H	-7.59638100	1.71339100	1.79286100
C	-7.36143900	4.26579400	2.79236900
H	-6.84740500	3.53236800	3.42217000
H	-6.86869500	5.23451900	2.92372200
H	-8.38810200	4.36147200	3.16089700
C	-8.14193800	4.90173100	0.50894700
H	-8.21308500	4.63228600	-0.54872400
H	-9.16167200	5.01946700	0.89420500
H	-7.63619300	5.87037000	0.57180000
C	4.01350700	-0.25078500	3.55196600
C	4.86708700	0.27242500	2.55869600
C	2.93320500	-1.09561000	3.31131300
H	4.20469000	0.03280900	4.57555100
C	4.58306600	-0.08804400	1.25555000
C	2.67147300	-1.48462600	1.95866200
C	3.50636700	-0.94338300	0.93551500
H	5.18252300	0.29017000	0.43442900
O	1.68256500	-2.32210300	1.70177500
C	3.28338100	-1.19188000	-0.45925400
Co	1.22731700	-3.10094200	0.03554600
N	2.41809100	-2.01138800	-0.95841100
H	3.89850200	-0.61279400	-1.14584800
N	0.83273200	-3.94815100	-1.62411900
C	2.21152200	-2.15821300	-2.40789600
C	-0.28220700	-4.54450100	-1.88133700
C	1.85271500	-3.63593600	-2.63156200
C	3.38147700	-1.73972700	-3.29287500
H	-0.48148400	-4.85255200	-2.90774800
C	-1.31145500	-4.83514400	-0.92123300
C	1.49398900	-3.90539400	-4.09084600
C	3.06845200	-2.03413600	-4.76549500
H	4.28247400	-2.28511000	-2.97948100
H	3.57340800	-0.67282700	-3.17611500
C	-2.55518200	-5.28638800	-1.41984900
C	-1.08351300	-4.71278500	0.48144700
C	2.67020700	-3.49670200	-4.99226000
H	1.25902800	-4.96526300	-4.23930500
H	0.60100500	-3.32658000	-4.36012800
H	3.93770300	-1.77617700	-5.37863600
H	2.25199200	-1.37995400	-5.09092600
C	-3.59552700	-5.60454800	-0.57083700
H	-2.67177000	-5.36061200	-2.49547700
C	-2.14513000	-5.05972700	1.37359800
O	0.08263300	-4.30625900	0.96187700
H	3.52745500	-4.14958900	-4.78011100
H	2.40185700	-3.66102300	-6.04066900
C	-3.34495600	-5.48318400	0.81476200
H	-4.15433000	-5.73143500	1.48823800
O	2.61525400	-4.47637500	0.48174400
H	2.97306400	-4.07117400	1.29199700
H	1.95684500	-5.12221400	0.80766800
C	-1.96662200	-4.93634000	2.89439200
C	-3.23219000	-5.35725900	3.66164600
H	-3.05048300	-5.25020200	4.73502400
H	-4.09232500	-4.72814000	3.41110000
H	-3.49964700	-6.40266300	3.47481000
C	-0.81014500	-5.84502800	3.36814300
H	-1.02063000	-6.89357900	3.13140500
H	0.13095300	-5.56183500	2.89732900
H	-0.69007000	-5.76009400	4.45334700
C	-1.66428000	-3.46549400	3.25124900

H	-0.75521200	-3.12354500	2.76103600
H	-2.49311300	-2.81678600	2.95008000
H	-1.52997300	-3.36073300	4.33276700
C	-4.97633000	-6.06066900	-1.05384600
C	-5.28508900	-7.46036700	-0.47947700
H	-5.28352000	-7.46048300	0.61432200
H	-6.27314600	-7.79728100	-0.81033600
H	-4.54351900	-8.19180100	-0.81614200
C	-6.04202200	-5.05545300	-0.56448900
H	-7.03830400	-5.36493200	-0.89756000
H	-6.06280600	-4.98524300	0.52685800
H	-5.84401400	-4.05467400	-0.96044900
C	-5.05135700	-6.13840700	-2.58708500
H	-4.87026900	-5.16362100	-3.05120000
H	-4.32891100	-6.85473300	-2.99219100
H	-6.04915700	-6.46793300	-2.89116600
C	2.02445600	-1.55564000	4.46386500
C	2.54052900	-1.07927600	5.83439000
H	3.54095800	-1.46586900	6.05566000
H	2.56630100	0.01259500	5.90861300
H	1.86525700	-1.44254400	6.61465800
C	0.62086100	-0.94379200	4.26340200
H	0.67593700	0.14903900	4.26919700
H	0.18189400	-1.25789900	3.31911900
H	-0.05027300	-1.25506400	5.07093300
C	1.93731600	-3.09826900	4.51674200
H	1.50216500	-3.50365100	3.60518600
H	2.93382100	-3.53199700	4.66194500
H	1.31312400	-3.40737100	5.36194400
C	6.05930100	1.18373500	2.88394700
C	7.36601500	0.42543100	2.56432600
H	8.23871400	1.05052700	2.78287800
H	7.44155800	-0.48932400	3.16097100
H	7.41059700	0.14212900	1.50815100
C	5.99738800	2.46677300	2.02831300
H	6.05004600	2.24792900	0.95878800
H	5.07372300	3.02210400	2.21642400
H	6.84104400	3.12246500	2.26755500
C	6.08145700	1.60071000	4.36424100
H	6.19830400	0.74065500	5.03108100
H	6.92672800	2.27163900	4.54381900
H	5.16742900	2.13361800	4.64672300
C	-1.50704300	0.21571400	0.08451000
C	-0.20570700	-0.55013700	0.32379100
O	-1.34541800	1.37598500	0.81250800
H	-1.62104000	0.39847400	-0.99172500
H	0.62878000	-0.02073300	-0.12241400
H	-0.05215200	-0.68449500	1.39159100
C	-2.74117200	-0.53924000	0.59068700
H	-3.62229200	0.08640400	0.42795900
H	-2.91180700	-1.49227200	0.06466100
H	-2.65353100	-0.73605900	1.66482300
O	-0.20420100	-1.88084500	-0.31636600
H	-1.03254200	-2.32274800	-0.06499700
H	0.49953900	4.90010300	2.02780800
H	0.24331900	1.95590800	2.70000600
H	2.73824600	-4.22935300	-2.36367600
H	1.33095500	-1.55404300	-2.66040100

Isolated molecular and some intermediates of structure, energy etc.

A~B means that the chemical entity, A~B, is formed by A weakly interacting with B via intermolecular forces and/or hydrogen bonds.

H_2O

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -76.416603
Thermal correction to Gibbs Free Energy (a.u.): 0.003709

No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -76.4711362 a.u.

O	0.00000000	0.00000000	0.11919600
H	0.00000000	0.75933400	-0.47678200
H	0.00000000	-0.75933400	-0.47678200

PO
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -193.066994
Thermal correction to Gibbs Free Energy (a.u.): 0.059302
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -193.2056507 a.u.

C	-0.15201300	-0.03917900	0.49087800
C	1.04225200	0.61600300	-0.06065700
O	0.82637400	-0.78932400	-0.24349500
H	-0.15457600	-0.25524000	1.56158900
H	1.87095300	0.88338100	0.59481000
H	0.94782200	1.22394600	-0.96079800
C	-1.50818000	0.10018800	-0.14891400
H	-2.07762600	-0.82981400	-0.05252800
H	-2.08280100	0.90031900	0.33021300
H	-1.40712400	0.32992900	-1.21316500

PG
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -269.509601
Thermal correction to Gibbs Free Energy (a.u.): 0.085173
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -269.7152886 a.u.

C	0.46407200	0.05096800	0.34340900
C	-0.70807200	-0.74715600	-0.22646300
O	0.41162200	1.37779600	-0.15683700
H	0.36386900	0.05724700	1.44687500
H	-0.73239200	-1.76458300	0.18912100
H	-0.60404000	-0.82052600	-1.31340000
C	1.81179000	-0.54837500	-0.02526600
H	2.61902500	0.07118700	0.37312100
H	1.91724700	-1.55936800	0.38122300
H	1.92096000	-0.59065200	-1.11335400
O	-1.93954000	-0.05540800	-0.00255800
H	-2.13603400	-0.10766700	0.94292100
H	-0.53202200	1.60264000	-0.18142200

$CH_3CHClCH_2OH$
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -653.908688
Thermal correction to Gibbs Free Energy (a.u.): 0.070477
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -654.0946971 a.u.

Cl	0.81054400	-1.23911000	0.06595800
C	0.24266000	0.45919100	-0.37506100
C	-1.11150000	0.69281300	0.28751900
O	-2.11219500	-0.19559900	-0.15398900
H	0.11576200	0.42212500	-1.45870800
H	-1.44643800	1.69955600	0.01147700
H	-0.98361500	0.67074900	1.38104100
C	1.29798100	1.46986800	0.03588600
H	2.25702100	1.25392300	-0.43867900
H	0.97883800	2.47212500	-0.27156100
H	1.43956700	1.46853800	1.12018700
H	-1.81766500	-1.08858900	0.07680100

Co^{III}(salen)-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1639.339142

Thermal correction to Gibbs Free Energy (a.u.): 0.318787
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2877.8318294 a.u.

C	4.71828000	-2.85691000	-0.28450700
C	5.40577200	-1.64253300	-0.06581200
C	3.34370100	-2.89308800	-0.39219000
H	5.28240100	-3.78214900	-0.36368400
C	4.68107000	-0.47531800	0.03692800
C	2.56883000	-1.70580300	-0.28635400
C	3.26858600	-0.47402100	-0.07077500
H	5.18778100	0.47202300	0.20580400
O	1.27970300	-1.79553100	-0.41938600
C	2.57812500	0.76752900	0.03090300
Co	0.00841400	-0.46857200	-0.16405600
N	1.29234300	0.92723100	-0.04827200
H	3.20049500	1.64811000	0.19198400
N	-1.27111300	0.92042800	-0.37653500
C	0.65045200	2.22173000	0.23528600
C	-2.55598900	0.76565300	-0.27770900
C	-0.64502200	2.23608800	-0.58653400
C	1.47998900	3.48015800	-0.02145600
H	-3.19241900	1.65007400	-0.30921500
C	-3.22343900	-0.48718700	-0.15701100
C	-1.49134400	3.46824800	-0.26634200
C	0.64245200	4.73139300	0.28416200
H	1.81215500	3.49126300	-1.06818100
H	2.37761900	3.48664500	0.60449500
C	-4.62479600	-0.49935600	0.04375800
C	-2.51382800	-1.72207900	-0.31965700
C	-0.67047800	4.74424300	-0.50662400
H	-2.39142200	3.49203500	-0.88915300
H	-1.81839600	3.41900200	0.78031300
H	1.22732000	5.63041300	0.06392700
H	0.41861800	4.75696100	1.35864600
C	-5.32888200	-1.68291000	0.09456800
H	-5.14002700	0.45128800	0.16013800
C	-3.26931600	-2.92496300	-0.27950100
O	-1.23555200	-1.79620200	-0.54274500
H	-0.44810500	4.83110300	-1.57856500
H	-1.26688500	5.62244100	-0.23873100
C	-4.63316400	-2.90049900	-0.07350100
H	-5.18213500	-3.83743900	-0.03605600
H	0.36268500	2.18569700	1.29529400
H	-0.35368800	2.27901600	-1.64756700
Cl	-0.19158900	-0.54441900	2.02500800
H	6.48668200	-1.63252600	0.02196000
H	2.80752900	-3.82145300	-0.55467300
H	-2.72704400	-3.85551200	-0.40485600
H	-6.40114100	-1.68241600	0.25740100

H_2O-Co^{III}-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1715.775582
Thermal correction to Gibbs Free Energy (a.u.): 0.343606
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2954.3231536 a.u.

C	4.74102300	-2.78048200	0.03670300
C	5.37513600	-1.57527800	0.40140700
C	3.39341400	-2.81972400	-0.26421400
H	5.32025800	-3.69907400	-0.00270300
C	4.62244800	-0.42125000	0.45444000
C	2.59492000	-1.64763600	-0.21761100
C	3.23888300	-0.42483100	0.15357500
H	5.08584400	0.52118400	0.73743300
O	1.33569200	-1.74140700	-0.55084400
C	2.53124800	0.81416700	0.23978000
Co	0.00811600	-0.40725000	-0.29584200
N	1.26805300	0.99039100	0.02554100

H	3.12952900	1.67811800	0.53290200
N	-1.31415000	0.96088500	-0.27607600
C	0.60161500	2.26701100	0.33089100
C	-2.57114100	0.77355300	-0.04389300
C	-0.70450800	2.27743500	-0.47856300
C	1.41233700	3.53765900	0.06622800
H	-3.21940800	1.64465700	0.05751500
C	-3.20124500	-0.50630100	0.07524600
C	-1.55893700	3.49777400	-0.13977000
C	0.56747600	4.78054700	0.38459000
H	1.72672000	3.54959000	-0.98568200
H	2.32084200	3.55436200	0.67572300
C	-4.55215000	-0.56039700	0.48674700
C	-2.51446400	-1.70903200	-0.28298100
C	-0.75584700	4.78298700	-0.38944100
H	-2.47066700	3.50740900	-0.74652200
H	-1.86657400	3.44577100	0.91281600
H	1.14128300	5.68529800	0.15842800
H	0.35673100	4.80284300	1.46192800
C	-5.22905700	-1.76055400	0.56966900
H	-5.05244300	0.36975400	0.74651400
C	-3.23565200	-2.92457800	-0.20001500
O	-1.28286000	-1.73491700	-0.72913600
H	-0.54823400	4.87322400	-1.46396200
H	-1.35701800	5.65498400	-0.11188200
C	-4.55369500	-2.94567100	0.21827200
H	-5.07531100	-3.89690000	0.28065500
Cl	-0.15490000	-0.70009100	1.91022100
O	0.13752700	-0.29749700	-2.34132200
H	-0.63862000	-0.88503400	-2.43949100
H	0.89036700	-0.91964900	-2.36906000
H	0.32440100	2.21943200	1.39338700
H	-0.42471000	2.32300600	-1.54111100
H	6.43285900	-1.55932800	0.64010700
H	2.89927100	-3.74581500	-0.53716800
H	-2.70977100	-3.83496300	-0.46601600
H	-6.26220800	-1.79234400	0.89796500

PO-Co^{III}-Cl

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1832.422024
Thermal correction to Gibbs Free Energy (a.u.): 0.401570
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3071.0652169 a.u.

C	-4.84127500	-2.28938200	-0.63609500
C	-5.42652400	-1.00967300	-0.53157100
C	-3.47104100	-2.45120600	-0.66816000
H	-5.48028700	-3.16645300	-0.69766900
C	-4.59815600	0.09030400	-0.46438700
C	-2.58830000	-1.33523900	-0.58813000
C	-3.18816100	-0.03664100	-0.48230300
H	-5.02264700	1.08949400	-0.39321000
O	-1.31252000	-1.56455000	-0.60427000
C	-2.40461500	1.15824000	-0.42542100
Co	0.04042600	-0.29678600	-0.24744100
N	-1.11673500	1.21243100	-0.35136700
H	-2.96320200	2.09471100	-0.45415400
N	1.39160500	0.95753800	0.25234300
C	-0.35802600	2.46590200	-0.39451000
C	2.66283200	0.72199400	0.21798300
C	0.82208400	2.27084700	0.57462200
C	-1.12663500	3.74923800	-0.08217200
H	3.35106700	1.54449800	0.41614300
C	3.26457300	-0.54623400	-0.05293600
C	1.77548500	3.46491500	0.53696800
C	-0.17493700	4.95415500	-0.11162100
H	-1.59526800	3.66419400	0.90776400
H	-1.92985200	3.90043300	-0.81049000

C	4.67471900	-0.61097800	-0.15501800
C	2.48392100	-1.74273900	-0.16946500
C	1.01055000	4.76166500	0.84072700
H	2.58383600	3.33603600	1.26469500
H	2.23703500	3.52512100	-0.45709800
H	-0.72384100	5.86638400	0.14464000
H	0.20024400	5.08909800	-1.13444000
C	5.32687000	-1.80558200	-0.37610600
H	5.24185500	0.31245200	-0.06009400
C	3.18402800	-2.95879700	-0.38953500
O	1.18977300	-1.78414800	-0.03474500
H	0.64355700	4.72929600	1.87552300
H	1.69256900	5.61595900	0.77716700
C	4.56088800	-2.98441100	-0.49089300
H	5.06227000	-3.93212000	-0.66856800
C	-0.74440600	-1.82013400	2.21184400
C	0.39041400	-1.03575000	2.71212800
O	-0.49866200	-0.46318900	1.71238400
H	-0.51203100	-2.55750700	1.44924800
H	1.38424600	-1.25891500	2.33991000
H	0.32273700	-0.52922000	3.67190500
C	-2.03604500	-1.98088500	2.95715300
H	-2.87027800	-2.00873900	2.25021700
H	-2.02845600	-2.92426400	3.51326300
H	-2.19339400	-1.15891800	3.66097500
H	0.39474100	2.18878400	1.58578700
H	0.06354300	2.52694700	-1.40657000
Cl	0.55481600	-0.04568200	-2.40987900
H	-6.50480600	-0.89574400	-0.51273100
H	-3.01702400	-3.43227500	-0.75881000
H	2.59026100	-3.86130100	-0.48579200
H	6.40748000	-1.84046600	-0.46117000

H_2O-Co^{III}-Cl~PO one intermediate structure in the formation of H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1908.838734
Thermal correction to Gibbs Free Energy (a.u.): 0.422398
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3147.5358591 a.u.

C	-1.82611100	4.86683000	-0.12089900
C	-0.58101600	5.40939200	-0.49627100
C	-1.95334400	3.53409800	0.22306300
H	-2.70550700	5.50499600	-0.10655800
C	0.52413200	4.58358200	-0.51683800
C	-0.83356200	2.66463800	0.20794900
C	0.43055400	3.21364500	-0.17430300
H	1.49526900	4.97798300	-0.80700400
O	-1.00609700	1.42356100	0.57993800
C	1.62208000	2.42211400	-0.23320500
Co	0.21933100	0.00003900	0.30363100
N	1.70969000	1.15376900	0.00258700
H	2.52731100	2.95570400	-0.52759000
N	1.47336800	-1.42505500	0.27476200
C	2.93627200	0.39182400	-0.28692200
C	1.18229900	-2.66070700	0.03178100
C	2.83057100	-0.92305900	0.50257700
C	4.26038600	1.09735200	0.01416200
H	1.99702300	-3.37966700	-0.06299700
C	-0.14513300	-3.17729500	-0.11582900
C	3.98504200	-1.86545000	0.16621500
C	5.43900700	0.16358800	-0.30094200
H	4.27778800	1.38991400	1.07224000
H	4.35742100	2.01337100	-0.57637800
C	-0.30940200	-4.50935700	-0.56025100
C	-1.29236900	-2.39717800	0.22644800
C	5.32537000	-1.16947200	0.44773400
H	3.91394600	-2.78417300	0.75800700
H	3.92458000	-2.15184600	-0.89187600

H	6.38182000	0.66055800	-0.04984300
H	5.46303100	-0.02891000	-1.38166100
C	-1.56509500	-5.06666100	-0.69391900
H	0.57772500	-5.08816300	-0.80703000
C	-2.56969300	-2.98663500	0.08493000
O	-1.21064300	-1.17594400	0.71098200
H	5.41545900	-0.98882900	1.52713400
H	6.15174500	-1.83220000	0.17088300
C	-2.69355200	-4.28881600	-0.36775000
H	-3.68654100	-4.71615600	-0.47805800
Cl	-0.06521900	-0.10907100	-1.90832700
O	0.33884600	0.09041700	2.35029500
H	-0.31030400	-0.63580500	2.44111100
H	-0.21426200	0.89422500	2.39303400
H	2.88870000	0.13387000	-1.35426700
H	2.88363900	-0.66296800	1.56977400
H	-0.49572500	6.45571300	-0.76806900
H	-2.90945000	3.10745100	0.50587500
H	-3.43703600	-2.37690000	0.32080700
H	-1.68258100	-6.08540000	-1.04739000
C	-4.62310700	0.59569200	-0.08993000
C	-4.09892400	0.43191500	1.27406300
O	-4.88399700	-0.60666700	0.65990900
H	-5.51554000	1.21489100	-0.21289900
H	-4.58529600	0.94001200	2.10820600
H	-3.04404500	0.20038100	1.38811400
C	-3.73528700	0.47397700	-1.29876100
H	-4.26732100	-0.01514800	-2.12201600
H	-3.42264200	1.46683300	-1.63920200
H	-2.83340200	-0.09261800	-1.06786500

$CH_3CHOAcCH_2OH$
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -422.156326
Thermal correction to Gibbs Free Energy (a.u.): 0.117498
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -422.4504619 a.u.

H	-0.19410800	1.93459200	0.43385000
C	-1.02363600	-0.39496600	0.30452800
C	-1.60311600	0.85470600	-0.35780300
O	-0.71885200	1.95507100	-0.38093000
H	-0.82982600	-0.19078100	1.36240200
H	-2.54633500	1.09379200	0.16259100
H	-1.85412000	0.62693500	-1.40065600
C	-1.91906800	-1.61163900	0.14498200
H	-2.06085100	-1.85059200	-0.91308600
H	-1.47864800	-2.48056600	0.63959900
H	-2.89903700	-1.42026600	0.59174100
C	2.57968200	-0.54569300	-0.57740600
H	2.58842900	-1.62690600	-0.73161600
H	3.46769700	-0.22579300	-0.03378100
H	2.56824000	-0.06996400	-1.56326200
C	1.34766500	-0.12343700	0.17898900
O	0.24852300	-0.72690700	-0.31467200
O	1.33900400	0.66380100	1.10716200

Co^{III}(salen)-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1407.569499
Thermal correction to Gibbs Free Energy (a.u.): 0.365073
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2646.1700493 a.u.

C	4.71980500	-2.74575300	-0.67220400
C	5.42578400	-1.55430900	-0.40168600
C	3.34141200	-2.76088300	-0.74688000
H	5.27000600	-3.67087000	-0.82017600
C	4.71573800	-0.38817000	-0.21226700

H	6.50848900	-1.55939700	-0.34067900
C	2.58439900	-1.57520800	-0.55375000
H	2.79248800	-3.67323700	-0.95289700
C	3.30179000	-0.36673600	-0.28533500
H	5.23643900	0.54255400	0.00034200
O	1.28607100	-1.64877000	-0.64963100
C	2.62598900	0.87300700	-0.07834900
Co	0.02672900	-0.30538700	-0.37402400
N	1.34383300	1.05069400	-0.13595000
H	3.25989800	1.72993500	0.15134600
N	-1.21105300	1.13702600	-0.55761800
C	0.70666400	2.31362500	0.26562600
C	-2.49763400	1.01050100	-0.48049900
C	-0.54365900	2.44786300	-0.61610100
C	1.56922700	3.57420000	0.20978400
H	-3.11220900	1.91049600	-0.45362000
C	-3.20144000	-0.23158200	-0.45253600
C	-1.37935200	3.66477800	-0.21885800
C	0.73446100	4.80291100	0.60081700
H	1.97057600	3.69837700	-0.80522900
H	2.42276200	3.48574700	0.88923100
C	-4.60495700	-0.21603600	-0.27544400
C	-2.52423100	-1.47271600	-0.67624200
C	-0.51875900	4.93569900	-0.27077600
H	-2.23911000	3.77699300	-0.88764900
H	-1.77005800	3.51655700	0.79616100
H	1.34868300	5.70602700	0.52438900
H	0.43644100	4.71236600	1.65339300
C	-5.34378600	-1.38034400	-0.30573600
H	-5.09573200	0.74032200	-0.11086700
C	-3.31224400	-2.65293300	-0.72279400
O	-1.23909300	-1.57397400	-0.86457500
H	-0.22091800	5.12747600	-1.31035100
H	-1.11472500	5.79695200	0.04811500
C	-4.68004900	-2.60325400	-0.53636600
H	-6.41798200	-1.35798300	-0.15886100
H	-2.79536600	-3.58938900	-0.90169900
H	-5.25402300	-3.52531300	-0.56540600
O	-0.23960100	-0.27333100	1.44162400
C	-0.30845400	-1.28403300	2.30769800
O	-0.35930200	-1.01168400	3.49676900
C	-0.37443300	-2.71137800	1.80519500
H	-0.13567500	-3.37689400	2.63559400
H	-1.39435800	-2.92142400	1.46912500
H	0.28833000	-2.88026600	0.95764000
H	-0.19747400	2.58181100	-1.65262700
H	0.36013000	2.14715700	1.29507600

H_2O-Co^{III}-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1484.005932
Thermal correction to Gibbs Free Energy (a.u.): 0.389430
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2722.6625802 a.u.

C	4.74089900	-2.62222600	-0.35182800
C	5.37409400	-1.45805700	0.12477500
C	3.39368800	-2.62910400	-0.66251000
H	5.31780900	-3.53504200	-0.47244800
C	4.62272800	-0.31119900	0.27982600
C	2.59975200	-1.46497800	-0.51098200
C	3.24218700	-0.28352100	-0.02859000
H	5.08627200	0.59955300	0.65168300
O	1.33451800	-1.52786700	-0.84531900
C	2.53311700	0.94463800	0.17218000
Co	0.00430900	-0.21149900	-0.50518300
N	1.27734900	1.14609100	-0.04987000
H	3.12827400	1.76992800	0.56580400
N	-1.30498400	1.17014300	-0.39583600

C	0.60475700	2.38134000	0.38509400
C	-2.55198500	0.97101900	-0.13428500
C	-0.67835600	2.49247100	-0.45435000
C	1.42911300	3.66792700	0.29628800
H	-3.19062600	1.83148400	0.06874800
C	-3.19087800	-0.31288300	-0.11396200
C	-1.53203800	3.68130100	-0.01657300
C	0.57936100	4.87694500	0.71540500
H	1.78638000	3.79364600	-0.73444800
H	2.31165300	3.60868800	0.94029100
C	-4.53180800	-0.39379800	0.32180600
C	-2.52673600	-1.48180100	-0.59959500
C	-0.71127800	4.97608800	-0.10518800
H	-2.42567800	3.76118400	-0.64503100
H	-1.87010600	3.52597900	1.01632900
H	1.16754800	5.79466600	0.61173500
H	0.32552400	4.78422900	1.77950000
C	-5.22253600	-1.59003000	0.30455300
H	-5.01525700	0.51175000	0.68086500
C	-3.26303500	-2.69083100	-0.62528200
O	-1.29568400	-1.48268600	-1.05204100
H	-0.46120500	5.17326500	-1.15614500
H	-1.31622000	5.82183900	0.23758600
C	-4.57271000	-2.74032500	-0.17973000
H	-5.10492100	-3.68733900	-0.20136300
O	-0.18890600	-0.42855800	1.32553800
C	-0.09000300	-1.50477300	2.09619500
O	0.03955900	-1.36261200	3.30339400
C	-0.22483500	-2.88440800	1.47586600
H	0.19827200	-3.61670500	2.16491500
H	-1.29060300	-3.10365800	1.35172000
H	0.24310400	-2.94654900	0.49519300
H	-0.37079900	2.63915000	-1.49973600
H	0.29703100	2.20392200	1.42472800
O	0.17283800	0.06352700	-2.54829000
H	-0.61556800	-0.48880600	-2.71310100
H	0.91074000	-0.57203100	-2.61358700
H	-6.24769000	-1.64240300	0.65416700
H	-2.75693900	-3.57571800	-0.99563900
H	2.90037500	-3.52516500	-1.02356200
H	6.43015700	-1.46622600	0.37074300

PO-Co^{III}-OAc

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -1600.652466

Thermal correction to Gibbs Free Energy (a.u.): 0.447883

No imaginary frequency

Calculation of single point energy based on the optimized structure, E = -2839.4045331 a.u.

C	4.82779100	-2.29748200	0.41210600
C	5.43519800	-1.02689700	0.35485600
C	3.45329600	-2.43391200	0.44617000
H	5.44984000	-3.18839600	0.43334200
C	4.62672000	0.09133600	0.34022500
C	2.59456000	-1.29990300	0.41638100
C	3.21635000	-0.01089600	0.36099200
H	5.06967500	1.08442400	0.31012100
O	1.30954600	-1.50306700	0.43758500
C	2.44843400	1.19928700	0.37617000
Co	-0.01290100	-0.21271800	0.03281600
N	1.16459200	1.26757500	0.28506200
H	3.01575200	2.12483700	0.48423800
N	-1.30636300	1.09815000	-0.50072700
C	0.40223600	2.51024900	0.41542700
C	-2.58012700	0.88965800	-0.52160300
C	-0.70530000	2.42862000	-0.65373200
C	1.18904100	3.81509000	0.30923600
H	-3.24747500	1.73733000	-0.68154900
C	-3.21770400	-0.38337300	-0.36240100

C	-1.65353600	3.62414100	-0.56335300
C	0.23651900	5.01589700	0.39782100
H	1.73281100	3.84011300	-0.64531400
H	1.93327000	3.87506700	1.11013000
C	-4.63113500	-0.42354700	-0.33529100
C	-2.46849900	-1.60086800	-0.28065500
C	-0.86530400	4.93813300	-0.66480000
H	-2.40391300	3.58111800	-1.36033600
H	-2.18938500	3.58436100	0.39374700
H	0.80274300	5.94703700	0.29109500
H	-0.22172400	5.03730000	1.39495600
C	-5.31793900	-1.61535200	-0.22353900
H	-5.17507200	0.51613500	-0.39996100
C	-3.20127200	-2.81267400	-0.17864600
O	-1.16695400	-1.66246100	-0.32805400
H	-0.41379000	5.01304000	-1.66339300
H	-1.55029300	5.78666500	-0.56637500
C	-4.58324100	-2.81500200	-0.14821600
H	-5.11037800	-3.76102000	-0.05881000
O	-0.59886600	0.09783600	1.76931600
C	-0.74898500	-0.69115300	2.82400900
O	-0.96055500	-0.18485100	3.91749600
C	-0.72146900	-2.19786700	2.64436200
H	-0.59569500	-2.65907000	3.62497800
H	-1.67929500	-2.52245100	2.22574400
H	0.06338400	-2.50799000	1.95628500
H	-0.20645500	2.43980200	-1.63478600
H	-0.09046700	2.44703900	1.39428300
C	0.92547800	-1.63423200	-2.46087900
C	-0.16653700	-0.80593900	-2.98494900
O	0.66780400	-0.30270700	-1.90533000
H	0.63980400	-2.40829500	-1.75477100
H	-1.18473400	-1.02982500	-2.68663100
H	-0.03275700	-0.25408200	-3.91221800
C	2.25398400	-1.77746400	-3.14317600
H	3.04932700	-1.85727900	-2.39685700
H	2.26242100	-2.68898700	-3.75012900
H	2.45973900	-0.92157200	-3.79188000
H	6.51520100	-0.93180200	0.33318800
H	2.98211600	-3.40989700	0.49692200
H	-2.63127100	-3.73337900	-0.11537100
H	-6.40182500	-1.63001100	-0.19421700

H_2O-Co^{III}-OAc~PO one intermediate structure in the formation of H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1677.065877
Thermal correction to Gibbs Free Energy (a.u.): 0.466541
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2915.8744208 a.u.

C	-0.78738500	-5.17102100	0.06105500
C	0.56094400	-5.50106200	0.29685900
C	-1.17305800	-3.86507700	-0.17947400
H	-1.54112900	-5.95351100	0.07353500
C	1.50260800	-4.49205000	0.28645300
C	-0.22499200	-2.81205400	-0.19681000
C	1.14316700	-3.14565300	0.04305000
H	2.54927200	-4.72043700	0.47327200
O	-0.65001100	-1.59962300	-0.45622800
C	2.18138900	-2.15677100	0.07162500
Co	0.35886600	0.01019700	-0.34011500
N	2.03431100	-0.89027600	-0.12751400
H	3.17902400	-2.53246000	0.30365200
N	1.37802200	1.61476500	-0.44229600
C	3.11825400	0.07140100	0.13271700
C	0.91676600	2.78182700	-0.14113900
C	2.79163800	1.32608900	-0.69483000
C	4.54049800	-0.41678900	-0.15053900
H	1.61527700	3.61490300	-0.05488300

C	-0.46891800	3.09549000	0.05660800
C	3.78587200	2.45184800	-0.41567800
C	5.55215600	0.71023300	0.10619400
H	4.60354100	-0.75316500	-1.19404200
H	4.78952800	-1.27382300	0.48254100
C	-0.81476400	4.39612300	0.48799200
C	-1.49814400	2.16126700	-0.27133600
C	5.21600700	1.97010200	-0.69936900
H	3.55615900	3.32571300	-1.03485500
H	3.69926600	2.76119100	0.63408600
H	6.56147700	0.36175300	-0.13610700
H	5.55170600	0.95402600	1.17662800
C	-2.13492800	4.78493600	0.60284900
H	-0.01516900	5.09171100	0.73175500
C	-2.84372800	2.59187800	-0.18659200
O	-1.25473400	0.93800800	-0.68574900
H	5.31833100	1.75578900	-1.77154800
H	5.92797300	2.76952400	-0.46977100
C	-3.14580300	3.87144500	0.24800700
H	-4.18734800	4.17386100	0.31418500
O	0.42091100	0.21385000	1.50438600
C	-0.44656800	-0.07111400	2.46495900
O	-0.06947700	-0.08685500	3.62757700
C	-1.90144900	-0.30068100	2.10137000
H	-2.41811000	-0.71744200	2.96649600
H	-2.35669600	0.66111700	1.84579300
H	-1.99940100	-0.95267000	1.23475700
H	2.86127400	1.04295200	-1.75515600
H	3.01926900	0.34751000	1.19127300
O	0.34339700	-0.15835500	-2.40181500
H	-0.40399300	0.46791600	-2.46874700
H	-0.09471900	-1.02907500	-2.38619600
H	-2.38945100	5.78141200	0.94699600
H	-3.61863200	1.89360900	-0.48855100
H	-2.21147400	-3.60449800	-0.35567600
H	0.85144000	-6.52778500	0.48976800
C	-5.12788500	-0.97772100	-0.81047400
C	-3.82534300	-0.94612100	-1.49124100
O	-4.76650200	0.13650600	-1.64149200
H	-5.90717300	-1.60576600	-1.24934200
H	-3.68180000	-1.55026100	-2.38885300
H	-2.92135300	-0.69993100	-0.94199200
C	-5.27552100	-0.70226100	0.66264800
H	-6.22045800	-0.18740700	0.86678600
H	-5.27042100	-1.63799300	1.23236100
H	-4.45547800	-0.07733000	1.02075600

$CH_3CHOTsCH_2OH$
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1088.406997
Thermal correction to Gibbs Free Energy (a.u.): 0.187996
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -1088.9507578 a.u.

H	-2.95601300	1.65618700	-0.41734000
C	-2.68301200	-1.01501000	-0.06148300
C	-3.63610200	-0.11919500	-0.85166600
O	-3.79188300	1.17129300	-0.31201200
H	-2.86774300	-0.89261800	1.00976900
H	-4.62688000	-0.58726700	-0.82883000
H	-3.30101500	-0.10406800	-1.90120500
C	-2.75220000	-2.47518100	-0.47190200
H	-2.56093000	-2.58637700	-1.54349300
H	-2.01067600	-3.06114400	0.07517700
H	-3.74561400	-2.87670300	-0.25251900
O	-1.03037100	1.88316500	-0.12662100
O	-1.28684400	-0.61523400	-0.32506200
S	-0.65981000	0.62214000	0.53468700
O	-0.95955900	0.42703500	1.95178500

C	1.05605700	0.30326100	0.22065500
C	1.77401800	-0.47660900	1.12602900
C	1.65564200	0.84146000	-0.91714200
C	3.11921500	-0.72679100	0.87343100
H	1.28529500	-0.86088200	2.01382000
C	3.00137500	0.57736400	-1.15180700
H	1.07773200	1.46472500	-1.58930600
C	3.74998800	-0.21137500	-0.26725400
H	3.69158800	-1.32616500	1.57516900
H	3.48165600	0.99552200	-2.03146400
C	5.19943900	-0.51485500	-0.54755300
H	5.67879900	0.29931500	-1.09762800
H	5.75884500	-0.68132400	0.37678000
H	5.29466400	-1.42194800	-1.15648400

Co^{III}(salen)-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2073.832422
Thermal correction to Gibbs Free Energy (a.u.): 0.436437
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3312.6846426 a.u.

S	0.61899800	-0.29270700	-1.41761100
O	-0.23773300	-1.21315000	-2.18205500
O	0.58308700	1.12651700	-1.82718400
O	0.41749400	-0.45296900	0.12924800
C	2.30860800	-0.85446900	-1.49116800
C	2.63078400	-1.96136900	-2.26799400
C	3.28541600	-0.15616100	-0.77558500
C	3.96248300	-2.37399700	-2.33364900
H	1.84635400	-2.48250000	-2.80479200
C	4.60422500	-0.58499800	-0.85029300
H	3.01395800	0.70003300	-0.16913400
C	4.96342300	-1.69829500	-1.62804200
H	4.22571700	-3.23618600	-2.93997000
H	5.36959300	-0.05078000	-0.29365600
C	6.39926700	-2.15677000	-1.68256200
H	6.72253000	-2.55280800	-0.71274800
H	6.54005000	-2.94390900	-2.42769100
H	7.07133100	-1.32877900	-1.93217600
N	-2.35672700	-0.00133200	-0.15152800
N	-0.88156100	1.99999100	0.54111800
C	-2.88869900	-1.14495600	-0.46314900
H	-3.51837000	-1.19566700	-1.35136100
C	0.19069000	2.71715600	0.62954600
H	0.23863800	3.66266600	0.09122400
C	-2.73701300	-2.35787600	0.26776300
C	-3.37680700	-3.52414200	-0.21652600
C	-1.99838500	-2.40896200	1.49434100
C	-3.31379000	-4.71448200	0.47544000
H	-3.92217200	-3.46254800	-1.15491200
C	-1.96617300	-3.64352900	2.19518000
C	-2.60343600	-4.76057300	1.69449400
H	-3.80230500	-5.60351700	0.09185500
H	-1.41083200	-3.67188300	3.12611500
H	-2.55061200	-5.69504800	2.24634100
C	1.33600500	2.35256400	1.40522200
C	2.52727900	3.09881300	1.26288700
C	1.26742800	1.28342100	2.35885200
C	3.64613500	2.80935600	2.01904600
H	2.55193100	3.90123300	0.52979100
C	2.42124400	1.03357300	3.14631900
C	3.57684600	1.77001000	2.97023600
H	4.56174100	3.37641800	1.89075400
H	2.36434500	0.22689600	3.86869300
H	4.45105900	1.53888200	3.57279200
O	-1.38135900	-1.38545100	2.01049400
O	0.20038200	0.56013200	2.55217800
C	-2.49332800	1.16668500	-1.04476700

C	-3.87254500	1.40147400	-1.66268100
C	-2.06959300	2.39428900	-0.22619900
C	-3.81558900	2.64589400	-2.56429400
H	-4.61493200	1.53486000	-0.86455900
H	-4.18705500	0.53931900	-2.25823100
C	-1.94934300	3.62035200	-1.12795700
C	-3.30164600	3.88088300	-1.81210800
H	-4.80699500	2.84613000	-2.98403400
H	-3.14994800	2.43594700	-3.41126400
H	-1.65698600	4.50191900	-0.54706300
H	-1.16701900	3.43531600	-1.87354100
H	-4.03635800	4.17194500	-1.04932900
H	-3.21099800	4.72919000	-2.49840800
Co	-0.98493400	0.20787300	1.14986900
H	-2.86130300	2.58008600	0.51618000
H	-1.76001100	1.03894600	-1.84825600

H_2O-Co^{III}-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2150.274119
Thermal correction to Gibbs Free Energy (a.u.): 0.462327
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3389.1814283 a.u.

S	-0.69864000	0.31915800	-1.40001300
O	-0.00579900	1.40841100	-2.11179200
O	-0.48999300	-1.04020900	-1.94563500
O	-0.45388500	0.36909000	0.13708200
C	-2.44964300	0.65897600	-1.40003500
C	-2.93282700	1.77149100	-2.07932900
C	-3.31104300	-0.21035500	-0.72582000
C	-4.30719900	2.01569400	-2.08533400
H	-2.23584300	2.42832900	-2.58701600
C	-4.67511700	0.05099000	-0.73929500
H	-2.91879700	-1.07018600	-0.19752700
C	-5.19457000	1.16591400	-1.41715100
H	-4.69409200	2.88209900	-2.61470800
H	-5.34946900	-0.61941200	-0.21284200
C	-6.67778600	1.44066600	-1.40691400
H	-7.02076000	1.71476800	-0.40228200
H	-6.93757800	2.25983100	-2.08244000
H	-7.24805800	0.55641100	-1.71126100
N	2.27542700	0.35959400	-0.24189900
N	1.15010800	-1.90971000	0.30480300
C	2.46910700	1.60098200	-0.55213500
H	2.99059000	1.82067900	-1.48437900
C	0.17407900	-2.74922500	0.28875300
H	0.24411400	-3.62689500	-0.35282700
C	2.05761600	2.73536800	0.21535500
C	2.32793400	4.02161600	-0.30544800
C	1.41094600	2.60357700	1.48309000
C	1.98748000	5.16555500	0.38741000
H	2.80818500	4.09276500	-1.27810100
C	1.08348700	3.79213200	2.17980000
C	1.36350100	5.03565000	1.64302300
H	2.19333000	6.14635800	-0.02695200
H	0.59209000	3.68711100	3.14105200
H	1.08735200	5.92761700	2.19897000
C	-1.02125800	-2.60754000	1.07330800
C	-2.11636800	-3.45357900	0.80052400
C	-1.09884700	-1.65377600	2.13671600
C	-3.28857300	-3.36658200	1.53011400
H	-2.02996600	-4.16609600	-0.01591000
C	-2.30098900	-1.59954700	2.87981600
C	-3.36690900	-2.43050900	2.57778500
H	-4.13139900	-4.00941500	1.30071300
H	-2.36077500	-0.86941000	3.67943500
H	-4.28239200	-2.35107200	3.15772700
O	1.13649800	1.45312800	2.04726300

O	-0.10518100	-0.86249300	2.46902200
C	2.60640700	-0.71567600	-1.19469400
C	4.01471400	-0.67842200	-1.79045700
C	2.38778200	-2.04880000	-0.46253300
C	4.17820500	-1.85014300	-2.77241800
H	4.75361800	-0.74517000	-0.98112000
H	4.19164900	0.26623600	-2.31372000
C	2.47925100	-3.21270600	-1.44548900
C	3.86426900	-3.20147900	-2.11445000
H	5.19509000	-1.85741700	-3.17888100
H	3.49945400	-1.69547200	-3.62100100
H	2.32569800	-4.16733500	-0.92989000
H	1.68775400	-3.10777300	-2.19730700
H	4.62707300	-3.41955200	-1.35495500
H	3.92322200	-4.00436200	-2.85666600
Co	1.05378900	-0.19745000	1.11457800
H	3.18868900	-2.14562100	0.28425700
H	1.86910800	-0.66248200	-2.00419700
O	2.47443400	-0.69557000	2.45759300
H	1.83339200	-1.14597200	3.04310800
H	2.51542400	0.21638900	2.81159700

PO-Co^{III}-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2266.919573
Thermal correction to Gibbs Free Energy (a.u.): 0.518947
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3505.922625 a.u.

C	2.18752000	4.92328000	1.18601500
C	2.69412000	4.98430600	-0.12870000
C	1.69149500	3.74606300	1.70924800
H	2.17940800	5.82094500	1.79882800
C	2.69338900	3.83517000	-0.89041700
C	1.66864300	2.54754600	0.94333100
C	2.19911100	2.60827700	-0.38589000
H	3.07770000	3.85356100	-1.90756200
O	1.18807000	1.47611800	1.49908800
C	2.27209900	1.46058200	-1.23269300
Co	0.94360500	-0.19172700	0.65810800
N	1.90585700	0.25894300	-0.92645900
H	2.68638700	1.63250700	-2.22654600
N	0.77858000	-1.92331700	-0.10898200
C	1.92955300	-0.83032900	-1.91710700
C	-0.23631400	-2.69280300	0.09051400
C	1.79904100	-2.14671500	-1.13264800
C	3.15212000	-0.89051100	-2.83475600
H	-0.35973400	-3.57441300	-0.53731000
C	-1.23494300	-2.47042900	1.09656100
C	1.58837500	-3.31771500	-2.08873500
C	3.00562000	-2.07704300	-3.80121800
H	4.06061500	-0.99585700	-2.22668600
H	3.25269000	0.03363500	-3.41151600
C	-2.40247900	-3.26347200	1.07712900
C	-1.05137100	-1.48664400	2.12159900
C	2.77734900	-3.40100000	-3.05951200
H	1.49640100	-4.25829700	-1.53373900
H	0.65320800	-3.16189200	-2.63968600
H	3.89358100	-2.15022300	-4.43817200
H	2.15405100	-1.88554300	-4.46651900
C	-3.39725000	-3.10086500	2.02336500
H	-2.51623800	-3.99682700	0.28257700
C	-2.07737700	-1.35701800	3.09056600
O	0.01870300	-0.74334600	2.22393000
H	3.68267800	-3.66000500	-2.49365900
H	2.61412000	-4.21209500	-3.77689000
C	-3.21780700	-2.13849100	3.03585300
H	-3.99282600	-1.99894400	3.78480100
C	2.86896800	-0.33082000	2.90630400

C	2.73839200	-1.75071200	2.55836100
O	2.67659000	-0.73868300	1.50929300
H	1.97541700	0.14686300	3.29521600
H	1.78819900	-2.24019400	2.74104600
H	3.62206600	-2.37860400	2.47657600
C	4.17909200	0.34774200	3.17177200
H	4.14332900	1.37256000	2.79072200
H	4.36492100	0.39003100	4.25008800
H	5.00708000	-0.18105500	2.69187900
H	2.74406300	-2.29526800	-0.58940100
H	1.02702600	-0.72775100	-2.52964300
S	-1.25252500	0.37942700	-1.47164500
O	-0.64060500	1.41548400	-2.32213800
O	-1.24881500	-0.99348200	-2.02694500
O	-0.71515600	0.41448900	-0.01414400
C	-2.94605400	0.83360700	-1.13894900
C	-3.48570400	1.96133800	-1.74652200
C	-3.70960400	0.03544700	-0.28302900
C	-4.81777800	2.29411400	-1.49383500
H	-2.86316800	2.56159800	-2.40015900
C	-5.03196800	0.38427900	-0.04019800
H	-3.27318700	-0.83693100	0.18714400
C	-5.60656700	1.51684500	-0.63986500
H	-5.24811100	3.17346900	-1.96526800
H	-5.62926500	-0.23025700	0.62843800
C	-7.04059600	1.88629900	-0.35195700
H	-7.16812600	2.18622900	0.69485600
H	-7.37318600	2.71730700	-0.97944300
H	-7.71250900	1.03916500	-0.52772300
H	3.07348800	5.91719100	-0.53101900
H	1.28733200	3.69785800	2.71488100
H	-1.94193400	-0.60538600	3.86062700
H	-4.29821400	-3.70357200	1.98855200

H_2O-Co^{III}-OTs~PO one intermediate structure in the formation of H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2343.337427
Thermal correction to Gibbs Free Energy (a.u.): 0.542421
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -3582.3961885 a.u.

S	0.09122100	-0.22951500	1.73171700
O	-0.47041900	0.85280500	2.55779600
O	-0.47592900	-1.57825500	1.94263500
O	0.12739600	0.15246500	0.22225400
C	1.85084100	-0.31784300	2.01310800
C	2.48709200	0.67850900	2.74452200
C	2.56753100	-1.38229200	1.46076700
C	3.86866800	0.60159800	2.93116400
H	1.90181200	1.49186800	3.15814400
C	3.94091300	-1.44264500	1.65696900
H	2.05696000	-2.14525000	0.88650700
C	4.61291100	-0.45341400	2.39299100
H	4.37462200	1.37401400	3.50370400
H	4.50381100	-2.26530200	1.22414400
C	6.10813100	-0.52692100	2.57596300
H	6.62620700	-0.41348700	1.61641700
H	6.46897800	0.25796900	3.24557300
H	6.41067400	-1.49367500	2.99253900
N	-2.59285100	0.57885800	0.18099700
N	-1.74561100	-1.70612100	-0.70274700
C	-2.64605800	1.74500500	0.73922400
H	-3.28610100	1.86649100	1.61403700
C	-0.94213600	-2.71138000	-0.75856000
H	-1.27794600	-3.67474100	-0.37567700
C	-1.93989900	2.91486300	0.31465000
C	-2.10356500	4.09951200	1.06819500
C	-1.11674400	2.92480000	-0.85347700
C	-1.49442700	5.28105400	0.69575200

H	-2.72247700	4.06034900	1.96100200
C	-0.52464000	4.15567100	-1.22999700
C	-0.70681700	5.29798500	-0.47091300
H	-1.62210200	6.18060900	1.28773800
H	0.08315400	4.16250700	-2.12843800
H	-0.22668500	6.22230200	-0.78063600
C	0.39022700	-2.64706700	-1.29035900
C	1.26189200	-3.73630900	-1.07516100
C	0.83282200	-1.51457400	-2.04277100
C	2.56272100	-3.71348300	-1.54466000
H	0.89692500	-4.58947500	-0.50844100
C	2.16641300	-1.51305200	-2.51441300
C	3.00564600	-2.58615400	-2.26219600
H	3.23091800	-4.54795400	-1.36072000
H	2.51638600	-0.62433200	-3.02924700
H	4.03089700	-2.54873200	-2.62060800
O	-0.90487400	1.87513200	-1.60796200
O	0.05303400	-0.49657800	-2.33453500
C	-3.26219200	-0.58363100	0.79323400
C	-4.73580200	-0.39569700	1.15759500
C	-3.11553000	-1.75473200	-0.19100500
C	-5.26669900	-1.68924500	1.79682600
H	-5.30534200	-0.14918300	0.25186400
H	-4.86128700	0.43754500	1.85585200
C	-3.57738500	-3.05526800	0.46076200
C	-5.04652900	-2.91055500	0.89280600
H	-6.33133800	-1.58098300	2.02932700
H	-4.74909500	-1.84856600	2.75154700
H	-3.47934300	-3.89385400	-0.23762200
H	-2.94002400	-3.26657700	1.32793200
H	-5.67223800	-2.81341900	-0.00455100
H	-5.37295800	-3.82179400	1.40467000
Co	-1.23822900	0.08330600	-1.07218700
H	-3.76094500	-1.53747000	-1.05402000
H	-2.69411600	-0.84234400	1.69434600
O	-2.42774300	0.12855500	-2.69775800
H	-1.75794800	-0.30665600	-3.26271300
H	-2.27102500	1.08374500	-2.84394800
C	3.91516300	1.90908300	-1.49866700
C	2.45559500	1.82664100	-1.36781600
O	3.09415400	1.64559300	-2.64819500
H	4.36775900	2.90393300	-1.51100300
H	1.86579400	2.73533300	-1.27144600
H	1.99437200	0.94005400	-0.94480300
C	4.82189600	0.79602700	-1.04253300
H	5.67709700	0.68718800	-1.71921900
H	5.20275800	1.00743600	-0.03817100
H	4.27856800	-0.15037500	-1.00614600

Co^{III}(salen)-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1254.924656
Thermal correction to Gibbs Free Energy (a.u.): 0.330682
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2493.426736 a.u.

C	4.74225300	-2.85189200	-0.17013600
C	5.42373100	-1.61735200	-0.09779900
C	3.36403200	-2.91101800	-0.17161500
H	5.31355800	-3.77485300	-0.22220500
C	4.68598600	-0.45582000	-0.02937000
H	6.50783500	-1.58716200	-0.09287000
C	2.57472500	-1.72937400	-0.10363600
H	2.83509300	-3.85638000	-0.22558900
C	3.26931200	-0.47752300	-0.03439300
H	5.18624800	0.50818500	0.03116500
O	1.28016300	-1.85164600	-0.12091400
C	2.57079400	0.76309300	0.05497600
Co	0.00182900	-0.49357800	-0.05517000

N	1.28304800	0.90629000	0.02238400
H	3.19151000	1.65273000	0.16916300
N	-1.27552500	0.88955200	-0.34116600
C	0.62638100	2.18705800	0.31430700
C	-2.55851700	0.73345500	-0.24309100
C	-0.65068400	2.20621000	-0.53904600
C	1.45299400	3.45681600	0.11105900
H	-3.19888300	1.61447000	-0.29741600
C	-3.22799900	-0.51699600	-0.09354400
C	-1.50792900	3.43420000	-0.23127500
C	0.59816900	4.69742800	0.40978700
H	1.81969700	3.49178000	-0.92377800
H	2.32996600	3.45441200	0.76620400
C	-4.63395700	-0.51661400	0.07338800
C	-2.51947500	-1.75952600	-0.18632900
C	-0.68520600	4.71599500	-0.42788100
H	-2.38932900	3.46248300	-0.88032200
H	-1.86665500	3.37139200	0.80431800
H	1.18470000	5.60391700	0.22726400
H	0.33506900	4.70209500	1.47570800
C	-5.34777500	-1.69276400	0.15680700
H	-5.14645400	0.44079200	0.13605300
C	-3.28530200	-2.95537500	-0.11375200
O	-1.23558200	-1.85317800	-0.36597500
H	-0.42435700	4.81692700	-1.48996300
H	-1.29449500	5.58884000	-0.17121300
C	-4.65412800	-2.91819200	0.05682000
H	-6.42383200	-1.67988000	0.29195100
H	-2.74689700	-3.89373800	-0.19140900
H	-5.20784900	-3.85133900	0.11733400
O	-0.22806700	-0.43130300	1.73802300
H	-0.03956000	-1.34411500	2.00365300
H	-0.33433200	2.25493500	-1.59274700
H	0.31037800	2.11837100	1.36504200

H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1331.359753
Thermal correction to Gibbs Free Energy (a.u.): 0.355388
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2569.9169091 a.u.

C	-4.78468700	-2.76198600	-0.11713900
C	-5.42885400	-1.52013700	-0.28788400
C	-3.41231400	-2.84435000	0.01661600
H	-5.37590700	-3.67358700	-0.09379600
C	-4.65895500	-0.37600000	-0.32245700
C	-2.59447500	-1.68243300	-0.00881000
C	-3.25115400	-0.42204400	-0.18463000
H	-5.13022600	0.59458800	-0.46122100
O	-1.30636600	-1.82938600	0.14732400
C	-2.52939000	0.81358000	-0.26449700
Co	0.00128600	-0.45032500	0.13833300
N	-1.25392800	0.95676500	-0.13016900
H	-3.13389700	1.69692400	-0.47606400
N	1.31001100	0.92468500	0.27982200
C	-0.57159700	2.22776400	-0.40697900
C	2.57046500	0.75419200	0.06286400
C	0.68798200	2.23530700	0.47711500
C	-1.39313000	3.50342700	-0.21173700
H	3.21850100	1.63048700	0.01563400
C	3.21606900	-0.51500700	-0.10174400
C	1.55584200	3.46291400	0.20427900
C	-0.52491300	4.74436400	-0.46677600
H	-1.78850600	3.52338900	0.81269300
H	-2.25152700	3.51805600	-0.89070900
C	4.58316400	-0.53124400	-0.45651700
C	2.52968900	-1.74400200	0.15392200
C	0.73500000	4.74445200	0.40607200

H	2.42723700	3.46985800	0.86791600
H	1.93075000	3.42025600	-0.82680700
H	-1.11338000	5.65011600	-0.28643000
H	-0.23176000	4.76527100	-1.52475300
C	5.28176700	-1.71634100	-0.58105400
H	5.08189900	0.41847000	-0.63725900
C	3.27333700	-2.94379700	0.03054400
O	1.27936700	-1.81223900	0.53521100
H	0.44623500	4.82562900	1.46251500
H	1.35324100	5.61997400	0.18176200
C	4.60903100	-2.92705900	-0.32933700
H	5.14602700	-3.86739200	-0.42180700
O	-0.22751700	-0.52968500	2.23391300
O	0.28744200	-0.51482800	-1.65842300
H	0.01447900	-1.41715000	-1.87917100
H	0.34843700	2.26305600	1.52284800
H	-0.23102900	2.16008000	-1.44967300
H	-0.97237200	-1.15408700	2.19837600
H	0.55229900	-1.11929600	2.25992800
H	6.32885200	-1.71556300	-0.86382900
H	2.75122400	-3.87485400	0.22408600
H	-2.91186600	-3.79858600	0.14356300
H	-6.50668700	-1.46751600	-0.39567400

PO-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1448.006408
Thermal correction to Gibbs Free Energy (a.u.): 0.414285
No imaginary frequency
Calculation of single point energy based on the optimized structure, E = -2686.6581627 a.u.

C	-4.83987400	-2.18324000	-0.69303800
C	-5.40100500	-0.91614300	-0.43584300
C	-3.47662800	-2.34453500	-0.84951500
H	-5.48961000	-3.05102400	-0.77234400
C	-4.55780100	0.17349000	-0.34979100
C	-2.57934200	-1.24386000	-0.74587000
C	-3.15705000	0.04387900	-0.48974400
H	-4.96615200	1.16524100	-0.16666300
O	-1.30686800	-1.46998300	-0.88841300
C	-2.35650900	1.23332500	-0.42904900
Co	0.06412300	-0.26772400	-0.36778200
N	-1.06835400	1.25824200	-0.41756000
H	-2.90274400	2.17794700	-0.40549900
N	1.42290000	0.93581500	0.21911000
C	-0.27212800	2.48318400	-0.46843700
C	2.68765100	0.67631300	0.17457500
C	0.88428200	2.26424800	0.52775200
C	-1.00400000	3.79679800	-0.20014900
H	3.39486800	1.47880600	0.38969500
C	3.26758100	-0.59799600	-0.12268000
C	1.86973800	3.43269900	0.50001300
C	-0.01385700	4.97001500	-0.22569100
H	-1.49734100	3.74794300	0.78036800
H	-1.78663500	3.95602100	-0.94953000
C	4.67801500	-0.68641700	-0.18975200
C	2.46829800	-1.77543100	-0.30115800
C	1.13637100	4.75565600	0.76457700
H	2.65620200	3.29072800	1.24913600
H	2.35776800	3.46638200	-0.48270100
H	-0.53901200	5.90468200	-0.00217100
H	0.39505400	5.07270400	-1.23939100
C	5.31792400	-1.88415300	-0.43269800
H	5.25811400	0.22303400	-0.04763400
C	3.15726100	-2.99563100	-0.54251800
O	1.17172400	-1.79893500	-0.21261000
H	0.73745800	4.74920100	1.78803600
H	1.84562800	5.58830800	0.71052000
C	4.53581100	-3.04442000	-0.60647200

H	5.02531300	-3.99558100	-0.79922800
C	-0.82389300	-1.92993100	2.00805200
C	0.31446500	-1.19876200	2.57608400
O	-0.55180400	-0.54911700	1.60824600
H	-0.59297200	-2.61879100	1.20041600
H	1.31176700	-1.40700500	2.20394500
H	0.23861400	-0.76694100	3.57139800
C	-2.12245400	-2.12569700	2.73470900
H	-2.95495600	-2.09050500	2.02636700
H	-2.13137100	-3.10579200	3.22350800
H	-2.27026700	-1.35305900	3.49441700
O	0.58788600	0.05862400	-2.08511000
H	0.16985500	-0.66777000	-2.56928600
H	0.43419100	2.20068200	1.53041900
H	0.17042800	2.49754400	-1.47336500
H	2.55202600	-3.88544100	-0.68038900
H	6.39993000	-1.93460700	-0.48799900
H	-3.04107100	-3.31758900	-1.05160400
H	-6.47286000	-0.80002100	-0.31817600

The basis set for Sb is Lanl2DZ.

$CH_3CHSbF_6CH_2OH$

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -798.235181

Thermal correction to Gibbs Free Energy (a.u.): 0.074753

No imaginary frequency

Calculation of single point energy based on the optimized structure, E = -1033.6376489 a.u.

C	2.35630200	0.56374600	0.43197000
C	2.69088600	-0.57840400	-0.50707800
O	2.64432200	-1.82286200	0.14387100
H	2.93700600	0.49202800	1.35186500
H	3.72085200	-0.40663100	-0.84406600
H	2.03838700	-0.53342200	-1.38496800
C	2.28629100	1.94952000	-0.14519400
H	1.95408100	2.66589100	0.60856900
H	3.28766700	2.23890600	-0.47966300
H	1.60456200	1.97901000	-0.99556700
H	1.71145000	-2.08458200	0.17520900
Sb	-0.88938400	-0.02118000	-0.02956600
F	0.01897300	0.42555800	-1.58674500
F	-1.04604700	1.77909700	0.32071800
F	0.97672000	0.26152200	0.99107700
F	-1.38910900	-0.44104300	1.68673600
F	-0.17450000	-1.73197900	-0.22152000
F	-2.50280300	-0.32618900	-0.82945000

Salen ligand structure is unsimplified and represented by aCo^{III}.

H_2O-aCo^{III}-SbF_6

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2488.886482

Thermal correction to Gibbs Free Energy (a.u.): 0.775762

No imaginary frequency

Calculation of single point energy based on the optimized structure, E = -3963.2503729 a.u.

C	-5.03016300	1.66026800	0.21289100
C	-5.61928900	0.37380600	0.20218000
C	-3.68970600	1.92398800	-0.02437700
H	-5.67605100	2.49912700	0.43646000
C	-4.77752700	-0.68458000	-0.05587400
C	-2.83160600	0.81577600	-0.33301400
C	-3.40038800	-0.49036800	-0.32686800
H	-5.14965700	-1.70342500	-0.06020500
O	-1.56557500	1.04353400	-0.61647700
C	-2.62535400	-1.66591900	-0.57261400
Co	-0.25127600	-0.20609100	-1.14629300
N	-1.38005100	-1.71743000	-0.91074800
H	-3.15950600	-2.60890800	-0.46037800

N	1.03534100	-1.45180500	-1.76812500
C	-0.65123800	-2.98772700	-1.06099500
C	2.30582000	-1.27352900	-1.62355300
C	0.42162800	-2.73241300	-2.13078700
C	-1.48610300	-4.22001100	-1.40570900
H	2.97112200	-2.11512000	-1.80699100
C	2.92303800	-0.05062900	-1.21205500
C	1.35859500	-3.93125900	-2.25709700
C	-0.56364600	-5.43828200	-1.57046200
H	-2.04892800	-4.03754300	-2.33139800
H	-2.21223300	-4.42576000	-0.61333800
C	4.27109600	-0.11624300	-0.80408000
C	2.20402500	1.17681300	-1.19775200
C	0.54190000	-5.18551300	-2.60241800
H	2.11246700	-3.75015000	-3.03129500
H	1.88145000	-4.07227200	-1.30397700
H	-1.15670900	-6.31330700	-1.85577900
H	-0.10592800	-5.66885300	-0.60014400
C	4.93606600	1.00825800	-0.36186700
H	4.75231500	-1.08758200	-0.80345100
C	2.90168700	2.36065700	-0.81858200
O	0.92592200	1.23012100	-1.55625700
H	0.09253500	-5.06216100	-3.59708000
H	1.20698500	-6.05292100	-2.66408100
C	4.22420400	2.22589100	-0.41010200
H	4.74224900	3.11670000	-0.08058000
H	-0.13609900	-3.15808300	-0.11264900
H	-0.09429300	-2.57177600	-3.08825700
Sb	1.07737200	-1.38084800	2.10438300
F	1.79328500	-2.54668000	0.81815300
F	-0.53762600	-2.29849300	1.92401200
F	0.41865000	-0.24299000	0.62506300
F	0.27194200	-0.12782500	3.19446100
F	2.62912300	-0.37724800	1.98867600
F	1.66729400	-2.43920600	3.49231800
C	2.19532300	3.72299900	-0.79934600
C	3.14488800	4.86674800	-0.40207200
H	2.59317100	5.81155100	-0.42137100
H	3.53885800	4.73985100	0.61121100
H	3.98924300	4.96081800	-1.09352700
C	1.05239200	3.66926200	0.23374400
H	0.34915300	2.87574000	-0.00695900
H	1.44883600	3.48334500	1.23709700
H	0.51273300	4.62229600	0.25052900
C	1.63223600	4.05485200	-2.19932500
H	2.43830000	4.10189900	-2.93986400
H	0.90846400	3.30569500	-2.51945600
H	1.13300800	5.02974100	-2.17952200
C	6.34544000	0.97409100	0.23511100
C	6.97428400	-0.42545400	0.14129500
H	6.39542600	-1.16585800	0.70194000
H	7.05554400	-0.76314900	-0.89750200
H	7.98319300	-0.40581100	0.56454700
C	6.24031500	1.36199100	1.72749900
H	7.22204500	1.30489700	2.21082100
H	5.86438000	2.38230100	1.84911500
H	5.55107200	0.69053300	2.24832600
C	7.26481300	1.96994700	-0.50188500
H	6.88867000	2.99521400	-0.44216200
H	8.26722400	1.95971600	-0.06048100
H	7.35519900	1.70703400	-1.56092100
C	-3.11845500	3.34249900	0.11900300
C	-2.17321400	3.34568000	1.34280400
H	-1.69291000	4.32352800	1.45255900
H	-2.74325700	3.14225200	2.25504300
H	-1.39586900	2.58792300	1.25217500
C	-2.37174400	3.78008800	-1.16250000
H	-1.51907300	3.13779800	-1.37104700
H	-3.05209000	3.76301400	-2.02264200

H	-2.00691400	4.80622200	-1.04733500
C	-4.21906800	4.38783000	0.37653600
H	-4.94314100	4.43311700	-0.44436300
H	-4.76182200	4.19606100	1.30742100
H	-3.75785800	5.37582600	0.46703300
C	-7.11673700	0.22294600	0.48925100
C	-7.56653700	-1.24580500	0.43501600
H	-7.38937300	-1.68636500	-0.55165900
H	-7.04814200	-1.85468100	1.18266500
H	-8.63936400	-1.31228400	0.64006200
C	-7.42790600	0.77382900	1.89801100
H	-7.16358800	1.83146300	1.98691900
H	-8.49661300	0.67753400	2.11883100
H	-6.86836900	0.22439400	2.66130600
C	-7.92249700	1.01687700	-0.56187500
H	-8.99693000	0.92882900	-0.36706200
H	-7.66775000	2.08058200	-0.54848900
H	-7.72492100	0.63802400	-1.56977800
O	-0.85731500	0.16291100	-2.97651500
H	-0.09508400	0.75960400	-3.14753600
H	-1.58743700	0.77100200	-2.75323400

(salen)aCo^{III}(S,S)-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2702.579765
No imaginary frequency

S	-0.73545600	1.38121100	2.28437700
O	0.02429500	1.70384300	3.50103700
O	-1.36241800	2.51960900	1.56897800
O	0.10580600	0.51023300	1.33365600
C	-2.05229600	0.25584900	2.73517100
C	-1.83656600	-0.66288100	3.76250300
C	-3.24242200	0.24965100	2.01213100
C	-2.82064300	-1.60386800	4.05342600
H	-0.91007000	-0.62617800	4.32449600
C	-4.21701700	-0.69923100	2.31329300
H	-3.39869000	0.97717900	1.22591200
C	-4.01878100	-1.64470600	3.32616300
H	-2.65604000	-2.32179200	4.85257900
H	-5.14067500	-0.71210600	1.74472800
C	-5.05340400	-2.70755400	3.60026900
H	-4.82531600	-3.62558200	3.04397000
H	-5.08768400	-2.97191800	4.66138800
H	-6.05225200	-2.38096100	3.29682500
N	1.87092200	2.01610500	-0.25969800
N	-0.51803800	2.12171200	-1.19691600
C	3.12686000	1.80384700	-0.02210500
H	3.74217200	2.65813400	0.25886600
C	-1.78922300	2.02618100	-1.44303700
H	-2.33257500	2.93773600	-1.68546000
C	3.80510600	0.55139400	-0.11029100
C	5.19066900	0.53116200	0.17811800
C	3.12972100	-0.63155100	-0.52772900
C	5.92906300	-0.62667000	0.06348400
H	5.65343100	1.45910300	0.49588200
C	3.88981600	-1.83843900	-0.67703300
C	5.24009200	-1.78657500	-0.37066800
H	5.81522100	-2.69829600	-0.46556300
C	-2.56647700	0.83556300	-1.39769200
C	-3.96821900	0.95791600	-1.56653700
C	-1.96533200	-0.44061900	-1.18552500
C	-4.79570400	-0.14015400	-1.49295900
H	-4.36942200	1.94966400	-1.74357500
C	-2.82079900	-1.58625700	-1.05849600
C	-4.18104100	-1.39018900	-1.22095100
H	-4.83043300	-2.24999700	-1.12089800
O	1.84725700	-0.64771400	-0.79356000
O	-0.66956500	-0.59614400	-1.11975200

C	1.23640600	3.33484400	-0.10792200
C	2.15373400	4.55474000	-0.10644500
C	0.19253600	3.41506700	-1.22907300
C	1.30308500	5.82654200	0.03978800
H	2.73450000	4.58852300	-1.03869800
H	2.86545300	4.49858100	0.72338500
C	-0.66988300	4.66732500	-1.07028300
C	0.22539200	5.91606400	-1.04648900
H	1.94989800	6.70941700	0.00683100
H	0.82369300	5.81956700	1.02650500
H	-1.38604700	4.75558600	-1.89402500
H	-1.23644500	4.57642400	-0.13645500
H	0.70665100	6.03420200	-2.02709500
H	-0.39314600	6.80622300	-0.89243100
Co	0.57329100	0.68192900	-0.61951600
H	0.73237700	3.46174500	-2.18735100
H	0.67623700	3.30294600	0.83344200
C	3.21055600	-3.13682900	-1.13675600
C	4.20903300	-4.30342500	-1.23618300
H	4.66596200	-4.53712500	-0.26882000
H	3.67881700	-5.19904200	-1.57343200
H	5.00815300	-4.10174400	-1.95763300
C	2.58628700	-2.93480200	-2.53671400
H	1.84246600	-2.13882800	-2.52650700
H	3.36098500	-2.68315900	-3.26955300
H	2.09932000	-3.86003200	-2.86326000
C	2.11782600	-3.53580200	-0.11966800
H	2.55760100	-3.70544800	0.86895700
H	1.35689000	-2.76311100	-0.03249900
H	1.63258000	-4.46446200	-0.43938400
C	7.42656300	-0.71305600	0.37636700
C	7.99965600	0.64044600	0.82580800
H	7.89034900	1.40384000	0.04852900
H	7.51221100	1.00296200	1.73649100
H	9.06768200	0.53693700	1.04022000
C	8.18978300	-1.16832300	-0.88667500
H	9.26260400	-1.24292400	-0.67807500
H	7.84960200	-2.14754700	-1.23555000
H	8.04839000	-0.45420500	-1.70414700
C	7.65294100	-1.73663400	1.51053400
H	7.29677500	-2.73309300	1.23398600
H	8.72004000	-1.81661600	1.74504200
H	7.12347800	-1.43237800	2.41869600
C	-2.23201800	-2.95697100	-0.69838300
C	-3.32677100	-4.02904100	-0.55648000
H	-4.04402300	-3.77594000	0.23180500
H	-3.87702400	-4.18695900	-1.49057200
H	-2.86067800	-4.98057200	-0.28381300
C	-1.25625900	-3.42072100	-1.80278500
H	-1.77467600	-3.50502700	-2.76458000
H	-0.42624900	-2.72530400	-1.91279300
H	-0.85092100	-4.40643700	-1.54951500
C	-1.50431800	-2.85629000	0.66297400
H	-1.03111300	-3.81589700	0.89874900
H	-0.73773100	-2.08307900	0.66035000
H	-2.21570500	-2.62202400	1.45824200
C	-6.31434200	-0.07187200	-1.68828300
C	-6.79083300	1.35602900	-1.99898700
H	-6.55760500	2.04646600	-1.18204100
H	-6.33644200	1.74192200	-2.91719000
H	-7.87625100	1.36214200	-2.13761700
C	-6.71402400	-0.98496100	-2.86829400
H	-6.43740600	-2.02728900	-2.68614600
H	-7.79712300	-0.94965700	-3.02836100
H	-6.22007700	-0.66426700	-3.79081300
C	-7.02998900	-0.55042500	-0.40665600
H	-8.11562200	-0.55055500	-0.55269900
H	-6.73151200	-1.56547200	-0.12863300
H	-6.80192400	0.11227100	0.43405700

(salen)aCo^{III}(R,S)-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2702.578609
No imaginary frequency

S	0.28364700	0.77604400	2.86287000
O	1.13467100	0.34492600	3.97835700
O	-0.18339500	2.18285100	2.86568000
O	0.94437300	0.39462700	1.52844900
C	-1.19276100	-0.23965800	2.88441700
C	-1.07531700	-1.60660300	3.13596200
C	-2.43541500	0.32426300	2.60771700
C	-2.21031900	-2.40974500	3.07766700
H	-0.10488900	-2.02460900	3.37959700
C	-3.56164600	-0.49296200	2.53807400
H	-2.50454000	1.39435900	2.45602500
C	-3.46363700	-1.87188000	2.75312500
H	-2.12196900	-3.47572400	3.26919900
H	-4.52645100	-0.05555000	2.29871000
C	-4.66821900	-2.76336400	2.59214600
H	-4.81226100	-3.02324200	1.53574000
H	-4.55611800	-3.69722000	3.15008400
H	-5.58435800	-2.26991200	2.92997500
N	1.74162100	2.26164500	-0.41964500
N	-0.79833400	2.26383100	-0.20092500
C	3.01565700	2.08627500	-0.25007500
H	3.63589200	2.97745000	-0.12301200
C	-2.08646000	2.12422900	-0.29101600
H	-2.70168200	3.00763400	-0.12555000
C	3.68046900	0.82939700	-0.26269800
C	5.05911300	0.80089000	0.05374300
C	3.00237100	-0.34640200	-0.71214000
C	5.79108700	-0.36070100	-0.05091600
H	5.51821600	1.72329200	0.39147900
C	3.77016500	-1.54715700	-0.88222800
C	5.10920800	-1.50715100	-0.53208200
H	5.68318700	-2.41918600	-0.62903100
C	-2.80060400	0.93025700	-0.58411900
C	-4.21425800	1.01331500	-0.62916100
C	-2.12990900	-0.30866300	-0.80770700
C	-4.98730500	-0.09232000	-0.89795400
H	-4.66806400	1.97893600	-0.43438600
C	-2.92432700	-1.46018600	-1.14033400
C	-4.29968100	-1.30593300	-1.15749400
H	-4.90151500	-2.17436400	-1.39082400
O	1.72686700	-0.34504700	-1.01056500
O	-0.83097400	-0.42228000	-0.72308500
C	1.15995400	3.59577800	-0.55845200
C	0.97563500	3.93438500	-2.04706500
C	-0.17431600	3.55137700	0.19649400
C	0.18312300	5.23238100	-2.23687200
H	0.44214200	3.10318300	-2.52522800
H	1.95968700	3.99482500	-2.52462600
C	-0.99868800	4.81878600	-0.04909500
C	-1.17907000	5.14899000	-1.53606800
H	0.05447400	5.43468700	-3.30527600
H	0.75324700	6.07570200	-1.82327900
H	-1.95754100	4.76469500	0.47602200
H	-0.45288400	5.63725700	0.43652800
H	-1.78840700	4.37787800	-2.02417300
H	-1.72281600	6.09345400	-1.64329300
Co	0.46632500	0.86774800	-0.39073500
H	1.81763900	4.33845700	-0.08882600
C	3.11199600	-2.82877700	-1.40953700
C	4.11112100	-3.99506300	-1.50538900
H	4.52618400	-4.26144000	-0.52778600
H	3.59250600	-4.87710500	-1.89292600
H	4.94007800	-3.77423200	-2.18640300

C	2.55404600	-2.57458600	-2.82854900
H	1.82531800	-1.76483200	-2.82870100
H	3.36521900	-2.31591100	-3.51810200
H	2.06479500	-3.47935100	-3.20519200
C	1.97738800	-3.25693000	-0.45425400
H	2.37666700	-3.47307100	0.54222400
H	1.22490400	-2.47764800	-0.36087900
H	1.49526700	-4.16483800	-0.83244500
C	7.27456900	-0.46569300	0.31544100
C	7.84155100	0.87553200	0.80729900
H	7.77081800	1.65115700	0.03756500
H	7.32134400	1.22913800	1.70305800
H	8.89916300	0.75825500	1.06227000
C	8.08126700	-0.90964300	-0.92440900
H	9.14439400	-0.99703200	-0.67544400
H	7.74701800	-1.88074400	-1.30067100
H	7.97818100	-0.18238700	-1.73608800
C	7.44589400	-1.50827500	1.44209300
H	7.09323800	-2.49727200	1.13577600
H	8.50206500	-1.60078800	1.71775500
H	6.88216900	-1.21319900	2.33224500
C	-2.26346400	-2.81230700	-1.44396300
C	-3.28984400	-3.86690900	-1.89514400
H	-4.02704700	-4.08673200	-1.11565300
H	-3.82362600	-3.56075200	-2.80129800
H	-2.76565500	-4.80098200	-2.11805000
C	-1.23042500	-2.65535400	-2.58275600
H	-1.71476700	-2.28467800	-3.49320600
H	-0.43457600	-1.96814600	-2.30442000
H	-0.78276500	-3.62840500	-2.81141600
C	-1.58004500	-3.34116500	-0.16570800
H	-1.02980500	-4.26184900	-0.38706600
H	-0.88612500	-2.61227700	0.24957000
H	-2.32900700	-3.56511400	0.59788700
C	-6.51835200	-0.06776200	-0.94365800
C	-7.08028800	1.32741000	-0.62745800
H	-6.78803900	1.66284700	0.37297400
H	-6.74213200	2.07373800	-1.35356800
H	-8.17362800	1.30309800	-0.66266800
C	-6.99587600	-0.47689300	-2.35421100
H	-6.65645000	-1.48173100	-2.62126500
H	-8.09013700	-0.46983100	-2.40417200
H	-6.61356000	0.21718600	-3.10926900
C	-7.07970500	-1.06162600	0.09603800
H	-8.17464400	-1.06758100	0.06624800
H	-6.73555400	-2.08275700	-0.09007100
H	-6.76674700	-0.78416600	1.10715400
H	0.03138600	3.43523700	1.26521300

(salen)aCo^{III}(S,R)-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2702.571131
No imaginary frequency

S	-0.76331200	1.40755800	2.14904200
O	-0.01904500	1.84071400	3.34107800
O	-1.52920000	2.45384800	1.43009500
O	0.15179300	0.61341300	1.20164100
C	-1.95393000	0.17316500	2.66435500
C	-1.60971900	-0.72393300	3.67580200
C	-3.18812500	0.08662100	2.02507700
C	-2.51027600	-1.72189000	4.03775000
H	-0.65224700	-0.62419800	4.17482300
C	-4.07921600	-0.91781700	2.39796300
H	-3.44312100	0.79939200	1.25088300
C	-3.75304800	-1.84026400	3.39884200
H	-2.24602400	-2.42240700	4.82553500
H	-5.03898700	-0.99097000	1.89696200
C	-4.69930300	-2.96054000	3.75199200

H	-4.46202800	-3.86591500	3.17906800
H	-4.63539500	-3.22199800	4.81242800
H	-5.73614800	-2.69399100	3.52757300
N	1.89265000	2.10220200	-0.61177700
N	-0.55718100	2.17557300	-1.29861400
C	3.15131400	1.89386600	-0.35214800
H	3.77648600	2.77829500	-0.20545200
C	-1.83308500	2.03983300	-1.50352900
H	-2.40328200	2.93360300	-1.75156200
C	3.81348100	0.64129100	-0.27276200
C	5.19724200	0.64024200	0.03620600
C	3.12896100	-0.57216200	-0.58551700
C	5.92597600	-0.52641800	0.03910200
H	5.66168000	1.59124000	0.27281300
C	3.89255800	-1.78912300	-0.63838700
C	5.23558800	-1.71576100	-0.31398700
H	5.80914000	-2.63318500	-0.33033700
C	-2.58512800	0.83631000	-1.41726500
C	-3.99369100	0.93262200	-1.53187100
C	-1.95157100	-0.42695300	-1.23112300
C	-4.79636400	-0.18177600	-1.43016600
H	-4.42043600	1.91724400	-1.68672300
C	-2.77794000	-1.59229200	-1.08990900
C	-4.14727800	-1.42169500	-1.19703300
H	-4.77500800	-2.29544700	-1.08161200
O	1.85155000	-0.59925900	-0.84940200
O	-0.65031300	-0.54872700	-1.20596100
C	1.41412200	3.49376700	-0.67218000
C	1.28662600	4.13021900	0.71719400
C	0.07355100	3.50954700	-1.44008700
C	0.94864200	5.62791500	0.57928700
H	2.21888200	3.99186900	1.27278400
H	0.50400500	3.61720000	1.27475600
C	-0.82690200	4.66644600	-0.96134500
C	0.02291900	5.89901100	-0.62954200
H	1.86615900	6.21866000	0.47654200
H	0.46341600	5.95820900	1.50262900
H	-1.56460700	4.91568100	-1.73052300
H	-1.36455600	4.33111200	-0.06881500
H	0.61835700	6.17270600	-1.51060000
H	-0.62870500	6.75415700	-0.42689700
Co	0.58018700	0.76422500	-0.77133400
H	0.30223300	3.64018200	-2.50641200
C	3.22541200	-3.11491200	-1.02937200
C	4.22771500	-4.28221500	-1.04579400
H	4.66817500	-4.45996000	-0.05907500
H	3.70449100	-5.19675100	-1.34055500
H	5.03880000	-4.11986300	-1.76381500
C	2.62525100	-2.99340900	-2.44903000
H	1.88504800	-2.19549800	-2.49782600
H	3.41320900	-2.78757000	-3.18199200
H	2.13905900	-3.93393200	-2.72933300
C	2.11769100	-3.45568500	-0.00972600
H	2.54191100	-3.57483300	0.99297500
H	1.36178200	-2.67507500	0.02461400
H	1.63123300	-4.39721400	-0.28714200
C	7.41606500	-0.59732700	0.38730300
C	7.99077800	0.78429100	0.73815600
H	7.90593200	1.48232300	-0.10114000
H	7.48588400	1.22330900	1.60456600
H	9.05273800	0.69124700	0.98490800
C	8.20036800	-1.15769800	-0.81934100
H	9.26814700	-1.22178300	-0.58338500
H	7.86004600	-2.15985700	-1.09530500
H	8.08095100	-0.51080500	-1.69423900
C	7.61101200	-1.52788500	1.60444100
H	7.25153800	-2.54085300	1.40193000
H	8.67260600	-1.59636400	1.86586500
H	7.06681600	-1.14757100	2.47440100

C	-2.15227200	-2.95527600	-0.76559800
C	-3.21813200	-4.05647700	-0.62705700
H	-3.92483600	-3.83983500	0.18119500
H	-3.78320400	-4.20609100	-1.55365200
H	-2.72361600	-5.00214100	-0.38571900
C	-1.18143500	-3.37703500	-1.89050600
H	-1.71015400	-3.45549600	-2.84720200
H	-0.36865000	-2.66162300	-1.99774800
H	-0.75157400	-4.35802400	-1.66042500
C	-1.40979400	-2.85739900	0.58709000
H	-0.89692400	-3.80229000	0.79640100
H	-0.67388400	-2.05482400	0.59040400
H	-2.11834100	-2.66730500	1.39548500
C	-6.32343100	-0.13941800	-1.55045000
C	-6.83954000	1.28180900	-1.82658800
H	-6.57860100	1.97066000	-1.01677900
H	-6.43769400	1.68201800	-2.76301000
H	-7.93037900	1.26933000	-1.91191800
C	-6.76715700	-1.05258900	-2.71433300
H	-6.46225200	-2.09069000	-2.55452200
H	-7.85760200	-1.03675200	-2.81729400
H	-6.32846500	-0.71686800	-3.65919300
C	-6.96255800	-0.63761000	-0.23616200
H	-8.05470400	-0.64373200	-0.32048200
H	-6.64236800	-1.65396300	0.01124100
H	-6.69010500	0.01621700	0.59827600
H	2.14428800	4.07332800	-1.25238500

(salen)aCo^{III}(R,R)-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2702.570789
No imaginary frequency

S	0.55844000	1.72089200	2.17086600
O	1.04489900	1.48548400	3.53403100
O	0.95943500	2.99907000	1.52861500
O	0.85179100	0.50742900	1.27880800
C	-1.23864600	1.73492800	2.20117200
C	-1.92625700	0.52844500	2.35140900
C	-1.93652800	2.93111800	2.05790600
C	-3.31613700	0.52341900	2.32967900
H	-1.37022800	-0.39551500	2.45090400
C	-3.33247100	2.91259700	2.03299700
H	-1.38402300	3.85920200	1.96064800
C	-4.04066700	1.71260300	2.16302900
H	-3.84841800	-0.42005800	2.41362700
H	-3.87942700	3.84494800	1.91688600
C	-5.54581900	1.68491800	2.09255300
H	-5.87743700	1.25036400	1.14308600
H	-5.97209600	1.07088500	2.89256300
H	-5.97240500	2.68852500	2.17117300
N	1.55411700	1.69428000	-1.20070400
N	-0.99792500	1.54244100	-1.06023100
C	2.83385000	1.64773300	-1.00224600
H	3.41119900	2.55534000	-1.17340400
C	-2.27089000	1.27456500	-1.13226200
H	-2.94633200	2.10003300	-1.35020400
C	3.57615700	0.49556900	-0.61314100
C	4.95345400	0.66152100	-0.34017400
C	2.97979100	-0.80034500	-0.61593900
C	5.76105600	-0.41824200	-0.05592600
H	5.35163400	1.66990300	-0.35144500
C	3.81754800	-1.93641900	-0.36287200
C	5.15381600	-1.69796700	-0.08520500
H	5.78377100	-2.55014000	0.13297100
C	-2.88807900	0.01452300	-0.92114800
C	-4.29887400	-0.05548800	-1.04396200
C	-2.12672500	-1.12861100	-0.53627700
C	-4.98285400	-1.21922200	-0.77914000

H	-4.82239500	0.84487800	-1.34664300
C	-2.83440100	-2.33965400	-0.21859700
C	-4.21108200	-2.33266700	-0.35377200
H	-4.74549600	-3.24347500	-0.11793200
O	1.70676300	-0.97579200	-0.87915600
O	-0.82545000	-1.10503600	-0.44930900
C	0.89484800	2.89934200	-1.72743700
C	1.60262700	4.23175700	-1.41841100
C	-0.51909400	2.93067300	-1.15291900
C	0.59645500	5.40830900	-1.43643200
H	2.40066100	4.40647600	-2.14785000
H	2.04908000	4.15863800	-0.42376800
C	-1.39932900	3.90932100	-1.94261000
C	-0.57326000	5.14070800	-2.39163200
H	1.11294900	6.33190600	-1.71433000
H	0.20791600	5.56289600	-0.42361400
H	-1.82466100	3.40805300	-2.82039800
H	-2.23687600	4.22905700	-1.31362400
H	-0.17889500	4.97062400	-3.40084100
H	-1.22390100	6.01770300	-2.46061400
Co	0.37878500	0.29446900	-0.70226900
C	3.23267400	-3.35490500	-0.35086300
C	4.30553400	-4.42100500	-0.06766300
H	4.76589400	-4.28971100	0.91699000
H	3.83707600	-5.40971800	-0.08078600
H	5.09741900	-4.42040000	-0.82444400
C	2.60654900	-3.67936100	-1.72626900
H	1.81969500	-2.97063900	-1.98158900
H	3.37099000	-3.65062700	-2.51069300
H	2.17542400	-4.68619200	-1.71102200
C	2.16832700	-3.44780000	0.76415000
H	2.62137300	-3.25666400	1.74229200
H	1.37224300	-2.72342100	0.60911400
H	1.72943500	-4.45124600	0.78105600
C	7.24998200	-0.29797200	0.28305500
C	7.72913500	1.16226300	0.25870300
H	7.60163400	1.61320700	-0.73097100
H	7.19226200	1.77533800	0.98939800
H	8.79385100	1.20570600	0.50739500
C	8.07824300	-1.09894100	-0.74521700
H	9.14609900	-1.02901200	-0.51128500
H	7.80714400	-2.15857100	-0.74848400
H	7.92297200	-0.71032300	-1.75675700
C	7.49616100	-0.86644100	1.69795100
H	7.20947400	-1.91971000	1.76683000
H	8.55741100	-0.79117500	1.95909500
H	6.91785000	-0.31307800	2.44398600
C	-2.07623300	-3.57772100	0.27794800
C	-3.02285100	-4.75554300	0.56903300
H	-3.75308600	-4.51485200	1.34896200
H	-3.56488100	-5.07890500	-0.32607300
H	-2.43395600	-5.60695100	0.92272800
C	-1.06970600	-4.04194500	-0.79850700
H	-1.59675600	-4.31336600	-1.71990800
H	-0.34502100	-3.26325900	-1.02641200
H	-0.52810300	-4.92622100	-0.44642600
C	-1.34553900	-3.23061000	1.59585700
H	-0.78322600	-4.09921600	1.95382500
H	-0.64829000	-2.40443100	1.46352300
H	-2.07075800	-2.95754700	2.37058900
C	-6.50160800	-1.36855100	-0.91708300
C	-7.16686700	-0.07540000	-1.41514000
H	-7.01829500	0.75625600	-0.71913100
H	-6.78092500	0.22418500	-2.39478200
H	-8.24540600	-0.22990000	-1.51562600
C	-6.81141500	-2.48933900	-1.93412700
H	-6.39490500	-3.45013000	-1.61892700
H	-7.89390900	-2.61522600	-2.04469900
H	-6.39191600	-2.24872500	-2.91600300

C	-7.11190600	-1.73854000	0.45258400
H	-8.19690400	-1.86172100	0.36629500
H	-6.70056100	-2.67545900	0.83890900
H	-6.91467000	-0.95681600	1.19210200
H	-0.41676300	3.27071100	-0.11921500
H	0.81657500	2.75659300	-2.81535300

PO(R)-aCo^{III}(S,S)-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2895.653423
No imaginary frequency

C	4.94989400	-1.90070800	0.06007300
C	5.67475700	-0.73505600	0.39198400
C	3.57572800	-1.94843900	-0.14100200
H	5.50040300	-2.82542000	-0.03047900
C	4.93497400	0.41902700	0.55991300
C	2.83161600	-0.72122000	-0.06215700
C	3.53990100	0.45328300	0.34637800
H	5.42063300	1.34358300	0.86256900
O	1.56068900	-0.72002200	-0.35434400
C	2.87635400	1.69522900	0.60636200
Co	0.44776600	0.80227000	-0.54584100
N	1.63560800	1.96434000	0.37975800
H	3.49910200	2.47591000	1.04353900
N	-0.62587900	2.34973400	-0.79871000
C	1.02140400	3.25922800	0.69290900
C	-1.90080200	2.30406100	-0.98869800
C	0.10502400	3.58619200	-0.50105300
C	1.96497600	4.42178800	0.99292900
H	-2.46516700	3.23436700	-0.94866400
C	-2.66505800	1.11416700	-1.21778300
C	-0.73446600	4.82849900	-0.21009300
C	1.14259500	5.68966400	1.27052200
H	2.63958300	4.58547000	0.14090600
H	2.58544300	4.19202100	1.86510300
C	-4.07106400	1.23603900	-1.15365800
C	-2.04054300	-0.14406000	-1.46695000
C	0.18763800	6.01345400	0.11520900
H	-1.36544000	5.07884000	-1.07036000
H	-1.39376100	4.61241100	0.63875700
H	1.81470600	6.53437600	1.45513400
H	0.56121800	5.54003900	2.18895100
C	-4.89619300	0.13928300	-1.29836000
H	-4.48150900	2.22003500	-0.95506000
C	-2.88901000	-1.29171400	-1.60667700
O	-0.73794100	-0.25809000	-1.59169300
H	0.77266600	6.27150600	-0.77837300
H	-0.41605000	6.89391500	0.35897300
C	-4.26177600	-1.10446200	-1.52359300
H	-4.89675900	-1.97591900	-1.61741900
C	1.82490200	0.18182200	-3.12499900
C	0.87723200	1.22715600	-3.52797600
O	1.47981900	1.26935800	-2.20103800
H	1.38581100	-0.75482400	-2.80257200
H	-0.18213200	0.99592600	-3.51192800
H	1.20589300	2.04967300	-4.15799100
C	3.26781100	0.14897400	-3.53024700
H	3.87261800	-0.24454300	-2.70829500
H	3.39285600	-0.51240000	-4.39390200
H	3.63000500	1.14637300	-3.79393600
H	0.75693100	3.78233500	-1.36575800
H	0.37662900	3.10337000	1.56298800
S	-0.99057300	0.93239600	2.23415800
O	0.09940100	1.11372100	3.20712000
O	-1.78249900	2.14192700	1.91680700
O	-0.51669000	0.19588400	0.95333000
C	-2.10680500	-0.32894100	2.82763300
C	-1.82363500	-0.99964200	4.01159300

C	-3.22431700	-0.65894200	2.05621100
C	-2.67853200	-2.01997000	4.43258200
H	-0.94125400	-0.72603200	4.57895100
C	-4.05894600	-1.68336100	2.48578000
H	-3.42711600	-0.13242700	1.13213600
C	-3.80062600	-2.37840500	3.67859800
H	-2.46387300	-2.55094100	5.35598500
H	-4.92095700	-1.95443200	1.88300000
C	-4.72706500	-3.47798400	4.13460300
H	-4.95956300	-4.16628100	3.31529400
H	-4.28851400	-4.05785100	4.95095800
H	-5.67971000	-3.06854400	4.49174300
C	-2.28150300	-2.69117500	-1.76824900
C	-3.35770200	-3.78677400	-1.86460600
H	-4.01572500	-3.64753200	-2.72942400
H	-2.86798600	-4.75919000	-1.97523300
H	-3.97580100	-3.83202500	-0.96185400
C	-1.41210700	-2.99586700	-0.52821600
H	-0.62877000	-2.25256900	-0.40016500
H	-2.02882700	-2.99639700	0.37618800
H	-0.94903200	-3.98348000	-0.62896100
C	-1.43583400	-2.75812600	-3.05922500
H	-2.06714700	-2.59354100	-3.93991400
H	-0.65059400	-2.00385700	-3.04979800
H	-0.97067600	-3.74536800	-3.15473900
C	-6.42372000	0.20650900	-1.19802800
C	-6.92146400	1.64135800	-0.96128800
H	-6.53406900	2.05309300	-0.02398300
H	-6.62843400	2.30918200	-1.77795000
H	-8.01421900	1.64962200	-0.90106900
C	-6.89739200	-0.66903300	-0.01705700
H	-7.98934700	-0.64159600	0.06924400
H	-6.60009700	-1.71415100	-0.14641100
H	-6.46990300	-0.31082500	0.92459300
C	-7.05149900	-0.31595000	-2.50819200
H	-6.75918700	-1.34986900	-2.71296200
H	-8.14510300	-0.28326100	-2.44944100
H	-6.73564500	0.29538000	-3.35955000
C	7.19675900	-0.72615300	0.59271100
C	7.52565000	-0.27388900	2.03181800
H	7.14271200	0.73023900	2.23623200
H	7.07993700	-0.95535700	2.76299000
H	8.60953400	-0.25748800	2.19288400
C	7.82231600	-2.11329500	0.37080300
H	7.64045800	-2.48278300	-0.64356800
H	8.90593500	-2.05601700	0.51408500
H	7.43322200	-2.85178000	1.07886000
C	7.83759900	0.25714200	-0.41068900
H	8.92559100	0.28692100	-0.28250500
H	7.62247200	-0.04541300	-1.44070800
H	7.45640500	1.27364900	-0.27501900
C	2.85173700	-3.28339900	-0.37714500
C	1.87383300	-3.51763300	0.79831300
H	1.17077600	-2.69123800	0.89941600
H	1.30491900	-4.44061600	0.64030900
H	2.43001900	-3.61748100	1.73636700
C	2.08051800	-3.27307500	-1.71500200
H	1.28696300	-2.53087700	-1.69951800
H	2.75901900	-3.06017600	-2.54976800
H	1.62737400	-4.25423000	-1.89439200
C	3.82722000	-4.47323700	-0.41980000
H	4.54342300	-4.38953800	-1.24472900
H	4.38758900	-4.58039300	0.51442400
H	3.25837500	-5.39614000	-0.56888100

PO(S)-aCo^{III}(S,S)-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2895.652709

No imaginary frequency

Co	0.46376600	0.87224800	-0.49814700
N	1.67726400	1.91161400	0.53212100
N	-0.64950300	2.41234000	-0.45956100
C	-1.93308300	2.36341500	-0.57299800
H	-2.50782000	3.26391800	-0.36196500
C	2.91642400	1.60356200	0.72416500
H	3.54071800	2.31434800	1.26573900
C	-2.69180600	1.20244700	-0.93165000
C	-2.06592800	0.01329500	-1.41185600
C	-4.09296400	1.27998400	-0.76678900
C	-2.90899900	-1.11092700	-1.70062000
C	-4.91105200	0.20275600	-1.03911600
H	-4.50317900	2.20980800	-0.38818900
C	-4.27614700	-0.97093600	-1.50777000
H	-4.90508200	-1.82769700	-1.71249800
C	3.57408300	0.40423800	0.30973300
C	2.86908200	-0.68660100	-0.28524300
C	4.96441500	0.31868900	0.56948100
C	3.60191700	-1.90572900	-0.51467400
C	5.68990100	-0.81230700	0.27066400
H	5.44252500	1.18342900	1.01790600
C	4.96201700	-1.90800200	-0.25546800
H	5.51221100	-2.81934100	-0.45138600
O	-0.77057000	-0.05683200	-1.61571300
O	1.60941600	-0.62821800	-0.61592000
O	1.36392900	1.63748900	-2.12698500
C	0.64304600	1.74909200	-3.39885600
C	1.70776400	0.75329600	-3.23419700
H	-0.37037600	1.37063900	-3.30814100
H	1.44621900	-0.28163100	-3.05229900
C	0.08364100	3.61122200	-0.04177100
C	1.06994700	3.14625400	1.04420500
H	0.68264700	3.92926300	-0.90826800
H	0.47731300	2.87037000	1.92217200
C	2.02043800	4.27624800	1.43590100
H	2.69141400	3.95020200	2.23679700
H	2.64432300	4.55333100	0.57472400
C	-0.74914100	4.79128700	0.45364000
H	-1.43392100	5.13715000	-0.32903500
H	-1.35404300	4.46000000	1.30593700
C	1.20685000	5.48755700	1.91762700
C	0.18125000	5.94025200	0.87141100
H	-0.41308900	6.77378000	1.26012900
H	0.70896900	6.31755800	-0.01545400
H	1.88277000	6.31224100	2.16746200
H	0.68281500	5.21584400	2.84260900
H	2.70216200	0.94867400	-3.62634800
C	0.84234400	3.05616200	-4.10820200
H	0.51648000	2.96661500	-5.14971300
H	0.24498400	3.84158300	-3.63469300
H	1.89332200	3.35693600	-4.09423100
C	-2.29722800	-2.44850000	-2.13635200
C	-3.36638200	-3.52745900	-2.38177500
H	-2.87350800	-4.45460600	-2.69013500
H	-3.94040100	-3.74788800	-1.47573000
H	-4.06633700	-3.24448000	-3.17570200
C	-1.36975400	-2.95115800	-1.00901500
H	-0.59007500	-2.22605900	-0.78812100
H	-1.94319100	-3.12215600	-0.09225100
H	-0.90025300	-3.89631800	-1.30227900
C	-1.50686500	-2.27249000	-3.45211300
H	-2.17437200	-1.95471200	-4.26133500
H	-0.72041100	-1.52822800	-3.33714800
H	-1.04769700	-3.22309700	-3.74492200
C	-6.42939100	0.21550200	-0.83395300
C	-6.93037800	1.58031500	-0.33513700
H	-6.48719200	1.84429400	0.63026400
H	-6.70175000	2.37863500	-1.04875900

H	-8.01670800	1.55172200	-0.20521900
C	-6.81047500	-0.85136600	0.21604100
H	-7.89450600	-0.86581600	0.37504700
H	-6.50707900	-1.85383600	-0.10088200
H	-6.32597100	-0.63969700	1.17428300
C	-7.13559100	-0.10333300	-2.16929100
H	-6.84367000	-1.08316100	-2.55795700
H	-8.22320200	-0.10711300	-2.03679500
H	-6.88542000	0.64508500	-2.92798000
C	2.86905400	-3.18404700	-0.94999300
C	1.88720200	-3.57493000	0.17971900
H	2.44259700	-3.81832900	1.09157500
H	1.19659800	-2.76227500	0.40363100
H	1.30456400	-4.45643800	-0.10962100
C	2.10522800	-2.97579600	-2.27640900
H	1.64968400	-3.91899500	-2.59753300
H	1.31527300	-2.23832300	-2.16032600
H	2.79086900	-2.64883700	-3.06736300
C	3.83564100	-4.36329900	-1.16069400
H	4.56366900	-4.16115500	-1.95416400
H	4.38218300	-4.61714800	-0.24686700
H	3.26198000	-5.24754600	-1.45491900
C	7.19755600	-0.94776700	0.50732800
C	7.80674100	0.33975700	1.08501900
H	7.66244500	1.19115500	0.41179900
H	7.36967600	0.59201400	2.05650400
H	8.88368800	0.20868200	1.22993800
C	7.46410200	-2.09779900	1.50308000
H	7.08584700	-3.05320400	1.12826300
H	8.53950200	-2.21110800	1.68071900
H	6.97610800	-1.89905000	2.46231900
C	7.90063900	-1.25770500	-0.83214100
H	8.98036200	-1.37114500	-0.68324200
H	7.52624100	-2.18305300	-1.27950600
H	7.73684000	-0.44876200	-1.55144400
S	-0.78867500	0.55513100	2.35028600
O	0.35973100	0.61146200	3.26957200
O	-1.61120000	1.78270700	2.26546800
O	-0.39222300	0.02420900	0.94668200
C	-1.85167000	-0.80185000	2.81803400
C	-1.50591800	-1.60974700	3.89473800
C	-2.99656500	-1.05685900	2.05803800
C	-2.32462100	-2.69352100	4.21830300
H	-0.60402300	-1.39064800	4.45504800
C	-3.79457700	-2.14499500	2.38886200
H	-3.24836700	-0.42335400	1.21697000
C	-3.47283300	-2.97859700	3.47262100
H	-2.06077200	-3.33151400	5.05736400
H	-4.67772500	-2.35686500	1.79286300
C	-4.35983200	-4.14722300	3.82312300
H	-4.59947400	-4.74342200	2.93634900
H	-3.88449800	-4.80484700	4.55563000
H	-5.31125400	-3.80677700	4.24914100

(salen)aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2268.072187
No imaginary frequency

C	4.74077300	-1.62706400	-0.02318700
C	5.44460400	-0.39541800	-0.06469300
C	3.36320700	-1.75345400	-0.01332200
H	5.33138800	-2.53302000	0.01816500
C	4.68527200	0.75214600	-0.07589200
C	2.57748100	-0.54928300	-0.08286500
C	3.26877700	0.70203200	-0.08010400
H	5.15354700	1.73085000	-0.07842600
O	1.28012700	-0.63337400	-0.16618400
C	2.57029800	1.94175200	-0.04767900

Co	-0.00418900	0.71292900	-0.08004900
N	1.28125700	2.09819000	-0.05004000
H	3.19465700	2.83418600	-0.00165600
N	-1.26594300	2.08881600	-0.40666100
C	0.64981600	3.40718800	0.17687000
C	-2.55338900	1.93834800	-0.33880100
C	-0.63729600	3.39686300	-0.65607900
C	1.48798300	4.65126400	-0.11480200
H	-3.18298600	2.82417400	-0.42203000
C	-3.24106100	0.69969000	-0.19426400
C	-1.48318300	4.64074700	-0.38317600
C	0.65209600	5.91420600	0.14415000
H	1.82770700	4.62922300	-1.15907000
H	2.38076400	4.67216100	0.51804000
C	-4.64707200	0.74457500	-0.03261900
C	-2.55097000	-0.54741600	-0.30330700
C	-0.65513100	5.90570600	-0.65648600
H	-2.37736200	4.64871300	-1.01471300
H	-1.81992000	4.62514500	0.66141100
H	1.24113900	6.80421900	-0.10029000
H	0.42047100	5.97460500	1.21556800
C	-5.39888600	-0.40730000	0.02573400
H	-5.11411200	1.72059400	0.04626300
C	-3.33281500	-1.75446300	-0.28377600
O	-1.25788600	-0.61269100	-0.46352800
H	-0.42426100	5.95803500	-1.72894400
H	-1.25029700	6.79405500	-0.42119500
C	-4.70093000	-1.63445300	-0.11313600
H	-5.28765000	-2.54330200	-0.08166600
C	-2.65733800	-3.12267500	-0.44651400
C	-3.66977900	-4.27986600	-0.38778400
H	-3.13578500	-5.22710800	-0.51009600
H	-4.19294700	-4.31916500	0.57353400
H	-4.41652600	-4.21702500	-1.18674200
C	-1.63362300	-3.33296900	0.68965000
H	-0.87983000	-2.54960600	0.68860900
H	-2.13572600	-3.33046700	1.66294500
H	-1.13372000	-4.30009100	0.56727000
C	-1.95439500	-3.18682200	-1.82185100
H	-2.68638300	-3.08217100	-2.63047700
H	-1.21007700	-2.39760000	-1.92103000
H	-1.45264900	-4.15321900	-1.94132600
C	2.67906100	-3.12024600	0.12656900
C	1.73467300	-3.38359100	-1.06706500
H	0.95244800	-2.63059700	-1.12521900
H	2.29677300	-3.38124700	-2.00788000
H	1.26465000	-4.36713600	-0.95780700
C	1.89004700	-3.13274100	1.45671200
H	1.16929500	-2.31689600	1.50179200
H	1.35049800	-4.07959400	1.56587600
H	2.57681000	-3.03314300	2.30412600
C	3.69632800	-4.27402300	0.17461400
H	4.29125700	-4.33600300	-0.74319800
H	4.37980300	-4.18748400	1.02581600
H	3.15709800	-5.21997400	0.28269300
C	6.97650900	-0.40280300	-0.06996800
C	7.55875100	1.01887100	-0.11743300
H	7.24049800	1.55521800	-1.01734900
H	7.26123900	1.60641200	0.75717400
H	8.65203600	0.97140500	-0.12811300
C	7.48040900	-1.17469800	-1.30901600
H	8.57563000	-1.19939800	-1.32522900
H	7.12331600	-2.20844500	-1.31462400
H	7.13423800	-0.69658900	-2.23082500
C	7.49231100	-1.09527900	1.21060000
H	7.14062600	-2.12837300	1.28230000
H	8.58773800	-1.11413900	1.22065600
H	7.14961100	-0.56309000	2.10347200
C	-6.91840400	-0.42296800	0.21964100

C	-7.49746900	0.99530200	0.34466900
H	-7.07702800	1.52820700	1.20356400
H	-7.30873700	1.58936100	-0.55555300
H	-8.58148300	0.94180700	0.48505900
C	-7.26074000	-1.20195600	1.50853900
H	-8.34527300	-1.23066800	1.66161600
H	-6.90239900	-2.23435500	1.46441100
H	-6.80262400	-0.72664500	2.38143100
C	-7.58520500	-1.11392800	-0.98999400
H	-7.23839400	-2.14419800	-1.11019300
H	-8.67314600	-1.14069900	-0.86332700
H	-7.36083400	-0.57548600	-1.91626500
H	0.35279600	3.41228200	1.23499900
H	-0.33668600	3.40480000	-1.71555500
Cl	-0.26326300	0.74001400	2.10319600

(salen)aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2268.079933
No imaginary frequency

C	4.75261700	-1.62201700	-0.05363900
C	5.44943100	-0.38769000	-0.12215600
C	3.37680600	-1.75492900	0.01022400
H	5.34769000	-2.52576300	-0.03992200
C	4.68663200	0.75709700	-0.10587500
C	2.58771300	-0.55284700	-0.01059300
C	3.27127600	0.69977900	-0.04599000
H	5.14996200	1.73750500	-0.13456600
O	1.28498000	-0.64108000	0.00059300
C	2.56404900	1.93321700	-0.00413100
Co	-0.00922000	0.69330200	0.02982600
N	1.27435700	2.08217100	0.03336000
H	3.18031900	2.83170700	0.01091900
N	-1.24890700	2.07071800	-0.43481100
C	0.63309500	3.39392400	0.21178400
C	-2.53697600	1.92207900	-0.40688400
C	-0.60476800	3.36764900	-0.69354200
C	1.48798900	4.63301300	-0.04545200
H	-3.16259000	2.80383400	-0.54296100
C	-3.22810400	0.68824100	-0.23961800
C	-1.46310100	4.61702300	-0.49515000
C	0.63584800	5.89724200	0.14679200
H	1.88898400	4.60200900	-1.06780500
H	2.34088100	4.66035900	0.64031300
C	-4.63880000	0.73444800	-0.13112000
C	-2.53585600	-0.55860400	-0.29157500
C	-0.61693300	5.87652500	-0.73628500
H	-2.31670000	4.61434700	-1.18083600
H	-1.86203100	4.61856900	0.52724600
H	1.23833900	6.78536300	-0.06996000
H	0.33637400	5.96849700	1.20035100
C	-5.38912200	-0.41794300	-0.06151900
H	-5.10978500	1.71082800	-0.09631300
C	-3.31181500	-1.76638300	-0.27506300
O	-1.23199300	-0.62886700	-0.39483400
H	-0.31763300	5.91169500	-1.79246600
H	-1.22502300	6.76847100	-0.55374900
C	-4.68529100	-1.64560900	-0.14573700
H	-5.27001600	-2.55519400	-0.10537000
C	-2.63014300	-3.13626800	-0.39259500
C	-3.64293900	-4.29337800	-0.33326700
H	-3.10539800	-5.24189000	-0.42593900
H	-4.18597700	-4.31484900	0.61744700
H	-4.37243100	-4.24730200	-1.14907700
C	-1.63104700	-3.32664100	0.76936700
H	-0.87233000	-2.54790900	0.77213500
H	-2.15371100	-3.30191000	1.73118400
H	-1.13424500	-4.29865500	0.67682700

C	-1.90220500	-3.22354700	-1.75351900
H	-2.62099400	-3.14359700	-2.57659700
H	-1.16346300	-2.42982900	-1.85845300
H	-1.38905200	-4.18697700	-1.84339900
C	2.70295200	-3.12647500	0.15273800
C	1.72480700	-3.36794100	-1.01770200
H	0.94508400	-2.61054100	-1.04206900
H	2.25991800	-3.35459900	-1.97396300
H	1.25161700	-4.34990200	-0.90952000
C	1.95261200	-3.17092800	1.50438600
H	1.22099500	-2.36760500	1.58465000
H	1.43027700	-4.12764100	1.61176400
H	2.66103100	-3.07585100	2.33419900
C	3.72602200	-4.27603000	0.14752200
H	4.29263300	-4.31836100	-0.78910500
H	4.43480100	-4.20213200	0.97899400
H	3.19416800	-5.22621800	0.25425100
C	6.97993400	-0.38977300	-0.18982700
C	7.55467200	1.03403100	-0.25906800
H	7.20021500	1.56971400	-1.14577500
H	7.28940300	1.62007300	0.62682000
H	8.64680100	0.99029700	-0.31223800
C	7.43559400	-1.15892600	-1.44907800
H	8.52927200	-1.17934400	-1.50956700
H	7.08279500	-2.19415300	-1.44118500
H	7.05072900	-0.68145800	-2.35575400
C	7.54860300	-1.08178600	1.06837500
H	7.20365900	-2.11619600	1.15295200
H	8.64351700	-1.09690200	1.03421400
H	7.24042600	-0.55169500	1.97492500
C	-6.91350700	-0.43222400	0.08977400
C	-7.49818600	0.98761700	0.15749400
H	-7.10286600	1.54615800	1.01194500
H	-7.28611300	1.55585000	-0.75417600
H	-8.58549300	0.93511600	0.26934200
C	-7.28928800	-1.17456700	1.39091600
H	-8.37750600	-1.20031800	1.51511600
H	-6.92936700	-2.20734900	1.38601000
H	-6.85523200	-0.67391300	2.26181900
C	-7.54413500	-1.15989700	-1.11765200
H	-7.19256400	-2.19245900	-1.19790500
H	-8.63504600	-1.18573900	-1.02065800
H	-7.29505100	-0.64809100	-2.05268700
H	0.27648800	3.40049500	1.25053800
H	-0.24850100	3.34459300	-1.73492100
Cl	-0.46888200	0.92024500	2.33986700

(salen)aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2268.075405
No imaginary frequency

C	4.85278300	-1.60103500	-0.35388800
C	5.53462800	-0.36123300	-0.29519200
C	3.47653600	-1.74635600	-0.27606700
H	5.45302100	-2.49438600	-0.46720300
C	4.76266600	0.77614500	-0.15292000
C	2.69280600	-0.55614500	-0.12157000
C	3.35631400	0.70532700	-0.06018100
H	5.22323200	1.75702000	-0.10237300
O	1.39231800	-0.64719000	-0.05063100
C	2.63326000	1.93834600	0.09222500
Co	-0.00798700	0.49857500	0.45002400
N	1.35500300	2.04848600	0.23795300
H	3.25231000	2.83934100	0.09053000
N	-1.20072400	2.00420100	-0.35011000
C	0.67937000	3.33488500	0.38737600
C	-2.47583300	1.87400300	-0.54741000
C	-0.52331000	3.29070400	-0.57984500

C	1.51884700	4.59605400	0.18267500
H	-3.05096200	2.74983000	-0.85649900
C	-3.25807300	0.68173800	-0.39312200
C	-1.38785700	4.54854000	-0.43801100
C	0.64710000	5.84838500	0.34156000
H	1.96681900	4.58287300	-0.82060500
H	2.34192500	4.62105300	0.90487400
C	-4.65681300	0.79103600	-0.57099600
C	-2.66915900	-0.58110300	-0.09118900
C	-0.54423200	5.81790000	-0.62045300
H	-2.19638400	4.54788900	-1.17577300
H	-1.85536800	4.54504800	0.55536100
H	1.25065400	6.74647300	0.17318200
H	0.28035800	5.90377400	1.37483900
C	-5.48802900	-0.30194700	-0.43339500
H	-5.06007600	1.76847400	-0.81361500
C	-3.51702300	-1.72410000	0.07106500
O	-1.37473300	-0.70700000	0.01710000
H	-0.17590100	5.86058900	-1.65445500
H	-1.17493200	6.70149800	-0.47664800
C	-4.87873300	-1.53886500	-0.10620800
H	-5.52782700	-2.39649700	0.01470700
C	-2.91557400	-3.08491000	0.45191700
C	-3.99703700	-4.17182600	0.58033300
H	-3.52263000	-5.11829100	0.85640200
H	-4.72983800	-3.93233900	1.35807300
H	-4.53180000	-4.33309400	-0.36199600
C	-2.19888900	-2.96624500	1.81736500
H	-1.40997000	-2.21489800	1.79547800
H	-2.91084400	-2.69036100	2.60216800
H	-1.75326800	-3.93030600	2.08688400
C	-1.91209200	-3.54419500	-0.63037700
H	-2.40873700	-3.64211800	-1.60205000
H	-1.08848100	-2.83917400	-0.72896300
H	-1.49964100	-4.52295400	-0.36102000
C	2.79174600	-3.11855500	-0.36711700
C	1.86959800	-3.15141700	-1.60795700
H	1.10511900	-2.37687100	-1.55096900
H	2.45194000	-3.00306700	-2.52400500
H	1.37142900	-4.12460300	-1.67649100
C	1.96473100	-3.38976400	0.91134200
H	1.17947300	-2.64759000	1.04554800
H	1.49813900	-4.37884400	0.84503100
H	2.60929700	-3.37813900	1.79661500
C	3.81464400	-4.25888500	-0.51282200
H	4.41576400	-4.15955600	-1.42295600
H	4.49228400	-4.31378700	0.34578100
H	3.28168100	-5.21240500	-0.57348300
C	7.06402300	-0.33873900	-0.38862900
C	7.62653900	1.08945100	-0.30742800
H	7.25800600	1.71631000	-1.12595300
H	7.36771900	1.57240700	0.64031400
H	8.71818700	1.06115900	-0.37763900
C	7.50484200	-0.95762100	-1.73332600
H	8.59735900	-0.95627100	-1.81393200
H	7.16446000	-1.99201000	-1.83454700
H	7.09822000	-0.38767200	-2.57471400
C	7.65976000	-1.16122700	0.77507700
H	7.32480900	-2.20196500	0.74892100
H	8.75395200	-1.16091700	0.72132000
H	7.36325800	-0.73876300	1.74015100
C	-7.00932700	-0.23613800	-0.60706200
C	-7.48910500	1.18102800	-0.95937400
H	-7.23831800	1.89971100	-0.17251700
H	-7.05281700	1.53312500	-1.89983900
H	-8.57709200	1.18460400	-1.07681100
C	-7.69451600	-0.66655300	0.70847100
H	-8.78424000	-0.63113900	0.60106400
H	-7.42052800	-1.68632900	0.99324200

H	-7.40846200	-0.00218300	1.52980800
C	-7.43704300	-1.18922000	-1.74456900
H	-7.15323400	-2.22425200	-1.53410900
H	-8.52410000	-1.16154800	-1.87789200
H	-6.96795900	-0.89959000	-2.69019900
H	0.27110500	3.33675900	1.40809200
H	-0.10893400	3.25767200	-1.59952700
Cl	-0.19696900	0.68262900	2.69995900

H_2O-aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2344.508164
No imaginary frequency

C	4.76466300	-1.62350400	0.07840300
C	5.44840400	-0.38296600	0.11798000
C	3.38839100	-1.76895800	0.02755100
H	5.36708800	-2.52240700	0.10262600
C	4.66747400	0.75078000	0.12485500
C	2.58550100	-0.57722200	-0.02333600
C	3.25327700	0.68189400	0.05844000
H	5.11848200	1.73595800	0.18363000
O	1.28939300	-0.68851800	-0.16360800
C	2.54275800	1.92106700	0.12241700
Co	-0.00606700	0.69551800	-0.20143500
N	1.26240800	2.08261600	0.04956800
H	3.16277100	2.80677000	0.26483600
N	-1.28340900	2.08562700	-0.42524000
C	0.60648700	3.37664400	0.27844400
C	-2.56284100	1.93336800	-0.32629700
C	-0.63322700	3.38430600	-0.63080600
C	1.45767800	4.62807300	0.06334900
H	-3.19292500	2.82267300	-0.35817200
C	-3.25189500	0.68663500	-0.18676100
C	-1.48784400	4.62956500	-0.39819300
C	0.60757900	5.88835200	0.28354400
H	1.86504900	4.62058300	-0.95663400
H	2.30732000	4.63890200	0.75333700
C	-4.64220200	0.73935300	0.06635400
C	-2.58399600	-0.56061500	-0.35887300
C	-0.64066400	5.89361600	-0.60602000
H	-2.34284800	4.64235100	-1.08236700
H	-1.88671100	4.60875800	0.62436100
H	1.21348400	6.78044100	0.09371900
H	0.30185100	5.93387900	1.33703300
C	-5.39831900	-0.40882800	0.17182100
H	-5.09629300	1.71776700	0.18336400
C	-3.35978700	-1.76067700	-0.26319300
O	-1.30291400	-0.63026200	-0.64969000
H	-0.33620000	5.95339200	-1.65952000
H	-1.24757900	6.78236200	-0.40439500
C	-4.71694800	-1.63634600	-0.00322100
H	-5.30125200	-2.54381500	0.07748900
Cl	-0.37725400	0.60704200	1.99475800
O	0.29197300	0.61257600	-2.23811000
H	-0.49367900	0.03467700	-2.32561800
H	1.03228300	-0.01903500	-2.20160600
H	0.24673700	3.35164500	1.31619200
H	-0.27102300	3.38908900	-1.66948200
C	-2.69454700	-3.13557500	-0.42603900
C	-3.69929400	-4.28915900	-0.25997600
H	-4.49377700	-4.25811600	-1.01360100
H	-3.17241500	-5.24130400	-0.37532200
H	-4.16265700	-4.28799900	0.73203100
C	-1.59919100	-3.30251400	0.64871300
H	-0.85522500	-2.51253700	0.57688000
H	-2.03821300	-3.27096300	1.65118400
H	-1.09878900	-4.26949500	0.52593700
C	-2.07692700	-3.25989200	-1.83728700

H	-2.84926600	-3.15624200	-2.60764700
H	-1.31568700	-2.49755500	-1.99911100
H	-1.60832100	-4.24296700	-1.95628300
C	2.72106400	-3.15153300	0.08645100
C	1.90314000	-3.23564700	1.39600900
H	2.57090500	-3.17051400	2.26155500
H	1.17442300	-2.42829000	1.46315300
H	1.37003000	-4.19115900	1.44880900
C	1.80409000	-3.38132400	-1.13675400
H	0.98540900	-2.66538500	-1.15635800
H	2.37729700	-3.29628900	-2.06774400
H	1.37847800	-4.38996200	-1.09704700
C	3.75492600	-4.29156900	0.10314800
H	4.37242800	-4.30027300	-0.80186000
H	4.41702600	-4.23512100	0.97322300
H	3.22924600	-5.24988000	0.15437500
C	6.97958900	-0.36465100	0.17340400
C	7.53651100	1.06738600	0.21356300
H	7.24419800	1.63884300	-0.67350600
H	7.19292000	1.60922500	1.10068400
H	8.63012200	1.03942400	0.24529700
C	7.45908800	-1.10615400	1.44041300
H	7.12409500	-2.14726300	1.45125500
H	8.55354200	-1.10713100	1.49330800
H	7.07181000	-0.62166500	2.34215300
C	7.54636400	-1.06989200	-1.07802100
H	8.64173100	-1.07704800	-1.05189100
H	7.20759800	-2.10775600	-1.14511200
H	7.22839300	-0.55503300	-1.99026900
C	-6.90282700	-0.41340800	0.46338300
C	-7.46336700	1.00955100	0.61715000
H	-6.98742800	1.54297500	1.44624400
H	-7.32578000	1.59855000	-0.29563800
H	-8.53712900	0.96465000	0.82403600
C	-7.16794900	-1.18289500	1.77577700
H	-8.24052700	-1.20221200	1.99907000
H	-6.82116000	-2.21835600	1.71408800
H	-6.65022600	-0.70729400	2.61448900
C	-7.65071600	-1.10556500	-0.69692900
H	-7.31808200	-2.13849700	-0.83366100
H	-8.72853500	-1.12519100	-0.50084000
H	-7.48314700	-0.57309500	-1.63862300

H_2O-aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2344.504465
No imaginary frequency

C	4.75720900	-1.61918400	0.03464300
C	5.44400500	-0.37881200	-0.00079400
C	3.38176900	-1.76177000	0.09328800
H	5.35829000	-2.51904000	0.02292200
C	4.67115700	0.75950000	0.03741200
C	2.58353100	-0.56591700	0.10222900
C	3.25623500	0.69315400	0.08782900
H	5.12795500	1.74332800	0.03007700
O	1.28072600	-0.66934300	0.11522900
C	2.54425700	1.92720300	0.15229500
Co	-0.01307800	0.68234600	0.02661700
N	1.25715400	2.07603600	0.16276300
H	3.16152100	2.82337700	0.21105800
N	-1.25692300	2.07455000	-0.39375800
C	0.60188400	3.37996600	0.33774900
C	-2.54153000	1.92591600	-0.38301500
C	-0.59379200	3.36344800	-0.62667800
C	1.46695000	4.62255500	0.13703400
H	-3.16680100	2.80938400	-0.51206200
C	-3.23597700	0.68658400	-0.22858100
C	-1.45482800	4.61653600	-0.47172300

C	0.60673000	5.88618300	0.29104200
H	1.92027900	4.59829900	-0.86327700
H	2.28294300	4.64336400	0.86678300
C	-4.64137200	0.73892100	-0.08223400
C	-2.55456100	-0.56223100	-0.30795700
C	-0.59230700	5.87310200	-0.66351500
H	-2.27100000	4.61588100	-1.20182100
H	-1.90753500	4.62042900	0.52826300
H	1.22196800	6.77488100	0.11638000
H	0.24662700	5.95001600	1.32604300
C	-5.39587200	-0.41089200	0.01150600
H	-5.10713300	1.71716900	-0.03309900
C	-3.32832600	-1.76490100	-0.24274700
O	-1.25128700	-0.63301400	-0.48381800
H	-0.23208400	5.90784500	-1.70038700
H	-1.20635100	6.76730100	-0.51483300
C	-4.69969300	-1.63989000	-0.07763600
H	-5.28481200	-2.54734900	-0.00674700
Cl	-0.59606700	0.78488200	2.32895500
O	0.42411500	0.36381200	-2.45248600
H	-0.35617500	-0.18890300	-2.27725400
H	1.15959600	-0.22967000	-2.24439700
H	0.19846400	3.36804600	1.35909500
H	-0.18888100	3.32556000	-1.64824700
C	-2.65027600	-3.13968600	-0.33356000
C	-3.66136900	-4.29258300	-0.20257800
H	-4.41089700	-4.27916000	-1.00126300
H	-3.12677100	-5.24498500	-0.26871300
H	-4.18055700	-4.27327700	0.76114200
C	-1.61958400	-3.28600100	0.80719100
H	-0.86595600	-2.50312000	0.76586100
H	-2.11685800	-3.22962600	1.78071200
H	-1.12018400	-4.25852300	0.73509000
C	-1.95904500	-3.28663700	-1.70798500
H	-2.69303400	-3.21369300	-2.51801000
H	-1.20177500	-2.51740900	-1.85397800
H	-1.46958900	-4.26386100	-1.77992300
C	2.71335900	-3.14084300	0.18585000
C	1.96250100	-3.24076900	1.53398700
H	2.67094700	-3.17525900	2.36648500
H	1.22789900	-2.44379200	1.64449100
H	1.44417800	-4.20318900	1.60440700
C	1.73435800	-3.34402400	-0.99256800
H	0.93431800	-2.60747800	-0.96988200
H	2.26406300	-3.27055700	-1.94976000
H	1.28292100	-4.34017600	-0.93527900
C	3.74155300	-4.28458000	0.13439800
H	4.30712500	-4.28817200	-0.80385000
H	4.45133800	-4.23785100	0.96674800
H	3.21527900	-5.24108400	0.20653900
C	6.97482000	-0.36634400	-0.06408000
C	7.53773600	1.06354500	-0.09411300
H	7.18282600	1.61893800	-0.96840800
H	7.26358400	1.62434100	0.80529100
H	8.63041100	1.03031500	-0.14337700
C	7.54594500	-1.08649500	1.17704300
H	7.20933900	-2.12559500	1.23342500
H	8.64102100	-1.09180800	1.14565300
H	7.23101400	-0.58302500	2.09634400
C	7.44070300	-1.09805200	-1.34178500
H	8.53464900	-1.10720500	-1.39985400
H	7.09736600	-2.13633200	-1.36203000
H	7.05405700	-0.60028000	-2.23674500
C	-6.91612100	-0.41645500	0.20291100
C	-7.49260200	1.00677200	0.27066200
H	-7.07523300	1.57142100	1.11047900
H	-7.29907000	1.56546700	-0.65097500
H	-8.57724500	0.96046100	0.40825300
C	-7.26154200	-1.14316200	1.52112900

H	-8.34621300	-1.16137800	1.67446800
H	-6.90757900	-2.17803000	1.51740900
H	-6.80151600	-0.63623600	2.37487900
C	-7.58109300	-1.15363200	-0.97998100
H	-7.23577500	-2.18849000	-1.05841200
H	-8.66923000	-1.17382700	-0.85452900
H	-7.35439500	-0.65267100	-1.92653400

H_2O-aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2344.496738
No imaginary frequency

C	4.95372000	-1.54038500	0.01887400
C	5.58286600	-0.27513400	0.07846800
C	3.58020000	-1.73252600	-0.01371000
H	5.59108000	-2.41490100	0.00200600
C	4.75986200	0.83545300	0.11689700
C	2.74918800	-0.56846600	-0.00127400
C	3.35400500	0.71798400	0.08274200
H	5.18025300	1.83356200	0.17807100
O	1.44919000	-0.70697000	-0.08414100
C	2.58545800	1.93604600	0.16881400
Co	-0.03261000	0.43625600	0.02664900
N	1.30006200	2.03145700	0.16512300
H	3.18878900	2.84172800	0.26944300
N	-1.27732100	2.02188800	-0.47006600
C	0.60315800	3.30886400	0.32769300
C	-2.56399700	1.92309500	-0.42859500
C	-0.58043700	3.29337500	-0.66897900
C	1.44879600	4.57516600	0.17311700
H	-3.17117200	2.82778600	-0.50903700
C	-3.31877900	0.70497000	-0.27533900
C	-1.43100900	4.56057200	-0.54956200
C	0.58137600	5.83387700	0.29896500
H	1.94238100	4.56361600	-0.80841800
H	2.23804700	4.59621800	0.93201400
C	-4.71189400	0.82433800	-0.08218200
C	-2.71449100	-0.58224500	-0.35838600
C	-0.56792500	5.81791300	-0.71245700
H	-2.22352700	4.55606100	-1.30563600
H	-1.92001700	4.57443400	0.43371600
H	1.20143800	6.72593500	0.16076200
H	0.17035800	5.89016500	1.31561100
C	-5.51842000	-0.28802200	0.06484700
H	-5.13186800	1.82356200	-0.03952100
C	-3.52986200	-1.74523200	-0.21100100
O	-1.42656800	-0.70286900	-0.60068300
H	-0.15760200	5.84767600	-1.73079600
H	-1.19104400	6.71126600	-0.59881200
C	-4.88834600	-1.55239600	-0.00222500
H	-5.51305200	-2.42748200	0.12139000
Cl	-0.54355500	0.40037300	2.26930500
O	0.30711500	0.34967000	-2.41055100
H	-0.50930200	-0.17380000	-2.34087400
H	1.01130300	-0.30155500	-2.27629100
H	0.16861500	3.28079100	1.33711600
H	-0.14397000	3.24644900	-1.67716700
C	-2.90133900	-3.14695900	-0.25651000
C	-3.95288600	-4.25243300	-0.05623700
H	-4.71844100	-4.24004700	-0.83957700
H	-3.45911600	-5.22816600	-0.09275300
H	-4.45033800	-4.17167900	0.91570800
C	-1.85178900	-3.28304100	0.87026200
H	-1.05938500	-2.54345900	0.77037700
H	-2.31860700	-3.14768600	1.85071400
H	-1.40220100	-4.28209600	0.84006600
C	-2.23129900	-3.38361600	-1.62926000
H	-2.96444800	-3.29884100	-2.43888400

H	-1.43192200	-2.66420400	-1.80534300
H	-1.80134000	-4.39066600	-1.66528100
C	2.94712500	-3.13278200	-0.03672700
C	2.09972600	-3.32834000	1.24214200
H	2.73375000	-3.27361400	2.13313200
H	1.32196700	-2.56956400	1.32717400
H	1.62129800	-4.31393000	1.22584800
C	2.05343300	-3.30782800	-1.28747700
H	1.20095200	-2.62986200	-1.26179400
H	2.62748800	-3.12726100	-2.20353500
H	1.66989400	-4.33297600	-1.32809400
C	4.01461400	-4.24047900	-0.07206200
H	4.63988000	-4.18035200	-0.96950800
H	4.66678600	-4.20913300	0.80671000
H	3.51974900	-5.21616900	-0.07831200
C	7.11323200	-0.19510800	0.10880500
C	7.61441000	1.25656100	0.17453000
H	7.28861900	1.83645800	-0.69511200
H	7.26392400	1.76463700	1.07869100
H	8.70850000	1.26939300	0.19056100
C	7.64195100	-0.94674000	1.35014100
H	7.35020900	-2.00073500	1.34048100
H	8.73605800	-0.90346100	1.38550600
H	7.25072600	-0.50012100	2.26951300
C	7.68528100	-0.84780700	-1.16871300
H	8.78002800	-0.80744500	-1.16111100
H	7.39093700	-1.89776100	-1.25365100
H	7.32920700	-0.32705000	-2.06324800
C	-7.03134300	-0.21132100	0.29836700
C	-7.53610100	1.24003200	0.33760900
H	-7.06997900	1.80770000	1.14929800
H	-7.34016500	1.76178000	-0.60487500
H	-8.61769200	1.25098300	0.50380300
C	-7.37524300	-0.88032300	1.64725600
H	-8.45459400	-0.83802300	1.83066700
H	-7.07451900	-1.93168200	1.66591400
H	-6.86582000	-0.37287100	2.47222800
C	-7.76554200	-0.94885500	-0.84270400
H	-7.47343600	-2.00137500	-0.89856000
H	-8.84937500	-0.91100000	-0.68723700
H	-7.54168000	-0.48781700	-1.80997500

PO-aCo^{III}-Cl

Charge: 0

Spin Multiplicity: 1

Sum of electronic and thermal Free Energies (a.u.): -2461.155374

No imaginary frequency

C	-4.69003300	-1.58258100	-0.25508500
C	-5.35754000	-0.33983200	-0.11297200
C	-3.32277900	-1.73484300	-0.41013200
H	-5.30157800	-2.47572800	-0.25511200
C	-4.57265000	0.78994200	-0.17436200
C	-2.50002200	-0.55141800	-0.37220800
C	-3.16413300	0.71388500	-0.30569600
H	-5.01681800	1.77865600	-0.11923300
O	-1.20606300	-0.67967000	-0.39885500
C	-2.45552000	1.95078900	-0.43065600
Co	0.06687200	0.69537300	-0.13517000
N	-1.17300100	2.09303800	-0.45840800
H	-3.07674400	2.84248900	-0.52574200
N	1.31715300	2.08226600	0.23262800
C	-0.49370800	3.37210000	-0.66777700
C	2.59888900	1.91627500	0.28157700
C	0.66581900	3.39245800	0.34611700
C	-1.34476700	4.63597900	-0.56383000
H	3.23024300	2.79806300	0.39682900
C	3.28937300	0.66805800	0.18657000
C	1.55133800	4.62288900	0.15011100
C	-0.46209300	5.87768500	-0.75867600

H	-1.83042500	4.67378400	0.42092500
H	-2.13834700	4.62345800	-1.31821500
C	4.70206600	0.71730200	0.10838400
C	2.59692900	-0.58136500	0.19397700
C	0.70464700	5.90186700	0.23546100
H	2.34160200	4.65507600	0.90770500
H	2.04085800	4.55994600	-0.83029400
H	-1.06785400	6.78400400	-0.65487700
H	-0.06637400	5.87866300	-1.78265900
C	5.46022600	-0.42908900	0.01415600
H	5.17152800	1.69565200	0.11326100
C	3.37811600	-1.78189400	0.08891400
O	1.29935500	-0.66166200	0.33804100
H	0.30958700	6.00422700	1.25532100
H	1.33878000	6.77645200	0.05655000
C	4.75555600	-1.65775400	0.00596100
H	5.34071100	-2.56449400	-0.07928700
C	-0.85917100	-0.44827300	2.50889300
C	0.29186300	0.36542900	2.91626600
O	-0.54729200	0.79939100	1.80968000
H	-0.63708500	-1.30824400	1.88826600
H	1.28440000	0.05138800	2.61235900
H	0.21709000	1.02082900	3.78051600
C	-2.18018800	-0.45258500	3.21898500
H	-2.99068200	-0.55903600	2.49224000
H	-2.22643500	-1.30152400	3.90900000
H	-2.32964500	0.47078300	3.78537400
C	-2.68900600	-3.11337600	-0.65608100
C	-1.96878400	-3.09438100	-2.02476300
H	-2.69059900	-2.92575800	-2.83098800
H	-1.21410800	-2.30901300	-2.06482500
H	-1.47860700	-4.05791300	-2.20392900
C	-1.67897000	-3.46306500	0.45825700
H	-0.83578100	-2.77743900	0.44148300
H	-2.15867400	-3.42565900	1.44359600
H	-1.29483000	-4.47840800	0.31110700
C	-3.74329900	-4.23377700	-0.69346800
H	-4.27108600	-4.33558500	0.26134800
H	-4.48486700	-4.07403600	-1.48291900
H	-3.24533500	-5.18648400	-0.89771900
C	2.68889300	-3.15364900	0.05736000
C	3.69430300	-4.30510600	-0.11993100
H	4.25348600	-4.21774400	-1.05720900
H	4.41072900	-4.36113400	0.70694500
H	3.14976400	-5.25400500	-0.14832800
C	1.94836400	-3.38971600	1.39311500
H	2.65959100	-3.40836500	2.22674400
H	1.21832400	-2.60336200	1.57747800
H	1.42433000	-4.35151600	1.37170000
C	1.70028500	-3.20845000	-1.12945700
H	1.18227200	-4.17406700	-1.13955300
H	0.96028700	-2.41314700	-1.07169600
H	2.24003300	-3.10248700	-2.07606200
C	6.98914500	-0.43349300	-0.08818500
C	7.57180500	0.98856100	-0.05939300
H	7.20770600	1.59029700	-0.89830700
H	7.32145500	1.50840600	0.87129200
H	8.66301500	0.94411700	-0.13155400
C	7.58281300	-1.22360900	1.09844600
H	7.22894500	-2.25845700	1.11246000
H	8.67662300	-1.24551600	1.03668000
H	7.30229300	-0.76171000	2.05054600
C	7.41344900	-1.10360500	-1.41325400
H	7.05684400	-2.13562100	-1.47636400
H	7.00682700	-0.55760400	-2.27011900
H	8.50552200	-1.12111100	-1.50226900
C	-6.87866400	-0.31460700	0.06792900
C	-7.41882400	1.11855400	0.19714000
H	-6.98476500	1.63673100	1.05854700

H	-7.21090100	1.71027000	-0.70019800
H	-8.50438000	1.09555800	0.33491200
C	-7.25324200	-1.09033600	1.34973300
H	-8.33948000	-1.09514200	1.49415900
H	-6.91776300	-2.13049200	1.30407200
H	-6.79256900	-0.62899600	2.22936500
C	-7.55794300	-0.97955000	-1.14918900
H	-7.24071100	-2.01902900	-1.27194000
H	-8.64742700	-0.97477100	-1.03160600
H	-7.30935200	-0.44401600	-2.07074100
H	0.21177300	3.43568700	1.34799300
H	-0.04614200	3.31370100	-1.66867200
Cl	0.66217000	0.66648300	-2.29133400

PO-aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2461.151444
No imaginary frequency

C	-4.65791300	-1.57698700	-0.28080700
C	-5.31930100	-0.34261000	-0.05284600
C	-3.30005300	-1.71841600	-0.50729200
H	-5.26739500	-2.47123900	-0.28703700
C	-4.54404200	0.79393400	-0.10527100
C	-2.48458000	-0.53235800	-0.46204400
C	-3.14392300	0.72681200	-0.31102000
H	-4.98708600	1.77671700	0.01628500
O	-1.19077600	-0.64456000	-0.56155900
C	-2.43437400	1.96078500	-0.41146700
Co	0.10020900	0.69289500	-0.30038500
N	-1.15066400	2.09711200	-0.50303400
H	-3.04956300	2.86059900	-0.43021000
N	1.32645800	2.08254800	0.19137800
C	-0.47713800	3.38634800	-0.68147600
C	2.60451000	1.91669700	0.29613100
C	0.66815100	3.38624400	0.34520400
C	-1.33543800	4.64297200	-0.56323000
H	3.22941200	2.79205300	0.47489500
C	3.29294500	0.66870400	0.19794300
C	1.55264500	4.62336400	0.18898100
C	-0.45184400	5.88884700	-0.72685600
H	-1.82890100	4.66520300	0.41818300
H	-2.12155300	4.64003000	-1.32570100
C	4.70688200	0.70331400	0.18367500
C	2.59089400	-0.57229200	0.17858800
C	0.69961600	5.89765100	0.28515200
H	2.32926000	4.64426700	0.96084600
H	2.05787000	4.58015600	-0.78435000
H	-1.06053100	6.79237900	-0.61674500
H	-0.04177700	5.90605600	-1.74483700
C	5.45366900	-0.45334300	0.12199700
H	5.18685100	1.67576500	0.20773600
C	3.35633400	-1.78343400	0.12594600
O	1.28178700	-0.63547400	0.25024300
H	0.28886800	5.97993900	1.30058000
H	1.33381900	6.77697400	0.13185000
C	4.73756700	-1.67455200	0.09424100
H	5.31547000	-2.58778400	0.03722000
C	-1.09176600	-0.49087400	2.52505600
C	0.09470400	0.19770600	3.04520400
O	-0.69528600	0.80056600	1.99644700
H	-0.91197700	-1.29109800	1.81460300
H	1.07996900	-0.13126300	2.72576000
H	0.04034500	0.72071800	3.99841400
C	-2.41653200	-0.52058000	3.23333500
H	-3.23114000	-0.48413300	2.50327600
H	-2.51700200	-1.44759700	3.80775400
H	-2.51741100	0.32845500	3.91546400
C	-2.67188300	-3.08505400	-0.82008200

C	-1.97305000	-3.02007200	-2.19851300
H	-2.70434100	-2.81066400	-2.98638700
H	-1.20672400	-2.24563500	-2.22367800
H	-1.50115500	-3.98332700	-2.42172300
C	-1.64742300	-3.46819800	0.26862800
H	-0.82051200	-2.76290100	0.28638000
H	-2.12154900	-3.49428200	1.25672000
H	-1.23937600	-4.46426300	0.06584600
C	-3.72804200	-4.20258300	-0.88054400
H	-4.23514700	-4.34446300	0.08022000
H	-4.48587100	-4.01016500	-1.64706400
H	-3.23508400	-5.14589200	-1.13392000
C	2.65288000	-3.14692000	0.08082300
C	3.65344800	-4.31195800	-0.01967400
H	4.25917200	-4.25313800	-0.92980200
H	4.32683400	-4.35550200	0.84328300
H	3.10014900	-5.25545300	-0.05341200
C	1.83938600	-3.34865900	1.37943700
H	2.50597000	-3.35865000	2.24926200
H	1.10767300	-2.55360100	1.51305300
H	1.30846100	-4.30618000	1.34802900
C	1.73387600	-3.21210400	-1.16060000
H	1.21015300	-4.17413300	-1.18658600
H	0.99650800	-2.41214700	-1.16032800
H	2.32823400	-3.12322700	-2.07545100
C	6.98504900	-0.47472400	0.07582300
C	7.58199500	0.94092300	0.12192500
H	7.25558200	1.54413200	-0.73123500
H	7.30493800	1.46634200	1.04184400
H	8.67437300	0.88343000	0.08912800
C	7.52543800	-1.26822800	1.28543000
H	7.16127100	-2.29955300	1.28870800
H	8.62032200	-1.30107000	1.26323800
H	7.21556600	-0.80105600	2.22575100
C	7.44759600	-1.15359400	-1.23194500
H	7.08359600	-2.18239300	-1.30424800
H	7.07667100	-0.60657300	-2.10409500
H	8.54177000	-1.18170700	-1.28212400
C	-6.82838500	-0.33292700	0.21034800
C	-7.36485600	1.09054200	0.42998300
H	-6.88695700	1.57351600	1.28857300
H	-7.20829400	1.72133100	-0.45100700
H	-8.44113500	1.05524300	0.62492100
C	-7.12830500	-1.16460500	1.47671700
H	-8.20468600	-1.17950700	1.68050900
H	-6.79466400	-2.20059400	1.36818900
H	-6.62034700	-0.73922800	2.34837200
C	-7.56938000	-0.94964200	-0.99604700
H	-7.25705200	-1.98155300	-1.17961500
H	-8.65061500	-0.95491900	-0.81924300
H	-7.37299700	-0.37437700	-1.90615100
H	0.20719200	3.39226000	1.34377800
H	-0.02067600	3.33922700	-1.67894400
Cl	0.86100300	0.81786200	-2.56993900

PO-aCo^{III}-Cl
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2461.143048
No imaginary frequency

C	-4.83223800	-1.49387000	-0.18951200
C	-5.42661700	-0.23715300	0.07514200
C	-3.49262900	-1.67900600	-0.49828500
H	-5.47243200	-2.36589300	-0.15511100
C	-4.61098200	0.87534700	-0.01876700
C	-2.64795500	-0.52161200	-0.50255800
C	-3.23434700	0.76343300	-0.30675200
H	-5.01326700	1.87118700	0.13423700
O	-1.36348600	-0.66508400	-0.68342800

C	-2.47867700	1.98570800	-0.43473700
Co	0.11112600	0.47016100	-0.48058100
N	-1.20640200	2.06955100	-0.61689400
H	-3.07799400	2.89885900	-0.38584100
N	1.30677300	2.03075500	0.20843400
C	-0.49611800	3.33767500	-0.74500200
C	2.58674200	1.90706000	0.33440900
C	0.62310900	3.32125100	0.32596800
C	-1.33232200	4.61446600	-0.65216400
H	3.19306200	2.79969100	0.50630400
C	3.33875800	0.68198200	0.25860300
C	1.50430300	4.56998700	0.22157300
C	-0.43760400	5.85326900	-0.78155400
H	-1.85513000	4.64495000	0.31380400
H	-2.09835600	4.61631100	-1.43537800
C	4.74755600	0.78412900	0.28470100
C	2.71343700	-0.59798800	0.19446400
C	0.66033600	5.84993500	0.28654000
H	2.24574900	4.58192700	1.02765300
H	2.05663500	4.53623200	-0.72670500
H	-1.04400900	6.76185800	-0.70279200
H	0.02240300	5.86576800	-1.77832100
C	5.55556600	-0.33391000	0.22059000
H	5.17954600	1.77748500	0.34476300
C	3.53404600	-1.76816200	0.12872600
O	1.40887800	-0.71019800	0.22981500
H	0.19865200	5.92927000	1.28021700
H	1.30922000	6.72475700	0.17223200
C	4.90909100	-1.59045600	0.14059100
H	5.53631600	-2.47062800	0.08109400
C	-1.00842000	-0.64785800	2.42232600
C	0.12920800	0.15193300	2.89213800
O	-0.68636400	0.61768200	1.79608500
H	-0.77446500	-1.49166100	1.78047700
H	1.13557000	-0.13666900	2.60328600
H	0.03113700	0.74436300	3.80014800
C	-2.33441400	-0.70164200	3.12789000
H	-3.14610900	-0.77487800	2.39785400
H	-2.38105100	-1.58145400	3.77853700
H	-2.49019800	0.19373000	3.73631000
C	-2.91673000	-3.06032200	-0.85066200
C	-2.32573000	-3.01282800	-2.27953200
H	-3.10452600	-2.76749800	-3.00918500
H	-1.53103800	-2.27002600	-2.35683000
H	-1.91111200	-3.99230900	-2.54258700
C	-1.81003400	-3.47174200	0.14643100
H	-0.95592300	-2.79951400	0.08382500
H	-2.19156800	-3.47416700	1.17384700
H	-1.46152800	-4.48450500	-0.08342900
C	-4.00043500	-4.15229800	-0.82139500
H	-4.43660700	-4.27279100	0.17633400
H	-4.80938400	-3.94541300	-1.52956200
H	-3.55283300	-5.11002700	-1.10295400
C	2.88918700	-3.15884600	0.02694600
C	3.94401400	-4.27580200	-0.05922300
H	4.58035000	-4.16917800	-0.94377900
H	4.58613100	-4.30572800	0.82774700
H	3.43767600	-5.24309500	-0.13270800
C	2.02596300	-3.42864400	1.28062500
H	2.64366600	-3.41096600	2.18551600
H	1.23951900	-2.68199500	1.38215500
H	1.55849700	-4.41694100	1.20827100
C	2.01505900	-3.23774800	-1.24632600
H	1.54611600	-4.22609700	-1.31369600
H	1.23267700	-2.48054200	-1.24695500
H	2.62779900	-3.08914000	-2.14090000
C	7.08709700	-0.27380100	0.22513700
C	7.60762600	1.16948200	0.31861900
H	7.27756800	1.77331700	-0.53270600

H	7.27455200	1.66036600	1.23897300
H	8.70202600	1.16878000	0.32051800
C	7.62927500	-1.06330500	1.43665500
H	7.32006600	-2.11202400	1.40769100
H	8.72454900	-1.03842600	1.45093000
H	7.26437500	-0.63286300	2.37473700
C	7.62792600	-0.89976700	-1.07905500
H	7.32145600	-1.94440500	-1.18384900
H	7.25761900	-0.35438200	-1.95255200
H	8.72313200	-0.86964100	-1.09265300
C	-6.91642800	-0.16753800	0.42762000
C	-7.38428800	1.27562600	0.67468700
H	-6.84023100	1.74010300	1.50351800
H	-7.25480000	1.90028300	-0.21497600
H	-8.44814700	1.28106400	0.93113100
C	-7.17254700	-0.98615500	1.71214600
H	-8.23420200	-0.95623000	1.98105700
H	-6.88934400	-2.03504900	1.58600800
H	-6.59518500	-0.58220800	2.55006700
C	-7.75121700	-0.75589800	-0.73079500
H	-7.49073200	-1.79940000	-0.92917500
H	-8.81935200	-0.71858200	-0.48997200
H	-7.58726100	-0.18955800	-1.65285000
H	0.11805500	3.31746400	1.30355000
H	-0.00055100	3.29688900	-1.72469200
Cl	0.90803400	0.58964400	-2.64616100

(salen)aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2036.298120
No imaginary frequency

C	4.79727700	-1.62570000	-0.07356100
C	5.49890100	-0.39412000	-0.07142800
C	3.41910800	-1.75683100	-0.05137500
H	5.38964800	-2.53101500	-0.09288900
C	4.73511400	0.75041000	-0.06616000
C	2.62873300	-0.55392200	-0.01771900
C	3.31906300	0.69681700	-0.05412800
H	5.19984100	1.73070700	-0.07658900
O	1.32444700	-0.63798600	0.02099900
C	2.62375700	1.94088200	-0.09393800
Co	0.04276800	0.72165300	-0.09348600
N	1.33999300	2.09971200	-0.16992000
H	3.25043500	2.83286500	-0.06951700
N	-1.19962100	2.05724700	-0.62554000
C	0.69426900	3.41371100	-0.04596800
C	-2.48297700	1.92006700	-0.52030600
C	-0.55631700	3.34442900	-0.93403900
C	1.54150700	4.64177600	-0.37530400
H	-3.11254000	2.80145700	-0.64286300
C	-3.17619300	0.68823500	-0.31154100
C	-1.41329800	4.60090200	-0.78373500
C	0.69104200	5.91417000	-0.23885700
H	1.93252900	4.55608800	-1.39836200
H	2.40166500	4.70727900	0.29843700
C	-4.58154900	0.74253400	-0.15464100
C	-2.49344200	-0.56361700	-0.39315000
C	-0.57380500	5.84737300	-1.10214600
H	-2.27878400	4.56157400	-1.45349700
H	-1.79468300	4.65521700	0.24406000
H	1.28967400	6.79003800	-0.50969000
H	0.40537800	6.04032600	0.81345800
C	-5.34081400	-0.40570200	-0.09817400
H	-5.04292700	1.72143300	-0.07965300
C	-3.28653100	-1.76068700	-0.45715900
O	-1.18920900	-0.63907500	-0.44157500
H	-0.28961500	5.82805400	-2.16289700
H	-1.18061500	6.74707700	-0.95712500

C	-4.65518800	-1.63262200	-0.28063500
H	-5.25218100	-2.53505300	-0.29088300
O	-0.23630900	1.25655700	1.65045300
C	-0.69003000	0.60590300	2.71459200
O	-0.87927300	1.23756100	3.74306500
C	-0.96468600	-0.87690400	2.61845700
H	-0.95455500	-1.30141300	3.62292400
H	-1.95445000	-1.03793000	2.18250300
H	-0.23916100	-1.37460000	1.97974300
H	-0.21046500	3.27803400	-1.97746400
H	0.35018900	3.46975000	0.99545500
C	-2.63938400	-3.12170700	-0.76131700
C	-1.61190300	-3.50310600	0.32385300
H	-0.80566900	-2.77672500	0.36745300
H	-2.08793600	-3.55965300	1.30832900
H	-1.18246800	-4.48559600	0.09892900
C	-1.93731700	-3.03875200	-2.13673100
H	-2.66447300	-2.82132800	-2.92659200
H	-1.17349200	-2.26101100	-2.14161000
H	-1.45646800	-3.99479200	-2.37076900
C	-3.68203400	-4.25110600	-0.83610800
H	-4.19904800	-4.39630500	0.11838800
H	-4.43245100	-4.06995300	-1.61275600
H	-3.17459900	-5.18919000	-1.08031700
C	-6.85795600	-0.41323600	0.11496200
C	-7.42100100	1.00655100	0.28727600
H	-6.97698200	1.51428600	1.14945000
H	-7.24718200	1.62120200	-0.60208900
H	-8.50212600	0.95886800	0.44977600
C	-7.18748200	-1.22361500	1.38767300
H	-8.26976000	-1.24846300	1.55593800
H	-6.83786500	-2.25718700	1.31051700
H	-6.71347300	-0.77508900	2.26623600
C	-7.54944000	-1.06505100	-1.10241500
H	-7.21771000	-2.09620400	-1.25398500
H	-8.63566200	-1.08212000	-0.96097300
H	-7.33163300	-0.50555600	-2.01771000
C	2.75011800	-3.13992900	-0.05786800
C	1.98861400	-3.34228700	1.26967700
H	2.68438300	-3.33001900	2.11530000
H	1.25222400	-2.55623400	1.42047400
H	1.46964100	-4.30687500	1.26780200
C	3.77567900	-4.28110400	-0.18247700
H	4.35705000	-4.21142900	-1.10801200
H	4.47123700	-4.30689800	0.66284700
H	3.24388700	-5.23729700	-0.19725900
C	1.78405500	-3.25417700	-1.25878800
H	1.00427400	-2.49687900	-1.21384200
H	2.33201600	-3.13884200	-2.20062400
H	1.30982800	-4.24160600	-1.26319700
C	7.60857200	1.02708100	-0.07718500
H	7.29606500	1.59254700	-0.96117500
H	7.30177200	1.58377800	0.81417600
H	8.70204100	0.98353400	-0.08124800
C	7.03089300	-0.39722200	-0.08196400
C	7.55037700	-1.13528800	1.17120900
H	7.19919100	-2.17054700	1.20583500
H	8.64579900	-1.15390200	1.17794200
H	7.20974000	-0.63631300	2.08381300
C	7.53539600	-1.12099800	-1.34947400
H	8.63065100	-1.13920400	-1.36952500
H	7.18432600	-2.15600800	-1.39188000
H	7.18413100	-0.61161600	-2.25242800

(salen)aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2036.315681
No imaginary frequency

C	4.87004100	-1.61951900	0.04515700
C	5.54754100	-0.37472200	-0.03437400
C	3.49587900	-1.77511700	0.07354400
H	5.47981200	-2.51229100	0.09310500
C	4.76501500	0.75547900	-0.07760100
C	2.68587200	-0.58760700	0.00735600
C	3.34910700	0.67495300	-0.05814200
H	5.21179500	1.74272200	-0.12728100
O	1.38566000	-0.69658900	0.01194500
C	2.61985600	1.89573600	-0.09043800
Co	0.06815200	0.61599200	-0.15550600
N	1.32695800	2.02865500	-0.11254100
H	3.22087000	2.80470800	-0.08852400
N	-1.16116600	1.96107800	-0.72783200
C	0.66465800	3.34194200	-0.03997300
C	-2.44320400	1.79635400	-0.70374300
C	-0.52383100	3.25615100	-1.00604600
C	1.51861700	4.57577100	-0.31630000
H	-3.08231200	2.66284000	-0.86603000
C	-3.10831400	0.54981200	-0.49328500
C	-1.41141600	4.49358000	-0.88171200
C	0.64152000	5.83416600	-0.21138300
H	1.96628400	4.50940700	-1.31816400
H	2.33989400	4.64641200	0.40477500
C	-4.51179900	0.57306100	-0.32352400
C	-2.39494800	-0.68382700	-0.56055000
C	-0.57689800	5.75755500	-1.13877300
H	-2.23871400	4.45232700	-1.59854400
H	-1.83718300	4.50923800	0.12812800
H	1.23932200	6.72199400	-0.44307100
H	0.30012600	5.94175500	0.82568300
C	-5.23761200	-0.59257100	-0.20231100
H	-4.99742200	1.54165000	-0.27781300
C	-3.14699600	-1.90350800	-0.49701400
O	-1.09129400	-0.72742200	-0.70752300
H	-0.23852200	5.76072000	-2.18404600
H	-1.20524300	6.64515300	-1.01097100
C	-4.51659500	-1.80701000	-0.30595900
H	-5.08060300	-2.72697700	-0.22486700
O	-0.60763500	0.57897000	1.71277700
C	-1.34738500	1.45565300	2.32180400
O	-1.38554000	2.67296900	2.09536400
C	-2.25742800	0.83993800	3.37903800
H	-2.71303000	1.61725900	3.99437100
H	-3.04350000	0.27043300	2.87086700
H	-1.69865300	0.13745400	4.00249500
H	-0.12326100	3.19716600	-2.03012400
H	0.22457000	3.39344700	0.96402400
C	2.84103500	-3.15674200	0.20497300
C	1.91139200	-3.41888800	-1.00091500
H	1.12585200	-2.66949100	-1.06643800
H	2.48576900	-3.40945000	-1.93407200
H	1.44326700	-4.40433200	-0.90321000
C	3.88230600	-4.28920900	0.24196700
H	4.56061200	-4.19893200	1.09697300
H	3.36304900	-5.24779000	0.33533600
H	4.48177600	-4.32654200	-0.67404300
C	2.04474200	-3.20924300	1.52950400
H	2.72220600	-3.09394700	2.38252600
H	1.29386500	-2.42137500	1.57612000
H	1.53952500	-4.17627800	1.62587300
C	7.07926500	-0.35141000	-0.05718400
C	7.63162600	1.08030300	-0.14322500
H	7.29728100	1.58792100	-1.05387600
H	7.32739600	1.68291100	0.71871200
H	8.72551000	1.05484900	-0.16016700
C	7.62217000	-1.00390100	1.23305900
H	7.29163700	-2.04172700	1.33254900
H	8.71772200	-1.00143500	1.23097900

H	7.27924900	-0.45772700	2.11737100
C	7.58538700	-1.14129000	-1.28393900
H	8.68057300	-1.14308400	-1.31242300
H	7.25084700	-2.18237200	-1.26163300
H	7.21878400	-0.69217300	-2.21238800
C	-2.44214800	-3.26255300	-0.60076300
C	-1.71097200	-3.36398000	-1.95874900
H	-2.42939100	-3.30721500	-2.78403500
H	-0.98183200	-2.56341400	-2.07677400
H	-1.18729300	-4.32336200	-2.03074900
C	-1.44083800	-3.40831700	0.56567000
H	-0.70564000	-2.60710900	0.55735000
H	-1.96763500	-3.38456700	1.52560200
H	-0.91496500	-4.36627300	0.49040900
C	-3.43274500	-4.43732400	-0.51966300
H	-3.96441500	-4.46195400	0.43737100
H	-4.17254900	-4.40971700	-1.32694900
H	-2.87937700	-5.37686900	-0.61100600
C	-6.75130100	-0.63034300	0.03087700
C	-7.35730200	0.78026500	0.10449900
H	-6.92749500	1.36181200	0.92631100
H	-7.20402400	1.33487200	-0.82702800
H	-8.43600900	0.71114800	0.27520900
C	-7.43349600	-1.39240900	-1.12606400
H	-7.06842200	-2.42031300	-1.20602500
H	-8.51690500	-1.43460800	-0.96920000
H	-7.24472200	-0.89503400	-2.08269900
C	-7.04165000	-1.35332900	1.36444000
H	-6.66209300	-2.37912800	1.35941100
H	-6.57084400	-0.82678900	2.20054300
H	-8.12064800	-1.39666700	1.54928800

(salen)aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2036.311726
No imaginary frequency

C	4.90002700	-1.63021600	-0.44825700
C	5.58176800	-0.39331100	-0.33703800
C	3.52175100	-1.77141000	-0.44118200
H	5.50306300	-2.52367700	-0.54532500
C	4.80710600	0.74315100	-0.20608200
C	2.73177900	-0.58108200	-0.30740100
C	3.39742600	0.67604700	-0.17606800
H	5.26737900	1.72130700	-0.11476600
O	1.43078300	-0.67253600	-0.32473800
C	2.67225400	1.91017100	-0.04184000
Co	0.04830100	0.46516300	0.29109500
N	1.39226900	2.01629500	0.09330900
H	3.28688800	2.81453300	-0.05588400
N	-1.11661500	1.89818600	-0.63632300
C	0.69214000	3.29689700	0.15956500
C	-2.38769600	1.75108300	-0.84763500
C	-0.45290200	3.19177400	-0.87317900
C	1.52331600	4.56063500	-0.05227500
H	-2.96097300	2.61180900	-1.19775800
C	-3.17212900	0.56704800	-0.64921800
C	-1.34698900	4.43478100	-0.81378000
C	0.62401100	5.80133900	0.02150100
H	2.01835400	4.52112300	-1.03281000
H	2.31190900	4.62438600	0.70586600
C	-4.56698400	0.66415300	-0.86366200
C	-2.59391000	-0.66970400	-0.24022400
C	-0.51874300	5.71474500	-0.99517100
H	-2.11668100	4.39657000	-1.59137900
H	-1.86069200	4.44793800	0.15573700
H	1.21857400	6.70513600	-0.14926100
H	0.20603300	5.88286200	1.03316500
C	-5.40570400	-0.41246500	-0.65861500

H	-4.96155900	1.62119200	-1.18823700
C	-3.45237900	-1.78914300	0.00838700
O	-1.30300000	-0.79620400	-0.10343700
H	-0.10093000	5.73350200	-2.01108300
H	-1.17232200	6.58938300	-0.91010200
C	-4.80946600	-1.61835000	-0.21281700
H	-5.46479500	-2.46060000	-0.03028300
O	0.08220500	0.26085700	2.18223100
C	-0.67614400	1.05606000	2.90310100
O	-1.21689500	2.07439400	2.47090700
C	-0.84443000	0.59149400	4.33726000
H	-1.39387300	1.33509700	4.91521000
H	-1.38912000	-0.35802900	4.34271000
H	0.13377000	0.40492000	4.78911100
H	0.01668100	3.13446600	-1.86775100
H	0.21419700	3.32651300	1.14707500
C	2.83816000	-3.14196900	-0.56396700
C	1.95206200	-3.17550200	-1.83086500
H	1.17751700	-2.41022100	-1.78987500
H	2.55874400	-3.01426400	-2.72881600
H	1.46910900	-4.15484900	-1.91994100
C	3.86398400	-4.28316400	-0.67947700
H	4.51226200	-4.34318700	0.20122400
H	3.33238200	-5.23579400	-0.76260900
H	4.49589500	-4.18003300	-1.56813000
C	1.97298100	-3.41255000	0.68964500
H	2.59289300	-3.40767400	1.59268400
H	1.18902300	-2.66520900	0.80269700
H	1.50140700	-4.39807100	0.60739500
C	7.11383400	-0.37435600	-0.36233400
C	7.67612200	1.05059300	-0.23565900
H	7.34406700	1.69076400	-1.05943500
H	7.37830200	1.52023200	0.70732500
H	8.76973100	1.01997300	-0.25975900
C	7.65578700	-1.21558600	0.81423000
H	7.31871300	-2.25449900	0.75849200
H	8.75133000	-1.21883200	0.80853000
H	7.31871700	-0.80562400	1.77142200
C	7.61223600	-0.97511100	-1.69511000
H	8.70729400	-0.97635800	-1.72744500
H	7.27360900	-2.00667300	-1.82659900
H	7.24466200	-0.39152100	-2.54504300
C	-2.86097600	-3.10577100	0.53290600
C	-1.84037400	-3.67492300	-0.47931600
H	-2.32468500	-3.87545900	-1.44133700
H	-1.01648300	-2.98196300	-0.64172800
H	-1.43196700	-4.61966400	-0.10293900
C	-2.16819800	-2.84876700	1.89301900
H	-1.37651700	-2.10404400	1.80885600
H	-2.89821800	-2.49787200	2.63120900
H	-1.72941500	-3.77990100	2.26887000
C	-3.94721500	-4.17255600	0.75423300
H	-4.69390900	-3.85228800	1.48861700
H	-4.46533400	-4.42902800	-0.17607400
H	-3.48150100	-5.08660400	1.13498800
C	-6.92245400	-0.35734600	-0.87267400
C	-7.38643100	1.02515000	-1.35865500
H	-7.15218100	1.80864500	-0.63081200
H	-6.92393900	1.29324300	-2.31414000
H	-8.47109300	1.02152000	-1.50428800
C	-7.32952900	-1.40454000	-1.93226800
H	-7.05558300	-2.41811800	-1.62588000
H	-8.41318500	-1.38549500	-2.09288800
H	-6.83730500	-1.20004600	-2.88830900
C	-7.64099200	-0.66851400	0.45852500
H	-7.37934600	-1.66056400	0.83746000
H	-7.37005700	0.06417600	1.22513000
H	-8.72785600	-0.63870100	0.32310000

H_2O-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2112.732725
No imaginary frequency

C	4.79952100	-1.61866800	0.01744100
C	5.49161200	-0.38488000	0.04680700
C	3.42088300	-1.75712800	0.06524600
H	5.39562200	-2.51920700	-0.05277600
C	4.71703100	0.75373900	0.09791100
C	2.62293900	-0.56401300	0.16990800
C	3.30353600	0.69226700	0.13677100
H	5.17553600	1.73714300	0.10130400
O	1.32056200	-0.66460000	0.27643500
C	2.60245500	1.94329900	0.14116800
Co	0.06086700	0.69668800	-0.13674800
N	1.32867000	2.10011400	0.01861700
H	3.22563400	2.83327400	0.23781000
N	-1.17320900	2.04718400	-0.66851300
C	0.65250200	3.39827400	0.10419900
C	-2.45067500	1.91334100	-0.55071200
C	-0.50362300	3.32846700	-0.91315900
C	1.51732000	4.63741400	-0.12049600
H	-3.07799800	2.79921600	-0.65418300
C	-3.15520800	0.68171200	-0.33174200
C	-1.37316800	4.58301100	-0.84877900
C	0.64834000	5.90303200	-0.07175200
H	2.01816400	4.56310100	-1.09556400
H	2.29859300	4.70131800	0.64386700
C	-4.55119100	0.76693600	-0.12781800
C	-2.50515700	-0.58400300	-0.42554900
C	-0.51013200	5.83324000	-1.07335300
H	-2.16733200	4.53773500	-1.60196900
H	-1.85598800	4.63728900	0.13553500
H	1.26774900	6.78447100	-0.26762600
H	0.24413300	6.02015600	0.94205000
C	-5.33523600	-0.36341000	-0.02669600
H	-4.98867400	1.75638600	-0.04782000
C	-3.32195600	-1.76247900	-0.43662900
O	-1.19863500	-0.68682500	-0.54190900
H	-0.10810900	5.81599500	-2.09531800
H	-1.13320600	6.73030500	-0.99669200
C	-4.68358900	-1.60388200	-0.21350200
H	-5.29828600	-2.49386100	-0.18645000
O	-0.42448500	1.17137600	1.59911600
C	-0.80112500	0.50519600	2.67653800
O	-1.03210100	1.11703000	3.71051600
C	-0.97420700	-0.99468700	2.58396400
H	-0.92028900	-1.42327900	3.58557200
H	-1.95971300	-1.21586100	2.16413500
H	-0.22726700	-1.43577400	1.92924000
H	-0.05172000	3.25597700	-1.91331500
H	0.20141800	3.42901300	1.10384800
O	0.55234200	0.33630800	-2.11552900
H	-0.19280000	-0.29546400	-2.17570300
H	1.34046000	-0.22495200	-2.03831800
C	2.75530900	-3.14117800	-0.00599400
C	1.75944700	-3.18394100	-1.18885900
H	0.95574700	-2.46294900	-1.05120600
H	2.27864000	-2.97605900	-2.13264000
H	1.31044500	-4.17950400	-1.26853100
C	3.78053900	-4.26677200	-0.23301700
H	4.49725800	-4.34317200	0.59090500
H	3.25289800	-5.22328600	-0.29631100
H	4.33873800	-4.13293000	-1.16583400
C	2.02266900	-3.43665900	1.32006800
H	2.73768300	-3.47857900	2.14828600
H	1.28683100	-2.66709700	1.54236600
H	1.50879200	-4.40261800	1.26356700

C	7.02344100	-0.37354000	0.00621100
C	7.58899200	1.05502000	0.05012700
H	7.25734800	1.64761700	-0.80880700
H	7.29196000	1.57823000	0.96474700
H	8.68259900	1.02170200	0.02683500
C	7.57381000	-1.14981200	1.22247800
H	7.23180500	-2.18875300	1.22742800
H	8.66932100	-1.15882800	1.20800000
H	7.24637100	-0.68622200	2.15824200
C	7.51045600	-1.04780700	-1.29492900
H	8.60525800	-1.05549800	-1.33658700
H	7.16746700	-2.08399400	-1.36687100
H	7.13790200	-0.51034600	-2.17285300
C	-2.72076800	-3.14809500	-0.73718400
C	-2.07118400	-3.12208200	-2.13988700
H	-2.81026700	-2.86316500	-2.90542500
H	-1.25717300	-2.39819100	-2.18103100
H	-1.65897900	-4.10751700	-2.38271000
C	-1.66304000	-3.54113900	0.31401000
H	-0.85168800	-2.81935800	0.34238700
H	-2.11016300	-3.59979800	1.31117100
H	-1.24727400	-4.52576300	0.07184700
C	-3.79457000	-4.25125400	-0.75136100
H	-4.28345900	-4.35847300	0.22237200
H	-4.56515800	-4.06903700	-1.50770100
H	-3.32003900	-5.20865900	-0.98684900
C	-6.84354000	-0.33230500	0.24253700
C	-7.36699500	1.10293900	0.41205400
H	-6.88000000	1.61307500	1.24918600
H	-7.21163100	1.69959700	-0.49290900
H	-8.44230600	1.08342800	0.61439600
C	-7.59510000	-0.98636800	-0.93731100
H	-7.29243600	-2.02718900	-1.08411500
H	-8.67548000	-0.97637300	-0.75572500
H	-7.39919500	-0.44637000	-1.86919700
C	-7.14415900	-1.11431500	1.53975900
H	-6.82223100	-2.15716900	1.46624600
H	-6.62610300	-0.66419100	2.39215300
H	-8.21958300	-1.11035000	1.74919700

H_2O-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2112.740367
No imaginary frequency

C	4.86613200	-1.60092600	0.13142900
C	5.53166400	-0.34998000	0.08599900
C	3.49221600	-1.76601700	0.16923400
H	5.48232900	-2.49056600	0.13981900
C	4.73766500	0.77477800	0.08016600
C	2.67181100	-0.58471200	0.15247500
C	3.32385600	0.68458000	0.10502500
H	5.17682700	1.76624100	0.05235200
O	1.37062900	-0.70760200	0.18157100
C	2.58835500	1.90825600	0.11039900
Co	0.07261400	0.60660900	-0.14884200
N	1.30042600	2.03482500	0.05957300
H	3.18704000	2.81721600	0.16769500
N	-1.15022900	1.96536600	-0.71453600
C	0.61438400	3.33255800	0.13090500
C	-2.42899600	1.79806400	-0.73544000
C	-0.49723700	3.26276900	-0.92846600
C	1.47295200	4.58177200	-0.04013800
H	-3.06497500	2.66557200	-0.90559600
C	-3.10251400	0.54848700	-0.53929900
C	-1.39735200	4.49466400	-0.85017600
C	0.57847400	5.82976000	0.02438400
H	1.99990800	4.54700200	-1.00428200
H	2.23289500	4.63616800	0.74695000

C	-4.50073400	0.58695700	-0.34498100
C	-2.40104400	-0.69037300	-0.59229400
C	-0.55323700	5.76841200	-1.00796900
H	-2.16393300	4.46413300	-1.63234200
H	-1.90424600	4.48944000	0.12196200
H	1.18521000	6.72825000	-0.13039200
H	0.14695400	5.90582900	1.03023400
C	-5.23273300	-0.57003400	-0.17213600
H	-4.97832900	1.55996200	-0.31205900
C	-3.15338000	-1.89940700	-0.45544500
O	-1.09752500	-0.73869800	-0.78958600
H	-0.12494400	5.79574200	-2.01926300
H	-1.19686400	6.64957800	-0.91649700
C	-4.52087000	-1.78962500	-0.24232700
H	-5.08646200	-2.70268000	-0.11044800
O	-0.73823300	0.46544100	1.68265700
C	-1.52388800	1.30724100	2.27802700
O	-1.54477300	2.53718800	2.11904800
C	-2.51943400	0.63902000	3.22160200
H	-3.03460800	1.38367600	3.83045900
H	-3.25230900	0.08869300	2.62104900
H	-2.01028600	-0.08809500	3.85948000
H	-0.01948100	3.21254900	-1.91766400
H	0.09862900	3.34038800	1.10017500
O	0.77602800	0.24360800	-2.50000400
H	-0.00315700	-0.33389300	-2.41788600
H	1.51643100	-0.34317200	-2.29191100
C	2.84635800	-3.15650200	0.24340000
C	1.90428800	-3.36497200	-0.96444300
H	1.10222600	-2.62982200	-0.97123500
H	2.46617700	-3.29352200	-1.90341100
H	1.45225600	-4.36142300	-0.92075200
C	3.89363700	-4.28345500	0.21133400
H	4.58127100	-4.23060000	1.06176300
H	3.38119600	-5.24876500	0.26388600
H	4.48298800	-4.27190300	-0.71194500
C	2.06351300	-3.27954700	1.57080600
H	2.74919500	-3.19951900	2.42111400
H	1.30718500	-2.50098800	1.66166700
H	1.56747800	-4.25460700	1.62593200
C	7.06303100	-0.31101400	0.05112300
C	7.60112800	1.12802600	0.00609600
H	7.25603500	1.66058700	-0.88610500
H	7.29706600	1.70053300	0.88834000
H	8.69504800	1.11366900	-0.01873500
C	7.62265800	-0.99873300	1.31561200
H	7.30224800	-2.04221100	1.38480700
H	8.71806900	-0.98602900	1.30484300
H	7.28216000	-0.48403800	2.21950300
C	7.56670000	-1.05663000	-1.20401000
H	8.66153000	-1.04607900	-1.24168700
H	7.24328200	-2.10147500	-1.21168100
H	7.18783000	-0.58231700	-2.11488900
C	-2.45486900	-3.26579600	-0.49469600
C	-1.75509700	-3.45899300	-1.85864000
H	-2.48764400	-3.43602500	-2.67288000
H	-1.01390400	-2.68121200	-2.03658600
H	-1.24746000	-4.42925200	-1.88610600
C	-1.42892900	-3.34256500	0.65695500
H	-0.69946200	-2.53848400	0.59350100
H	-1.93704600	-3.26737200	1.62394500
H	-0.90002000	-4.30139100	0.62453400
C	-3.44583300	-4.43015900	-0.31948300
H	-3.95903100	-4.39011400	0.64681100
H	-4.20090200	-4.45313000	-1.11267400
H	-2.89609800	-5.37546000	-0.35922800
C	-6.74114500	-0.58809100	0.09602100
C	-7.33709500	0.82842500	0.12430700
H	-6.88860700	1.43929000	0.91420400

H	-7.19778700	1.34431500	-0.83136600
H	-8.41279300	0.77344900	0.31768300
C	-7.45391000	-1.39311800	-1.01218600
H	-7.09615400	-2.42573400	-1.05745600
H	-8.53362800	-1.42210100	-0.82908700
H	-7.28473500	-0.93716400	-1.99285500
C	-7.00460300	-1.25256900	1.46516900
H	-6.63244000	-2.28072200	1.49386400
H	-6.50958800	-0.69552400	2.26683400
H	-8.07908500	-1.27945300	1.67758900

H_2O-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2112.731673
No imaginary frequency

C	5.03476600	-1.53887000	0.13675200
C	5.64782900	-0.26502600	0.17355600
C	3.66351200	-1.74775200	0.10573100
H	5.68269700	-2.40583300	0.13332400
C	4.81137600	0.83637700	0.17692000
C	2.81898300	-0.59373500	0.10371700
C	3.40733800	0.70135100	0.13955500
H	5.21930200	1.84104900	0.20680600
O	1.51838900	-0.74552000	0.05815100
C	2.61964600	1.91115600	0.15506700
Co	0.04217700	0.37451000	-0.17470500
N	1.33434400	1.99003600	0.09392200
H	3.20693900	2.82914600	0.23405700
N	-1.15266300	1.93671700	-0.82356100
C	0.62115600	3.26923200	0.13745300
C	-2.43723800	1.82908100	-0.79255900
C	-0.45887800	3.21633200	-0.97116400
C	1.47139300	4.53445800	0.02119300
H	-3.05231400	2.72706500	-0.87399800
C	-3.17389800	0.60013100	-0.61216600
C	-1.33699300	4.46876500	-0.93299100
C	0.58482900	5.78635700	0.04891600
H	2.04698300	4.51034300	-0.91520700
H	2.19352800	4.58037300	0.84387100
C	-4.55046700	0.70649500	-0.32435500
C	-2.55361600	-0.67801700	-0.70476100
C	-0.48137200	5.73642700	-1.04948500
H	-2.07195000	4.44115400	-1.74541500
H	-1.89032300	4.48171000	0.01447000
H	1.20472300	6.68285600	-0.05995600
H	0.09347300	5.85678600	1.02780100
C	-5.32601800	-0.41347100	-0.08708100
H	-4.97859000	1.70126900	-0.26622600
C	-3.33935000	-1.84704800	-0.47988400
O	-1.27109600	-0.77490100	-0.99929500
H	0.00700200	5.75726500	-2.03333000
H	-1.12366000	6.62214500	-0.99912400
C	-4.68324200	-1.66903700	-0.17521200
H	-5.28186400	-2.55000500	0.01709700
O	-0.80375100	0.13555800	1.55453800
C	-1.52949200	0.98684500	2.22973900
O	-1.45640200	2.21603500	2.16453600
C	-2.56164500	0.30526000	3.11759200
H	-3.04159100	1.03090200	3.77567900
H	-3.31568300	-0.16511800	2.47714900
H	-2.09188000	-0.48843100	3.70453600
H	0.06596500	3.16884400	-1.93655800
H	0.07183500	3.25713600	1.08735500
O	0.69397000	0.22875800	-2.46535800
H	-0.14524800	-0.26228800	-2.52912200
H	1.36547000	-0.45826300	-2.34736600
C	3.04622400	-3.15478600	0.08124600
C	2.16179900	-3.33278500	-1.17633700

H	1.31003200	-2.65314000	-1.16323100
H	2.74692600	-3.15955100	-2.08716700
H	1.77433500	-4.35639200	-1.21745100
C	4.12522900	-4.25109200	0.04692900
H	4.77197800	-4.21651300	0.92959900
H	3.64116600	-5.23215800	0.03298900
H	4.75522300	-4.17959400	-0.84622500
C	2.19473200	-3.36521200	1.35460500
H	2.82314400	-3.29781600	2.24889500
H	1.40231600	-2.62095500	1.43119300
H	1.73497800	-4.35959300	1.33699200
C	7.17710700	-0.16547500	0.20946400
C	7.66007300	1.29332300	0.24835600
H	7.33448000	1.85073000	-0.63589100
H	7.29577100	1.81602400	1.13859700
H	8.75377000	1.32003100	0.27277200
C	7.70847500	-0.88523300	1.46837700
H	7.42824200	-1.94238200	1.47931800
H	8.80186500	-0.82916900	1.50781700
H	7.30821000	-0.42391400	2.37658000
C	7.76429800	-0.83659900	-1.05151900
H	8.85836100	-0.78123600	-1.03981600
H	7.48467900	-1.89203500	-1.11617100
H	7.40560800	-0.33920200	-1.95822100
C	-2.69286600	-3.24025900	-0.52682200
C	-2.08489300	-3.49617000	-1.92423000
H	-2.85942300	-3.45238800	-2.69761100
H	-1.31765200	-2.75859700	-2.15874300
H	-1.62904700	-4.49202900	-1.95661600
C	-1.58906100	-3.33482200	0.55121300
H	-0.81111200	-2.59128400	0.39137200
H	-2.01011100	-3.17451900	1.54868900
H	-1.13111600	-4.33033400	0.52896100
C	-3.71483100	-4.35750700	-0.25273900
H	-4.15882500	-4.27055000	0.74432200
H	-4.52310800	-4.36641000	-0.99184700
H	-3.20960100	-5.32679800	-0.30348400
C	-6.81312500	-0.35013500	0.27889100
C	-7.33637300	1.09468900	0.31566200
H	-6.80987800	1.69595000	1.06368300
H	-7.23241000	1.58660500	-0.65695500
H	-8.39914900	1.09669200	0.57671100
C	-7.63659500	-1.13771200	-0.76310100
H	-7.33386000	-2.18769700	-0.80955800
H	-8.70213000	-1.10862700	-0.50993100
H	-7.50987800	-0.70860700	-1.76211700
C	-7.01874000	-0.97519600	1.67629300
H	-6.69769200	-2.02048200	1.70269900
H	-6.44405700	-0.42996400	2.43167900
H	-8.07670600	-0.94272900	1.95934800

PO-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2229.378271
No imaginary frequency

C	-4.72305300	-1.54598200	-0.22134100
C	-5.37562800	-0.32115600	0.05480300
C	-3.37313800	-1.68286100	-0.50690100
H	-5.33056500	-2.44148000	-0.21527300
C	-4.59548400	0.81370000	-0.00039600
C	-2.54818300	-0.50028400	-0.47945100
C	-3.20591500	0.74998600	-0.25524000
H	-5.02966200	1.79465800	0.16357700
O	-1.25709800	-0.60171500	-0.65926300
C	-2.50406100	1.99950800	-0.31621600
Co	0.01754300	0.71935800	-0.14538500
N	-1.22509000	2.14001300	-0.34603000
H	-3.12674200	2.89512400	-0.34014500

N	1.23705400	2.06496400	0.43553100
C	-0.53129300	3.42014800	-0.46597700
C	2.51717800	1.90218300	0.42500700
C	0.58949700	3.37298700	0.59225600
C	-1.37728500	4.68280800	-0.32684200
H	3.15167300	2.77880800	0.55948800
C	3.21538000	0.65931600	0.28747500
C	1.48904500	4.60466300	0.49349800
C	-0.47843900	5.92429700	-0.42310900
H	-1.89879600	4.67586100	0.64048600
H	-2.14201100	4.71430500	-1.11015500
C	4.62820600	0.73455000	0.25160600
C	2.54038700	-0.60249300	0.27992800
C	0.64820000	5.88452700	0.61617300
H	2.25348800	4.58848700	1.27803800
H	2.00952000	4.59125200	-0.47268600
H	-1.08033100	6.83012000	-0.29545600
H	-0.04275200	5.97321700	-1.42929600
C	5.41306700	-0.39673800	0.23131300
H	5.07664200	1.72246700	0.23850400
C	3.35532200	-1.78797300	0.36765900
O	1.23554900	-0.69866500	0.23750800
H	0.21438800	5.93579400	1.62414700
H	1.29522400	6.76137000	0.50913300
C	4.73295600	-1.63380200	0.31593900
H	5.34150100	-2.52761800	0.34940000
O	0.59477700	1.18181900	-1.85992200
C	0.93307500	0.51809100	-2.94960500
O	1.13421500	1.13010200	-3.99042400
C	1.12305200	-0.97939200	-2.85865400
H	1.06783400	-1.41267400	-3.85821000
H	2.11369300	-1.18503000	-2.44244200
H	0.38766500	-1.42732400	-2.19588000
H	0.09944700	3.36576700	1.57788700
H	-0.04755900	3.39746700	-1.45006800
C	-2.77874900	-3.05433700	-0.86708200
C	-1.66163700	-3.44285300	0.12380100
H	-0.84841900	-2.72173100	0.09344800
H	-2.05667700	-3.49959300	1.14503600
H	-1.25604000	-4.42759900	-0.13153100
C	-3.83222900	-4.17616700	-0.83084200
H	-4.64837600	-3.99825200	-1.53838300
H	-3.35600000	-5.12106400	-1.10982100
H	-4.26230400	-4.30619600	0.16827200
C	-2.21462000	-2.99194200	-2.30396200
H	-3.02260600	-2.81833900	-3.02229800
H	-1.48734300	-2.18892600	-2.40735000
H	-1.72693300	-3.93867600	-2.56198700
C	-6.87390600	-0.31422200	0.37426300
C	-7.39876700	1.10632200	0.63687100
H	-6.88994700	1.57360300	1.48639200
H	-7.27033800	1.75178200	-0.23800400
H	-8.46783000	1.07042600	0.86838300
C	-7.66124400	-0.90965900	-0.81322700
H	-7.35666700	-1.93843700	-1.02568600
H	-8.73531900	-0.91765300	-0.59665200
H	-7.49810200	-0.31934100	-1.72025900
C	-7.12963600	-1.16619000	1.63677600
H	-8.19780100	-1.18368300	1.88035700
H	-6.80165400	-2.20056000	1.49866000
H	-6.58910400	-0.75589900	2.49611500
C	2.73203000	-3.18503700	0.54482700
C	1.84312600	-3.19513500	1.80809700
H	2.43488900	-2.95644600	2.69900000
H	1.03785500	-2.46965100	1.71832700
H	1.40015200	-4.18690800	1.95045100
C	1.88921000	-3.56742000	-0.68748400
H	1.08654100	-2.85378100	-0.84727400
H	2.51204100	-3.59418900	-1.58719700

H	1.45017800	-4.56175400	-0.54845200
C	3.80025200	-4.27845100	0.73209500
H	4.44125400	-4.38321800	-0.14914900
H	4.43666600	-4.08960500	1.60305900
H	3.30119800	-5.23975600	0.88808600
C	6.94293500	-0.37499000	0.15272600
C	7.49301000	1.05800000	0.07246300
H	7.11757100	1.58447200	-0.81078200
H	7.22890800	1.64256500	0.95997200
H	8.58510700	1.03284900	0.00591000
C	7.53671100	-1.05287900	1.40680000
H	7.20908300	-2.09247000	1.49899800
H	8.63144700	-1.05147700	1.36169400
H	7.23037600	-0.52390300	2.31501900
C	7.39913800	-1.14063400	-1.10840500
H	7.06268500	-2.18137800	-1.09244100
H	6.99565700	-0.67332600	-2.01198100
H	8.49244500	-1.14368700	-1.18115400
C	-1.07909700	-0.64500600	2.39705100
C	0.08735800	0.09749000	2.88943400
O	-0.69541000	0.62516300	1.78505100
H	-0.87320100	-1.47741300	1.73529100
H	1.08064700	-0.23157000	2.60648100
H	0.00253900	0.69944800	3.79081500
C	-2.41607600	-0.64049700	3.07821200
H	-3.21705100	-0.68401600	2.33554800
H	-2.50142800	-1.51953600	3.72574500
H	-2.54459900	0.25832200	3.68755600

PO-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2229.387936
No imaginary frequency

C	4.76444200	-1.53771500	0.42248200
C	5.41162600	-0.29283100	0.21724100
C	3.39826300	-1.70552200	0.57102500
H	5.39070800	-2.41881000	0.47342400
C	4.60977300	0.82690200	0.20667500
C	2.56177600	-0.53854400	0.46377700
C	3.20235000	0.73155200	0.32966600
H	5.03772200	1.81746400	0.09485900
O	1.26515700	-0.67328000	0.49882300
C	2.46164700	1.95271300	0.36191400
Co	-0.02427300	0.62550700	0.06453400
N	1.17294200	2.06539600	0.36356900
H	3.05614000	2.86566000	0.40368500
N	-1.23490300	1.98349600	-0.53301300
C	0.46481900	3.34612600	0.45000100
C	-2.50658600	1.79637500	-0.64630100
C	-0.59614900	3.29944700	-0.66367300
C	1.30706000	4.61447300	0.36702100
H	-3.14454800	2.65666400	-0.84440400
C	-3.17161400	0.53593700	-0.50725300
C	-1.52160000	4.51218200	-0.57522000
C	0.38709800	5.84238500	0.44903000
H	1.87026400	4.63336300	-0.57708800
H	2.03659500	4.64260700	1.18394600
C	-4.58200500	0.55146500	-0.42339800
C	-2.44673200	-0.69194700	-0.48349000
C	-0.69654200	5.80683600	-0.63525900
H	-2.24948900	4.50568600	-1.39424700
H	-2.07337900	4.45160600	0.36991500
H	0.98119100	6.75832300	0.36139500
H	-0.08964600	5.86426900	1.43682800
C	-5.30641800	-0.61388800	-0.28225700
H	-5.07674200	1.51625000	-0.44752000
C	-3.18958400	-1.91046900	-0.35535900
O	-1.13839200	-0.72872200	-0.60154000

H	-0.22330500	5.88917800	-1.62354700
H	-1.36158600	6.67094100	-0.53391900
C	-4.57018700	-1.82187700	-0.25492400
H	-5.12824300	-2.74132000	-0.13433400
O	-0.92686200	0.46076900	1.87116500
C	-1.77468200	1.27028400	2.41863900
O	-1.81979500	2.50315800	2.27575600
C	-2.81810700	0.56297100	3.28034200
H	-3.39047300	1.28354400	3.86695500
H	-3.49648300	0.01009300	2.62080800
H	-2.33793700	-0.16678400	3.93747500
H	-0.06931400	3.30102300	-1.62935100
H	-0.09873600	3.31059600	1.39187200
C	2.78345000	-3.08405400	0.85710000
C	1.83743000	-3.49741800	-0.29003200
H	1.00305700	-2.80538400	-0.37285300
H	2.37700200	-3.52855700	-1.24367100
H	1.43191800	-4.49728900	-0.10150700
C	3.85782400	-4.17770100	0.99128100
H	4.56318700	-3.96335000	1.80085800
H	3.37078900	-5.13002000	1.22161800
H	4.42564100	-4.31485100	0.06452900
C	2.00251500	-3.02545300	2.19070100
H	2.68116900	-2.79217800	3.01812400
H	1.21884800	-2.26906000	2.16026600
H	1.54011500	-3.99735600	2.39543600
C	6.93297900	-0.25282600	0.04163500
C	7.45084100	1.17967600	-0.16357400
H	7.01437300	1.64252000	-1.05465500
H	7.22884900	1.81659900	0.69873700
H	8.53727600	1.16607800	-0.29438200
C	7.61583300	-0.84014600	1.29602400
H	7.31562700	-1.87673800	1.47351900
H	8.70537100	-0.82337100	1.18210100
H	7.35482000	-0.25958700	2.18634800
C	7.32359900	-1.09120400	-1.19524900
H	8.41006000	-1.08466000	-1.33644600
H	7.00631900	-2.13306500	-1.09380900
H	6.85802800	-0.68637000	-2.09972400
C	-2.46113300	-3.25807500	-0.26750000
C	-1.63668000	-3.49626400	-1.55263500
H	-2.29799500	-3.55079500	-2.42479300
H	-0.91720700	-2.69520800	-1.71335400
H	-1.09248500	-4.44418600	-1.48069300
C	-1.54850600	-3.24963700	0.98018000
H	-0.83952100	-2.42475300	0.95410200
H	-2.15338400	-3.14769100	1.88717400
H	-0.99288900	-4.19147900	1.04617200
C	-3.43744400	-4.43902000	-0.12462300
H	-4.03490500	-4.36928800	0.79018400
H	-4.11896400	-4.51701500	-0.97872300
H	-2.86559600	-5.37056600	-0.07186400
C	-6.83126200	-0.65346300	-0.13843000
C	-7.45173900	0.75122500	-0.20464000
H	-7.08273100	1.39377600	0.60106200
H	-7.23979400	1.24137100	-1.16055700
H	-8.53899100	0.68102100	-0.10154600
C	-7.43595600	-1.50514200	-1.27561800
H	-7.05739800	-2.53115600	-1.25905100
H	-8.52652500	-1.55043600	-1.18119700
H	-7.19418400	-1.07513300	-2.25285600
C	-7.19703300	-1.28130800	1.22447400
H	-6.81222500	-2.30106800	1.31586900
H	-6.77882800	-0.69156900	2.04618600
H	-8.28491600	-1.32166500	1.34850100
C	1.41561100	-0.58884500	-2.61295200
C	0.28036900	0.09941900	-3.23741700
O	0.96645200	0.69785300	-2.11440000
H	1.17200400	-1.39490800	-1.92864700

H	-0.72817000	-0.23552800	-3.01089800
H	0.42214600	0.63109800	-4.17651500
C	2.80091600	-0.60920800	-3.19440400
H	3.54445300	-0.57860000	-2.39208400
H	2.95599700	-1.53024300	-3.76640300
H	2.96195000	0.24667200	-3.85606100

PO-aCo^{III}-OAc
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2229.375092
No imaginary frequency

C	-4.91323600	-1.49115600	0.02728900
C	-5.48923100	-0.23421800	0.33273700
C	-3.59173000	-1.67830600	-0.34613700
H	-5.55543200	-2.36064100	0.08426800
C	-4.67494500	0.87460600	0.20411700
C	-2.73420400	-0.52614100	-0.37904900
C	-3.31391300	0.76158300	-0.15389800
H	-5.06555100	1.87110000	0.38204300
O	-1.46384600	-0.68427700	-0.61118700
C	-2.57454200	1.98656900	-0.32322100
Co	0.02273200	0.50718400	-0.54405700
N	-1.31643800	2.07554300	-0.58699200
H	-3.17262200	2.89826600	-0.23474900
N	1.20499800	2.03409900	0.19169600
C	-0.61086900	3.33953800	-0.75107100
C	2.44988400	1.88829400	0.51857200
C	0.53492500	3.33822300	0.28835600
C	-1.43774700	4.62218700	-0.66135100
H	3.02440200	2.77142500	0.80827500
C	3.20160300	0.66842200	0.52792400
C	1.42962200	4.57089000	0.10983600
C	-0.53830200	5.84792100	-0.86415800
H	-1.91997800	4.68412500	0.32387800
H	-2.23590900	4.60565500	-1.41179600
C	4.58753100	0.76723900	0.78052300
C	2.60645200	-0.60238400	0.26707600
C	0.60434300	5.86456000	0.15622000
H	2.19571800	4.60907300	0.89057500
H	1.95298100	4.48792900	-0.85149600
H	-1.13162900	6.76529200	-0.78706500
H	-0.12111400	5.82616200	-1.87955200
C	5.41045600	-0.34021100	0.74366500
H	4.99301700	1.75266400	0.98396400
C	3.44930500	-1.75818300	0.20214300
O	1.31443200	-0.72569300	0.12400900
H	0.18510600	5.98821200	1.16415100
H	1.25957200	6.72486300	-0.01723200
C	4.80246600	-1.58297700	0.44088100
H	5.44583700	-2.45191600	0.38901800
O	0.34945000	0.48797600	-2.43277500
C	1.53772200	0.32957600	-2.97250600
O	2.60023300	0.63564300	-2.44116800
C	1.48156100	-0.29825200	-4.35752700
H	2.46335800	-0.26184400	-4.83137400
H	1.16280100	-1.34140200	-4.25887900
H	0.73895900	0.21039400	-4.97829900
H	0.05691500	3.37859800	1.27885900
H	-0.14043100	3.28624700	-1.74326200
C	-1.00107100	-0.63407500	2.45771900
C	0.14576000	0.16554800	2.90492200
O	-0.70642200	0.64191600	1.84336500
H	-0.78281400	-1.46598500	1.79489900
H	1.14651800	-0.11195000	2.58682400
H	0.07315600	0.74034900	3.82690400
C	-2.30126700	-0.70896800	3.20873700
H	-3.13847900	-0.77374800	2.50745400
H	-2.32036000	-1.60047900	3.84486500

H	-2.44002600	0.17453100	3.83846700
C	2.85048500	-3.13027700	-0.13970400
C	3.93474100	-4.21570600	-0.25823300
H	3.46255100	-5.16998900	-0.51100300
H	4.65827800	-3.98408100	-1.04682100
H	4.48028300	-4.35804300	0.68068800
C	2.10926300	-3.06045200	-1.49621800
H	1.25986000	-2.38045900	-1.45228600
H	2.78601900	-2.71403600	-2.28374700
H	1.74360700	-4.05658900	-1.76999000
C	1.87267800	-3.56026100	0.97689500
H	2.40283600	-3.67453400	1.92890600
H	1.08174400	-2.82243200	1.10531200
H	1.41152500	-4.52234700	0.72699800
C	6.92167500	-0.28204100	0.99020500
C	7.40043200	1.14441200	1.30435800
H	7.19972000	1.82896600	0.47412000
H	6.91908900	1.54296600	2.20349500
H	8.48083200	1.14234600	1.47924100
C	7.66537800	-0.77551000	-0.27029100
H	8.74930600	-0.74283500	-0.11276300
H	7.39553300	-1.80512200	-0.52188200
H	7.42258600	-0.14720600	-1.13265000
C	7.28296400	-1.18848600	2.18726800
H	6.99531000	-2.22852400	2.00866300
H	8.36285500	-1.16763400	2.37161000
H	6.77359000	-0.85210000	3.09605000
C	-3.04363900	-3.05948400	-0.74056400
C	-2.51759500	-2.99770000	-2.19428800
H	-3.32702400	-2.73874600	-2.88506400
H	-1.72403100	-2.25633900	-2.29420500
H	-2.12074600	-3.97594300	-2.48830100
C	-4.13194500	-4.14533100	-0.67688000
H	-4.52218300	-4.27717200	0.33821100
H	-4.97171800	-3.92401500	-1.34371800
H	-3.70393900	-5.10184600	-0.99152900
C	-1.89537300	-3.48927500	0.19922000
H	-1.04441800	-2.81755300	0.10387000
H	-2.22885000	-3.50042900	1.24311400
H	-1.56338700	-4.50149200	-0.05688000
C	-6.95863300	-0.16233900	0.76121100
C	-7.40743300	1.28024300	1.04424700
H	-6.81861800	1.73580700	1.84699200
H	-7.32207700	1.91187200	0.15414300
H	-8.45641300	1.28738300	1.35613400
C	-7.85437600	-0.73749600	-0.35766200
H	-7.60852400	-1.78011100	-0.57819900
H	-8.90868600	-0.69859100	-0.06212500
H	-7.73564400	-0.16353200	-1.28199100
C	-7.15225200	-0.99123200	2.05011600
H	-8.19880200	-0.96064100	2.37303400
H	-6.87908900	-2.03975200	1.90073800
H	-6.53151800	-0.59626000	2.86083600

(salen)aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2702.579765
No imaginary frequency

S	-0.73545600	1.38121100	2.28437700
O	0.02429500	1.70384300	3.50103700
O	-1.36241800	2.51960900	1.56897800
O	0.10580600	0.51023300	1.33365600
C	-2.05229600	0.25584900	2.73517100
C	-1.83656600	-0.66288100	3.76250300
C	-3.24242200	0.24965100	2.01213100
C	-2.82064300	-1.60386800	4.05342600
H	-0.91007000	-0.62617800	4.32449600
C	-4.21701700	-0.69923100	2.31329300

H	-3.39869000	0.97717900	1.22591200
C	-4.01878100	-1.64470600	3.32616300
H	-2.65604000	-2.32179200	4.85257900
H	-5.14067500	-0.71210600	1.74472800
C	-5.05340400	-2.70755400	3.60026900
H	-4.82531600	-3.62558200	3.04397000
H	-5.08768400	-2.97191800	4.66138800
H	-6.05225200	-2.38096100	3.29682500
N	1.87092200	2.01610500	-0.25969800
N	-0.51803800	2.12171200	-1.19691600
C	3.12686000	1.80384700	-0.02210500
H	3.74217200	2.65813400	0.25886600
C	-1.78922300	2.02618100	-1.44303700
H	-2.33257500	2.93773600	-1.68546000
C	3.80510600	0.55139400	-0.11029100
C	5.19066900	0.53116200	0.17811800
C	3.12972100	-0.63155100	-0.52772900
C	5.92906300	-0.62667000	0.06348400
H	5.65343100	1.45910300	0.49588200
C	3.88981600	-1.83843900	-0.67703300
C	5.24009200	-1.78657500	-0.37066800
H	5.81522100	-2.69829600	-0.46556300
C	-2.56647700	0.83556300	-1.39769200
C	-3.96821900	0.95791600	-1.56653700
C	-1.96533200	-0.44061900	-1.18552500
C	-4.79570400	-0.14015400	-1.49295900
H	-4.36942200	1.94966400	-1.74357500
C	-2.82079900	-1.58625700	-1.05849600
C	-4.18104100	-1.39018900	-1.22095100
H	-4.83043300	-2.24999700	-1.12089800
O	1.84725700	-0.64771400	-0.79356000
O	-0.66956500	-0.59614400	-1.11975200
C	1.23640600	3.33484400	-0.10792200
C	2.15373400	4.55474000	-0.10644500
C	0.19253600	3.41506700	-1.22907300
C	1.30308500	5.82654200	0.03978800
H	2.73450000	4.58852300	-1.03869800
H	2.86545300	4.49858100	0.72338500
C	-0.66988300	4.66732500	-1.07028300
C	0.22539200	5.91606400	-1.04648900
H	1.94989800	6.70941700	0.00683100
H	0.82369300	5.81956700	1.02650500
H	-1.38604700	4.75558600	-1.89402500
H	-1.23644500	4.57642400	-0.13645500
H	0.70665100	6.03420200	-2.02709500
H	-0.39314600	6.80622300	-0.89243100
Co	0.57329100	0.68192900	-0.61951600
H	0.73237700	3.46174500	-2.18735100
H	0.67623700	3.30294600	0.83344200
C	3.21055600	-3.13682900	-1.13675600
C	4.20903300	-4.30342500	-1.23618300
H	4.66596200	-4.53712500	-0.26882000
H	3.67881700	-5.19904200	-1.57343200
H	5.00815300	-4.10174400	-1.95763300
C	2.58628700	-2.93480200	-2.53671400
H	1.84246600	-2.13882800	-2.52650700
H	3.36098500	-2.68315900	-3.26955300
H	2.09932000	-3.86003200	-2.86326000
C	2.11782600	-3.53580200	-0.11966800
H	2.55760100	-3.70544800	0.86895700
H	1.35689000	-2.76311100	-0.03249900
H	1.63258000	-4.46446200	-0.43938400
C	7.42656300	-0.71305600	0.37636700
C	7.99965600	0.64044600	0.82580800
H	7.89034900	1.40384000	0.04852900
H	7.51221100	1.00296200	1.73649100
H	9.06768200	0.53693700	1.04022000
C	8.18978300	-1.16832300	-0.88667500
H	9.26260400	-1.24292400	-0.67807500

H	7.84960200	-2.14754700	-1.23555000
H	8.04839000	-0.45420500	-1.70414700
C	7.65294100	-1.73663400	1.51053400
H	7.29677500	-2.73309300	1.23398600
H	8.72004000	-1.81661600	1.74504200
H	7.12347800	-1.43237800	2.41869600
C	-2.23201800	-2.95697100	-0.69838300
C	-3.32677100	-4.02904100	-0.55648000
H	-4.04402300	-3.77594000	0.23180500
H	-3.87702400	-4.18695900	-1.49057200
H	-2.86067800	-4.98057200	-0.28381300
C	-1.25625900	-3.42072100	-1.80278500
H	-1.77467600	-3.50502700	-2.76458000
H	-0.42624900	-2.72530400	-1.91279300
H	-0.85092100	-4.40643700	-1.54951500
C	-1.50431800	-2.85629000	0.66297400
H	-1.03111300	-3.81589700	0.89874900
H	-0.73773100	-2.08307900	0.66035000
H	-2.21570500	-2.62202400	1.45824200
C	-6.31434200	-0.07187200	-1.68828300
C	-6.79083300	1.35602900	-1.99898700
H	-6.55760500	2.04646600	-1.18204100
H	-6.33644200	1.74192200	-2.91719000
H	-7.87625100	1.36214200	-2.13761700
C	-6.71402400	-0.98496100	-2.86829400
H	-6.43740600	-2.02728900	-2.68614600
H	-7.79712300	-0.94965700	-3.02836100
H	-6.22007700	-0.66426700	-3.79081300
C	-7.02998900	-0.55042500	-0.40665600
H	-8.11562200	-0.55055500	-0.55269900
H	-6.73151200	-1.56547200	-0.12863300
H	-6.80192400	0.11227100	0.43405700

(salen)aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2702.573385
No imaginary frequency

S	-0.64390100	1.33471700	2.55551300
O	-0.03957500	1.53223900	3.87691100
O	-1.05592700	2.53716700	1.79591600
O	0.27710600	0.42870200	1.69419600
C	-2.11063100	0.33189000	2.76206000
C	-2.12363100	-0.67299600	3.73035600
C	-3.21302300	0.54376800	1.93916400
C	-3.24993200	-1.48152500	3.85431200
H	-1.26518400	-0.80263800	4.37986500
C	-4.32979400	-0.27866900	2.06915300
H	-3.19238300	1.34434600	1.21189400
C	-4.36226900	-1.30694800	3.01715100
H	-3.26557200	-2.26581200	4.60643000
H	-5.18206100	-0.12409500	1.41669100
C	-5.54872800	-2.23345100	3.10732500
H	-5.35521400	-3.16555200	2.56123200
H	-5.76992200	-2.50617300	4.14372300
H	-6.44404000	-1.77930500	2.67375300
N	1.96738300	1.97152300	-0.19933100
N	-0.49473700	2.02721700	-1.12098700
C	3.24819000	1.81807500	-0.16502400
H	3.88990100	2.69665300	-0.06152200
C	-1.74679700	1.95424800	-1.43901200
H	-2.26138600	2.86293100	-1.75689800
C	3.94803800	0.56181200	-0.23900900
C	5.35303700	0.58535600	-0.13193700
C	3.26325100	-0.67722200	-0.42175000
C	6.10146100	-0.57690300	-0.18751800
H	5.83345900	1.54818800	0.00375200
C	4.02137800	-1.89239500	-0.48840600
C	5.39816400	-1.79289500	-0.36673400

H	5.98105900	-2.70351200	-0.41033800
C	-2.58596100	0.78629900	-1.40376400
C	-3.95565800	0.95866700	-1.70456300
C	-2.08558100	-0.50504000	-1.07087400
C	-4.84188300	-0.10109000	-1.66638500
H	-4.29473600	1.95673100	-1.96030200
C	-2.98466800	-1.61766300	-1.03170000
C	-4.31650100	-1.37099300	-1.32399900
H	-5.00809200	-2.20259400	-1.28563900
O	1.96515800	-0.72221100	-0.53734500
O	-0.81876200	-0.68093800	-0.80568700
C	1.32327500	3.28056600	-0.11361400
C	2.22291700	4.51285200	-0.19364300
C	0.23936100	3.30117200	-1.21375200
C	1.37573600	5.78730000	-0.07986200
H	2.77552400	4.51410000	-1.14408100
H	2.96329500	4.49109700	0.61334600
C	-0.60582900	4.57444900	-1.10346000
C	0.28358600	5.82464900	-1.15294300
H	2.01827900	6.67069600	-0.15881200
H	0.91103000	5.81918100	0.91356300
H	-1.33647300	4.62841400	-1.91711600
H	-1.16069600	4.53363600	-0.15851800
H	0.75160200	5.89643100	-2.14453000
H	-0.33637800	6.71958900	-1.03438200
Co	0.54278100	0.46089500	-0.23937100
H	0.76147400	3.29435000	-2.18352000
H	0.78368800	3.28622200	0.84138600
C	3.31131500	-3.23878400	-0.69458900
C	4.30768900	-4.41123800	-0.71751900
H	4.85872700	-4.49920100	0.22474400
H	3.75807500	-5.34541500	-0.86613800
H	5.03090900	-4.32137000	-1.53503300
C	2.56426600	-3.22814500	-2.04852500
H	1.81869500	-2.43401300	-2.08139200
H	3.26783000	-3.08352300	-2.87570800
H	2.05532900	-4.18625000	-2.19988600
C	2.30980100	-3.49496200	0.45610700
H	2.82720500	-3.51125400	1.42111400
H	1.53602200	-2.72959800	0.49135600
H	1.82692400	-4.46804000	0.31387600
C	7.62821900	-0.60373000	-0.06264200
C	8.21797600	0.80344300	0.12390300
H	7.98934700	1.45402900	-0.72647500
H	7.84327900	1.28139200	1.03464500
H	9.30702400	0.73881900	0.20785900
C	8.23561800	-1.21881400	-1.34282300
H	9.32792500	-1.25185100	-1.26763200
H	7.88197700	-2.24014700	-1.50985200
H	7.97048300	-0.62438000	-2.22284500
C	8.02537900	-1.46220700	1.15857500
H	7.66583500	-2.49085000	1.06553000
H	9.11546700	-1.49721400	1.26059700
H	7.60763200	-1.04365000	2.07940700
C	-2.47009900	-3.01487500	-0.65636300
C	-3.60294900	-4.05581000	-0.65440900
H	-4.38239000	-3.80749300	0.07424200
H	-4.07037700	-4.16036900	-1.63947200
H	-3.19315900	-5.03187900	-0.37833600
C	-1.40606000	-3.47067200	-1.68092200
H	-1.83047500	-3.51066000	-2.69013400
H	-0.55198800	-2.79462400	-1.68743200
H	-1.04946100	-4.47409900	-1.42308600
C	-1.85715500	-2.99000000	0.76248000
H	-1.47630900	-3.98593700	1.01531300
H	-1.03608200	-2.27856600	0.83667200
H	-2.61083300	-2.71433000	1.50292900
C	-6.33580900	0.03434600	-1.98341400
C	-6.71945900	1.47638300	-2.35187700

H	-6.51123100	2.17166300	-1.53227900
H	-6.18351800	1.82193200	-3.24169200
H	-7.79077200	1.53064300	-2.56809300
C	-6.68797400	-0.88144600	-3.17647600
H	-6.48035900	-1.93239800	-2.95642000
H	-7.75195800	-0.79550600	-3.42252500
H	-6.10747900	-0.60411700	-4.06187700
C	-7.16952400	-0.38656500	-0.75321900
H	-8.23932600	-0.34767700	-0.98545400
H	-6.93431500	-1.40492200	-0.43073500
H	-6.98348800	0.28607600	0.09022000

H_2O-aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2779.006845
No imaginary frequency

S	-0.51846900	0.91269200	1.98183200
O	0.71338900	1.09296600	2.76680800
O	-1.36322200	2.11708100	1.81897100
O	-0.25073600	0.20947400	0.62069700
C	-1.50720000	-0.37397700	2.72851000
C	-1.17173000	-0.85489200	3.98871500
C	-2.61248300	-0.87309100	2.03360700
C	-1.96164100	-1.85180700	4.56522100
H	-0.30046500	-0.45649400	4.49623600
C	-3.38116200	-1.87135200	2.61856800
H	-2.85500600	-0.49787300	1.04901300
C	-3.07026300	-2.37524800	3.89231100
H	-1.70664700	-2.23273500	5.55030900
H	-4.23285600	-2.27218100	2.07474000
C	-3.90947900	-3.46915600	4.50395600
H	-3.80187900	-4.40674500	3.94597000
H	-3.62074500	-3.66312600	5.54017500
H	-4.97307800	-3.20768100	4.49151700
N	1.67646600	2.10701200	-0.16686300
N	-0.72913700	2.40103800	-1.04697500
C	2.88908700	1.80826500	0.16327000
H	3.48883600	2.58136500	0.64300400
C	-2.01169800	2.30139700	-1.00864900
H	-2.60141700	3.20404400	-0.85712600
C	3.55058400	0.55549100	-0.02460200
C	4.90191800	0.48678900	0.39466600
C	2.89761800	-0.58090400	-0.58571000
C	5.63653300	-0.67229900	0.28262300
H	5.34226100	1.38621700	0.81169000
C	3.63311600	-1.81371300	-0.64292800
C	4.95696500	-1.80180900	-0.23212800
H	5.51181000	-2.72905000	-0.29145900
C	-2.74556500	1.07449700	-1.14139100
C	-4.10581700	1.09688500	-0.78674600
C	-2.12137000	-0.11941100	-1.61156400
C	-4.89212400	-0.04156000	-0.85835100
H	-4.51826700	2.03066100	-0.41506900
C	-2.93342300	-1.28524200	-1.74198600
C	-4.27204900	-1.20237100	-1.35837400
H	-4.86938700	-2.09846200	-1.43605100
O	1.67531700	-0.53586800	-1.06390300
O	-0.84129800	-0.14203700	-1.94158200
C	1.07373500	3.40922000	0.16573500
C	2.02481800	4.60193600	0.26701500
C	-0.00117500	3.66412000	-0.90184400
C	1.22305100	5.87416400	0.58513600
H	2.57139400	4.71819300	-0.67876300
H	2.76525600	4.44063300	1.05624600
C	-0.82618600	4.90124000	-0.55688400
C	0.10349700	6.11824900	-0.43391300
H	1.89732900	6.73629000	0.62116500
H	0.78417400	5.77362000	1.58597900

H	-1.58213700	5.08762500	-1.32786300
H	-1.34956000	4.72543900	0.39070600
H	0.54535800	6.33390100	-1.41616200
H	-0.47893300	7.00138300	-0.15145000
Co	0.43954500	0.90803000	-0.97481400
H	0.51728000	3.82867000	-1.85739600
H	0.55567500	3.28402900	1.12286900
O	1.08536900	1.27879000	-2.85734200
H	0.28951100	0.85271100	-3.23798300
H	1.75055000	0.56442600	-2.85323900
C	-2.32936200	-2.61217000	-2.22110700
C	-3.37722000	-3.73538700	-2.31057500
H	-4.18335800	-3.49480900	-3.01222500
H	-2.89072400	-4.64908000	-2.66554800
H	-3.82223300	-3.96046600	-1.33583300
C	-1.70724400	-2.44474800	-3.62517200
H	-2.46931300	-2.14503400	-4.35320900
H	-0.91904400	-1.69267500	-3.61456100
H	-1.27516900	-3.39489300	-3.95809900
C	-1.24819000	-3.04640600	-1.21182200
H	-0.47395800	-2.28808000	-1.12652400
H	-1.68603400	-3.20032700	-0.21991200
H	-0.78663400	-3.98638000	-1.53311800
C	2.93727200	-3.12241500	-1.04651500
C	1.88728700	-3.43576100	0.04505100
H	1.19267100	-2.60705100	0.17921200
H	1.31449400	-4.33110200	-0.21878600
H	2.38812300	-3.62091500	1.00106700
C	2.27322300	-3.01477700	-2.43817000
H	1.49452000	-2.25591300	-2.45296600
H	3.02338300	-2.76952800	-3.19953800
H	1.82466400	-3.97663300	-2.70968200
C	3.91807400	-4.30784000	-1.10650900
H	4.70939000	-4.14879100	-1.84734400
H	4.38623400	-4.50756800	-0.13750300
H	3.36996000	-5.20995300	-1.39494900
C	7.10400300	-0.79709000	0.70509700
C	7.66308400	0.53148500	1.23881200
H	7.61601200	1.32165500	0.48229700
H	7.11860500	0.87121400	2.12568900
H	8.71255100	0.40501300	1.52238400
C	7.23107400	-1.85858500	1.81960800
H	6.88275500	-2.84004600	1.48519300
H	8.27614400	-1.96383900	2.13165200
H	6.63794200	-1.57395000	2.69418200
C	7.95270500	-1.22684900	-0.51118900
H	9.00549200	-1.33256900	-0.22659800
H	7.61919300	-2.18589600	-0.91802100
H	7.88699900	-0.48322000	-1.31187600
C	-6.35166300	-0.00932100	-0.38598400
C	-6.39326500	0.41635600	1.09840300
H	-5.82160200	-0.27861300	1.72084900
H	-5.96659900	1.41264100	1.24433600
H	-7.42648200	0.43714400	1.46264900
C	-7.03495200	-1.38087100	-0.51202000
H	-8.06805100	-1.31109000	-0.15777300
H	-7.06290000	-1.72869500	-1.54960400
H	-6.52888000	-2.14237100	0.09041200
C	-7.14502500	1.00788400	-1.23376600
H	-7.13488200	0.72437500	-2.29106200
H	-8.18798100	1.05575100	-0.90136100
H	-6.72256400	2.01379300	-1.15298100

H_2O-aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2779.004576
No imaginary frequency

S	-0.79035400	1.14653500	2.24995400

O	0.13080000	1.39926600	3.37030700
O	-1.49478400	2.33176700	1.70256900
O	-0.11014400	0.32251500	1.14680600
C	-2.03951300	-0.01485600	2.78995700
C	-1.72485900	-0.93729900	3.78626100
C	-3.26418700	-0.06909500	2.12705500
C	-2.64613300	-1.93037800	4.11183300
H	-0.76907500	-0.86599300	4.29328800
C	-4.17418000	-1.06820800	2.46271900
H	-3.49423700	0.65704400	1.35714100
C	-3.87715000	-2.01836200	3.44829000
H	-2.40508600	-2.65165900	4.88828900
H	-5.12546700	-1.11853100	1.94354500
C	-4.84664900	-3.13157400	3.75922000
H	-4.65212400	-4.00672000	3.12646700
H	-4.76330400	-3.45815700	4.79989500
H	-5.88081800	-2.82320900	3.57966100
N	1.80737500	2.03513500	-0.12038900
N	-0.58142900	2.23833400	-1.06592200
C	3.03869500	1.78582900	0.19692400
H	3.63030200	2.60219600	0.61010600
C	-1.85683300	2.15646700	-1.25557700
H	-2.42193700	3.08094600	-1.36129000
C	3.72568200	0.54329500	0.04962300
C	5.09506900	0.51178900	0.40971400
C	3.08206600	-0.61902200	-0.46917800
C	5.85344800	-0.62757500	0.25635800
H	5.53009700	1.42041600	0.81130700
C	3.86805500	-1.80538000	-0.66203300
C	5.20163700	-1.76104600	-0.29066600
H	5.79403500	-2.65684200	-0.42332200
C	-2.62137000	0.94969800	-1.30130800
C	-4.02949200	1.07573400	-1.34018800
C	-2.00216600	-0.33347600	-1.29531700
C	-4.84937800	-0.03324400	-1.31956200
H	-4.44485100	2.07682200	-1.37171500
C	-2.84028100	-1.48925000	-1.18124900
C	-4.21334500	-1.29367400	-1.21394600
H	-4.84958600	-2.16564800	-1.13801600
O	1.81342100	-0.63524400	-0.78927900
O	-0.69901700	-0.47487900	-1.41336300
C	1.16819800	3.33853600	0.13350700
C	2.09344300	4.54900400	0.24023800
C	0.14070400	3.51670500	-0.99312700
C	1.25297800	5.81615200	0.46278900
H	2.69002400	4.64177300	-0.67773300
H	2.79015400	4.42887300	1.07579900
C	-0.71045800	4.76368800	-0.75838400
C	0.19708000	5.99707200	-0.63329800
H	1.90969600	6.69130700	0.50633600
H	0.75470700	5.74344700	1.43758700
H	-1.41403500	4.91342200	-1.58438900
H	-1.29195700	4.61732200	0.15946000
H	0.69740500	6.17645200	-1.59472000
H	-0.41349600	6.88237300	-0.42767500
Co	0.55316700	0.75077700	-0.72471400
H	0.69447800	3.61727400	-1.93777900
H	0.60129900	3.23397600	1.06580700
C	3.23285300	-3.07777000	-1.24429100
C	2.64698600	-2.78656000	-2.64550300
H	1.83924000	-2.05774100	-2.58696100
H	3.42441000	-2.41070900	-3.32056000
H	2.23970000	-3.70584600	-3.07936200
C	2.11518500	-3.57473900	-0.30183000
H	2.52669600	-3.82609100	0.68129300
H	1.34551400	-2.81730900	-0.17151400
H	1.64878900	-4.47564100	-0.71591400
C	4.26015300	-4.21261300	-1.40214800
H	3.76146000	-5.09026900	-1.82401600

H	5.07713900	-3.93861300	-2.07838400
H	4.69135500	-4.51138200	-0.44126400
C	7.33461400	-0.72016600	0.63757400
C	7.86422600	0.60320800	1.21266100
H	7.78450000	1.41976400	0.48758200
H	7.32496100	0.89367700	2.11993400
H	8.92109600	0.49574800	1.47508000
C	8.16673700	-1.07291100	-0.61461100
H	9.22889200	-1.15027700	-0.35797100
H	7.85932400	-2.02794900	-1.05027500
H	8.05539800	-0.30248900	-1.38421400
C	7.51974900	-1.82127200	1.70458800
H	7.19282500	-2.79896500	1.33902400
H	8.57494800	-1.90616700	1.98647300
H	6.94126700	-1.59024500	2.60436500
C	-2.22809300	-2.87822700	-0.94682300
C	-1.29654800	-3.27355400	-2.11351900
H	-1.84542800	-3.28183900	-3.06223900
H	-0.46026900	-2.58258400	-2.19752700
H	-0.89842600	-4.28018800	-1.94505700
C	-3.30876200	-3.96696300	-0.82244500
H	-3.98528700	-3.77437200	0.01683000
H	-3.90542500	-4.06641300	-1.73601700
H	-2.82394000	-4.93031400	-0.63794600
C	-1.44370100	-2.84694300	0.38609200
H	-0.94608900	-3.80998400	0.54502300
H	-0.69291800	-2.05810900	0.39742000
H	-2.12384100	-2.67144900	1.22339300
C	-6.37836100	0.04285000	-1.39753500
C	-6.87583200	1.49104800	-1.53154900
H	-6.58806100	2.09867600	-0.66760000
H	-6.48506800	1.96963000	-2.43528600
H	-7.96820000	1.50273400	-1.59515000
C	-7.00221800	-0.56414800	-0.12271600
H	-8.09562100	-0.55028300	-0.18843600
H	-6.69135500	-1.60226500	0.02696900
H	-6.70850700	0.00916200	0.76203100
C	-6.86033000	-0.75261100	-2.63071800
H	-6.56901700	-1.80521700	-2.57219400
H	-7.95221900	-0.71130900	-2.70940600
H	-6.43421700	-0.33837000	-3.54985100
O	1.10073600	0.80106300	-3.09829600
H	1.83796500	0.18576900	-2.97352900
H	0.32628600	0.21368000	-3.12784500

H_2O-aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2778.995533
No imaginary frequency

S	-0.11392800	0.32137700	2.01041400
O	1.11209900	0.32312400	2.82699500
O	-0.96128900	1.53203600	2.08135000
O	0.20274600	-0.07452400	0.55359300
C	-1.12465800	-1.07443600	2.48408600
C	-0.51688600	-2.20755200	3.02034700
C	-2.48744400	-1.06165000	2.19005300
C	-1.28666700	-3.34440000	3.25804000
H	0.54368800	-2.18586200	3.24511500
C	-3.24233800	-2.20617600	2.43222600
H	-2.94242900	-0.17180400	1.77147100
C	-2.65519000	-3.36465900	2.95851800
H	-0.81864400	-4.23082200	3.67800600
H	-4.30208200	-2.20431900	2.19943100
C	-3.47427600	-4.61472600	3.16441100
H	-3.47730800	-5.23365900	2.25845500
H	-3.07327300	-5.22826300	3.97630200
H	-4.51586600	-4.37608900	3.39893500
N	1.62976600	2.34666600	-0.05762300

N	-0.91364000	2.61717900	-0.71568700
C	2.70523000	1.89622200	0.49848400
H	3.13963200	2.44823300	1.33632900
C	-2.17886900	2.46955400	-0.54725000
H	-2.77861400	3.31149700	-0.19495100
C	3.41494800	0.69667900	0.13518100
C	4.55204900	0.37022300	0.90153600
C	3.02489900	-0.12941100	-0.95768500
C	5.31863800	-0.74533200	0.62156900
H	4.80015800	1.01999300	1.73296500
C	3.82094300	-1.26929700	-1.28420900
C	4.92386700	-1.53314000	-0.48227100
H	5.52105300	-2.40633200	-0.70985300
C	-2.90910000	1.23929900	-0.75001600
C	-4.25236900	1.21548500	-0.32698300
C	-2.31868400	0.08513300	-1.34061800
C	-5.02162000	0.06896300	-0.42381100
H	-4.66357200	2.12639700	0.09361300
C	-3.07495400	-1.12645300	-1.39167200
C	-4.38906400	-1.08225700	-0.94150700
H	-4.96951000	-1.99437200	-0.98216200
O	1.95209700	0.15449800	-1.66951800
O	-1.09910700	0.14187900	-1.84416000
C	0.96721400	3.54302400	0.47775400
C	1.87823400	4.76608400	0.62721800
C	-0.20811500	3.87017400	-0.46483800
C	1.07887200	5.96502800	1.15511900
H	2.31870500	5.00187600	-0.35089300
H	2.70683500	4.54519900	1.30722700
C	-1.02763600	5.03888300	0.08185000
C	-0.13034700	6.27236900	0.26314400
H	1.72824700	6.84400400	1.22936800
H	0.73084600	5.74183000	2.17218200
H	-1.85416700	5.27657400	-0.59755300
H	-1.46658600	4.75222000	1.04610900
H	0.22158200	6.60758900	-0.72185500
H	-0.71431700	7.09737400	0.68487200
Co	0.37597000	1.03626900	-1.08850100
H	0.22777200	4.15976900	-1.43234800
H	0.53593000	3.27120100	1.44964000
C	3.44726900	-2.17706100	-2.46750100
C	3.49035200	-1.36724600	-3.78288200
H	2.77831500	-0.54165600	-3.75726500
H	4.49092700	-0.95677800	-3.95422900
H	3.23678900	-2.01279700	-4.63098500
C	2.03342200	-2.76277200	-2.25915400
H	1.98668700	-3.33577100	-1.32790200
H	1.28138300	-1.97809100	-2.20900200
H	1.78059300	-3.43586100	-3.08643600
C	4.42485200	-3.35614100	-2.61962700
H	4.11915500	-3.96797500	-3.47373700
H	5.45075100	-3.02040500	-2.80405300
H	4.42578800	-4.00162800	-1.73543500
C	6.54451900	-1.15681700	1.44412100
C	6.82118600	-0.17634500	2.59511400
H	7.02326900	0.83411800	2.22504800
H	5.97968700	-0.12570100	3.29304200
H	7.70057100	-0.50533500	3.15739400
C	7.78907000	-1.19758000	0.53086600
H	8.67342900	-1.49797100	1.10352500
H	7.66679700	-1.90959500	-0.29049800
H	7.98223200	-0.21263500	0.09395700
C	6.30386500	-2.55769100	2.04840700
H	6.13797200	-3.31006100	1.27186700
H	7.17058600	-2.87291100	2.63992300
H	5.42552500	-2.55092100	2.70103400
C	-2.42776100	-2.44071200	-1.85491500
C	-1.87062700	-2.30525600	-3.28966900
H	-2.66863600	-2.03709800	-3.99124000

H	-1.09225600	-1.54545100	-3.34122500
H	-1.44384400	-3.26134000	-3.61178800
C	-3.43359600	-3.60602300	-1.85801900
H	-3.83243000	-3.80217400	-0.85744900
H	-4.27288900	-3.42738300	-2.53913200
H	-2.92442200	-4.51560000	-2.19056900
C	-1.29400800	-2.80819800	-0.86936500
H	-0.77553500	-3.70752200	-1.22023000
H	-0.56682500	-2.00520500	-0.76423500
H	-1.70367800	-3.01388900	0.12314500
C	-6.49421700	0.00406700	-0.00231900
C	-7.00429200	1.35652100	0.52096700
H	-6.44878500	1.68285400	1.40597500
H	-6.92881000	2.13872600	-0.24115800
H	-8.05771800	1.26980300	0.80432900
C	-6.67338600	-1.04300700	1.11774300
H	-7.72759800	-1.11794700	1.40595600
H	-6.34448200	-2.03669900	0.79974700
H	-6.09771000	-0.76221700	2.00517400
C	-7.35189600	-0.40004200	-1.22161300
H	-7.05993900	-1.37792400	-1.61492300
H	-8.41032000	-0.45287600	-0.94388900
H	-7.24532600	0.33065800	-2.02949500
O	0.61891900	1.89787400	-3.17829000
H	1.41426200	1.35897200	-3.32382400
H	-0.11511800	1.38476300	-3.55047800

PO-aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -2895.652497
No imaginary frequency

C	5.05925300	-1.77752000	0.66100000
C	5.77228100	-0.55751400	0.66146300
C	3.68119600	-1.88838000	0.52319200
H	5.62424600	-2.68910500	0.78628700
C	5.02139800	0.59772500	0.55862900
C	2.92608500	-0.68645400	0.31444100
C	3.62123700	0.56143800	0.38907700
H	5.50097000	1.57211200	0.60010200
O	1.64277100	-0.76200200	0.07882200
C	2.92709400	1.81130300	0.36213800
Co	0.52790800	0.60770900	-0.54287700
N	1.67216800	1.97819200	0.10245900
H	3.52390200	2.69103800	0.60234600
N	-0.52058200	2.04522200	-1.23041500
C	0.99937400	3.28201200	0.14469500
C	-1.77786000	1.92221600	-1.49949600
C	0.15886400	3.34509400	-1.14281200
C	1.88319000	4.51707200	0.29252900
H	-2.35610900	2.82076400	-1.70233500
C	-2.49980100	0.68789900	-1.54602500
C	-0.73492300	4.58434800	-1.14091000
C	0.99848300	5.77352300	0.28840300
H	2.60638700	4.56302000	-0.53388100
H	2.45062300	4.46791000	1.22784700
C	-3.90551400	0.76879800	-1.64736400
C	-1.83754900	-0.57210100	-1.48441700
C	0.12562200	5.84578400	-0.97032900
H	-1.30252900	4.65209700	-2.07582500
H	-1.44900000	4.48989500	-0.31508500
H	1.62547500	6.66785000	0.36780200
H	0.35429300	5.75540200	1.17610700
C	-4.69143000	-0.36494200	-1.66745900
H	-4.35060400	1.75672400	-1.67246400
C	-2.64118500	-1.75811800	-1.51166800
O	-0.52636900	-0.66456400	-1.41966400
H	0.76961200	5.96837200	-1.85225600
H	-0.52178200	6.72795000	-0.93032100

C	-4.01823300	-1.60693100	-1.60214000
H	-4.62588100	-2.50236500	-1.60005400
C	2.35678700	-0.55784700	-2.93016100
C	1.38576200	0.22545000	-3.70216200
O	1.87511300	0.72048500	-2.43282200
H	1.95782700	-1.38905300	-2.35810300
H	0.33993800	-0.06844200	-3.68539500
H	1.71988900	0.80778600	-4.55841100
C	3.82445400	-0.61260700	-3.24485500
H	4.40338400	-0.66891100	-2.31798600
H	4.04808800	-1.50410300	-3.84036200
H	4.14037700	0.27240500	-3.80426600
H	0.85982100	3.39327400	-1.98898300
H	0.30601400	3.24427600	0.99146200
S	-1.41290300	1.45303500	1.99139200
O	-0.52069000	1.96927100	3.04838900
O	-2.09263500	2.50648600	1.19147400
O	-0.73152200	0.40961000	1.10978900
C	-2.69325900	0.47034700	2.76521200
C	-2.94443700	0.60989600	4.12614700
C	-3.44742400	-0.40961700	1.98475700
C	-3.96629000	-0.13932000	4.71209300
H	-2.33454100	1.29026900	4.70997100
C	-4.45666400	-1.15468900	2.58466500
H	-3.23395500	-0.51984900	0.92976200
C	-4.73344900	-1.03106600	3.95518000
H	-4.16596700	-0.03318100	5.77519200
H	-5.03767800	-1.84686600	1.98122100
C	-5.81573700	-1.86526300	4.59481200
H	-5.47856200	-2.89739800	4.75081300
H	-6.10708400	-1.46352200	5.56916800
H	-6.70955400	-1.91017300	3.96409200
C	-1.99448900	-3.14044400	-1.35387700
C	-3.03224800	-4.27606000	-1.39409900
H	-3.58022700	-4.30217500	-2.34228000
H	-2.51631600	-5.23472400	-1.28368000
H	-3.75660800	-4.19860700	-0.57674500
C	-1.28978600	-3.19787600	0.02085400
H	-0.54066100	-2.41545600	0.12058200
H	-2.01998500	-3.06905600	0.82633300
H	-0.80275500	-4.17004400	0.15336900
C	-0.99066900	-3.39253700	-2.50094300
H	-1.50895500	-3.40015400	-3.46650000
H	-0.22099700	-2.62288600	-2.52727300
H	-0.50574800	-4.36583400	-2.36938200
C	-6.22228400	-0.33351300	-1.72093200
C	-6.76464300	1.10279900	-1.79410000
H	-6.47638800	1.68752100	-0.91500100
H	-6.40699200	1.62420100	-2.68806100
H	-7.85801500	1.08332800	-1.83633300
C	-6.78832900	-0.99864200	-0.44699800
H	-7.88377000	-0.98411300	-0.46181000
H	-6.47073700	-2.04251100	-0.36260400
H	-6.44682800	-0.47089100	0.44817600
C	-6.71175000	-1.10369500	-2.96617000
H	-6.38331200	-2.14701500	-2.95295600
H	-7.80629200	-1.09925900	-3.01251100
H	-6.32831700	-0.64378600	-3.88261600
C	7.30009200	-0.48610000	0.79279300
C	7.67262400	0.32384300	2.05330800
H	7.28138300	1.34436900	2.00816500
H	7.26674900	-0.14969600	2.95255000
H	8.76111200	0.38812600	2.16035200
C	7.94184700	-1.87872000	0.90868600
H	7.73163300	-2.49708600	0.03012100
H	9.02840900	-1.77684300	0.99007600
H	7.59224100	-2.41453100	1.79679500
C	7.88292400	0.21155300	-0.45555400
H	8.97412300	0.28033300	-0.38456600

H	7.63367800	-0.34689600	-1.36370800
H	7.48989400	1.22618600	-0.56912500
C	2.97450900	-3.24939800	0.61662600
C	1.96019600	-3.20993000	1.78378800
H	1.22941600	-2.41246900	1.65296200
H	1.42541200	-4.16398500	1.84686900
H	2.48149700	-3.05026200	2.73348300
C	2.24878900	-3.57332200	-0.70651700
H	1.46948500	-2.84371200	-0.91199200
H	2.95824600	-3.58916200	-1.54212200
H	1.78054900	-4.56162200	-0.64613700
C	3.96313900	-4.39562000	0.89493900
H	4.69284600	-4.51763000	0.08698600
H	4.50724000	-4.25020300	1.83376000
H	3.40641200	-5.33377800	0.97894700

PO-aCo^{III}-OTs
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2895.642332
No imaginary frequency

C	5.20603500	-1.79107100	0.36203000
C	5.87696100	-0.56674100	0.55351500
C	3.83091700	-1.90829600	0.17559700
H	5.79315700	-2.69730300	0.37017800
C	5.09663700	0.58122300	0.58679500
C	3.06285300	-0.70584900	0.13330200
C	3.70707000	0.54224000	0.38629300
H	5.55515400	1.54892600	0.77261100
O	1.78249200	-0.76193500	-0.12795500
C	2.97699700	1.78485000	0.50733000
Co	0.46990300	0.49025300	-0.52674100
N	1.71638700	1.94520100	0.30627500
H	3.58472000	2.63755300	0.81970300
N	-0.54458100	2.20951700	-1.04534200
C	1.04382700	3.23239200	0.47860400
C	-1.82105900	2.16984100	-1.23566900
C	0.17577600	3.45800500	-0.78587400
C	1.93047300	4.44554000	0.76013400
H	-2.38971000	3.10003700	-1.22783100
C	-2.61693400	0.98211200	-1.42176000
C	-0.67992900	4.71656400	-0.62630500
C	1.07234700	5.70882000	0.90856600
H	2.65000600	4.58021000	-0.06010300
H	2.50699200	4.28170900	1.67696500
C	-4.01835000	1.14325200	-1.40470500
C	-2.04265200	-0.31349100	-1.57816000
C	0.20084100	5.93743500	-0.33041100
H	-1.26495400	4.89589800	-1.53566000
H	-1.38493300	4.55438300	0.19780500
H	1.71581900	6.57668500	1.08902400
H	0.42817500	5.60135300	1.79036200
C	-4.87324000	0.06116200	-1.49991600
H	-4.40695300	2.14792200	-1.28180100
C	-2.91004900	-1.44771200	-1.65302500
O	-0.73934900	-0.45819100	-1.65537600
H	0.84570500	6.14039600	-1.19676300
H	-0.42951400	6.82275400	-0.19474000
C	-4.27876300	-1.21689000	-1.61543100
H	-4.94015600	-2.07260000	-1.66007300
C	2.00401000	-0.27795300	-3.21185800
C	1.12582200	0.78166000	-3.72284300
O	1.69565900	0.88382300	-2.39642300
H	1.51125200	-1.17384300	-2.84652700
H	0.05225500	0.61870100	-3.72487800
H	1.51711700	1.51620700	-4.42342600
C	3.44982800	-0.42159900	-3.59172700
H	4.02923600	-0.75756000	-2.72619900
H	3.55993900	-1.16631600	-4.38699600

H	3.86070800	0.52993600	-3.94026500
H	0.87015800	3.59454900	-1.62868500
H	0.34827600	3.09970500	1.31487900
S	-1.19911800	0.97342600	2.17718700
O	-0.14867300	1.16410100	3.19169700
O	-1.84502400	2.21158300	1.68047800
O	-0.72843000	0.08537300	1.01058900
C	-2.47622000	-0.07045400	2.86686500
C	-2.47328700	-0.35699600	4.22713100
C	-3.45932100	-0.59494500	2.02267300
C	-3.47212300	-1.17990300	4.75175500
H	-1.68729400	0.05086300	4.85272100
C	-4.44010600	-1.42063200	2.55946900
H	-3.44333200	-0.37564600	0.96289000
C	-4.46520200	-1.72274700	3.93072400
H	-3.47281700	-1.41000500	5.81384300
H	-5.19645300	-1.84342300	1.90418700
C	-5.54930700	-2.60607900	4.49672600
H	-5.67274300	-3.51630300	3.90033800
H	-5.32743100	-2.90253800	5.52533400
H	-6.51711500	-2.09029200	4.50068700
C	-2.32479200	-2.86722700	-1.69244500
C	-3.42510200	-3.94157000	-1.74008100
H	-4.05686500	-3.84558900	-2.62975400
H	-2.95961600	-4.93143000	-1.77010100
H	-4.06710400	-3.90732800	-0.85377500
C	-1.49060900	-3.10637600	-0.41195000
H	-0.66832300	-2.39862700	-0.33017900
H	-2.11523300	-2.99632100	0.47984600
H	-1.07763700	-4.12153900	-0.42058900
C	-1.43996100	-3.04723000	-2.94614100
H	-2.03354800	-2.92268500	-3.85866500
H	-0.62884900	-2.32005700	-2.95920700
H	-1.00729200	-4.05387400	-2.95770400
C	-6.40029300	0.18488200	-1.45508600
C	-6.85602500	1.64794300	-1.33462300
H	-6.48638300	2.11088300	-0.41430100
H	-6.51410800	2.24823500	-2.18400700
H	-7.94925300	1.69421800	-1.31372600
C	-6.94133900	-0.58960600	-0.23334500
H	-8.03344500	-0.51580800	-0.18510000
H	-6.68198700	-1.65159400	-0.28243400
H	-6.52730800	-0.18447100	0.69470800
C	-7.00280200	-0.40747900	-2.74738600
H	-6.73996500	-1.46212200	-2.87041600
H	-8.09589400	-0.33563500	-2.72820600
H	-6.63929600	0.13249900	-3.62748900
C	7.39700200	-0.47395400	0.74482500
C	7.70434000	0.15206700	2.12260500
H	7.28200700	1.15691400	2.21339200
H	7.28675000	-0.45955600	2.92830300
H	8.78651100	0.22924600	2.27537300
C	8.07973300	-1.85019000	0.67885200
H	7.91527100	-2.33911200	-0.28672400
H	9.15956700	-1.73105700	0.81057800
H	7.72212500	-2.51938400	1.46772600
C	7.99546100	0.41505300	-0.36720300
H	9.08120600	0.50039600	-0.24782500
H	7.79208700	-0.01005400	-1.35532100
H	7.57606500	1.42508800	-0.34514300
C	3.13812800	-3.27624700	0.06126600
C	2.12587100	-3.42554900	1.22206600
H	1.37375100	-2.63645500	1.19978900
H	1.61507900	-4.39212800	1.14879300
H	2.64129700	-3.38605300	2.18724100
C	2.39650500	-3.41425700	-1.28756700
H	1.58149900	-2.69678300	-1.36112300
H	3.08353400	-3.26445000	-2.12804000
H	1.97168700	-4.41999800	-1.37614800

C	4.14516800	-4.43574100	0.15848700
H	4.87590900	-4.41557600	-0.65741200
H	4.68827500	-4.42845900	1.10890800
H	3.60586500	-5.38552200	0.09496800

(salen)aCo^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1883.656145
No imaginary frequency

C	4.76174200	-1.58797800	-0.15311000
C	5.45113800	-0.36600900	0.05571100
C	3.38673800	-1.71609100	-0.24293300
H	5.36093100	-2.48452100	-0.24673300
C	4.68108800	0.77045500	0.15707800
C	2.58869800	-0.52682500	-0.10230900
C	3.26735600	0.71814000	0.07419600
H	5.13968700	1.74287800	0.30351600
O	1.28927000	-0.61496200	-0.16245200
C	2.56033500	1.95416800	0.15053500
Co	-0.00192800	0.72345100	0.01143800
N	1.27639100	2.10966300	0.05620800
H	3.17738400	2.84199500	0.29350000
N	-1.26626600	2.08281800	-0.37967400
C	0.61551300	3.39758500	0.30327100
C	-2.55154900	1.91889600	-0.40979700
C	-0.63398500	3.39661500	-0.58892400
C	1.44944500	4.66108300	0.09326200
H	-3.18036200	2.79159400	-0.58972700
C	-3.24983400	0.68697500	-0.23112500
C	-1.50139100	4.62945300	-0.33122600
C	0.58738500	5.90757000	0.34309600
H	1.84317500	4.67289900	-0.93213400
H	2.30881800	4.67276000	0.77102600
C	-4.66594400	0.73937500	-0.22450600
C	-2.56207000	-0.55744100	-0.09048800
C	-0.67354500	5.90822800	-0.52826900
H	-2.36247000	4.64752100	-1.00700100
H	-1.89168500	4.58390500	0.69371700
H	1.17832800	6.81050100	0.15708000
H	0.29634900	5.93424800	1.40141600
C	-5.42929300	-0.39554300	-0.06798200
H	-5.13249300	1.71156500	-0.34538700
C	-3.35049200	-1.74589300	0.09976400
O	-1.26176600	-0.65278300	-0.14979300
H	-0.38435400	5.98967800	-1.58473700
H	-1.29019900	6.78501300	-0.30458000
C	-4.72871100	-1.61732400	0.09722200
H	-5.32104300	-2.51220800	0.23818100
O	-0.20552100	0.87744100	1.80568400
H	-0.68286900	0.06774300	2.03950600
C	-2.66755400	-3.10175300	0.33591100
C	-3.68813000	-4.23898200	0.51877800
H	-3.15130700	-5.17761400	0.68657900
H	-4.34017900	-4.07369400	1.38301800
H	-4.31651100	-4.37237200	-0.36828300
C	-1.82278400	-3.02221000	1.62842000
H	-1.05994500	-2.24812300	1.55130500
H	-2.46263100	-2.80434800	2.49051600
H	-1.32031800	-3.97816000	1.81103500
C	-1.76876700	-3.46829200	-0.86579700
H	-2.36649200	-3.54497700	-1.78084100
H	-0.99204700	-2.72168800	-1.01634000
H	-1.29097200	-4.43891400	-0.69177400
C	2.71736700	-3.07521500	-0.49604700
C	1.92507400	-3.01741200	-1.82237300
H	1.16666100	-2.23572900	-1.79214600
H	2.60011200	-2.81986800	-2.66247400
H	1.42817300	-3.97662700	-2.00461600

C	1.76908600	-3.41990900	0.67317900
H	0.99429200	-2.66435700	0.77966800
H	1.28973800	-4.38872300	0.49326500
H	2.32752300	-3.48658300	1.61327700
C	3.74559100	-4.21352300	-0.61659800
H	4.43907800	-4.05643000	-1.44966900
H	4.32994100	-4.33804000	0.30132200
H	3.21749900	-5.15411800	-0.80070400
C	6.98045300	-0.36995800	0.15021500
C	7.54704100	1.04111600	0.37454800
H	7.29073000	1.71465700	-0.44974800
H	7.17658300	1.48086300	1.30618600
H	8.63866100	0.99654700	0.43927100
C	7.57678700	-0.92839700	-1.16035900
H	8.67105400	-0.94561500	-1.10686300
H	7.23672600	-1.94908100	-1.35735300
H	7.28464000	-0.30841300	-2.01387000
C	7.41831700	-1.26128200	1.33298500
H	7.07141100	-2.29157400	1.21284800
H	8.51092300	-1.28353700	1.41264600
H	7.01273300	-0.88032600	2.27549200
C	-6.96151000	-0.39697000	-0.05385900
C	-7.54028300	1.01370500	-0.24726200
H	-7.22559900	1.69212400	0.55235000
H	-7.23569600	1.44657300	-1.20569900
H	-8.63380100	0.97087600	-0.23476300
C	-7.46325100	-0.94466800	1.30022600
H	-8.55856900	-0.95970900	1.32577800
H	-7.11170900	-1.96477500	1.47948700
H	-7.10903900	-0.31945700	2.12587400
C	-7.48477300	-1.29588800	-1.19539000
H	-7.13124600	-2.32590600	-1.09341700
H	-8.58028300	-1.31710700	-1.19553900
H	-7.14852000	-0.92226600	-2.16774700
H	0.26819100	3.35421200	1.34540900
H	-0.28540500	3.42376000	-1.63345300

(salen)aCo^{III}-OH
Charge: 0
Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -1883.661608
No imaginary frequency

C	4.69362400	-1.63220100	-0.39572200
C	5.42490700	-0.43832500	-0.18129600
C	3.31077200	-1.72461600	-0.39511900
H	5.26139000	-2.53728000	-0.56969400
C	4.69100400	0.70484500	0.05320900
C	2.55686900	-0.52673100	-0.15603400
C	3.27667400	0.68192100	0.08167200
H	5.18286300	1.65604000	0.22850700
O	1.24913300	-0.57483100	-0.17809700
C	2.59771800	1.92419200	0.29073000
Co	0.02127100	0.69344700	0.49137400
N	1.32294700	2.07454000	0.43864000
H	3.22716900	2.81489100	0.30843400
N	-1.12806400	2.03658900	-0.36116600
C	0.65305400	3.37250400	0.52971200
C	-2.40450900	1.88067600	-0.53493100
C	-0.45098400	3.32853700	-0.55022800
C	1.52294300	4.61924600	0.39002700
H	-2.99002600	2.73219400	-0.88764100
C	-3.15566700	0.68956200	-0.29937600
C	-1.32741200	4.58092800	-0.48727200
C	0.64317500	5.87576100	0.46366000
H	2.05268300	4.59725600	-0.57199900
H	2.28118000	4.64194300	1.18009200
C	-4.55081100	0.75805700	-0.55137300
C	-2.55848300	-0.52561500	0.16715200
C	-0.46349700	5.84666600	-0.59714500

H	-2.06946100	4.57575200	-1.29244600
H	-1.87811100	4.58153000	0.46257700
H	1.26231700	6.77055400	0.34131700
H	0.19004400	5.93972600	1.46155000
C	-5.37625800	-0.32595700	-0.36515300
H	-4.94922900	1.70586800	-0.89810800
C	-3.41213000	-1.67197600	0.34496200
O	-1.28605000	-0.64800400	0.42090800
H	-0.00801600	5.88561300	-1.59585300
H	-1.09849400	6.73436500	-0.50875200
C	-4.76184200	-1.52440100	0.08049900
H	-5.40204500	-2.38546000	0.22216900
O	-0.13803500	0.90791500	2.29298800
H	-0.75509600	0.22020100	2.58425000
C	-2.81950600	-3.01979500	0.78642700
C	-3.90312500	-4.10203600	0.94032500
H	-3.43120700	-5.03843000	1.25285700
H	-4.64536200	-3.83611900	1.70073900
H	-4.42689300	-4.29699800	-0.00134600
C	-2.10904300	-2.88080700	2.15271700
H	-1.27403000	-2.18409000	2.09576300
H	-2.81127800	-2.52982300	2.91707200
H	-1.72346400	-3.85551700	2.47118100
C	-1.81750900	-3.50616400	-0.28491200
H	-2.32707400	-3.65935800	-1.24246700
H	-1.01488700	-2.78507200	-0.42806300
H	-1.37505100	-4.46094400	0.02015700
C	2.58784400	-3.06330000	-0.60604200
C	1.67226100	-2.98113400	-1.84866700
H	0.93454900	-2.18692200	-1.74127500
H	2.26688800	-2.78812600	-2.74856000
H	1.14585700	-3.93188000	-1.98840400
C	1.75402200	-3.39513000	0.65334100
H	1.01342900	-2.62150600	0.85114000
H	1.23260400	-4.34881900	0.51681400
H	2.40698900	-3.48756400	1.52803300
C	3.57390300	-4.22294100	-0.83151200
H	4.19134600	-4.07031200	-1.72328500
H	4.23720500	-4.37188400	0.02712400
H	3.00984500	-5.14948400	-0.97590500
C	6.95662300	-0.47466200	-0.21401600
C	7.57097600	0.91261800	0.03210700
H	7.25892100	1.63322300	-0.73094100
H	7.29254400	1.30876300	1.01399800
H	8.66286900	0.84585900	-0.00130700
C	7.42992500	-0.97535800	-1.59612600
H	8.52418200	-1.01638500	-1.63528000
H	7.05058600	-1.97762200	-1.81487000
H	7.08290900	-0.30646900	-2.39011300
C	7.47137100	-1.43342300	0.88183000
H	7.09410800	-2.45007800	0.73909400
H	8.56613200	-1.47830400	0.86918700
H	7.15273000	-1.09522800	1.87280300
C	-6.88788500	-0.30028800	-0.61398000
C	-7.36877400	1.07888900	-1.09252700
H	-7.16118300	1.85781300	-0.35165300
H	-6.89445500	1.36640200	-2.03652200
H	-8.45042600	1.05775000	-1.25777800
C	-7.62969100	-0.64426300	0.69611100
H	-8.71359900	-0.63922300	0.53595400
H	-7.35258400	-1.63411900	1.06990400
H	-7.39461300	0.08550100	1.47730800
C	-7.24942700	-1.34132500	-1.69592400
H	-6.96202900	-2.35322200	-1.39624300
H	-8.32927700	-1.34234300	-1.88152900
H	-6.73942700	-1.11440200	-2.63745400
H	0.15361600	3.38199600	1.50729600
H	0.05678600	3.29440100	-1.52642000

(salen)aCo^{III}-OH
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -1883.658593
No imaginary frequency

C	4.77056100	-1.61089300	-0.32873600
C	5.48720000	-0.39685000	-0.17969900
C	3.39043400	-1.71994400	-0.30434600
H	5.34952300	-2.51399300	-0.47407900
C	4.74168500	0.74847800	0.00185400
C	2.62279100	-0.52143200	-0.10215900
C	3.32782700	0.71434200	0.05341800
H	5.22487700	1.71331500	0.11729100
O	1.32142200	-0.59053100	-0.09379500
C	2.64656700	1.96436200	0.21892900
Co	0.00810600	0.61004500	0.65233300
N	1.36972800	2.11076500	0.36923200
H	3.28850100	2.84995300	0.20741800
N	-1.18139200	2.05046100	-0.21904800
C	0.70701700	3.40730800	0.46688400
C	-2.45273400	1.89918500	-0.42983400
C	-0.50439000	3.32868800	-0.49079800
C	1.55270100	4.65120700	0.19252700
H	-3.03312400	2.76039500	-0.77088300
C	-3.22002100	0.70074100	-0.26430400
C	-1.36373300	4.59323300	-0.38711000
C	0.69180000	5.91673500	0.30146600
H	1.98758400	4.58278000	-0.81401400
H	2.38611300	4.70462500	0.90127500
C	-4.62026200	0.80496400	-0.45241600
C	-2.62116100	-0.56244100	0.03966500
C	-0.51747200	5.84956300	-0.63711900
H	-2.18472300	4.56514300	-1.11042500
H	-1.81577600	4.63305400	0.61287300
H	1.29824600	6.80093400	0.07845500
H	0.34326600	6.02732300	1.33687300
C	-5.45184800	-0.28662300	-0.32578700
H	-5.02250100	1.78282100	-0.69651300
C	-3.47938400	-1.70726900	0.17810700
O	-1.33303000	-0.70016400	0.16901900
H	-0.16707200	5.84498600	-1.67810900
H	-1.14059400	6.74269300	-0.52128300
C	-4.83953200	-1.52449600	-0.00485600
H	-5.48708800	-2.38554500	0.10089400
O	-0.12055700	0.60237800	2.44590700
H	-0.66531900	-0.11975100	2.78862300
C	-2.88122000	-3.07961300	0.52455200
C	-3.96509600	-4.16448000	0.65076300
H	-3.49095300	-5.11869700	0.89976200
H	-4.68562400	-3.93669900	1.44368200
H	-4.51500800	-4.30482300	-0.28578600
C	-2.13961400	-3.00093300	1.87938600
H	-1.31778200	-2.28663000	1.83217300
H	-2.82718500	-2.70159500	2.67826000
H	-1.72612400	-3.98184300	2.13800300
C	-1.89829000	-3.51852900	-0.58454600
H	-2.41903700	-3.60942900	-1.54399400
H	-1.08626700	-2.80179300	-0.69386900
H	-1.46963300	-4.49655400	-0.33806700
C	2.67722100	-3.06796900	-0.49409700
C	1.79496700	-3.01108000	-1.76260900
H	1.05193200	-2.21772500	-1.68561900
H	2.41154900	-2.83098600	-2.65019300
H	1.27438300	-3.96551600	-1.89949200
C	1.80158900	-3.38510600	0.74031500
H	1.03119600	-2.62851600	0.87863500
H	1.31395300	-4.35771500	0.60996000
H	2.41647700	-3.43270900	1.64577800
C	3.67478200	-4.22649400	-0.66846800

H	4.30902600	-4.09421500	-1.55152900
H	4.32196900	-4.34625700	0.20705400
H	3.12019100	-5.16072100	-0.79917100
C	7.01875800	-0.41566500	-0.22833000
C	7.61855500	0.98870500	-0.05368100
H	7.29149600	1.66875900	-0.84698900
H	7.34373100	1.42769100	0.91083300
H	8.71083500	0.93286900	-0.09397700
C	7.48369200	-0.97423600	-1.59109800
H	8.57792400	-1.00289900	-1.64054900
H	7.11566300	-1.99041600	-1.75894400
H	7.11935800	-0.34743300	-2.41119500
C	7.55715400	-1.31636000	0.90486400
H	7.19070500	-2.34287500	0.81409100
H	8.65216300	-1.34895300	0.88136000
H	7.24572400	-0.93595200	1.88276000
C	-6.97189400	-0.22381900	-0.51081800
C	-7.45259900	1.19500700	-0.85496900
H	-7.20746400	1.90799000	-0.06109900
H	-7.01063500	1.55520800	-1.78964700
H	-8.53991100	1.19790900	-0.97937300
C	-7.66729400	-0.66694000	0.79502500
H	-8.75639300	-0.63610000	0.67909000
H	-7.39066800	-1.68754800	1.07461600
H	-7.39150600	-0.00714600	1.62371600
C	-7.38931000	-1.16804900	-1.65943700
H	-7.10399600	-2.20406700	-1.45567100
H	-8.47547200	-1.14251800	-1.80127700
H	-6.91330700	-0.86921400	-2.59868200
H	0.30332000	3.47354900	1.48845900
H	-0.09311600	3.26178700	-1.51006700

H_2O-aCo^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -1960.090547
No imaginary frequency

C	-4.74399700	-1.59526500	-0.07089800
C	-5.42441100	-0.35428700	-0.03972300
C	-3.36930100	-1.74228500	-0.16584300
H	-5.34647700	-2.49299900	-0.01850000
C	-4.64321600	0.77902300	-0.11031900
C	-2.56127100	-0.55337100	-0.22583100
C	-3.23192300	0.70828800	-0.19197200
H	-5.09493500	1.76570800	-0.10095400
O	-1.25881900	-0.66594400	-0.30672000
C	-2.52277300	1.95245200	-0.29311800
Co	0.01257000	0.70802100	0.01805800
N	-1.24222800	2.09721400	-0.25328500
H	-3.14412500	2.84047800	-0.41883700
N	1.25915000	2.08689900	0.41079000
C	-0.55714600	3.37398500	-0.46393600
C	2.53976900	1.93268000	0.36807800
C	0.60293600	3.39001100	0.55095100
C	-1.40775900	4.63896800	-0.36502300
H	3.17242300	2.81732300	0.45237300
C	3.23656000	0.68779900	0.22370100
C	1.48072600	4.62851800	0.37309300
C	-0.52622700	5.88466400	-0.53736800
H	-1.90711100	4.66846800	0.61309600
H	-2.19143100	4.63289800	-1.13000300
C	4.63832700	0.75405300	0.05581100
C	2.56472100	-0.56776600	0.29368700
C	0.62786600	5.90175200	0.47121600
H	2.26982500	4.65146200	1.13230100
H	1.97197600	4.58391000	-0.60769600
H	-1.13649900	6.78790600	-0.43286800
H	-0.11732800	5.89665900	-1.55625600
C	5.40639600	-0.38534700	-0.06778300

H	5.09442100	1.73794000	0.01791800
C	3.35224500	-1.75873700	0.17176400
O	1.27038500	-0.65446400	0.50356000
H	0.22074900	5.98641900	1.48777800
H	1.25893700	6.78243400	0.31225000
C	4.72203100	-1.62076900	-0.00280100
H	5.31379400	-2.52174000	-0.10142500
O	-0.44813400	0.47943000	2.06446800
O	0.53203000	0.80290200	-1.72573100
H	0.06519400	0.05459400	-2.12439500
C	-2.71070300	-3.12969900	-0.21633400
C	-1.99035900	-3.30184400	-1.57266600
H	-2.71327600	-3.25627800	-2.39426600
H	-1.24305200	-2.52376900	-1.72168900
H	-1.48918900	-4.27509900	-1.61416700
C	-1.70440400	-3.28401600	0.94716800
H	-0.90798800	-2.54582200	0.87699400
H	-2.21595500	-3.17395200	1.91099100
H	-1.25049400	-4.28052000	0.92210700
C	-3.74092900	-4.26577700	-0.08856500
H	-4.28532400	-4.22203700	0.86092800
H	-4.46989700	-4.25453700	-0.90552200
H	-3.22002400	-5.22736100	-0.12690000
C	2.68717300	-3.14272100	0.22801000
C	3.69987500	-4.28351000	0.02440500
H	4.19882100	-4.21829600	-0.94810600
H	4.46684700	-4.30025700	0.80614400
H	3.17206600	-5.24157300	0.06072500
C	2.03082300	-3.34919000	1.61157500
H	2.78552200	-3.30622300	2.40458000
H	1.27810300	-2.58596400	1.80494500
H	1.54513400	-4.33031900	1.65715400
C	1.62539100	-3.25423000	-0.88819200
H	1.13572200	-4.23355200	-0.84413700
H	0.86755700	-2.48052000	-0.78566600
H	2.09580100	-3.15439900	-1.87230000
C	6.92577900	-0.37049600	-0.26841400
C	7.48725900	1.05980800	-0.30871300
H	7.05927400	1.63773600	-1.13413100
H	7.29106800	1.59673200	0.62516700
H	8.57189700	1.02878600	-0.45212000
C	7.60688900	-1.12496300	0.89419300
H	7.27139600	-2.16437300	0.95292100
H	8.69477800	-1.13193400	0.76286900
H	7.38000600	-0.64630300	1.85218500
C	7.27423100	-1.06478100	-1.60311900
H	6.92924800	-2.10258000	-1.62040200
H	6.80574200	-0.54363800	-2.44382300
H	8.35849600	-1.06993000	-1.76204600
C	-6.95334100	-0.33118500	0.06242500
C	-7.50750100	1.10242300	0.07740400
H	-7.12935900	1.67235200	0.93237700
H	-7.24945400	1.64420300	-0.83832200
H	-8.59913800	1.07758400	0.15170800
C	-7.39258400	-1.03349200	1.36577500
H	-8.48490800	-1.03507800	1.45220100
H	-7.05405800	-2.07307900	1.39852500
H	-6.98024500	-0.52006100	2.24025400
C	-7.56170500	-1.07244700	-1.14808700
H	-7.23026200	-2.11383200	-1.19273700
H	-8.65581400	-1.07244700	-1.08830900
H	-7.26892400	-0.58862500	-2.08521700
H	0.15288000	3.41102600	1.55455900
H	-0.10733700	3.30012500	-1.46298200
H	-1.22433900	-0.09982500	2.01613500
H	0.31102900	-0.13804500	2.10657000

H_2O-aCo^{III}-OH
Charge: 0

Spin Multiplicity: 3
Sum of electronic and thermal Free Energies (a.u.): -1960.077484
No imaginary frequency

C	-4.70339900	-1.62541900	-0.08654800
C	-5.40351900	-0.40049300	0.04220200
C	-3.33433900	-1.74201900	-0.25760000
H	-5.28681000	-2.53612900	-0.04642500
C	-4.64676300	0.74845400	-0.00112500
C	-2.55121500	-0.53490500	-0.31510600
C	-3.23962400	0.71025100	-0.16574300
H	-5.11204000	1.72398100	0.09400100
O	-1.25950700	-0.62330400	-0.49817500
C	-2.56026700	1.96797900	-0.20889800
Co	0.03491800	0.73488700	-0.28438800
N	-1.28017600	2.13841400	-0.25523400
H	-3.20304200	2.84992800	-0.20728800
N	1.26972600	2.12076400	0.17283600
C	-0.63877100	3.44437800	-0.42816200
C	2.54832400	1.95573200	0.22416200
C	0.61411800	3.40420500	0.45851700
C	-1.48838200	4.68111400	-0.13922300
H	3.17750900	2.83159100	0.38772700
C	3.24044800	0.70441000	0.12439900
C	1.46418900	4.66264200	0.27905000
C	-0.64275700	5.95103100	-0.31701300
H	-1.87388900	4.62701500	0.88779600
H	-2.35272700	4.71797400	-0.81054100
C	4.64808500	0.75104800	0.00992300
C	2.55307500	-0.53749500	0.25092100
C	0.61837400	5.91516000	0.55351700
H	2.32373700	4.64917300	0.95687500
H	1.85608800	4.68656400	-0.74612100
H	-1.24472400	6.83389000	-0.07773200
H	-0.35320000	6.04367000	-1.37205400
C	5.40783000	-0.40003100	-0.01355700
H	5.11470500	1.72737200	-0.06820400
C	3.33291200	-1.73943000	0.24873000
O	1.24479500	-0.59981800	0.39430900
H	0.32806600	5.92710200	1.61258800
H	1.22279700	6.81244200	0.38436500
C	4.70898700	-1.62257400	0.11019900
H	5.29465100	-2.53249100	0.09329700
O	-0.49887500	0.34220500	2.25599200
O	0.52289900	0.85077900	-2.07930400
H	0.11085000	0.09129200	-2.51668300
C	-2.65327800	-3.11447100	-0.36667800
C	-1.94449400	-3.24366000	-1.73389900
H	-2.67522300	-3.17947200	-2.54743700
H	-1.20212300	-2.45876400	-1.86957900
H	-1.44108400	-4.21391600	-1.80584500
C	-1.63599700	-3.27169900	0.78591900
H	-0.87123700	-2.49901300	0.74163800
H	-2.14632500	-3.21652600	1.75455200
H	-1.14010500	-4.24601000	0.72331200
C	-3.66042800	-4.27286500	-0.25676800
H	-4.18739800	-4.27071000	0.70331200
H	-4.40440200	-4.24901200	-1.05999600
H	-3.12239300	-5.22248300	-0.33494000
C	2.65580800	-3.11261600	0.37320900
C	3.66972600	-4.26902600	0.31023300
H	4.21521400	-4.28475700	-0.63904600
H	4.39774700	-4.22532200	1.12730600
H	3.13373900	-5.21914200	0.39746100
C	1.92844700	-3.21358700	1.73265500
H	2.64362000	-3.11648000	2.55665000
H	1.17282400	-2.43668500	1.83719400
H	1.43393500	-4.18674400	1.82508300
C	1.65910800	-3.30249800	-0.79177000
H	1.15907900	-4.27344700	-0.70494800

H	0.90219600	-2.52115600	-0.79411800
H	2.18824700	-3.27864700	-1.75051400
C	6.93329500	-0.41063800	-0.15974100
C	7.51032200	1.00949600	-0.27331300
H	7.11668200	1.53597800	-1.14872100
H	7.28865500	1.60765500	0.61661700
H	8.59873000	0.96017000	-0.37691200
C	7.56427500	-1.09263200	1.07375900
H	7.21691400	-2.12349200	1.18790700
H	8.65591400	-1.11625500	0.98250100
H	7.30819900	-0.55058000	1.98965400
C	7.32068500	-1.19417500	-1.43285400
H	6.96590300	-2.22811800	-1.39441000
H	6.88792700	-0.72567500	-2.32226300
H	8.40968900	-1.21852400	-1.55182300
C	-6.92520400	-0.41422400	0.22100500
C	-7.50317100	1.00502100	0.33969300
H	-7.09467400	1.53614500	1.20558300
H	-7.29934500	1.59983100	-0.55660200
H	-8.58926200	0.95388100	0.46408300
C	-7.28515200	-1.19302600	1.50507300
H	-8.37146700	-1.22078000	1.64508700
H	-6.92791600	-2.22610800	1.46529900
H	-6.83795200	-0.71833100	2.38418300
C	-7.57909800	-1.10355000	-0.99645300
H	-7.23100800	-2.13388800	-1.11321000
H	-8.66853000	-1.13002200	-0.88281900
H	-7.34316400	-0.56477300	-1.91953800
H	0.26744300	3.34757600	1.50092000
H	-0.29598300	3.47024000	-1.47225900
H	-1.23548500	-0.25192800	2.05943900
H	0.28344000	-0.17249800	1.98598600

H_2O-aCo^{III}-OH
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -1960.080677
No imaginary frequency

C	-4.81927800	-1.57231000	0.14550200
C	-5.50579200	-0.35536800	-0.08329500
C	-3.44150200	-1.69571600	0.24214500
H	-5.41850300	-2.46706700	0.25400800
C	-4.73412900	0.78024600	-0.21765300
C	-2.65239900	-0.50889400	0.08864900
C	-3.32240500	0.72961800	-0.14803900
H	-5.19487000	1.74755900	-0.38895200
O	-1.34814100	-0.58105400	0.20413300
C	-2.61537100	1.97247900	-0.28113100
Co	0.01093000	0.58075500	-0.56359600
N	-1.33213600	2.11258900	-0.35821700
H	-3.25068200	2.86153700	-0.31795600
N	1.23683000	2.05826200	0.17618900
C	-0.66835400	3.41309700	-0.44022200
C	2.51614200	1.91855200	0.30722200
C	0.55161700	3.31508600	0.50277600
C	-1.51823400	4.64538100	-0.12651800
H	3.11599400	2.78868200	0.58499500
C	3.26827300	0.70612100	0.13363500
C	1.39861200	4.58963800	0.45005800
C	-0.66511200	5.91923800	-0.18661200
H	-1.95508600	4.53660100	0.87540000
H	-2.34952000	4.72323500	-0.83535800
C	4.67827400	0.81301700	0.15850000
C	2.64233800	-0.56982000	0.00527400
C	0.54096700	5.82574600	0.75325100
H	2.21958000	4.53487700	1.17207100
H	1.84924800	4.67924500	-0.54766800
H	-1.27955200	6.78969200	0.06634200
H	-0.31383000	6.07071700	-1.21605000

C	5.49073400	-0.29486000	0.02861500
H	5.10566300	1.80299200	0.27866900
C	3.47218700	-1.72925300	-0.13384300
O	1.33724400	-0.70173900	0.04744600
H	0.18781400	5.77221800	1.79165500
H	1.15534100	6.72909500	0.67732100
C	4.84691900	-1.54658200	-0.12020000
H	5.47707500	-2.42013500	-0.22737800
O	0.04594500	0.15088500	2.57453100
O	0.14247800	0.41826300	-2.34492300
H	0.58974600	-0.38803400	-2.63805700
C	-2.76486900	-3.05017500	0.51232000
C	-1.76540500	-3.38231500	-0.61880500
H	-2.27621600	-3.41943100	-1.58725700
H	-0.97236700	-2.63921400	-0.66860600
H	-1.31126100	-4.36281000	-0.43707100
C	-2.02400600	-3.00495200	1.86866600
H	-1.25331300	-2.23547300	1.88426200
H	-2.72714200	-2.80641500	2.68470900
H	-1.54482000	-3.97090100	2.06355100
C	-3.78861100	-4.19754600	0.58044500
H	-4.50732100	-4.06128000	1.39539700
H	-4.34468000	-4.30675700	-0.35678800
H	-3.26071400	-5.13836600	0.76308100
C	2.83717200	-3.11750100	-0.31281000
C	3.89965500	-4.22264000	-0.44615200
H	4.54694900	-4.06927400	-1.31616300
H	4.53062000	-4.29285300	0.44608700
H	3.40011100	-5.18777100	-0.57330400
C	1.95027800	-3.46259600	0.90551300
H	2.54629100	-3.46884100	1.82442600
H	1.13958100	-2.74502200	1.01997700
H	1.51501500	-4.46007600	0.77829300
C	1.98552600	-3.12993400	-1.60329700
H	1.53043500	-4.11599400	-1.74585700
H	1.18401600	-2.39351100	-1.54712200
H	2.60906500	-2.91367300	-2.47780700
C	7.02210600	-0.23054100	0.03942100
C	7.53727400	1.20735200	0.21178700
H	7.20576800	1.85589800	-0.60561600
H	7.20179800	1.64585900	1.15719600
H	8.63161000	1.21059400	0.21475800
C	7.56346600	-1.08231100	1.20837700
H	7.25876700	-2.12916500	1.12158500
H	8.65853700	-1.05378800	1.22781500
H	7.19322100	-0.70501200	2.16677800
C	7.56877800	-0.78409800	-1.29466200
H	7.26441400	-1.82199000	-1.45741900
H	7.20244000	-0.19190500	-2.13917800
H	8.66390000	-0.75230400	-1.30229600
C	-7.03614900	-0.35708400	-0.16732000
C	-7.60114400	1.05065400	-0.41572900
H	-7.33606800	1.74044100	0.39214200
H	-7.23878100	1.47031100	-1.35975400
H	-8.69333800	1.00721200	-0.46952700
C	-7.62368200	-0.88754900	1.15875100
H	-8.71829300	-0.90224800	1.11372200
H	-7.28528100	-1.90523500	1.37321900
H	-7.32322000	-0.25188200	1.99762600
C	-7.48461000	-1.27084700	-1.32878200
H	-7.14102800	-2.29988300	-1.18979700
H	-8.57772400	-1.29042800	-1.40064600
H	-7.08418900	-0.91079700	-2.28168500
H	0.15572400	3.18617200	1.52089000
H	-0.27700400	3.50225300	-1.46510500
H	-0.73329500	-0.08541200	2.04866800
H	0.74558300	-0.25940700	2.04455000

PO-aCo^{III}-OH

Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2076.737918
No imaginary frequency

C	-4.65784500	-1.55187200	-0.29126900
C	-5.31407500	-0.31316700	-0.09320900
C	-3.29917800	-1.70141700	-0.52179600
H	-5.26874300	-2.44507000	-0.26801500
C	-4.53019600	0.81805800	-0.17717900
C	-2.47425300	-0.52023300	-0.51324500
C	-3.13304700	0.74302700	-0.38267800
H	-4.96904100	1.80585000	-0.07883000
O	-1.17944300	-0.63862100	-0.63061300
C	-2.42678100	1.98608500	-0.52141300
Co	0.08934700	0.72281100	-0.22816900
N	-1.14616100	2.11807700	-0.55761200
H	-3.04941900	2.87746700	-0.61754900
N	1.32440300	2.10036400	0.20043300
C	-0.44655400	3.37968400	-0.78372100
C	2.60436900	1.92920700	0.24057200
C	0.68079200	3.41573400	0.26916800
C	-1.28480800	4.65530500	-0.75118200
H	3.24226900	2.80742600	0.35135400
C	3.29229300	0.67739500	0.14882200
C	1.58008700	4.63641900	0.07398600
C	-0.38286400	5.88267100	-0.94669700
H	-1.80593500	4.72865300	0.21335300
H	-2.05148300	4.62607700	-1.53296100
C	4.70566700	0.72718700	0.09772000
C	2.59959100	-0.57299500	0.13627400
C	0.74249400	5.92360400	0.09378600
H	2.34407900	4.68156100	0.85760800
H	2.10336400	4.54528500	-0.88666800
H	-0.98238500	6.79763300	-0.89404700
H	0.05473100	5.84974800	-1.95308500
C	5.46927500	-0.41683500	0.01193300
H	5.17365800	1.70621400	0.11851200
C	3.38871000	-1.77097800	0.03825900
O	1.30191100	-0.65747100	0.25042200
H	0.30666300	6.05511300	1.09352800
H	1.39080300	6.78873400	-0.08094200
C	4.76737900	-1.64613000	-0.01700700
H	5.35564600	-2.55164100	-0.09510100
C	-0.92885300	-0.49262400	2.39503000
C	0.21182700	0.31053800	2.84974600
O	-0.60702300	0.77322600	1.74335100
H	-0.69326200	-1.33437800	1.75455500
H	1.21228600	0.01194000	2.55539100
H	0.11704200	0.93146600	3.73746600
C	-2.25906900	-0.52502100	3.08908900
H	-3.06245900	-0.61093000	2.35187300
H	-2.31044600	-1.39421700	3.75329900
H	-2.41759900	0.38034400	3.68164700
O	0.68523400	0.79831000	-1.95281000
H	0.21050500	0.06611100	-2.37098800
C	-2.68392800	-3.08363600	-0.79778700
C	-2.01425700	-3.07369800	-2.19110700
H	-2.75790800	-2.87963400	-2.97141900
H	-1.24083400	-2.30828000	-2.24641800
H	-1.55343200	-4.04676400	-2.39435300
C	-1.63506800	-3.43756000	0.27768900
H	-0.80432600	-2.73698500	0.24888600
H	-2.08607700	-3.42503100	1.27675900
H	-1.23927000	-4.44380500	0.10154700
C	-3.74370300	-4.19965000	-0.79808600
H	-4.23485900	-4.30139100	0.17577000
H	-4.51458700	-4.03482200	-1.55798200
H	-3.25792300	-5.15421000	-1.02233800
C	2.70420300	-3.14493400	-0.01323300

C	3.71449500	-4.29418600	-0.17671800
H	4.29201300	-4.20196900	-1.10242900
H	4.41506100	-4.35145400	0.66332900
H	3.17277300	-5.24433900	-0.21874000
C	1.93639100	-3.38960600	1.30540300
H	2.63180000	-3.41420400	2.15196000
H	1.20501100	-2.60247800	1.48055600
H	1.41203300	-4.35096700	1.26823200
C	1.73993000	-3.19760800	-1.22030500
H	1.22946600	-4.16678900	-1.25235700
H	0.99167800	-2.40968500	-1.16181700
H	2.29878900	-3.07744200	-2.15455200
C	7.00005800	-0.41709300	-0.05884100
C	7.57883300	1.00605900	-0.01071000
H	7.23010600	1.61150200	-0.85350700
H	7.30794800	1.52033900	0.91725400
H	8.67149000	0.96468200	-0.06083800
C	7.57171000	-1.21179300	1.13552200
H	7.21968500	-2.24738300	1.13703400
H	8.66673500	-1.23108700	1.09645800
H	7.27022900	-0.75539500	2.08383600
C	7.45432200	-1.07918700	-1.37800300
H	7.10077100	-2.11142000	-1.45414600
H	7.06491100	-0.52912000	-2.24034000
H	8.54814800	-1.09452200	-1.44428500
C	-6.82228000	-0.28894400	0.17590300
C	-7.35174000	1.14287000	0.35514300
H	-6.86871200	1.64862400	1.19758300
H	-7.19374900	1.74680900	-0.54426100
H	-8.42781100	1.11908300	0.55387300
C	-7.12231700	-1.08076400	1.46748300
H	-8.19803000	-1.08550800	1.67644100
H	-6.79266000	-2.12075600	1.38830100
H	-6.60868300	-0.63184400	2.32389200
C	-7.57301200	-0.93741800	-1.00754400
H	-7.26494500	-1.97538500	-1.16226400
H	-8.65369400	-0.93359400	-0.82606900
H	-7.37861600	-0.38992300	-1.93514600
H	0.19409800	3.48382800	1.25428800
H	0.03600400	3.27042500	-1.76393400

PO-aCo^{III}-OH

Charge: 0

Spin Multiplicity: 3

Sum of electronic and thermal Free Energies (a.u.): -2076.723971

No imaginary frequency

C	-4.61717400	-1.57653900	-0.28650600
C	-5.27562500	-0.35702200	0.00701100
C	-3.27459000	-1.69717900	-0.60404800
H	-5.21449000	-2.47873900	-0.26384000
C	-4.51184200	0.78674800	-0.06668200
C	-2.46572700	-0.50395800	-0.60482700
C	-3.12861100	0.74197400	-0.36545300
H	-4.95271300	1.76179400	0.11318700
O	-1.18301600	-0.60248800	-0.82337300
C	-2.44603300	1.99731500	-0.45553800
Co	0.12981000	0.73806400	-0.53143200
N	-1.17194600	2.15239300	-0.58282300
H	-3.08117500	2.88458100	-0.42286100
N	1.35100600	2.11855900	-0.02280200
C	-0.50856000	3.44042000	-0.77220700
C	2.61979900	1.93795800	0.12925700
C	0.69900900	3.41988300	0.17912400
C	-1.35349100	4.69741000	-0.57714600
H	3.24625100	2.80680700	0.33640300
C	3.30447300	0.68140900	0.07471000
C	1.57425200	4.65972000	-0.01279500
C	-0.48185400	5.94636500	-0.77450600
H	-1.78305400	4.69908300	0.43393200

H	-2.18840800	4.70860900	-1.28599400
C	4.71808300	0.71629000	0.10088000
C	2.59788200	-0.55891900	0.07984600
C	0.73439100	5.93471600	0.15865900
H	2.39833500	4.66936200	0.70791900
H	2.01836400	4.62956600	-1.01611900
H	-1.07989500	6.84842500	-0.60742400
H	-0.13954600	5.98338200	-1.81699900
C	5.47007400	-0.43901500	0.10188200
H	5.19602800	1.69039100	0.10991800
C	3.37310300	-1.76841000	0.08806200
O	1.28944100	-0.62312200	0.10533300
H	0.39146300	6.00120700	1.20006900
H	1.36035800	6.81507700	-0.02129200
C	4.75503200	-1.66003400	0.09367300
H	5.33435700	-2.57435900	0.08752000
C	-1.02995800	-0.45124600	2.35946500
C	0.16165100	0.21918000	2.89174900
O	-0.63804300	0.85561200	1.87357000
H	-0.85730200	-1.22731800	1.62093300
H	1.14422300	-0.09818400	2.55362800
H	0.11423700	0.70450400	3.86557700
C	-2.34428800	-0.50973000	3.08640900
H	-3.17147700	-0.44993500	2.37246500
H	-2.43356800	-1.45610100	3.63065400
H	-2.43548200	0.31499000	3.79927700
O	0.67105800	0.89067900	-2.32549100
H	0.28134800	0.13366300	-2.78624700
C	-2.65555400	-3.06332800	-0.94140200
C	-2.01882300	-3.01587700	-2.34925500
H	-2.78015400	-2.79993300	-3.10657000
H	-1.24511500	-2.25096600	-2.40373700
H	-1.56744800	-3.98517800	-2.58829000
C	-1.58197200	-3.42688700	0.10515700
H	-0.77370600	-2.69998200	0.09603100
H	-2.01914500	-3.46579600	1.10939400
H	-1.15725200	-4.41239900	-0.11492800
C	-3.70436400	-4.18969500	-0.94510300
H	-4.16418100	-4.32863800	0.03922900
H	-4.49966800	-4.00851700	-1.67575000
H	-3.21612700	-5.13129000	-1.21417900
C	2.67669700	-3.13669300	0.06827500
C	3.68129400	-4.30225000	0.03626400
H	4.31475900	-4.27311200	-0.85640800
H	4.32865000	-4.31405900	0.91968000
H	3.13094400	-5.24810000	0.01894000
C	1.82311700	-3.29901200	1.34601900
H	2.46406100	-3.28344700	2.23469000
H	1.09163300	-2.49783000	1.43313300
H	1.29047300	-4.25613400	1.32861600
C	1.79699100	-3.24759900	-1.19820900
H	1.28163800	-4.21423300	-1.21554900
H	1.05203700	-2.45495800	-1.23447700
H	2.42070600	-3.17972600	-2.09600500
C	7.00231000	-0.45840000	0.10844400
C	7.59570600	0.95943900	0.12318200
H	7.29616400	1.53096700	-0.76116400
H	7.28704600	1.51674000	1.01374800
H	8.68880100	0.90420400	0.12855300
C	7.50319100	-1.20563100	1.36364500
H	7.13951800	-2.23676800	1.39230400
H	8.59838200	-1.23709600	1.38051300
H	7.16035800	-0.70513100	2.27489300
C	7.51194500	-1.18315300	-1.15642900
H	7.14978600	-2.21407900	-1.20467700
H	7.17269700	-0.66781700	-2.06039000
H	8.60732200	-1.21260700	-1.16723200
C	-6.76421500	-0.36816800	0.36862900
C	-7.29905900	1.04580400	0.64599400

H	-6.77247800	1.51922200	1.48105100
H	-7.20300300	1.69275400	-0.23200100
H	-8.36072500	0.99661100	0.90726400
C	-6.97308300	-1.22242200	1.63827400
H	-8.03353100	-1.25206900	1.91263700
H	-6.63709300	-2.25291100	1.49105800
H	-6.41222900	-0.80553900	2.48108700
C	-7.57756200	-0.97396700	-0.79585500
H	-7.26599400	-1.99872100	-1.01739000
H	-8.64474000	-0.99588200	-0.54829900
H	-7.44864300	-0.38149500	-1.70709600
H	0.29755100	3.41345800	1.20336500
H	-0.11265400	3.41680600	-1.79691500

PO-aCo^{III}-OH
Charge: 0
Spin Multiplicity: 5
Sum of electronic and thermal Free Energies (a.u.): -2076.724621
No imaginary frequency

C	-4.75817800	-1.53114800	-0.13642800
C	-5.35605400	-0.27093000	0.11166800
C	-3.43003100	-1.71748500	-0.48237200
H	-5.39009100	-2.40607100	-0.05176900
C	-4.55091800	0.83824600	-0.04139400
C	-2.58091100	-0.55827200	-0.55718000
C	-3.18069200	0.72882800	-0.37805200
H	-4.95186600	1.83639600	0.10228100
O	-1.30779000	-0.71384900	-0.76681400
C	-2.45683800	1.95991600	-0.53487300
Co	0.15538700	0.55342500	-0.82118800
N	-1.19685900	2.08630900	-0.78996500
H	-3.06818600	2.86003800	-0.42785200
N	1.32081300	2.07413700	-0.01846200
C	-0.52502100	3.37949300	-0.88558200
C	2.58459400	1.93404300	0.20212300
C	0.62272500	3.35108400	0.15241600
C	-1.38592100	4.63187100	-0.71520000
H	3.18130000	2.81303200	0.46243200
C	3.32831100	0.70184000	0.14238000
C	1.48258800	4.61552300	0.05764900
C	-0.52088100	5.89320200	-0.83429900
H	-1.87035300	4.61541500	0.27049500
H	-2.18245100	4.64461900	-1.46731900
C	4.73508500	0.79638000	0.24430600
C	2.69407400	-0.57372200	0.03623500
C	0.61939600	5.87810300	0.18906100
H	2.24872900	4.61894400	0.84004800
H	2.00663400	4.61680500	-0.90743900
H	-1.14104100	6.78590100	-0.69995900
H	-0.10144400	5.95044800	-1.84749900
C	5.54298700	-0.32259800	0.21423500
H	5.16606300	1.78790100	0.33795800
C	3.52107300	-1.74538600	0.01466200
O	1.39106700	-0.69480100	-0.01109600
H	0.19560200	5.92029300	1.20158700
H	1.24744700	6.76820700	0.07550400
C	4.89488000	-1.57480300	0.09647300
H	5.51997900	-2.45830300	0.07166000
C	-0.92566600	-0.47475200	2.30540100
C	0.24190100	0.28556600	2.76700200
O	-0.61538500	0.81750800	1.73955300
H	-0.73266800	-1.28212000	1.60597800
H	1.23236700	0.00056500	2.42239400
H	0.19457800	0.81987900	3.71537700
C	-2.21608400	-0.55848700	3.07300500
H	-3.06437900	-0.57622600	2.38190100
H	-2.24501400	-1.47714200	3.66904000
H	-2.32897400	0.29842000	3.74365500
O	0.68481600	0.53238300	-2.55585300

H	1.11238700	-0.30245300	-2.79566100
C	-2.86209300	-3.11208300	-0.79517500
C	-2.31237800	-3.12421800	-2.24053600
H	-3.11389900	-2.91986100	-2.95829300
H	-1.53255800	-2.37279600	-2.36661600
H	-1.89102400	-4.10892600	-2.47291300
C	-1.72722500	-3.47863400	0.18694200
H	-0.88585300	-2.79690000	0.07945000
H	-2.08362700	-3.44555100	1.22269500
H	-1.37386700	-4.49647500	-0.01349000
C	-3.93881500	-4.20664100	-0.69257800
H	-4.34542900	-4.28917400	0.32122600
H	-4.76942700	-4.03155000	-1.38424100
H	-3.49428400	-5.17328900	-0.94846400
C	2.88031300	-3.13879000	-0.08756400
C	3.93650200	-4.25621100	-0.14943300
H	4.58928000	-4.15483300	-1.02297300
H	4.56283500	-4.28065500	0.74848600
H	3.43184000	-5.22430200	-0.22426400
C	2.00154200	-3.39121000	1.15873300
H	2.61404900	-3.38065800	2.06697100
H	1.22886400	-2.62909300	1.25072400
H	1.51632000	-4.37102800	1.08731200
C	2.01935400	-3.24086100	-1.36843300
H	1.59373200	-4.24685800	-1.45324000
H	1.19988100	-2.52363400	-1.35133400
H	2.63361800	-3.05932800	-2.25766100
C	7.07238300	-0.26893000	0.30165000
C	7.59257100	1.17191300	0.42841300
H	7.30930400	1.78077100	-0.43619400
H	7.21316000	1.66014900	1.33200200
H	8.68539800	1.16751900	0.48774300
C	7.54615900	-1.06459200	1.53756400
H	7.23521100	-2.11205000	1.48790500
H	8.63918500	-1.04382700	1.61161500
H	7.13197000	-0.63638400	2.45590900
C	7.68151100	-0.89262200	-0.97311200
H	7.37475000	-1.93487200	-1.09941700
H	7.36406900	-0.34085900	-1.86350400
H	8.77602300	-0.86963400	-0.92646300
C	-6.83290200	-0.20205400	0.51448100
C	-7.30308000	1.24452700	0.73550700
H	-6.73368300	1.73631700	1.53088300
H	-7.20776800	1.84349300	-0.17594300
H	-8.35768100	1.25141200	1.02828200
C	-7.03859100	-0.98368900	1.83061200
H	-8.09071300	-0.95499400	2.13560100
H	-6.74964400	-2.03342700	1.72576500
H	-6.43598800	-0.55034700	2.63540400
C	-7.70414600	-0.82975000	-0.59532000
H	-7.44039500	-1.87610800	-0.77387700
H	-8.76362700	-0.79534200	-0.31770500
H	-7.57846300	-0.28834900	-1.53823500
H	0.14369200	3.31006500	1.14156000
H	-0.05780300	3.40532900	-1.88067400

LanL2TZ(f) basis set for Co and 6-311G(d,p) for all non-metal C, H, O, N and S
PO-Co^{III}-Cl + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3164.416210
Thermal correction to Gibbs Free Energy (a.u.): 0.777242
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -5640.9971787 a.u.

C	5.98768300	-3.24918500	-3.03410200

C	5.29305100	-4.25086500	-2.33447700
C	5.87089500	-1.92014000	-2.68255000
H	6.62324600	-3.52241900	-3.86975600
C	4.49226800	-3.88194100	-1.27565800
H	5.38782900	-5.29030000	-2.62152400
C	5.04538400	-1.51011900	-1.60671000
H	6.39893000	-1.14453500	-3.22355600
C	4.34875200	-2.53165700	-0.88912300
H	3.94837300	-4.63663800	-0.71609700
O	4.98436900	-0.23942100	-1.31730300
C	3.51952800	-2.24453200	0.24409100
Co	3.67766000	0.56257200	-0.18309000
N	3.25914800	-1.07693000	0.71587800
H	3.07333300	-3.11093100	0.73319200
N	2.51222600	1.37165300	1.08374400
C	2.29450200	-0.90140100	1.81848800
C	1.86318400	2.46448400	0.90143100
C	2.42431700	0.54993200	2.29108200
C	2.47769900	-1.83805600	3.01581000
H	1.13434900	2.77798600	1.64472700
C	2.03867300	3.32997800	-0.22996100
C	1.33380300	0.88095800	3.30175900
C	1.43463800	-1.52090600	4.09939000
H	3.49135800	-1.70592500	3.41138400
H	2.39168500	-2.88414600	2.71352900
C	1.12084400	4.38311000	-0.41472500
C	3.15030800	3.17751600	-1.11675100
C	1.47256000	-0.04735100	4.51625300
H	1.41752800	1.92240400	3.62566700
H	0.35298500	0.74362100	2.83579500
H	1.59933700	-2.16556800	4.96709700
H	0.43397100	-1.74832700	3.72009900
C	1.25271900	5.27151300	-1.46238900
H	0.28820000	4.47063500	0.27470900
C	3.26350100	4.11075000	-2.17364800
O	4.07142300	2.25937400	-0.97753400
H	2.41769400	0.16713100	5.02997200
H	0.66977900	0.15789700	5.22873000
C	2.33817800	5.12431500	-2.34044700
H	0.53242000	6.06732700	-1.60357400
H	4.10261900	3.99659400	-2.84886600
H	2.45477600	5.81562500	-3.16848700
O	2.30919900	0.25161500	-1.37098100
H	2.75161300	0.36652600	-2.22033800
O	5.34162200	1.02810100	0.98182700
H	5.39922100	1.92375600	0.60654300
H	5.95505100	0.51042300	0.43502200
C	-0.43452600	0.91397700	-1.35684600
C	-0.38956300	-0.49207000	-1.70498300
O	-1.67818800	0.10786500	-1.32739000
H	-0.10371800	1.15889400	-0.35917600
H	-0.00311800	-1.19166400	-0.98128000
H	-0.36221900	-0.78844000	-2.74759700
C	-0.42319300	2.00850100	-2.37411700
H	-0.99581400	2.86964800	-2.02463900
H	0.60855900	2.32723600	-2.52880100
H	-0.83876400	1.66060600	-3.32256100
C	-1.59025300	4.43788800	2.30774400
C	-2.50922300	5.04523800	1.43342500
C	-1.39133000	3.07413900	2.30271300
H	-1.03153800	5.05086100	3.00736800
C	-3.25749600	4.23413000	0.60950200
H	-2.65315000	6.11780600	1.43937100
C	-2.08314600	2.21624400	1.40176200
H	-0.71031200	2.61251400	3.00190400
C	-3.08695700	2.83226900	0.58618900
H	-4.01805100	4.66761700	-0.03279100
O	-1.76868200	0.96213800	1.36387600
C	-4.02423300	2.06076300	-0.17061500

Co	-2.66202900	-0.39496300	0.34964800
N	-4.03275100	0.78101700	-0.28042500
H	-4.82306600	2.62765500	-0.64559100
N	-3.51198600	-1.71303500	-0.74674500
C	-5.12874700	0.04378800	-0.91965900
C	-3.30583600	-2.98033800	-0.67818300
C	-4.46518400	-1.10854400	-1.68514200
C	-6.06646400	0.84452800	-1.81899600
H	-3.90789500	-3.63921900	-1.30111400
C	-2.32439800	-3.62196600	0.13725100
C	-5.50435000	-2.03960400	-2.30428100
C	-7.11298700	-0.08469800	-2.44831800
H	-5.48542800	1.33975100	-2.60647600
H	-6.57156500	1.62590100	-1.24569500
C	-2.29680600	-5.03409200	0.14660500
C	-1.34467400	-2.87866700	0.86777000
C	-6.45664300	-1.24238700	-3.20562300
H	-5.01780500	-2.82290700	-2.89124100
H	-6.06999800	-2.53263900	-1.50530400
H	-7.75962300	0.48848200	-3.11798700
H	-7.75655100	-0.48724200	-1.65762500
C	-1.34472800	-5.73672600	0.84969700
H	-3.05455900	-5.56523100	-0.42117000
C	-0.37022400	-3.63499700	1.56895000
O	-1.26515100	-1.58224300	0.88760600
H	-5.89552400	-0.84510800	-4.05989800
H	-7.21999000	-1.90913300	-3.61519800
C	-0.37297400	-5.01297200	1.56249500
H	-1.34152300	-6.81902700	0.85306000
H	0.36954200	-3.08720500	2.12903000
H	0.38630400	-5.54614300	2.12542700
H	-5.70030100	-0.39997700	-0.09579000
H	-3.86050300	-0.65819900	-2.48224400
H	3.40585700	0.64520800	2.77280400
H	1.28882800	-1.02366500	1.39744600
Cl	-3.94699700	-0.96447900	2.10151900

PO-Co^{III}-Cl + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3164.401681
Thermal correction to Gibbs Free Energy (a.u.): 0.780627
Imaginary frequencies: -448.91
Calculation of single point energy based on the optimized structure, Et = -5640.9834404 a.u.

C	5.80102700	-3.10154100	-3.10845700
C	5.10943300	-4.10603900	-2.41087600
C	5.71315000	-1.77691300	-2.72956600
H	6.41049300	-3.36783600	-3.96539600
C	4.34306400	-3.74768300	-1.32313600
H	5.18068700	-5.14063500	-2.72096600
C	4.92035500	-1.37787500	-1.62819000
H	6.23890900	-0.99943700	-3.26990900
C	4.22969700	-2.40268800	-0.91001900
H	3.80286700	-4.50463000	-0.76347800
O	4.88643900	-0.11126600	-1.30786700
C	3.44940800	-2.12414100	0.25814500
Co	3.52640700	0.66958800	-0.22258000
N	3.20170700	-0.95582000	0.73939700
H	3.03196200	-2.99065900	0.77192500
N	2.33447000	1.45651500	1.03509300
C	2.29819800	-0.78639100	1.89449000
C	1.63149600	2.51325200	0.84231700
C	2.34966400	0.69135100	2.28525100
C	2.62154700	-1.64265200	3.12074800
H	0.91374400	2.81725900	1.60016900
C	1.73419300	3.34966400	-0.32073700
C	1.28238300	0.99963500	3.32640400
C	1.60693000	-1.34901000	4.23789900
H	3.63930900	-1.41050500	3.45476200
H	2.60412600	-2.70571700	2.87047600

C	0.76008900	4.35042100	-0.51267900
C	2.82494700	3.22139300	-1.23418300
C	1.54156200	0.14450700	4.57575500
H	1.31112100	2.05827700	3.59939100
H	0.29477100	0.77927000	2.90936800
H	1.86387900	-1.92769400	5.12921400
H	0.61267200	-1.67817800	3.92135300
C	0.82300600	5.20979300	-1.59034500
H	-0.05771900	4.42119400	0.19602000
C	2.86845600	4.12438900	-2.32065900
O	3.79144700	2.34231500	-1.10235000
H	2.48557300	0.45835500	5.03807500
H	0.75337400	0.32385600	5.31096100
C	1.89165500	5.08842500	-2.49189200
H	0.06056200	5.96408400	-1.73648400
H	3.69521400	4.02977900	-3.01386600
H	1.95404000	5.75846000	-3.34268400
O	2.21880900	0.17359100	-1.44125700
H	2.44386000	0.64184700	-2.25361500
O	5.14329400	1.25286700	0.89214500
H	5.18639900	2.14378700	0.50468600
H	5.77543700	0.73602300	0.36218900
C	-0.55530200	1.00804700	-1.33990700
C	0.22210700	-0.22167500	-1.32010200
O	-1.56626700	0.00550800	-1.26444100
H	-0.48324800	1.60150000	-0.43558900
H	0.38610900	-0.70857800	-0.37768100
H	0.32127800	-0.79254900	-2.22818100
C	-0.61850000	1.84348500	-2.59350100
H	-1.46903800	2.52699100	-2.54289100
H	0.28900900	2.44148400	-2.69860500
H	-0.73263800	1.20386600	-3.47208900
C	-1.79108000	4.41756100	2.38632600
C	-2.71032400	4.97330400	1.47982500
C	-1.51662500	3.06613800	2.38880200
H	-1.29331500	5.05939400	3.10590000
C	-3.38541700	4.12022600	0.63319300
H	-2.91505200	6.03601700	1.47940900
C	-2.12576100	2.17095900	1.46310100
H	-0.83846400	2.64313600	3.11499300
C	-3.13703300	2.73143200	0.61646200
H	-4.14846400	4.51096500	-0.03329100
O	-1.73198500	0.94059600	1.42433300
C	-4.00941000	1.90874300	-0.16860400
Co	-2.52152600	-0.46711900	0.37903400
N	-3.94303400	0.63260400	-0.27846000
H	-4.82650300	2.43217000	-0.66232500
N	-3.28515600	-1.83754700	-0.71533200
C	-4.97830200	-0.16325000	-0.94760100
C	-2.99308300	-3.08568200	-0.66042200
C	-4.23332700	-1.28225100	-1.68674800
C	-5.92758900	0.58650300	-1.87823400
H	-3.52968600	-3.77442900	-1.31065600
C	-1.99503800	-3.67610600	0.17733800
C	-5.20474400	-2.26464400	-2.33649100
C	-6.90552100	-0.39531600	-2.53696800
H	-5.34754600	1.10866700	-2.64893000
H	-6.48979300	1.34250600	-1.32425100
C	-1.87808900	-5.08227600	0.16509300
C	-1.09506300	-2.88605300	0.96003200
C	-6.16710900	-1.51842300	-3.26999700
H	-4.66084100	-3.02250800	-2.90611500
H	-5.76974900	-2.78561800	-1.55484100
H	-7.55977200	0.14331800	-3.22783000
H	-7.55165500	-0.82960700	-1.76532000
C	-0.91789300	-5.74128000	0.90101400
H	-2.57451200	-5.64794700	-0.44641400
C	-0.12018700	-3.59854000	1.70831200
O	-1.08945500	-1.58923900	0.99658200

H	-5.59950100	-1.09328300	-4.10641800
H	-6.88198300	-2.22357100	-3.70249700
C	-0.03566600	-4.97432000	1.67997000
H	-0.84787100	-6.82125400	0.88499500
H	0.54366000	-3.02159900	2.33128600
H	0.71978000	-5.47063800	2.28091900
H	-5.54949300	-0.63233100	-0.13756700
H	-3.61848900	-0.80567700	-2.45962200
H	3.34099400	0.87833800	2.71680600
H	1.27737900	-1.00277700	1.55805500
Cl	-3.83680400	-1.09656900	2.11842700

PO-Co^{III}-OAc + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2932.689039
Thermal correction to Gibbs Free Energy (a.u.): 0.822133
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -5409.337591 a.u.

C	6.17160100	-3.28720100	-3.10695000
C	5.41218200	-4.30905400	-2.51140900
C	6.08501600	-1.98304100	-2.66551100
H	6.83429200	-3.52440800	-3.93245500
C	4.57722600	-3.98582700	-1.46427000
H	5.48411200	-5.32848900	-2.86827500
C	5.22691900	-1.61929100	-1.59837300
H	6.66338800	-1.19148900	-3.12593200
C	4.46267100	-2.66170400	-0.98750600
H	3.98310800	-4.75745700	-0.98453500
O	5.19876800	-0.37115600	-1.22011700
C	3.58998800	-2.42433800	0.12453200
Co	3.88556800	0.39890400	-0.07203200
N	3.34943200	-1.28506300	0.67011200
H	3.08970500	-3.30598100	0.52622300
N	2.71022700	1.16142500	1.21357700
C	2.33926400	-1.14865100	1.73754900
C	2.12561600	2.29937800	1.10198700
C	2.52901100	0.24687600	2.34079400
C	2.40813100	-2.19595800	2.85272900
H	1.38308700	2.58845500	1.84134300
C	2.39213100	3.24636100	0.05741600
C	1.42037500	0.55636000	3.33810900
C	1.34827900	-1.90338400	3.92708100
H	3.41196100	-2.17293800	3.29241800
H	2.26115300	-3.20279800	2.45498200
C	1.53864800	4.36067200	-0.06825700
C	3.53032600	3.10841800	-0.79746600
C	1.46130500	-0.47661200	4.47201500
H	1.55011000	1.56053200	3.75199800
H	0.45246100	0.51718700	2.82843300
H	1.44097300	-2.62972300	4.73931300
H	0.35027200	-2.03221000	3.49848000
C	1.76015800	5.32613900	-1.02895600
H	0.68409000	4.43525200	0.59556900
C	3.73549500	4.12010400	-1.76442200
O	4.39626000	2.13248600	-0.70418300
H	2.39945200	-0.36615600	5.02946800
H	0.64883000	-0.28217300	5.17677500
C	2.87183500	5.19385900	-1.87609900
H	1.08907200	6.17003400	-1.12665500
H	4.59465000	4.01739700	-2.41585200
H	3.05834400	5.94543800	-2.63602400
O	2.55432700	0.25758200	-1.33159800
H	3.03910500	0.40386000	-2.15258700
O	5.51975800	0.68187300	1.19184700
H	5.63318700	1.60110400	0.89394600
H	6.13137100	0.18136500	0.62748000
C	-0.12930500	1.05700600	-1.39885500

C	-0.19264400	-0.30813700	-1.88323300
O	-1.43782000	0.36287000	-1.48131000
H	0.18557200	1.17517000	-0.37372100
H	0.10430900	-1.10647700	-1.22164500
H	-0.15665200	-0.50325300	-2.94944400
C	0.00275400	2.24014700	-2.30218100
H	-0.51828000	3.10475000	-1.88694600
H	1.06021500	2.49247500	-2.39124600
H	-0.40067100	2.01905500	-3.29297800
C	-1.27428000	4.35921900	2.59000200
C	-2.13391500	5.09727500	1.75795300
C	-1.12967900	2.99635000	2.44007300
H	-0.71769300	4.86714800	3.37080500
C	-2.87924800	4.41405900	0.82198800
H	-2.23477900	6.16826000	1.87630500
C	-1.82106800	2.27244600	1.42775500
H	-0.49253100	2.43309500	3.10534900
C	-2.76616600	3.01709200	0.65128000
H	-3.59234000	4.94881300	0.20197900
O	-1.55884500	1.01710400	1.26048800
C	-3.68585800	2.38145800	-0.24348400
Co	-2.51126100	-0.19764100	0.11581000
N	-3.76828500	1.12220500	-0.48335100
H	-4.40167800	3.04608900	-0.72423600
N	-3.41313900	-1.37190800	-1.07959000
C	-4.83586100	0.54969300	-1.31940900
C	-3.40920800	-2.65120800	-0.98485800
C	-4.20917100	-0.63533900	-2.06633400
C	-5.53836200	1.49414700	-2.29013000
H	-4.07443600	-3.22418600	-1.62656600
C	-2.57154000	-3.40915400	-0.10492000
C	-5.27436200	-1.42576700	-2.81875200
C	-6.60355900	0.72079600	-3.08136700
H	-4.80523800	1.93890000	-2.97469100
H	-6.02097800	2.31386600	-1.75187100
C	-2.77503600	-4.80302400	-0.03085400
C	-1.48215700	-2.80187900	0.59607300
C	-6.01186900	-0.49867400	-3.79493100
H	-4.82148600	-2.25243900	-3.37329400
H	-5.97686800	-1.85315300	-2.09562100
H	-7.08249400	1.38662100	-3.80453000
H	-7.38597600	0.38878600	-2.38981500
C	-1.94431500	-5.61908500	0.70598900
H	-3.61231600	-5.22828200	-0.57529900
C	-0.62364500	-3.67617600	1.30974300
O	-1.21143500	-1.53007900	0.57087800
H	-5.31153500	-0.16159300	-4.56881000
H	-6.80091900	-1.05532100	-4.30761900
C	-0.85217500	-5.03514400	1.36877100
H	-2.11987500	-6.68563500	0.76218500
H	0.21624300	-3.23532000	1.82190800
H	-0.17580500	-5.66087900	1.94201800
C	-4.95099500	-1.68873800	3.17345900
H	-4.39423000	-2.61421000	3.34354100
H	-6.01546700	-1.87797000	3.30491600
H	-4.59734300	-0.95272700	3.89640000
C	-4.67900200	-1.21444200	1.75109100
O	-3.48641300	-0.71201000	1.64060700
O	-5.52349500	-1.34621300	0.86966300
H	-5.55492800	0.12062900	-0.61659600
H	-3.48616500	-0.22574600	-2.78243800
H	3.49427400	0.24264400	2.86320600
H	1.35153400	-1.17246100	1.26001500

PO-Co^{III}-OAc + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -2932.674315
Thermal correction to Gibbs Free Energy (a.u.): 0.825531

Imaginary frequencies: -447.88
Calculation of single point energy based on the optimized structure, Et = -5409.3236578 a.u.

C	6.00044000	-3.11991800	-3.20881900
C	5.23209600	-4.15163900	-2.64365100
C	5.94704000	-1.83341600	-2.71139400
H	6.64319900	-3.33392600	-4.05600300
C	4.42364900	-3.85975200	-1.56679100
H	5.27757000	-5.15562600	-3.04555500
C	5.11407100	-1.50138200	-1.61722700
H	6.53259100	-1.03441500	-3.14906800
C	4.34283500	-2.55450400	-1.03485500
H	3.82444000	-4.64001100	-1.10832700
O	5.11811700	-0.27009000	-1.17991200
C	3.50941700	-2.34903800	0.11168300
Co	3.74722600	0.47220300	-0.08144400
N	3.28325800	-1.22122300	0.68997200
H	3.02884800	-3.24008900	0.51705400
N	2.54023300	1.19711900	1.19758200
C	2.32404800	-1.11514800	1.80810200
C	1.90939400	2.30998600	1.08861300
C	2.44991100	0.30678000	2.35813800
C	2.52126500	-2.11883600	2.94674500
H	1.17410300	2.57818900	1.84288600
C	2.11708500	3.25437500	0.02676800
C	1.36083100	0.58023200	3.38578000
C	1.48702600	-1.86394600	4.05569400
H	3.53875500	-2.01020100	3.33947800
H	2.42853800	-3.14473300	2.58246200
C	1.21254900	4.32832700	-0.09954800
C	3.24194300	3.15303800	-0.84756000
C	1.51284900	-0.41291300	4.54688300
H	1.44703300	1.60134800	3.76766900
H	0.38001300	0.47319100	2.91195800
H	1.66754700	-2.54934100	4.88830600
H	0.48544700	-2.08428800	3.67552000
C	1.37746900	5.28796400	-1.07713700
H	0.36711200	4.37745100	0.57789500
C	3.39065200	4.15822300	-1.82987400
O	4.14921100	2.20676100	-0.76735100
H	2.45805300	-0.21689900	5.06790700
H	0.71215700	-0.25309400	5.27328000
C	2.48024200	5.19355600	-1.94000500
H	0.66787600	6.09942600	-1.17513100
H	4.24351300	4.08401600	-2.49328900
H	2.62242800	5.94217500	-2.71202300
O	2.47952100	0.18105100	-1.40366200
H	2.77502800	0.71128000	-2.15300600
O	5.33492900	0.84299700	1.16116400
H	5.44258700	1.76522900	0.87172100
H	5.96489000	0.34916300	0.60723700
C	-0.23129900	1.20449500	-1.36456800
C	0.46017900	-0.07540600	-1.41611600
O	-1.31252100	0.27730500	-1.42956700
H	-0.17149100	1.71098800	-0.40844800
H	0.53276100	-0.65738500	-0.51695500
H	0.56861700	-0.57055100	-2.36679100
C	-0.16452900	2.14718200	-2.53973400
H	-0.96915800	2.88287300	-2.47327700
H	0.78562500	2.68548400	-2.54211500
H	-0.26919800	1.59591600	-3.47743600
C	-1.42990900	4.30905800	2.74724200
C	-2.26356400	5.03330500	1.87890900
C	-1.23224800	2.95359700	2.58305500
H	-0.93686600	4.81995700	3.56784600
C	-2.93463900	4.34104100	0.89267300
H	-2.40715500	6.09824400	2.00773900
C	-1.83837800	2.22586100	1.51895000
H	-0.61787200	2.39954000	3.27732500
C	-2.76681400	2.95313300	0.70588000

H	-3.63138100	4.86332100	0.24395800
O	-1.51201600	0.98922500	1.33170300
C	-3.62164800	2.30298100	-0.24553800
Co	-2.38074300	-0.24272100	0.12742100
N	-3.65227200	1.04744100	-0.50596600
H	-4.33542000	2.95363700	-0.74838700
N	-3.22374200	-1.44121300	-1.08422000
C	-4.66535600	0.45408300	-1.39350200
C	-3.18028600	-2.71813700	-1.00275400
C	-3.98189600	-0.71899800	-2.10841400
C	-5.33668800	1.38654100	-2.39739700
H	-3.79806300	-3.30583400	-1.67812100
C	-2.35605200	-3.46181800	-0.09464200
C	-4.99512400	-1.52732200	-2.91177400
C	-6.34738800	0.59518300	-3.24044600
H	-4.57779000	1.84399400	-3.04454100
H	-5.86032100	2.19747500	-1.88462600
C	-2.52411800	-4.86021600	-0.04495000
C	-1.31688200	-2.83325300	0.66246600
C	-5.69930800	-0.61289400	-3.92361600
H	-4.50077700	-2.34511700	-3.44351100
H	-5.72531100	-1.96827500	-2.22485900
H	-6.80219700	1.25303700	-3.98638000
H	-7.15675700	0.24843300	-2.58813500
C	-1.70957900	-5.66582200	0.72279200
H	-3.32234000	-5.30040900	-0.63456300
C	-0.47730700	-3.69579400	1.41503300
O	-1.07767600	-1.55665600	0.66344700
H	-4.96665600	-0.26235400	-4.66071600
H	-6.45196200	-1.18237700	-4.47576800
C	-0.67138300	-5.06153400	1.44886700
H	-1.86011800	-6.73714700	0.75758900
H	0.31771100	-3.24149200	1.98460000
H	-0.01132000	-5.67499000	2.05387400
C	-4.91278600	-1.81512600	3.09510600
H	-4.35061900	-2.73764600	3.26436400
H	-5.97858900	-2.01981300	3.18851900
H	-4.59210600	-1.09080700	3.84504700
C	-4.59795700	-1.30636000	1.69234500
O	-3.41228000	-0.78810000	1.62680500
O	-5.41604700	-1.43146300	0.78284600
H	-5.40742700	0.01206700	-0.72271800
H	-3.22558600	-0.29921300	-2.78155200
H	3.43077000	0.37871000	2.84468000
H	1.31288900	-1.22282400	1.39718000

PO-Co^{III}-OTs + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3599.035779
Thermal correction to Gibbs Free Energy (a.u.): 0.898344
No imaginary frequency
Calculation of single point energy based on the optimized structure, Er = -6075.8623111 a.u.

C	6.83252100	-3.53972200	-1.41340300
C	5.96994900	-4.36959400	-0.67763600
C	6.71178300	-2.16522300	-1.37052500
H	7.60435600	-3.98457000	-2.03259300
C	4.99861400	-3.78401200	0.10596500
H	6.06958800	-5.44657800	-0.72346800
C	5.71285500	-1.53702600	-0.58812700
H	7.36993300	-1.52270900	-1.94251300
C	4.84756900	-2.38260900	0.17224200
H	4.32160600	-4.40115800	0.68832300
O	5.64940300	-0.23265800	-0.58268300
C	3.83855600	-1.85707600	1.04414600
Co	4.14548500	0.77116500	0.02261100
N	3.53930900	-0.61482200	1.18995900
H	3.28001600	-2.59392600	1.62128700
N	2.73782200	1.81038500	0.77618600

C	2.39764400	-0.21714100	2.03392100
C	2.17707700	2.81433900	0.20598900
C	2.38761800	1.31184300	2.10837200
C	2.40772800	-0.76792100	3.46329300
H	1.31887500	3.27891300	0.68417800
C	2.61485900	3.39971900	-1.02955600
C	1.08201000	1.77907200	2.74504500
C	1.14251700	-0.30481600	4.20249200
H	3.30990500	-0.40443600	3.96911100
H	2.46676900	-1.85808000	3.46774500
C	1.78768500	4.35946200	-1.64592000
C	3.88655900	3.07585500	-1.59808100
C	0.99775100	1.22162200	4.17496500
H	1.03157500	2.87174200	2.77692000
H	0.23911900	1.40894000	2.15368900
H	1.17135700	-0.65759700	5.23719300
H	0.25656700	-0.74819600	3.73998000
C	2.16188200	4.98479700	-2.81714300
H	0.82771800	4.57999800	-1.19166500
C	4.24824400	3.74398700	-2.79217400
O	4.73173200	2.23823500	-1.05910400
H	1.78588700	1.68157300	4.78399300
H	0.04410400	1.50961600	4.62478800
C	3.40702200	4.66666400	-3.38367800
H	1.50939600	5.70747400	-3.29051500
H	5.20995400	3.49829800	-3.22552300
H	3.71587300	5.15091300	-4.30411100
O	3.05628000	0.13352500	-1.31647000
H	3.66968500	0.06450500	-2.05756000
O	5.52876300	1.55737400	1.36465900
H	5.70167300	2.32827300	0.79731400
H	6.22623900	0.92826600	1.11704900
C	0.39739300	0.35033100	-1.99039200
C	0.49050800	-1.06376800	-2.30134600
O	-0.84242300	-0.47343900	-2.10569500
H	0.59569700	0.61324300	-0.96341900
H	0.79358200	-1.73796800	-1.51488700
H	0.64579000	-1.38445700	-3.32585200
C	0.51070800	1.42592900	-3.02009700
H	-0.12347000	2.27594100	-2.76187100
H	1.54559000	1.76777700	-3.04669200
H	0.22382500	1.05397900	-4.00629600
C	-1.78057600	4.39123800	-0.04071600
C	-2.70690500	4.56388800	-1.08389600
C	-1.42081500	3.13539500	0.39513200
H	-1.35102800	5.26193300	0.44410200
C	-3.27734100	3.44156000	-1.64115800
H	-2.98156800	5.55458000	-1.42231900
C	-1.94505600	1.95550000	-0.19613500
H	-0.74611900	3.01051200	1.22634000
C	-2.92532200	2.14094400	-1.22043000
H	-4.02674100	3.54277500	-2.42004200
O	-1.52695400	0.80483800	0.23474000
C	-3.66087300	1.04317400	-1.76563300
Co	-1.95687200	-0.89414100	-0.52853100
N	-3.44183500	-0.19784200	-1.51973200
H	-4.49458300	1.30757400	-2.41402500
N	-2.37682600	-2.55497500	-1.39183500
C	-4.29582900	-1.28086700	-2.01181100
C	-1.97627700	-3.71067800	-0.99238800
C	-3.32700200	-2.37348500	-2.49408200
C	-5.31765900	-0.91645600	-3.08431800
H	-2.35154000	-4.59595000	-1.50223900
C	-1.07742800	-3.94821200	0.08909400
C	-4.07564500	-3.61937400	-2.96103800
C	-6.06946800	-2.17068500	-3.54798700
H	-4.80502600	-0.45724400	-3.93829600
H	-6.02868900	-0.18127100	-2.69780200
C	-0.85517000	-5.28704500	0.48361100

C	-0.41684300	-2.87942100	0.76861500
C	-5.10282800	-3.25181100	-4.03950700
H	-3.37576200	-4.36007800	-3.35688700
H	-4.58517700	-4.07586300	-2.10475100
H	-6.77633600	-1.90514500	-4.33835600
H	-6.66207100	-2.56495000	-2.71453400
C	-0.03172900	-5.59953100	1.54038600
H	-1.36486100	-6.07521200	-0.06174300
C	0.39134200	-3.23367100	1.87470400
O	-0.48123600	-1.62991600	0.40711900
H	-4.57813300	-2.89132400	-4.93237200
H	-5.65463200	-4.14609800	-4.34022900
C	0.58160000	-4.54725900	2.24369300
H	0.12216800	-6.62808400	1.83995800
H	0.81663200	-2.42911600	2.44699600
H	1.19864300	-4.76941900	3.10821800
H	-4.80926000	-1.67683600	-1.12732900
H	-2.75996200	-1.95244000	-3.33417200
H	3.22794500	1.61195600	2.74723800
H	1.48530800	-0.53219200	1.51322100
S	-3.20754400	-1.02120300	2.33136400
O	-4.30733800	-1.77592900	2.93139700
O	-1.89348100	-1.09204500	2.97348400
O	-3.17751800	-1.41805600	0.82786900
C	-3.68295900	0.70870700	2.30909200
C	-4.75842700	1.12013000	1.52923200
C	-2.98917300	1.61813300	3.09541500
C	-5.11707100	2.46208400	1.51718500
H	-5.29470400	0.39578600	0.92992200
C	-3.36606400	2.95648800	3.08225300
H	-2.15422600	1.27068100	3.68846700
C	-4.42463000	3.40158700	2.28672600
H	-5.94379700	2.78961800	0.89578400
H	-2.81947100	3.67071800	3.68913500
C	-4.77784200	4.86385800	2.21828500
H	-4.49615000	5.38586300	3.13515700
H	-4.25095700	5.34148000	1.38582900
H	-5.84845700	5.00948200	2.05750000

PO-Co^{III}-OTs + H_2O-Co^{III}-OH
Charge: 0
Spin Multiplicity: 1
Sum of electronic and thermal Free Energies (a.u.): -3599.022647
Thermal correction to Gibbs Free Energy (a.u.): 0.900871
Imaginary frequencies: -447.39
Calculation of single point energy based on the optimized structure, Et = -6075.8481186 a.u.

C	-7.19673700	2.89214400	-1.33780100
C	-6.41000600	3.83350300	-0.65397600
C	-6.92529100	1.54036200	-1.25913000
H	-8.02939600	3.23052000	-1.94521500
C	-5.35924100	3.38286900	0.11626400
H	-6.62810400	4.89118400	-0.72783400
C	-5.84286400	1.05127900	-0.49183300
H	-7.52571800	0.81258200	-1.79090700
C	-5.05352400	2.00903000	0.21640900
H	-4.73905100	4.08821800	0.66015700
O	-5.64180600	-0.24027500	-0.44362600
C	-3.97536700	1.62277200	1.07789000
Co	-3.98326800	-1.02641200	0.07194100
N	-3.52852100	0.42578500	1.23361800
H	-3.49941800	2.42617300	1.64094600
N	-2.43271300	-1.86580400	0.79385700
C	-2.34857100	0.16406100	2.08243400
C	-1.74145700	-2.77865300	0.21517400
C	-2.16165100	-1.35177100	2.14088000
C	-2.42359900	0.70448300	3.51265200
H	-0.82641500	-3.12608000	0.68737300
C	-2.10153300	-3.40069500	-1.02896700
C	-0.82235600	-1.68214300	2.78833200

C	-1.11548400	0.37508100	4.25163400
H	-3.28147900	0.24485100	4.01747600
H	-2.59719000	1.78259100	3.51613100
C	-1.15033400	-4.22282100	-1.66566400
C	-3.41027000	-3.25176700	-1.58273700
C	-0.81030400	-1.12674300	4.22087000
H	-0.66818700	-2.76495500	2.81851500
H	-0.01531800	-1.22984900	2.20482600
H	-1.18172700	0.72274500	5.28625400
H	-0.27730400	0.90380900	3.78937900
C	-1.44681200	-4.88038300	-2.84209100
H	-0.16463200	-4.31164000	-1.22200200
C	-3.68718000	-3.94679800	-2.78239900
O	-4.36335900	-2.54203600	-1.02718700
H	-1.54858400	-1.67023300	4.82395600
H	0.16726800	-1.31126900	4.67285000
C	-2.72947200	-4.73548600	-3.39315500
H	-0.70289100	-5.49615200	-3.33116100
H	-4.67870700	-3.83586900	-3.20384000
H	-2.97691700	-5.24737300	-4.31698200
O	-3.10831600	-0.18053600	-1.32889500
H	-3.56289100	-0.48973600	-2.12090100
O	-5.18145400	-1.99093400	1.42764100
H	-5.27325600	-2.79531300	0.88904100
H	-5.96833200	-1.46498100	1.20030500
C	-0.31820800	-0.59048300	-2.02613600
C	-1.18428800	0.51682000	-1.66553700
O	0.56379000	0.54225600	-2.01527200
H	-0.11761300	-1.28885300	-1.22308500
H	-1.19677200	0.85857200	-0.64914000
H	-1.58107000	1.15182300	-2.44056700
C	-0.43925700	-1.24354100	-3.37781900
H	0.46247900	-1.81938000	-3.59780100
H	-1.28995500	-1.92722800	-3.39011600
H	-0.57402700	-0.48682100	-4.15432700
C	2.18260700	-4.27790500	0.31303300
C	2.96582600	-4.44515200	-0.84117900
C	1.74186900	-3.03234900	0.70474500
H	1.93025300	-5.14115900	0.92003000
C	3.32927700	-3.32005800	-1.54862500
H	3.30314100	-5.42767400	-1.14510900
C	2.03326100	-1.86019300	-0.04423400
H	1.18774000	-2.91018100	1.62108800
C	2.89612100	-2.03146900	-1.17202200
H	3.98136500	-3.40890100	-2.41212500
O	1.51940000	-0.72932600	0.33110600
C	3.46984900	-0.91217800	-1.85512500
Co	1.75540800	0.96857600	-0.53783200
N	3.19322900	0.32045600	-1.63333000
H	4.24282900	-1.15182500	-2.58344400
N	2.02447400	2.62646500	-1.46359200
C	3.92135000	1.42723200	-2.25983900
C	1.60004700	3.77240500	-1.06956400
C	2.84583300	2.44756500	-2.66284800
C	4.83428300	1.07155300	-3.42951200
H	1.87929100	4.65525300	-1.64164800
C	0.77971300	4.00724000	0.07461000
C	3.46510300	3.70849100	-3.26095000
C	5.45536100	2.34155500	-4.02463600
H	4.25360100	0.54996100	-4.20003800
H	5.62648800	0.39237800	-3.10284500
C	0.51116000	5.34733900	0.42962300
C	0.22447500	2.93489100	0.83654600
C	4.37844900	3.34765600	-4.43928400
H	2.68308800	4.39385500	-3.59819700
H	4.04515300	4.22850700	-2.48974400
H	6.08090700	2.07845900	-4.88171700
H	6.11646500	2.80253200	-3.28173200
C	-0.26360900	5.66511200	1.52194900

H	0.94250800	6.13574400	-0.17945100
C	-0.54131200	3.29728100	1.97205300
O	0.34362500	1.67565600	0.53040800
H	3.77435000	2.92021600	-5.24847900
H	4.83979900	4.25493200	-4.83795200
C	-0.78000200	4.61455200	2.29968500
H	-0.45286000	6.69678000	1.78895900
H	-0.89193000	2.50150200	2.60454000
H	-1.35907500	4.84066900	3.18918100
H	4.50923900	1.88376100	-1.45395400
H	2.20138300	1.96337100	-3.40635100
H	-2.97228500	-1.75693200	2.75932900
H	-1.47280800	0.58590500	1.57596300
S	3.20199600	1.27807200	2.23454800
O	4.25357300	2.15511800	2.75127200
O	1.92667000	1.24670000	2.95670400
O	3.05688400	1.59414200	0.72465200
C	3.84200700	-0.40010300	2.25754700
C	4.84396100	-0.77383400	1.36794000
C	3.35766500	-1.30221700	3.19480500
C	5.33781900	-2.07126400	1.40148900
H	5.21316600	-0.05586100	0.64732900
C	3.87077700	-2.59508400	3.22669400
H	2.57505400	-0.98730800	3.87231000
C	4.85723300	-3.00321000	2.32651700
H	6.10384400	-2.37086100	0.69402800
H	3.48761300	-3.30374400	3.95363800
C	5.35656700	-4.42406100	2.31383800
H	4.85143000	-4.99742500	1.52954900
H	6.42979300	-4.46876400	2.11330100
H	5.16726800	-4.92203700	3.26692400