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Quantum Chemical Characterization of the Mechanism of a Supported Cobalt-based Water Oxidation Catalyst

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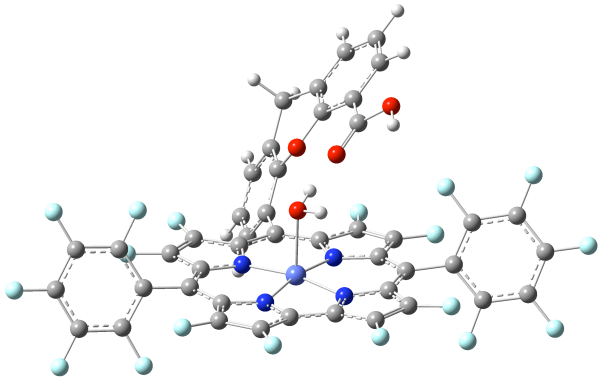
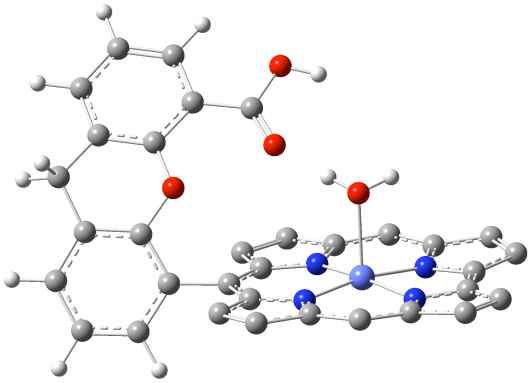
SUPPORTING INFORMATION

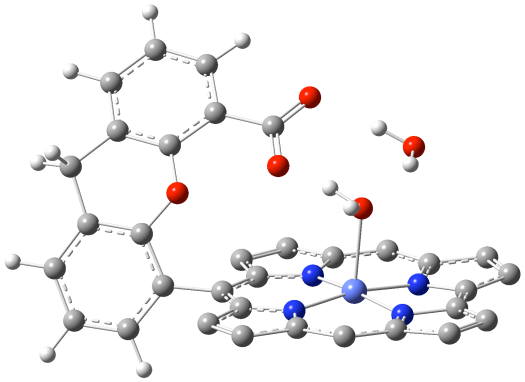
The following table lists the figures for all the structures investigated in the present study followed by the cartesian coordinates and gas phase electronic energies at M06-L level of theory. (6-31G(d) basis set on C, H, N, O and F, and Stuttgart [8s7p6d2f | 6s5p3d2f] ECP10MDF contracted pseudopotential basis on Co). C_6F_5 and F atoms are omitted for clarity.



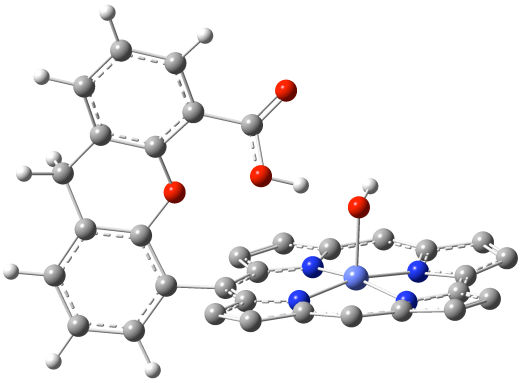
Model Compound



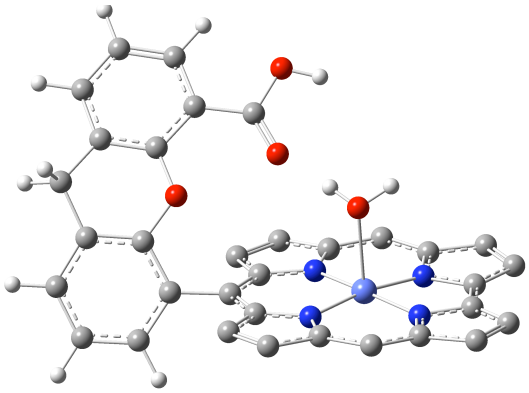
{H$_8^F$CX–CO$_2$H–Co^{III}–OH$_2$}



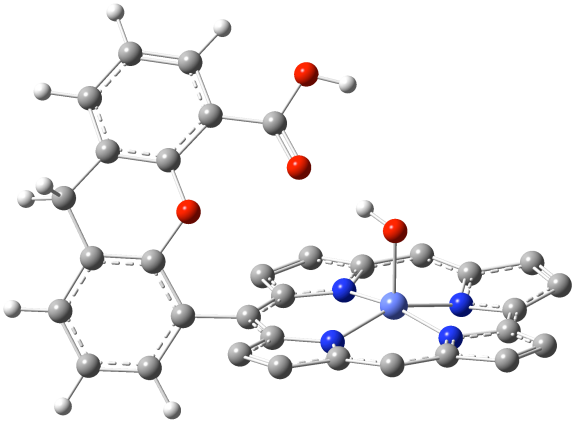
{H$_8^F$CX–CO$_2$–Co^{III}–(OH$_2$)$_2$}$^-$



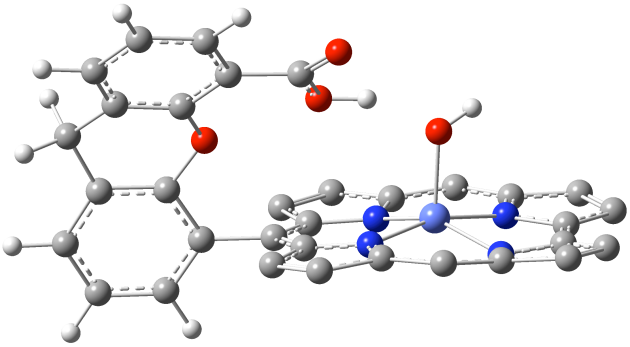
$\{H^{\beta F}CX–CO_2H–Co^{III}–OH\}^-$



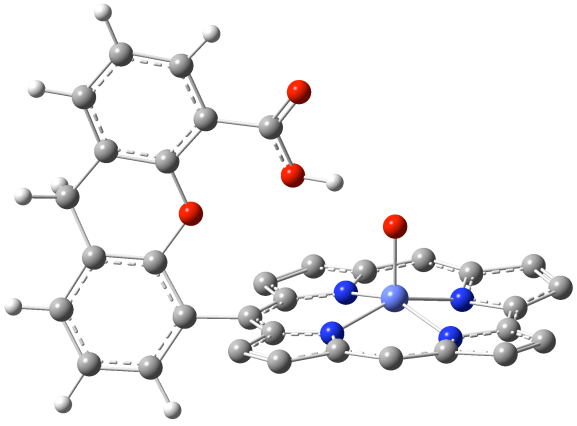
$\{H^{+\bullet\beta F}CX–CO_2H–Co^{III}–OH_2\}^+$



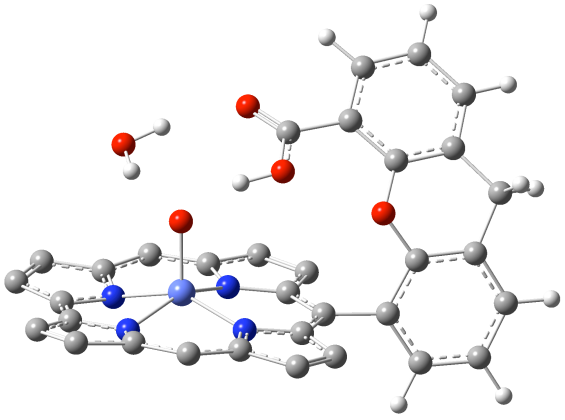
$\{H^{+\bullet\beta F}CX–CO_2H–Co^{III}–OH\}$ Conformer 1



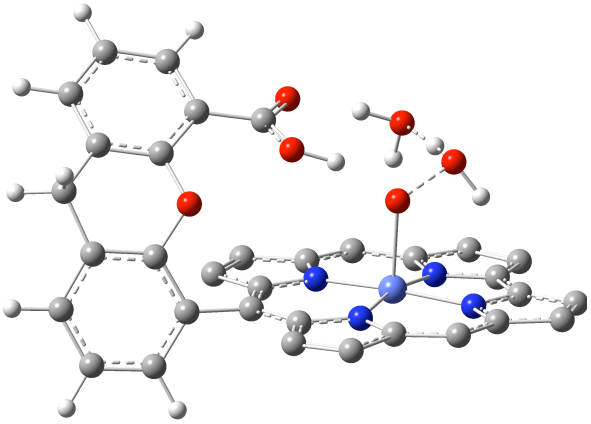
$\{H^{+\bullet\beta F}CX–CO_2H–Co^{III}–OH\}$ Conformer 2



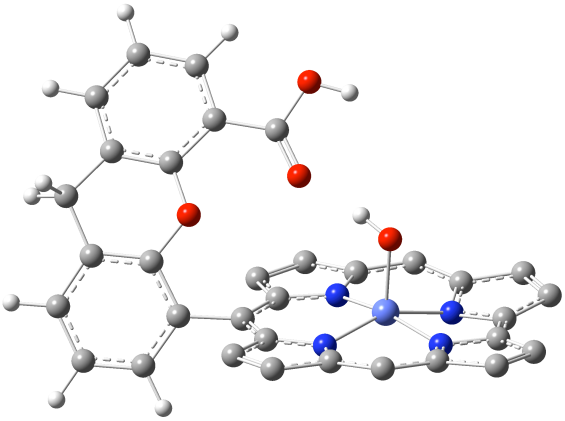
$\{H^{\beta F}CX–CO_2H–Co^{III}–O^{\bullet-}\}^-$



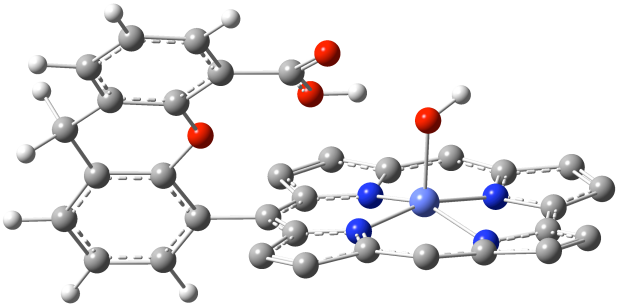
$\{H^{\beta F}CX–CO_2H–Co^{III}–O^{\bullet-}(H_2O)\}^-$



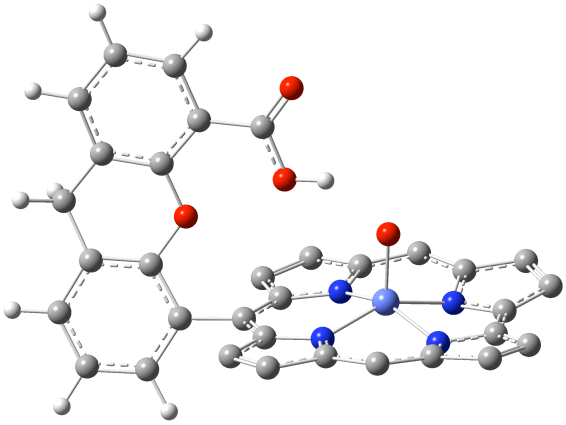
$\{H_{\beta}^{F}CX–CO_2H–Co^{III}–O^{\bullet-}\}\bullet H_2O^{\ddagger}$



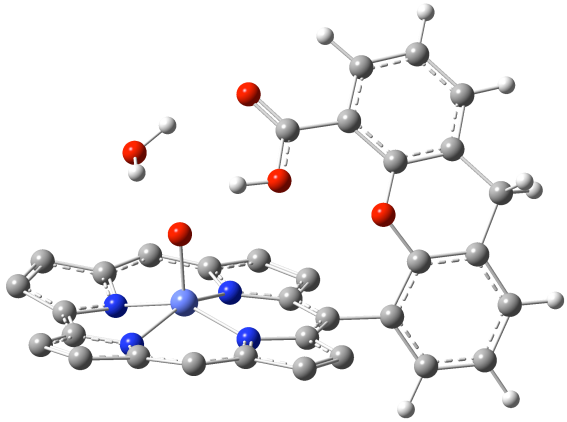
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{IV}–OH\}^{+}$ Conformer 1



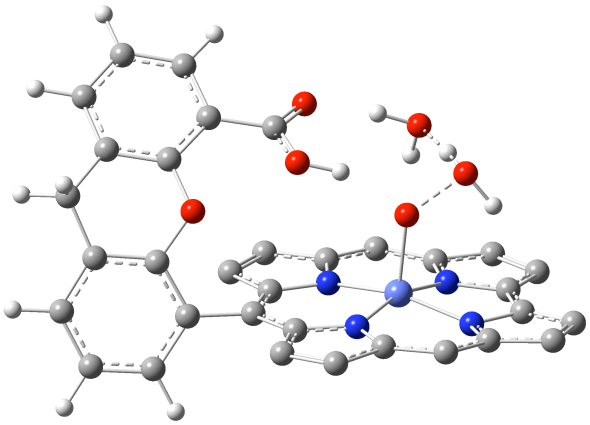
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{IV}–OH\}^{+}$ Conformer 2



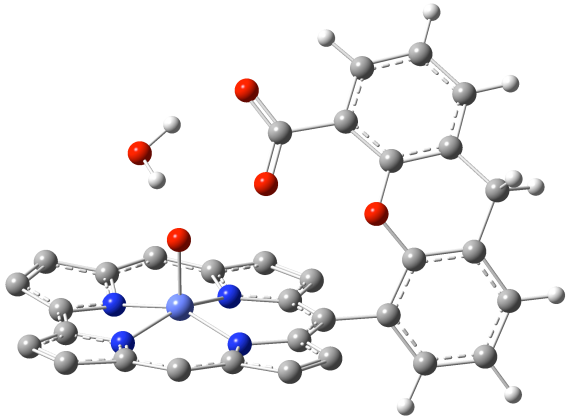
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{III}–O^{\bullet-}\}$



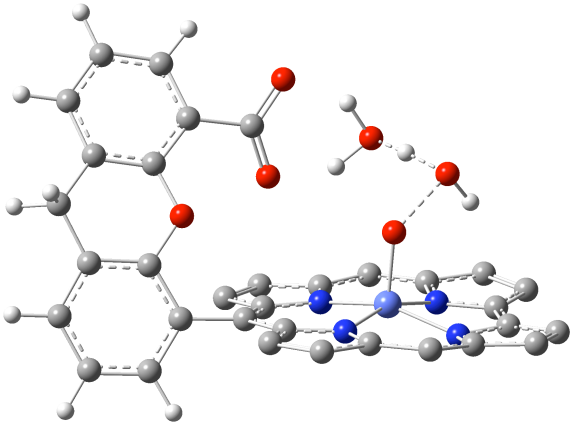
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{III}–O^{\bullet-}(H_2O)\}$



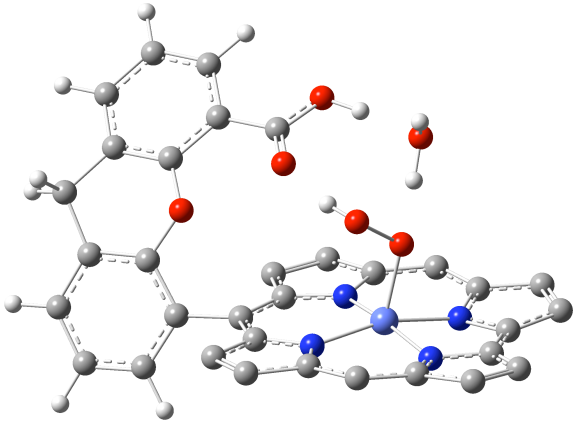
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{III}–O^{\bullet-}\}\bullet H_2O^{\ddagger}$ (triplet)



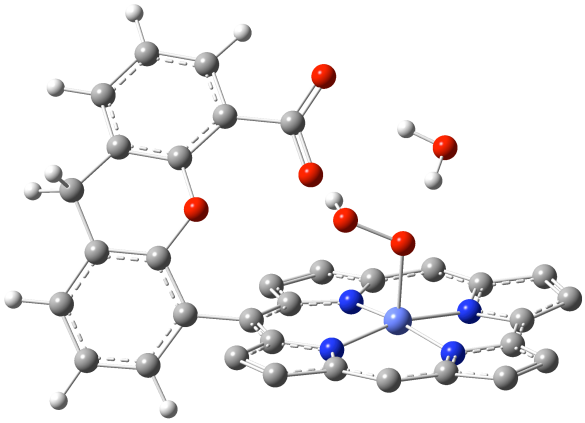
$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2–Co^{III}–O^{\bullet-}(H_2O)\}^-$ (triplet)



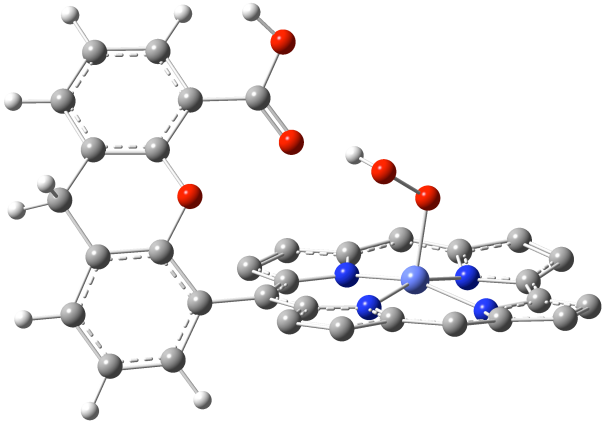
$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2–Co^{III}–O^{\bullet-}\}\bullet H_2O^{\ddagger}$ (triplet)



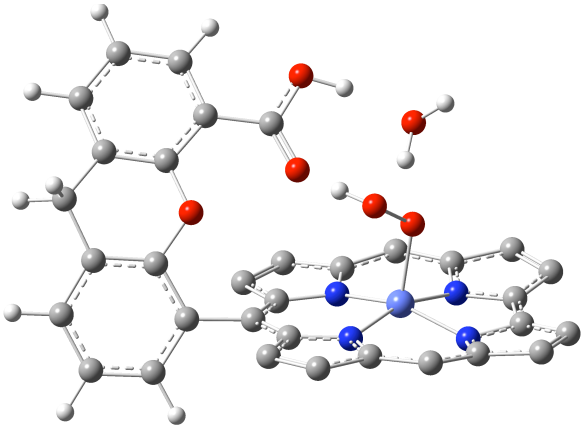
$\{H_{\beta}{}^{F}CX–CO_2H–Co^{III}–OOH(H_2O)\}^-$



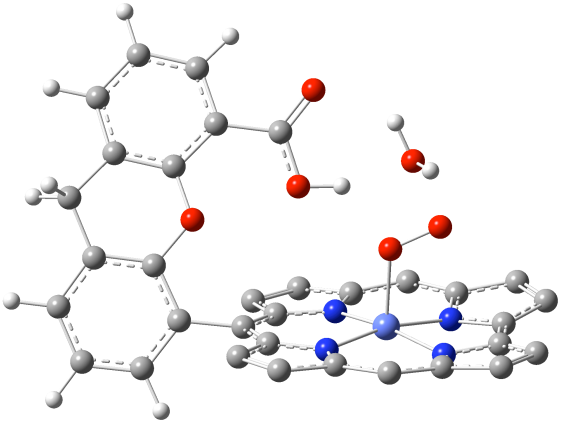
$\{H_{\beta}{}^{F}CX–CO_2H–Co^{III}–OOH(H_2O)\}^{2-}$



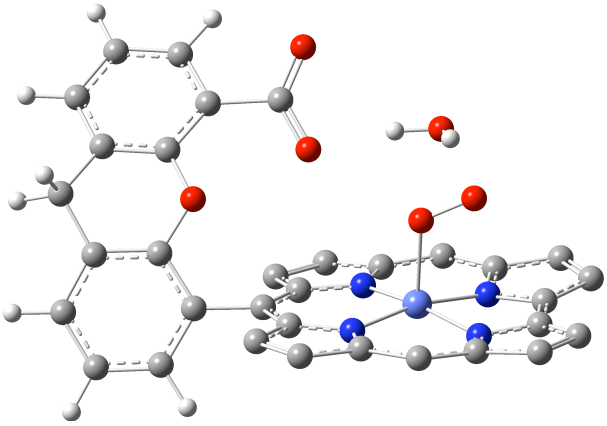
$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{III}–OOH\}$



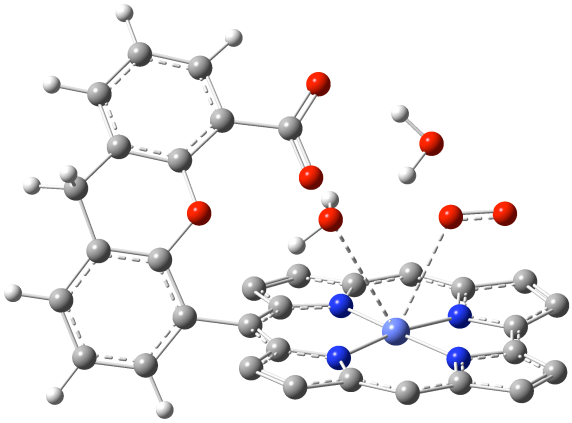
$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{III}–OOH(H_2O)\}$



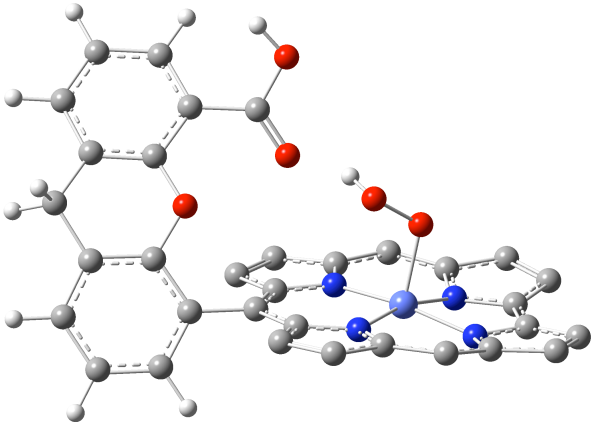
$\{H_{\beta}^{F}CX–CO_2H–Co^{III}–OO^{\bullet-}(H_2O)\}^{-}$



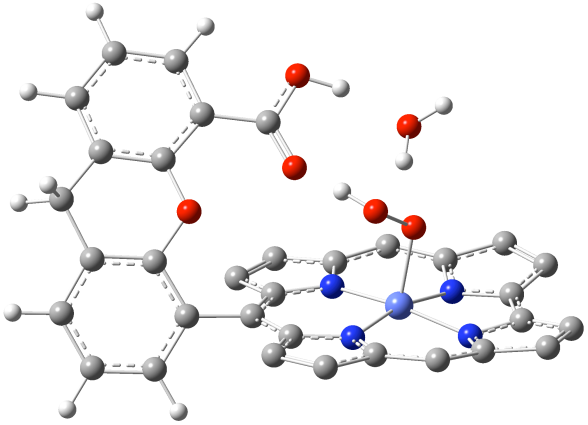
$\{H_{\beta}^{F}CX–CO_2–Co^{III}–OO^{\bullet-}(H_2O)\}^{2-}$



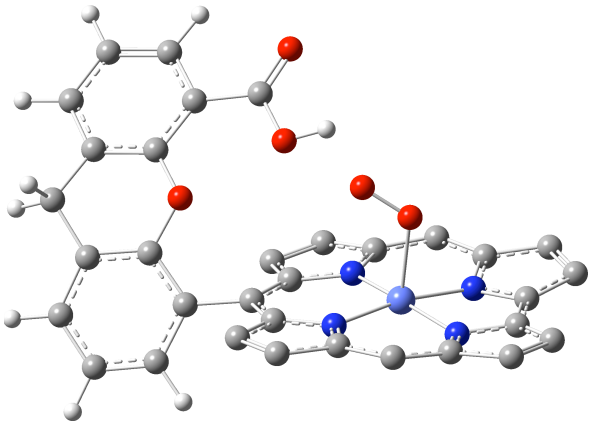
$\{H_{\beta}^{F}CX–CO_2–Co^{III}–OO^{\bullet-}\}\bullet H_2O^{\ddagger}$



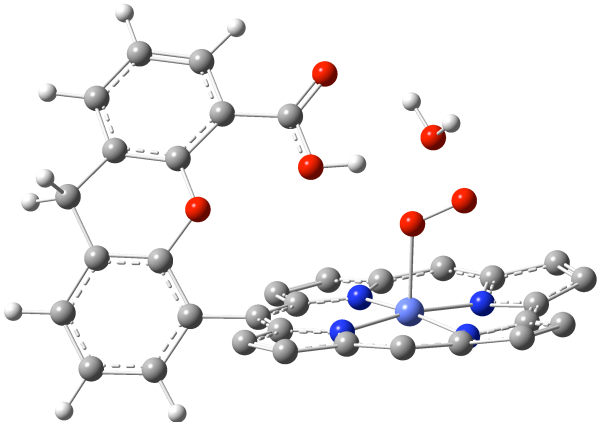
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{IV}–OOH\}^{+}$



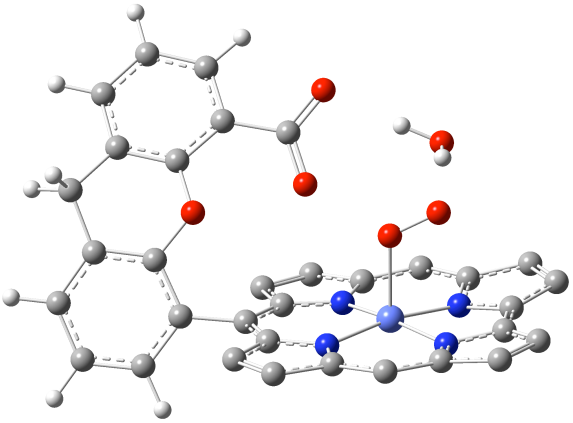
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{IV}–OOH(H_2O)\}^{+}$



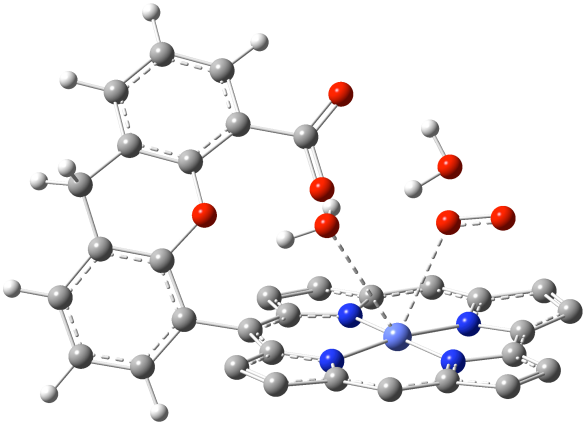
$\{H^{+\bullet}{}_{\beta}^{F}CX–CO_2H–Co^{III}–OO^{\bullet-}\}$



$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{III}–OO^{\bullet-}(H_2O)\}$



$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2–Co^{III}–OO^{\bullet-}(H_2O)\}^{-}$



$\{H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2–Co^{III}–OO^{\bullet-}\}\bullet H_2O$

Cartesian Coordinates and Energies

{$H_9^F CX–CO_2H–Co^{III}–OH_2$} (Singlet)

Energy: -4183.87627387 a.u.

C	-3.98045600	-3.08985200	0.46927100
C	-2.98414300	-4.03404000	0.54493000
C	-1.77682000	-3.39129800	0.16874400
N	-2.05621600	-2.10115700	-0.14363700
C	-0.38625000	-3.68129500	0.10492500
C	0.49969800	-4.75214600	0.37738800
N	0.35173600	-2.59727900	-0.25341600
C	1.77851400	-4.27407500	0.19220500
C	1.68504900	-2.90125800	-0.20379900
C	2.65017200	-1.92078400	-0.47023100
C	-3.38843800	-1.85295100	0.04269600
C	-3.91042000	-0.56950500	-0.12261500
C	-3.09962200	0.54048800	-0.50157100
C	-3.55188600	1.87472200	-0.74753500
N	-1.74155300	0.51925400	-0.71173400
C	-2.47108100	2.63901200	-1.06826600
C	-1.31945900	1.78809300	-1.04977200
C	0.01932800	2.15364900	-1.27850500
C	1.12015700	1.27406700	-1.19500300
C	2.49789600	1.58484200	-1.41961200
N	1.03806100	-0.05241600	-0.84933600
C	3.21976900	0.45576900	-1.17949800
C	2.31156900	-0.58378000	-0.80701500
C	0.30378800	3.57306600	-1.60802100
C	1.00491200	4.37731300	-0.70330300
C	-0.08710000	4.14072600	-2.82133500
C	1.32326900	5.70316500	-0.97582900
C	0.23072300	5.46014500	-3.12462300
H	-0.63762400	3.52792800	-3.53345200
C	2.43078700	4.27579300	1.17297900
C	0.93417200	6.23206100	-2.20594700
C	3.10002000	3.43312700	2.08781600
C	2.83418300	5.60523900	0.98999200
H	1.18577600	7.26705600	-2.43782000
C	4.19269500	3.95844800	2.79645500
C	3.93169300	6.07629100	1.70370200
C	4.61281300	5.26402300	2.60591600
H	4.71164600	3.31389400	3.49875800
H	4.24787300	7.10877500	1.55141100
C	2.04822100	6.49691800	0.06989200
O	1.37771700	3.76369600	0.47717700
C	2.69532800	2.03452300	2.31954000

O	1.74245000	1.45281300	1.82423600
O	3.52167200	1.41127500	3.19085800
H	3.21469500	0.49026300	3.23762300
Co	-0.57462600	-0.95201500	-0.37759300
O	-0.32770700	-0.49126800	1.71625500
H	0.11072100	-1.27585400	2.07887600
H	0.35945500	0.21023800	1.74697700
C	-5.35346300	-0.36276200	0.12439300
C	-6.32351500	-1.03650100	-0.62099600
C	-5.80688700	0.48897700	1.13430800
C	-7.68120000	-0.86975800	-0.38218100
C	-7.15778900	0.67255100	1.39132000
C	-8.09878400	-0.01128200	0.62861700
C	4.07527100	-2.30043800	-0.36891200
C	4.92639700	-1.69180200	0.55441200
C	4.62467500	-3.30456700	-1.16888800
C	6.25954200	-2.05031100	0.68251200
C	5.95661700	-3.68381400	-1.06052500
C	6.77652100	-3.05351900	-0.13119800
F	-4.92560000	1.15809700	1.88267300
F	-7.55854500	1.49098000	2.36473200
F	-9.39693800	0.15669100	0.86584000
F	-8.58366500	-1.52101200	-1.11615000
F	-5.95532700	-1.86588400	-1.60126300
F	4.45386300	-0.72137700	1.35250400
F	7.04255100	-1.45045200	1.57986300
F	8.05338000	-3.40790200	-0.01875200
F	6.45349200	-4.64099500	-1.84270800
F	3.86637600	-3.92465800	-2.07494200
F	-5.26707000	-3.29502100	0.74864400
F	-3.11319000	-5.30958100	0.90100800
F	0.15411100	-5.98343000	0.74566000
F	2.90154600	-4.97704400	0.35603200
F	4.54462700	0.34598200	-1.30669700
F	3.01202700	2.75713500	-1.79570300
F	-2.51118200	3.94272800	-1.33768700
F	-4.81075100	2.31331700	-0.69547800
H	5.46533500	5.65074000	3.15865200
H	2.70935600	7.23954900	-0.39781500
H	1.32317600	7.08346400	0.66083900
H	-0.06891900	5.88560800	-4.07956100

{H$_{6}$^{F}CX–CO$_2$H–Co^{III}–OH$_2$} (Triplet)

Energy: -4183.88028722 a.u.

C	-3.99448900	-3.04872700	0.51620700

C	-3.00921000	-4.00258100	0.61737000
C	-1.78790800	-3.36705700	0.30686500
N	-2.06445200	-2.03551500	0.01481400
C	-0.43167100	-3.66223900	0.23461800
C	0.44800800	-4.74573000	0.44539300
N	0.33637100	-2.55754300	-0.11810700
C	1.72376600	-4.27750600	0.22835400
C	1.64802500	-2.88901100	-0.13355900
C	2.63846900	-1.93189000	-0.44046200
C	-3.38907000	-1.79935500	0.13356000
C	-3.92875700	-0.51498800	-0.06838600
C	-3.11223100	0.56644300	-0.43119300
C	-3.54161800	1.90491100	-0.68280100
N	-1.73288200	0.53946600	-0.63235900
C	-2.45107000	2.65518500	-0.99666300
C	-1.29973800	1.79769800	-0.97667800
C	0.03148600	2.16011400	-1.23270300
C	1.10710000	1.26253300	-1.15594100
C	2.48924300	1.54905900	-1.40918500
N	1.02125600	-0.05755000	-0.79221000
C	3.20635800	0.41863800	-1.17129700
C	2.30241500	-0.61248900	-0.77158300
C	0.32524800	3.57528100	-1.57876900
C	1.03962100	4.38715000	-0.69052000
C	-0.07848400	4.13793600	-2.79017600
C	1.34387300	5.71500100	-0.97188800
C	0.22369300	5.45909400	-3.10323800
H	-0.63517800	3.51924200	-3.49272000
C	2.51465700	4.30267400	1.15018800
C	0.93240200	6.23953100	-2.19660700
C	3.22440000	3.46711800	2.04151400
C	2.89653400	5.63782500	0.95960300
H	1.17257700	7.27615300	-2.43346300
C	4.33032400	4.00564800	2.71924000
C	4.00735600	6.12246900	1.64275300
C	4.72575900	5.31785200	2.52261100
H	4.87910400	3.36534800	3.40256200
H	4.30467200	7.15955700	1.48367900
C	2.07534700	6.51887000	0.06122100
O	1.44937800	3.77865100	0.48329500
C	2.85152600	2.06069300	2.27797900
O	1.88066200	1.47046400	1.83012000
O	3.73462400	1.43765000	3.09205700
H	3.44426500	0.51126800	3.14062100
Co	-0.58552800	-0.93627700	-0.29856800
O	-0.29203600	-0.37235600	1.82800100

H	0.13525900	-1.13566400	2.24369400
H	0.40691600	0.31647100	1.80952700
C	-5.38371200	-0.32592900	0.11935300
C	-6.30767000	-1.00366700	-0.67822000
C	-5.89818800	0.50313000	1.11824100
C	-7.67773500	-0.86689500	-0.49995600
C	-7.26353400	0.66410700	1.31091500
C	-8.15653400	-0.02609800	0.49828500
C	4.05661100	-2.34354700	-0.38561200
C	4.95033600	-1.76319500	0.51509800
C	4.55940400	-3.35261300	-1.20880600
C	6.27881400	-2.15251000	0.59843400
C	5.88276100	-3.76913100	-1.14083400
C	6.74611900	-3.16416400	-0.23428500
F	-5.06533100	1.17800700	1.91595600
F	-7.72366900	1.46640600	2.27219600
F	-9.46777400	0.11804500	0.67559300
F	-8.53386900	-1.52785500	-1.28024800
F	-5.87630400	-1.81978400	-1.64618100
F	4.52747600	-0.78307400	1.33063700
F	7.10459400	-1.57527700	1.47261300
F	8.01725200	-3.55076200	-0.16226300
F	6.33112900	-4.73511800	-1.94222100
F	3.75573500	-3.94798700	-2.09444000
F	-5.28805700	-3.25061100	0.74584200
F	-3.16380900	-5.28110100	0.94716700
F	0.10012100	-5.98033800	0.79510200
F	2.83945200	-4.99521600	0.34688700
F	4.52577200	0.29641800	-1.32468800
F	3.00482700	2.70898400	-1.80833600
F	-2.47684500	3.95689400	-1.26372600
F	-4.79406700	2.35717700	-0.63828200
H	5.58823700	5.71499100	3.05204600
H	2.71257700	7.27568000	-0.41673900
H	1.35194200	7.08925800	0.66988400
H	-0.09209200	5.87881600	-4.05564500

$\{H_6{}^{F}CX–CO_2–Co^{III}–(OH_2)_2\}^-$ (Triplet)

Energy: -4183.88028722 a.u.

C	-3.85475300	-3.10048400	0.46496400
C	-2.82681200	-4.01205800	0.55611700
C	-1.64250100	-3.33724300	0.19835500
N	-1.98571700	-2.02740700	-0.11719500
C	-0.27443200	-3.57439900	0.11148300
C	0.65394400	-4.60677600	0.37333500

N	0.43980600	-2.45928100	-0.29222300
C	1.90537100	-4.08931400	0.14711800
C	1.76261900	-2.72166000	-0.27090100
C	2.70952200	-1.71956500	-0.56064100
C	-3.31763900	-1.83925700	0.04192300
C	-3.91087100	-0.57521000	-0.14979900
C	-3.14231800	0.54431200	-0.51640700
C	-3.63247200	1.85429800	-0.80861800
N	-1.76363600	0.58174400	-0.68716500
C	-2.57544500	2.64878400	-1.12910700
C	-1.38647000	1.85387600	-1.05997400
C	-0.07525600	2.27392900	-1.30398400
C	1.03786400	1.41929600	-1.21264600
C	2.40653500	1.76998600	-1.44949900
N	1.00919300	0.08990400	-0.87163200
C	3.17114200	0.66567900	-1.23452600
C	2.31592600	-0.41000100	-0.85754100
C	0.19840900	3.71073100	-1.58833800
C	0.84213800	4.47007900	-0.60151500
C	-0.05950800	4.32220100	-2.81382000
C	1.27066700	5.77767800	-0.81862500
C	0.34199300	5.63511500	-3.05238000
H	-0.56231900	3.74951700	-3.59275200
C	2.15196900	4.19148100	1.33382400
C	1.01668500	6.34879200	-2.06469500
C	2.71147700	3.22982900	2.19280000
C	2.67468700	5.48482800	1.20972400
H	1.35235900	7.36885000	-2.25853500
C	3.83920600	3.61540600	2.92180400
C	3.80363500	5.81801900	1.95503700
C	4.38663600	4.88880100	2.81221500
H	4.27635200	2.85647200	3.56769200
H	4.22196400	6.82185400	1.85877700
C	1.97751300	6.47418000	0.31031800
O	1.05886600	3.82858400	0.58151300
C	2.18987600	1.80753700	2.36844900
O	2.91324100	1.02544900	3.02137400
O	1.06169500	1.55902400	1.84151900
Co	-0.54500200	-0.86121300	-0.37788100
C	-5.36900100	-0.44586300	0.04820400
C	-6.27590500	-1.19015300	-0.71064600
C	-5.91382800	0.39668900	1.02099500
C	-7.64836000	-1.10844300	-0.51694400
C	-7.28263500	0.50682600	1.22463500
C	-8.15420300	-0.25281400	0.45339100
C	4.14014400	-2.08024300	-0.50846600

C	5.03663400	-1.46173100	0.36951400
C	4.64914800	-3.10006500	-1.31528500
C	6.37061600	-1.84668100	0.43875300
C	5.97506600	-3.50406200	-1.25639100
C	6.84003600	-2.87216700	-0.37247400
F	-5.10760400	1.13463200	1.79072100
F	-7.76933000	1.32420200	2.16444900
F	-9.47292600	-0.16054600	0.64337900
F	-8.48689100	-1.83478300	-1.26413600
F	-5.83044400	-2.01670100	-1.66367900
F	4.63872700	-0.46407300	1.14710900
F	7.21036300	-1.23845700	1.28141800
F	8.12180900	-3.24483600	-0.30828700
F	6.42634800	-4.48507500	-2.04835100
F	3.84542900	-3.72804000	-2.18501800
F	-5.13727300	-3.35747100	0.73960200
F	-2.93037900	-5.29259200	0.91671400
F	0.35841700	-5.84545600	0.77274600
F	3.05006400	-4.75221700	0.30187300
F	4.49301000	0.60339000	-1.41002500
F	2.88055800	2.95411400	-1.83516500
F	-2.65727200	3.93756400	-1.45817900
F	-4.91439500	2.24119000	-0.80404400
H	0.14416700	6.09630800	-4.01838300
H	1.24687700	7.05817900	0.89943900
H	2.69376500	7.21278900	-0.07872800
H	5.27016600	5.15813500	3.38953000
O	2.30704900	-1.71597800	2.52116900
H	1.34175600	-1.64754000	2.46863400
H	2.56957300	-0.78851200	2.72101300
O	-0.29386600	-0.57950900	1.75732400
H	0.34230300	0.24211000	1.84585700
H	-1.14148800	-0.24528000	2.08594700

{H$_6^F$CX–CO$_2$H–Co^{III}–OH}$^-$ (Singlet)

Energy: -4183.37719258 a.u.

C	-2.93887000	-3.76265900	0.43874000
C	-1.77965400	-4.48766800	0.59560600
C	-0.70976900	-3.65898700	0.18670400
N	-1.23890800	-2.47606600	-0.24926200
C	0.69518900	-3.65340100	0.21166800
C	1.76374700	-4.48877500	0.60903800
N	1.22778700	-2.45944000	-0.19232600
C	2.92572600	-3.76357800	0.46487900
C	2.58586500	-2.46821400	-0.03220300

C	3.35383300	-1.32684200	-0.30857900
C	-2.59304000	-2.47451600	-0.07408700
C	-3.35553400	-1.32752100	-0.33326900
C	-2.76726500	-0.12177700	-0.76792700
C	-3.45458000	1.07214100	-1.14689300
N	-1.41491900	0.11429500	-0.94380500
C	-2.53357200	2.00264400	-1.51624400
C	-1.23864700	1.41175300	-1.38252300
C	0.00048200	2.03085700	-1.59361200
C	1.23368300	1.41089100	-1.35393700
C	2.52770900	1.98863600	-1.53013100
N	1.40900700	0.12119400	-0.89555900
C	3.45249600	1.06151600	-1.16096800
C	2.76530100	-0.12201600	-0.74768400
C	-0.00371000	3.47601300	-1.96053900
C	0.20902900	4.42018000	-0.94934200
C	-0.26510100	3.95050000	-3.24335900
C	0.13343200	5.79403300	-1.16479100
C	-0.34047600	5.31952500	-3.49380700
H	-0.44124900	3.23242900	-4.04352500
C	0.19700200	4.65142300	1.38970600
C	-0.15349000	6.23067500	-2.45834600
C	0.00868500	3.95561300	2.59158600
C	0.13732500	6.04548300	1.31654800
H	-0.22376600	7.30221800	-2.65163100
C	-0.18432300	4.70012300	3.75475300
C	-0.11744500	6.75052800	2.49227900
C	-0.26513300	6.08833700	3.70889300
H	-0.29025400	4.15744700	4.69246400
H	-0.17943900	7.83927500	2.44987400
C	0.39140200	6.72034900	-0.00675500
O	0.49450400	3.90267400	0.28547900
C	0.02835000	2.45789900	2.67941600
O	0.52776600	1.88050500	3.63231500
O	-0.57583000	1.88179700	1.65449300
H	-0.42207600	0.86679300	1.65833700
Co	-0.00979000	-1.05352400	-0.39945600
O	-0.09909900	-0.66291900	1.42195800
H	0.81178100	-0.76463600	1.74335900
C	-4.81731400	-1.39557800	-0.12184200
C	-5.61295500	-2.30155000	-0.82693900
C	-5.46947600	-0.58178800	0.80839100
C	-6.98269700	-2.40183900	-0.62158400
C	-6.83889600	-0.65763200	1.02488100
C	-7.59856600	-1.57413800	0.30830700
C	4.81804700	-1.40286900	-0.12126800

C	5.49174900	-0.57694900	0.78255000
C	5.59619800	-2.32568800	-0.82457300
C	6.86392500	-0.65695100	0.97759700
C	6.96850900	-2.43148800	-0.63956900
C	7.60526200	-1.59170100	0.26520100
F	-4.77573100	0.30923000	1.51941500
F	-7.43237800	0.13534700	1.92398700
F	-8.91681800	-1.65703100	0.51197000
F	-7.71491700	-3.27823100	-1.31984100
F	-5.06186700	-3.10786700	-1.74080300
F	4.81393700	0.33053200	1.49023500
F	7.47736000	0.14802800	1.85196900
F	8.92585700	-1.68034000	0.44889300
F	7.68354300	-3.32412200	-1.33456600
F	5.02556000	-3.14162700	-1.71719100
F	-4.17376800	-4.20730600	0.71437600
F	-1.67965500	-5.74138900	1.04797500
F	1.66318600	-5.75024700	1.03859700
F	4.15938900	-4.21444900	0.73740500
F	4.78099800	1.22567700	-1.22493200
F	2.79679700	3.21477200	-1.99018900
F	-2.81792000	3.24036500	-1.93277100
F	-4.78242800	1.24868700	-1.17863800
H	-0.55755100	5.67636600	-4.49900300
H	-0.22156100	7.62977800	-0.09681700
H	1.43797700	7.07246800	-0.04393300
H	-0.44391500	6.65644300	4.62002800

$\{H_9^F CX–CO_2H–Co^{III}–OH\}^-$ (Triplet)

Energy: -4183.37719258 a.u.

C	-3.13970600	-3.64646900	0.50992200
C	-2.00836500	-4.41432700	0.69556800
C	-0.90474100	-3.62526200	0.32216200
N	-1.38642200	-2.41714700	-0.13022500
C	0.49594400	-3.66758700	0.39162100
C	1.53359300	-4.58560200	0.67303600
N	1.07643400	-2.46986700	0.07730700
C	2.72470000	-3.91239800	0.51593100
C	2.43220500	-2.57102900	0.11254800
C	3.24706100	-1.48634900	-0.25469300
C	-2.74473500	-2.37126200	0.01050900
C	-3.47482000	-1.19940800	-0.25248300
C	-2.83958900	-0.00582500	-0.64468700
C	-3.48068600	1.19175500	-1.09136100
N	-1.47813800	0.20706800	-0.74329200

C	-2.52165500	2.08662200	-1.44964000
C	-1.24678100	1.46652700	-1.24784300
C	0.01585800	2.01505400	-1.51358100
C	1.21911400	1.32435500	-1.31252300
C	2.53425600	1.82681400	-1.54076200
N	1.34765800	0.03533200	-0.83487500
C	3.42438400	0.86279800	-1.17477300
C	2.69749000	-0.27507400	-0.71474600
C	0.08599200	3.44060000	-1.94486000
C	0.43891700	4.41707000	-1.00432300
C	-0.21248100	3.86672200	-3.23708200
C	0.47279200	5.77724600	-1.30290900
C	-0.18890100	5.22039200	-3.56657000
H	-0.49451900	3.12296100	-3.98151500
C	0.64655700	4.78148000	1.31387400
C	0.14346900	6.16602200	-2.60145700
C	0.51633400	4.18601800	2.57841500
C	0.70566000	6.16926300	1.15016400
H	0.15828400	7.22722500	-2.85493700
C	0.49560000	5.02275800	3.69487800
C	0.62709000	6.96976800	2.28867600
C	0.53411500	6.40583700	3.55842900
H	0.43024700	4.54887200	4.67259400
H	0.65977700	8.05433700	2.17084700
C	0.89653100	6.74219600	-0.22975300
O	0.76082300	3.94487800	0.23917300
C	0.40589600	2.70564100	2.80625400
O	0.81301100	2.19186000	3.83742700
Co	-0.11411500	-1.00747500	-0.15178900
O	-0.17876800	-0.48656400	1.70708400
H	0.50631900	-0.96181000	2.20090600
C	-4.94370800	-1.23583400	-0.10511900
C	-5.72996200	-2.13491300	-0.83097500
C	-5.61937400	-0.39130400	0.78109900
C	-7.10920700	-2.20149900	-0.68478800
C	-6.99837500	-0.43213400	0.93649600
C	-7.74690100	-1.34406000	0.20256300
C	4.71495300	-1.64491700	-0.16422900
C	5.48949500	-0.86809000	0.70088500
C	5.39260500	-2.60002400	-0.92480300
C	6.86486600	-1.02700000	0.80682400
C	6.76540800	-2.78660900	-0.82716600
C	7.50482600	-1.99466400	0.04187200
F	-4.93890300	0.49664500	1.50905600
F	-7.61256700	0.38998900	1.79462900
F	-9.07442700	-1.39378200	0.34886900

F	-7.82974000	-3.07273000	-1.40149800
F	-5.15943200	-2.96740600	-1.70917100
F	4.90992900	0.07115600	1.45249900
F	7.57786600	-0.26605500	1.64447500
F	8.82711700	-2.16124300	0.13974500
F	7.38285500	-3.71110900	-1.57199800
F	4.72036900	-3.36944300	-1.78756100
O	-0.20094300	2.07897300	1.81679400
H	-0.18268500	1.05904800	1.93511400
F	-4.38998000	-4.04610100	0.77677200
F	-1.96458900	-5.66487600	1.16476900
F	1.38068600	-5.86885700	1.01402800
F	3.94427200	-4.44772900	0.67130800
F	4.75568100	0.96967600	-1.27158300
F	2.85915200	3.02737500	-2.02760000
F	-2.75682000	3.31071200	-1.93046600
F	-4.80077700	1.39357600	-1.19561800
H	-0.43695700	5.53823700	-4.57765100
H	0.34936100	7.69207500	-0.32780700
H	1.95970100	7.00667200	-0.37325000
H	0.49128100	7.04536900	4.43825200

$\{H^{+\bullet,F}CX–CO_2H–Co^{III}–OH_2\}^+$ (doublet)

Energy: -4183.64991740 a.u.

C	-4.02017700	-3.03637000	0.46133800
C	-3.03374500	-3.99125200	0.54624600
C	-1.81911000	-3.34770700	0.21756000
N	-2.08673200	-2.02698500	-0.07372800
C	-0.45157900	-3.64920600	0.15067500
C	0.41321100	-4.74116700	0.38559300
N	0.31229900	-2.55355000	-0.19496800
C	1.69573100	-4.27861500	0.18935200
C	1.62519100	-2.88939400	-0.18184000
C	2.62015300	-1.93042100	-0.45388400
C	-3.41271700	-1.78628900	0.06864300
C	-3.94277600	-0.49710600	-0.09119300
C	-3.11448900	0.60006700	-0.45049600
C	-3.55048900	1.93553200	-0.69128100
N	-1.74685600	0.56114900	-0.67263900
C	-2.45791700	2.68648300	-1.01482200
C	-1.31457800	1.82016300	-1.01195600
C	0.02789200	2.18375700	-1.23690900
C	1.11298000	1.27684000	-1.15362000
C	2.49155700	1.55761000	-1.42441300
N	1.01506400	-0.03719600	-0.79558500

C	3.20361300	0.41952200	-1.18761000
C	2.29118100	-0.59628700	-0.77962200
C	0.33340200	3.59123900	-1.56579900
C	1.12962600	4.35209900	-0.69522000
C	-0.12011600	4.19118700	-2.74444100
C	1.48997500	5.66539700	-0.97666900
C	0.24148000	5.49530500	-3.05332400
H	-0.73811200	3.61332100	-3.42947800
C	2.60826100	4.18796800	1.14273100
C	1.04203800	6.22160100	-2.17392100
C	3.23730900	3.32754700	2.07029500
C	3.06253500	5.49606000	0.94308900
H	1.32387900	7.24593500	-2.41566800
C	4.35108200	3.81564100	2.77341400
C	4.17987800	5.92889700	1.65295900
C	4.82635900	5.09952200	2.56384800
H	4.84149200	3.16245300	3.48779300
H	4.53887100	6.94515400	1.49076200
C	2.31970900	6.41963200	0.01866800
O	1.53051400	3.70510100	0.45043600
C	2.77176700	1.95488100	2.33088400
O	1.83458300	1.37917900	1.78912800
O	3.51342100	1.34470900	3.27647100
H	3.17357200	0.43767900	3.35551900
Co	-0.59785600	-0.91738500	-0.32158600
O	-0.36913200	-0.34914900	1.75497000
H	-0.15385500	-1.09806000	2.33015100
H	0.40106100	0.26295200	1.82105900
C	-5.38579000	-0.29320700	0.12582200
C	-6.33449900	-0.99123700	-0.62904000
C	-5.86266400	0.57531800	1.11353500
C	-7.69664000	-0.82884700	-0.42365700
C	-7.21896300	0.74980900	1.34155500
C	-8.13865100	0.04506600	0.56716300
C	4.03478600	-2.33540000	-0.37590100
C	4.91840000	-1.71982100	0.51526500
C	4.54282900	-3.36630100	-1.17219000
C	6.24549500	-2.10432800	0.61815100
C	5.86939900	-3.76699300	-1.09270700
C	6.72231500	-3.13322300	-0.19234000
F	-4.99480800	1.25557000	1.86597000
F	-7.64430600	1.57479500	2.29109300
F	-9.43522300	0.20622400	0.77352400
F	-8.57576000	-1.49416500	-1.16270100
F	-5.92865400	-1.83135600	-1.58419500
F	4.47691200	-0.72744200	1.30270300

F	7.05911000	-1.50681700	1.48175100
F	7.98812700	-3.50711600	-0.10459600
F	6.32713700	-4.74139600	-1.86798200
F	3.74227700	-3.97965400	-2.04520200
F	-5.29967100	-3.23036600	0.71806700
F	-3.17567100	-5.26311300	0.87467400
F	0.04929100	-5.96318400	0.73299600
F	2.80011900	-4.99034500	0.33567500
F	4.51272300	0.28861600	-1.35407800
F	3.01292600	2.70238700	-1.83576300
F	-2.48431600	3.98307500	-1.26530400
F	-4.79357500	2.39061200	-0.64047600
H	-0.09320600	5.94605700	-3.98397500
H	1.67073300	7.08560900	0.61231800
H	3.02323400	7.08767600	-0.49642400
H	5.69366100	5.45721600	3.11220800

$\{H^{+\bullet,F}CX–CO_2H–Co^{III}–OH_2\}^+$ (quartet)

Energy: -4183.65022203 a.u.

C	-4.03288700	-3.02453800	0.48237700
C	-3.04763500	-3.98400400	0.57186500
C	-1.83224700	-3.34312200	0.25379300
N	-2.09532800	-2.01831100	-0.03374800
C	-0.46292000	-3.64663000	0.18724500
C	0.39569700	-4.74189800	0.41345700
N	0.30510900	-2.55135600	-0.15839600
C	1.68075500	-4.28324600	0.21010300
C	1.61523000	-2.89162200	-0.15910400
C	2.61349100	-1.94117600	-0.44244600
C	-3.42064100	-1.77687100	0.09354100
C	-3.94811300	-0.48591300	-0.08149100
C	-3.11746400	0.60565100	-0.43954700
C	-3.54763600	1.94159300	-0.68529900
N	-1.74503900	0.56575200	-0.64760500
C	-2.45020900	2.69140000	-0.99661500
C	-1.30908300	1.82338900	-0.98689200
C	0.03530500	2.18304300	-1.21631300
C	1.11527300	1.27409700	-1.13489100
C	2.49223500	1.54726100	-1.41801300
N	1.01591100	-0.03977300	-0.77044500
C	3.20030200	0.40385400	-1.18975700
C	2.28626800	-0.60534000	-0.76993500
C	0.34227300	3.58922800	-1.55150600
C	1.14200400	4.35378800	-0.68739300
C	-0.11498800	4.18411600	-2.73126300

C	1.49810000	5.66712200	-0.97514400
C	0.24354200	5.48743700	-3.04695300
H	-0.73507900	3.60293000	-3.41165000
C	2.63619000	4.19828400	1.13854800
C	1.04532100	6.21845300	-2.17275500
C	3.27861500	3.34048700	2.05919100
C	3.08428100	5.50763300	0.93326900
H	1.32435300	7.24254800	-2.41875200
C	4.39800800	3.83289700	2.75021900
C	4.20780600	5.94480900	1.63058000
C	4.86666100	5.11829600	2.53514700
H	4.89817700	3.18147600	3.45946300
H	4.56166600	6.96209700	1.46359500
C	2.32825800	6.42700500	0.01552100
O	1.55213100	3.71199900	0.45813000
C	2.82114200	1.96574000	2.32452600
O	1.87896500	1.38682000	1.79618100
O	3.57833600	1.35676400	3.25917100
H	3.23962400	0.44959800	3.34230200
Co	-0.60584200	-0.92086900	-0.32231800
O	-0.37608500	-0.29884700	1.77687000
H	-0.17506100	-1.03112800	2.37744200
H	0.40308500	0.30065800	1.82909500
C	-5.39317400	-0.28167500	0.12148800
C	-6.33373900	-0.98486500	-0.63877800
C	-5.88036300	0.59094100	1.10066200
C	-7.69791600	-0.82371800	-0.44713400
C	-7.23917700	0.76407300	1.31505400
C	-8.15042100	0.05429500	0.53532200
C	4.02675200	-2.35369700	-0.37894800
C	4.92312500	-1.74029800	0.50092300
C	4.52162100	-3.38804200	-1.17884900
C	6.24975800	-2.13026100	0.58945200
C	5.84711700	-3.79483800	-1.11323600
C	6.71287300	-3.16316300	-0.22376900
F	-5.02106300	1.27559600	1.85837900
F	-7.67488800	1.59279200	2.25651300
F	-9.44907600	0.21432500	0.72853300
F	-8.56910900	-1.49379000	-1.19116500
F	-5.91728500	-1.82882700	-1.58613400
F	4.49535900	-0.74340700	1.28996300
F	7.07582500	-1.53409400	1.44203000
F	7.97777900	-3.54305500	-0.14897900
F	6.29150100	-4.77326200	-1.89136400
F	3.70829800	-4.00056600	-2.04122500
F	-5.31440100	-3.21916600	0.72720100

F	-3.19768700	-5.25522900	0.89920500
F	0.03150100	-5.96343100	0.76103100
F	2.78018800	-5.00078200	0.34882000
F	4.50685900	0.26607300	-1.36865000
F	3.01629800	2.68820100	-1.83494800
F	-2.47370300	3.98845600	-1.24594900
F	-4.78979600	2.39973300	-0.64492700
H	-0.09508300	5.93396900	-3.97822700
H	1.67751800	7.08655800	0.61446300
H	3.02284300	7.10156700	-0.50311300
H	5.73861600	5.47919700	3.07397600

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OH$} Conformer 1 (doublet)

Energy: -4183.24482007 a.u.

C	-3.99184700	-3.08165600	0.41014800
C	-3.00825200	-4.04073500	0.41398700
C	-1.79597900	-3.39138300	0.06559000
N	-2.06383000	-2.07879700	-0.15687100
C	-0.42767000	-3.68612900	-0.05655300
C	0.45315200	-4.74025900	0.26996100
N	0.31539100	-2.60861400	-0.46229900
C	1.73369700	-4.26212500	0.11130400
C	1.65479000	-2.90390800	-0.31727700
C	2.63755200	-1.93172400	-0.49752500
C	-3.39254900	-1.83169200	0.04663500
C	-3.91088600	-0.55023500	-0.11772300
C	-3.09136400	0.53183300	-0.52128100
C	-3.51880000	1.87757600	-0.71557500
N	-1.73491200	0.48300800	-0.80039000
C	-2.43603400	2.62969400	-1.05927100
C	-1.29991600	1.76861700	-1.09701700
C	0.03247400	2.14591600	-1.31093500
C	1.12367400	1.26753400	-1.20753300
C	2.49867000	1.56421900	-1.45201200
N	1.03875200	-0.05360900	-0.83267600
C	3.21686200	0.43736200	-1.19388900
C	2.30762600	-0.59024100	-0.80253200
C	0.32214000	3.56505300	-1.63508900
C	1.04432100	4.35601800	-0.73342700
C	-0.07299300	4.14115500	-2.84294700
C	1.38846300	5.67486200	-1.01012000
C	0.26507600	5.45535900	-3.14708800
H	-0.63967900	3.53871400	-3.55141600
C	2.46390200	4.23166700	1.14832600
C	0.99576100	6.21123900	-2.23603000

C	3.09374100	3.38216000	2.08350000
C	2.89775700	5.54990200	0.96081900
H	1.26630600	7.24075900	-2.47113300
C	4.18233700	3.88876400	2.80928400
C	3.99401300	6.00177200	1.68992100
C	4.63854600	5.18217200	2.61173000
H	4.67012200	3.23886600	3.52906600
H	4.33695800	7.02531100	1.53492600
C	2.14484000	6.45435300	0.02475500
O	1.40720600	3.73611000	0.44255800
C	2.64677900	1.99311200	2.31339600
O	1.74607500	1.41059000	1.73454600
O	3.36916800	1.38598100	3.28411000
H	3.02987900	0.47511400	3.32970100
Co	-0.56009500	-0.93664900	-0.27410600
O	-0.36991500	-0.64448300	1.49813300
H	0.36314800	0.00029400	1.59156500
C	-5.34694300	-0.32727400	0.16059500
C	-6.33679600	-0.95759400	-0.59492900
C	-5.76880100	0.49118400	1.20989400
C	-7.68803800	-0.78280600	-0.32648900
C	-7.11302900	0.68315800	1.49610000
C	-8.07577800	0.04140200	0.72403100
C	4.05556900	-2.30707400	-0.33343800
C	4.86924300	-1.67697300	0.61112900
C	4.64272000	-3.31502200	-1.10237400
C	6.20004400	-2.02341500	0.78951200
C	5.97261000	-3.68125700	-0.94233000
C	6.75366500	-3.03228800	0.00761900
F	-4.86434500	1.12205500	1.96266700
F	-7.48653100	1.47141500	2.50403500
F	-9.36709200	0.21758500	0.98996500
F	-8.61183500	-1.39313700	-1.06874300
F	-5.99236500	-1.75462200	-1.61054700
F	4.36473800	-0.70027200	1.37767300
F	6.94615100	-1.40462000	1.70460800
F	8.02816800	-3.37468100	0.16897400
F	6.50566100	-4.64258700	-1.69496200
F	3.92278600	-3.95155400	-2.02903900
F	-5.28285700	-3.29084000	0.65834000
F	-3.15282800	-5.33500200	0.67341100
F	0.10016700	-5.95570900	0.67018700
F	2.84923900	-4.94834400	0.35172300
F	4.53567600	0.30760100	-1.34195000
F	3.01088100	2.72167000	-1.86726200
F	-2.46114200	3.94032200	-1.28073400

F	-4.76311000	2.33872500	-0.60492400
H	-0.03736700	5.88838300	-4.09768100
H	1.44357600	7.07852100	0.60570300
H	2.83317400	7.16409300	-0.45511900
H	5.49000300	5.55415900	3.17622500

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OH$} Conformer 1 (quartet)

Energy: -4183.23159721 a.u.

C	-4.01733900	-3.04511400	0.40638000
C	-3.03548900	-4.01350500	0.43885700
C	-1.82566300	-3.37465600	0.10812700
N	-2.09200900	-2.04130000	-0.11995200
C	-0.46741500	-3.69098700	-0.01900300
C	0.39908200	-4.75482400	0.29347800
N	0.29664200	-2.60928000	-0.39293500
C	1.68806000	-4.27644100	0.15273600
C	1.61442800	-2.91592200	-0.25910000
C	2.61465900	-1.93874500	-0.46865800
C	-3.41358200	-1.78989800	0.05110400
C	-3.94334500	-0.50417500	-0.09036500
C	-3.11496000	0.57757400	-0.45917200
C	-3.53978000	1.92230800	-0.68237100
N	-1.75227200	0.53542300	-0.68790900
C	-2.44832800	2.67094300	-1.00039000
C	-1.30751800	1.80626800	-1.00234700
C	0.02349700	2.16894400	-1.22921000
C	1.09931800	1.26101700	-1.15023600
C	2.47578900	1.53428300	-1.44119100
N	1.00965800	-0.04564600	-0.75636300
C	3.19146200	0.40893400	-1.18331800
C	2.28782000	-0.61182700	-0.76158500
C	0.33404500	3.57843500	-1.57436300
C	1.10854700	4.36146800	-0.70865100
C	-0.08923600	4.15489700	-2.77298400
C	1.46849200	5.67111700	-1.00898900
C	0.26216100	5.45982000	-3.10034800
H	-0.69157200	3.55839400	-3.45662000
C	2.59874100	4.22533500	1.11924300
C	1.04029300	6.20761600	-2.22278600
C	3.24601400	3.37569000	2.04301600
C	3.04795300	5.53455400	0.90507200
H	1.32280100	7.22977200	-2.47544300
C	4.36686600	3.87080300	2.72613200
C	4.17595800	5.97473700	1.59170700
C	4.83843200	5.15382100	2.49928200

H	4.86695800	3.21973100	3.43637800
H	4.52985200	6.99094500	1.41449000
C	2.27911500	6.44478000	-0.01173700
O	1.51134400	3.73974200	0.45431200
C	2.78348000	1.99790500	2.30605800
O	1.86356900	1.41907000	1.75476200
O	3.51560700	1.39633600	3.27347200
H	3.16114800	0.49270400	3.34231700
Co	-0.58112000	-0.91494500	-0.18084500
O	-0.32687900	-0.57755200	1.62808300
H	0.41022000	0.05415400	1.74990800
C	-5.38476000	-0.29085100	0.15693300
C	-6.35720800	-0.93211700	-0.61293300
C	-5.83574400	0.53878300	1.18608400
C	-7.71481700	-0.76109600	-0.37707400
C	-7.18702900	0.73075700	1.43780000
C	-8.13007800	0.07584700	0.65271100
C	4.02966200	-2.33689900	-0.34918300
C	4.88795500	-1.72161700	0.56598200
C	4.56878100	-3.36378400	-1.12877700
C	6.21434800	-2.10235200	0.70544900
C	5.89218800	-3.76481700	-1.00669300
C	6.71822600	-3.13013800	-0.08536200
F	-4.95277700	1.18326000	1.95280600
F	-7.58598100	1.53004500	2.42738500
F	-9.42805500	0.25065200	0.88626700
F	-8.61887100	-1.38561100	-1.13230900
F	-5.98795400	-1.74126500	-1.61163600
F	4.43433400	-0.72823100	1.34193600
F	7.00445300	-1.49778800	1.59269900
F	7.98820300	-3.50323300	0.03944800
F	6.37659400	-4.74353200	-1.76978400
F	3.80451300	-3.98401500	-2.03113200
F	-5.30195400	-3.25014500	0.65964100
F	-3.19846800	-5.30271500	0.70967600
F	0.04354800	-5.97705500	0.66943300
F	2.79688400	-4.98248300	0.36742700
F	4.50283300	0.26534500	-1.37211600
F	2.98721400	2.67897400	-1.88731900
F	-2.46903000	3.97630600	-1.24679800
F	-4.78855200	2.37918700	-0.61779000
H	-0.06520000	5.89108800	-4.04353500
H	1.61345700	7.08941700	0.58844300
H	2.96352500	7.13479400	-0.52490300
H	5.71489600	5.51687700	3.03039200

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OH$} Conformer 2 (doublet)

Energy: -4183.24568473 a.u.

C	-1.85669500	-4.20098500	0.16161600
C	-0.58425400	-4.70201700	0.32615700
C	0.31318900	-3.65985600	0.01330700
N	-0.40849100	-2.56770900	-0.38807800
C	1.68934700	-3.38460400	0.15378000
C	2.89762100	-4.06453600	0.45464000
N	1.97445000	-2.07027500	-0.03056400
C	3.90034200	-3.12401600	0.44385000
C	3.31761200	-1.85431100	0.12038500
C	3.86237100	-0.58822500	-0.08242000
C	-1.75223100	-2.84047600	-0.25706900
C	-2.72089400	-1.84989800	-0.43381100
C	-2.36733400	-0.50581700	-0.71647400
C	-3.25656500	0.53390800	-1.12477700
N	-1.09041400	0.00821300	-0.74299200
C	-2.51564600	1.64519800	-1.39226600
C	-1.14621500	1.32190900	-1.14467200
C	-0.03345400	2.17061700	-1.29823400
C	1.29086200	1.76358000	-1.08550200
C	2.44920600	2.59225500	-1.12420200
N	1.69247000	0.48828500	-0.71873900
C	3.51981200	1.82913500	-0.76039100
C	3.05799100	0.50904200	-0.48722200
C	-0.31074600	3.58418400	-1.66208400
C	-0.96469100	4.39458900	-0.72684100
C	-0.03905500	4.11889300	-2.92133800
C	-1.40611700	5.67968300	-1.02267300
C	-0.45770600	5.40759700	-3.23940100
H	0.47585700	3.50663900	-3.66047700
C	-2.21896800	4.24548300	1.26092400
C	-1.14921800	6.17183800	-2.30159800
C	-2.72309700	3.36253200	2.23293500
C	-2.76762800	5.51587400	1.05443400
H	-1.49320700	7.17294400	-2.56230700
C	-3.82312300	3.78718200	2.98519300
C	-3.86642200	5.89154100	1.82347500
C	-4.39616500	5.03525400	2.78580300
H	-4.21357800	3.09260400	3.72559200
H	-4.30578300	6.87721500	1.66573000
C	-2.12822100	6.44284300	0.05219500
O	-1.16249400	3.82113000	0.49801500
C	-2.19928600	1.99308800	2.52433500
O	-2.77523200	1.22015400	3.26897000

Co	0.48885500	-0.90479400	-0.16965100
O	0.19991700	-0.64572800	1.64235300
H	0.89125200	-1.09411600	2.15523300
C	-4.14457400	-2.21917800	-0.32714800
C	-4.69208900	-3.23132700	-1.12184200
C	-5.00310500	-1.58220900	0.57559300
C	-6.02613200	-3.60011600	-1.02684600
C	-6.33990100	-1.93756400	0.68909400
C	-6.85210400	-2.95024500	-0.11570800
C	5.31579600	-0.40195200	0.12021600
C	5.81200600	0.43196900	1.12384800
C	6.24802900	-1.07778500	-0.66896400
C	7.17352800	0.59390900	1.33719600
C	7.61515100	-0.93333400	-0.47379900
C	8.07774800	-0.09346700	0.53344700
F	-4.54159500	-0.60577700	1.35337000
F	-7.13385800	-1.31916200	1.56069000
F	-8.13157700	-3.29468500	-0.01602000
F	-6.52014700	-4.56293200	-1.80424100
F	-3.92777800	-3.86613500	-2.01502800
F	4.96148900	1.10498400	1.90339900
F	7.61854800	1.39524200	2.30380100
F	9.38429300	0.05365800	0.72738000
F	8.48249200	-1.58720500	-1.24486300
F	5.83060200	-1.88711000	-1.64627800
O	-1.04680300	1.71707700	1.90760300
H	-0.76464000	0.78514300	2.09594200
F	-2.98016500	-4.87213700	0.39197400
F	-0.25362800	-5.92372100	0.72562000
F	3.02404000	-5.36637600	0.67942500
F	5.19136100	-3.36298000	0.65622400
F	4.77826200	2.25790600	-0.69991100
F	2.49878200	3.88184500	-1.43138400
F	-3.00475800	2.80119500	-1.83103000
F	-4.57280700	0.42911700	-1.28948600
H	-5.25350100	5.34478300	3.37920600
H	-1.41876600	7.11028000	0.57201500
H	-2.88259900	7.10868100	-0.38960100
H	-0.25918400	5.81192400	-4.22926900

{$H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{III}–OH$} Conformer 2 (quartet)

Energy: -4183.23468952 a.u.

C	-3.35853500	-3.51412200	0.45103300
C	-2.25966500	-4.33442800	0.60438200
C	-1.13532500	-3.58647500	0.20181200

N	-1.55963100	-2.36518600	-0.23980500
C	0.27751700	-3.69252700	0.26849400
C	1.26542600	-4.65476200	0.58516400
N	0.89966000	-2.52640000	-0.04020600
C	2.48621800	-4.02708700	0.46251600
C	2.25269600	-2.67550700	0.04477300
C	3.11163800	-1.62105500	-0.29004700
C	-2.91208500	-2.25264400	-0.06046100
C	-3.58308100	-1.04378900	-0.26263500
C	-2.89256600	0.13908700	-0.65996800
C	-3.49447000	1.36888200	-1.05891100
N	-1.53458300	0.28256300	-0.79112400
C	-2.49989300	2.23337500	-1.41487900
C	-1.25437000	1.54651300	-1.26057300
C	0.03633200	2.04915500	-1.50432700
C	1.22004500	1.29434100	-1.31943200
C	2.54833100	1.72788200	-1.58651300
N	1.28912200	0.01034700	-0.83527200
C	3.39798500	0.71558400	-1.22877500
C	2.61625100	-0.36997400	-0.74643600
C	0.17951900	3.47090000	-1.90710400
C	0.73689400	4.37208400	-0.98755500
C	-0.23696800	3.96952100	-3.14199300
C	0.86110000	5.73485500	-1.24844100
C	-0.11429400	5.32444800	-3.43205100
H	-0.67209300	3.28741300	-3.87083400
C	1.18024800	4.63454300	1.30578400
C	0.41964300	6.19821600	-2.48668400
C	1.06057000	4.00140900	2.54916700
C	1.36565500	6.01153100	1.17783100
H	0.50532700	7.26080900	-2.71507000
C	1.20608300	4.78503800	3.69509500
C	1.44851100	6.76747500	2.34645100
C	1.38712800	6.16030900	3.59875900
H	1.14873900	4.28690800	4.66089500
H	1.58218200	7.84692800	2.26797200
C	1.49813500	6.60732700	-0.20016200
O	1.15074000	3.82968400	0.19306600
C	0.77590400	2.54188800	2.71333400
O	1.19858200	1.89696000	3.65658500
Co	-0.22381800	-1.01211300	-0.24034300
O	-0.29976900	-0.54081200	1.61079900
H	0.32032700	-1.06475600	2.14237300
C	-5.04153100	-0.99576800	-0.05216200
C	-5.90711400	-1.84422900	-0.74961400
C	-5.62002600	-0.11257100	0.86571200

C	-7.27988000	-1.82088500	-0.54848600
C	-6.98937400	-0.07258900	1.08413500
C	-7.82204100	-0.93118300	0.37298900
C	4.56926600	-1.82971000	-0.17975000
C	5.35488100	-1.04740900	0.67153400
C	5.21810200	-2.82935800	-0.90890400
C	6.72121500	-1.25062200	0.80139800
C	6.58366900	-3.05067900	-0.79540800
C	7.33649100	-2.25804100	0.06451800
F	-4.84641200	0.72378900	1.55897600
F	-7.51022500	0.77487300	1.96941100
F	-9.13502200	-0.90083600	0.57273800
F	-8.07934600	-2.63679000	-1.23374100
F	-5.41883100	-2.70270200	-1.64920800
F	4.78870300	-0.07107800	1.38261200
F	7.44449100	-0.49409700	1.62437100
F	8.64440600	-2.46098500	0.17993600
F	7.17634700	-4.00735800	-1.50773600
F	4.52334200	-3.59430300	-1.75525300
O	-0.01899300	2.06160600	1.75942700
H	-0.13338400	1.06417700	1.87410900
F	-4.60783000	-3.84949400	0.74606200
F	-2.25351300	-5.57733900	1.06946100
F	1.04874600	-5.91942400	0.92643900
F	3.67018500	-4.59746000	0.66298000
F	4.72118300	0.75214000	-1.35597900
F	2.92871500	2.89412300	-2.09139700
F	-2.69386000	3.47591600	-1.83631000
F	-4.79719700	1.63495600	-1.12135100
H	1.47497600	6.76346100	4.49971400
H	2.56670900	6.74474700	-0.44124400
H	1.06406400	7.61686800	-0.22451900
H	-0.44055700	5.70263100	-4.39805700

$\{H_6^F CX–CO_2H–Co^{III}–O^{\bullet -}\}^-$ (quartet)

Energy: -4182.72289952 a.u.

C	-3.28868200	-3.59227200	0.44413400
C	-2.18250100	-4.40658100	0.55867800
C	-1.06135500	-3.63563700	0.18781200
N	-1.51196300	-2.39696000	-0.19126600
C	0.33678300	-3.72201600	0.21313900
C	1.34206200	-4.63786300	0.58200400
N	0.95383900	-2.55164700	-0.15607500
C	2.55080300	-3.98496300	0.46483200
C	2.30523600	-2.65846200	0.00082000

C	3.16255100	-1.58648400	-0.29738000
C	-2.85927200	-2.31145400	-0.01948200
C	-3.54822500	-1.11001000	-0.25692400
C	-2.86890300	0.05515600	-0.65993300
C	-3.46761900	1.29118800	-1.04987200
N	-1.50169000	0.20731400	-0.81531500
C	-2.48197900	2.15412100	-1.41884000
C	-1.22844600	1.48240300	-1.27022800
C	0.04586200	2.00558700	-1.53028500
C	1.23339600	1.28297600	-1.34072700
C	2.56232200	1.74094000	-1.59804900
N	1.32771600	0.00558800	-0.84445500
C	3.42354600	0.75585300	-1.22404200
C	2.65907400	-0.35096400	-0.74331700
C	0.15852200	3.42955900	-1.95432500
C	0.61262400	4.38256400	-1.03273800
C	-0.17159900	3.87578900	-3.23244600
C	0.73265000	5.73467400	-1.34061400
C	-0.07154600	5.22425600	-3.56793500
H	-0.53169600	3.15129300	-3.96199100
C	0.96293200	4.72736700	1.27607700
C	0.37363900	6.14501900	-2.62446000
C	0.82691900	4.15851600	2.55692300
C	1.10057500	6.11043400	1.09650200
H	0.45525900	7.20166300	-2.88384100
C	0.84033500	5.02146300	3.65644400
C	1.09958500	6.92976700	2.22238700
C	0.97764000	6.39388500	3.50173300
H	0.71698200	4.56651700	4.63693300
H	1.20138900	8.00779400	2.08524900
C	1.27976300	6.66305100	-0.29304600
O	0.94509500	3.88836700	0.20100300
C	0.59689500	2.70553700	2.85158800
O	0.28978700	2.32616900	3.96941100
Co	-0.17116100	-1.00830700	-0.10909300
O	-0.12894900	-0.57601200	1.56081800
C	-5.01134700	-1.08107300	-0.05920200
C	-5.86246600	-1.92753400	-0.77458500
C	-5.61585200	-0.22552100	0.86678200
C	-7.23722800	-1.93539900	-0.57904800
C	-6.98891800	-0.20719400	1.07141400
C	-7.80350600	-1.06878500	0.34694600
C	4.61930900	-1.77553800	-0.14528200
C	5.38074300	-0.98328000	0.71890600
C	5.30536100	-2.76720400	-0.85105800
C	6.74756700	-1.16703500	0.87975300

C	6.66944400	-2.97728900	-0.69826400
C	7.39435700	-2.17180800	0.17060100
F	-4.86946900	0.61655500	1.58475200
F	-7.53381800	0.62367700	1.96688800
F	-9.12609500	-1.06198900	0.53825900
F	-8.02174300	-2.75813800	-1.28547600
F	-5.36197700	-2.76334600	-1.69124000
F	4.79776700	-0.00707800	1.41781300
F	7.44606800	-0.39338200	1.71798000
F	8.70866000	-2.36027200	0.32167300
F	7.29325700	-3.93667300	-1.39203600
F	4.65067000	-3.54880100	-1.71671000
O	0.75862500	1.91580900	1.79697400
H	0.47044100	0.97650900	1.99454000
F	-4.54920500	-3.96740100	0.69742700
F	-2.17178400	-5.68041500	0.96163300
F	1.15753500	-5.90407100	0.96518000
F	3.74747500	-4.53362700	0.71146800
F	4.75622100	0.80404000	-1.34742800
F	2.91679200	2.91830100	-2.12213600
F	-2.68223200	3.40266400	-1.84964500
F	-4.77930100	1.55269700	-1.10979300
H	-0.34277300	5.55715200	-4.56812600
H	0.80942200	7.65465900	-0.37170400
H	2.35412000	6.83750600	-0.48338200
H	0.98077000	7.04733200	4.37211200

$\{H_6^F CX–CO_2H–Co^{III}–O^{\bullet -}(H_2O)\}^-$ (quartet)

Energy: -4259.14949872 a.u.

C	-2.03873100	-4.11326400	-0.00439900
C	-0.78864400	-4.66672200	0.15822800
C	0.15194800	-3.64608900	-0.09782000
N	-0.53941700	-2.51967900	-0.46434400
C	1.52699200	-3.41958600	0.04361200
C	2.68090900	-4.10514200	0.46761200
N	1.89216400	-2.12185100	-0.23756300
C	3.71851200	-3.19556500	0.47243300
C	3.21962200	-1.93572300	0.03290000
C	3.83956700	-0.68971600	-0.15987300
C	-1.87848700	-2.74477900	-0.38304700
C	-2.80053700	-1.70635000	-0.57279200
C	-2.37537600	-0.38957900	-0.82950300
C	-3.20934700	0.71703000	-1.16783100
N	-1.06764100	0.06884900	-0.87767200
C	-2.41896200	1.79856700	-1.41562000

C	-1.05854800	1.40673600	-1.22472700
C	0.07934400	2.21260100	-1.38604900
C	1.38757300	1.75701300	-1.17918000
C	2.59502000	2.50492500	-1.33651300
N	1.73331500	0.50205200	-0.73547900
C	3.63272000	1.70188100	-0.97227700
C	3.10474500	0.43198700	-0.58538100
C	-0.15491500	3.64818800	-1.71198100
C	-0.65267800	4.48495800	-0.70830400
C	-0.00981000	4.19232900	-2.98704900
C	-1.06313900	5.79404800	-0.93933600
C	-0.38758800	5.50836600	-3.24638400
H	0.38091900	3.56302000	-3.78580000
C	-1.77223400	4.33625400	1.34674800
C	-0.92858500	6.29594100	-2.23304800
C	-2.29501900	3.42194700	2.27700300
C	-2.28250300	5.63348300	1.21503700
H	-1.25169100	7.31633400	-2.44396000
C	-3.37062500	3.83805100	3.06603100
C	-3.34850600	6.00895100	2.02823700
C	-3.89300600	5.11996000	2.95329800
H	-3.79161700	3.11222800	3.75875000
H	-3.75641500	7.01627300	1.92981400
C	-1.63362200	6.56294100	0.22127300
O	-0.76044300	3.91326900	0.53429700
C	-1.82276700	2.01076300	2.42559200
O	-2.55349600	1.14461000	2.88863200
Co	0.44953800	-0.87220700	-0.15142800
O	0.26385700	-0.60991800	1.54278600
C	-4.23867300	-2.00841400	-0.44023900
C	-4.85360400	-2.97118400	-1.24435200
C	-5.04488400	-1.38000800	0.51475800
C	-6.19315800	-3.30818400	-1.10792700
C	-6.38961800	-1.69575700	0.66209200
C	-6.96511000	-2.66614300	-0.14862700
C	5.29114300	-0.56975000	0.08066600
C	5.81450100	0.33025900	1.01391000
C	6.21461300	-1.36022700	-0.60921400
C	7.17757000	0.43869700	1.25461800
C	7.58105900	-1.27795700	-0.37734500
C	8.06504000	-0.37288400	0.55844400
F	-4.54375000	-0.43147700	1.30167300
F	-7.13686800	-1.07565900	1.58181800
F	-8.25814900	-2.97621800	-0.01055400
F	-6.74854400	-4.23423800	-1.89984600
F	-4.14867000	-3.60360900	-2.19107600

F	4.99617600	1.12819500	1.70433300
F	7.64369100	1.30921900	2.15705100
F	9.37862500	-0.28105500	0.78468900
F	8.43607400	-2.04955000	-1.05840900
F	5.79491300	-2.22629300	-1.53769600
O	-0.57132400	1.83103200	2.03943000
H	-0.32335800	0.85137100	2.01789000
F	-3.19169200	-4.76964300	0.14369400
F	-0.51531500	-5.92451300	0.51372900
F	2.76127000	-5.39743200	0.79227500
F	4.98448700	-3.47777800	0.80563400
F	4.92766900	2.04031800	-1.02130900
F	2.70387100	3.76471300	-1.76844100
F	-2.86885900	3.00263300	-1.78563000
F	-4.53829300	0.69108100	-1.30871000
H	-0.27973100	5.91501800	-4.25030900
H	-2.35329000	7.31664500	-0.12866900
H	-0.82995000	7.13204100	0.72221900
H	-4.72987600	5.42642200	3.57778200
O	-2.13494800	-1.78928200	2.57962200
H	-1.21190100	-1.64053800	2.30612900
H	-2.43167000	-0.87785200	2.74090300

{H$_9^F$CX–CO$_2$H–Co^{III}–O$^{\bullet-}$}•H$_2$O‡ (doublet)

Energy: -4335.51443352 a.u.

C	-3.85310800	-3.09557800	0.45070600
C	-2.82709800	-4.00855500	0.56338600
C	-1.62500700	-3.32861400	0.25289400
N	-1.95060900	-2.03057500	-0.04864400
C	-0.23221200	-3.56874100	0.17485100
C	0.69205000	-4.62765500	0.32192600
N	0.47653300	-2.44014000	-0.14992400
C	1.94879100	-4.11253100	0.07990400
C	1.80887200	-2.72339800	-0.22872100
C	2.74968300	-1.70635600	-0.50210700
C	-3.29392000	-1.83846700	0.05863600
C	-3.86857600	-0.57717100	-0.19206100
C	-3.10077600	0.54239500	-0.57190000
C	-3.59907200	1.84230000	-0.91787100
N	-1.72569400	0.59106500	-0.70586600
C	-2.54262700	2.63939700	-1.22659300
C	-1.35026300	1.85526400	-1.09486400
C	-0.02888000	2.28179300	-1.29429300
C	1.10020500	1.45666300	-1.13114200
C	2.47330700	1.81478200	-1.34260200

N	1.07420500	0.13111200	-0.76128500
C	3.23362900	0.71046400	-1.11482700
C	2.36615300	-0.36988100	-0.75345500
C	0.23752400	3.71104700	-1.62390600
C	0.80736500	4.52912600	-0.64427600
C	0.06138100	4.26688100	-2.89083100
C	1.27114100	5.81657300	-0.89198100
C	0.48343600	5.56620100	-3.16553100
H	-0.38826000	3.65636300	-3.67299500
C	2.02372300	4.31192700	1.34362100
C	1.10503600	6.32741400	-2.17840800
C	2.55441000	3.35719600	2.22747400
C	2.60371800	5.57613600	1.18365000
H	1.46773500	7.33108100	-2.40458100
C	3.71100100	3.69199800	2.93682300
C	3.74736100	5.87373400	1.91949000
C	4.30225100	4.94066300	2.79461000
H	4.13799300	2.93573100	3.59226000
H	4.21054800	6.85440600	1.79958200
C	1.93931200	6.54768000	0.24153900
O	0.94019400	3.95736000	0.59970300
C	1.98446000	1.98983600	2.39003700
O	2.70909000	1.04965500	2.72743500
Co	-0.51155000	-0.82847100	-0.31499900
O	-0.57066100	-0.27583600	1.69742800
C	-5.33520200	-0.44473000	-0.04941400
C	-6.21598600	-1.19401700	-0.83308500
C	-5.91265100	0.40836100	0.89484100
C	-7.59461400	-1.10982900	-0.68749100
C	-7.28790100	0.51887200	1.05104600
C	-8.13315400	-0.24720400	0.25809000
C	4.18073700	-2.08272300	-0.53575300
C	5.10408800	-1.55315600	0.36913200
C	4.66886700	-3.01789700	-1.45130000
C	6.44408000	-1.91514400	0.36017100
C	6.00244800	-3.40561500	-1.47294100
C	6.89447100	-2.84852400	-0.56555600
F	-5.13632400	1.15838200	1.68144500
F	-7.80749700	1.34660700	1.96599500
F	-9.45903700	-0.15294900	0.40298900
F	-8.40877900	-1.84109800	-1.45877900
F	-5.74216000	-2.02551400	-1.76730500
F	4.69997000	-0.66472000	1.28278400
F	7.30185200	-1.38801100	1.24115500
F	8.18135500	-3.21018500	-0.58171800
F	6.43867300	-4.30057400	-2.36758400

F	3.84618100	-3.57033100	-2.34861300
O	0.69327300	1.92082100	2.17948700
H	0.33044600	0.96276700	2.13269100
F	-5.15130100	-3.36233000	0.66987400
F	-2.94075000	-5.29792500	0.90732400
F	0.39995100	-5.89583800	0.63573500
F	3.09514700	-4.81276100	0.11642700
F	4.56555700	0.65032300	-1.25577200
F	2.95274100	3.00759900	-1.72242400
F	-2.61894500	3.92253700	-1.60059600
F	-4.88629100	2.21719700	-0.95972000
H	0.34994100	5.97889100	-4.16401400
H	1.19139500	7.14144800	0.79712500
H	2.66896600	7.27507000	-0.14133600
H	5.20070000	5.18706300	3.35684700
O	2.05308900	-1.57735100	2.70363400
H	2.32970300	-1.80295300	1.79725500
H	2.29371900	-0.61390200	2.77746200
O	-0.45553800	-1.49138000	2.69917900
H	-0.82420400	-2.18136000	2.10168500
H	0.60275200	-1.61148700	2.69562100

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OH\}^+$ Conformer 1 (singlet)

Energy: -4183.00245169 a.u.

C	-3.97723200	-3.08354800	0.38800200
C	-2.99338200	-4.03685100	0.40199000
C	-1.78657000	-3.38506700	0.02077200
N	-2.06585000	-2.06444800	-0.22718400
C	-0.43348700	-3.67258800	-0.10361600
C	0.44786700	-4.73748600	0.23416500
N	0.31708600	-2.59248500	-0.51409600
C	1.72333100	-4.26099000	0.08307600
C	1.63950700	-2.88975600	-0.35280100
C	2.63879800	-1.91341100	-0.51404200
C	-3.37751200	-1.82869300	-0.00953400
C	-3.90901300	-0.53165900	-0.15632200
C	-3.09321300	0.53827300	-0.56911600
C	-3.52723600	1.89187400	-0.77404500
N	-1.73096900	0.49273500	-0.84814100
C	-2.44512000	2.64282400	-1.10209200
C	-1.30073200	1.77434100	-1.13234600
C	0.03328700	2.16354400	-1.33645800
C	1.12138900	1.27830600	-1.21359800
C	2.51287200	1.57775700	-1.45686500
N	1.03025600	-0.03875700	-0.85830600

C	3.22557800	0.45435100	-1.20234800
C	2.30442800	-0.57948900	-0.81947700
C	0.32987800	3.57902000	-1.65492800
C	1.09348500	4.33735500	-0.75437100
C	-0.08691200	4.18397300	-2.84128400
C	1.46396200	5.65263100	-1.01341800
C	0.27422700	5.49683500	-3.12461000
H	-0.68059300	3.61081000	-3.55154400
C	2.48299200	4.16615000	1.15528600
C	1.04530300	6.21862900	-2.21775100
C	3.03883400	3.30917000	2.13127900
C	2.94218300	5.47771300	0.98719100
H	1.33053100	7.24556200	-2.44368800
C	4.08666200	3.80309700	2.92042500
C	3.99581800	5.91773500	1.78584300
C	4.57006600	5.09205400	2.74632800
H	4.52090900	3.15355000	3.67380600
H	4.36165600	6.93572600	1.65302800
C	2.27371200	6.39764300	0.00451100
O	1.46199800	3.67392500	0.39038600
C	2.55921400	1.92840600	2.33970500
O	1.72157600	1.33824400	1.67140300
O	3.16754900	1.33870300	3.38684700
H	2.81520900	0.43293700	3.43577800
Co	-0.56515800	-0.92388100	-0.33239400
O	-0.40269200	-0.66209300	1.44562200
H	0.33041300	-0.02006600	1.57789400
C	-5.33283100	-0.31097700	0.15788600
C	-6.33623300	-0.99075500	-0.53871800
C	-5.73042000	0.55393500	1.18201200
C	-7.67982000	-0.82017700	-0.23815700
C	-7.06651900	0.73702100	1.50444100
C	-8.04370600	0.04661600	0.79005400
C	4.05031600	-2.28801600	-0.32869800
C	4.85579000	-1.63931200	0.61285800
C	4.63807500	-3.31379100	-1.07616600
C	6.18179500	-1.98920400	0.81066800
C	5.96469300	-3.68070600	-0.90008500
C	6.73787800	-3.01507600	0.04837400
F	-4.80604500	1.22643200	1.87164700
F	-7.41803900	1.55976900	2.48524600
F	-9.32122100	0.21702200	1.08851700
F	-8.61349100	-1.46951400	-0.92239200
F	-5.99953600	-1.82351000	-1.52715100
F	4.34001600	-0.64753700	1.35259200
F	6.91907000	-1.35968600	1.71858800

F	8.00313900	-3.35627000	0.22635200
F	6.49931700	-4.65196900	-1.62839400
F	3.91273800	-3.95733400	-1.99297000
F	-5.25159300	-3.27843900	0.67584500
F	-3.11227500	-5.31849900	0.68704400
F	0.07500700	-5.93523400	0.63408700
F	2.83507900	-4.92596100	0.34314500
F	4.53376000	0.31543700	-1.35070200
F	3.01539500	2.72477200	-1.88138100
F	-2.45889900	3.94505400	-1.32269100
F	-4.76665200	2.34030200	-0.67925200
H	-0.03925500	5.95566100	-4.05868500
H	1.62437100	7.10294500	0.55071100
H	3.02317600	7.02900700	-0.49292400
H	5.38780200	5.45538100	3.36298900

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OH\}^+$ Conformer 1 (triplet)

Energy: -4183.00514425 a.u.

C	-3.97815900	-3.08888200	0.38842600
C	-2.98973400	-4.04274000	0.36648100
C	-1.80289300	-3.38405800	-0.04777700
N	-2.07730000	-2.08647300	-0.30026300
C	-0.42196700	-3.68257500	-0.15932100
C	0.43682300	-4.73603300	0.20529600
N	0.32268700	-2.60977200	-0.55511200
C	1.72751000	-4.25773100	0.07356400
C	1.65585100	-2.90566600	-0.37677700
C	2.64127300	-1.92249400	-0.51251400
C	-3.39844100	-1.83575300	-0.02993200
C	-3.91519700	-0.55748000	-0.14323800
C	-3.08706900	0.54135600	-0.56372500
C	-3.53459200	1.87146500	-0.78832900
N	-1.73857100	0.49644300	-0.83772100
C	-2.45241900	2.63213200	-1.13808600
C	-1.30937600	1.77867600	-1.15863100
C	0.02712600	2.16643400	-1.32479700
C	1.13004000	1.28310100	-1.19823900
C	2.50156700	1.58004700	-1.45280700
N	1.04019400	-0.03493200	-0.83576200
C	3.22053400	0.44967000	-1.19916000
C	2.30864000	-0.57340900	-0.80550000
C	0.32085400	3.57617200	-1.63910900
C	1.10753300	4.33104100	-0.75049500
C	-0.11579100	4.18405400	-2.82072100
C	1.49926700	5.63691500	-1.02760400

C	0.27020700	5.48256000	-3.12022600
H	-0.72727800	3.61423000	-3.51785300
C	2.49418800	4.15758600	1.15739600
C	1.07518500	6.19610900	-2.23115100
C	3.02553800	3.29935600	2.14423900
C	2.99257700	5.44940700	0.96178900
H	1.37775100	7.21435100	-2.47364600
C	4.09668000	3.77137500	2.91561200
C	4.06894600	5.86704900	1.74167400
C	4.62352500	5.03851300	2.71171000
H	4.51438600	3.12149200	3.67799000
H	4.46771600	6.86965900	1.58830600
C	2.33721400	6.37513900	-0.02568300
O	1.45251600	3.68480300	0.40411400
C	2.49224800	1.94248800	2.38671300
O	1.62854000	1.37113600	1.73739600
O	3.08057100	1.35768900	3.44905300
H	2.68576600	0.47178500	3.52827700
Co	-0.56675400	-0.94048000	-0.35498500
O	-0.41566700	-0.70580000	1.42575300
H	0.29736300	-0.04601300	1.57920800
C	-5.33290800	-0.32125000	0.17407500
C	-6.35112300	-1.00723900	-0.49838400
C	-5.71507000	0.57656500	1.17766200
C	-7.69017700	-0.80486900	-0.19708300
C	-7.04545600	0.78696000	1.50297400
C	-8.03644700	0.09288500	0.81060300
C	4.05063000	-2.28724000	-0.31937900
C	4.85658900	-1.61135700	0.60645600
C	4.64504600	-3.32817800	-1.04577300
C	6.18321300	-1.95114700	0.81122700
C	5.97583600	-3.67682700	-0.86774400
C	6.74558300	-2.98759700	0.06701500
F	-4.77772600	1.24961100	1.84768900
F	-7.37977300	1.63706800	2.46562200
F	-9.30885500	0.28884800	1.11136800
F	-8.63689200	-1.45546500	-0.86119800
F	-6.04078700	-1.86608100	-1.47093600
F	4.33737400	-0.61626100	1.33408500
F	6.91667900	-1.30315700	1.70820000
F	8.01216300	-3.31612700	0.24919400
F	6.51855200	-4.65421400	-1.58057800
F	3.93328500	-3.99181500	-1.95558100
F	-5.23918100	-3.29001500	0.71860700
F	-3.09705500	-5.32390900	0.66411900
F	0.06890500	-5.93659400	0.60982200

F	2.82627100	-4.93884800	0.34770800
F	4.53096000	0.32028600	-1.35626900
F	3.01551600	2.73122000	-1.86576700
F	-2.49558100	3.93024200	-1.37575500
F	-4.77635200	2.32348200	-0.70483700
H	-0.04287800	5.93943000	-4.05533200
H	1.70859600	7.09999300	0.51854100
H	3.09665700	6.98265300	-0.53704800
H	5.45957200	5.38425000	3.31381700

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OH\}^+$ Conformer 1 (quintet)

Energy: -4182.99313910 a.u.

C	-4.00024300	-3.04246800	0.42889900
C	-3.01259000	-4.00719000	0.46547900
C	-1.81251200	-3.36192300	0.11878800
N	-2.08257800	-2.02593900	-0.11725000
C	-0.45480300	-3.66843100	-0.02425600
C	0.40537400	-4.74746800	0.29186600
N	0.30409100	-2.59878000	-0.43242700
C	1.68970400	-4.28068600	0.13706200
C	1.61896000	-2.90838800	-0.29972600
C	2.62258400	-1.94263300	-0.48879800
C	-3.40028700	-1.78824400	0.04636800
C	-3.93663000	-0.49306700	-0.10950200
C	-3.11435700	0.58734500	-0.50167600
C	-3.54755700	1.92695700	-0.74164600
N	-1.75261500	0.54621700	-0.74346100
C	-2.45445700	2.67630400	-1.07082700
C	-1.31747400	1.80842900	-1.06861500
C	0.03118000	2.17933800	-1.27146000
C	1.10515100	1.27090600	-1.16658800
C	2.48683500	1.54026500	-1.46162700
N	1.01553200	-0.03413200	-0.78514300
C	3.20011000	0.40394400	-1.21679400
C	2.28953800	-0.60226200	-0.79306600
C	0.34434100	3.58511600	-1.59758000
C	1.15693600	4.33564700	-0.72866100
C	-0.10775000	4.19421600	-2.77185200
C	1.53732300	5.64406000	-1.01172900
C	0.26864400	5.49451800	-3.07908300
H	-0.73563300	3.62638500	-3.45620000
C	2.59868800	4.16937800	1.14355000
C	1.08653200	6.20773200	-2.20411500
C	3.16449200	3.31982600	2.11970800
C	3.07135500	5.47099200	0.94716700

H	1.38117800	7.22814100	-2.44730800
C	4.23616900	3.81087400	2.87872400
C	4.15074000	5.90715500	1.71296600
C	4.73560300	5.08829700	2.67277300
H	4.67668900	3.16606900	3.63252300
H	4.52710100	6.91787700	1.55581600
C	2.38991700	6.38908100	-0.02843600
O	1.55043900	3.68046600	0.40942100
C	2.67138500	1.94927500	2.36345600
O	1.84833500	1.33973400	1.69548100
O	3.25116300	1.39359500	3.44596100
H	2.89199900	0.49194600	3.51662400
Co	-0.58003400	-0.90828300	-0.25468300
O	-0.38278000	-0.59097500	1.56607700
H	0.39079100	-0.00290500	1.70581200
C	-5.37020200	-0.28293400	0.15095900
C	-6.34489400	-0.98697400	-0.56517700
C	-5.81253900	0.60235700	1.14090500
C	-7.69914100	-0.81983700	-0.31759300
C	-7.16043300	0.78024100	1.41161600
C	-8.10641900	0.06652900	0.67756100
C	4.03424500	-2.32962700	-0.34971900
C	4.88518500	-1.67445300	0.54793500
C	4.58164500	-3.37588300	-1.10146500
C	6.21360300	-2.03775900	0.69926600
C	5.90978100	-3.75535100	-0.97195500
C	6.72767100	-3.08312100	-0.06636700
F	-4.92122900	1.29394100	1.85233800
F	-7.55358900	1.61821300	2.36267500
F	-9.39445400	0.23261900	0.92550800
F	-8.60280000	-1.48993600	-1.02127800
F	-5.97049000	-1.83396300	-1.52714000
F	4.41132500	-0.66666400	1.29134100
F	6.99362300	-1.40303300	1.56660400
F	7.99472300	-3.43622300	0.06760800
F	6.40404000	-4.74413000	-1.70508800
F	3.81725400	-4.02452900	-1.98196800
F	-5.27349300	-3.24599600	0.69892900
F	-3.15676500	-5.28708200	0.75226400
F	0.02770400	-5.94492500	0.69246700
F	2.79158700	-4.96871500	0.36577400
F	4.50216700	0.26047700	-1.41378100
F	3.00098100	2.66975400	-1.91005800
F	-2.48068300	3.97330000	-1.32232200
F	-4.78746100	2.38225400	-0.68568400
H	-0.06544200	5.95206700	-4.00661400

H	1.76777300	7.11176000	0.52616800
H	3.13487500	7.00060900	-0.55637600
H	5.57294500	5.44877400	3.26431600

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OH\}^+$ Conformer 2 (singlet)

Energy: -4182.99809158 a.u.

C	-1.78299700	-4.22474900	0.11184700
C	-0.50873800	-4.71447400	0.24720400
C	0.37594200	-3.65513000	-0.08775200
N	-0.36310300	-2.56875700	-0.48564700
C	1.73913700	-3.37620800	0.04887400
C	2.94705400	-4.04945100	0.37676700
N	2.02019700	-2.05129600	-0.14480200
C	3.94127500	-3.10231600	0.37281800
C	3.34762000	-1.83246900	0.03163500
C	3.88774600	-0.54320000	-0.12240000
C	-1.69237800	-2.85416900	-0.32085600
C	-2.68213800	-1.87089100	-0.47422800
C	-2.33458900	-0.52946800	-0.77286000
C	-3.24231700	0.49951900	-1.19376600
N	-1.06224900	0.00271600	-0.79332100
C	-2.51587200	1.61498400	-1.45837200
C	-1.13400000	1.31259800	-1.18537100
C	-0.03516600	2.18577400	-1.31687400
C	1.29402200	1.78956200	-1.09092900
C	2.44600300	2.64009600	-1.09404600
N	1.70711900	0.51296900	-0.76255000
C	3.52388400	1.88298400	-0.75304500
C	3.07422400	0.54386000	-0.51526500
C	-0.33065200	3.59970300	-1.65753300
C	-1.10879900	4.34707000	-0.75574300
C	0.05723500	4.21437300	-2.84495700
C	-1.54888600	5.64259600	-1.01487800
C	-0.35390400	5.51757800	-3.12371300
H	0.66068600	3.66367100	-3.56413000
C	-2.40964900	4.12567800	1.21402100
C	-1.15377900	6.21742600	-2.22251900
C	-2.84587700	3.23762100	2.21951800
C	-2.96239900	5.40455600	1.04135000
H	-1.48128800	7.22856400	-2.46103800
C	-3.89119900	3.66072500	3.03728800
C	-3.99817700	5.78344200	1.89220000
C	-4.46604900	4.92067500	2.87969100
H	-4.23951400	2.97041700	3.80203300
H	-4.44162100	6.77188800	1.77623700

C	-2.40713600	6.33764700	0.00045900
O	-1.42129700	3.68036900	0.38825900
C	-2.29182500	1.87166900	2.48150800
O	-2.82727800	1.09094300	3.24233200
Co	0.52594600	-0.90180200	-0.24989000
O	0.22240200	-0.67478900	1.56322900
H	0.90482900	-1.11026800	2.09976900
C	-4.09661300	-2.23680200	-0.32016300
C	-4.66276800	-3.28422300	-1.05806000
C	-4.93300200	-1.55406000	0.57339000
C	-5.99316300	-3.64617400	-0.91347700
C	-6.26398200	-1.90372100	0.73958800
C	-6.79478200	-2.95349100	-0.00807700
C	5.32445100	-0.33969700	0.13948700
C	5.76586100	0.51967800	1.15021000
C	6.29656900	-1.02381400	-0.59661600
C	7.11355400	0.69399900	1.42418900
C	7.65139700	-0.86103400	-0.34566800
C	8.05895800	0.00023100	0.67081400
F	-4.44532500	-0.54138200	1.28947400
F	-7.03273500	-1.24741000	1.59961600
F	-8.06474600	-3.29021900	0.13834700
F	-6.50710400	-4.63549700	-1.63295500
F	-3.91500300	-3.94740300	-1.94296900
F	4.86998500	1.19393100	1.87630300
F	7.50607400	1.50995800	2.39477600
F	9.34750200	0.16211800	0.92069700
F	8.55496000	-1.51249600	-1.06665900
F	5.92010800	-1.84734900	-1.57748400
O	-1.15707100	1.61881600	1.81897400
H	-0.83090500	0.70589900	2.02624500
F	-2.89335100	-4.88418800	0.38450200
F	-0.14363300	-5.91719500	0.64230300
F	3.06450700	-5.34183700	0.61312400
F	5.22114700	-3.32074800	0.61956600
F	4.76928900	2.32106400	-0.68012200
F	2.47224300	3.93523200	-1.35670500
F	-3.00601200	2.75639700	-1.91793800
F	-4.54659300	0.36893500	-1.37426700
H	-5.27877500	5.23162900	3.53131300
H	-1.82093900	7.12847200	0.49967500
H	-3.22581500	6.87382200	-0.50099500
H	-0.06138600	5.98422300	-4.06080800

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OH\}^+$ Conformer 2 (triplet)

Energy: -4183.00072876 a.u.

C	-1.80126300	-4.19980800	0.13817000
C	-0.51655100	-4.69469600	0.27209900
C	0.35564400	-3.65058500	-0.08433100
N	-0.37706900	-2.56613600	-0.47745800
C	1.73794400	-3.36562800	0.03834500
C	2.93385400	-4.05031400	0.38595900
N	2.01876400	-2.06009900	-0.16276800
C	3.93472100	-3.11010300	0.40019600
C	3.35736800	-1.83627400	0.04150600
C	3.89446100	-0.56838700	-0.10647200
C	-1.71292500	-2.84819700	-0.31179500
C	-2.69299600	-1.85602500	-0.46399700
C	-2.34356900	-0.50641200	-0.74404000
C	-3.23720900	0.51865100	-1.17770600
N	-1.07183000	0.02270800	-0.75163500
C	-2.50135700	1.63873400	-1.43026500
C	-1.13766400	1.33291200	-1.14307500
C	-0.02095000	2.20180400	-1.28567900
C	1.30964400	1.79519900	-1.11157100
C	2.46709500	2.62768500	-1.13041000
N	1.71739500	0.51717600	-0.75218800
C	3.54171200	1.85845200	-0.77618200
C	3.07429900	0.54189600	-0.51236700
C	-0.30598600	3.61166400	-1.61558300
C	-1.09709700	4.35617700	-0.71714700
C	0.10525800	4.23621500	-2.79555800
C	-1.54907700	5.64698000	-0.98292300
C	-0.32310400	5.52700200	-3.07930500
H	0.72023200	3.69001600	-3.50784000
C	-2.40790600	4.12026400	1.23784500
C	-1.14924900	6.21830700	-2.18688000
C	-2.84860700	3.21312400	2.22173500
C	-2.99009600	5.38090400	1.04980100
H	-1.48616100	7.22418500	-2.43497000
C	-3.93366800	3.60033500	3.00715800
C	-4.06432800	5.72433100	1.86670800
C	-4.53802300	4.84279700	2.83626200
H	-4.28917600	2.89452000	3.75418600
H	-4.53324100	6.69975400	1.74070900
C	-2.41979200	6.33303600	0.03177700
O	-1.38191900	3.70607000	0.43562300
C	-2.26988000	1.85712000	2.48027100
O	-2.82945800	1.03785400	3.18169000
Co	0.52337200	-0.90228100	-0.24681900
O	0.24788800	-0.66689500	1.56813100

H	0.92906300	-1.11594500	2.09524000
C	-4.10583100	-2.22142600	-0.33046200
C	-4.65281600	-3.28950900	-1.05917500
C	-4.96763000	-1.52461000	0.53216900
C	-5.98450100	-3.65198200	-0.93843100
C	-6.29799800	-1.88221300	0.67979600
C	-6.80790600	-2.94802200	-0.06054200
C	5.33123100	-0.36036500	0.14019200
C	5.77652700	0.52784600	1.12538000
C	6.30261600	-1.06189400	-0.58265900
C	7.12420100	0.71490000	1.38740400
C	7.65796900	-0.88406200	-0.34483200
C	8.06809700	0.00519900	0.64632300
F	-4.50434200	-0.50228700	1.24514300
F	-7.08749800	-1.21874900	1.51399100
F	-8.07724600	-3.28894600	0.06580300
F	-6.48088100	-4.65243900	-1.65350900
F	-3.89179400	-3.96158500	-1.92262300
F	4.88136400	1.21432400	1.83987400
F	7.51901400	1.55583500	2.33484200
F	9.35675400	0.17797700	0.88446200
F	8.56004300	-1.54939600	-1.05431600
F	5.92986400	-1.91030900	-1.54224500
O	-1.08878300	1.65547800	1.88507700
H	-0.76890700	0.73426100	2.06242600
F	-2.90525200	-4.86979200	0.41510700
F	-0.16301900	-5.89925800	0.67844500
F	3.03363600	-5.34246200	0.63448000
F	5.20633400	-3.33556700	0.67130600
F	4.79163900	2.29159300	-0.72141100
F	2.52445500	3.91727000	-1.40868800
F	-2.99393700	2.78857400	-1.87556200
F	-4.54204700	0.40081600	-1.37347800
H	-5.37999400	5.12758900	3.46223600
H	-1.83301800	7.10913100	0.55198300
H	-3.23004000	6.88033400	-0.46998500
H	-0.03423600	5.99558900	-4.01653900

{$H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{IV}–OH$} Conformer 2 (quintet)

Energy: -4182.99082521 a.u.

C	-1.79214800	-4.20619000	0.18953800
C	-0.51673700	-4.69668000	0.33790100
C	0.36362600	-3.63376500	0.01980700
N	-0.37738000	-2.54923200	-0.38572100
C	1.72882400	-3.35623200	0.15776600

C	2.92947300	-4.03181000	0.46596000
N	2.01743800	-2.02455200	-0.05029900
C	3.93193200	-3.08691000	0.43175700
C	3.34494800	-1.81526900	0.08522300
C	3.89902600	-0.52872800	-0.09358600
C	-1.69970200	-2.83327700	-0.24891600
C	-2.69362800	-1.85574800	-0.43569400
C	-2.34216200	-0.51275000	-0.72413900
C	-3.23899800	0.50566500	-1.16727300
N	-1.06564300	0.03356700	-0.71305100
C	-2.50592200	1.62404300	-1.42523900
C	-1.12684100	1.33060300	-1.12441400
C	-0.03075600	2.20975500	-1.26583900
C	1.30710600	1.81120000	-1.04925600
C	2.46286700	2.64985400	-1.09545100
N	1.71658300	0.54942600	-0.68642200
C	3.54541100	1.88763500	-0.75778100
C	3.08889800	0.56397600	-0.47750700
C	-0.32662700	3.61906900	-1.61286300
C	-1.11733000	4.36699600	-0.71913500
C	0.07338800	4.23650000	-2.79730100
C	-1.56310900	5.65961900	-0.98584000
C	-0.34450700	5.53364600	-3.08300400
H	0.68581300	3.68764400	-3.51012400
C	-2.43312300	4.14508600	1.23888900
C	-1.16029900	6.23124300	-2.19093900
C	-2.87774500	3.24799700	2.23067600
C	-2.99772100	5.41526000	1.05513900
H	-1.49163700	7.23938000	-2.43713400
C	-3.94798400	3.65241600	3.02578300
C	-4.05502700	5.77867600	1.88629200
C	-4.53263700	4.90648200	2.86142100
H	-4.30867900	2.95271800	3.77623300
H	-4.50903500	6.76160300	1.76407800
C	-2.43235900	6.35361800	0.02311800
O	-1.42705800	3.70813500	0.42667000
C	-2.31424500	1.88271100	2.47959800
O	-2.90250400	1.05241800	3.14405200
Co	0.52985000	-0.88106300	-0.19884400
O	0.21164100	-0.60875000	1.64664900
H	0.92194800	-0.94245200	2.21778800
C	-4.10766800	-2.24209000	-0.34415600
C	-4.61602200	-3.30383800	-1.10447500
C	-5.00135500	-1.57729100	0.50738700
C	-5.94270900	-3.69604800	-1.02371900
C	-6.33079300	-1.95737000	0.60970200

C	-6.80199600	-3.02023800	-0.15887200
C	5.34468200	-0.34507100	0.11869500
C	5.83705400	0.53454100	1.08935900
C	6.28034100	-1.06894400	-0.62884400
C	7.19626200	0.68778200	1.31459400
C	7.64510100	-0.92771600	-0.42655900
C	8.10262600	-0.04678300	0.55130200
F	-4.57324100	-0.55420800	1.24334300
F	-7.15515100	-1.31766300	1.42954400
F	-8.06920100	-3.38567600	-0.07081600
F	-6.39848800	-4.69789300	-1.76495600
F	-3.81132400	-3.95438700	-1.94903300
F	4.98092800	1.24579600	1.82649500
F	7.63757200	1.52122300	2.24825700
F	9.40112900	0.09500700	0.75391500
F	8.51181600	-1.61625900	-1.15768400
F	5.85752100	-1.90710100	-1.57778400
O	-1.11681700	1.69357900	1.91876900
H	-0.79220400	0.76613300	2.07873900
F	-2.90172700	-4.87285400	0.43468200
F	-0.15830900	-5.89922700	0.73976900
F	3.05046800	-5.32107600	0.72113800
F	5.21115300	-3.31621000	0.66195200
F	4.79412400	2.31929700	-0.72962100
F	2.50646400	3.93609800	-1.39349600
F	-2.99457100	2.75767300	-1.89732400
F	-4.53951000	0.37952900	-1.37609500
H	-5.36251900	5.20585100	3.49669800
H	-1.84873700	7.14065500	0.53084000
H	-3.24558700	6.89201900	-0.48426300
H	-0.04974800	5.99927300	-4.01994100

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$O^{\bullet-}$} (singlet)

Energy: -4182.58057488 a.u.

C	-3.38971400	-3.48373300	0.41635000
C	-2.30030500	-4.32287500	0.48376500
C	-1.19246400	-3.58869600	0.00334800
N	-1.61554800	-2.35785700	-0.38674400
C	0.21389400	-3.72776100	-0.02807500
C	1.17808400	-4.64900300	0.42060900
N	0.85049000	-2.59177100	-0.43503200
C	2.40627600	-4.02188800	0.32193400
C	2.19374400	-2.71002500	-0.19536700
C	3.06251000	-1.62928000	-0.40430300
C	-2.94936200	-2.22244700	-0.11174000

C	-3.59999100	-1.00656200	-0.28940700
C	-2.89897500	0.14983200	-0.74509300
C	-3.48820600	1.39864700	-1.08759600
N	-1.54150400	0.26024100	-0.95387300
C	-2.49194500	2.25607400	-1.45930300
C	-1.25433100	1.55004000	-1.37008000
C	0.03481300	2.05953700	-1.59034600
C	1.21151200	1.30182600	-1.40963300
C	2.54914200	1.74236400	-1.63687800
N	1.26255300	0.00900200	-0.94987400
C	3.38456500	0.73229400	-1.26639500
C	2.58583600	-0.36627200	-0.82810600
C	0.18260200	3.49694400	-1.93161200
C	0.75219700	4.35112900	-0.97373100
C	-0.23436400	4.05446400	-3.14029300
C	0.89429000	5.72084100	-1.17456400
C	-0.09495000	5.41949800	-3.37030400
H	-0.67926400	3.41051000	-3.89733700
C	1.27885000	4.47870700	1.32369900
C	0.45509200	6.24342200	-2.39010500
C	1.20226800	3.79177900	2.54831300
C	1.45545400	5.86419700	1.25430700
H	0.55504700	7.31361100	-2.57261700
C	1.32625900	4.54463700	3.71987800
C	1.56539700	6.57224500	2.44894100
C	1.51106900	5.91966600	3.67819900
H	1.25093800	4.00827900	4.66311700
H	1.69894800	7.65392700	2.40837600
C	1.54757400	6.53588700	-0.09240000
O	1.15449100	3.74112500	0.17620700
C	0.92123500	2.33083500	2.71330400
O	0.66489600	1.84371100	3.79902100
Co	-0.24210300	-1.04319700	-0.44398000
O	-0.19465000	-0.77974500	1.24764800
C	-5.04139200	-0.91587500	0.01199000
C	-5.96859000	-1.74280700	-0.62878700
C	-5.53864700	-0.01909900	0.96279100
C	-7.32516600	-1.68733500	-0.34120700
C	-6.89048800	0.05461800	1.26613300
C	-7.78639800	-0.78516300	0.61145800
C	4.50468700	-1.82034800	-0.16690500
C	5.21136200	-1.01867700	0.73624000
C	5.22299200	-2.82223300	-0.82723700
C	6.56363900	-1.20868700	0.98134400
C	6.57650500	-3.02698600	-0.60085700
C	7.24762100	-2.21738700	0.30972500

F	-4.70180300	0.79913400	1.60316900
F	-7.33494800	0.91663300	2.17846800
F	-9.08288500	-0.72413500	0.89492700
F	-8.18515900	-2.48426400	-0.97337500
F	-5.55747500	-2.61264100	-1.55573400
F	4.58276600	-0.04207200	1.39066200
F	7.20990000	-0.43734600	1.85299000
F	8.54271800	-2.40493200	0.53676400
F	7.23526000	-3.98389200	-1.25222500
F	4.60961900	-3.60532700	-1.71835100
O	0.97182300	1.63824400	1.57240000
H	0.63842600	0.70584400	1.70772500
F	-4.62619700	-3.79549700	0.78140500
F	-2.27757100	-5.57730500	0.91351700
F	0.94358400	-5.88037500	0.85334600
F	3.57309500	-4.56667000	0.64803300
F	4.71172800	0.75127400	-1.36480300
F	2.93062800	2.91500300	-2.13121000
F	-2.68174000	3.51372100	-1.83464900
F	-4.78602000	1.69195400	-1.08999900
H	-0.41948000	5.84433700	-4.31729400
H	1.10316200	7.54027000	-0.04732600
H	2.60831900	6.70043100	-0.35049800
H	1.60168600	6.48768100	4.60132900

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$O^{\bullet-}$} (triplet)

Energy: -4182.59986430 a.u.

C	-3.44947100	-3.46360000	0.40498600
C	-2.37758400	-4.32615900	0.44615000
C	-1.24663600	-3.59857400	0.01646500
N	-1.64597500	-2.33765000	-0.32920700
C	0.14544400	-3.75481300	-0.01179600
C	1.10353400	-4.70694900	0.39863000
N	0.79827700	-2.61549100	-0.39276400
C	2.33539500	-4.09837600	0.31515400
C	2.14495500	-2.76564200	-0.16514200
C	3.03050400	-1.71158100	-0.38462800
C	-2.98692600	-2.19490400	-0.06534400
C	-3.62963900	-0.97151500	-0.24124000
C	-2.91528600	0.17530100	-0.66653100
C	-3.47797600	1.44320700	-0.99494700
N	-1.55456300	0.25752200	-0.88145500
C	-2.46909300	2.27430700	-1.38083500
C	-1.24695900	1.54139600	-1.29982500
C	0.04625500	2.02176600	-1.55080500

C	1.20504000	1.24978500	-1.37892500
C	2.54810100	1.66949700	-1.60635600
N	1.24437500	-0.05428300	-0.92608400
C	3.37130900	0.65018900	-1.23374500
C	2.56336000	-0.44199800	-0.80126100
C	0.20678800	3.44265700	-1.95591000
C	0.77471300	4.34682600	-1.04758400
C	-0.19443000	3.92335000	-3.20138300
C	0.94093600	5.69641000	-1.34185000
C	-0.04117100	5.26933400	-3.51986400
H	-0.63985500	3.23393200	-3.91718000
C	1.36473700	4.61574500	1.22658900
C	0.51577100	6.14504100	-2.59230000
C	1.35709200	4.01755400	2.50052100
C	1.56963500	5.98944100	1.05806200
H	0.63440900	7.19976800	-2.84161400
C	1.57837100	4.84170200	3.60937000
C	1.76886400	6.77130900	2.19375500
C	1.78234200	6.20603200	3.46565200
H	1.56686700	4.36779400	4.58800700
H	1.92301200	7.84390800	2.06956600
C	1.60474000	6.58221800	-0.32608300
O	1.16242200	3.80238600	0.14495400
C	1.08669100	2.58074300	2.79649200
O	1.03719000	2.14632900	3.93165600
Co	-0.26161500	-1.02997200	-0.23889800
O	-0.17410200	-0.72711300	1.40607500
C	-5.07606000	-0.87674100	0.03825800
C	-5.99816600	-1.67326200	-0.64550300
C	-5.58104300	-0.00413500	1.00620200
C	-7.35928900	-1.61297500	-0.38081200
C	-6.93769200	0.07466200	1.28681800
C	-7.82924100	-0.73513900	0.59004800
C	4.47340300	-1.92594600	-0.16511800
C	5.19874900	-1.15002300	0.74397200
C	5.17126600	-2.92421000	-0.85037600
C	6.55138600	-1.35932000	0.97134800
C	6.52427400	-3.15106600	-0.63982400
C	7.21533600	-2.36540800	0.27645800
F	-4.74727200	0.78618700	1.68534100
F	-7.39056600	0.91378600	2.21656500
F	-9.13049200	-0.66878100	0.85062400
F	-8.21515500	-2.38196500	-1.05209200
F	-5.57656700	-2.51825600	-1.59044100
F	4.58766600	-0.17461000	1.41881000
F	7.21604500	-0.60921800	1.84814600

F	8.51067700	-2.57346000	0.48665300
F	7.16356400	-4.10674400	-1.31243200
F	4.53724200	-3.68531100	-1.74667300
O	0.89031000	1.81535900	1.70949100
H	0.64278600	0.91119900	2.00995600
F	-4.70034800	-3.77253500	0.72776200
F	-2.38311200	-5.59810300	0.82047000
F	0.84369500	-5.94487100	0.79664600
F	3.49814100	-4.66635600	0.61525600
F	4.69787700	0.65321400	-1.33334700
F	2.94720800	2.83752600	-2.09526000
F	-2.62569900	3.53985700	-1.74872400
F	-4.77026400	1.75925000	-0.98403800
H	-0.35818800	5.63602700	-4.49330800
H	1.13760200	7.57773000	-0.32301500
H	2.65284200	6.75820100	-0.62471300
H	1.94499000	6.83102200	4.34066900

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$O^{\bullet-}$} (quintet)

Energy: -4182.58459559 a.u.

C	-3.43283600	-3.47531300	0.46004600
C	-2.35272700	-4.33253900	0.51379400
C	-1.22843700	-3.59363000	0.09493500
N	-1.63404800	-2.33794200	-0.24623200
C	0.17643700	-3.75761900	0.04232900
C	1.13094900	-4.71492200	0.43852700
N	0.82640900	-2.62740200	-0.35117600
C	2.36671500	-4.10812600	0.32863700
C	2.16782900	-2.77627700	-0.15621100
C	3.04974800	-1.70767700	-0.37045800
C	-2.97441400	-2.20263800	-0.01361200
C	-3.62936300	-0.98568200	-0.21873900
C	-2.92426200	0.16795300	-0.66758200
C	-3.50497200	1.40964200	-1.05473800
N	-1.56619000	0.27644500	-0.83949100
C	-2.49707200	2.25058000	-1.43475600
C	-1.26509000	1.53872200	-1.29715800
C	0.03693100	2.03029200	-1.51525000
C	1.20808700	1.26409900	-1.31631500
C	2.54614100	1.68101600	-1.57774300
N	1.26105100	-0.02387900	-0.84526200
C	3.37758900	0.65650100	-1.22439200
C	2.57575600	-0.42654700	-0.76263900
C	0.19833200	3.44507600	-1.93119700
C	0.78101900	4.35428100	-1.03434200

C	-0.21228700	3.92259600	-3.17634100
C	0.95232200	5.70136600	-1.33943200
C	-0.05174100	5.26434100	-3.50542600
H	-0.66624300	3.23157600	-3.88498000
C	1.34951800	4.64487300	1.24099000
C	0.51946800	6.14380300	-2.58876300
C	1.30916600	4.06009600	2.51991100
C	1.56572300	6.01499700	1.05995300
H	0.64250400	7.19579400	-2.84723900
C	1.51519600	4.89556800	3.62269700
C	1.74566500	6.80957000	2.18994200
C	1.73096400	6.25729900	3.46761800
H	1.48135300	4.43247800	4.60606700
H	1.90784900	7.87992600	2.05723800
C	1.63097100	6.58619100	-0.33233600
O	1.16966200	3.82180900	0.16071600
C	1.01770600	2.62648700	2.82539900
O	0.98032800	2.20130600	3.96471800
Co	-0.25027000	-1.02490100	-0.19918600
O	-0.15329700	-0.67577900	1.48111200
C	-5.08054400	-0.90138100	0.02933500
C	-5.98319000	-1.72940400	-0.64464800
C	-5.61352300	0.00080200	0.95558300
C	-7.34948600	-1.67263600	-0.40840400
C	-6.97559500	0.07477100	1.20860600
C	-7.84616100	-0.76734400	0.52336000
C	4.49431000	-1.92208900	-0.17893400
C	5.24119100	-1.13792600	0.70767000
C	5.17817000	-2.93048500	-0.86633300
C	6.59683400	-1.34960900	0.91180700
C	6.53425600	-3.15795600	-0.67990400
C	7.24503200	-2.36469300	0.21476300
F	-4.80143300	0.82326300	1.62164900
F	-7.45373200	0.93962000	2.10103900
F	-9.15246900	-0.70536400	0.75651200
F	-8.18569300	-2.47002900	-1.07089300
F	-5.53822300	-2.59797400	-1.55671200
F	4.64806600	-0.15568200	1.38693800
F	7.27964500	-0.59394900	1.76926000
F	8.54321700	-2.57393400	0.40184200
F	7.15863600	-4.12074500	-1.35586200
F	4.52872200	-3.69668300	-1.74652200
O	0.78669700	1.87043400	1.74378600
H	0.53105400	0.95883700	2.02975700
F	-4.68242000	-3.79842800	0.76627500
F	-2.35832600	-5.60552200	0.88720700

F	0.87977100	-5.95006600	0.85367500
F	3.53034600	-4.68357700	0.60633800
F	4.70064700	0.65836800	-1.36282600
F	2.94111000	2.84199700	-2.08626700
F	-2.67231100	3.49957200	-1.84662200
F	-4.80168700	1.70742200	-1.08701900
H	-0.37234100	5.62580200	-4.47963600
H	1.19163400	7.59389200	-0.34973900
H	2.68649000	6.72733400	-0.62348600
H	1.88058300	6.89082700	4.33889200

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$O^{\bullet-}$(H_2O)} (triplet)

Energy: -4259.02474795 a.u.

C	-1.83260400	-4.14242300	-0.00572100
C	-0.56192800	-4.66692200	0.07527600
C	0.33110900	-3.63657300	-0.28288000
N	-0.39565900	-2.52897700	-0.63658000
C	1.70752600	-3.38335800	-0.20168300
C	2.87306000	-4.05433300	0.22945900
N	2.02701800	-2.07959500	-0.46203100
C	3.87995700	-3.11741100	0.27943100
C	3.34348600	-1.85767800	-0.13487800
C	3.90265500	-0.58402000	-0.20624100
C	-1.73017800	-2.78708800	-0.44417200
C	-2.68412100	-1.78191900	-0.60210800
C	-2.29754400	-0.45628000	-0.91845900
C	-3.16848000	0.60081200	-1.30917600
N	-1.00919000	0.03553700	-0.95851100
C	-2.41284200	1.70674600	-1.56507500
C	-1.05057000	1.36882100	-1.31713100
C	0.05593800	2.23316500	-1.38545100
C	1.37272800	1.82443200	-1.14812200
C	2.53967600	2.64406600	-1.16411100
N	1.76190500	0.53981600	-0.81090000
C	3.59900900	1.86213900	-0.81161500
C	3.11929600	0.53881300	-0.57673500
C	-0.22936300	3.66505900	-1.66936600
C	-0.89686400	4.41302900	-0.69330700
C	0.03718000	4.27371600	-2.89504100
C	-1.35281200	5.70713100	-0.91611500
C	-0.39390100	5.57463600	-3.13980200
H	0.56058500	3.71070700	-3.66640100
C	-2.16821400	4.13258700	1.27059000
C	-1.09712500	6.27599100	-2.16327300
C	-2.67023300	3.19319600	2.19236200

C	-2.72999300	5.40716200	1.13563200
H	-1.45218900	7.28624100	-2.36737100
C	-3.77709000	3.56381500	2.96504500
C	-3.83737200	5.72589300	1.91771100
C	-4.36340400	4.81321400	2.82936700
H	-4.16124300	2.82956200	3.66916200
H	-4.28644500	6.71418000	1.81289000
C	-2.09175300	6.39791100	0.19561000
O	-1.10137800	3.76617000	0.49755900
C	-2.12862000	1.82555300	2.41359500
O	-2.65018400	1.03146700	3.18463000
Co	0.54556700	-0.88611900	-0.29749600
O	0.41387100	-0.74375800	1.38026500
C	-4.10711200	-2.09524700	-0.39770100
C	-4.72778500	-3.13462000	-1.09848500
C	-4.89732200	-1.38106900	0.51151900
C	-6.05864000	-3.46949200	-0.89579300
C	-6.22897100	-1.70286500	0.73165100
C	-6.81079800	-2.75172200	0.02743000
C	5.32772600	-0.40439900	0.13281400
C	5.73221800	0.44054700	1.17000800
C	6.33079500	-1.08440000	-0.56288800
C	7.06857600	0.60400500	1.50492400
C	7.67421800	-0.93618000	-0.24627300
C	8.04288500	-0.08879900	0.79322800
F	-4.39122500	-0.34819800	1.18217500
F	-6.95561100	-1.00977200	1.60675400
F	-8.08760300	-3.06071500	0.22829500
F	-6.62108300	-4.46153600	-1.58506900
F	-4.03979200	-3.82878800	-2.01056700
F	4.81822100	1.11997000	1.86618900
F	7.42358200	1.41299000	2.50151700
F	9.32570100	0.06056800	1.10602700
F	8.60866300	-1.59182600	-0.93281700
F	6.00678400	-1.89883600	-1.57095200
O	-1.02580900	1.55708300	1.71269000
H	-0.71954300	0.63381100	1.88113000
F	-2.94964300	-4.80079800	0.26724800
F	-0.22262200	-5.89473900	0.44523600
F	2.96110300	-5.34217100	0.53116000
F	5.13799100	-3.35647800	0.63108600
F	4.86697000	2.26217700	-0.75584900
F	2.59916700	3.93701600	-1.45846800
F	-2.89258200	2.87673300	-1.97569600
F	-4.48406500	0.51463700	-1.48044100
H	-0.19581700	6.03746300	-4.10377700

H	-2.84939900	7.08109600	-0.21252500
H	-1.39444000	7.03998400	0.76154600
H	-5.22685500	5.08079900	3.43376800
O	-2.12116300	-1.69927400	2.31670900
H	-1.15284500	-1.63379300	2.28619600
H	-2.39333300	-0.88174900	2.77237000

$\{H^{+\bullet,F}CX–CO_2H–Co^{III}–O^{\bullet-}\}\bullet H_2O^{\ddagger}$ (triplet)

Energy: -4335.39582496 a.u.

C	-3.82593300	-3.11159600	0.37234500
C	-2.79809100	-4.02903200	0.45386900
C	-1.61042800	-3.35058100	0.11907600
N	-1.94322800	-2.04140800	-0.18900200
C	-0.22963000	-3.58329600	0.07544600
C	0.69225900	-4.64426400	0.23106600
N	0.48621100	-2.44065600	-0.20074800
C	1.95107300	-4.11563300	0.04411900
C	1.81744100	-2.71724600	-0.23642800
C	2.76215300	-1.70485900	-0.48205300
C	-3.28340900	-1.84910100	-0.01945000
C	-3.87512300	-0.58937100	-0.19911500
C	-3.10394300	0.53178700	-0.54805800
C	-3.60040000	1.82706100	-0.89520500
N	-1.72367000	0.57920800	-0.67828100
C	-2.54392300	2.62187800	-1.21811800
C	-1.35278800	1.84459900	-1.08423600
C	-0.04275800	2.27399000	-1.31083200
C	1.07475800	1.44130500	-1.15487200
C	2.44279500	1.80204100	-1.34064400
N	1.04903100	0.10698800	-0.78382500
C	3.21294700	0.70662900	-1.07909800
C	2.35883200	-0.37995500	-0.73694300
C	0.21773300	3.69854800	-1.66447900
C	0.75880700	4.53338700	-0.68504100
C	0.06176900	4.22349100	-2.94676600
C	1.20999200	5.82252800	-0.94306300
C	0.47417700	5.52345400	-3.23075000
H	-0.36249200	3.59632900	-3.72969000
C	1.95840600	4.35030500	1.31505900
C	1.06259800	6.30832900	-2.24144500
C	2.50371500	3.40713300	2.20320800
C	2.51861800	5.62117100	1.14914800
H	1.41418300	7.31273900	-2.47759800
C	3.65277100	3.76296600	2.91866900
C	3.65456900	5.93903800	1.88864300

C	4.22094900	5.02015500	2.77202400
H	4.08752900	3.02182200	3.58555300
H	4.10318900	6.92541300	1.76711900
C	1.84840800	6.57532400	0.19316000
O	0.88176300	3.97376900	0.56615000
C	1.96638400	2.03700400	2.36756400
O	2.68254000	1.10697300	2.74249300
Co	-0.51011400	-0.82279900	-0.22838500
O	-0.50045700	-0.46039600	1.63405600
C	-5.33659800	-0.45982100	-0.02385900
C	-6.23006700	-1.20195800	-0.79972100
C	-5.88824900	0.39169300	0.93666800
C	-7.60490100	-1.11180800	-0.62998300
C	-7.25936200	0.50463100	1.12041900
C	-8.12068700	-0.25312600	0.33410600
C	4.19719600	-2.06901400	-0.50036600
C	5.10175500	-1.53856200	0.42080200
C	4.70057200	-2.98471000	-1.42667300
C	6.44548600	-1.88303800	0.42267400
C	6.03947500	-3.35357100	-1.44157300
C	6.91476300	-2.79724200	-0.51506600
F	-5.08631100	1.13472100	1.70416600
F	-7.75512100	1.32652400	2.04581200
F	-9.43658500	-0.15533600	0.50251900
F	-8.43107100	-1.83327900	-1.38779300
F	-5.76595000	-2.03020900	-1.74119600
F	4.66612000	-0.66270900	1.33668200
F	7.28292100	-1.35635300	1.31522500
F	8.19947500	-3.14074900	-0.52326600
F	6.49142200	-4.22825100	-2.33951900
F	3.88417200	-3.53318300	-2.33067100
O	0.67529500	1.92256400	2.10113600
H	0.37863600	0.97197300	2.12233100
F	-5.10219000	-3.37057000	0.63831700
F	-2.89791300	-5.31058600	0.79071600
F	0.38745200	-5.91004100	0.49612800
F	3.09366700	-4.79830300	0.09734700
F	4.53855700	0.66586900	-1.18664500
F	2.91903600	2.98839000	-1.70482800
F	-2.61777100	3.89010000	-1.60649500
F	-4.87997000	2.19005700	-0.94487500
H	0.35702900	5.91934600	-4.23709300
H	1.08133800	7.15627500	0.73408700
H	2.56823000	7.31338200	-0.18480800
H	5.10976700	5.28646700	3.33893500
O	2.16427000	-1.53027000	2.77177400

H	2.54156300	-1.75502900	1.90435900
H	2.35505100	-0.55350500	2.85770200
O	-0.30648800	-1.67991400	2.71139100
H	-0.59367300	-2.42560400	2.14046300
H	0.78481500	-1.68359200	2.73204100

$\{H^{+\bullet,F}CX–CO_2–Co^{III}–O^{\bullet-}(H_2O)\}^-$ (triplet)

Energy: -4258.49256134 a.u.

C	-1.83710300	-4.11045900	0.12416100
C	-0.57203800	-4.62778400	0.28460200
C	0.34136900	-3.61042100	-0.05500200
N	-0.37503600	-2.51309700	-0.46777400
C	1.71576800	-3.35985600	0.03140200
C	2.90160200	-4.02566400	0.41593700
N	2.03408900	-2.06259700	-0.25623900
C	3.91666300	-3.09739200	0.38463200
C	3.36651600	-1.84572100	-0.02442400
C	3.92787900	-0.57807300	-0.17744400
C	-1.71771400	-2.76822900	-0.33571400
C	-2.66708100	-1.77317500	-0.57565700
C	-2.27768600	-0.46581800	-0.92461900
C	-3.14423200	0.59210200	-1.32817100
N	-0.98628600	0.02240000	-0.96997000
C	-2.39119200	1.69930200	-1.55757500
C	-1.02953400	1.35986800	-1.30194100
C	0.06953900	2.22551700	-1.35684400
C	1.38716000	1.81850200	-1.12431300
C	2.55096100	2.64287400	-1.11033000
N	1.78336200	0.52546100	-0.82375000
C	3.61244700	1.85880600	-0.77729400
C	3.14509400	0.52895800	-0.56539000
C	-0.20970500	3.66512700	-1.60469400
C	-0.89239600	4.39817100	-0.62291300
C	0.11427300	4.30438200	-2.79992300
C	-1.27224600	5.72517400	-0.82080900
C	-0.25647000	5.62804500	-3.02082200
H	0.64785400	3.74491700	-3.56773700
C	-2.26254400	4.12920000	1.27846700
C	-0.95339500	6.32546900	-2.03765200
C	-2.85864900	3.19029800	2.13619000
C	-2.72060300	5.44897400	1.17957300
H	-1.25423900	7.36018300	-2.20958900
C	-3.94909100	3.62618900	2.89245200
C	-3.82596900	5.82863700	1.93802500
C	-4.44071500	4.92302500	2.79683600

H	-4.39531000	2.88726400	3.55492600
H	-4.19398200	6.85316800	1.85534400
C	-1.98599500	6.42560400	0.29898600
O	-1.17794500	3.72550900	0.52677300
C	-2.43029700	1.72435100	2.29410600
O	-3.00729600	1.08193600	3.20026800
Co	0.55606400	-0.86335000	-0.28808400
O	0.39703200	-0.57565400	1.34640900
C	-4.09795300	-2.10765300	-0.44158700
C	-4.65594600	-3.16342800	-1.16741000
C	-4.95423400	-1.40888700	0.41837900
C	-5.98539400	-3.53648100	-1.03438400
C	-6.29006900	-1.76627800	0.56189800
C	-6.80576400	-2.83434300	-0.16127300
C	5.36907300	-0.40477600	0.10660800
C	5.82266300	0.41490600	1.14256400
C	6.34046500	-1.08075600	-0.63398800
C	7.17351200	0.56391100	1.42667500
C	7.69668800	-0.95307100	-0.36414800
C	8.11417300	-0.12537100	0.67056700
F	-4.52523500	-0.35679800	1.09912800
F	-7.08834200	-1.08399500	1.38700700
F	-8.08965500	-3.17778300	-0.02818200
F	-6.48369300	-4.55366900	-1.74785200
F	-3.90457000	-3.85130700	-2.03761200
F	4.94767500	1.09062600	1.88907200
F	7.57621900	1.35629000	2.42426900
F	9.41527100	0.00864400	0.93670600
F	8.60186100	-1.61087300	-1.09614200
F	5.97728200	-1.88093300	-1.64179500
O	-1.55559500	1.31266100	1.48191600
F	-2.96824300	-4.77344100	0.36039700
F	-0.25969400	-5.85758400	0.69330600
F	3.01384600	-5.31579700	0.73030600
F	5.20130800	-3.34417500	0.66312200
F	4.88210500	2.27336400	-0.70308600
F	2.61669300	3.94842000	-1.36934800
F	-2.86412200	2.87465400	-1.97198100
F	-4.46136900	0.50279000	-1.52207400
H	-0.00993700	6.11221000	-3.96385900
H	-2.67902900	7.18196400	-0.09856300
H	-1.25418000	6.99184800	0.90369400
H	-5.30124100	5.22969700	3.39027800
O	-2.22044000	-1.50702000	2.36912300
H	-1.40211500	-1.10387700	2.03069200
H	-2.62751500	-0.70998500	2.77772000

{$H^{+\bullet,F}CX–CO_2–Co^{III}–O^{\bullet-}$}•$H_2O^{\ddagger}$ (triplet)

Energy: -4334.88962874 a.u.

C	-3.87498700	-3.12825000	0.40248500
C	-2.85759600	-4.05289200	0.50064300
C	-1.66898700	-3.40648200	0.10977900
N	-1.98981000	-2.12283200	-0.26612100
C	-0.28833500	-3.64913400	0.10773600
C	0.62343600	-4.68231600	0.41484100
N	0.44119300	-2.54151600	-0.24154400
C	1.89280600	-4.16644500	0.25546700
C	1.77694600	-2.80931100	-0.17001900
C	2.72490300	-1.83491100	-0.52130600
C	-3.32244000	-1.89596100	-0.05288300
C	-3.88713500	-0.62464500	-0.22329200
C	-3.10198400	0.48632400	-0.58030400
C	-3.56962600	1.80561100	-0.85915500
N	-1.72993300	0.49919700	-0.76745600
C	-2.50173700	2.58655200	-1.17823200
C	-1.32981700	1.76950700	-1.12535400
C	-0.01106200	2.15512600	-1.40031700
C	1.07844000	1.28141800	-1.32947400
C	2.43456900	1.59163900	-1.64703200
N	1.03394600	-0.04044500	-0.93414000
C	3.18551700	0.48928800	-1.39759700
C	2.32846800	-0.54599800	-0.91644100
C	0.24992100	3.57428300	-1.76531500
C	0.88590100	4.42586200	-0.84798300
C	-0.10829500	4.09141100	-3.00801500
C	1.14175200	5.76511400	-1.14389300
C	0.15915200	5.41779200	-3.33549500
H	-0.60417800	3.43515000	-3.72273500
C	2.11341700	4.50212400	1.17618800
C	0.77882300	6.24247100	-2.40345000
C	2.66602300	3.75223000	2.22816100
C	2.39887200	5.86158700	1.01164900
H	0.98397300	7.28654600	-2.64599300
C	3.49526500	4.41669900	3.13248000
C	3.26948800	6.47240300	1.91449000
C	3.81265700	5.76185000	2.97836900
H	3.89024600	3.82996400	3.95914400
H	3.50361300	7.53011600	1.77933700
C	1.74994900	6.64852200	-0.09380200
O	1.23544800	3.85260400	0.34029400
C	2.46412000	2.26463600	2.41112400

O	2.53809700	1.83704600	3.59957200
Co	-0.52895200	-0.90416100	-0.26148700
O	-0.51449900	-0.50874300	1.41186000
C	-5.33873600	-0.46414300	0.00299000
C	-6.27352300	-1.18569000	-0.74346200
C	-5.84612400	0.38717400	0.98847800
C	-7.64024600	-1.07412800	-0.52637000
C	-7.20905700	0.52309700	1.21696500
C	-8.10999600	-0.21343900	0.45740600
C	4.15801100	-2.19508400	-0.48121100
C	5.07684900	-1.51436700	0.32439100
C	4.65511900	-3.25606000	-1.24229300
C	6.41691500	-1.87705600	0.37732200
C	5.98825500	-3.64070400	-1.19830600
C	6.87300800	-2.94710100	-0.38267800
F	-5.01319900	1.10715800	1.74204200
F	-7.66189600	1.34713500	2.16737600
F	-9.42290200	-0.09331600	0.67046800
F	-8.50711100	-1.77819100	-1.26281200
F	-5.86370300	-2.01758100	-1.70735500
F	4.68443200	-0.47537000	1.05672800
F	7.27245100	-1.20896000	1.15673400
F	8.15921300	-3.30420700	-0.33339800
F	6.42850000	-4.66141500	-1.94356400
F	3.83968300	-3.93687400	-2.05649200
O	2.29720200	1.56844200	1.36894000
F	-5.15961600	-3.36389300	0.69299200
F	-2.97092200	-5.32251700	0.89627600
F	0.31143400	-5.92855400	0.77798000
F	3.02822300	-4.84982200	0.43793600
F	4.50184600	0.39013300	-1.60229300
F	2.90091200	2.75290400	-2.10275400
F	-2.56961600	3.88054100	-1.49446300
F	-4.84491000	2.21053000	-0.85630100
H	-0.11815200	5.80623900	-4.31364700
H	0.96977100	7.30764800	0.32819800
H	2.48099200	7.33462100	-0.55004800
H	4.47928800	6.25533500	3.68412100
O	2.21227400	-0.57009200	2.74881600
H	2.19048200	0.06059300	1.93801700
H	2.32328500	0.20284800	3.40840200
O	-0.03082000	-1.57739700	2.87104100
H	0.02880500	-2.37576600	2.31789500
H	1.19544100	-1.01759000	2.84249300

{H$_9$^{F}CX–CO$_2$H–Co^{III}–OOH(H$_2$O)}$^-$ (singlet)

Energy: -4334.93634400 a.u.

C	-3.95482400	-3.10577000	0.29580800
C	-2.95903000	-4.05579200	0.31050300
C	-1.75784000	-3.40753700	-0.05656700
N	-2.05266800	-2.09903700	-0.32184900
C	-0.38031900	-3.68002200	-0.11467900
C	0.51129800	-4.74050400	0.16662900
N	0.36692700	-2.58060900	-0.43494700
C	1.78843500	-4.24133300	0.04904400
C	1.69715900	-2.86105100	-0.31043000
C	2.66953100	-1.86349600	-0.47816800
C	-3.37486900	-1.85747400	-0.08887100
C	-3.90593000	-0.56461500	-0.20604000
C	-3.10315200	0.54140100	-0.55167700
C	-3.55571000	1.87416200	-0.79957500
N	-1.73363600	0.53258000	-0.74651500
C	-2.47934200	2.64266200	-1.11664800
C	-1.31895200	1.80753400	-1.07570500
C	0.00987400	2.19940800	-1.28841300
C	1.11238600	1.33873700	-1.14406100
C	2.49323100	1.65816100	-1.33540000
N	1.04209900	0.00631800	-0.79484100
C	3.22233400	0.53735200	-1.08141500
C	2.32326200	-0.51921100	-0.73992400
C	0.28697700	3.60841700	-1.68578100
C	0.94304900	4.47267700	-0.80385300
C	-0.01801100	4.10404600	-2.95379000
C	1.35023400	5.75612800	-1.15394600
C	0.35369600	5.39304100	-3.32871800
H	-0.53824400	3.45404900	-3.65639200
C	2.30377400	4.40553400	1.10607000
C	1.04929200	6.20659800	-2.43870700
C	2.90250800	3.53837700	2.03748700
C	2.82735900	5.67568000	0.83856400
H	1.36494100	7.20693300	-2.73838800
C	4.06519500	3.96807200	2.68424700
C	3.98485800	6.06574200	1.50710200
C	4.60520500	5.22197400	2.42624000
H	4.53989100	3.29018000	3.38921800
H	4.40301900	7.05235800	1.30108300
C	2.09210200	6.56750600	-0.12722600
O	1.20495500	3.95490100	0.44220900
C	2.31106700	2.20592100	2.32997900
O	1.13918600	1.93102000	2.11312400

Co	-0.56657600	-0.93879400	-0.38534300
O	-0.33585500	-0.98412700	1.45855500
C	-5.34745300	-0.37125500	0.05691000
C	-6.32288900	-1.03342000	-0.69240200
C	-5.80567600	0.46018700	1.08253900
C	-7.68036700	-0.88630200	-0.43880500
C	-7.15757900	0.63048600	1.34907900
C	-8.09976500	-0.04855500	0.58647500
C	4.09190000	-2.25959900	-0.40290000
C	4.97721400	-1.70841000	0.52791900
C	4.61430000	-3.23711900	-1.25500100
C	6.30692400	-2.10118300	0.60733100
C	5.93743000	-3.65250100	-1.18785700
C	6.78916800	-3.07979300	-0.25245200
F	-4.93430800	1.12894100	1.84096200
F	-7.56131900	1.43366900	2.34071100
F	-9.40405000	0.10581100	0.83667300
F	-8.58744200	-1.53256200	-1.18178700
F	-5.96437200	-1.83745000	-1.69929400
F	4.55935700	-0.76604000	1.37333400
F	7.12696800	-1.55352200	1.51170000
F	8.06726100	-3.46583100	-0.18139300
F	6.40136000	-4.58835900	-2.02553800
F	3.83629200	-3.80519500	-2.18309700
O	3.18313100	1.36023100	2.86782400
H	2.70905600	0.47065200	2.97169400
F	-5.24676800	-3.33333800	0.57909500
F	-3.09983900	-5.35101000	0.61249600
F	0.17335000	-5.99460200	0.48461800
F	2.91520900	-4.94419700	0.23756200
F	4.55339500	0.44284400	-1.20136400
F	3.01051000	2.83636900	-1.71119400
F	-2.52212700	3.94834000	-1.40735000
F	-4.82549600	2.30375300	-0.76687400
H	0.11624300	5.75727700	-4.32662400
H	1.38240300	7.20423100	0.43114400
H	2.78896900	7.26436100	-0.61456200
H	5.51087300	5.54264300	2.93714700
O	1.86186800	-0.95038900	3.05351100
H	1.27558800	-0.98549400	2.25612900
O	-0.97746900	0.09583500	2.12393000
H	-0.29392700	0.80051500	2.05989200
H	1.20298900	-0.86253700	3.75688500

{H$_6$^{F}CX–CO$_2$H–Co^{III}–OOH(H$_2$O)}$^-$ (triplet)

Energy: -4334.92783241 a.u.

C	-3.96764300	-3.09678100	0.21372600
C	-2.98759300	-4.06602800	0.16822900
C	-1.78812100	-3.42788700	-0.20049900
N	-2.07183900	-2.09849000	-0.42352700
C	-0.41534700	-3.71401000	-0.24401100
C	0.46182700	-4.80467100	-0.03792300
N	0.35059600	-2.60151700	-0.45223900
C	1.74485600	-4.30909900	-0.09395500
C	1.67124500	-2.90339200	-0.35381600
C	2.65173000	-1.90642600	-0.49353200
C	-3.38344100	-1.84479700	-0.13869700
C	-3.90552500	-0.53963300	-0.16867700
C	-3.09040700	0.57326300	-0.45377800
C	-3.53781100	1.90247900	-0.73465700
N	-1.71850300	0.56649600	-0.61143400
C	-2.45919100	2.65476700	-1.08014100
C	-1.30065800	1.81606500	-1.01484400
C	0.02142800	2.18374700	-1.29906200
C	1.11426300	1.30677200	-1.17903100
C	2.49879800	1.61669600	-1.34011800
N	1.03381600	-0.02943200	-0.84693900
C	3.21947800	0.49283900	-1.06277400
C	2.31207200	-0.56398700	-0.76010000
C	0.30460700	3.57891200	-1.74125500
C	0.96338100	4.46508900	-0.88426200
C	0.00639600	4.03677100	-3.02478700
C	1.38390400	5.73312700	-1.27273900
C	0.38683000	5.31212200	-3.43695600
H	-0.51511500	3.36891500	-3.70952500
C	2.33135900	4.43303700	1.01932800
C	1.08753500	6.14692200	-2.57080700
C	2.92299500	3.58299800	1.97053700
C	2.86969700	5.68827800	0.71365400
H	1.41225200	7.13468600	-2.90093700
C	4.09497600	4.01530100	2.59881100
C	4.03735900	6.08022500	1.36315800
C	4.65155800	5.25321900	2.30148900
H	4.56248300	3.35186100	3.32199400
H	4.46770100	7.05495000	1.12760400
C	2.13801700	6.56360900	-0.27041100
O	1.22085500	3.98120200	0.37525100
C	2.31113500	2.26972600	2.30984500
O	1.13928200	1.99941500	2.08531000

Co	-0.56926100	-0.94662800	-0.32997100
O	-0.28063700	-1.04878900	1.57174900
C	-5.34325100	-0.34403600	0.10010900
C	-6.32740000	-0.98981000	-0.65407200
C	-5.79485400	0.48500600	1.13206500
C	-7.68286800	-0.83377000	-0.39658500
C	-7.14476800	0.66446300	1.40179200
C	-8.09416800	-0.00082100	0.63602600
C	4.07274200	-2.29422500	-0.37005900
C	4.89406400	-1.77117600	0.63203700
C	4.65515300	-3.22178800	-1.23661500
C	6.22426700	-2.14514700	0.76813500
C	5.98040400	-3.61883500	-1.11489600
C	6.76861200	-3.07608600	-0.10821500
F	-4.91840000	1.14234100	1.89449800
F	-7.53974400	1.46344800	2.39996300
F	-9.39655800	0.16229900	0.88956100
F	-8.59626400	-1.46468200	-1.14487600
F	-5.97908300	-1.78476700	-1.67219200
F	4.40532900	-0.87604000	1.49309400
F	6.98435500	-1.62780100	1.73919600
F	8.04697100	-3.44593500	0.01661200
F	6.50724500	-4.50743000	-1.96627200
F	3.93578900	-3.75474400	-2.23017400
O	3.16457600	1.44102300	2.90032400
H	2.66463100	0.57604300	3.08377500
F	-5.24707400	-3.31452100	0.54608200
F	-3.14262600	-5.36383900	0.44713500
F	0.10850900	-6.07671500	0.17028400
F	2.86319900	-5.03744600	0.03332300
F	4.55360500	0.40197000	-1.12645900
F	3.03447500	2.79498700	-1.68262000
F	-2.49407500	3.94774100	-1.42059400
F	-4.80680500	2.33277500	-0.71914000
H	0.15356900	5.64800600	-4.44574400
H	1.43691500	7.22022600	0.27556700
H	2.83876800	7.24156700	-0.77832200
H	5.56467800	5.57525600	2.79812700
O	1.73829400	-0.75399000	3.38028600
H	1.46856900	-1.13167200	2.51768800
O	-0.81536400	0.01178100	2.39493200
H	-0.26714700	0.77350000	2.10507700
H	0.87270400	-0.38185000	3.63331300

{H$_6^F$CX–CO$_2$–Co^{III}–OOH(H$_2$O)}$^{2-}$ (singlet)

Energy: -4334.32152344 a.u.

C	-4.07963700	-3.00822400	0.39051800
C	-3.08828100	-3.96154500	0.47900900
C	-1.87184200	-3.33312200	0.13630300
N	-2.15089300	-2.03216100	-0.17950500
C	-0.49522600	-3.62378100	0.08832600
C	0.38428700	-4.69299400	0.36325900
N	0.26193800	-2.54875000	-0.28574900
C	1.66620600	-4.22850400	0.17152800
C	1.58803700	-2.86395900	-0.24085400
C	2.56480800	-1.90351700	-0.54967400
C	-3.47906300	-1.77818100	-0.01424000
C	-3.99243100	-0.47913400	-0.17658100
C	-3.17124800	0.61525400	-0.51861000
C	-3.59065900	1.96772900	-0.70220700
N	-1.80695600	0.58282700	-0.74748600
C	-2.49645500	2.72645100	-0.97937700
C	-1.35815200	1.85897600	-1.01113000
C	-0.01588500	2.21450800	-1.23433800
C	1.05450000	1.30565500	-1.21369400
C	2.42370200	1.57653500	-1.53320200
N	0.96236300	-0.02250400	-0.87376700
C	3.12786900	0.43508700	-1.33731200
C	2.22690700	-0.58085600	-0.88971200
C	0.30472200	3.63758200	-1.52253100
C	1.11097800	4.38855700	-0.64823300
C	-0.13960500	4.26083400	-2.68948600
C	1.46346900	5.71050800	-0.92729900
C	0.20704700	5.57428900	-2.99233100
H	-0.76502500	3.68566200	-3.37187100
C	2.68701700	4.19585500	1.10737300
C	1.01116800	6.28989700	-2.11184700
C	3.37175500	3.31291400	1.96393000
C	3.12047600	5.51529300	0.90996900
H	1.29579600	7.32055300	-2.33471400
C	4.52265400	3.80209600	2.58743700
C	4.29138500	5.94337100	1.53239600
C	4.99963900	5.08966400	2.37134300
H	5.02322200	3.10413200	3.25656800
H	4.63124200	6.96778000	1.36087100
C	2.28749400	6.45337100	0.08141600
O	1.54012400	3.75027500	0.48100900
C	2.96920500	1.86189200	2.27217300
O	2.13278000	1.33246300	1.49121400
Co	-0.64671200	-0.88896900	-0.35111900
O	-0.48790000	-0.63004600	1.48445700

C	-5.43647000	-0.27378700	0.05871700
C	-6.40155100	-0.93576300	-0.70592900
C	-5.91850700	0.55300100	1.07911500
C	-7.76369200	-0.79011300	-0.47787400
C	-7.27607000	0.72498400	1.31693800
C	-8.20448900	0.04757300	0.53728600
C	3.98431300	-2.30570900	-0.48536500
C	4.90703400	-1.66959000	0.35639200
C	4.46823800	-3.36943900	-1.25118800
C	6.23141800	-2.08820100	0.43503800
C	5.78313400	-3.80730300	-1.17777600
C	6.66957300	-3.16291500	-0.32700800
F	-5.06806200	1.21226300	1.86699600
F	-7.70211600	1.52495000	2.30653000
F	-9.51828600	0.20314000	0.76190700
F	-8.65997600	-1.43674500	-1.24121200
F	-6.03038500	-1.74004300	-1.70939400
F	4.55316700	-0.62274800	1.08485800
F	7.09815200	-1.46423200	1.24431200
F	7.94665700	-3.57054200	-0.24983600
F	6.20875500	-4.83390500	-1.93511300
F	3.65937500	-4.00612200	-2.11091100
O	3.53570000	1.33623200	3.25382200
H	2.58546400	-0.58913500	2.76718800
F	-5.38963700	-3.22682400	0.63059200
F	-3.25305100	-5.24969300	0.82296700
F	0.03364000	-5.93496300	0.73643000
F	2.78081500	-4.96240700	0.33228800
F	4.44295100	0.28662200	-1.56674100
F	2.94348600	2.73623400	-1.96298900
F	-2.52774100	4.05221200	-1.18735500
F	-4.85332400	2.43425600	-0.64151200
H	-0.14373600	6.03410400	-3.91559000
H	1.62177200	7.04021300	0.74256500
H	2.92689700	7.19947100	-0.41641000
H	5.91315000	5.43149000	2.85921000
O	2.17809900	-1.47113700	2.67135900
H	1.33557900	-1.25464300	2.23484700
O	-0.42975600	0.73577800	1.79396300
H	0.55293000	0.93362000	1.73613700

{H$_6^F$CX–CO$_2$–Co^{III}–OOH(H$_2$O)}$^{2-}$ (triplet)

Energy: -4334.30977513 a.u.

C	-4.09632900	-3.00430500	0.32982400
C	-3.11224900	-3.96960900	0.39370100

C	-1.89417800	-3.34487200	0.06462100
N	-2.16858000	-2.03083300	-0.23250800
C	-0.51917000	-3.63446300	0.05800600
C	0.35083400	-4.72315700	0.28978300
N	0.25328200	-2.54382600	-0.22735300
C	1.63699800	-4.25411300	0.15016200
C	1.57358600	-2.86781600	-0.19806600
C	2.55708800	-1.91150100	-0.50893500
C	-3.49286200	-1.76944500	-0.04779400
C	-4.00037800	-0.45820700	-0.15083100
C	-3.16550100	0.64372700	-0.43051100
C	-3.58393100	1.99291800	-0.64880100
N	-1.79611300	0.61811000	-0.60675500
C	-2.48749600	2.74634700	-0.92863900
C	-1.34607700	1.88036500	-0.92126600
C	-0.01184900	2.22485600	-1.19403700
C	1.05252200	1.30578100	-1.17891600
C	2.42061100	1.56860600	-1.49822000
N	0.96002400	-0.02218900	-0.83997700
C	3.12392100	0.42333400	-1.30014300
C	2.22271300	-0.58878900	-0.85311000
C	0.31097100	3.63870400	-1.52715000
C	1.12653500	4.40666600	-0.67784000
C	-0.12853200	4.23358200	-2.71043100
C	1.50576700	5.71146400	-0.99715100
C	0.23645300	5.53346500	-3.05087200
H	-0.76216500	3.64816200	-3.37638000
C	2.71153600	4.21910200	1.06566500
C	1.05797600	6.26231400	-2.19692900
C	3.38725700	3.33074800	1.92359700
C	3.18086000	5.51897600	0.82497400
H	1.36040900	7.27965500	-2.45484000
C	4.56987700	3.79494700	2.50521000
C	4.37719800	5.92372000	1.41350400
C	5.07810500	5.06437000	2.25347700
H	5.07072800	3.09086500	3.16771600
H	4.74608500	6.93257600	1.21210100
C	2.35794100	6.45870000	-0.01395000
O	1.54361100	3.79492900	0.46802400
C	2.93276700	1.90282800	2.27671000
O	1.95379300	1.44847700	1.62884700
Co	-0.64902600	-0.87866900	-0.23217100
O	-0.37464800	-0.68955400	1.66398000
C	-5.44513700	-0.25411900	0.06304700
C	-6.40163600	-0.91401800	-0.71632000
C	-5.94385100	0.57646900	1.07400000

C	-7.76652000	-0.76641400	-0.50881100
C	-7.30447100	0.75147100	1.28968500
C	-8.22241300	0.07401600	0.49752400
C	3.97506500	-2.32183700	-0.46674700
C	4.91686400	-1.68812100	0.35605600
C	4.44150500	-3.38645600	-1.24277600
C	6.23844800	-2.11835600	0.41685800
C	5.75341000	-3.83577100	-1.18667300
C	6.65657600	-3.19892300	-0.34802900
F	-5.10570800	1.23564600	1.87547600
F	-7.74424400	1.55344900	2.27180400
F	-9.53950200	0.23213600	0.70119000
F	-8.65170700	-1.41134000	-1.28659000
F	-6.01816300	-1.71590300	-1.71756400
F	4.58741100	-0.62938600	1.07758700
F	7.12262700	-1.49782600	1.20959600
F	7.93095800	-3.61737500	-0.28769500
F	6.16063700	-4.86423100	-1.95144200
F	3.61870300	-4.01094800	-2.09850300
O	3.59819200	1.32884600	3.16818200
H	2.75257300	-0.55227600	2.84219800
F	-5.40158700	-3.21785800	0.58971800
F	-3.28662400	-5.25924700	0.72626400
F	-0.01261000	-5.98232000	0.58337700
F	2.74373500	-5.00280900	0.28744600
F	4.43812600	0.27934200	-1.53275500
F	2.95177600	2.72171400	-1.92893000
F	-2.51548600	4.06391200	-1.18061100
F	-4.84876400	2.45479600	-0.62903400
H	-0.11103800	5.97153300	-3.98591700
H	1.71321200	7.07367500	0.64241800
H	3.00736200	7.17955200	-0.53529800
H	6.01331200	5.38734700	2.71231300
O	2.34671400	-1.43330000	2.72059800
H	1.47059100	-1.20261500	2.36420100
O	-0.53490700	0.64420300	2.11720800
H	0.40927200	0.96907400	2.04678800

{$H^{+\bullet}{}_{\beta}{}^{F}CX–CO_2H–Co^{III}–OOH$} (doublet)

Energy: -4258.36780648 a.u.

C	-4.04634900	-3.02184700	0.27026300
C	-3.08520100	-4.00750600	0.28038300
C	-1.86759900	-3.40420100	-0.09655800
N	-2.10992100	-2.07922200	-0.37323700
C	-0.50518300	-3.72894400	-0.13418400

C	0.34062100	-4.82253000	0.17567800
N	0.27935000	-2.65548800	-0.43787100
C	1.63427700	-4.36553500	0.09193200
C	1.59673200	-2.98445700	-0.28313900
C	2.59590700	-2.02988200	-0.47975400
C	-3.42898500	-1.79210800	-0.11059000
C	-3.91803500	-0.48601100	-0.16021900
C	-3.07360000	0.60286500	-0.47153700
C	-3.47591000	1.95863300	-0.66845400
N	-1.71432600	0.53639800	-0.69631600
C	-2.37229700	2.68806900	-0.98968900
C	-1.25465200	1.79867800	-1.00706200
C	0.08211900	2.12642600	-1.27559400
C	1.13660200	1.20367900	-1.22961000
C	2.51915200	1.46027100	-1.45774900
N	1.01324700	-0.13428800	-0.89288500
C	3.20919600	0.31645700	-1.19196100
C	2.28023600	-0.69626700	-0.82338000
C	0.40519800	3.52307700	-1.67136900
C	1.17549300	4.34884200	-0.84673700
C	0.00765600	4.02792700	-2.91025300
C	1.59412800	5.61611600	-1.23974700
C	0.39630400	5.29841100	-3.32134500
H	-0.59883800	3.39938000	-3.56062100
C	2.63347500	4.29904100	1.00649400
C	1.19599000	6.07858900	-2.49360200
C	3.18492700	3.52067200	2.04285700
C	3.16553500	5.55404700	0.68667900
H	1.52141900	7.06707300	-2.81808200
C	4.32353500	3.99897800	2.70522700
C	4.31209100	5.97955500	1.35349500
C	4.90363000	5.20796000	2.34977900
H	4.79332800	3.38204700	3.47146400
H	4.74010600	6.94674800	1.08914400
C	2.45265000	6.42426300	-0.31036500
O	1.53269500	3.80889000	0.37459800
C	2.57655500	2.22795900	2.44078300
O	2.02610900	1.45252700	1.68418500
Co	-0.59047500	-0.97498800	-0.32510600
O	-0.33051400	-0.93060700	1.49145000
C	-5.34525800	-0.24820000	0.13673900
C	-6.35427600	-0.85014400	-0.61891700
C	-5.74770100	0.57055200	1.19502000
C	-7.69997100	-0.65113900	-0.34190300
C	-7.08648600	0.78659900	1.48942100
C	-8.06626800	0.17126500	0.71764300

C	4.00852600	-2.42104500	-0.30048300
C	4.82218600	-1.79496100	0.64765100
C	4.58606600	-3.44405100	-1.05601200
C	6.14434400	-2.16740000	0.84255200
C	5.90590400	-3.83653800	-0.87605400
C	6.68736600	-3.19469800	0.07806800
F	-4.83057400	1.17643700	1.95265500
F	-7.43915400	1.57311300	2.50663700
F	-9.35262000	0.37037500	0.99240800
F	-8.63984400	-1.23515300	-1.08573700
F	-6.03409700	-1.64228500	-1.64638200
F	4.33104100	-0.79957600	1.39166900
F	6.89483200	-1.55150500	1.75793300
F	7.95426300	-3.55978900	0.25762100
F	6.43007900	-4.81371300	-1.61601300
F	3.86675600	-4.06931400	-1.99209200
F	-5.32694800	-3.19375800	0.58792200
F	-3.25865400	-5.28686500	0.59054500
F	-0.05522400	-6.05280200	0.48221000
F	2.72868600	-5.09272600	0.30856500
F	4.52927100	0.17610600	-1.30733500
F	3.07799600	2.61009100	-1.83373400
F	-2.35939400	3.99624500	-1.23726400
F	-4.71903300	2.43393200	-0.59786700
H	0.08798000	5.67330400	-4.29452200
H	1.83271700	7.15944400	0.23182100
H	3.17645900	7.02288100	-0.88104600
H	5.80545200	5.55199500	2.84964800
O	-0.46562600	0.34300700	2.03756400
H	0.47491800	0.65833000	2.03857200
O	2.65803900	1.91583200	3.75325800
H	2.99698200	2.67635000	4.25318900

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OOH$} (quartet)

Energy: -4258.35789897 a.u.

C	-4.01996500	-3.03789400	0.41602900
C	-3.04473300	-4.00216300	0.51027100
C	-1.81522600	-3.37316400	0.21906000
N	-2.08011200	-2.03429900	-0.05911000
C	-0.46209900	-3.67803800	0.16939300
C	0.40490400	-4.76329300	0.43483200
N	0.32139400	-2.58788500	-0.17866900
C	1.68850600	-4.30243200	0.26632500
C	1.62751300	-2.91940100	-0.12147600
C	2.63503200	-1.96885300	-0.41277900

C	-3.39992000	-1.78543900	0.05805000
C	-3.92541500	-0.49003400	-0.11300900
C	-3.09244400	0.58854400	-0.44884600
C	-3.50682100	1.93526600	-0.69766700
N	-1.71467900	0.54817800	-0.63497400
C	-2.40688600	2.67302200	-1.00325600
C	-1.26471200	1.80225800	-0.97280600
C	0.06821100	2.14731800	-1.23415100
C	1.13323400	1.23453900	-1.14000900
C	2.50521200	1.47470900	-1.48712500
N	1.04044000	-0.05861100	-0.69661600
C	3.21233500	0.34389800	-1.23419200
C	2.31294900	-0.64875400	-0.74213800
C	0.38069900	3.53861500	-1.65513200
C	1.14638300	4.37517500	-0.83363700
C	-0.03341700	4.04421200	-2.88761800
C	1.51398200	5.66372500	-1.20774100
C	0.31711900	5.32932600	-3.28874400
H	-0.63028300	3.40731100	-3.53895700
C	2.55346800	4.39598400	1.06628600
C	1.09119300	6.12705400	-2.45401900
C	3.10399400	3.64419200	2.12271100
C	2.99973400	5.69424000	0.79652600
H	1.37609900	7.13215800	-2.76571700
C	4.12947100	4.21094600	2.88913700
C	4.04088400	6.20987100	1.56684000
C	4.61148600	5.48152400	2.60611600
H	4.59443200	3.62059200	3.67883800
H	4.40177300	7.21492800	1.34689700
C	2.32495200	6.51113300	-0.26957300
O	1.53698700	3.82174000	0.37094600
C	2.64911200	2.25973800	2.39628200
O	2.32357700	1.46011800	1.54071400
Co	-0.58024000	-0.92958500	-0.22902200
O	-0.54010100	-0.74649800	1.77316100
C	-5.37769700	-0.28596900	0.07422500
C	-6.30906800	-0.94310300	-0.73214700
C	-5.88343500	0.54079200	1.07980000
C	-7.67756000	-0.79130500	-0.55431700
C	-7.24694800	0.71659600	1.27215800
C	-8.14732300	0.04542600	0.45171100
C	4.04690000	-2.39759400	-0.37578900
C	4.97563600	-1.78712000	0.47129400
C	4.51147700	-3.44743200	-1.17133600
C	6.29934300	-2.19909600	0.53086700
C	5.82893900	-3.88249200	-1.12467100

C	6.72644800	-3.25398700	-0.26861500
F	-5.04370000	1.19895100	1.88388400
F	-7.69835300	1.51556800	2.24013200
F	-9.45681900	0.20434800	0.62866900
F	-8.54056900	-1.43317800	-1.34283400
F	-5.88603600	-1.75290100	-1.70922500
F	4.59668500	-0.76869000	1.24873800
F	7.16206000	-1.59629000	1.35083100
F	7.99306700	-3.65850100	-0.21607500
F	6.24004000	-4.88641700	-1.89980400
F	3.67517000	-4.06172800	-2.01430800
F	-5.31618000	-3.23250700	0.62779200
F	-3.21610800	-5.28378100	0.81351300
F	0.03579900	-5.98972800	0.78559100
F	2.79646800	-5.01880500	0.44061400
F	4.51645000	0.18432000	-1.45622000
F	3.01725700	2.60395700	-1.96857100
F	-2.40893600	3.97517100	-1.27164600
F	-4.75614900	2.39639000	-0.66583800
H	-0.00615200	5.70487500	-4.25690100
H	1.67667300	7.26625600	0.20776200
H	3.07227500	7.09153300	-0.83014700
H	5.42738600	5.90139200	3.18882700
O	0.55301300	-0.38895700	2.48937300
H	1.17195500	0.08795000	1.86974200
O	2.63626100	1.87890400	3.69153700
H	2.79112000	2.64880700	4.26305900

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OOH(H_2O)$} (doublet)

Energy: -4334.81070112 a.u.

C	-3.96292200	-3.06938600	0.27703200
C	-2.95888600	-4.01022300	0.33227500
C	-1.77011400	-3.37268600	-0.07863500
N	-2.06922500	-2.07806300	-0.42334500
C	-0.39115200	-3.64069800	-0.09805600
C	0.49926300	-4.69468200	0.22345700
N	0.34632600	-2.54762900	-0.43577200
C	1.77425200	-4.19542300	0.09702600
C	1.67841900	-2.82923200	-0.32124300
C	2.63503400	-1.84980300	-0.59481600
C	-3.39958700	-1.83429400	-0.16398500
C	-3.93927100	-0.55123000	-0.24737600
C	-3.14063600	0.56650100	-0.58927500
C	-3.59835000	1.90319400	-0.79221100
N	-1.78253900	0.55180000	-0.81513100

C	-2.52258700	2.67839000	-1.10217800
C	-1.37097400	1.83315100	-1.11595800
C	-0.04357800	2.21112500	-1.36729400
C	1.03765100	1.31719300	-1.34863700
C	2.40416700	1.62847700	-1.59867200
N	0.96716000	-0.02424700	-1.01334200
C	3.14032000	0.50655200	-1.36097100
C	2.25731000	-0.53691800	-0.96449900
C	0.25586500	3.64171500	-1.64054700
C	0.98744800	4.38986500	-0.70981000
C	-0.11785300	4.26344200	-2.83214300
C	1.36746800	5.70724900	-0.94451100
C	0.25112400	5.57925900	-3.09211200
H	-0.69030600	3.69636700	-3.56464600
C	2.41560200	4.16223500	1.15698500
C	0.99523400	6.28978500	-2.15546200
C	3.03109500	3.25818000	2.04929800
C	2.88555700	5.47250800	1.01037500
H	1.29310500	7.31843300	-2.35941600
C	4.14341500	3.70234400	2.77729100
C	4.00545100	5.86269700	1.74004800
C	4.63608300	4.98890100	2.62153600
H	4.61848800	3.00567400	3.46180700
H	4.37904200	6.88006000	1.61854400
C	2.14450000	6.42995200	0.11722000
O	1.33127900	3.72794100	0.44746300
C	2.54235700	1.87297000	2.22579400
O	1.61180700	1.37878600	1.59182600
Co	-0.59855600	-0.90272700	-0.39515700
O	-0.39867000	-0.79347300	1.45619500
C	-5.37096700	-0.36186400	0.06163100
C	-6.36491800	-1.02115400	-0.66567100
C	-5.79033500	0.46511000	1.10711000
C	-7.71363400	-0.86586700	-0.37593000
C	-7.13246400	0.63593900	1.41504600
C	-8.09754400	-0.03338300	0.66971200
C	4.06446300	-2.19782800	-0.47124600
C	4.91859100	-1.51426200	0.39906100
C	4.61867300	-3.24801400	-1.20825200
C	6.25409200	-1.86308800	0.54198800
C	5.95102000	-3.61584200	-1.08031500
C	6.77126000	-2.92036400	-0.19912000
F	-4.88695100	1.12029200	1.83913200
F	-7.50182700	1.42965900	2.41987400
F	-9.38639200	0.12311600	0.95701200
F	-8.63923100	-1.50230800	-1.09331200

F	-6.02680400	-1.82681600	-1.67648600
F	4.46250800	-0.48082300	1.10911300
F	7.04291100	-1.19265500	1.38183700
F	8.05021400	-3.26131600	-0.06976400
F	6.44916600	-4.62058800	-1.80059300
F	3.86215500	-3.92525000	-2.07684500
O	3.21327000	1.18350100	3.14374700
H	2.84774900	0.24787700	3.11296100
F	-5.23218200	-3.28014600	0.61256800
F	-3.07483500	-5.27769300	0.70937600
F	0.15531400	-5.92946400	0.57219100
F	2.89558400	-4.88054900	0.30596800
F	4.45805400	0.41080600	-1.52398400
F	2.90821300	2.79691600	-1.98569600
F	-2.56447500	3.98307300	-1.35586300
F	-4.86001300	2.32673400	-0.73388400
H	-0.03557800	6.04802900	-4.03059200
H	1.45792700	7.04186000	0.72808500
H	2.84294100	7.14612400	-0.33770000
H	5.50666600	5.31387800	3.18617800
O	2.10179000	-1.26326300	2.77717900
H	1.36594700	-0.99040900	2.18861800
O	-0.87499900	0.40658400	2.01925700
H	-0.06756000	0.97328200	1.94090800
H	1.65235900	-1.70107200	3.51272700

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OOH(H_2O)$} (quartet)

Energy: -4334.79863092 a.u.

C	-3.99126200	-3.06658800	0.25589900
C	-2.99131200	-4.01893900	0.29377700
C	-1.80483200	-3.37758400	-0.10750400
N	-2.09791200	-2.08163900	-0.43153700
C	-0.41278400	-3.64920000	-0.10996500
C	0.46106900	-4.71785200	0.19168000
N	0.33441600	-2.55404900	-0.40449000
C	1.74398400	-4.22244100	0.08809500
C	1.66063700	-2.84458500	-0.29935300
C	2.63061800	-1.86600200	-0.54785000
C	-3.41777100	-1.83051000	-0.17511600
C	-3.94294800	-0.53316900	-0.23442100
C	-3.13081700	0.59025400	-0.54692300
C	-3.58612700	1.92621500	-0.77448300
N	-1.76881700	0.58140200	-0.72178100
C	-2.50507500	2.69861200	-1.07175200
C	-1.35089800	1.85240500	-1.05273500

C	-0.02124100	2.22278200	-1.31092100
C	1.06971800	1.32439900	-1.26946300
C	2.43475100	1.62524000	-1.53893400
N	0.99690200	-0.00076400	-0.91301300
C	3.16470700	0.49292500	-1.30610700
C	2.27221500	-0.53522000	-0.89476400
C	0.28078800	3.64270300	-1.62998900
C	1.02887200	4.40732000	-0.72615900
C	-0.09261100	4.23665100	-2.83627800
C	1.44034400	5.70667000	-1.00239100
C	0.30186100	5.53665500	-3.13613700
H	-0.67931400	3.65998200	-3.54978500
C	2.45964000	4.19226200	1.13583200
C	1.07157300	6.25899400	-2.22842900
C	3.05573900	3.28586700	2.03691700
C	2.97145400	5.48030700	0.94502600
H	1.39127400	7.27316400	-2.46862800
C	4.19655600	3.70507900	2.73332400
C	4.11604700	5.84767800	1.64810700
C	4.72945600	4.97121900	2.53960300
H	4.66034900	3.00694600	3.42436400
H	4.52468700	6.84742000	1.49686700
C	2.24757500	6.43563900	0.03384700
O	1.35352500	3.77624000	0.44947600
C	2.51178600	1.92334900	2.24531400
O	1.50966900	1.48866700	1.68551900
Co	-0.60822200	-0.90797900	-0.39385600
O	-0.46631700	-0.77553800	1.54014200
C	-5.37461000	-0.33596400	0.05930500
C	-6.36693000	-0.99986500	-0.66814700
C	-5.79964900	0.50534300	1.09275600
C	-7.71678400	-0.83564800	-0.39070900
C	-7.14319000	0.68271100	1.38948700
C	-8.10518400	0.00887300	0.64388900
C	4.05491000	-2.23390900	-0.44248600
C	4.92697100	-1.56633900	0.42396700
C	4.59013500	-3.28276600	-1.19672700
C	6.25960100	-1.93275200	0.54881300
C	5.91982900	-3.66513400	-1.08880000
C	6.75694100	-2.98795200	-0.20892000
F	-4.90086700	1.16358900	1.82560100
F	-7.51733800	1.48648100	2.38393200
F	-9.39502100	0.17260800	0.91999600
F	-8.63950300	-1.47415300	-1.10949200
F	-6.02636200	-1.81360800	-1.67132500
F	4.49097700	-0.53655600	1.14887400

F	7.06533300	-1.28096800	1.38657500
F	8.03292400	-3.34387700	-0.09690200
F	6.39924800	-4.66594300	-1.82670200
F	3.81884300	-3.94126300	-2.06656400
O	3.21930700	1.19190500	3.10186200
H	2.81212200	0.27144800	3.08103700
F	-5.26078900	-3.27951400	0.58356300
F	-3.11868700	-5.28919500	0.66022400
F	0.11007300	-5.95901100	0.51033100
F	2.85485300	-4.92232000	0.29194900
F	4.47993900	0.38674400	-1.48196000
F	2.94866600	2.78395800	-1.94190500
F	-2.54137300	3.99969100	-1.34322600
F	-4.84934600	2.34925500	-0.74593500
H	0.01770700	5.98351100	-4.08602800
H	1.58355200	7.08120600	0.63483900
H	2.96053700	7.12050900	-0.44600700
H	5.62026700	5.27839000	3.08237600
O	2.03024000	-1.21372600	2.75773600
H	1.24196200	-0.95181500	2.22518400
O	-0.97268000	0.42212000	2.10155300
H	-0.18172500	1.00503200	2.01999600
H	1.64182600	-1.66201400	3.52095100

{$H^{+\bullet}{}_{\delta}{}^{F}CX–CO_2H–Co^{III}–OOH(H_2O)$} (sextet)

Energy: -4334.78922355 a.u.

C	-4.10280900	-3.03603000	0.42182800
C	-3.10331900	-3.97796800	0.55314800
C	-1.87418200	-3.29657400	0.38110700
N	-2.13707900	-1.99014000	0.14467100
C	-0.47770200	-3.60028100	0.36871000
C	0.35772500	-4.73233600	0.43816400
N	0.30169300	-2.50821000	0.14570500
C	1.65368300	-4.28797800	0.22908200
C	1.60844900	-2.87641800	0.00850400
C	2.59159100	-1.93292800	-0.33812700
C	-3.48276400	-1.77011000	0.14639300
C	-3.99782300	-0.49071100	-0.08983800
C	-3.16283300	0.62427300	-0.41420100
C	-3.59631500	1.94872000	-0.71823000
N	-1.79430700	0.60125200	-0.53440000
C	-2.49172300	2.70376200	-1.00103400
C	-1.34620700	1.85133100	-0.90543500
C	0.00613700	2.19902100	-1.11488800
C	1.11088000	1.30944200	-0.99078600

C	2.46652500	1.56298100	-1.35228700
N	1.03710100	0.01578800	-0.54379400
C	3.18046200	0.41587100	-1.12451600
C	2.28498700	-0.57014700	-0.61731000
C	0.31331800	3.58664300	-1.54187400
C	1.11279200	4.40942200	-0.73799100
C	-0.11777100	4.09676100	-2.76914900
C	1.50299000	5.68700900	-1.12639200
C	0.26225500	5.36802300	-3.18354900
H	-0.73905600	3.47167500	-3.40859100
C	2.67637100	4.31608400	1.01926100
C	1.07346600	6.15260900	-2.36805300
C	3.36846800	3.45089600	1.88911900
C	3.16982600	5.58707500	0.70682400
H	1.37891200	7.14692000	-2.69416200
C	4.58458200	3.89012300	2.42770900
C	4.38372200	5.98216200	1.26317300
C	5.09169900	5.14439000	2.12106300
H	5.12415800	3.21983700	3.09105700
H	4.77443100	6.97046300	1.01890400
C	2.35624100	6.48655700	-0.18363900
O	1.50925800	3.86779300	0.46286000
C	2.84220600	2.11219400	2.23911800
O	1.68567900	1.74969300	2.04894600
Co	-0.58227500	-0.74070500	0.35496900
O	-0.39916000	-0.37601500	2.18164600
C	-5.46223300	-0.29926700	-0.01863200
C	-6.32677400	-0.98081400	-0.87799100
C	-6.04206200	0.54846600	0.92834500
C	-7.70493100	-0.82884200	-0.80567300
C	-7.41630900	0.71811300	1.01838100
C	-8.25025300	0.02430200	0.14734700
C	3.98555700	-2.40215300	-0.48950400
C	5.03010200	-1.88039300	0.27891500
C	4.31445500	-3.40243400	-1.40917800
C	6.33464100	-2.33736200	0.15188600
C	5.61162800	-3.87469500	-1.55336700
C	6.62569300	-3.34017800	-0.76659800
F	-5.26319300	1.22538300	1.77500100
F	-7.94151200	1.53356700	1.93230600
F	-9.56881500	0.17775900	0.22527100
F	-8.50494100	-1.48705000	-1.64409900
F	-5.83135500	-1.80119100	-1.80877800
F	4.79131300	-0.90595200	1.15562400
F	7.30818200	-1.82202100	0.90259300
F	7.87261400	-3.78344500	-0.89589800

F	5.89105700	-4.82642500	-2.44350500
F	3.36813900	-3.92633700	-2.19383200
O	3.75169000	1.31602800	2.79236000
H	3.30030800	0.43041600	2.93825300
F	-5.40594300	-3.28103900	0.52290500
F	-3.26285200	-5.27497100	0.79632300
F	-0.01631000	-5.99004200	0.64881300
F	2.73024500	-5.06840200	0.22650700
F	4.47612300	0.26773200	-1.39476200
F	2.98706000	2.68092700	-1.85537200
F	-2.52626200	3.99825400	-1.30203700
F	-4.84968000	2.40018600	-0.75346800
H	-0.06661300	5.74466300	-4.14925400
H	1.71489600	7.13560000	0.43790400
H	3.01138300	7.17014500	-0.74060700
H	6.03704700	5.47102500	2.54769700
O	2.31665800	-0.97057300	2.90244000
H	1.46133200	-0.58954500	2.60677700
O	-0.88196200	0.95517700	2.33422800
H	-0.03545200	1.46173400	2.28367500
H	2.09947400	-1.40562300	3.73777400

{H$_{\beta}^{F}$CX–CO$_2$H–Co^{III}–OO$^{\bullet-}$(H$_2$O)}$^{-}$ (doublet)

Energy: -4334.32635317 a.u.

C	-3.93446300	-3.06540600	0.40187300
C	-2.92375200	-3.99441900	0.49632400
C	-1.73660200	-3.36664500	0.05422900
N	-2.05585000	-2.09344600	-0.33076000
C	-0.35498400	-3.62485200	0.00692700
C	0.55336400	-4.63653800	0.39255800
N	0.37387600	-2.55365300	-0.43216900
C	1.82250700	-4.13953500	0.20140700
C	1.71065300	-2.81275600	-0.31688500
C	2.66723000	-1.84062700	-0.64730100
C	-3.37717300	-1.84682100	-0.09584700
C	-3.92104900	-0.56362600	-0.25917700
C	-3.13130000	0.54214000	-0.63979100
C	-3.58250300	1.88153800	-0.84748400
N	-1.76635000	0.53615200	-0.86975200
C	-2.50659500	2.65921700	-1.14586700
C	-1.34918500	1.81807100	-1.16436400
C	-0.01972400	2.19419400	-1.41654700
C	1.06595700	1.30655600	-1.40475800
C	2.42344000	1.60882200	-1.73321900
N	1.01071000	-0.01738300	-1.03165300

C	3.16184300	0.48855800	-1.51952600
C	2.29198100	-0.54202600	-1.04644800
C	0.27476800	3.62782500	-1.67716100
C	1.00266100	4.38529300	-0.74530100
C	-0.13460600	4.26058300	-2.84997000
C	1.29980400	5.72944400	-0.95464200
C	0.16669700	5.59703300	-3.09271600
H	-0.70024400	3.68125500	-3.57843000
C	2.31873600	4.26844000	1.23001100
C	0.87970800	6.32184800	-2.14605100
C	2.88136300	3.45114600	2.23567100
C	2.66413300	5.62459800	1.13627100
H	1.11719500	7.37244300	-2.32046700
C	3.77742400	4.03381000	3.13798500
C	3.58555000	6.14983700	2.03894200
C	4.14248200	5.36793500	3.04436200
H	4.18549200	3.38642000	3.91024000
H	3.85480600	7.20382100	1.94934400
C	2.01939100	6.50803800	0.10564600
O	1.40619400	3.70881300	0.38530500
C	2.63292100	1.99344600	2.43825700
O	2.97643200	1.42982000	3.47605300
Co	-0.58466300	-0.92676900	-0.51288700
O	-0.50158600	-0.55421300	1.36789300
C	-5.35922100	-0.37704000	0.02899400
C	-6.34031600	-1.07297500	-0.68150700
C	-5.80884800	0.46734600	1.04762200
C	-7.69444200	-0.93756100	-0.40447900
C	-7.15722000	0.62760500	1.33654400
C	-8.10519200	-0.08052400	0.60831500
C	4.09850600	-2.17899300	-0.51576500
C	4.96928300	-1.44778800	0.30122300
C	4.65117300	-3.27113900	-1.19143100
C	6.30732600	-1.79061400	0.44610400
C	5.98302800	-3.63752700	-1.05302900
C	6.81608700	-2.89299600	-0.22882600
F	-4.93114500	1.15743800	1.78131700
F	-7.55137300	1.44628800	2.31907500
F	-9.40598700	0.06266900	0.88116800
F	-8.60644300	-1.61589000	-1.11160800
F	-5.99009200	-1.90382200	-1.66920500
F	4.54116600	-0.36942900	0.96074100
F	7.11178000	-1.07020200	1.23629100
F	8.10217300	-3.23145500	-0.09127300
F	6.47432900	-4.69006900	-1.71904000
F	3.89411500	-4.00175400	-2.01817400

O	2.06350600	1.37214500	1.41987500
H	2.02470400	0.39454400	1.64590200
F	-5.21909600	-3.28100100	0.72428200
F	-3.04105500	-5.25689400	0.92030300
F	0.23634300	-5.85162300	0.85222100
F	2.95720700	-4.80778300	0.45124800
F	4.47643900	0.37112400	-1.75077200
F	2.90107400	2.77535700	-2.18476400
F	-2.55853800	3.97556700	-1.38332200
F	-4.84970800	2.31582300	-0.78621000
H	-0.15497600	6.07067000	-4.01833300
H	1.31310100	7.19654400	0.60300900
H	2.77626500	7.16419700	-0.35210700
H	4.85478300	5.79573400	3.74686900
O	2.22544800	-1.10867300	2.51035200
H	2.51934300	-0.53716500	3.24508600
O	-0.60882400	-1.52452100	2.18607800
H	1.31364900	-1.37092000	2.72517600

{H$_6$^{F}CX–CO$_2$H–Co^{III}–OO$^{\bullet-}$(H$_2$O)}$^{-}$ (quartet)

Energy: -4334.31567786 a.u.

C	-3.90972600	-3.04325800	0.43714300
C	-2.89696300	-3.97098000	0.54292600
C	-1.71189400	-3.34474400	0.10269300
N	-2.03652500	-2.06819700	-0.29263100
C	-0.33378500	-3.60446700	0.04196700
C	0.57767600	-4.63362700	0.36900200
N	0.39221500	-2.52350500	-0.38616100
C	1.84311600	-4.14278900	0.14301800
C	1.72453700	-2.80198200	-0.34059400
C	2.67844600	-1.82696700	-0.67526200
C	-3.35813500	-1.82666600	-0.07222900
C	-3.91202600	-0.54865400	-0.25938500
C	-3.12503700	0.55584000	-0.64728900
C	-3.58263000	1.89025700	-0.87781100
N	-1.75724800	0.55886900	-0.86038300
C	-2.50879500	2.67106300	-1.17459800
C	-1.34597500	1.83659500	-1.17407000
C	-0.01679900	2.21910100	-1.41609200
C	1.07304200	1.33609800	-1.38744100
C	2.43735400	1.65012900	-1.66551000
N	1.01691500	0.00317400	-1.03992800
C	3.17717500	0.52716600	-1.46039000
C	2.30458400	-0.52093500	-1.04131100
C	0.27893500	3.65661700	-1.65387700

C	0.98599800	4.40100100	-0.69667500
C	-0.09958400	4.30741700	-2.82751500
C	1.30363100	5.74327000	-0.88499800
C	0.21690600	5.64456700	-3.04716500
H	-0.65060400	3.74081400	-3.57685000
C	2.32451900	4.22321500	1.25496000
C	0.91751700	6.35326000	-2.07864500
C	2.91096500	3.36947100	2.21603500
C	2.70508200	5.57117600	1.16998200
H	1.17093600	7.40247700	-2.23794000
C	3.88034100	3.90527000	3.07162600
C	3.69510800	6.04865100	2.02416900
C	4.28589600	5.22721700	2.97832300
H	4.31104000	3.22995200	3.80672100
H	3.99191400	7.09561400	1.94011100
C	2.01109000	6.49110500	0.20521900
O	1.35735000	3.71409700	0.44052200
C	2.61422200	1.92155800	2.41864700
O	3.05662200	1.31185900	3.39154500
Co	-0.57759000	-0.92326400	-0.60675000
O	-0.72854500	-0.51114000	1.71022200
C	-5.35539000	-0.37231800	0.00543500
C	-6.31892000	-1.09556300	-0.70243400
C	-5.83034800	0.48663100	1.00062800
C	-7.67814600	-0.97297300	-0.44567700
C	-7.18455700	0.63613900	1.26747100
C	-8.11372700	-0.09968200	0.54242500
C	4.10920100	-2.17013100	-0.55121300
C	4.96432100	-1.47822500	0.31338300
C	4.67174600	-3.22864600	-1.26876000
C	6.30277100	-1.81926200	0.45697000
C	6.00416500	-3.59471000	-1.13282300
C	6.82456000	-2.88491300	-0.26599200
F	-4.97199500	1.20185400	1.73322600
F	-7.60259500	1.47011100	2.22743000
F	-9.42011100	0.03209300	0.79469900
F	-8.57182700	-1.67903300	-1.14945800
F	-5.94567000	-1.94327100	-1.66765000
F	4.51417600	-0.44140400	1.02489600
F	7.09400600	-1.13572100	1.29207100
F	8.11136000	-3.22269500	-0.13120800
F	6.50786400	-4.61407000	-1.83994900
F	3.92286500	-3.92675600	-2.13011200
O	1.87675700	1.35861200	1.47624400
H	1.81419200	0.37991700	1.68238400
F	-5.19081000	-3.25834800	0.76915400

F	-3.01235600	-5.22642700	0.98876400
F	0.26408700	-5.85305200	0.82110200
F	2.98240700	-4.82045400	0.34514400
F	4.50048000	0.43262900	-1.64818500
F	2.92988900	2.83076100	-2.06077100
F	-2.56514900	3.98452100	-1.42754400
F	-4.85217600	2.31921300	-0.82824100
H	-0.08049900	6.13105700	-3.97428800
H	1.28674600	7.11856000	0.75525600
H	2.73317800	7.20202900	-0.22452000
H	5.05390100	5.61671200	3.64341800
O	2.07163000	-1.16066300	2.48827500
H	2.51409200	-0.61126100	3.16465400
O	-0.95347800	-1.49735000	2.45435600
H	1.20707500	-1.39095800	2.86182000

{H$_6$^{F}CX–CO$_2$–Co^{III}–OO$^{\bullet-}$(H$_2$O)}$^{2-}$ (doublet)

Energy: -4333.69760314 a.u.

C	-4.13381700	-2.94535300	0.33338900
C	-3.16124200	-3.91858700	0.40925500
C	-1.93662800	-3.31583500	0.05084200
N	-2.19476900	-2.00997400	-0.26840800
C	-0.56335700	-3.62620700	0.02996200
C	0.29241400	-4.71200400	0.31360200
N	0.22061000	-2.55734500	-0.30593600
C	1.58547700	-4.26534700	0.15643200
C	1.54043100	-2.89399900	-0.23807400
C	2.54103700	-1.94777900	-0.51514800
C	-3.51437600	-1.72583200	-0.07363900
C	-4.00005900	-0.41048900	-0.18840000
C	-3.15339100	0.68050200	-0.48263400
C	-3.54558900	2.04127500	-0.65731000
N	-1.78255800	0.63258600	-0.67065900
C	-2.43397100	2.78708300	-0.90293100
C	-1.30722100	1.90315000	-0.91997800
C	0.04268700	2.23346800	-1.13935000
C	1.09759400	1.30920400	-1.09012700
C	2.46993900	1.55493000	-1.41684900
N	0.97945600	-0.02045800	-0.75890400
C	3.14900200	0.39558100	-1.24823100
C	2.23080500	-0.60712300	-0.80589800
C	0.36361200	3.64044800	-1.49065900
C	1.17810800	4.43562500	-0.66496700
C	-0.11844100	4.20513000	-2.67274700
C	1.48517300	5.75624200	-1.00446700

C	0.19308800	5.51099800	-3.03793800
H	-0.74859500	3.58944900	-3.31456100
C	2.80588500	4.35391600	1.05094600
C	0.99481700	6.27827100	-2.20010100
C	3.53974800	3.52365600	1.91619700
C	3.18950400	5.67845800	0.78993400
H	1.24804400	7.30714000	-2.46536000
C	4.69828400	4.07578700	2.47298000
C	4.36874600	6.16693700	1.34786900
C	5.13269200	5.36466500	2.18818300
H	5.23488100	3.41950600	3.15631200
H	4.66855300	7.19414400	1.12492100
C	2.30097600	6.56104800	-0.04008800
O	1.65299600	3.84897000	0.47082700
C	3.21124400	2.06460200	2.33309100
O	3.83294800	1.67124700	3.34211300
Co	-0.66582000	-0.89070900	-0.35056300
O	-0.68525500	-0.60106600	1.58339800
C	-5.43866600	-0.18117600	0.05026400
C	-6.41883900	-0.81499200	-0.72002900
C	-5.90368000	0.64481500	1.07956000
C	-7.77725100	-0.64182500	-0.48950300
C	-7.25656900	0.84413300	1.32031400
C	-8.19982800	0.19519100	0.53418900
C	3.95037300	-2.38556200	-0.46907000
C	4.90624700	-1.77708800	0.35851300
C	4.39367600	-3.46020200	-1.24599500
C	6.21794300	-2.23826500	0.41748500
C	5.69504800	-3.93838200	-1.19204900
C	6.61237600	-3.32432200	-0.35184800
F	-5.03849600	1.27556200	1.87679400
F	-7.66393200	1.64184800	2.31910000
F	-9.50946100	0.37667100	0.76130400
F	-8.68729800	-1.26078000	-1.25881200
F	-6.06567100	-1.61700600	-1.73154100
F	4.60218400	-0.71949800	1.09066400
F	7.11446900	-1.64252800	1.21420100
F	7.87666200	-3.77195200	-0.29266600
F	6.07862400	-4.97448500	-1.95880900
F	3.55637000	-4.06914100	-2.09942600
O	2.39126000	1.43349700	1.61536100
F	-5.44311100	-3.13542000	0.59609200
F	-3.34806400	-5.20223500	0.75615700
F	-0.08590800	-5.95331300	0.66062900
F	2.68320400	-5.01943300	0.33494500
F	4.45573800	0.22073000	-1.49727700

F	3.00959200	2.70580300	-1.83742700
F	-2.44259200	4.11630800	-1.07997000
F	-4.80106100	2.52736100	-0.61183100
H	-0.18605700	5.92504000	-3.97154400
H	1.62685200	7.13986000	0.62008000
H	2.89764500	7.31718400	-0.57458800
H	6.05471700	5.74876800	2.62720200
O	2.27470100	-1.29179100	2.49904500
H	2.40882400	-0.34082000	2.26724000
O	-0.92704600	-1.58317200	2.33662600
H	1.33104700	-1.32117800	2.69486100

$\{H^{F}CX–CO_2–Co^{III}–OO^{\bullet-}(H_2O)\}^{2-}$ (quartet)

Energy: -4333.69018491 a.u.

C	-4.07471200	-2.98115500	0.35614000
C	-3.10844000	-3.95934800	0.45034500
C	-1.87307600	-3.35858100	0.13240300
N	-2.11998900	-2.04371400	-0.18097400
C	-0.50382600	-3.67575500	0.11871400
C	0.34665800	-4.77816900	0.35215100
N	0.28722800	-2.60110700	-0.19078400
C	1.64006100	-4.33835700	0.18229900
C	1.60058400	-2.95381100	-0.17137700
C	2.60496300	-2.01433400	-0.46155400
C	-3.44317500	-1.75969100	-0.02796500
C	-3.92590100	-0.44396200	-0.16445600
C	-3.07037300	0.64154400	-0.45438400
C	-3.46205500	1.99225200	-0.70135800
N	-1.69441200	0.59214100	-0.60311800
C	-2.34912600	2.72628400	-0.97550200
C	-1.22125800	1.84594500	-0.93038900
C	0.12639700	2.16930800	-1.16723800
C	1.18292400	1.25199300	-1.06195300
C	2.56388700	1.49460800	-1.34482100
N	1.05594700	-0.07499500	-0.71500300
C	3.23632800	0.33304000	-1.15850400
C	2.30777200	-0.66909900	-0.74164500
C	0.43359900	3.55064800	-1.62608500
C	1.17574700	4.44530300	-0.83538600
C	-0.00234000	3.98918700	-2.87685100
C	1.46697200	5.73900600	-1.27849900
C	0.29017300	5.26728900	-3.34395300
H	-0.58065400	3.29727600	-3.48937600
C	2.64613300	4.61077500	1.01189200
C	1.02496300	6.13200900	-2.54125200

C	3.29040400	3.90982500	2.04280600
C	3.00386600	5.91953500	0.66528700
H	1.26253400	7.14043200	-2.88752400
C	4.32361400	4.57475300	2.70772400
C	4.07608300	6.52079400	1.32425900
C	4.74162200	5.85111100	2.34576300
H	4.78173400	4.03621600	3.53629900
H	4.36592300	7.53473600	1.03765800
C	2.20456900	6.66899400	-0.36251100
O	1.59412800	3.97690100	0.37303600
C	2.96291000	2.47772400	2.50304200
O	3.08235100	2.28778300	3.72922300
Co	-0.58934400	-0.94664400	-0.35843300
O	-1.04321400	-0.74129900	2.09909300
C	-5.37146900	-0.21312100	0.01962800
C	-6.32445900	-0.86539100	-0.76975100
C	-5.87353100	0.63543600	1.01308300
C	-7.69017600	-0.69265300	-0.58770300
C	-7.23425000	0.83613500	1.20352600
C	-8.14917200	0.16598400	0.40170000
C	4.00987300	-2.46911500	-0.43773400
C	4.96048700	-1.90986600	0.42687200
C	4.45017200	-3.51103400	-1.25811300
C	6.27195500	-2.37081100	0.46942400
C	5.75146900	-3.99263200	-1.22120100
C	6.66763900	-3.41841200	-0.35162100
F	-5.03714200	1.28740600	1.82398900
F	-7.67709500	1.65543300	2.16947500
F	-9.46642400	0.34790600	0.58049100
F	-8.57245000	-1.33154000	-1.37309100
F	-5.93657300	-1.68510500	-1.75434600
F	4.63707100	-0.90344100	1.22478100
F	7.16316100	-1.82065000	1.30548800
F	7.93067700	-3.87080900	-0.30913100
F	6.13639600	-4.99552900	-2.02947900
F	3.61024600	-4.08312300	-2.13281100
O	2.66631900	1.66634600	1.58436800
F	-5.38862700	-3.16742200	0.59336300
F	-3.30739700	-5.24328900	0.79001100
F	-0.03807900	-6.02315200	0.67890000
F	2.73804400	-5.10255200	0.32455500
F	4.55524900	0.16722400	-1.34435600
F	3.12095100	2.65045200	-1.71942500
F	-2.35179800	4.04332000	-1.22671500
F	-4.71841500	2.47742500	-0.69311300
H	-0.05171200	5.58353900	-4.32878600

H	1.48281900	7.33951400	0.14201100
H	2.85729300	7.34132700	-0.94280800
H	5.57222400	6.33043100	2.86600000
O	1.96104500	-0.89248500	2.46060700
H	2.31265800	-0.00315900	2.20263700
O	-1.57812500	-1.71507800	2.65509300
H	1.06099500	-0.67262700	2.73059600

{H$_b$^{F}CX–CO$_2$–Co^{III}– OO$^{\bullet-}$}•H$_2$O‡ (doublet)

Energy: -4410.11841395 a.u.

C	-4.10341200	-2.95851200	0.33139600
C	-3.11762600	-3.91855200	0.40860800
C	-1.88992100	-3.28435700	0.11754500
N	-2.15477100	-1.96685100	-0.13543600
C	-0.51421300	-3.58440000	0.05633800
C	0.35917000	-4.66305500	0.31583200
N	0.25112500	-2.49926700	-0.26855100
C	1.64458200	-4.19852500	0.15212700
C	1.57644500	-2.82408900	-0.23358600
C	2.56043900	-1.87336000	-0.56334400
C	-3.48932500	-1.71671500	-0.01791800
C	-3.99868600	-0.41733800	-0.19537700
C	-3.17137100	0.67981000	-0.51905800
C	-3.58860900	2.03050600	-0.72245600
N	-1.80100000	0.65047700	-0.71472100
C	-2.49191400	2.78911600	-0.99228700
C	-1.35036000	1.92227700	-1.00281300
C	-0.00119900	2.26938000	-1.22053200
C	1.06649500	1.35688800	-1.17714000
C	2.43271300	1.61857400	-1.51961200
N	0.97199900	0.03239900	-0.82409600
C	3.12915200	0.46850500	-1.35292400
C	2.22983800	-0.54148200	-0.88368700
C	0.32444500	3.68955300	-1.51253200
C	1.13097300	4.44211600	-0.63909400
C	-0.12854500	4.31452400	-2.67568000
C	1.45937500	5.77179200	-0.90957100
C	0.20272500	5.63269400	-2.97341800
H	-0.75157400	3.73638200	-3.35760200
C	2.73624000	4.25817100	1.09424500
C	0.99716400	6.35376000	-2.08889300
C	3.46667700	3.37952400	1.91831100
C	3.13786500	5.58939900	0.90334000
H	1.26570300	7.39042400	-2.30326500
C	4.62670100	3.88873400	2.51012100

C	4.31583200	6.03750500	1.49647300
C	5.06824900	5.18923600	2.30071300
H	5.16575400	3.19121200	3.14853400
H	4.62617400	7.07166600	1.32788000
C	2.26627400	6.51948400	0.10756200
O	1.58046900	3.80257600	0.48519100
C	3.11487100	1.91348500	2.23213000
O	2.20176700	1.38710100	1.54518800
Co	-0.65823800	-0.85007300	-0.41722300
O	-0.49401200	-1.47973600	2.44798000
C	-5.45134400	-0.21659500	-0.01332900
C	-6.38462900	-0.87734700	-0.81749300
C	-5.97392600	0.60380000	0.99199700
C	-7.75485600	-0.73710300	-0.63985900
C	-7.34002800	0.77119500	1.17918800
C	-8.23604500	0.09464000	0.36166800
C	3.97317100	-2.30707600	-0.57894000
C	4.96753000	-1.68826100	0.19239400
C	4.38270500	-3.38935800	-1.36469500
C	6.28230600	-2.14247900	0.19251400
C	5.68717400	-3.86305500	-1.36780100
C	6.64299600	-3.23669400	-0.58150700
F	-5.15492400	1.26121100	1.81447600
F	-7.80600700	1.56563900	2.15519100
F	-9.55785600	0.24521400	0.53698100
F	-8.61981500	-1.38315600	-1.43870200
F	-5.97341400	-1.67464400	-1.81056600
F	4.69585400	-0.62028300	0.92502300
F	7.21427800	-1.53243900	0.93786400
F	7.91091400	-3.67851800	-0.58035600
F	6.03743100	-4.90604800	-2.14078900
F	3.50998500	-4.00849700	-2.17318100
O	3.79879400	1.38498700	3.14179700
F	-5.41885500	-3.17651500	0.54141800
F	-3.29421700	-5.21667300	0.70545000
F	-0.00074700	-5.90944300	0.66319600
F	2.75551600	-4.93847200	0.31364700
F	4.43491200	0.31107800	-1.62471800
F	2.95302100	2.77546900	-1.95606300
F	-2.52363700	4.11425500	-1.20749000
F	-4.85071500	2.49907100	-0.67628700
H	-0.15511400	6.09293100	-3.89371000
H	1.58659700	7.06581800	0.78882800
H	2.87530800	7.29851600	-0.37714400
H	5.98859700	5.54383000	2.76605100
O	2.58579500	-1.23762700	2.73693800

H	3.11888500	-0.48172900	3.06003300
O	-0.47877200	-2.64628100	2.81468500
H	2.09083900	-0.76024200	2.05197100
O	-0.49417900	1.26740500	2.03326400
H	0.48005800	1.14572600	2.05548800
H	-0.57129200	1.88956600	1.29763200

{$H_{\beta}^{F}CX–CO_2–Co^{III}–OO^{\bullet -}$}•$H_2O^{\ddagger}$ (quartet)

Energy: -4410.11744097 a.u.

C	-4.05422900	-2.98710200	0.39471100
C	-3.05168400	-3.92636700	0.50317000
C	-1.83412900	-3.27732600	0.20235200
N	-2.12125200	-1.97084600	-0.08299800
C	-0.45572700	-3.56040200	0.12905800
C	0.43600400	-4.62035100	0.40137600
N	0.29011700	-2.47574300	-0.24421400
C	1.71193800	-4.14474500	0.20040200
C	1.61972400	-2.78320200	-0.22414200
C	2.58717600	-1.82923300	-0.59164300
C	-3.46087800	-1.74416700	0.01469600
C	-3.99359000	-0.46089300	-0.20582100
C	-3.18429400	0.64024500	-0.55833000
C	-3.62101400	1.98229100	-0.77636200
N	-1.81446800	0.62725100	-0.76331500
C	-2.53578300	2.75359800	-1.05598100
C	-1.38207400	1.90308300	-1.06142500
C	-0.03745600	2.26816900	-1.27194800
C	1.04227100	1.37070600	-1.22752700
C	2.40305400	1.65329900	-1.57304100
N	0.96799900	0.04653800	-0.87365500
C	3.11542800	0.51092600	-1.41659400
C	2.23380900	-0.50954100	-0.93566000
C	0.27843400	3.69712700	-1.52473300
C	1.06151000	4.42939400	-0.61290600
C	-0.15912100	4.35172800	-2.67699500
C	1.37050100	5.77289800	-0.83221600
C	0.16000300	5.68280200	-2.92650000
H	-0.76191600	3.78758800	-3.38808400
C	2.63262200	4.21723900	1.15150100
C	0.92346100	6.38615300	-2.00160600
C	3.36746000	3.32815700	1.96142300
C	3.00855100	5.56311800	1.01285500
H	1.17877200	7.43374000	-2.17511800
C	4.50504300	3.84635500	2.58976700
C	4.16230900	6.01969600	1.64497400

C	4.91908400	5.16290800	2.43508300
H	5.05077400	3.13771000	3.20956000
H	4.45011000	7.06602100	1.51608600
C	2.13723200	6.50163400	0.22760000
O	1.50253600	3.75730300	0.49705100
C	3.05563800	1.84132700	2.23476100
O	2.11346000	1.31501900	1.58807300
Co	-0.64728800	-0.84668900	-0.44054600
O	-0.26968500	-1.33002400	2.46561300
C	-5.45018300	-0.28210900	-0.03000300
C	-6.36960900	-0.97820500	-0.81999400
C	-5.98914200	0.54795800	0.95856300
C	-7.74242500	-0.86153900	-0.64539700
C	-7.35848100	0.69268400	1.14157600
C	-8.24036400	-0.01863000	0.33832900
C	4.00468800	-2.24649400	-0.61572300
C	5.00599100	-1.59640200	0.12031800
C	4.41191300	-3.34828400	-1.37529700
C	6.32401900	-2.04112900	0.11325700
C	5.71970300	-3.81237300	-1.38467700
C	6.68230900	-3.15530600	-0.63270400
F	-5.18344900	1.23676300	1.76812600
F	-7.84112000	1.49807300	2.10040900
F	-9.56501400	0.10921300	0.51011100
F	-8.59419400	-1.54137400	-1.43028000
F	-5.94216500	-1.78906000	-1.79512800
F	4.74216200	-0.50504000	0.82033700
F	7.26264000	-1.40084300	0.82432800
F	7.95419800	-3.58606600	-0.63890000
F	6.06589100	-4.87547000	-2.13187700
F	3.53210700	-3.99851700	-2.15158000
O	3.80420100	1.29825200	3.08360900
F	-5.36639400	-3.22180700	0.60684400
F	-3.20558100	-5.21874500	0.83533200
F	0.09877600	-5.85968300	0.79384800
F	2.83393500	-4.86541300	0.36418200
F	4.41783900	0.36903600	-1.71138800
F	2.90186900	2.81723800	-2.01652400
F	-2.58751900	4.07585600	-1.28490500
F	-4.88911400	2.43385000	-0.73095200
H	-0.18527500	6.16738400	-3.83906000
H	1.43022000	7.01157100	0.90924500
H	2.74182800	7.30805200	-0.21610300
H	5.82185000	5.52196000	2.93046700
O	2.78393700	-1.35461600	2.64549100
H	3.28666900	-0.58623100	2.98801100

O	-0.34349300	-2.49513200	2.83132500
H	2.20937800	-0.86111600	2.03758900
O	-0.60852300	1.45830000	2.01666900
H	0.36109900	1.29911000	2.01060500
H	-0.69495400	2.05131000	1.25905100

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OOH\}^+$ (singlet)

Energy: -4258.13215186 a.u.

C	-4.07961700	-3.02497300	0.29243600
C	-3.11548700	-4.00252800	0.32081600
C	-1.90095400	-3.38145000	-0.06050800
N	-2.13969700	-2.06892000	-0.35159700
C	-0.52533300	-3.70525200	-0.08587500
C	0.30162000	-4.79918500	0.26492100
N	0.26033600	-2.64232800	-0.42357000
C	1.59977900	-4.35447700	0.16133400
C	1.56852800	-2.97567700	-0.26213800
C	2.58568200	-2.02704200	-0.44009900
C	-3.45312500	-1.78704700	-0.11339200
C	-3.93441400	-0.47778400	-0.16676400
C	-3.07711300	0.61708200	-0.49794300
C	-3.48512000	1.96989800	-0.69765500
N	-1.72066700	0.54669300	-0.72401000
C	-2.37685300	2.70269500	-1.00556100
C	-1.25557900	1.80796600	-1.02592700
C	0.09157300	2.14687500	-1.24498500
C	1.16157300	1.22308200	-1.15404500
C	2.54449600	1.46854700	-1.42637600
N	1.03321100	-0.08960700	-0.79015000
C	3.22753500	0.31336000	-1.17499900
C	2.28650100	-0.67188700	-0.76295000
C	0.41405800	3.53524800	-1.63600600
C	1.25733300	4.32687600	-0.84035200
C	-0.05629200	4.07155900	-2.83952600
C	1.68294000	5.59005400	-1.23788000
C	0.35007700	5.33229100	-3.25360300
H	-0.71525000	3.47137700	-3.46463900
C	2.72743600	4.26383200	1.00959700
C	1.22085000	6.07635000	-2.46041000
C	3.24095200	3.49482600	2.07168100
C	3.26941700	5.51059300	0.68622000
H	1.54895900	7.06117700	-2.79165300
C	4.35474500	3.98084200	2.76881700
C	4.39175700	5.94473800	1.39075400
C	4.94486500	5.18692300	2.41826000

H	4.79720200	3.37670800	3.56073000
H	4.83066900	6.90763400	1.13064600
C	2.60797500	6.37371300	-0.35212500
O	1.63934200	3.75961100	0.35082800
C	2.62269500	2.20493300	2.45753500
O	2.10901800	1.41999400	1.67845400
Co	-0.61879100	-0.96720700	-0.41022100
O	-0.45169000	-0.86220700	1.44490100
C	-5.35256000	-0.22758500	0.12933800
C	-6.36722200	-0.87172800	-0.59009400
C	-5.74382700	0.64451000	1.15326600
C	-7.70901000	-0.65435000	-0.31622700
C	-7.07825400	0.86749100	1.45274100
C	-8.06383200	0.21599300	0.71276600
C	3.98687100	-2.44545500	-0.29562500
C	4.85971000	-1.79897700	0.58976900
C	4.50303400	-3.51883500	-1.03404400
C	6.17587000	-2.20358400	0.74473500
C	5.81959100	-3.93388500	-0.90305800
C	6.65756600	-3.27462600	-0.00608100
F	-4.81433700	1.27424700	1.87222700
F	-7.42237100	1.68931000	2.43620400
F	-9.33950800	0.42558800	0.98822700
F	-8.65104900	-1.26320000	-1.02503700
F	-6.04671300	-1.70332500	-1.58292400
F	4.42174700	-0.76976500	1.31644000
F	6.97764200	-1.58037200	1.60086300
F	7.91351400	-3.66319500	0.13155100
F	6.28451700	-4.94406300	-1.62649200
F	3.72393900	-4.15349300	-1.91125800
F	-5.35221700	-3.18774300	0.60201900
F	-3.26510000	-5.27404400	0.64272500
F	-0.10955300	-6.00237500	0.61842300
F	2.67978100	-5.06618000	0.42397200
F	4.53329600	0.15093100	-1.33504400
F	3.10180500	2.59598500	-1.83966800
F	-2.36754900	4.00558000	-1.22840700
F	-4.72023800	2.44724000	-0.63410400
H	0.00231800	5.73097500	-4.20297200
H	2.04864000	7.17998500	0.15139700
H	3.36734900	6.88795700	-0.95766200
H	5.82581800	5.54004300	2.94736900
O	-0.41326200	0.43999600	1.88233900
H	0.56190600	0.62849500	1.96353600
O	2.64571400	1.89569400	3.76638400
H	2.96341600	2.65082500	4.28940300

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OOH\}^+$ (triplet)

Energy: -4258.13339314 a.u.

C	-4.05035100	-3.02023000	0.22593600
C	-3.08344900	-4.00343800	0.20894800
C	-1.88281600	-3.38184900	-0.18769600
N	-2.12503200	-2.06298700	-0.45430600
C	-0.50780000	-3.71027800	-0.22564800
C	0.31690500	-4.80489200	0.12517300
N	0.27368200	-2.64502200	-0.53470600
C	1.61640000	-4.35085700	0.06704500
C	1.58876900	-2.97400600	-0.33639800
C	2.58929700	-2.01554400	-0.48606900
C	-3.44229300	-1.78096800	-0.16659000
C	-3.92870300	-0.47841100	-0.16832800
C	-3.07488000	0.62676600	-0.48282100
C	-3.49097700	1.97466400	-0.68377900
N	-1.72509700	0.55942700	-0.71603900
C	-2.38836100	2.71130100	-1.01243600
C	-1.26944700	1.82379800	-1.03551700
C	0.07058300	2.15925300	-1.28380300
C	1.13475400	1.23174900	-1.22473700
C	2.51018600	1.48302200	-1.47667500
N	1.01133300	-0.09780900	-0.87434400
C	3.20219300	0.32991600	-1.21321000
C	2.27227900	-0.66558300	-0.82331600
C	0.39771800	3.55385800	-1.65548300
C	1.22994500	4.32741700	-0.83432500
C	-0.04520900	4.10873800	-2.85993000
C	1.68197200	5.58804600	-1.20736200
C	0.38178500	5.37192200	-3.24808400
H	-0.69837100	3.52429300	-3.50562500
C	2.68965800	4.19433200	1.01699500
C	1.24850200	6.09545700	-2.43200000
C	3.19141700	3.38652300	2.05637800
C	3.26576800	5.43088900	0.71203000
H	1.59579500	7.07914200	-2.74649800
C	4.33424200	3.82047200	2.74258800
C	4.41365200	5.81178300	1.40505400
C	4.95927500	5.01216600	2.40554300
H	4.77164700	3.18622600	3.51358600
H	4.88038300	6.76522800	1.15897800
C	2.60831400	6.33692900	-0.29276700
O	1.58212600	3.74016200	0.35790600
C	2.52134400	2.12250600	2.43653400

O	1.92215500	1.39213400	1.66284100
Co	-0.60245900	-0.96450200	-0.39508200
O	-0.36167400	-0.97612200	1.42448900
C	-5.34064500	-0.23479000	0.15753400
C	-6.37074800	-0.86415300	-0.55368300
C	-5.71161300	0.62712600	1.19790100
C	-7.70669200	-0.64374800	-0.25412300
C	-7.03955100	0.85271000	1.52263000
C	-8.04045100	0.21464200	0.79160500
C	3.99421900	-2.39708200	-0.28490600
C	4.80831100	-1.72580600	0.63697100
C	4.57263800	-3.45404500	-1.00014600
C	6.12729600	-2.09140300	0.85094700
C	5.89444000	-3.82971700	-0.80974600
C	6.67245900	-3.14754700	0.12289100
F	-4.76748900	1.24584700	1.90788700
F	-7.36336100	1.66480400	2.52101700
F	-9.31032700	0.42604700	1.09122800
F	-8.66341900	-1.23854900	-0.95516700
F	-6.07367900	-1.68223400	-1.56442000
F	4.30898200	-0.70852800	1.34317500
F	6.87108300	-1.44512400	1.74224400
F	7.93211700	-3.49972200	0.31568000
F	6.42153200	-4.82424800	-1.51177900
F	3.85502300	-4.10745600	-1.91417500
F	-5.31102300	-3.19561900	0.57095900
F	-3.23256300	-5.27780900	0.51637700
F	-0.09662400	-6.01644500	0.44697400
F	2.69442500	-5.06660600	0.33331600
F	4.51149600	0.18621300	-1.35287200
F	3.07246800	2.61415500	-1.87210600
F	-2.38695900	4.01125800	-1.25415500
F	-4.72811500	2.44473400	-0.61241900
H	0.05387200	5.78743100	-4.19733200
H	2.05065500	7.12383100	0.24245000
H	3.36919700	6.87194400	-0.87755600
H	5.86146000	5.32323400	2.92509100
O	-0.50209900	0.26255500	2.00841400
H	0.44195400	0.59553900	2.03366000
O	2.58484200	1.77061400	3.73234700
H	2.96868100	2.48837600	4.26361100

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OOH(H_2O)\}^+$ (singlet)

Energy: -4334.57136168 a.u.

C	-4.01087200	-3.06184000	0.27002200

C	-3.00895000	-3.99881200	0.31490100
C	-1.82694500	-3.34378800	-0.11621600
N	-2.11943400	-2.06227800	-0.45699400
C	-0.43637200	-3.62236600	-0.14365300
C	0.42885600	-4.67200600	0.23680900
N	0.30811900	-2.54565000	-0.52088400
C	1.71305700	-4.18628200	0.10632200
C	1.63027300	-2.83142600	-0.36928500
C	2.60875900	-1.84818100	-0.58797900
C	-3.43798700	-1.81674900	-0.19309300
C	-3.96082500	-0.52791500	-0.25400700
C	-3.14305000	0.59816500	-0.61576200
C	-3.60519900	1.93555000	-0.79734900
N	-1.79343200	0.57679600	-0.85689700
C	-2.52538200	2.71572400	-1.09206000
C	-1.37347500	1.86234600	-1.13366100
C	-0.03539500	2.25147700	-1.31481600
C	1.06377300	1.35023800	-1.25809500
C	2.42990400	1.64898300	-1.55250800
N	0.98143700	0.02881400	-0.92129000
C	3.15458400	0.51155200	-1.34278600
C	2.25545700	-0.50995800	-0.91835000
C	0.26725600	3.67124100	-1.57857900
C	1.09897200	4.38001600	-0.69017500
C	-0.19586000	4.33465800	-2.72048900
C	1.50838000	5.68812900	-0.92984800
C	0.20764700	5.63555800	-2.98356200
H	-0.83974000	3.80486700	-3.41988200
C	2.55716600	4.10156800	1.15272500
C	1.05673200	6.30033900	-2.09668200
C	3.12170900	3.18011200	2.06133500
C	3.07367900	5.39042600	0.99198800
H	1.37118800	7.32105200	-2.31230300
C	4.24124000	3.58748200	2.79680800
C	4.19532000	5.74641100	1.73869100
C	4.77937800	4.85703600	2.63586600
H	4.68398600	2.88300000	3.49482100
H	4.60919100	6.74725700	1.61681400
C	2.39134200	6.36966100	0.07558000
O	1.46933700	3.68832500	0.42662400
C	2.57330600	1.81797700	2.24038300
O	1.60247300	1.37807200	1.62437800
Co	-0.62875800	-0.90358000	-0.52985100
O	-0.46860800	-0.83623900	1.33192600
C	-5.37743000	-0.31745500	0.07592000
C	-6.39068800	-1.00682400	-0.60318000

C	-5.76797000	0.55977800	1.09625000
C	-7.73068200	-0.82447400	-0.29678700
C	-7.09976200	0.74743800	1.42855400
C	-8.08434100	0.05319900	0.72658100
C	4.02238100	-2.21846500	-0.46263700
C	4.90543100	-1.50991400	0.36545100
C	4.54420600	-3.31815900	-1.16060300
C	6.23069500	-1.88664100	0.51215900
C	5.87027600	-3.70260900	-1.04067100
C	6.71481600	-2.98641500	-0.19443000
F	-4.83861900	1.22893000	1.77868600
F	-7.44252200	1.57479000	2.40740100
F	-9.35753700	0.22842200	1.03370300
F	-8.67199300	-1.47483000	-0.96814200
F	-6.07222800	-1.84801300	-1.58806800
F	4.47648100	-0.44563200	1.04150600
F	7.04042200	-1.20734800	1.31525300
F	7.97943300	-3.34630300	-0.06667700
F	6.33938900	-4.73649400	-1.72642100
F	3.76141100	-4.00543000	-1.99321400
O	3.23449700	1.08464600	3.12595300
H	2.84311800	0.16256800	3.07297900
F	-5.26876700	-3.25980300	0.61375000
F	-3.09960900	-5.26177700	0.68781300
F	0.06521400	-5.87628800	0.63930200
F	2.81620700	-4.85843500	0.38113100
F	4.45693200	0.38832900	-1.55437000
F	2.93490200	2.80195700	-1.96580400
F	-2.56998700	4.02052300	-1.29418100
F	-4.85642800	2.36665700	-0.72636500
H	-0.12554500	6.13293100	-3.89065800
H	1.78953200	7.07179100	0.67700700
H	3.13711200	6.99552500	-0.43359100
H	5.65127200	5.15666300	3.21149700
O	2.08173500	-1.33749800	2.61655000
H	1.28561100	-1.04958300	2.12092300
O	-0.89318600	0.38838100	1.85191500
H	-0.04103800	0.89481200	1.88288900
H	1.73017400	-1.86548700	3.34695900

$\{H^{+\bullet,F}CX–CO_2H–Co^{IV}–OOH(H_2O)\}^+$ (triplet)

Energy: -4334.57124510 a.u.

C	-3.98295000	-3.06557300	0.24847300
C	-2.97639800	-4.00357400	0.28849300

C	-1.79761000	-3.35055200	-0.13160000
N	-2.09194300	-2.06234400	-0.47406300
C	-0.41070700	-3.62838900	-0.14620400
C	0.45814200	-4.68580800	0.21002600
N	0.32892100	-2.54538800	-0.49074300
C	1.74144300	-4.19408400	0.09903900
C	1.65772700	-2.83453700	-0.34680900
C	2.62274600	-1.85355200	-0.59221300
C	-3.42300000	-1.82028000	-0.20182100
C	-3.95841900	-0.54234400	-0.24658300
C	-3.14565400	0.59001700	-0.59204300
C	-3.61270200	1.92185700	-0.79094400
N	-1.79789900	0.57038300	-0.82475900
C	-2.53572600	2.70339200	-1.09473900
C	-1.38308800	1.85669500	-1.12152000
C	-0.05269000	2.23893400	-1.33523700
C	1.04065400	1.33492600	-1.30374500
C	2.39650800	1.63455600	-1.59413100
N	0.96506600	0.00139700	-0.96563100
C	3.13212200	0.49987400	-1.37081600
C	2.24873800	-0.52606900	-0.94631600
C	0.24939900	3.65965900	-1.60570700
C	1.06219200	4.37620200	-0.70893800
C	-0.20265100	4.31291500	-2.75634700
C	1.45985800	5.68834600	-0.94599600
C	0.19067800	5.61813600	-3.01763800
H	-0.83365600	3.77507500	-3.46134000
C	2.50985300	4.11329500	1.14404500
C	1.01862400	6.29393800	-2.12052100
C	3.08417500	3.19911900	2.05426900
C	3.01052300	5.40962100	0.98805000
H	1.32505800	7.31769700	-2.33304700
C	4.19537700	3.62215200	2.79502600
C	4.12411800	5.78024800	1.73909200
C	4.71703200	4.89841800	2.63789800
H	4.64521200	2.92366600	3.49423600
H	4.52432300	6.78690100	1.61936100
C	2.31993000	6.38140100	0.07048500
O	1.43058100	3.68755000	0.41365400
C	2.55829100	1.82920200	2.23666000
O	1.59520000	1.36487700	1.62219700
Co	-0.61556400	-0.89629000	-0.43438200
O	-0.43861500	-0.81384700	1.42050900
C	-5.37790700	-0.34327800	0.07766100
C	-6.38568800	-1.02955500	-0.61224500
C	-5.77659000	0.52770600	1.09988400

C	-7.72794300	-0.85090200	-0.31267500
C	-7.11070200	0.71220300	1.42477700
C	-8.08974000	0.02047300	0.71298100
C	4.04304000	-2.20356800	-0.46736200
C	4.91211100	-1.48363400	0.36409700
C	4.58178300	-3.29413400	-1.16518900
C	6.24240700	-1.84039200	0.51529000
C	5.91319600	-3.65992100	-1.03939200
C	6.74450600	-2.93284000	-0.18993900
F	-4.85227000	1.19560800	1.79134600
F	-7.46047800	1.53427000	2.40582600
F	-9.36537300	0.19187000	1.01302100
F	-8.66395600	-1.49945400	-0.99339400
F	-6.06099800	-1.86519500	-1.59978700
F	4.46383800	-0.42381900	1.03683000
F	7.03921000	-1.14888900	1.32133900
F	8.01413100	-3.27483500	-0.05827500
F	6.39945900	-4.68659900	-1.72420500
F	3.81276900	-3.99000900	-2.00306600
O	3.23236700	1.11565100	3.12754700
H	2.86216200	0.18428500	3.08830500
F	-5.23659100	-3.27306800	0.59915700
F	-3.06851500	-5.26530400	0.66313700
F	0.09376300	-5.90141700	0.57610600
F	2.84744400	-4.87360700	0.34951000
F	4.43611100	0.39703500	-1.57125500
F	2.90539900	2.78807400	-1.99706400
F	-2.58480100	4.00441700	-1.32138400
F	-4.86730900	2.34435700	-0.73111400
H	-0.13605200	6.10964500	-3.93028200
H	1.69948300	7.06936400	0.66945100
H	3.05919300	7.02315900	-0.42814500
H	5.58256800	5.20904200	3.21723400
O	2.13343800	-1.33346100	2.68641200
H	1.32650500	-1.05962000	2.20568500
O	-0.87896400	0.38976500	1.97566100
H	-0.03730600	0.91981500	1.96479800
H	1.80510400	-1.85449700	3.43258600

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OO^{\bullet-}$} (singlet)

Energy: -4257.76612943 a.u.

C	-4.19602200	-2.95413000	0.24519200
C	-3.25511000	-3.95859200	0.24951000
C	-2.01645600	-3.35995800	-0.08543000
N	-2.22304000	-2.03964900	-0.32220100

C	-0.63981800	-3.71813300	-0.11766700
C	0.16988400	-4.83901800	0.17675800
N	0.16767600	-2.66119500	-0.38987900
C	1.47995400	-4.41544100	0.10270800
C	1.47753200	-3.02848000	-0.25163200
C	2.50435000	-2.09029900	-0.41827500
C	-3.53504400	-1.72485700	-0.09633800
C	-3.97757400	-0.40255000	-0.12277400
C	-3.09428400	0.68763900	-0.39275400
C	-3.46271600	2.05926600	-0.52507500
N	-1.73900400	0.60138200	-0.60421400
C	-2.33479200	2.77973600	-0.79449700
C	-1.24006100	1.86120100	-0.85592100
C	0.11605900	2.16108100	-1.10239500
C	1.16214600	1.21162600	-1.04975500
C	2.54330100	1.42295700	-1.34809500
N	1.00656600	-0.10632300	-0.69009300
C	3.19891100	0.25041000	-1.11978000
C	2.23950700	-0.72223300	-0.70665000
C	0.44732100	3.54526500	-1.51199500
C	1.31679600	4.35128100	-0.76213300
C	-0.08580300	4.07297900	-2.69239700
C	1.66547500	5.63588800	-1.17190900
C	0.26152200	5.34495500	-3.12737500
H	-0.76551800	3.45624900	-3.27879400
C	2.96644200	4.29597200	0.93070200
C	1.13616200	6.11630200	-2.36826000
C	3.68384700	3.49477300	1.84159600
C	3.41717600	5.57634200	0.58670200
H	1.41362000	7.11674400	-2.70079100
C	4.87900100	4.00305500	2.36667100
C	4.62016100	6.03128200	1.11982300
C	5.35749000	5.25177800	2.00531600
H	5.41590300	3.37064000	3.06932300
H	4.97187600	7.02468900	0.83904700
C	2.57358500	6.44869000	-0.29929200
O	1.80443000	3.79807400	0.39621500
C	3.29689600	2.15122600	2.34456700
O	2.15259200	1.66125100	1.82761600
Co	-0.66956100	-0.96432300	-0.39505900
O	-0.60162400	-0.87783500	1.61241200
C	-5.40267700	-0.13145700	0.15354700
C	-6.41268500	-0.68339200	-0.63883100
C	-5.80220100	0.66139000	1.23288500
C	-7.75713400	-0.45570800	-0.37905600
C	-7.13934000	0.90281800	1.51244800

C	-8.12031000	0.34018000	0.70192400
C	3.90370500	-2.53390300	-0.28357600
C	4.76657300	-1.93879500	0.64302500
C	4.42308900	-3.57093700	-1.06402400
C	6.07999100	-2.35765100	0.79710400
C	5.73456400	-4.00430300	-0.92946700
C	6.56420900	-3.39561700	0.00631800
F	-4.88069100	1.21104100	2.02742900
F	-7.48987600	1.66107600	2.55016300
F	-9.40454600	0.56345500	0.96070200
F	-8.69804800	-0.98852800	-1.15736700
F	-6.09488200	-1.44897700	-1.68620400
F	4.32774500	-0.93779800	1.41009200
F	6.87741800	-1.78049600	1.69279900
F	7.82148600	-3.80299400	0.14370400
F	6.20402600	-4.98932300	-1.69365900
F	3.65801900	-4.16161300	-1.98535000
O	3.94756500	1.53832400	3.16971300
F	-5.48870700	-3.10544500	0.51485900
F	-3.45693800	-5.24308900	0.51982800
F	-0.25832700	-6.06156200	0.47144100
F	2.55011800	-5.17596700	0.31866500
F	4.50397100	0.05127300	-1.29841100
F	3.12048200	2.54526500	-1.77112300
F	-2.29886200	4.09972700	-0.94369100
F	-4.68923100	2.57062900	-0.42826200
H	-0.14521000	5.73279200	-4.05825000
H	1.97216600	7.13217300	0.32538200
H	3.21080500	7.10223500	-0.91130500
H	6.29332300	5.62207800	2.41693400
O	-0.37779200	0.23314000	2.13498300
H	2.01424000	0.80008900	2.26308400

{$H^{+\bullet,F}CX–CO_2H–Co^{III}–OO^{\bullet-}$} (triplet)

Energy: -4257.76634408 a.u.

C	-4.19661000	-2.95667800	0.23067600
C	-3.25782800	-3.96389600	0.22338900
C	-2.01861100	-3.36638900	-0.10865100
N	-2.22294200	-2.04292500	-0.33360300
C	-0.64305200	-3.72428300	-0.14195100
C	0.16526300	-4.84616700	0.15137800
N	0.16650200	-2.66585000	-0.40655100
C	1.47572400	-4.42175100	0.08782700
C	1.47602900	-3.03261100	-0.25968300
C	2.50380000	-2.09513600	-0.41492300

C	-3.53418400	-1.72751900	-0.10130700
C	-3.97352900	-0.40263700	-0.11867800
C	-3.09056400	0.68647300	-0.38625100
C	-3.45785800	2.05849900	-0.52094800
N	-1.73478600	0.59900700	-0.59848400
C	-2.33051400	2.77713000	-0.79541500
C	-1.23588600	1.85851200	-0.85540800
C	0.11894300	2.15719000	-1.10898500
C	1.16348100	1.20790100	-1.05291800
C	2.54499100	1.41763800	-1.34886700
N	1.00765100	-0.10989200	-0.69017200
C	3.20020300	0.24526400	-1.11538600
C	2.23966900	-0.72582300	-0.70286000
C	0.44954300	3.54032400	-1.52445500
C	1.31401200	4.35109000	-0.77443700
C	-0.08041700	4.06220100	-2.70857100
C	1.66090200	5.63516800	-1.18718900
C	0.26474900	5.33396400	-3.14650100
H	-0.75667200	3.44179800	-3.29513000
C	2.95928100	4.30461000	0.92283600
C	1.13445900	6.11028400	-2.38700100
C	3.67674800	3.50754600	1.83734600
C	3.40775000	5.58519100	0.57647900
H	1.41034600	7.11038200	-2.72186900
C	4.86945400	4.02014500	2.36393300
C	4.60836000	6.04445100	1.11120400
C	5.34557500	5.26914400	2.00052500
H	5.40651800	3.39081100	3.06921700
H	4.95833300	7.03795400	0.82857500
C	2.56410900	6.45291300	-0.31404400
O	1.79990800	3.80253200	0.38728600
C	3.29263100	2.16396300	2.34184200
O	2.14920800	1.67019700	1.82567000
Co	-0.66852900	-0.96779700	-0.37555300
O	-0.60090600	-0.88028100	1.59000700
C	-5.39727000	-0.13009400	0.16296800
C	-6.41070000	-0.67682600	-0.62867000
C	-5.79179300	0.66065600	1.24568300
C	-7.75385200	-0.44714300	-0.36410800
C	-7.12759100	0.90385800	1.53007200
C	-8.11211900	0.34581500	0.72066400
C	3.90276500	-2.53735500	-0.27195100
C	4.75923500	-1.94162100	0.66011200
C	4.42935500	-3.57128800	-1.05169400
C	6.07287600	-2.35730600	0.82079000
C	5.74110200	-4.00183800	-0.91034500

C	6.56405100	-3.39280400	0.03107800
F	-4.86672100	1.20631100	2.03889100
F	-7.47349900	1.65975600	2.57104900
F	-9.39509000	0.57092100	0.98394200
F	-8.69818400	-0.97486500	-1.14168800
F	-6.09760700	-1.43803600	-1.68049200
F	4.31389300	-0.94226700	1.42587800
F	6.86381700	-1.77952100	1.72184600
F	7.82157100	-3.79740000	0.17485600
F	6.21737400	-4.98427200	-1.67371600
F	3.67125000	-4.16186400	-1.97896000
O	3.94442900	1.55313000	3.16766300
F	-5.48988900	-3.10863800	0.49971600
F	-3.46360200	-5.25048200	0.48080700
F	-0.26370200	-6.07059000	0.43625600
F	2.54393300	-5.18359800	0.30571200
F	4.50543000	0.04521800	-1.29111600
F	3.12315100	2.53840900	-1.77352800
F	-2.29324600	4.09644700	-0.95145200
F	-4.68447200	2.56976600	-0.42407800
H	-0.14013600	5.71769500	-4.07989200
H	1.95894800	7.13620300	0.30723100
H	3.20116800	7.10678400	-0.92587900
H	6.27953700	5.64285900	2.41330800
O	-0.38811300	0.23352400	2.11232900
H	2.01529000	0.80855400	2.26146900

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$OO^{\bullet-}$(H_2O)} (singlet)

Energy: -4334.19758370 a.u.

C	-3.99608800	-3.03409500	0.31527500
C	-2.99435800	-3.97245700	0.37854100
C	-1.81416800	-3.33977600	-0.08339300
N	-2.11584100	-2.06853300	-0.45826900
C	-0.42357600	-3.62225300	-0.11791200
C	0.45131200	-4.65691100	0.27985200
N	0.31839700	-2.55219600	-0.50691300
C	1.73367100	-4.17024400	0.13770200
C	1.64614100	-2.83123900	-0.35403000
C	2.61890900	-1.85039400	-0.60884600
C	-3.42953500	-1.80581100	-0.17957200
C	-3.95163600	-0.51879000	-0.26321100
C	-3.13768200	0.60336900	-0.61670900
C	-3.58786100	1.94417700	-0.80471900
N	-1.78124600	0.58695600	-0.82612500
C	-2.50286200	2.72189100	-1.08579900

C	-1.35346400	1.86956300	-1.10646400
C	-0.01727900	2.23883700	-1.32774400
C	1.07403000	1.34029600	-1.29534300
C	2.43905100	1.64078100	-1.58892200
N	0.99538000	0.01613700	-0.94376800
C	3.16323900	0.50674300	-1.38184700
C	2.26930600	-0.52178600	-0.95498600
C	0.28387900	3.66434300	-1.60269200
C	1.04466600	4.40902000	-0.68950600
C	-0.13885900	4.29086600	-2.77608200
C	1.38500000	5.73796400	-0.92316600
C	0.20629300	5.61120000	-3.03977500
H	-0.73127600	3.72177000	-3.49093800
C	2.47815500	4.22409600	1.18656400
C	0.96483900	6.32397100	-2.11669700
C	3.10464500	3.35737300	2.10676900
C	2.89740300	5.55338300	1.04603400
H	1.23552400	7.36108000	-2.31596400
C	4.16773100	3.86267100	2.86633000
C	3.97196400	6.00245900	1.80918900
C	4.61010700	5.16726200	2.72015000
H	4.63825700	3.18138400	3.57034800
H	4.30038400	7.03545400	1.68827500
C	2.15917700	6.48269700	0.12287400
O	1.43204900	3.73937700	0.44609800
C	2.76199000	1.93221100	2.35885900
O	3.34856900	1.27349900	3.21435500
Co	-0.62304100	-0.91382900	-0.57412200
O	-0.60177000	-0.67499600	1.41925800
C	-5.37714600	-0.31010700	0.05977300
C	-6.38643800	-0.97267800	-0.64418000
C	-5.77832300	0.53425000	1.09885700
C	-7.73023900	-0.79967700	-0.34150400
C	-7.11450100	0.72335500	1.41982900
C	-8.09453500	0.05210500	0.69564000
C	4.03991800	-2.22112600	-0.48475300
C	4.92217300	-1.52741100	0.35207300
C	4.56409600	-3.30939300	-1.19160700
C	6.25032800	-1.90397100	0.49175800
C	5.88964300	-3.70045500	-1.07016000
C	6.73545700	-2.99560800	-0.22091100
F	-4.85924400	1.18769800	1.81458800
F	-7.46417300	1.53352100	2.41814300
F	-9.37796500	0.22441100	0.99608200
F	-8.66951700	-1.43870200	-1.03794900
F	-6.06936700	-1.79882400	-1.64505400

F	4.50425400	-0.46521100	1.04235100
F	7.06332900	-1.22774300	1.30200900
F	8.00703600	-3.36039700	-0.09477500
F	6.35698500	-4.73677600	-1.76503400
F	3.78573300	-3.99738700	-2.03086300
O	1.79540900	1.42708200	1.59618000
H	1.72191100	0.45779000	1.82456300
F	-5.26066900	-3.22718400	0.67119700
F	-3.09532200	-5.23020800	0.79128300
F	0.09659700	-5.86489400	0.70558200
F	2.84789100	-4.84658900	0.40825800
F	4.47373700	0.38193200	-1.58730000
F	2.93936000	2.80485600	-1.99852000
F	-2.54315400	4.03332500	-1.29438500
F	-4.84556500	2.38041700	-0.74038300
H	-0.11399600	6.08309100	-3.96565400
H	1.47077200	7.11366700	0.71188600
H	2.86066500	7.18617300	-0.34794000
H	5.44445600	5.53456700	3.31290500
O	2.13963000	-1.13229800	2.49059600
H	2.77703100	-0.61582200	3.02472300
O	-0.76033800	-1.68647900	2.14350400
H	1.43621100	-1.38620900	3.10439700

{$H^{+\bullet}$,^{F}CX–CO_2H–Co^{III}–$OO^{\bullet-}$(H_2O)} (triplet)

Energy: -4334.19591727 a.u.

C	-4.03176500	-3.03221800	0.30859600
C	-3.03980500	-3.98380100	0.35397300
C	-1.84158400	-3.34762900	-0.05337100
N	-2.12277100	-2.05784600	-0.37057800
C	-0.45109400	-3.63304900	-0.08227700
C	0.42111200	-4.68967800	0.26315600
N	0.29744300	-2.55287900	-0.42936600
C	1.70577700	-4.20654700	0.13200800
C	1.62677200	-2.84757500	-0.30800900
C	2.60407700	-1.87694900	-0.56519900
C	-3.44518700	-1.79632900	-0.12939200
C	-3.95872000	-0.50466600	-0.22863100
C	-3.13971400	0.61256600	-0.58095700
C	-3.58199400	1.95442300	-0.77403000
N	-1.78257500	0.58893500	-0.79403400
C	-2.49253500	2.72496800	-1.06245200
C	-1.34866000	1.86702000	-1.08014400
C	-0.00765200	2.22946100	-1.30491700
C	1.07921000	1.32745000	-1.26235600

C	2.44391000	1.61561700	-1.56268000
N	0.99633800	0.00604800	-0.89831600
C	3.16192000	0.47611900	-1.34805300
C	2.26199700	-0.54041400	-0.90965900
C	0.29660300	3.64983600	-1.60157600
C	1.06913600	4.40675200	-0.70846900
C	-0.13618100	4.25976800	-2.78045200
C	1.41219100	5.73037000	-0.96750600
C	0.21097200	5.57419100	-3.06917500
H	-0.73799300	3.68157900	-3.48002000
C	2.53081000	4.24339800	1.14673100
C	0.98210800	6.29884900	-2.16589000
C	3.17188200	3.38532400	2.06485600
C	2.95508900	5.56787600	0.97862700
H	1.25480600	7.33144100	-2.38482300
C	4.25490500	3.89388800	2.79354500
C	4.04924200	6.02033000	1.71126000
C	4.70225700	5.19329900	2.61927600
H	4.73666100	3.21924400	3.49640900
H	4.38147800	7.04934500	1.56883400
C	2.20051200	6.48752100	0.05900000
O	1.46620800	3.75598700	0.43474600
C	2.82411400	1.96671800	2.34460800
O	3.42744900	1.31301400	3.19221300
Co	-0.62980600	-0.90790000	-0.49136800
O	-0.58219500	-0.56227200	1.43560000
C	-5.38907800	-0.28939600	0.07003700
C	-6.38973200	-0.93706900	-0.65905100
C	-5.80134100	0.54730500	1.11057300
C	-7.73729000	-0.75829900	-0.37685200
C	-7.14138700	0.74107700	1.41187900
C	-8.11319300	0.08401200	0.66388300
C	4.02457200	-2.25865600	-0.46448300
C	4.92027800	-1.58106000	0.37080100
C	4.53623400	-3.33471900	-1.19807700
C	6.24877500	-1.96408700	0.48751100
C	5.86183800	-3.73270900	-1.09948700
C	6.72075500	-3.04577500	-0.24882900
F	-4.88949000	1.18866300	1.84618300
F	-7.50271000	1.54298800	2.41272800
F	-9.40036000	0.26165700	0.94439900
F	-8.66912200	-1.38226500	-1.09642700
F	-6.06034300	-1.75093600	-1.66553500
F	4.51457100	-0.52574100	1.07960400
F	7.07489500	-1.30327800	1.29729200
F	7.99249700	-3.41727100	-0.14415700

F	6.31643200	-4.75812400	-1.81871200
F	3.74594300	-4.00404600	-2.04143300
O	1.83133400	1.46191100	1.61603400
H	1.75297000	0.49716900	1.86156600
F	-5.30950700	-3.23118000	0.61831000
F	-3.16867700	-5.25657800	0.71101400
F	0.06514400	-5.91385700	0.63830400
F	2.81535900	-4.90210600	0.36747400
F	4.47089600	0.34394500	-1.55690400
F	2.95386600	2.77014700	-1.98502600
F	-2.52794000	4.03558500	-1.27927700
F	-4.83650400	2.39960100	-0.71066700
H	-0.11736700	6.03223400	-3.99917900
H	1.51950600	7.12182200	0.65304200
H	2.89258800	7.18828000	-0.42927200
H	5.55205800	5.56314200	3.18802800
O	2.14569100	-1.08359800	2.55238700
H	2.81676300	-0.57538000	3.05191200
O	-0.77192700	-1.51591100	2.22470900
H	1.45640300	-1.29835400	3.19639900

$\{H^{+\bullet,F}CX–CO_2–Co^{III}–OO^{\bullet-}(H_2O)\}^-$ (singlet)

Energy: -4333.66922249 a.u.

C	-3.94649400	-3.02146600	0.44310900
C	-2.93064800	-3.93891400	0.56212600
C	-1.74047700	-3.29726100	0.14612000
N	-2.06817300	-2.01251200	-0.23662400
C	-0.36787900	-3.54616600	0.08596700
C	0.55210100	-4.56451200	0.44169400
N	0.35430300	-2.46643500	-0.36902700
C	1.80985000	-4.06907900	0.21280900
C	1.68049800	-2.72892700	-0.29585700
C	2.63848800	-1.75797500	-0.63871900
C	-3.38982700	-1.79027600	-0.04103600
C	-3.95403500	-0.51108600	-0.22616700
C	-3.16957700	0.59708200	-0.58869700
C	-3.63444900	1.93426300	-0.80874300
N	-1.79607800	0.60868500	-0.78799100
C	-2.56364700	2.72281300	-1.08014500
C	-1.39009200	1.89281500	-1.07138800
C	-0.06341100	2.29196600	-1.28586900
C	1.02704900	1.40355900	-1.26133700
C	2.40101800	1.72880200	-1.54300500
N	0.96741200	0.06807800	-0.97923000
C	3.13463500	0.59869000	-1.39976100

C	2.25953100	-0.45383200	-0.98881600
C	0.23006500	3.73335900	-1.50961900
C	0.95662800	4.45225700	-0.54799300
C	-0.14792400	4.40260200	-2.67334500
C	1.30255400	5.79118400	-0.72502800
C	0.19363200	5.73621300	-2.87867300
H	-0.71134700	3.85630400	-3.42899700
C	2.42021500	4.17989800	1.28478800
C	0.91897900	6.42046800	-1.90845500
C	3.08069900	3.24380400	2.09850400
C	2.83279500	5.51576400	1.21301600
H	1.19363100	7.46519600	-2.06226200
C	4.17358900	3.69174900	2.84368200
C	3.94491100	5.91055000	1.95387200
C	4.61477400	5.00756700	2.77358700
H	4.66809900	2.95421800	3.47277300
H	4.27585600	6.94875400	1.88920600
C	2.04503500	6.48839500	0.37808000
O	1.32571600	3.75313200	0.56978200
C	2.72439500	1.77694000	2.20176300
O	3.27290000	1.10049100	3.10638400
Co	-0.60891800	-0.85202500	-0.47793700
O	-0.48232600	-0.50169900	1.50416100
C	-5.40430300	-0.35257000	0.01254900
C	-6.34216200	-1.07802700	-0.72616200
C	-5.90798700	0.48572500	1.01074500
C	-7.70745500	-0.97701800	-0.49540100
C	-7.26927400	0.61281900	1.25284500
C	-8.17317700	-0.12438800	0.49737300
C	4.06473200	-2.13612800	-0.57934500
C	4.99115800	-1.47021800	0.23082100
C	4.54262100	-3.22351200	-1.31497100
C	6.31797300	-1.87649700	0.30851700
C	5.86100400	-3.64997700	-1.24610900
C	6.75340000	-2.97179800	-0.42655100
F	-5.07154400	1.20129900	1.76694300
F	-7.71746000	1.42655300	2.21461900
F	-9.48463800	-0.01353400	0.72413300
F	-8.57673400	-1.68405700	-1.22595200
F	-5.93421000	-1.90691500	-1.69360400
F	4.63550200	-0.40070300	0.93213200
F	7.18430400	-1.21994700	1.08589500
F	8.02833400	-3.36572700	-0.35285800
F	6.27893600	-4.69687300	-1.96929100
F	3.71508600	-3.89883900	-2.12523700
O	1.92204100	1.28506700	1.35952500

F	-5.23173700	-3.24330800	0.74454400
F	-3.04145300	-5.20135700	0.97940400
F	0.23870100	-5.77446600	0.90820200
F	2.94873100	-4.72180200	0.43703800
F	4.44577900	0.49528600	-1.63262300
F	2.88271200	2.91418400	-1.91554300
F	-2.62246900	4.03432600	-1.31634700
F	-4.90701300	2.34790200	-0.77634600
H	-0.10106000	6.23885300	-3.79796600
H	1.32725800	7.03050600	1.02035000
H	2.70675400	7.26491900	-0.03360800
H	5.47847400	5.32991500	3.35306100
O	2.62773300	-1.68275000	2.51056900
H	2.89530200	-0.75113400	2.66454300
O	-0.58047100	-1.47799300	2.27872600
H	1.66631600	-1.63366700	2.59349500

$\{H^{+\bullet,F}CX–CO_2–Co^{III}–OO^{\bullet-}\}\bullet H_2O$ (singlet)

Energy: -4410.08614764 a.u.

C	-3.97295800	-3.00160200	0.40167300
C	-2.96487300	-3.92806900	0.52513500
C	-1.76017500	-3.27759000	0.18110700
N	-2.07019400	-1.96474800	-0.14862800
C	-0.39492400	-3.53422500	0.12949100
C	0.51362700	-4.57203000	0.44356600
N	0.34251100	-2.43595700	-0.28069600
C	1.77512100	-4.08083800	0.22593100
C	1.66095500	-2.72605200	-0.25027900
C	2.62962800	-1.77686200	-0.63477000
C	-3.39973000	-1.75520700	-0.02461100
C	-3.96443300	-0.48353900	-0.25515500
C	-3.17362100	0.61042200	-0.63437000
C	-3.62720300	1.94998900	-0.84871600
N	-1.80053000	0.60817000	-0.85545200
C	-2.55063900	2.72852600	-1.12923800
C	-1.38396500	1.88759900	-1.13639800
C	-0.04922900	2.28245700	-1.32163400
C	1.03534500	1.39079500	-1.27273200
C	2.40438000	1.69570300	-1.58760000
N	0.96993800	0.06595000	-0.94864000
C	3.13070400	0.55954100	-1.44616000
C	2.25843800	-0.47580300	-0.99390400
C	0.25732200	3.72033200	-1.53471800
C	1.00156900	4.43100400	-0.57724300
C	-0.14419700	4.39769800	-2.68661300

C	1.31365200	5.77970600	-0.74765100
C	0.17811500	5.73563400	-2.88718000
H	-0.71623200	3.85118200	-3.43556900
C	2.51924400	4.17519100	1.22873100
C	0.90414700	6.41805100	-1.91715200
C	3.23518600	3.26413100	2.02899200
C	2.88806600	5.52526500	1.14917300
H	1.15858100	7.46973100	-2.05741100
C	4.33891100	3.76124400	2.72943600
C	4.01245400	5.96314400	1.84461900
C	4.74220500	5.08631300	2.63837300
H	4.87086500	3.04243600	3.34886400
H	4.30036500	7.01307700	1.76480500
C	2.04457400	6.48235400	0.35525800
O	1.40890300	3.72735500	0.52980400
C	2.94129100	1.77828500	2.20146500
O	2.11046300	1.24432900	1.40285200
Co	-0.62133400	-0.83815900	-0.49590400
O	-0.39856000	-1.29380500	2.38696900
C	-5.42038100	-0.32367200	-0.04833900
C	-6.33992200	-1.03908200	-0.81800700
C	-5.94457200	0.50308900	0.94851300
C	-7.71017700	-0.94158800	-0.61713400
C	-7.31159200	0.62687300	1.16067400
C	-8.19764000	-0.10129300	0.37574900
C	4.05010000	-2.18203500	-0.62895600
C	5.02568700	-1.52633800	0.13186800
C	4.47324900	-3.28558300	-1.37453300
C	6.34601400	-1.96150700	0.15329600
C	5.78359000	-3.74056100	-1.35908700
C	6.72557300	-3.07344500	-0.58740300
F	-5.12509400	1.21039500	1.72801500
F	-7.78259300	1.42953800	2.12043500
F	-9.51381600	0.00675500	0.57403000
F	-8.56258300	-1.64007600	-1.37519900
F	-5.90743100	-1.85673400	-1.78503400
F	4.73004300	-0.43963600	0.83149100
F	7.25985200	-1.31572600	0.88361200
F	7.99395300	-3.49324800	-0.56641000
F	6.14670600	-4.80275500	-2.08889300
F	3.59702400	-3.94838700	-2.14368000
O	3.56639500	1.18331600	3.10577600
F	-5.26728400	-3.23014600	0.64410800
F	-3.09374200	-5.20215000	0.89670200
F	0.19002700	-5.78978600	0.87856000
F	2.90724700	-4.74931300	0.42922300

F	4.43327400	0.44009200	-1.71171700
F	2.88826800	2.86762600	-1.99218200
F	-2.60371000	4.04163100	-1.35553200
F	-4.89341700	2.37849000	-0.79976700
H	-0.13569600	6.24296500	-3.79748200
H	1.31518800	6.97620800	1.02310100
H	2.66414900	7.29662100	-0.04847000
H	5.61695700	5.43613800	3.18477900
O	2.57230600	-1.44273000	2.36105200
H	3.12599300	-0.87275400	2.92592700
O	-0.55335400	-2.41903800	2.83319000
H	2.17377800	-0.72677500	1.83095300
O	-0.60919300	1.33534900	1.81202400
H	0.36318300	1.19718900	1.81648100
H	-0.67287500	2.15447800	1.30335000

$\{H^{+\bullet}{}_{,}{}^{F}CX–CO_2–Co^{III}–OO^{\bullet-}\}\bullet H_2O$ (triplet)

Energy: -4410.08167771 a.u.

C	-3.97251000	-3.02950600	0.41271200
C	-2.95359500	-3.95033400	0.52304000
C	-1.75848700	-3.28918400	0.15599300
N	-2.06372000	-2.00914700	-0.17304900
C	-0.35873500	-3.54535400	0.09957000
C	0.54484500	-4.58540400	0.42135500
N	0.35633500	-2.46533600	-0.30561000
C	1.81168600	-4.09407100	0.21242100
C	1.69452400	-2.74537900	-0.26053600
C	2.64300500	-1.78215000	-0.60594400
C	-3.40431000	-1.79280800	-0.02720300
C	-3.95110600	-0.52373800	-0.25501900
C	-3.16536400	0.58769000	-0.65132400
C	-3.63129500	1.91780700	-0.87449000
N	-1.80148100	0.58982900	-0.87040000
C	-2.55842800	2.70272000	-1.17347500
C	-1.39711200	1.86639200	-1.17482100
C	-0.04903500	2.25916100	-1.35577600
C	1.04853200	1.39100100	-1.29210800
C	2.41214900	1.70941200	-1.58990100
N	0.99376500	0.06101300	-0.94696300
C	3.14382900	0.57697900	-1.42276600
C	2.26480800	-0.45756000	-0.97457300
C	0.24325700	3.69807300	-1.56573900
C	0.97422300	4.41085800	-0.59970600
C	-0.15876000	4.37100100	-2.72032200
C	1.27632400	5.76226100	-0.76807300

C	0.16170600	5.70867300	-2.92005200
H	-0.72369400	3.82103900	-3.47179700
C	2.46190000	4.17053300	1.23410800
C	0.87494100	6.39534200	-1.94280500
C	3.17145000	3.26753600	2.04815100
C	2.81929900	5.52381300	1.15631400
H	1.12229400	7.44896900	-2.08079500
C	4.25693400	3.77961000	2.76669100
C	3.92578600	5.97570800	1.87107700
C	4.64870400	5.10828300	2.68067100
H	4.78487100	3.06595100	3.39536500
H	4.20420000	7.02831400	1.79308100
C	1.98453100	6.47266600	0.34388700
O	1.36585400	3.71151400	0.51442500
C	2.89343600	1.77597700	2.22573800
O	2.04760100	1.22862500	1.45358900
Co	-0.60914100	-0.84879100	-0.50081000
O	-0.42570300	-1.23580300	2.26063900
C	-5.40564600	-0.35394000	-0.03791800
C	-6.33630200	-1.06683400	-0.79597600
C	-5.91093600	0.48271500	0.96006700
C	-7.70371500	-0.95290700	-0.58366400
C	-7.27432700	0.61624400	1.18734100
C	-8.17368800	-0.10618300	0.41217300
C	4.06933500	-2.16654400	-0.59578300
C	5.03472500	-1.49413200	0.16484300
C	4.51130700	-3.26166500	-1.34502800
C	6.36069900	-1.91078600	0.19053600
C	5.82993000	-3.69216700	-1.33030300
C	6.75920300	-3.01403700	-0.55297100
F	-5.07686300	1.18533200	1.72651400
F	-7.72865000	1.42504900	2.14909900
F	-9.48621400	0.01386600	0.62264700
F	-8.56941500	-1.64477400	-1.33163800
F	-5.92222500	-1.88974500	-1.76471000
F	4.72380100	-0.41289000	0.86366100
F	7.26230700	-1.25276600	0.92432100
F	8.03330700	-3.41369100	-0.53057900
F	6.21239900	-4.74300000	-2.06594000
F	3.65451700	-3.93402600	-2.12502500
O	3.54980700	1.19393500	3.11646000
F	-5.26562400	-3.26625500	0.66707800
F	-3.06820000	-5.22509100	0.90145400
F	0.21905400	-5.80563800	0.85209600
F	2.94135800	-4.77050400	0.41445100
F	4.45174500	0.46359300	-1.67105600

F	2.89600800	2.88203200	-2.00130100
F	-2.62601100	4.01425900	-1.42043400
F	-4.89976400	2.34305600	-0.82152300
H	-0.14594400	6.21397000	-3.83339600
H	1.24036700	6.96498100	0.99630900
H	2.60646400	7.28880400	-0.05226800
H	5.50973000	5.46771700	3.24247600
O	2.57687700	-1.42523500	2.35920900
H	3.11748400	-0.85517000	2.93704000
O	-0.58148800	-2.37857200	2.66311900
H	2.15103500	-0.70410800	1.85542700
O	-0.67145700	1.44995900	1.79414900
H	0.29704000	1.28253100	1.79527700
H	-0.71333400	2.29055300	1.32006600