Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


*Supporting Information*

# Electrochemical, spectroscopic and theoretical studies of a simple bifunctional cobalt corrole catalyst for oxygen evolution and hydrogen production

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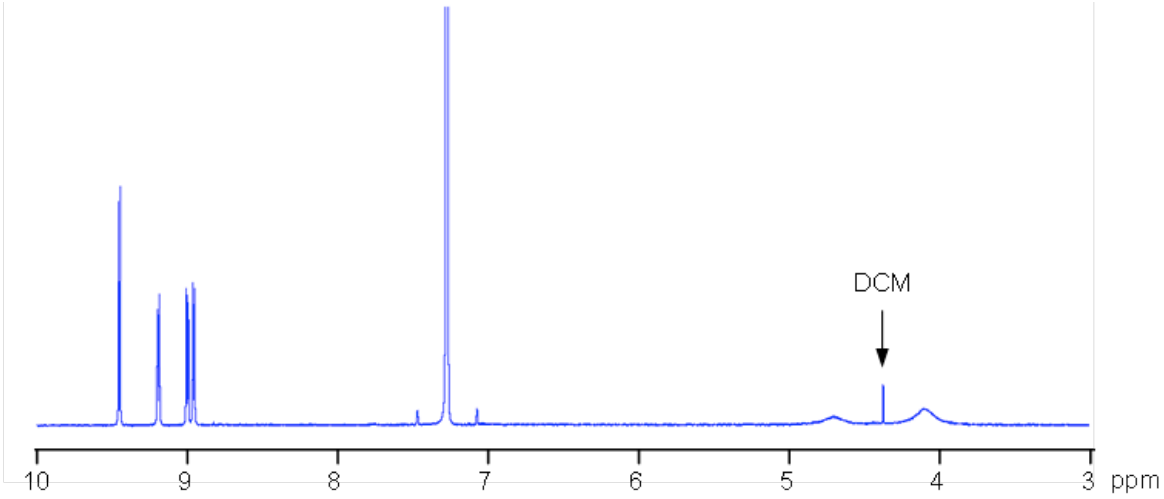


**Figure S1.** $^{1}$H NMR spectrum of complex **1** in $C_6D_6$.

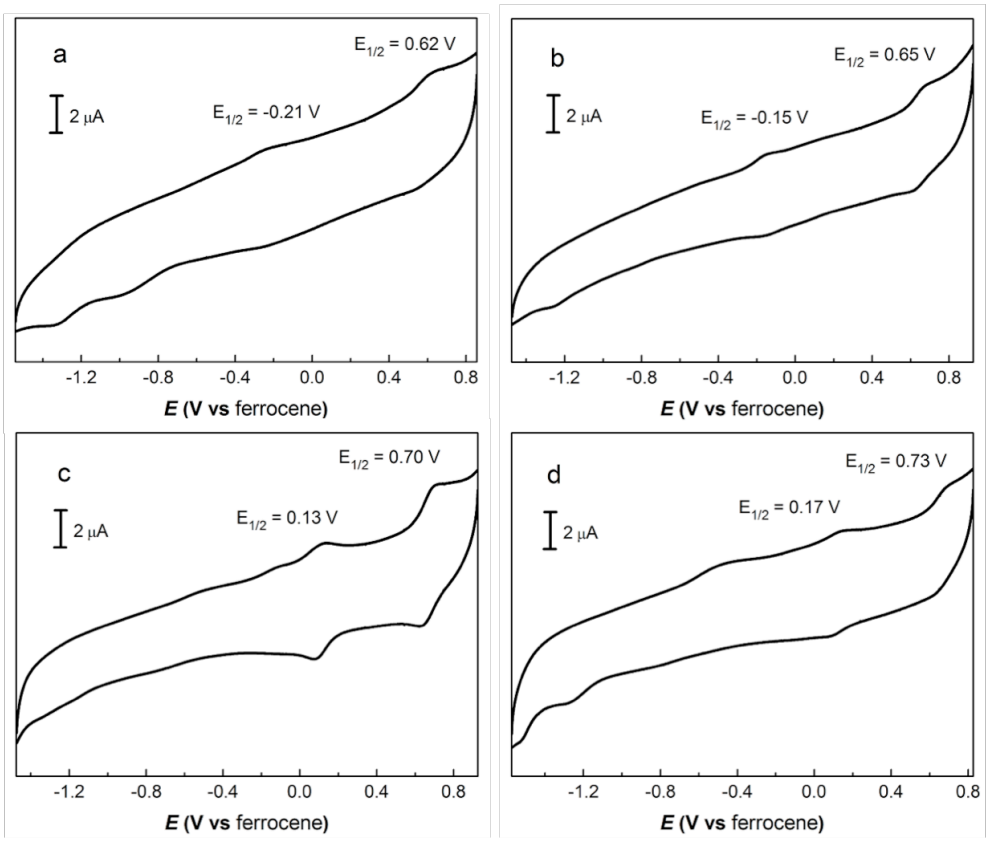


**Figure S2.** CVs of 0.02 mM complex **3** (a), **4** (b), **5** (c) and **6** (d) in acetonitrile. Conditions: 0.1 M $Bu_4NClO_4$, GC as the working electrode, Pt as the auxiliary electrode, Ag as the reference electrode (calibrated using $Fc^+/Fc$). Scan rate: 50 mV/s.

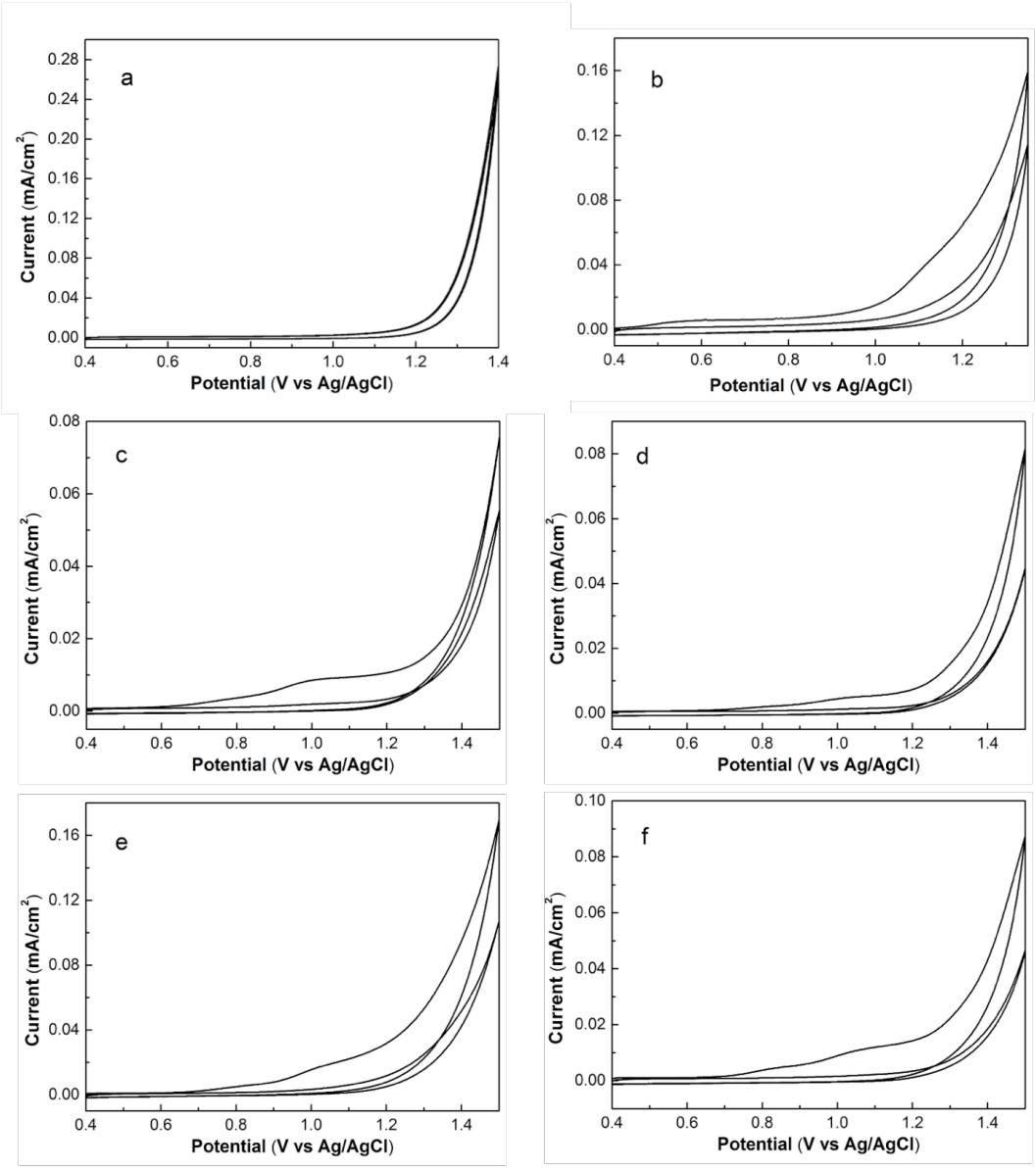


**Figure S3.** CVs of the ITO electrode coated with complex **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) and **6** (f) in 0.1 M phosphate buffer, pH = 7.0. The loaded catalyst was 2.5 nmol/cm$^2$.

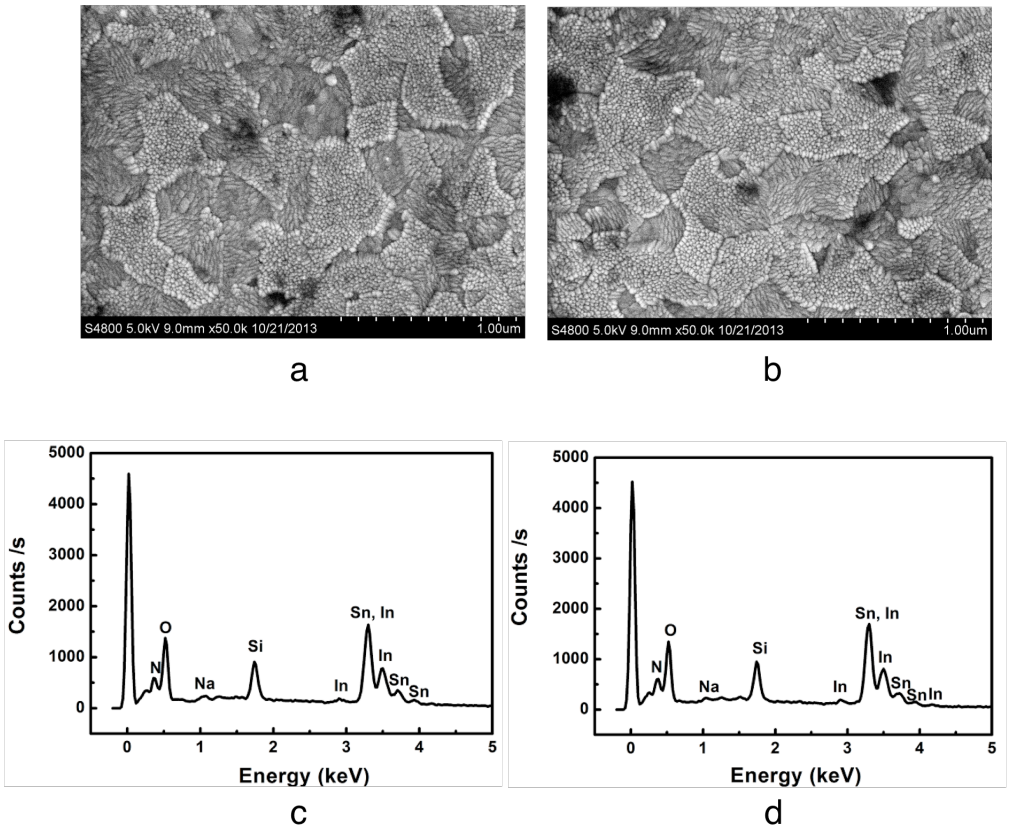


**Figure S4.** SEM images for ITO electrodes. (a) bare ITO; (b) ITO coated with **1** after bulk electrolysis and washed by DCM. EDX data for ITO electrodes. (c) bare ITO; (d) ITO coated with **1** after bulk electrolysis and washed by DCM.

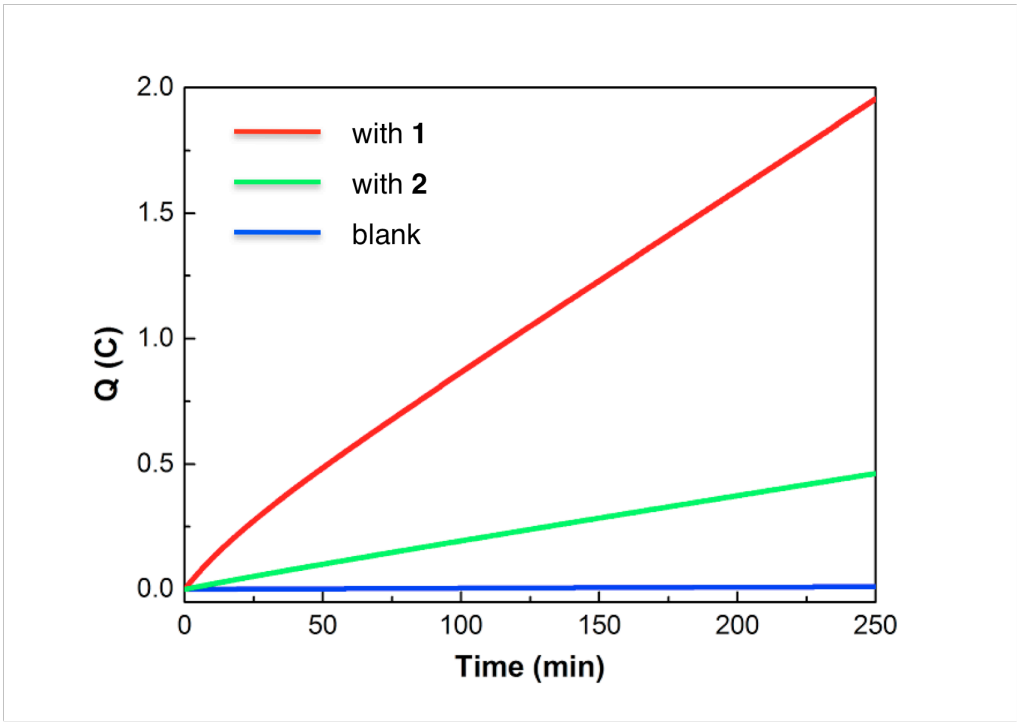


**Figure S5.** Electric charge curve of ITO coated with complex **1** (red) or **2** (green) and bare ITO (blue) during 250-min electrolysis at 1.40 V (vs Ag/AgCl).

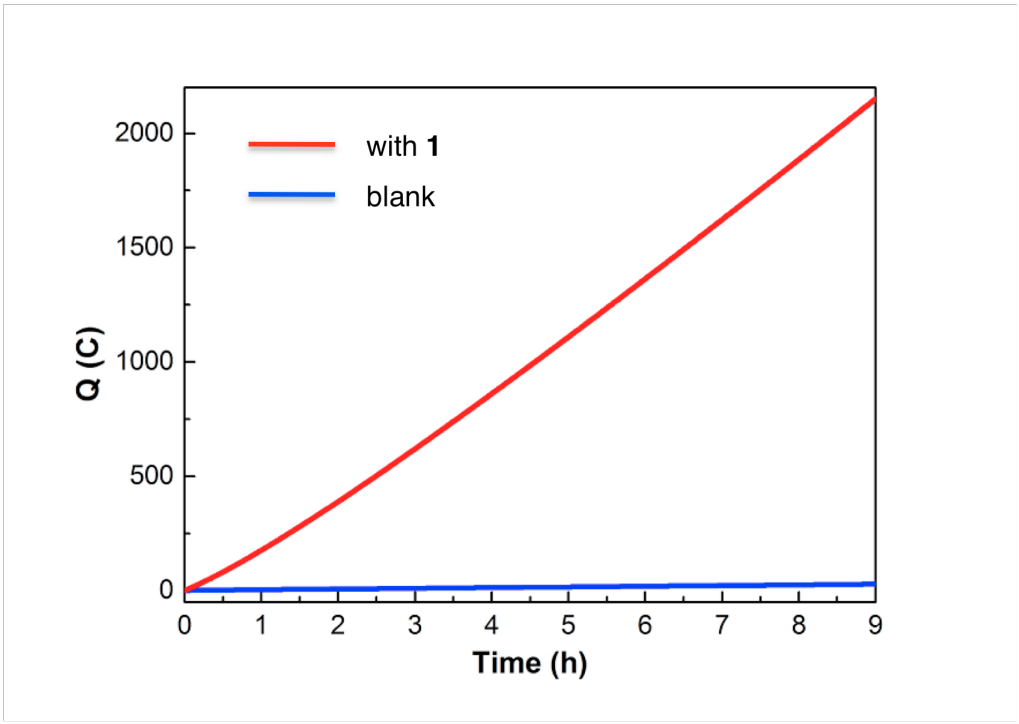


**Figure S6.** Electric charge curve of GC electrode coated with **1** (red) and bare GC electrode (blue) during 9.0-h electrolysis at −1.1 V vs Ag/AgCl.

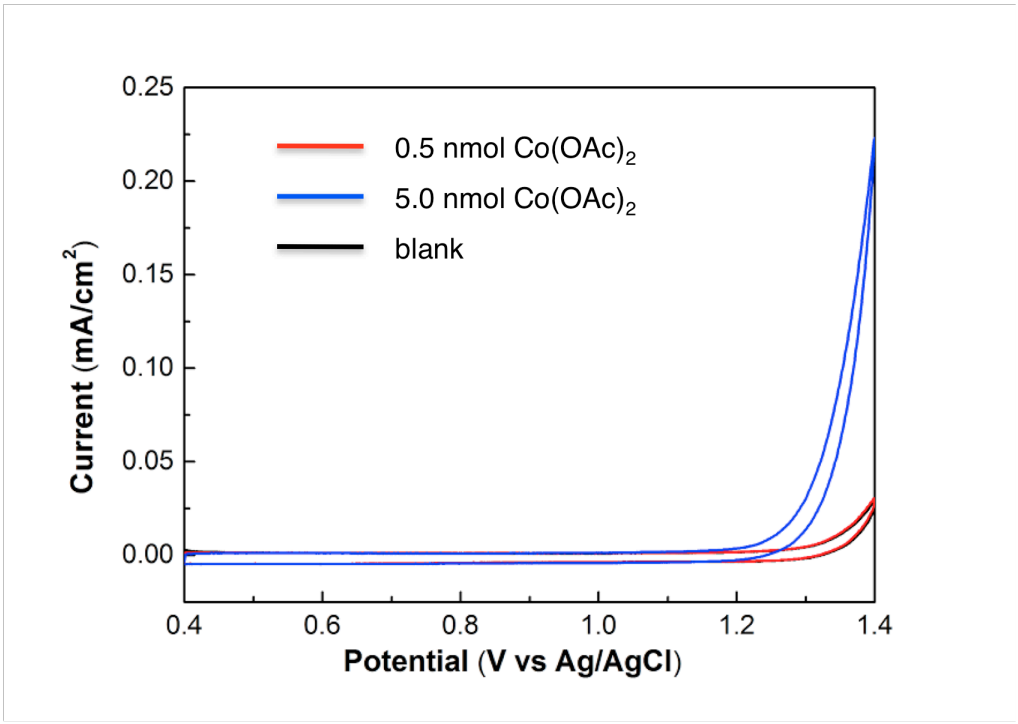


**Figure S7.** CVs of bare ITO electrode in 0.1 M phosphate buffer (20 mL, pH = 7) with addition of 0.5 nmol $Co(OAc)_2$ (red) or 5.0 nmol $Co(OAc)_2$ or without addition of any Co ions (black).

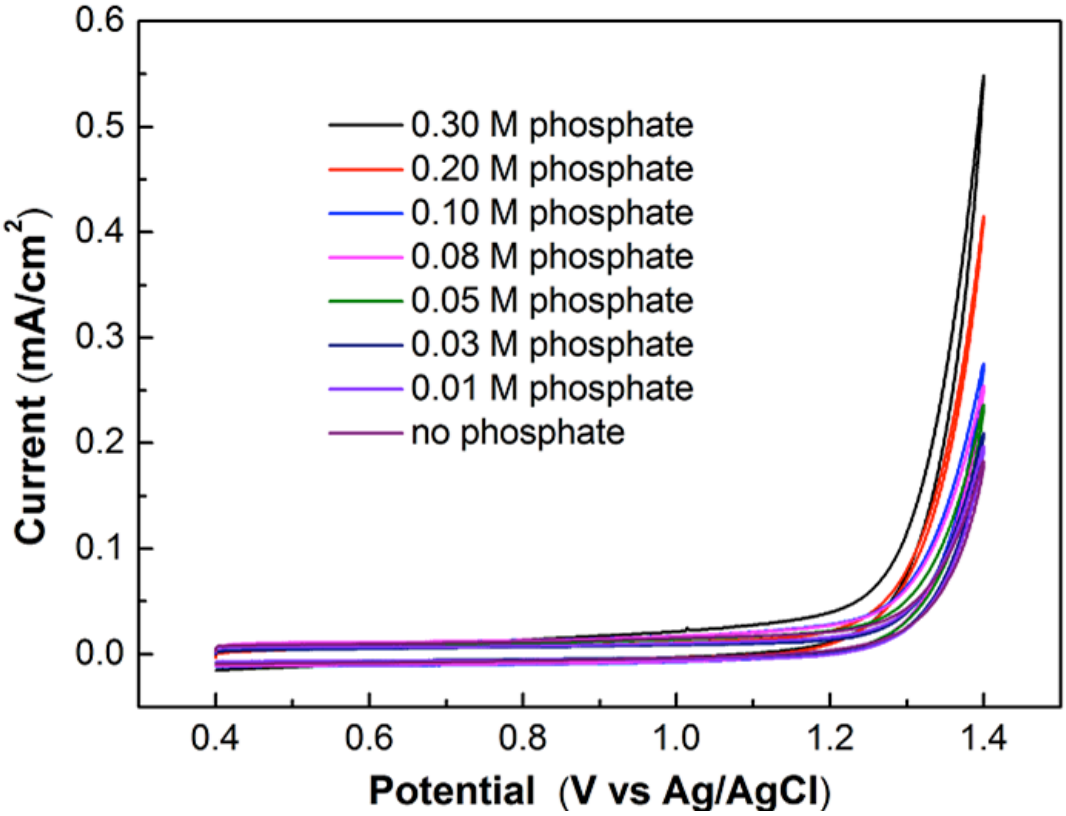


**Figure S8.** CVs of an ITO electrode coated with complex **1** in pH 7.0 buffer solutions with increasing amounts of phosphate. The loaded catalyst was 2.5 nmol/cm$^2$.

**Table S1.** Crystal data and structure refinement parameters for $[Co(tpfc)(py)_2]$ (**1**)

| Complex | **1** |
|---|---|
| molecular formula | $C_{47}H_{18}CoF_{15}N_6$ |
| formula wt. (g mol$^{-1}$) | 1010.60 |
| temperature (K) | 153(2) |
| radiation (λ, Å) | 0.71073 |
| crystal system | Triclinic |
| space group | $P\bar{1}$ (# 2) |
| $a$ (Å) | 13.638(4) |
| $b$ (Å) | 16.772(4) |
| $c$ (Å) | 20.382(5) |
| $\alpha$ (°) | 71.783(5) |
| $\beta$ (°) | 80.567(7) |
| $\gamma$ (°) | 87.282(7) |
| Volume (Å$^3$) | 4368.6(19) |
| $Z$ | 4 |
| $\rho_{calcd}$ (g cm$^{-3}$) | 1.537 |
| $\mu$ (mm$^{-1}$) | 0.499 |
| F(000) | 2016 |
| crystal size (mm$^3$) | 0.50 × 0.08 × 0.02 |
| Theta range | 1.90 to 23.26° |
| reflections collected | 23178 |
| independent reflections | 11608 [R(int) = 0.0576] |
| Completeness | 92.4% |
| goodness-of-fit on $F^2$ | 1.037 |
| final R indices | $R1^a$ = 0.0989 |
| [R > 2σ (I)] | $wR_2{}^b$ = 0.2547 |
| R indices (all data) | $R1^a$ = 0.1441 |
| | $wR_2{}^b$ = 0.2712 |
| largest diff. peak and hole (e Å$^{-3}$) | 1.374 and −0.582 |

$^aR_1 = \Sigma||F_o| - |F_c|| / |F_o|$, $^bwR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{0.5}$

## Energies, Spin Densities, and Key Geometrical Parameters

**Table S2.** Calculated absolute energies of the key species (a.u.)

| | $E$(B1) | $E$(B2) | $G_{corr}$ | D$\Delta E_{solv}$ |
|---|---|---|---|---|
| $^{1}$[Cor-Co$^{III}$-H$_2$O] | -4835.752528 | -4839.765682 | 0.408354 | -0.018535 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-H$_2$O]$^{+}$ | -4835.527211 | -4839.544204 | 0.407968 | -0.065754 |
| $^{1}$[Cor-Co$^{III}$-OH]$^{-}$ | -4835.218241 | -4839.237941 | 0.396227 | -0.070507 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-OH] | -4835.104030 | -4839.125696 | 0.395108 | -0.065754 |
| $^{1}$[Cor$^{\bullet+}$-Co$^{III}$-OH]$^{+}$ | -4834.871307 | -4838.896655 | 0.398038 | -0.064122 |
| $^{2}$[Cor-Co$^{III}$-O$^{\bullet-}$]$^{-}$ | -4834.551712 | -4838.570800 | 0.386686 | -0.064122 |
| $^{1}$[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] | -4834.434640 | -4838.456612 | 0.385958 | -0.023841 |
| $^{3}$[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] | -4834.440285 | -4838.460189 | 0.383635 | -0.019868 |
| $^{1}$[Cor-Co$^{III}$-OOH]$^{-}$ | -4910.294093 | -4914.398702 | 0.397157 | -0.055713 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-OOH]$^{-}$ | -4910.180338 | -4914.286610 | 0.395780 | -0.022133 |
| $^{1}$[Cor$^{\bullet-}$-Co$^{III}$-OO$^{\bullet-}$]$^{2-}$ | -4909.646023 | -4913.746282 | 0.381192 | -0.198096 |
| $^{2}$[Cor-Co$^{III}$-OO$^{\bullet-}$]$^{-}$ | -4909.688371 | -4913.790821 | 0.385826 | -0.066410 |
| $^{3}$[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$] | -4909.577579 | -4913.682001 | 0.385136 | -0.017867 |

| | $E_{solv}$(B1) | $E_{solv}$(B2) | $G_{corr}$ | D |
|---|---|---|---|---|
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} | -5139.960025 | -5144.336323 | 0.475444 | |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} | -5139.960265 | -5144.336323 | 0.474416 | |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O}$^{‡}$ | -5139.925102 | -5144.292460 | 0.478199 | |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$} | -5139.260575 | -5143.638629 | 0.449821 | |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$} | -5139.264804 | -5143.639952 | 0.449630 | |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$}$^{‡}$ | -5139.244331 | -5143.612743 | 0.451328 | |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$}$^{‡}$ | -5139.237937 | -5143.607626 | 0.449832 | |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·H$_2$O} | -4985.940316 | -4990.134217 | 0.408298 | |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·H$_2$O}$^{‡}$ | -4985.928934 | -4990.125212 | 0.404960 | |

**Table S3.** Mulliken spin densities of the key species.

| species | Co | Cor | py | L[a] |
|---|---|---|---|---|
| $^{1}$[Cor-Co$^{III}$-H$_2$O] | 0.00 | 0.00 | 0.00 | 0.00 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-H$_2$O]$^{+}$ | 0.00 | 1.00 | 0.00 | 0.01 |
| $^{1}$[Cor-Co$^{III}$-OH]$^{-}$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-OH] | 0.01 | 0.86 | 0.01 | 0.11 |
| $^{1}$[Cor$^{\bullet+}$-Co$^{III}$-OH]$^{+}$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $^{2}$[Cor-Co$^{III}$-O$^{\bullet-}$]$^{-}$ | 0.02 | 0.02 | -0.02 | 0.98 |
| $^{1}$[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] | 0.02 | -0.96 | -0.03 | 0.96 |
| $^{3}$[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] | 0.26 | 0.60 | 0.00 | 1.15 |
| $^{1}$[Cor-Co$^{III}$-OOH]$^{-}$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $^{2}$[Cor$^{\bullet+}$-Co$^{III}$-OOH]$^{-}$ | 0.04 | 0.72 | 0.01 | 0.23 |
| $^{1}$[Cor$^{\bullet-}$-Co$^{III}$-OO$^{\bullet-}$]$^{2-}$ | -0.31 | -0.96 | -0.01 | 1.29 |
| $^{2}$[Cor-Co$^{III}$-OO$^{\bullet-}$]$^{-}$ | -1.04 | 0.14 | -0.03 | 1.93 |
| $^{3}$[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$] | -0.19 | 0.63 | 0.01 | 1.54 |

| RCs and TSs[b] | Co | Cor | py | L[a] | $H_2O$ | other |
|---|---|---|---|---|---|---|
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} | 0.15 | -1.00 | -0.02 | 0.89 | -0.01 | -0.01 |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} | 0.10 | 1.01 | 0.00 | 0.91 | -0.01 | -0.01 |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O}$^{‡}$ | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$} | -0.11 | 0.91 | 0.02 | -0.91 | 0.07 | 0.01 |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$} | 0.05 | 0.92 | 0.00 | 0.95 | 0.07 | 0.01 |
| $^{1}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$}$^{‡}$ | -0.06 | -0.20 | -0.01 | 0.29 | -0.01 | 0.00 |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·[OAc]$^{-}$}$^{‡}$ | 1.15 | -0.05 | -0.05 | -0.01 | 0.00 | 0.00 |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·H$_2$O} | -0.17 | 0.73 | 0.01 | 1.44 | 0.00 | – |
| $^{3}${[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·H$_2$O}$^{‡}$ | -0.29 | 0.30 | 0.01 | 1.98 | 0.00 | – |

[a]The distal ligand. [b]Reactant complexes and transitions states for the O−O bond formation and $O_2$ release.

## Cartesian Coordinates

### [Cor-$Co^{III}$-$OH_2$] (singlet)

| | | | |
|---|---|---|---|
| C | 11.722397 | 3.923975 | 5.471347 |
| C | 12.658428 | 4.471308 | 4.533930 |
| H | 13.667971 | 4.800683 | 4.773347 |
| C | 12.049651 | 4.506124 | 3.306461 |
| H | 12.474065 | 4.873956 | 2.374079 |
| C | 10.729804 | 3.969000 | 3.466440 |
| C | 9.750074 | 3.808450 | 2.461951 |
| C | 8.454582 | 3.284239 | 2.667469 |
| C | 7.432768 | 3.092299 | 1.678993 |
| H | 7.512964 | 3.351730 | 0.625109 |
| C | 6.354033 | 2.528954 | 2.308506 |
| H | 5.399824 | 2.257879 | 1.859379 |
| C | 6.694510 | 2.355361 | 3.689816 |
| C | 5.886039 | 1.760387 | 4.687684 |
| C | 6.309451 | 1.602887 | 6.027395 |
| C | 5.667315 | 1.036816 | 7.179109 |
| H | 4.655496 | 0.634877 | 7.208378 |
| C | 6.557453 | 1.117154 | 8.236866 |
| H | 6.387599 | 0.790448 | 9.261090 |
| C | 7.744105 | 1.722837 | 7.734230 |
| C | 9.030991 | 2.122365 | 8.189336 |
| C | 9.792602 | 2.154617 | 9.392286 |
| H | 9.466754 | 1.800289 | 10.368375 |
| C | 11.009928 | 2.736610 | 9.081663 |
| H | 11.836720 | 2.927771 | 9.764725 |
| C | 10.992712 | 3.058881 | 7.683992 |
| C | 11.953977 | 3.664651 | 6.843005 |
| C | 10.110532 | 4.209795 | 1.082494 |
| C | 11.118788 | 3.552257 | 0.367347 |
| C | 11.452656 | 3.905539 | -0.938467 |
| C | 10.770606 | 4.946181 | -1.566410 |
| C | 9.761692 | 5.622794 | -0.882734 |
| C | 9.450960 | 5.254843 | 0.424723 |
| C | 4.576316 | 1.197966 | 4.298246 |
| C | 4.484546 | 0.153631 | 3.368876 |
| C | 3.266970 | -0.416082 | 3.006873 |
| C | 2.090795 | 0.052461 | 3.590165 |
| C | 2.146171 | 1.081687 | 4.528306 |
| C | 3.376460 | 1.642569 | 4.866576 |
| C | 13.281783 | 3.966830 | 7.414692 |
| C | 14.082087 | 2.940983 | 7.933782 |
| C | 15.332488 | 3.185524 | 8.495457 |
| C | 15.818271 | 4.491004 | 8.545196 |
| C | 15.052601 | 5.534449 | 8.026966 |
| C | 13.800847 | 5.265656 | 7.476297 |
| C | 11.001562 | 0.673640 | 5.271226 |
| H | 11.619881 | 1.450251 | 5.724216 |
| C | 11.531838 | -0.573668 | 4.967451 |
| H | 12.582058 | -0.769335 | 5.187185 |
| C | 10.711553 | -1.540839 | 4.394444 |
| H | 11.103734 | -2.528684 | 4.143702 |
| C | 9.379204 | -1.220638 | 4.151854 |
| H | 8.686887 | -1.937196 | 3.708101 |
| C | 8.914782 | 0.044984 | 4.484119 |
| H | 7.874088 | 0.320623 | 4.310706 |
| Co | 9.011536 | 2.738862 | 5.484089 |
| F | 11.784409 | 2.545351 | 0.924921 |
| F | 12.402575 | 3.249447 | -1.591946 |
| F | 11.077129 | 5.289357 | -2.807790 |
| F | 9.114163 | 6.618032 | -1.473648 |
| F | 8.496930 | 5.938025 | 1.051335 |
| F | 5.590918 | -0.348486 | 2.819285 |
| F | 3.220424 | -1.407432 | 2.126430 |
| F | 0.926709 | -0.483055 | 3.258523 |
| F | 1.028402 | 1.526137 | 5.085792 |
| F | 3.385380 | 2.632321 | 5.752778 |
| F | 13.667757 | 1.676265 | 7.868581 |
| F | 16.066290 | 2.185630 | 8.965684 |
| F | 17.005557 | 4.739607 | 9.075130 |
| F | 15.515838 | 6.776059 | 8.073955 |
| F | 13.092514 | 6.289345 | 7.009184 |
| N | 10.554646 | 3.641758 | 4.786901 |
| N | 7.973954 | 2.845113 | 3.874433 |
| N | 7.550140 | 1.994121 | 6.412130 |
| N | 9.788575 | 2.669137 | 7.197387 |
| N | 9.715440 | 0.976886 | 5.027040 |
| O | 8.275335 | 4.611570 | 5.946423 |
| H | 9.005367 | 5.196336 | 5.687834 |
| H | 7.599614 | 4.753072 | 5.264696 |

**$[Cor^{\bullet+}\text{-}Co^{III}\text{-}OH_2]^{+}$ (doublet)**

| | | | |
|---|---|---|---|
| C | 11.727959 | 3.904744 | 5.457082 |
| C | 12.664118 | 4.467963 | 4.533483 |
| H | 13.663894 | 4.817819 | 4.780693 |
| C | 12.063684 | 4.491062 | 3.299991 |
| H | 12.484565 | 4.873262 | 2.372645 |
| C | 10.757355 | 3.929772 | 3.455922 |
| C | 9.769296 | 3.778261 | 2.451957 |
| C | 8.462027 | 3.268377 | 2.661492 |
| C | 7.428009 | 3.117157 | 1.683363 |
| H | 7.498395 | 3.392977 | 0.633789 |
| C | 6.344482 | 2.570713 | 2.322107 |
| H | 5.376519 | 2.331704 | 1.886337 |
| C | 6.710280 | 2.365828 | 3.689989 |
| C | 5.892898 | 1.760889 | 4.699018 |
| C | 6.317782 | 1.588321 | 6.026708 |
| C | 5.677263 | 1.021563 | 7.182155 |
| H | 4.664440 | 0.624507 | 7.216367 |
| C | 6.570465 | 1.096104 | 8.233536 |
| H | 6.406305 | 0.767632 | 9.257401 |
| C | 7.759104 | 1.694141 | 7.719473 |
| C | 9.064108 | 2.089202 | 8.176157 |
| C | 9.804082 | 2.159280 | 9.396366 |
| H | 9.464998 | 1.826835 | 10.374866 |
| C | 11.014622 | 2.745746 | 9.089432 |
| H | 11.826802 | 2.969442 | 9.779046 |
| C | 11.012736 | 3.033777 | 7.679562 |
| C | 11.958095 | 3.653690 | 6.849617 |
| C | 10.128850 | 4.185119 | 1.076188 |
| C | 11.154051 | 3.537871 | 0.374234 |
| C | 11.485882 | 3.890328 | -0.931428 |
| C | 10.794898 | 4.927357 | -1.560473 |
| C | 9.773805 | 5.597369 | -0.883443 |
| C | 9.453992 | 5.221470 | 0.418600 |
| C | 4.574367 | 1.226677 | 4.305897 |
| C | 4.474423 | 0.205618 | 3.351098 |
| C | 3.251591 | -0.350677 | 2.989760 |
| C | 2.082396 | 0.119526 | 3.591132 |
| C | 2.148572 | 1.131774 | 4.550368 |
| C | 3.385529 | 1.670204 | 4.898582 |
| C | 13.275046 | 3.987707 | 7.422674 |
| C | 14.077102 | 2.978987 | 7.974526 |
| C | 15.325621 | 3.248865 | 8.526676 |
| C | 15.795830 | 4.563267 | 8.544531 |
| C | 15.021513 | 5.590060 | 7.999967 |
| C | 13.777977 | 5.294926 | 7.446590 |
| C | 11.011586 | 0.614059 | 5.247618 |
| H | 11.635247 | 1.376660 | 5.714960 |
| C | 11.535770 | -0.632192 | 4.932142 |
| H | 12.583507 | -0.837340 | 5.154229 |
| C | 10.712522 | -1.588238 | 4.344572 |
| H | 11.099731 | -2.575357 | 4.084910 |
| C | 9.383282 | -1.256933 | 4.099443 |
| H | 8.688799 | -1.964388 | 3.644888 |
| C | 8.925887 | 0.007913 | 4.442179 |
| H | 7.888363 | 0.286207 | 4.261067 |
| Co | 9.033271 | 2.708206 | 5.474791 |
| F | 11.820490 | 2.540511 | 0.944869 |
| F | 12.440838 | 3.246125 | -1.576465 |
| F | 11.103298 | 5.272154 | -2.792478 |
| F | 9.124633 | 6.583537 | -1.473411 |
| F | 8.492360 | 5.887177 | 1.049419 |
| F | 5.580383 | -0.286177 | 2.792814 |
| F | 3.194000 | -1.322931 | 2.098163 |
| F | 0.919229 | -0.398412 | 3.259301 |
| F | 1.043244 | 1.572711 | 5.120323 |
| F | 3.418958 | 2.639366 | 5.805419 |
| F | 13.666283 | 1.713269 | 7.938041 |
| F | 16.064020 | 2.271646 | 9.019781 |
| F | 16.972075 | 4.835281 | 9.067962 |
| F | 15.467023 | 6.831992 | 8.021398 |
| F | 13.053182 | 6.291171 | 6.950876 |
| N | 10.580489 | 3.591088 | 4.773489 |
| N | 7.996220 | 2.812786 | 3.866288 |
| N | 7.569713 | 1.972566 | 6.408993 |
| N | 9.820048 | 2.602563 | 7.182849 |
| N | 9.728029 | 0.930873 | 5.000379 |
| O | 8.326778 | 4.553306 | 5.990229 |
| H | 8.785246 | 5.233070 | 5.473094 |
| H | 7.391736 | 4.635746 | 5.749335 |

**[Cor-Co$^{III}$-OH]$^{-}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 11.777384 | 3.804158 | 5.428999 |
| C | 12.699665 | 4.399487 | 4.501978 |
| H | 13.696880 | 4.763507 | 4.746850 |
| C | 12.092692 | 4.420338 | 3.273344 |
| H | 12.502264 | 4.818091 | 2.345614 |
| C | 10.788760 | 3.836084 | 3.433853 |
| C | 9.788860 | 3.711166 | 2.440559 |
| C | 8.480887 | 3.213813 | 2.653986 |
| C | 7.419930 | 3.123910 | 1.683723 |
| H | 7.473928 | 3.443499 | 0.644095 |
| C | 6.337156 | 2.582349 | 2.322879 |
| H | 5.352473 | 2.391969 | 1.897006 |
| C | 6.726426 | 2.320590 | 3.682741 |
| C | 5.911284 | 1.750148 | 4.691468 |
| C | 6.351871 | 1.544009 | 6.021135 |
| C | 5.687868 | 1.027158 | 7.187204 |
| H | 4.653082 | 0.688674 | 7.237237 |
| C | 6.598144 | 1.068546 | 8.230880 |
| H | 6.425108 | 0.767609 | 9.263475 |
| C | 7.812494 | 1.593439 | 7.696247 |
| C | 9.112207 | 1.970801 | 8.144391 |
| C | 9.842293 | 2.065331 | 9.365037 |
| H | 9.498635 | 1.746091 | 10.348205 |
| C | 11.059148 | 2.654495 | 9.058407 |
| H | 11.866075 | 2.888893 | 9.752865 |
| C | 11.063201 | 2.914231 | 7.645592 |
| C | 12.005477 | 3.561362 | 6.807151 |
| C | 10.137362 | 4.156056 | 1.073685 |
| C | 11.151386 | 3.527560 | 0.337241 |
| C | 11.490270 | 3.922319 | -0.955015 |
| C | 10.807922 | 4.976721 | -1.556008 |
| C | 9.795138 | 5.626347 | -0.854775 |
| C | 9.479980 | 5.220456 | 0.440923 |
| C | 4.556067 | 1.291147 | 4.330800 |
| C | 4.358741 | 0.288529 | 3.369744 |
| C | 3.093647 | -0.188012 | 3.036147 |
| C | 1.971347 | 0.328422 | 3.678844 |
| C | 2.129197 | 1.315985 | 4.647810 |
| C | 3.403990 | 1.787940 | 4.956891 |
| C | 13.263773 | 4.027843 | 7.416880 |
| C | 14.132702 | 3.144289 | 8.075184 |
| C | 15.297566 | 3.573703 | 8.706780 |
| C | 15.636238 | 4.924477 | 8.685212 |
| C | 14.804949 | 5.829679 | 8.030735 |
| C | 13.638972 | 5.380281 | 7.415590 |
| C | 11.048864 | 0.427368 | 5.133601 |
| H | 11.682621 | 1.197634 | 5.583009 |
| C | 11.556899 | -0.828116 | 4.816339 |
| H | 12.607624 | -1.049151 | 5.012253 |
| C | 10.706445 | -1.777974 | 4.255873 |
| H | 11.074837 | -2.773194 | 3.994138 |
| C | 9.375663 | -1.430855 | 4.038522 |
| H | 8.664487 | -2.136084 | 3.604737 |
| C | 8.948688 | -0.152870 | 4.383956 |
| H | 7.911223 | 0.155255 | 4.229780 |
| Co | 9.060561 | 2.646727 | 5.454126 |
| F | 11.820907 | 2.501855 | 0.855729 |
| F | 12.447173 | 3.287084 | -1.629741 |
| F | 11.119417 | 5.360984 | -2.791184 |
| F | 9.150119 | 6.645359 | -1.419240 |
| F | 8.530105 | 5.895596 | 1.077635 |
| F | 5.403526 | -0.273678 | 2.762121 |
| F | 2.949093 | -1.153504 | 2.130310 |
| F | 0.757940 | -0.125373 | 3.376005 |
| F | 1.056733 | 1.809598 | 5.263069 |
| F | 3.495250 | 2.748846 | 5.867818 |
| F | 13.875387 | 1.838133 | 8.089610 |
| F | 16.101160 | 2.702230 | 9.314567 |
| F | 16.747759 | 5.347374 | 9.280718 |
| F | 15.120923 | 7.122616 | 8.021393 |
| F | 12.864085 | 6.292786 | 6.839083 |
| N | 10.639692 | 3.461939 | 4.736571 |
| N | 8.032715 | 2.707606 | 3.833845 |
| N | 7.622764 | 1.836520 | 6.374524 |
| N | 9.890348 | 2.463360 | 7.145024 |
| N | 9.769916 | 0.761490 | 4.916288 |
| O | 8.384548 | 4.316497 | 5.952114 |
| H | 9.172186 | 4.874024 | 5.994557 |

**[Cor$^{\bullet+}$-Co$^{III}$-OH] (doublet)**

| | | | |
|---|---|---|---|
| C | 11.771209 | 3.772145 | 5.440930 |
| C | 12.694300 | 4.370968 | 4.522223 |
| H | 13.685376 | 4.745051 | 4.772247 |
| C | 12.096518 | 4.377695 | 3.287927 |
| H | 12.507162 | 4.772150 | 2.360464 |
| C | 10.801499 | 3.784219 | 3.445685 |
| C | 9.800169 | 3.651418 | 2.451155 |
| C | 8.492012 | 3.158509 | 2.664043 |
| C | 7.420226 | 3.095828 | 1.708815 |
| H | 7.464935 | 3.424325 | 0.672635 |
| C | 6.337708 | 2.568749 | 2.360790 |
| H | 5.344763 | 2.397035 | 1.949334 |
| C | 6.746460 | 2.287172 | 3.709254 |
| C | 5.930868 | 1.706840 | 4.730427 |
| C | 6.379271 | 1.470527 | 6.037671 |
| C | 5.707019 | 0.976322 | 7.213391 |
| H | 4.666727 | 0.659366 | 7.266480 |
| C | 6.616623 | 1.006733 | 8.249715 |
| H | 6.442547 | 0.720871 | 9.285147 |
| C | 7.843455 | 1.502570 | 7.701480 |
| C | 9.153400 | 1.884058 | 8.151567 |
| C | 9.870127 | 2.010966 | 9.381734 |
| H | 9.522458 | 1.699673 | 10.364775 |
| C | 11.069811 | 2.623273 | 9.078234 |
| H | 11.865273 | 2.885710 | 9.774023 |
| C | 11.079587 | 2.865324 | 7.660339 |
| C | 11.992339 | 3.542112 | 6.833992 |
| C | 10.148282 | 4.103286 | 1.084094 |
| C | 11.144455 | 3.456340 | 0.343319 |
| C | 11.479739 | 3.854729 | -0.948466 |
| C | 10.817217 | 4.935201 | -1.528666 |
| C | 9.825821 | 5.605886 | -0.813920 |
| C | 9.505913 | 5.188533 | 0.476536 |
| C | 4.549546 | 1.317271 | 4.375171 |
| C | 4.312221 | 0.323906 | 3.417324 |
| C | 3.024710 | -0.072297 | 3.066442 |
| C | 1.930538 | 0.528089 | 3.688245 |
| C | 2.133258 | 1.514328 | 4.652082 |
| C | 3.431476 | 1.897248 | 4.986036 |
| C | 13.230575 | 4.062747 | 7.447039 |
| C | 14.132522 | 3.214001 | 8.102410 |
| C | 15.280758 | 3.696426 | 8.725574 |
| C | 15.552989 | 5.063266 | 8.703188 |
| C | 14.679662 | 5.934434 | 8.053948 |
| C | 13.537080 | 5.430711 | 7.437399 |
| C | 11.098465 | 0.386710 | 5.080492 |
| H | 11.723494 | 1.146722 | 5.557122 |
| C | 11.627569 | -0.844149 | 4.709910 |
| H | 12.683069 | -1.052340 | 4.890348 |
| C | 10.791460 | -1.785512 | 4.115956 |
| H | 11.176744 | -2.760931 | 3.810847 |
| C | 9.452743 | -1.457175 | 3.922172 |
| H | 8.752839 | -2.158684 | 3.466124 |
| C | 9.002628 | -0.203809 | 4.320598 |
| H | 7.957207 | 0.084169 | 4.184226 |
| Co | 9.096068 | 2.552895 | 5.469802 |
| F | 11.792771 | 2.418657 | 0.862271 |
| F | 12.414736 | 3.209200 | -1.631635 |
| F | 11.126382 | 5.323304 | -2.754829 |
| F | 9.202487 | 6.640687 | -1.358693 |
| F | 8.573328 | 5.864126 | 1.136158 |
| F | 5.339413 | -0.290318 | 2.831582 |
| F | 2.831803 | -1.022804 | 2.163014 |
| F | 0.700861 | 0.158482 | 3.369630 |
| F | 1.090405 | 2.082973 | 5.238956 |
| F | 3.586483 | 2.848461 | 5.896345 |
| F | 13.920931 | 1.901195 | 8.120867 |
| F | 16.118532 | 2.866577 | 9.331229 |
| F | 16.638625 | 5.532161 | 9.294542 |
| F | 14.935873 | 7.234009 | 8.040309 |
| F | 12.717376 | 6.292883 | 6.849221 |
| N | 10.642851 | 3.416568 | 4.752594 |
| N | 8.051747 | 2.649836 | 3.850430 |
| N | 7.666012 | 1.731429 | 6.387150 |
| N | 9.920193 | 2.367079 | 7.152106 |
| N | 9.811414 | 0.705033 | 4.883167 |
| O | 8.348399 | 4.191983 | 5.954168 |
| H | 8.951586 | 4.860443 | 5.600326 |

**[Cor$^{++}$-Co$^{III}$-OH]$^{+}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 11.745468 | 3.753315 | 5.466166 |
| C | 12.677825 | 4.358991 | 4.563534 |
| H | 13.655503 | 4.754371 | 4.830433 |
| C | 12.103381 | 4.345638 | 3.318988 |
| H | 12.521711 | 4.746351 | 2.398609 |
| C | 10.819718 | 3.728425 | 3.460946 |
| C | 9.825046 | 3.594494 | 2.461110 |
| C | 8.514537 | 3.100980 | 2.667634 |
| C | 7.451443 | 3.019282 | 1.710247 |
| H | 7.497867 | 3.331878 | 0.670033 |
| C | 6.367697 | 2.496195 | 2.366261 |
| H | 5.378427 | 2.315082 | 1.952736 |
| C | 6.777792 | 2.228490 | 3.713348 |
| C | 5.946700 | 1.651775 | 4.751513 |
| C | 6.402021 | 1.376863 | 6.033130 |
| C | 5.719833 | 0.912777 | 7.221303 |
| H | 4.668540 | 0.638474 | 7.283052 |
| C | 6.635311 | 0.912939 | 8.243963 |
| H | 6.463799 | 0.641168 | 9.282998 |
| C | 7.879333 | 1.356739 | 7.672215 |
| C | 9.202596 | 1.745609 | 8.132051 |
| C | 9.884379 | 1.905809 | 9.383504 |
| H | 9.522683 | 1.591601 | 10.359897 |
| C | 11.060182 | 2.560034 | 9.102354 |
| H | 11.826783 | 2.861630 | 9.813273 |
| C | 11.092194 | 2.791474 | 7.678657 |
| C | 11.960025 | 3.532633 | 6.881380 |
| C | 10.184037 | 4.036530 | 1.097900 |
| C | 11.228090 | 3.416876 | 0.396291 |
| C | 11.572788 | 3.803152 | -0.895493 |
| C | 10.882679 | 4.852261 | -1.506187 |
| C | 9.847609 | 5.498696 | -0.826613 |
| C | 9.506835 | 5.084373 | 0.458212 |
| C | 4.533480 | 1.377768 | 4.426400 |
| C | 4.192533 | 0.442080 | 3.441244 |
| C | 2.867254 | 0.155320 | 3.129785 |
| C | 1.844900 | 0.821562 | 3.810533 |
| C | 2.153875 | 1.760145 | 4.796316 |
| C | 3.487833 | 2.021851 | 5.102003 |
| C | 13.161013 | 4.117797 | 7.497053 |
| C | 14.077209 | 3.324137 | 8.206304 |
| C | 15.213138 | 3.868399 | 8.797568 |
| C | 15.445742 | 5.242501 | 8.705429 |
| C | 14.549910 | 6.060457 | 8.013296 |
| C | 13.427574 | 5.494751 | 7.415862 |
| C | 11.168726 | 0.346484 | 4.993271 |
| H | 11.773215 | 1.089777 | 5.519248 |
| C | 11.730506 | -0.848369 | 4.560862 |
| H | 12.788113 | -1.042397 | 4.743324 |
| C | 10.924114 | -1.772755 | 3.902974 |
| H | 11.335580 | -2.719955 | 3.548739 |
| C | 9.580438 | -1.464642 | 3.709565 |
| H | 8.904254 | -2.155618 | 3.204835 |
| C | 9.095059 | -0.247344 | 4.171406 |
| H | 8.044437 | 0.020406 | 4.033417 |
| Co | 9.134362 | 2.446600 | 5.464258 |
| F | 11.893850 | 2.410850 | 0.950521 |
| F | 12.540618 | 3.183948 | -1.543839 |
| F | 11.206004 | 5.231996 | -2.722496 |
| F | 9.205019 | 6.498382 | -1.397899 |
| F | 8.537884 | 5.730556 | 1.091942 |
| F | 5.156114 | -0.222101 | 2.806579 |
| F | 2.570555 | -0.745923 | 2.212784 |
| F | 0.588500 | 0.561335 | 3.523452 |
| F | 1.185996 | 2.392685 | 5.430107 |
| F | 3.757047 | 2.925138 | 6.032659 |
| F | 13.900015 | 2.010535 | 8.285356 |
| F | 16.071630 | 3.096574 | 9.435712 |
| F | 16.510935 | 5.765230 | 9.269245 |
| F | 14.765877 | 7.358823 | 7.939040 |
| F | 12.576921 | 6.295685 | 6.791003 |
| N | 10.642955 | 3.368618 | 4.773149 |
| N | 8.070696 | 2.607365 | 3.865535 |
| N | 7.715956 | 1.573864 | 6.369888 |
| N | 9.958768 | 2.233745 | 7.144324 |
| N | 9.875380 | 0.647028 | 4.797403 |
| O | 8.309486 | 4.010052 | 6.061173 |
| H | 8.466804 | 4.685325 | 5.385963 |

**[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]$^{-}$ (doublet)**

| | | | |
|---|---|---|---|
| C | 11.730691 | 3.914032 | 5.432951 |
| C | 12.659093 | 4.499492 | 4.504168 |
| H | 13.656091 | 4.863202 | 4.749369 |
| C | 12.053684 | 4.518724 | 3.275535 |
| H | 12.465944 | 4.910784 | 2.346695 |
| C | 10.748911 | 3.933741 | 3.435670 |
| C | 9.760601 | 3.782235 | 2.434332 |
| C | 8.462401 | 3.257001 | 2.635923 |
| C | 7.425158 | 3.110493 | 1.647837 |
| H | 7.493244 | 3.404941 | 0.601587 |
| C | 6.347210 | 2.546156 | 2.275974 |
| H | 5.380222 | 2.307517 | 1.834035 |
| C | 6.713488 | 2.328971 | 3.649420 |
| C | 5.898052 | 1.751643 | 4.654158 |
| C | 6.317568 | 1.599248 | 5.999284 |
| C | 5.667682 | 1.045496 | 7.154814 |
| H | 4.654496 | 0.645389 | 7.188798 |
| C | 6.558430 | 1.136189 | 8.213520 |
| H | 6.388324 | 0.818221 | 9.241406 |
| C | 7.748345 | 1.730211 | 7.700935 |
| C | 9.037618 | 2.133401 | 8.157270 |
| C | 9.786510 | 2.184793 | 9.369593 |
| H | 9.452457 | 1.843539 | 10.348608 |
| C | 11.010348 | 2.757585 | 9.059272 |
| H | 11.833154 | 2.957794 | 9.746005 |
| C | 10.999012 | 3.054830 | 7.654190 |
| C | 11.957623 | 3.665453 | 6.809046 |
| C | 10.113824 | 4.215158 | 1.064461 |
| C | 11.144239 | 3.596217 | 0.343034 |
| C | 11.485002 | 3.981348 | -0.951714 |
| C | 10.786451 | 5.014202 | -1.571083 |
| C | 9.755016 | 5.651784 | -0.886064 |
| C | 9.438351 | 5.256541 | 0.412647 |
| C | 4.575546 | 1.219002 | 4.276268 |
| C | 4.443871 | 0.197153 | 3.323521 |
| C | 3.211130 | -0.350621 | 2.978599 |
| C | 2.053443 | 0.111961 | 3.599155 |
| C | 2.145188 | 1.117276 | 4.558535 |
| C | 3.388405 | 1.660362 | 4.879061 |
| C | 13.275102 | 3.989439 | 7.387427 |
| C | 14.078001 | 2.979874 | 7.938690 |
| C | 15.321637 | 3.240015 | 8.508340 |
| C | 15.806928 | 4.545086 | 8.533927 |
| C | 15.042174 | 5.572318 | 7.986170 |
| C | 13.794347 | 5.291048 | 7.431642 |
| C | 11.034774 | 0.540696 | 5.276701 |
| H | 11.648911 | 1.331950 | 5.715842 |
| C | 11.563955 | -0.722445 | 5.029796 |
| H | 12.608384 | -0.925205 | 5.273940 |
| C | 10.741221 | -1.701356 | 4.477953 |
| H | 11.125560 | -2.703529 | 4.271560 |
| C | 9.416883 | -1.373511 | 4.197492 |
| H | 8.726922 | -2.100855 | 3.765789 |
| C | 8.969506 | -0.086175 | 4.476543 |
| H | 7.936794 | 0.206253 | 4.269621 |
| Co | 8.999176 | 2.791181 | 5.460359 |
| F | 11.828277 | 2.588918 | 0.878006 |
| F | 12.459667 | 3.357230 | -1.610840 |
| F | 11.100084 | 5.388801 | -2.808574 |
| F | 9.091462 | 6.647305 | -1.470063 |
| F | 8.466467 | 5.916122 | 1.031261 |
| F | 5.523773 | -0.317342 | 2.736035 |
| F | 3.132902 | -1.331058 | 2.080674 |
| F | 0.870780 | -0.407444 | 3.281699 |
| F | 1.039976 | 1.563529 | 5.151198 |
| F | 3.413844 | 2.635971 | 5.779239 |
| F | 13.680893 | 1.709209 | 7.894574 |
| F | 16.059032 | 2.248225 | 9.004407 |
| F | 16.995160 | 4.809033 | 9.070756 |
| F | 15.503224 | 6.820718 | 8.016296 |
| F | 13.093090 | 6.311341 | 6.950658 |
| N | 10.597127 | 3.570503 | 4.738621 |
| N | 8.003746 | 2.764023 | 3.818043 |
| N | 7.561053 | 1.973092 | 6.376934 |
| N | 9.806908 | 2.648579 | 7.164036 |
| N | 9.762319 | 0.855362 | 5.002767 |
| O | 8.370473 | 4.413432 | 5.844663 |

**[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] (singlet)**

| | | | |
|---|---|---|---|
| C | 11.733490 | 3.878230 | 5.423811 |
| C | 12.656270 | 4.485188 | 4.507855 |
| H | 13.644412 | 4.864685 | 4.760334 |
| C | 12.054585 | 4.500985 | 3.276365 |
| H | 12.460923 | 4.904789 | 2.351160 |
| C | 10.763161 | 3.895837 | 3.433099 |
| C | 9.770140 | 3.741820 | 2.433546 |
| C | 8.470783 | 3.215836 | 2.630577 |
| C | 7.422826 | 3.104379 | 1.653818 |
| H | 7.481877 | 3.414361 | 0.612654 |
| C | 6.342797 | 2.553183 | 2.290357 |
| H | 5.364714 | 2.343402 | 1.861329 |
| C | 6.730571 | 2.310149 | 3.651931 |
| C | 5.910954 | 1.728006 | 4.671463 |
| C | 6.330800 | 1.562556 | 6.000569 |
| C | 5.669994 | 1.031549 | 7.164935 |
| H | 4.652608 | 0.645737 | 7.201074 |
| C | 6.556908 | 1.121946 | 8.218992 |
| H | 6.382762 | 0.822411 | 9.250473 |
| C | 7.759056 | 1.693292 | 7.694719 |
| C | 9.062025 | 2.096947 | 8.154011 |
| C | 9.798764 | 2.178171 | 9.378133 |
| H | 9.455305 | 1.857520 | 10.359576 |
| C | 11.015201 | 2.752921 | 9.068444 |
| H | 11.829613 | 2.976114 | 9.756237 |
| C | 11.012293 | 3.022934 | 7.654789 |
| C | 11.954170 | 3.638373 | 6.816383 |
| C | 10.122136 | 4.187879 | 1.065162 |
| C | 11.139781 | 3.555044 | 0.341319 |
| C | 11.477004 | 3.945268 | -0.952351 |
| C | 10.794560 | 5.002833 | -1.551260 |
| C | 9.780074 | 5.657680 | -0.854192 |
| C | 9.457131 | 5.248487 | 0.438302 |
| C | 4.570040 | 1.235465 | 4.293533 |
| C | 4.422499 | 0.216378 | 3.343198 |
| C | 3.176760 | -0.297091 | 2.994653 |
| C | 2.030643 | 0.211418 | 3.604352 |
| C | 2.142755 | 1.222024 | 4.557903 |
| C | 3.400539 | 1.723120 | 4.890057 |
| C | 13.261009 | 4.006636 | 7.398574 |
| C | 14.098717 | 3.018314 | 7.930335 |
| C | 15.334406 | 3.321083 | 8.495910 |
| C | 15.758012 | 4.648650 | 8.544510 |
| C | 14.948338 | 5.655354 | 8.020064 |
| C | 13.717132 | 5.328855 | 7.454611 |
| C | 11.057727 | 0.482756 | 5.245020 |
| H | 11.674374 | 1.264316 | 5.696781 |
| C | 11.589465 | -0.773266 | 4.974587 |
| H | 12.635017 | -0.976691 | 5.210592 |
| C | 10.767736 | -1.744978 | 4.409909 |
| H | 11.154413 | -2.741379 | 4.184851 |
| C | 9.441265 | -1.418034 | 4.141305 |
| H | 8.752422 | -2.140704 | 3.701469 |
| C | 8.990763 | -0.137945 | 4.442500 |
| H | 7.955730 | 0.148986 | 4.242599 |
| Co | 9.030003 | 2.712293 | 5.454799 |
| F | 11.805831 | 2.537763 | 0.877178 |
| F | 12.432724 | 3.313696 | -1.619182 |
| F | 11.106518 | 5.383787 | -2.778731 |
| F | 9.136027 | 6.668529 | -1.418491 |
| F | 8.499353 | 5.904642 | 1.078570 |
| F | 5.498747 | -0.316993 | 2.767642 |
| F | 3.075665 | -1.273737 | 2.104490 |
| F | 0.841874 | -0.272264 | 3.286126 |
| F | 1.053997 | 1.700888 | 5.140728 |
| F | 3.463630 | 2.694798 | 5.789941 |
| F | 13.736923 | 1.738692 | 7.872835 |
| F | 16.108078 | 2.357555 | 8.975626 |
| F | 16.927084 | 4.953127 | 9.082382 |
| F | 15.348636 | 6.916623 | 8.071628 |
| F | 12.969581 | 6.313560 | 6.974929 |
| N | 10.611036 | 3.520117 | 4.734777 |
| N | 8.021527 | 2.712588 | 3.814245 |
| N | 7.587218 | 1.921985 | 6.378750 |
| N | 9.824055 | 2.586966 | 7.159027 |
| N | 9.782546 | 0.799090 | 4.980693 |
| O | 8.398852 | 4.346313 | 5.810101 |

**[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$] (triplet)**

| | | | |
|---|---|---|---|
| C | 11.729242 | 3.908329 | 5.432825 |
| C | 12.646589 | 4.514761 | 4.511003 |
| H | 13.634051 | 4.897267 | 4.761621 |
| C | 12.044409 | 4.524302 | 3.280150 |
| H | 12.449912 | 4.925595 | 2.353393 |
| C | 10.753179 | 3.916935 | 3.433634 |
| C | 9.769351 | 3.751245 | 2.430840 |
| C | 8.470698 | 3.229521 | 2.631056 |
| C | 7.426192 | 3.104751 | 1.653320 |
| H | 7.492747 | 3.403845 | 0.609430 |
| C | 6.341214 | 2.559382 | 2.286971 |
| H | 5.367488 | 2.341635 | 1.851859 |
| C | 6.712633 | 2.327156 | 3.653346 |
| C | 5.897403 | 1.742259 | 4.664673 |
| C | 6.320850 | 1.582666 | 5.997202 |
| C | 5.676533 | 1.017569 | 7.150785 |
| H | 4.669873 | 0.603394 | 7.176054 |
| C | 6.560661 | 1.107284 | 8.209626 |
| H | 6.392410 | 0.780300 | 9.233749 |
| C | 7.747639 | 1.717359 | 7.704651 |
| C | 9.040292 | 2.122711 | 8.162255 |
| C | 9.803544 | 2.154832 | 9.367225 |
| H | 9.478700 | 1.799374 | 10.342970 |
| C | 11.020508 | 2.731140 | 9.053524 |
| H | 11.851422 | 2.916287 | 9.732744 |
| C | 11.001218 | 3.050795 | 7.653766 |
| C | 11.952931 | 3.661477 | 6.816810 |
| C | 10.124608 | 4.186413 | 1.060044 |
| C | 11.147755 | 3.553813 | 0.343445 |
| C | 11.488749 | 3.936122 | -0.951749 |
| C | 10.802592 | 4.984266 | -1.562618 |
| C | 9.781729 | 5.638406 | -0.874465 |
| C | 9.458183 | 5.239170 | 0.420971 |
| C | 4.566448 | 1.225411 | 4.286825 |
| C | 4.433246 | 0.205266 | 3.335096 |
| C | 3.196004 | -0.330727 | 2.989672 |
| C | 2.042726 | 0.152997 | 3.605698 |
| C | 2.139892 | 1.162106 | 4.562508 |
| C | 3.389158 | 1.687000 | 4.889580 |
| C | 13.269004 | 3.998979 | 7.396369 |
| C | 14.090784 | 2.990880 | 7.916150 |
| C | 15.334683 | 3.264159 | 8.478572 |
| C | 15.787101 | 4.581760 | 8.532547 |
| C | 14.996169 | 5.607893 | 8.017424 |
| C | 13.753774 | 5.310798 | 7.459866 |
| C | 11.031921 | 0.548406 | 5.285097 |
| H | 11.645976 | 1.330578 | 5.737382 |
| C | 11.566172 | -0.707520 | 5.019028 |
| H | 12.610594 | -0.908402 | 5.261733 |
| C | 10.749397 | -1.680077 | 4.449333 |
| H | 11.139148 | -2.675738 | 4.226339 |
| C | 9.424195 | -1.355776 | 4.172558 |
| H | 8.738783 | -2.079042 | 3.728604 |
| C | 8.968677 | -0.076777 | 4.470900 |
| H | 7.934360 | 0.206770 | 4.266141 |
| Co | 8.994906 | 2.784769 | 5.475004 |
| F | 11.818864 | 2.544741 | 0.889303 |
| F | 12.451248 | 3.304556 | -1.609483 |
| F | 11.117131 | 5.356801 | -2.792511 |
| F | 9.133168 | 6.640691 | -1.449705 |
| F | 8.494382 | 5.897460 | 1.051785 |
| F | 5.516192 | -0.308773 | 2.753599 |
| F | 3.110366 | -1.306545 | 2.096433 |
| F | 0.861720 | -0.351144 | 3.289018 |
| F | 1.044582 | 1.619071 | 5.151318 |
| F | 3.437009 | 2.656914 | 5.793171 |
| F | 13.704046 | 1.718001 | 7.851401 |
| F | 16.090515 | 2.281171 | 8.947885 |
| F | 16.965792 | 4.858410 | 9.065407 |
| F | 15.425506 | 6.859936 | 8.071640 |
| F | 13.023577 | 6.314930 | 6.991359 |
| N | 10.608042 | 3.544078 | 4.738283 |
| N | 8.008019 | 2.733973 | 3.815802 |
| N | 7.565215 | 1.968597 | 6.386275 |
| N | 9.795266 | 2.650745 | 7.169643 |
| N | 9.757596 | 0.860233 | 5.012922 |
| O | 8.410694 | 4.393875 | 5.701914 |

**{[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} (singlet)**

| | | | |
|---|---|---|---|
| C | 2.695017 | 0.859974 | 0.730292 |
| C | 3.579332 | 1.527718 | -0.179038 |
| H | 4.560861 | 1.927193 | 0.069025 |
| C | 2.960618 | 1.557446 | -1.403541 |
| H | 3.341030 | 2.001834 | -2.321081 |
| C | 1.697553 | 0.897497 | -1.250928 |
| C | 0.683251 | 0.754943 | -2.235780 |
| C | -0.591246 | 0.181762 | -2.029244 |
| C | -1.663594 | 0.089540 | -2.980034 |
| H | -1.621063 | 0.405104 | -4.020649 |
| C | -2.736641 | -0.447107 | -2.320425 |
| H | -3.732657 | -0.625195 | -2.718769 |
| C | -2.320290 | -0.712026 | -0.972081 |
| C | -3.131234 | -1.271747 | 0.070316 |
| C | -2.653657 | -1.536813 | 1.358977 |
| C | -3.288350 | -2.094469 | 2.526189 |
| H | -4.319352 | -2.440953 | 2.579810 |
| C | -2.356939 | -2.096584 | 3.542369 |
| H | -2.496964 | -2.438268 | 4.565791 |
| C | -1.153959 | -1.548613 | 2.994399 |
| C | 0.151017 | -1.138817 | 3.438916 |
| C | 0.889363 | -1.040357 | 4.658106 |
| H | 0.571133 | -1.402937 | 5.633359 |
| C | 2.067403 | -0.384399 | 4.353132 |
| H | 2.869575 | -0.126243 | 5.042937 |
| C | 2.043351 | -0.090806 | 2.945317 |
| C | 2.935210 | 0.614843 | 2.118051 |
| C | 0.964304 | 1.328149 | -3.572035 |
| C | 2.005349 | 0.845926 | -4.373335 |
| C | 2.285198 | 1.390858 | -5.622948 |
| C | 1.517844 | 2.451849 | -6.098429 |
| C | 0.476801 | 2.957987 | -5.324315 |
| C | 0.214777 | 2.394910 | -4.079620 |
| C | -4.546255 | -1.570371 | -0.226723 |
| C | -4.909081 | -2.501043 | -1.205013 |
| C | -6.240411 | -2.779533 | -1.499752 |
| C | -7.249508 | -2.121764 | -0.800205 |
| C | -6.919422 | -1.194902 | 0.185323 |
| C | -5.582582 | -0.937227 | 0.468824 |
| C | 4.173678 | 1.141225 | 2.725578 |
| C | 5.098986 | 0.289521 | 3.342084 |
| C | 6.247169 | 0.775314 | 3.959533 |
| C | 6.492475 | 2.146169 | 3.974494 |
| C | 5.593631 | 3.020000 | 3.367001 |
| C | 4.453405 | 2.513360 | 2.752120 |
| C | 2.083668 | -2.537641 | 0.390877 |
| H | 2.706381 | -1.763894 | 0.846297 |
| C | 2.625507 | -3.768502 | 0.040340 |
| H | 3.684521 | -3.958947 | 0.216954 |
| C | 1.797067 | -4.732377 | -0.528103 |
| H | 2.192165 | -5.708772 | -0.814948 |
| C | 0.452829 | -4.425368 | -0.719555 |
| H | -0.240436 | -5.145245 | -1.155389 |
| C | -0.010748 | -3.170879 | -0.343277 |
| H | -1.061181 | -2.902892 | -0.478085 |
| Co | 0.029464 | -0.395287 | 0.766660 |
| F | 2.751579 | -0.169886 | -3.948903 |
| F | 3.271884 | 0.906057 | -6.363914 |
| F | 1.779481 | 2.977519 | -7.283525 |
| F | -0.245922 | 3.975084 | -5.772109 |
| F | -0.775869 | 2.923530 | -3.358965 |
| F | -3.966848 | -3.167667 | -1.871251 |
| F | -6.554513 | -3.678597 | -2.424170 |
| F | -8.519956 | -2.379502 | -1.069584 |
| F | -7.881110 | -0.563733 | 0.848092 |
| F | -5.310346 | -0.042674 | 1.411174 |
| F | 4.908507 | -1.026772 | 3.325903 |
| F | 7.109267 | -0.055020 | 4.530384 |
| F | 7.577988 | 2.617342 | 4.565564 |
| F | 5.821620 | 4.325978 | 3.394706 |
| F | 3.603692 | 3.376818 | 2.203782 |
| N | 1.578956 | 0.472774 | 0.039180 |
| N | -1.015629 | -0.341255 | -0.840193 |
| N | -1.361307 | -1.273853 | 1.692602 |
| N | 0.879957 | -0.587789 | 2.446528 |
| N | 0.790255 | -2.240273 | 0.196557 |
| O | -0.638082 | 1.202057 | 1.254426 |
| O | -2.650024 | 1.319796 | 3.102313 |
| H | -3.223711 | 1.815214 | 2.484872 |
| H | -1.791577 | 1.318506 | 2.639661 |
| O | -4.159365 | 2.984755 | 1.349418 |
| H | -4.662718 | 2.448470 | 0.708233 |
| H | -3.390802 | 3.217012 | 0.799675 |
| O | -2.147053 | 2.542293 | -0.537672 |
| H | -1.568642 | 2.882777 | -1.229720 |
| H | -1.543710 | 2.018253 | 0.058064 |
| O | -4.717094 | 1.542374 | -1.005624 |
| H | -5.083157 | 2.072637 | -1.722977 |
| H | -3.764037 | 1.774696 | -1.018613 |

**{[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O} (triplet)**

| | | | |
|---|---|---|---|
| C | 2.693837 | 0.866195 | 0.730091 |
| C | 3.577143 | 1.534107 | -0.180316 |
| H | 4.558570 | 1.934266 | 0.067031 |
| C | 2.957738 | 1.563108 | -1.404274 |
| H | 3.337591 | 2.007100 | -2.322234 |
| C | 1.694903 | 0.902691 | -1.250859 |
| C | 0.680886 | 0.758111 | -2.235170 |
| C | -0.592768 | 0.182773 | -2.028203 |
| C | -1.665380 | 0.088860 | -2.978509 |
| H | -1.624075 | 0.404718 | -4.019079 |
| C | -2.737128 | -0.449935 | -2.318467 |
| H | -3.733136 | -0.629283 | -2.716294 |
| C | -2.319707 | -0.714400 | -0.970329 |
| C | -3.129149 | -1.275584 | 0.072256 |
| C | -2.651196 | -1.538194 | 1.361483 |
| C | -3.284420 | -2.097277 | 2.528738 |
| H | -4.314661 | -2.446009 | 2.582630 |
| C | -2.352628 | -2.097882 | 3.544651 |
| H | -2.491724 | -2.440200 | 4.567986 |
| C | -1.150908 | -1.547200 | 2.996595 |
| C | 0.153758 | -1.136089 | 3.440091 |
| C | 0.894072 | -1.039011 | 4.658089 |
| H | 0.577335 | -1.402709 | 5.633415 |
| C | 2.071419 | -0.382146 | 4.352168 |
| H | 2.874608 | -0.124514 | 5.040981 |
| C | 2.045075 | -0.086779 | 2.944915 |
| C | 2.935790 | 0.619887 | 2.116961 |
| C | 0.961047 | 1.330633 | -3.571933 |
| C | 2.002195 | 0.848695 | -4.373217 |
| C | 2.281297 | 1.393087 | -5.623245 |
| C | 1.513007 | 2.453184 | -6.099191 |
| C | 0.471790 | 2.958982 | -5.325082 |
| C | 0.210613 | 2.396506 | -4.079936 |
| C | -4.543307 | -1.578313 | -0.225061 |
| C | -4.903291 | -2.510128 | -1.203325 |
| C | -6.233801 | -2.791434 | -1.499127 |
| C | -7.244869 | -2.135606 | -0.800596 |
| C | -6.917587 | -1.207734 | 0.184886 |
| C | -5.581539 | -0.947190 | 0.469519 |
| C | 4.175188 | 1.145402 | 2.723392 |
| C | 5.101336 | 0.292724 | 3.337258 |
| C | 6.250237 | 0.777567 | 3.954120 |
| C | 6.495461 | 2.148422 | 3.971034 |
| C | 5.595829 | 3.023182 | 3.366034 |
| C | 4.454966 | 2.517439 | 2.751590 |
| C | 2.086108 | -2.531255 | 0.392246 |
| H | 2.708071 | -1.756658 | 0.847163 |
| C | 2.629489 | -3.761282 | 0.041324 |
| H | 3.688932 | -3.949974 | 0.217177 |
| C | 1.802178 | -4.726491 | -0.526465 |
| H | 2.198616 | -5.702251 | -0.813585 |
| C | 0.457327 | -4.421638 | -0.716868 |
| H | -0.235170 | -5.142601 | -1.152105 |
| C | -0.008117 | -3.167954 | -0.340362 |
| H | -1.059048 | -2.901702 | -0.474502 |
| Co | 0.031522 | -0.395329 | 0.767053 |
| F | 2.749360 | -0.166261 | -3.948335 |
| F | 3.268239 | 0.908625 | -6.364120 |
| F | 1.773960 | 2.978414 | -7.284625 |
| F | -0.251787 | 3.975346 | -5.773212 |
| F | -0.780124 | 2.924859 | -3.359184 |
| F | -3.959062 | -3.174750 | -1.868757 |
| F | -6.545358 | -3.691279 | -2.423688 |
| F | -8.514566 | -2.396041 | -1.070947 |
| F | -7.881255 | -0.578458 | 0.846592 |
| F | -5.311925 | -0.051757 | 1.411736 |
| F | 4.910930 | -1.023575 | 3.318904 |
| F | 7.113067 | -0.053561 | 4.522695 |
| F | 7.581614 | 2.618657 | 4.561654 |
| F | 5.823603 | 4.329174 | 3.395793 |
| F | 3.604633 | 3.381645 | 2.205379 |
| N | 1.576836 | 0.478875 | 0.040025 |
| N | -1.015514 | -0.341035 | -0.839094 |
| N | -1.359662 | -1.271846 | 1.695095 |
| N | 0.880978 | -0.582942 | 2.447282 |
| N | 0.791959 | -2.236006 | 0.198775 |
| O | -0.643310 | 1.203239 | 1.252423 |
| O | -2.656257 | 1.321224 | 3.102145 |
| H | -3.229725 | 1.817704 | 2.485329 |
| H | -1.798011 | 1.319803 | 2.639351 |
| O | -4.168183 | 2.982771 | 1.348055 |
| H | -4.669963 | 2.443164 | 0.708405 |
| H | -3.400178 | 3.215897 | 0.797936 |
| O | -2.155267 | 2.541709 | -0.539720 |
| H | -1.578861 | 2.880993 | -1.234027 |
| H | -1.550225 | 2.019274 | 0.055378 |
| O | -4.722992 | 1.534494 | -1.003827 |
| H | -5.090669 | 2.059591 | -1.724143 |
| H | -3.770535 | 1.769232 | -1.018137 |

**{[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·4H$_2$O}$^{\ddagger}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 2.538418 | 1.039087 | 0.839313 |
| C | 3.402890 | 1.743762 | -0.065899 |
| H | 4.368895 | 2.174215 | 0.194495 |
| C | 2.799221 | 1.757288 | -1.296726 |
| H | 3.179850 | 2.210389 | -2.210839 |
| C | 1.549153 | 1.062588 | -1.168793 |
| C | 0.586345 | 0.840085 | -2.176231 |
| C | -0.676076 | 0.235976 | -1.973564 |
| C | -1.739846 | 0.111535 | -2.933865 |
| H | -1.695595 | 0.422887 | -3.975960 |
| C | -2.809923 | -0.438134 | -2.281873 |
| H | -3.797396 | -0.638422 | -2.692790 |
| C | -2.405285 | -0.696968 | -0.927256 |
| C | -3.187219 | -1.314056 | 0.079187 |
| C | -2.694649 | -1.625755 | 1.365111 |
| C | -3.282006 | -2.294922 | 2.485896 |
| H | -4.288803 | -2.710379 | 2.515837 |
| C | -2.342139 | -2.314207 | 3.508248 |
| H | -2.466691 | -2.739953 | 4.502229 |
| C | -1.180488 | -1.654450 | 3.019952 |
| C | 0.098526 | -1.209220 | 3.470685 |
| C | 0.879307 | -1.179634 | 4.663558 |
| H | 0.612271 | -1.630338 | 5.617796 |
| C | 2.025646 | -0.457277 | 4.372092 |
| H | 2.846105 | -0.229132 | 5.051980 |
| C | 1.941667 | -0.048985 | 2.997782 |
| C | 2.807325 | 0.723035 | 2.190897 |
| C | 0.921432 | 1.308494 | -3.541508 |
| C | 1.980385 | 0.741424 | -4.260103 |
| C | 2.314535 | 1.162870 | -5.543724 |
| C | 1.583014 | 2.182943 | -6.146313 |
| C | 0.523731 | 2.772070 | -5.460024 |
| C | 0.213984 | 2.333042 | -4.176518 |
| C | -4.601568 | -1.627615 | -0.204932 |
| C | -4.987797 | -2.546771 | -1.183765 |
| C | -6.326577 | -2.825190 | -1.446724 |
| C | -7.319347 | -2.182491 | -0.711433 |
| C | -6.966220 | -1.266661 | 0.276998 |
| C | -5.622463 | -1.005359 | 0.522884 |
| C | 4.077881 | 1.184432 | 2.788553 |
| C | 5.042626 | 0.267553 | 3.219929 |
| C | 6.236358 | 0.673974 | 3.808549 |
| C | 6.488229 | 2.032433 | 3.983559 |
| C | 5.550631 | 2.971432 | 3.560391 |
| C | 4.364760 | 2.540847 | 2.971907 |
| C | 2.065248 | -2.327778 | 0.420334 |
| H | 2.637264 | -1.543758 | 0.921457 |
| C | 2.673001 | -3.511756 | 0.021088 |
| H | 3.738712 | -3.653494 | 0.202933 |
| C | 1.902946 | -4.490449 | -0.601044 |
| H | 2.352536 | -5.430446 | -0.926405 |
| C | 0.546105 | -4.247343 | -0.795262 |
| H | -0.103140 | -4.983291 | -1.270282 |
| C | 0.009946 | -3.037443 | -0.371708 |
| H | -1.050992 | -2.815248 | -0.507498 |
| Co | -0.064121 | -0.353474 | 0.826521 |
| F | 2.699457 | -0.241315 | -3.722924 |
| F | 3.319419 | 0.596628 | -6.200078 |
| F | 1.893374 | 2.593893 | -7.366758 |
| F | -0.171881 | 3.750949 | -6.024402 |
| F | -0.797201 | 2.939850 | -3.544394 |
| F | -4.063711 | -3.199550 | -1.888880 |
| F | -6.661949 | -3.711938 | -2.377024 |
| F | -8.596572 | -2.444127 | -0.949326 |
| F | -7.912310 | -0.650679 | 0.977506 |
| F | -5.323294 | -0.122270 | 1.471490 |
| F | 4.844533 | -1.038102 | 3.045930 |
| F | 7.140071 | -0.219352 | 4.192971 |
| F | 7.619765 | 2.427917 | 4.547757 |
| F | 5.784293 | 4.266705 | 3.735626 |
| F | 3.482461 | 3.463706 | 2.595492 |
| N | 1.422498 | 0.649525 | 0.131548 |
| N | -1.103671 | -0.281809 | -0.785290 |
| N | -1.434224 | -1.260456 | 1.734649 |
| N | 0.779397 | -0.539513 | 2.503620 |
| N | 0.758588 | -2.093431 | 0.219560 |
| O | -0.553274 | 1.382574 | 1.210905 |
| O | -1.868527 | 1.484827 | 2.476705 |
| H | -2.597102 | 2.037845 | 2.013901 |
| H | -2.144853 | 0.555917 | 2.370765 |
| O | -3.681622 | 2.968781 | 1.370967 |
| H | -4.225100 | 2.437183 | 0.742693 |
| H | -3.125779 | 3.460069 | 0.741861 |
| O | -2.002612 | 2.718404 | -0.768407 |
| H | -1.430611 | 2.874015 | -1.530116 |
| H | -1.450995 | 2.179547 | -0.152993 |
| O | -4.608103 | 1.663665 | -0.843208 |
| H | -5.138769 | 2.245945 | -1.400543 |
| H | -3.686219 | 1.892698 | -1.085045 |

**{[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·H$_2$O·[OAc$^-$]} (singlet)**

| | | | |
|---|---|---|---|
| C | 2.633684 | 1.002006 | 0.456544 |
| C | 3.555089 | 1.581112 | -0.480848 |
| H | 4.552340 | 1.949163 | -0.246639 |
| C | 2.943152 | 1.576291 | -1.708567 |
| H | 3.346920 | 1.954720 | -2.645949 |
| C | 1.646974 | 0.985729 | -1.527177 |
| C | 0.639146 | 0.826830 | -2.509337 |
| C | -0.667588 | 0.326209 | -2.281674 |
| C | -1.723822 | 0.189818 | -3.243232 |
| H | -1.663926 | 0.444668 | -4.299500 |
| C | -2.809864 | -0.318723 | -2.576223 |
| H | -3.791033 | -0.541674 | -2.992095 |
| C | -2.419631 | -0.514626 | -1.210117 |
| C | -3.230788 | -1.073132 | -0.169715 |
| C | -2.787981 | -1.238183 | 1.150827 |
| C | -3.410932 | -1.817780 | 2.315492 |
| H | -4.422291 | -2.219895 | 2.363173 |
| C | -2.499805 | -1.747627 | 3.347751 |
| H | -2.642002 | -2.057368 | 4.380050 |
| C | -1.323912 | -1.130096 | 2.813910 |
| C | -0.015901 | -0.724564 | 3.250442 |
| C | 0.761554 | -0.686032 | 4.451224 |
| H | 0.434262 | -1.022621 | 5.432245 |
| C | 1.972832 | -0.114925 | 4.118985 |
| H | 2.810681 | 0.084514 | 4.786066 |
| C | 1.933026 | 0.191849 | 2.711911 |
| C | 2.868177 | 0.786041 | 1.852862 |
| C | 0.974247 | 1.238502 | -3.892030 |
| C | 1.971088 | 0.581607 | -4.621816 |
| C | 2.286721 | 0.941292 | -5.928727 |
| C | 1.606053 | 1.993878 | -6.535663 |
| C | 0.613353 | 2.673437 | -5.833256 |
| C | 0.311692 | 2.293486 | -4.528707 |
| C | -4.582864 | -1.558619 | -0.511579 |
| C | -4.770664 | -2.579009 | -1.452553 |
| C | -6.031402 | -3.085243 | -1.750860 |
| C | -7.150251 | -2.568432 | -1.101800 |
| C | -6.997528 | -1.558700 | -0.154559 |
| C | -5.726651 | -1.066095 | 0.128168 |
| C | 4.186481 | 1.151900 | 2.410034 |
| C | 5.029605 | 0.170603 | 2.944187 |
| C | 6.272944 | 0.480010 | 3.486785 |
| C | 6.700358 | 1.805682 | 3.508758 |
| C | 5.885311 | 2.805462 | 2.982602 |
| C | 4.646970 | 2.472163 | 2.441939 |
| C | 1.878345 | -2.375457 | 0.393490 |
| H | 2.519434 | -1.598171 | 0.816211 |
| C | 2.375678 | -3.652805 | 0.161967 |
| H | 3.416528 | -3.875307 | 0.400012 |
| C | 1.527238 | -4.621074 | -0.368471 |
| H | 1.886981 | -5.633696 | -0.561041 |
| C | 0.209084 | -4.268538 | -0.645264 |
| H | -0.499125 | -4.986936 | -1.059559 |
| C | -0.207937 | -2.968621 | -0.383675 |
| H | -1.236664 | -2.666710 | -0.590478 |
| Co | -0.095824 | -0.096226 | 0.548689 |
| F | 2.637213 | -0.433096 | -4.077576 |
| F | 3.222416 | 0.283375 | -6.601329 |
| F | 1.899394 | 2.347496 | -7.777218 |
| F | -0.030268 | 3.683134 | -6.404733 |
| F | -0.625413 | 2.979667 | -3.880065 |
| F | -3.719877 | -3.121342 | -2.065972 |
| F | -6.172815 | -4.065040 | -2.633683 |
| F | -8.354812 | -3.042375 | -1.378403 |
| F | -8.062930 | -1.070989 | 0.467484 |
| F | -5.623366 | -0.090128 | 1.026982 |
| F | 4.662838 | -1.108885 | 2.916722 |
| F | 7.050882 | -0.478510 | 3.973596 |
| F | 7.878432 | 2.116263 | 4.027062 |
| F | 6.287544 | 4.069143 | 3.011074 |
| F | 3.889568 | 3.454661 | 1.960600 |
| N | 1.504126 | 0.638472 | -0.215858 |
| N | -1.120177 | -0.116126 | -1.072148 |
| N | -1.530828 | -0.863988 | 1.509884 |
| N | 0.722950 | -0.217525 | 2.245065 |
| N | 0.609112 | -2.034695 | 0.123746 |
| O | -0.673156 | 1.560685 | 0.892867 |
| O | -0.359716 | 2.610142 | 3.477440 |
| H | -1.260206 | 2.283291 | 3.718152 |
| H | -0.320356 | 2.330354 | 2.547808 |
| O | -2.355653 | 0.394068 | 5.561232 |
| O | -2.957209 | 1.785299 | 3.902970 |
| C | -3.187728 | 0.907050 | 4.777749 |
| C | -4.644241 | 0.454407 | 4.892057 |
| H | -4.764896 | -0.427945 | 5.535296 |
| H | -5.254776 | 1.269115 | 5.310925 |
| H | -5.057218 | 0.235939 | 3.895780 |

**{[Cor$^{\bullet+}$-Co$^{III}$-O$^{\bullet-}$]·$H_2O$·[$OAc^-$]}$^{\ddagger}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 2.597380 | 1.056126 | 0.845176 |
| C | 3.493438 | 1.667377 | -0.097479 |
| H | 4.489668 | 2.043386 | 0.131186 |
| C | 2.864706 | 1.676063 | -1.315379 |
| H | 3.252089 | 2.073669 | -2.252185 |
| C | 1.574699 | 1.068146 | -1.132550 |
| C | 0.570305 | 0.906772 | -2.116696 |
| C | -0.721247 | 0.384635 | -1.886471 |
| C | -1.797397 | 0.266810 | -2.832576 |
| H | -1.759760 | 0.565209 | -3.878734 |
| C | -2.866702 | -0.274263 | -2.166911 |
| H | -3.852947 | -0.488016 | -2.576604 |
| C | -2.460227 | -0.515731 | -0.810296 |
| C | -3.244272 | -1.098415 | 0.216138 |
| C | -2.771841 | -1.303918 | 1.530207 |
| C | -3.389538 | -1.879526 | 2.695367 |
| H | -4.411061 | -2.254692 | 2.752980 |
| C | -2.458851 | -1.852122 | 3.718461 |
| H | -2.598317 | -2.188253 | 4.744525 |
| C | -1.273432 | -1.269890 | 3.179596 |
| C | 0.029095 | -0.874138 | 3.602644 |
| C | 0.825465 | -0.845159 | 4.781844 |
| H | 0.538366 | -1.231965 | 5.758205 |
| C | 2.017378 | -0.218134 | 4.449380 |
| H | 2.860568 | -0.021988 | 5.111194 |
| C | 1.949361 | 0.135945 | 3.062212 |
| C | 2.862536 | 0.795685 | 2.211542 |
| C | 0.896586 | 1.334572 | -3.496997 |
| C | 1.892649 | 0.689884 | -4.239166 |
| C | 2.202745 | 1.060414 | -5.544487 |
| C | 1.511859 | 2.110091 | -6.144073 |
| C | 0.517557 | 2.777095 | -5.432689 |
| C | 0.227560 | 2.389213 | -4.127336 |
| C | -4.608363 | -1.563278 | -0.109367 |
| C | -4.823810 | -2.578982 | -1.048585 |
| C | -6.096173 | -3.061227 | -1.339293 |
| C | -7.200288 | -2.527477 | -0.679233 |
| C | -7.020989 | -1.521840 | 0.267363 |
| C | -5.738953 | -1.050251 | 0.536204 |
| C | 4.178150 | 1.174673 | 2.767099 |
| C | 5.071251 | 0.197329 | 3.221066 |
| C | 6.312186 | 0.520728 | 3.761403 |
| C | 6.687845 | 1.858113 | 3.863289 |
| C | 5.824351 | 2.855119 | 3.416242 |
| C | 4.589578 | 2.506805 | 2.876101 |
| C | 1.931960 | -2.291515 | 0.594382 |
| H | 2.564536 | -1.511285 | 1.024901 |
| C | 2.459195 | -3.536518 | 0.270977 |
| H | 3.517450 | -3.733039 | 0.446872 |
| C | 1.618597 | -4.505528 | -0.270529 |
| H | 2.002914 | -5.492127 | -0.536851 |
| C | 0.276421 | -4.189509 | -0.461993 |
| H | -0.425962 | -4.912062 | -0.878950 |
| C | -0.174445 | -2.922832 | -0.110183 |
| H | -1.222809 | -2.646714 | -0.242898 |
| Co | -0.099778 | -0.126201 | 0.934741 |
| F | 2.570565 | -0.325018 | -3.706299 |
| F | 3.141592 | 0.412584 | -6.225290 |
| F | 1.797201 | 2.472847 | -7.386623 |
| F | -0.137985 | 3.785575 | -5.996151 |
| F | -0.713593 | 3.067322 | -3.472995 |
| F | -3.787919 | -3.135228 | -1.677098 |
| F | -6.263495 | -4.035394 | -2.225944 |
| F | -8.417321 | -2.979805 | -0.945770 |
| F | -8.073798 | -1.015861 | 0.899160 |
| F | -5.610724 | -0.072362 | 1.431789 |
| F | 4.754838 | -1.092568 | 3.114263 |
| F | 7.142497 | -0.434441 | 4.164556 |
| F | 7.864304 | 2.181484 | 4.381113 |
| F | 6.177398 | 4.130910 | 3.520399 |
| F | 3.787288 | 3.489266 | 2.470791 |
| N | 1.452739 | 0.700427 | 0.175515 |
| N | -1.153981 | -0.109036 | -0.687456 |
| N | -1.502289 | -0.977693 | 1.874650 |
| N | 0.739496 | -0.279164 | 2.601613 |
| N | 0.639349 | -1.988149 | 0.402955 |
| O | -0.896780 | 1.450908 | 1.130746 |
| O | -0.788677 | 2.264429 | 2.967846 |
| H | -1.810510 | 2.349589 | 3.013116 |
| H | -0.700961 | 1.482668 | 3.546767 |
| O | -2.249588 | 1.184628 | 5.065077 |
| O | -3.333500 | 2.170063 | 3.367094 |
| C | -3.287847 | 1.486786 | 4.437785 |
| C | -4.631986 | 1.021896 | 4.978483 |
| H | -4.523847 | 0.368683 | 5.853445 |
| H | -5.244479 | 1.890654 | 5.261210 |
| H | -5.192699 | 0.488611 | 4.198020 |

**[Cor-Co$^{III}$-OOH]$^{-}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 11.667603 | 3.933692 | 5.436799 |
| C | 12.602680 | 4.529393 | 4.519246 |
| H | 13.590776 | 4.908395 | 4.777545 |
| C | 12.017268 | 4.531426 | 3.281666 |
| H | 12.437078 | 4.924409 | 2.356448 |
| C | 10.717165 | 3.930093 | 3.427297 |
| C | 9.739990 | 3.773620 | 2.416598 |
| C | 8.436384 | 3.257809 | 2.614645 |
| C | 7.402223 | 3.114148 | 1.622970 |
| H | 7.477801 | 3.399349 | 0.574723 |
| C | 6.315121 | 2.569422 | 2.252027 |
| H | 5.347018 | 2.339345 | 1.808066 |
| C | 6.673628 | 2.359564 | 3.628622 |
| C | 5.851131 | 1.783983 | 4.628341 |
| C | 6.266373 | 1.608079 | 5.970746 |
| C | 5.601475 | 1.059338 | 7.121015 |
| H | 4.578824 | 0.683951 | 7.152018 |
| C | 6.493816 | 1.119870 | 8.179786 |
| H | 6.315179 | 0.800518 | 9.205852 |
| C | 7.697208 | 1.689997 | 7.670850 |
| C | 8.984890 | 2.089465 | 8.137815 |
| C | 9.718530 | 2.161544 | 9.355877 |
| H | 9.381666 | 1.817214 | 10.332964 |
| C | 10.935385 | 2.761225 | 9.057225 |
| H | 11.746529 | 2.978772 | 9.752665 |
| C | 10.934485 | 3.051645 | 7.652007 |
| C | 11.885821 | 3.688614 | 6.814679 |
| C | 10.108501 | 4.188403 | 1.045554 |
| C | 11.148127 | 3.561034 | 0.344406 |
| C | 11.500542 | 3.925687 | -0.953114 |
| C | 10.805821 | 4.946704 | -1.596288 |
| C | 9.766890 | 5.593165 | -0.931364 |
| C | 9.439049 | 5.219338 | 0.370914 |
| C | 4.522364 | 1.269676 | 4.243354 |
| C | 4.383479 | 0.245763 | 3.294415 |
| C | 3.145821 | -0.287097 | 2.943803 |
| C | 1.990906 | 0.193263 | 3.555820 |
| C | 2.090087 | 1.201024 | 4.511763 |
| C | 3.338451 | 1.729256 | 4.837914 |
| C | 13.187215 | 4.048109 | 7.408108 |
| C | 14.014583 | 3.062326 | 7.966066 |
| C | 15.243236 | 3.358819 | 8.550447 |
| C | 15.687496 | 4.678526 | 8.586148 |
| C | 14.896939 | 5.683165 | 8.033527 |
| C | 13.665982 | 5.364490 | 7.462406 |
| C | 10.990123 | 0.550806 | 5.232959 |
| H | 11.601695 | 1.338939 | 5.681775 |
| C | 11.521084 | -0.708783 | 4.971373 |
| H | 12.565396 | -0.913519 | 5.213909 |
| C | 10.700322 | -1.681248 | 4.406152 |
| H | 11.086705 | -2.680096 | 4.187687 |
| C | 9.375884 | -1.353242 | 4.128164 |
| H | 8.687974 | -2.076776 | 3.687034 |
| C | 8.925299 | -0.070372 | 4.422976 |
| H | 7.891935 | 0.223704 | 4.221015 |
| Co | 8.956798 | 2.766616 | 5.442249 |
| F | 11.829072 | 2.563997 | 0.902160 |
| F | 12.483123 | 3.292741 | -1.591977 |
| F | 11.130585 | 5.300603 | -2.837123 |
| F | 9.106725 | 6.576962 | -1.538689 |
| F | 8.461900 | 5.889845 | 0.969303 |
| F | 5.460576 | -0.285168 | 2.715928 |
| F | 3.059877 | -1.269982 | 2.049032 |
| F | 0.803499 | -0.313300 | 3.234966 |
| F | 0.987329 | 1.661701 | 5.098001 |
| F | 3.372255 | 2.705238 | 5.736422 |
| F | 13.656145 | 1.780721 | 7.914817 |
| F | 16.004701 | 2.388537 | 9.053015 |
| F | 16.860435 | 4.977774 | 9.138108 |
| F | 15.313917 | 6.946505 | 8.076343 |
| F | 12.939830 | 6.365109 | 6.975615 |
| N | 10.547943 | 3.572950 | 4.729954 |
| N | 7.966531 | 2.785805 | 3.801463 |
| N | 7.518589 | 1.947535 | 6.349995 |
| N | 9.753889 | 2.621746 | 7.149595 |
| N | 9.717671 | 0.864742 | 4.960118 |
| O | 8.309620 | 4.513547 | 5.790827 |
| O | 7.814149 | 4.680065 | 7.100202 |
| H | 8.621327 | 4.867779 | 7.607300 |

**[Cor$^{\bullet+}$-Co$^{III}$-OOH] (doublet)**

| | | | |
|---|---|---|---|
| C | 11.667820 | 3.898878 | 5.442146 |
| C | 12.595342 | 4.510671 | 4.532854 |
| H | 13.577962 | 4.897464 | 4.797373 |
| C | 12.011373 | 4.512003 | 3.294718 |
| H | 12.426886 | 4.910189 | 2.371057 |
| C | 10.720682 | 3.899024 | 3.436941 |
| C | 9.747405 | 3.729992 | 2.421858 |
| C | 8.453993 | 3.194027 | 2.611586 |
| C | 7.419727 | 3.053847 | 1.624224 |
| H | 7.493413 | 3.341367 | 0.577525 |
| C | 6.333669 | 2.513144 | 2.257604 |
| H | 5.362796 | 2.288961 | 1.819591 |
| C | 6.698615 | 2.302660 | 3.630971 |
| C | 5.865925 | 1.738301 | 4.642119 |
| C | 6.282321 | 1.557625 | 5.969943 |
| C | 5.591253 | 1.083121 | 7.142187 |
| H | 4.553589 | 0.755709 | 7.180706 |
| C | 6.476253 | 1.151320 | 8.198871 |
| H | 6.281946 | 0.887663 | 9.236485 |
| C | 7.707358 | 1.650150 | 7.668178 |
| C | 9.007249 | 2.044595 | 8.137954 |
| C | 9.731252 | 2.133241 | 9.361421 |
| H | 9.387261 | 1.801662 | 10.339149 |
| C | 10.946464 | 2.730242 | 9.063625 |
| H | 11.751050 | 2.960161 | 9.761000 |
| C | 10.953042 | 3.006943 | 7.656360 |
| C | 11.887155 | 3.656190 | 6.824177 |
| C | 10.116788 | 4.153696 | 1.051406 |
| C | 11.150714 | 3.518100 | 0.353050 |
| C | 11.499800 | 3.883764 | -0.944681 |
| C | 10.811754 | 4.918621 | -1.576098 |
| C | 9.780684 | 5.575440 | -0.905984 |
| C | 9.448394 | 5.192647 | 0.392328 |
| C | 4.510686 | 1.286846 | 4.260269 |
| C | 4.336347 | 0.247086 | 3.338597 |
| C | 3.075446 | -0.217681 | 2.976031 |
| C | 1.942293 | 0.358922 | 3.548157 |
| C | 2.081464 | 1.391053 | 4.474334 |
| C | 3.354341 | 1.843666 | 4.818810 |
| C | 13.177661 | 4.063921 | 7.418915 |
| C | 14.084112 | 3.101211 | 7.876727 |
| C | 15.303666 | 3.450523 | 8.451340 |
| C | 15.634426 | 4.798062 | 8.589027 |
| C | 14.752659 | 5.780629 | 8.140629 |
| C | 13.542260 | 5.406943 | 7.560028 |
| C | 11.035132 | 0.531290 | 5.194778 |
| H | 11.645482 | 1.317060 | 5.646967 |
| C | 11.579447 | -0.714715 | 4.905219 |
| H | 12.629539 | -0.905839 | 5.130499 |
| C | 10.766227 | -1.690050 | 4.335142 |
| H | 11.164530 | -2.678168 | 4.094650 |
| C | 9.433166 | -1.379020 | 4.081632 |
| H | 8.750532 | -2.105753 | 3.639164 |
| C | 8.964488 | -0.110771 | 4.402694 |
| H | 7.922909 | 0.163347 | 4.219961 |
| Co | 8.990867 | 2.674789 | 5.436466 |
| F | 11.822163 | 2.520239 | 0.918730 |
| F | 12.471814 | 3.249026 | -1.584967 |
| F | 11.134290 | 5.274870 | -2.808653 |
| F | 9.129500 | 6.563462 | -1.502132 |
| F | 8.474032 | 5.852136 | 1.004609 |
| F | 5.400364 | -0.349969 | 2.802167 |
| F | 2.945921 | -1.213512 | 2.110485 |
| F | 0.738243 | -0.080462 | 3.220081 |
| F | 1.003418 | 1.938356 | 5.016575 |
| F | 3.446691 | 2.835549 | 5.693791 |
| F | 13.803952 | 1.807560 | 7.736131 |
| F | 16.153004 | 2.515978 | 8.854566 |
| F | 16.786491 | 5.143852 | 9.139128 |
| F | 15.065097 | 7.060573 | 8.278928 |
| F | 12.720717 | 6.365093 | 7.150110 |
| N | 10.545939 | 3.536425 | 4.740185 |
| N | 7.987445 | 2.721462 | 3.803450 |
| N | 7.555448 | 1.846029 | 6.343414 |
| N | 9.772944 | 2.561631 | 7.147521 |
| N | 9.752465 | 0.829302 | 4.943300 |
| O | 8.139258 | 4.347110 | 5.799010 |
| O | 7.820734 | 4.582240 | 7.127908 |
| H | 8.686898 | 4.706295 | 7.558021 |

**$[Cor^{\bullet-}\text{-}Co^{III}\text{-}OO^{\bullet-}]^{2-}$ (singlet)**

| | | | |
|---|---|---|---|
| C | 11.659309 | 3.981960 | 5.442468 |
| C | 12.603430 | 4.528989 | 4.508424 |
| H | 13.611453 | 4.865293 | 4.748915 |
| C | 12.000778 | 4.549595 | 3.272722 |
| H | 12.427765 | 4.921568 | 2.340988 |
| C | 10.689666 | 3.995449 | 3.433208 |
| C | 9.700522 | 3.849610 | 2.429725 |
| C | 8.396900 | 3.324292 | 2.613965 |
| C | 7.386329 | 3.153090 | 1.613640 |
| H | 7.467164 | 3.442798 | 0.565724 |
| C | 6.305094 | 2.564904 | 2.228087 |
| H | 5.349492 | 2.308102 | 1.770526 |
| C | 6.649481 | 2.354599 | 3.604866 |
| C | 5.816218 | 1.762434 | 4.600769 |
| C | 6.214282 | 1.648495 | 5.975313 |
| C | 5.583003 | 1.053122 | 7.106235 |
| H | 4.585725 | 0.612185 | 7.125234 |
| C | 6.471279 | 1.160152 | 8.185235 |
| H | 6.306833 | 0.816214 | 9.206982 |
| C | 7.630264 | 1.801454 | 7.695002 |
| C | 8.928448 | 2.204964 | 8.164349 |
| C | 9.671822 | 2.221067 | 9.365738 |
| H | 9.332413 | 1.868231 | 10.340098 |
| C | 10.916635 | 2.788844 | 9.061162 |
| H | 11.739758 | 2.969717 | 9.754099 |
| C | 10.911237 | 3.102712 | 7.671575 |
| C | 11.895066 | 3.708631 | 6.822019 |
| C | 10.063076 | 4.272512 | 1.063103 |
| C | 11.104063 | 3.659709 | 0.346641 |
| C | 11.450639 | 4.041721 | -0.947632 |
| C | 10.747534 | 5.061550 | -1.581988 |
| C | 9.704726 | 5.690379 | -0.907218 |
| C | 9.383950 | 5.303116 | 0.392722 |
| C | 4.539522 | 1.179064 | 4.196083 |
| C | 4.443734 | 0.203019 | 3.177899 |
| C | 3.243755 | -0.385962 | 2.799372 |
| C | 2.059447 | -0.042102 | 3.451940 |
| C | 2.108632 | 0.902706 | 4.477495 |
| C | 3.316380 | 1.494248 | 4.830821 |
| C | 13.216809 | 3.981321 | 7.383608 |
| C | 13.974536 | 2.970225 | 8.015708 |
| C | 15.226839 | 3.199382 | 8.572662 |
| C | 15.799577 | 4.470226 | 8.507886 |
| C | 15.091933 | 5.496350 | 7.881464 |
| C | 13.830636 | 5.253075 | 7.348053 |
| C | 10.930793 | 0.609085 | 5.353003 |
| H | 11.543121 | 1.412782 | 5.773472 |
| C | 11.448053 | -0.671114 | 5.170612 |
| H | 12.484281 | -0.876328 | 5.447769 |
| C | 10.623983 | -1.661643 | 4.641717 |
| H | 10.999311 | -2.677518 | 4.487087 |
| C | 9.310467 | -1.330002 | 4.317860 |
| H | 8.619569 | -2.066066 | 3.901442 |
| C | 8.872604 | -0.026065 | 4.533851 |
| H | 7.847488 | 0.272914 | 4.295929 |
| Co | 8.909755 | 2.853227 | 5.460514 |
| F | 11.787864 | 2.648936 | 0.876435 |
| F | 12.435143 | 3.417192 | -1.602495 |
| F | 11.068611 | 5.432979 | -2.825596 |
| F | 9.037235 | 6.682276 | -1.505272 |
| F | 8.409002 | 5.974148 | 0.996361 |
| F | 5.548518 | -0.253335 | 2.578154 |
| F | 3.220094 | -1.335639 | 1.853286 |
| F | 0.894606 | -0.602694 | 3.093747 |
| F | 0.970612 | 1.268106 | 5.083305 |
| F | 3.273890 | 2.433036 | 5.775502 |
| F | 13.532340 | 1.710128 | 8.028187 |
| F | 15.925114 | 2.193784 | 9.117823 |
| F | 17.013017 | 4.698343 | 9.031312 |
| F | 15.620785 | 6.727240 | 7.848783 |
| F | 13.180371 | 6.296102 | 6.830134 |
| N | 10.517079 | 3.661628 | 4.750039 |
| N | 7.921745 | 2.832933 | 3.800521 |
| N | 7.439917 | 2.074420 | 6.370754 |
| N | 9.702430 | 2.737880 | 7.176072 |
| N | 9.668960 | 0.923381 | 5.037637 |
| O | 8.227284 | 4.664298 | 5.769771 |
| O | 7.816123 | 4.977437 | 6.917752 |

**[Cor-Co$^{III}$-OO$^{\bullet-}$]$^{-}$ (doublet)**

| | | | |
|---|---|---|---|
| C | 11.650490 | 3.953100 | 5.447782 |
| C | 12.591754 | 4.529997 | 4.526742 |
| H | 13.588478 | 4.888773 | 4.780402 |
| C | 11.999956 | 4.547050 | 3.291435 |
| H | 12.424529 | 4.932192 | 2.365189 |
| C | 10.690715 | 3.969336 | 3.440603 |
| C | 9.713298 | 3.811390 | 2.428959 |
| C | 8.413713 | 3.283988 | 2.620773 |
| C | 7.392640 | 3.112986 | 1.620721 |
| H | 7.473995 | 3.390757 | 0.570797 |
| C | 6.310904 | 2.547483 | 2.241850 |
| H | 5.353911 | 2.289717 | 1.788887 |
| C | 6.658137 | 2.353892 | 3.623192 |
| C | 5.837418 | 1.769100 | 4.620291 |
| C | 6.244365 | 1.614803 | 5.968904 |
| C | 5.588553 | 1.047996 | 7.114852 |
| H | 4.576609 | 0.643924 | 7.138979 |
| C | 6.471292 | 1.134994 | 8.180506 |
| H | 6.294779 | 0.809076 | 9.204832 |
| C | 7.661058 | 1.740551 | 7.681854 |
| C | 8.946494 | 2.145361 | 8.149034 |
| C | 9.692257 | 2.185221 | 9.362920 |
| H | 9.356258 | 1.833389 | 10.337487 |
| C | 10.914822 | 2.766353 | 9.062936 |
| H | 11.733825 | 2.963173 | 9.755087 |
| C | 10.906587 | 3.079397 | 7.661501 |
| C | 11.867827 | 3.697658 | 6.824872 |
| C | 10.080953 | 4.226250 | 1.057438 |
| C | 11.118948 | 3.600338 | 0.352908 |
| C | 11.467242 | 3.967058 | -0.945248 |
| C | 10.769109 | 4.987486 | -1.585613 |
| C | 9.730360 | 5.631310 | -0.917759 |
| C | 9.406745 | 5.255234 | 0.384838 |
| C | 4.523976 | 1.223156 | 4.227912 |
| C | 4.411074 | 0.197008 | 3.277692 |
| C | 3.186434 | -0.359958 | 2.918705 |
| C | 2.018294 | 0.096443 | 3.523981 |
| C | 2.091342 | 1.105402 | 4.481082 |
| C | 3.326748 | 1.657880 | 4.815266 |
| C | 13.183022 | 4.018385 | 7.410704 |
| C | 13.986322 | 3.007146 | 7.957887 |
| C | 15.228044 | 3.266651 | 8.532114 |
| C | 15.710628 | 4.572518 | 8.566653 |
| C | 14.945518 | 5.601377 | 8.022508 |
| C | 13.699906 | 5.320531 | 7.463043 |
| C | 10.979046 | 0.564152 | 5.273285 |
| H | 11.584935 | 1.359909 | 5.716938 |
| C | 11.513444 | -0.699324 | 5.037149 |
| H | 12.554861 | -0.900819 | 5.294938 |
| C | 10.698600 | -1.680016 | 4.477213 |
| H | 11.087062 | -2.682279 | 4.278949 |
| C | 9.377466 | -1.356204 | 4.177951 |
| H | 8.695168 | -2.086501 | 3.738994 |
| C | 8.924184 | -0.068693 | 4.448546 |
| H | 7.893489 | 0.224279 | 4.229516 |
| Co | 8.931884 | 2.798775 | 5.450302 |
| F | 11.801967 | 2.603056 | 0.907220 |
| F | 12.448808 | 3.336325 | -1.587546 |
| F | 11.089987 | 5.343176 | -2.826813 |
| F | 9.065848 | 6.613568 | -1.522740 |
| F | 8.427337 | 5.920691 | 0.986016 |
| F | 5.501489 | -0.312312 | 2.705189 |
| F | 3.125750 | -1.342200 | 2.021214 |
| F | 0.843115 | -0.432256 | 3.194393 |
| F | 0.975910 | 1.545433 | 5.058965 |
| F | 3.335319 | 2.635517 | 5.713478 |
| F | 13.592311 | 1.735783 | 7.904534 |
| F | 15.966341 | 2.273539 | 9.024251 |
| F | 16.896960 | 4.835647 | 9.108131 |
| F | 15.404198 | 6.850471 | 8.060227 |
| F | 12.998368 | 6.341704 | 6.984021 |
| N | 10.516655 | 3.621023 | 4.746603 |
| N | 7.938880 | 2.815424 | 3.809177 |
| N | 7.481526 | 2.000381 | 6.358776 |
| N | 9.713417 | 2.681662 | 7.162884 |
| N | 9.710202 | 0.872870 | 4.981996 |
| O | 8.235629 | 4.611225 | 5.810984 |
| O | 7.806840 | 4.870978 | 6.960920 |

**[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$] (triplet)**

| | | | |
|---|---|---|---|
| C | 11.667004 | 3.901850 | 5.434799 |
| C | 12.608018 | 4.476052 | 4.516191 |
| H | 13.605578 | 4.828505 | 4.771134 |
| C | 12.012666 | 4.505006 | 3.283644 |
| H | 12.434058 | 4.892145 | 2.358026 |
| C | 10.704034 | 3.937234 | 3.434303 |
| C | 9.728319 | 3.778596 | 2.425126 |
| C | 8.432925 | 3.248676 | 2.620024 |
| C | 7.414807 | 3.072360 | 1.624465 |
| H | 7.496855 | 3.346086 | 0.574622 |
| C | 6.334758 | 2.509443 | 2.249326 |
| H | 5.376927 | 2.250766 | 1.801369 |
| C | 6.683100 | 2.326091 | 3.628832 |
| C | 5.857850 | 1.738937 | 4.628553 |
| C | 6.260937 | 1.588713 | 5.967115 |
| C | 5.576712 | 1.102948 | 7.134183 |
| H | 4.551739 | 0.737287 | 7.166155 |
| C | 6.447702 | 1.217136 | 8.201188 |
| H | 6.249667 | 0.959738 | 9.239721 |
| C | 7.663924 | 1.754012 | 7.682462 |
| C | 8.956828 | 2.158919 | 8.149884 |
| C | 9.674218 | 2.269694 | 9.378863 |
| H | 9.310305 | 1.985087 | 10.364048 |
| C | 10.902752 | 2.823595 | 9.072214 |
| H | 11.705766 | 3.063588 | 9.767883 |
| C | 10.927375 | 3.056101 | 7.654401 |
| C | 11.885169 | 3.658814 | 6.819672 |
| C | 10.095688 | 4.186575 | 1.049254 |
| C | 11.116964 | 3.536582 | 0.345931 |
| C | 11.457817 | 3.890571 | -0.957486 |
| C | 10.772820 | 4.926334 | -1.590670 |
| C | 9.752476 | 5.595746 | -0.916631 |
| C | 9.429519 | 5.225116 | 0.387403 |
| C | 4.540113 | 1.203287 | 4.225899 |
| C | 4.448657 | 0.150624 | 3.306498 |
| C | 3.228270 | -0.400485 | 2.927044 |
| C | 2.050457 | 0.100148 | 3.480345 |
| C | 2.106297 | 1.142003 | 4.404394 |
| C | 3.340137 | 1.682459 | 4.763990 |
| C | 13.197751 | 3.997813 | 7.405969 |
| C | 14.005894 | 2.991529 | 7.950313 |
| C | 15.247478 | 3.263402 | 8.518500 |
| C | 15.710419 | 4.577866 | 8.555291 |
| C | 14.932740 | 5.602287 | 8.016883 |
| C | 13.692341 | 5.306729 | 7.454094 |
| C | 10.991863 | 0.581013 | 5.209487 |
| H | 11.602921 | 1.358932 | 5.673478 |
| C | 11.527465 | -0.666294 | 4.912817 |
| H | 12.574545 | -0.864975 | 5.145042 |
| C | 10.713022 | -1.632407 | 4.328866 |
| H | 11.107512 | -2.620690 | 4.083366 |
| C | 9.383745 | -1.311367 | 4.068686 |
| H | 8.697547 | -2.028300 | 3.615730 |
| C | 8.918689 | -0.043987 | 4.395335 |
| H | 7.880245 | 0.234980 | 4.205992 |
| Co | 8.984072 | 2.681283 | 5.428842 |
| F | 11.783903 | 2.535202 | 0.911044 |
| F | 12.418032 | 3.242018 | -1.602045 |
| F | 11.087324 | 5.270919 | -2.828684 |
| F | 9.102589 | 6.583620 | -1.514705 |
| F | 8.463568 | 5.895028 | 1.002926 |
| F | 5.557729 | -0.376412 | 2.787558 |
| F | 3.179625 | -1.402048 | 2.059272 |
| F | 0.883925 | -0.418901 | 3.135049 |
| F | 0.986814 | 1.615288 | 4.931379 |
| F | 3.351253 | 2.681856 | 5.636523 |
| F | 13.609844 | 1.721052 | 7.900692 |
| F | 15.991752 | 2.281931 | 9.009077 |
| F | 16.887481 | 4.853030 | 9.092707 |
| F | 15.372856 | 6.851371 | 8.054689 |
| F | 12.973396 | 6.309874 | 6.966318 |
| N | 10.523176 | 3.587920 | 4.744537 |
| N | 7.958390 | 2.795576 | 3.820382 |
| N | 7.515433 | 1.944898 | 6.350856 |
| N | 9.744304 | 2.618560 | 7.149948 |
| N | 9.711195 | 0.886392 | 4.948801 |
| O | 8.228028 | 4.548723 | 5.964539 |
| O | 7.775961 | 4.696318 | 7.104833 |

**{[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·$H_2O$} (triplet)**

| | | | |
|---|---|---|---|
| C | 11.794311 | 3.725813 | 5.415419 |
| C | 12.717531 | 4.358551 | 4.518494 |
| H | 13.692094 | 4.758095 | 4.792557 |
| C | 12.140384 | 4.369894 | 3.276980 |
| H | 12.555398 | 4.787836 | 2.362093 |
| C | 10.862935 | 3.730563 | 3.401575 |
| C | 9.892179 | 3.568910 | 2.385612 |
| C | 8.618515 | 2.985271 | 2.559942 |
| C | 7.599254 | 2.828436 | 1.561925 |
| H | 7.689972 | 3.104607 | 0.513003 |
| C | 6.505814 | 2.291433 | 2.186093 |
| H | 5.538309 | 2.069128 | 1.741550 |
| C | 6.851828 | 2.097163 | 3.563182 |
| C | 5.982977 | 1.625543 | 4.587562 |
| C | 6.391834 | 1.438176 | 5.914674 |
| C | 5.661888 | 1.071589 | 7.097557 |
| H | 4.604361 | 0.814512 | 7.133307 |
| C | 6.540773 | 1.130422 | 8.160491 |
| H | 6.319912 | 0.935369 | 9.207854 |
| C | 7.804109 | 1.525594 | 7.623733 |
| C | 9.096768 | 1.924473 | 8.100488 |
| C | 9.764689 | 2.115686 | 9.346152 |
| H | 9.375114 | 1.864764 | 10.330653 |
| C | 10.981255 | 2.702310 | 9.055220 |
| H | 11.748663 | 3.005514 | 9.765868 |
| C | 11.047506 | 2.870763 | 7.629937 |
| C | 11.985775 | 3.524516 | 6.811700 |
| C | 10.203629 | 4.121742 | 1.048010 |
| C | 11.270310 | 3.647685 | 0.275877 |
| C | 11.567678 | 4.180644 | -0.976547 |
| C | 10.787005 | 5.216439 | -1.487365 |
| C | 9.715714 | 5.710170 | -0.744675 |
| C | 9.440397 | 5.164230 | 0.506538 |
| C | 4.560406 | 1.412613 | 4.251650 |
| C | 4.152458 | 0.423033 | 3.352603 |
| C | 2.812831 | 0.227855 | 3.027867 |
| C | 1.842107 | 1.042546 | 3.609798 |
| C | 2.217222 | 2.036127 | 4.512581 |
| C | 3.564374 | 2.215975 | 4.821930 |
| C | 13.207858 | 4.057136 | 7.447746 |
| C | 14.096960 | 3.214348 | 8.127190 |
| C | 15.232427 | 3.701762 | 8.769387 |
| C | 15.502622 | 5.069040 | 8.744019 |
| C | 14.640481 | 5.934697 | 8.072941 |
| C | 13.509855 | 5.425762 | 7.438312 |
| C | 11.191322 | 0.339666 | 5.161496 |
| H | 11.795006 | 1.134103 | 5.607748 |
| C | 11.737558 | -0.907652 | 4.883836 |
| H | 12.788131 | -1.093823 | 5.110251 |
| C | 10.926903 | -1.891817 | 4.325263 |
| H | 11.328256 | -2.881453 | 4.096974 |
| C | 9.592574 | -1.588976 | 4.068307 |
| H | 8.912858 | -2.324060 | 3.635668 |
| C | 9.117977 | -0.319558 | 4.373511 |
| H | 8.075263 | -0.048595 | 4.188251 |
| Co | 9.150347 | 2.417757 | 5.375841 |
| F | 12.024968 | 2.650378 | 0.726873 |
| F | 12.579402 | 3.704483 | -1.688089 |
| F | 11.062773 | 5.729051 | -2.674509 |
| F | 8.980856 | 6.701791 | -1.225825 |
| F | 8.425909 | 5.677792 | 1.196876 |
| F | 5.059217 | -0.375607 | 2.789981 |
| F | 2.455333 | -0.725981 | 2.178255 |
| F | 0.565661 | 0.867902 | 3.307933 |
| F | 1.292325 | 2.805905 | 5.066701 |
| F | 3.885516 | 3.173465 | 5.677215 |
| F | 13.884267 | 1.901107 | 8.150641 |
| F | 16.060609 | 2.876372 | 9.394364 |
| F | 16.576284 | 5.543416 | 9.352909 |
| F | 14.894983 | 7.234541 | 8.055841 |
| F | 12.699226 | 6.282973 | 6.831485 |
| N | 10.686215 | 3.345301 | 4.701861 |
| N | 8.141509 | 2.514114 | 3.753190 |
| N | 7.683495 | 1.658510 | 6.284341 |
| N | 9.904644 | 2.353634 | 7.104041 |
| N | 9.906775 | 0.626969 | 4.904146 |
| O | 8.364363 | 4.246815 | 5.878830 |
| O | 7.913715 | 4.399949 | 7.031748 |
| O | 5.979004 | 4.948814 | 3.883988 |
| H | 6.618044 | 4.867983 | 4.603680 |
| H | 6.548406 | 4.953383 | 3.105608 |

**{[Cor$^{\bullet+}$-Co$^{III}$-OO$^{\bullet-}$]·$H_2O$}$^{\ddagger}$ (triplet)**

| | | | |
|---|---|---|---|
| C | 11.645903 | 3.916067 | 5.389413 |
| C | 12.585787 | 4.484472 | 4.467088 |
| H | 13.581864 | 4.841984 | 4.720999 |
| C | 11.989950 | 4.510645 | 3.234171 |
| H | 12.414289 | 4.889859 | 2.306317 |
| C | 10.685114 | 3.935777 | 3.383128 |
| C | 9.716598 | 3.764987 | 2.374063 |
| C | 8.434325 | 3.211945 | 2.564021 |
| C | 7.415391 | 3.039875 | 1.568959 |
| H | 7.497724 | 3.317324 | 0.519677 |
| C | 6.338543 | 2.467045 | 2.190697 |
| H | 5.380448 | 2.209828 | 1.742093 |
| C | 6.684335 | 2.282625 | 3.570547 |
| C | 5.851117 | 1.720380 | 4.572913 |
| C | 6.231842 | 1.641850 | 5.923427 |
| C | 5.570102 | 1.103199 | 7.076983 |
| H | 4.564885 | 0.685110 | 7.096667 |
| C | 6.432000 | 1.237597 | 8.149380 |
| H | 6.244238 | 0.945656 | 9.180901 |
| C | 7.619497 | 1.848210 | 7.651775 |
| C | 8.898438 | 2.257935 | 8.117402 |
| C | 9.641845 | 2.314539 | 9.332763 |
| H | 9.294596 | 1.994404 | 10.313252 |
| C | 10.868450 | 2.873235 | 9.026412 |
| H | 11.686222 | 3.078124 | 9.716077 |
| C | 10.872206 | 3.155933 | 7.619817 |
| C | 11.855184 | 3.699826 | 6.775890 |
| C | 10.056210 | 4.245504 | 1.014473 |
| C | 11.061350 | 3.649116 | 0.246341 |
| C | 11.380390 | 4.105348 | -1.031097 |
| C | 10.687782 | 5.188631 | -1.569303 |
| C | 9.681868 | 5.807759 | -0.828305 |
| C | 9.384256 | 5.332924 | 0.446515 |
| C | 4.551362 | 1.144956 | 4.170287 |
| C | 4.483466 | 0.082031 | 3.260213 |
| C | 3.275051 | -0.492578 | 2.876469 |
| C | 2.084866 | -0.008225 | 3.417448 |
| C | 2.116586 | 1.041360 | 4.333587 |
| C | 3.338252 | 1.605953 | 4.696602 |
| C | 13.184581 | 3.988914 | 7.353992 |
| C | 13.960925 | 2.954220 | 7.890484 |
| C | 15.215333 | 3.181676 | 8.450224 |
| C | 15.725575 | 4.478235 | 8.483247 |
| C | 14.981578 | 5.530363 | 7.950621 |
| C | 13.725835 | 5.278856 | 7.400154 |
| C | 10.929200 | 0.586096 | 5.419017 |
| H | 11.541670 | 1.394605 | 5.823568 |
| C | 11.444805 | -0.694318 | 5.264965 |
| H | 12.478493 | -0.886324 | 5.556033 |
| C | 10.630004 | -1.697421 | 4.747525 |
| H | 11.009653 | -2.712749 | 4.615791 |
| C | 9.319427 | -1.376850 | 4.403754 |
| H | 8.635035 | -2.120179 | 3.992723 |
| C | 8.868062 | -0.076767 | 4.588713 |
| H | 7.844464 | 0.204621 | 4.331966 |
| Co | 8.973541 | 2.671286 | 5.373062 |
| F | 11.740229 | 2.612590 | 0.726845 |
| F | 12.331457 | 3.514534 | -1.740545 |
| F | 10.984095 | 5.630621 | -2.780452 |
| F | 9.028556 | 6.844668 | -1.332632 |
| F | 8.432355 | 5.958126 | 1.139274 |
| F | 5.603952 | -0.433054 | 2.753909 |
| F | 3.249201 | -1.500952 | 2.014921 |
| F | 0.929252 | -0.548481 | 3.067046 |
| F | 0.985273 | 1.500759 | 4.848029 |
| F | 3.324184 | 2.613978 | 5.559263 |
| F | 13.518815 | 1.697523 | 7.845191 |
| F | 15.929095 | 2.175116 | 8.935479 |
| F | 16.916519 | 4.709559 | 9.011065 |
| F | 15.470807 | 6.761861 | 7.981087 |
| F | 13.037048 | 6.306650 | 6.917242 |
| N | 10.496324 | 3.598075 | 4.700283 |
| N | 7.960864 | 2.754523 | 3.766445 |
| N | 7.455002 | 2.092641 | 6.322330 |
| N | 9.661516 | 2.781305 | 7.120930 |
| N | 9.663190 | 0.885252 | 5.084956 |
| O | 7.797577 | 5.165159 | 7.225218 |
| O | 7.555475 | 4.923226 | 8.381851 |
| O | 8.221986 | 5.751110 | 4.481182 |
| H | 9.153762 | 5.965544 | 4.357168 |
| H | 7.914405 | 5.621474 | 3.576503 |