Supporting Information:

Cobalt Kβ Valence-to-Core X-ray Emission Spectroscopy: A Study of Low-Spin Octahedral Cobalt(III) Complexes

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Preparation and Characterization of Complexes

All reagents, including $[Co(NH_3)_6]Cl_3$ (**1**) and $[Co(acac)_3]$ (**5**), were purchased from commercial sources such as Sigma-Aldrich and used without further purification unless otherwise noted. Elemental analyses were performed at Atlantic Microlab, Inc. Abbreviations used: acac = acetylacetonate; dmgH = dimethylgloxime monoanion; $dmgH_2$ = neutral dimethylgloxime; en = ethane-1,2-diamine.

$[Co^{III}(NH_3)_5Cl]Cl_2$ (**2**) was synthesized according to an established procedure.[1,2] Anal. calcd. for $[Co^{III}(NH_3)_5Cl]Cl_2{\cdot}0.5H_2O$ ($CoN_5H_{16}Cl_3O_{0.5}$): C 0.00, H 6.22, N 26.99; found C 0.19, H 6.20, N 27.01.

$[Co^{III}(NH_3)_4CO_3]NO_3$ (**3**) was synthesized according to an established procedure.[1,3] Anal. calcd. for $[Co^{III}(NH_3)_4CO_3]NO_3{\cdot}0.5H_2O$ ($CoN_5H_{13}CO_{6.5}$): C 4.65, H 5.08, N 27.14; found C 5.04, H 4.74, N 27.24.

$[Co^{III}(en)_3]Cl_3$ (**4**) was synthesized following a published procedure.[1] Anal. calcd. for $[Co(en)_3]Cl_3{\cdot}\frac{1}{2}$ $NaCl{\cdot}3H_2O$ ($CoC_6N_6H_{30}O_3Cl_{3.5}Na_{0.5}$): C 16.80 H 7.05 N 19.60; found C 17.11, H 6.83, N 19.55.

$[Co^{III}(dmgH_2)(dmgH)Cl_2]$ (**6**) was made using a procedure previously described.[4] Anal calcd. for $[Co^{III}(dmgH_2)(dmgH)Cl_2]$ ($CoC_8H_{15}N_4O_4Cl_2$): C 26.61, H 4.19, N 15.52; found C 26.74, H 4.14, N 15.51. ^{1}H NMR (300MHz, d_6-DMSO): δ ppm 2.34 (12H, singlet, CH_3).

$[Co^{III}(dmgH)_2(py)Cl]$ (**7**) was synthesized using the method described by Trogler and co-workers.[5] Anal calcd. for $[Co^{III}(dmgH)_2(py)Cl]$ ($CoC_{13}H_{19}N_5O_4Cl$): C: 38.68, H: 4.74, N: 17.35; found: C: 38.70, H: 4.75, N: 17.25. ^{1}H NMR (300MHz, d_6-DMSO): δ ppm 2.40 (12H, singlet, CH_3), 7.25 (2H, m, py), 7.70 (1H, m, py), 8.29 (2H, m, py).

Synthesis of $[Co^{III}(dmgH)_2(py)_2]NO_3$ (**8**). Cobalt nitrate hexahydrate (1.18 g, 4.05 mmol) and dimethylgloxime (0.99 g, 8.53 mmol) were placed in a large test tube with a stir bar, and then dissolved with a minimum volume of boiling absolute ethanol. Pyridine (0.80 mL, 9.93 mmol) dissolved in a minimum volume of absolute ethanol was added to the reaction mixture with vigorous stirring. Heating and stirring was continued for 30 minutes. After the heat was turned off, the solution was allowed to cool while

a stream of air was bubbled into the solution for one hour. The air stream was then removed and the solution was allowed to sit at room temperatures for an additional hour while the precipitate formed. The complex was collected using vacuum filtration and washed with absolute ethanol and diethyl ether. Yield: 0.78 g (38%). Anal calc. for $[Co^{III}(dmgH)_2(py)_2]NO_3$ ($CoC_{18}H_{24}N_7O_7$): C: 42.44, H: 4.75, N: 19.25; found: C: 42.37, H: 4.78, N: 19.15. ^{1}H NMR (300 MHz, d_3-MeCN): δ ppm 2.24 (12H, s, CH_3), 7.40 (4H, m, py), 7.88 (2H, m, py), 8.26 (4H, m, py).

$[Co^{III}(dmgH)_2(^iPr)(py)]$ (**9**) was made using a procedure previously described.[1] Anal. calcd. For $[Co^{III}(dmgH)_2(^iPr)(py)]$ ($CoC_{16}H_{26}N_5O_4$): C 46.72, H 6.37, N 17.03; found: C 46.69, H 6.20, N 17.02. ^{1}H NMR (300MHz, $CDCl_3$): δ ppm 2.12 (12H, s, CH_3), 0.47 (6H, d, $(C\mathbf{H}_3)_2CH$], 1.94 (1H, sep, $(CH_3)_2C\mathbf{H}$). 7.28 (2H, m, py), 7.68 (1H, m, py), 8.58 (2H, m, py).

[$Co^{III}(dmgH)_2$(*cis*-1,2-dichlorovinyl)(py)] (**10**) was prepared using the procedure described by Follett *et al*.[6] Anal. Calcd. for $CoN_5Cl_2O_4C_{15}H_{20}$: C: 38.81, H: 4.34, N: 15.09; found C: 38.70, H: 4.38, N: 14.98. ^{1}H NMR (400MHz, $CDCl_3$): δ ppm 2.19 (12H, s, CH_3), 5.79 (1H, s, CCl=CHCl), 7.32 (2H, m, py), 7.74 (1H, m, py), 8.55 (2H, m, py).

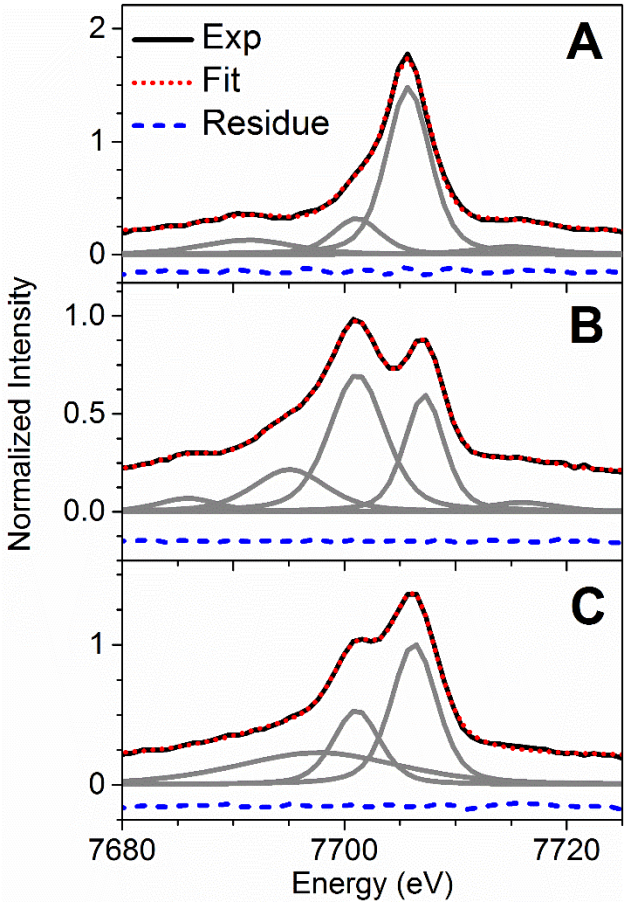

Figure S1. Fits to the background-subtracted normalized cobalt Kβ V2C X-ray emission spectra of $[Co^{III}(NH_3)_6]Cl_3$ (Panel A), $[Co^{III}(acac)_3]$ (Panel B), and $[Co^{III}(dmgH)(dmgH_2)(Cl)_2]$ (Panel C).

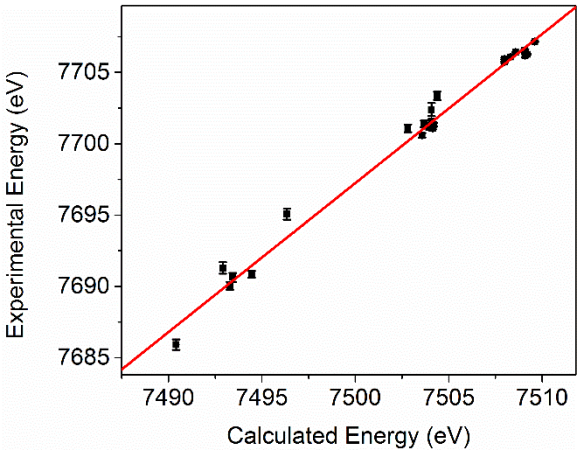

Figure S2. Correlation of calculated vs. experimental V2C X-ray emission energies for low-spin octahedral cobalt(III) complexes. The linear fit gives a slope of 1.045±0.029, and an intercept of −138.2±220.7. The width-modulated calculated spectra (hwhm: 2.0 eV) were curve-fitted with three to four pseudo-Voigt functions having a fixed 50:50 proportion of Gaussian and Lorentzian character in order to determine the center energies of K$\beta_{2,5}$ and Kβ'' peaks of the calculated spectra. The center energies of the K$\beta_{2,5}$ and Kβ'' peaks of the experimental spectra were obtained following procedures described in the experimental section of the text. Error bars of both experimental and calculated data shown in the figure represent the standard deviation.

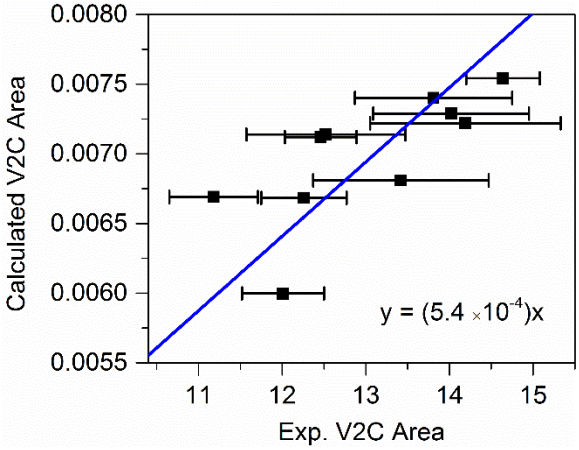

Figure S3. Correlation of calculated vs. experimental V2C areas for low-spin octahedral cobalt(III) complexes. The linear fit has been forced through the origin (intercept = 0), and the slope is (5.4±0.1)×10^{-4}. Error bars represent the standard deviation. The calculated V2C area is taken from the calculated oscillator strength that encompasses the electric dipole, magnetic dipole, and electric quadrupole contributions.

Table S1. Details of V2C XES curve-fitting results for complexes **1** – **10**.

$[Co(NH_3)_6]Cl_3$ (1)			
	Center (eV)[c]	Height	Area[c]
	7705.7(1)	1.48	8.79(33)
	7701.1(3)	0.32	2.05(22)
WSSR[a] =	7691.3(4)	0.13	1.62(16)
0.0151	7715.1(6)	0.07	0.70(12)[b]
			Total 12.5(4)
$[Co(NH_3)_5Cl]Cl_2$ (2)			
	Center (eV)[c]	Height	Area[c]
	7706.1(1)	1.09	5.58(32)
	7703.4(3)	0.42	5.30(37)
WSSR =	7690.8(2)	0.12	1.13(9)
0.00711	7715.7(3)	0.07	0.43(7)[b]
			Total 12.0(5)
$[Co(NH_3)_4(CO_3)]NO_3$ (3)			
	Center (eV)[c]	Height	Area[c]
	7706.0(1)	1.19	7.37(32)
	7701.4(2)	0.39	3.14(38)
WSSR =	7690.6(3)	0.13	1.75(13)
0.00599	7715.9(3)	0.07	0.59(06)[b]
			Total 12.3(5)
$[Co(en)_3]Cl_3$ (4)			
	Center (eV)[c]	Height	Area[c]
	7706.4(1)	1.08	5.78(57)
	7702.4(5)	0.48	5.48(76)
WSSR =	7689.0(3)	0.12	1.27(12)
0.00598	7716.0(5)	0.06	0.52(16)[b]
			Total 12.5(10)
$[Co(acac)_3]$ (5)			
	Center (eV)[c]	Height	Area[c]
	7707.2(1)	0.60	3.18(9)
	7701.1(1)	0.70	5.30(35)
	7695.1(4)	0.22	2.15(37)
WSSR =	7685.9(4)	0.07	0.56(9)
0.00282	7716.0(4)	0.05	0.45(5)[b]
			Total 11.2(5)

[Co(dmgH)(dmgH$_2$)Cl$_2$)] (6)			
	Center (eV)[c]	Height	Area[c]
	7706.5(1)	1.00	5.65(21)
	7701.6(1)	0.55	4.52(68)
WSSR =	7695.6(15)	0.18	3.25(77)
0.00584	7715.5(3)	0.05	0.22(5)[b]
			Total 13.4(10)

[Co(dmgH)$_2$(Cl)(py)] (7)			
	Center (eV)[c]	Height	Area[c]
	7706.3(1)	1.01	6.21(21)
WSSR =	7701.1(1)	0.53	3.35(22)
0.00713	7697.6(5)	0.23	5.08(31)
			Total 14.6(4)

[Co(dmgH)$_2$(py)$_2$] (8)			
	Center (eV)[c]	Height	Area[c]
	7706.5(1)	0.96	6.02(28)
	7701.4(1)	0.69	5.35(65)
WSSR =	7694.2(13)	0.15	2.65(60)
0.0119			**Total 14.0(9)**

[Co(dmgH)$_2$(^{i}Pr)(py)] (9)			
	Center (eV)[c]	Height	Area[c]
	7706.2(1)	0.889	4.867
	7700.6(2)	0.794	5.977
WSSR =	7692.9(17)	0.084	0.474
0.0200			**Total 14.2(11)**

[Co(dmgH)$_2$(cis-1,2-dichlorovinyl)(py)] (10)			
	Center (eV)[c]	Height	Area[c]
	7706.6(1)	1.01	6.09(26)
WSSR =	7701.2(1)	0.67	5.37(66)
0.0137	7693.7(16)	0.13	2.35(63)
			Total 13.8(9)

[a] Weighted Sum of Squared Residuals (WSSR), also called chi-square, is defined as $\chi^2(\boldsymbol{a}) = \sum_{i=1}^{N}[\frac{y_i - y(x_i;\boldsymbol{a})}{\sigma_i}]^2$, where σ is the standard deviation. [b] This high-energy peak above the K$\beta_{2,5}$ feature is not included in the V2C total area. [c] Uncertainties associated with the energy and area of each peak are determined using the Fityk program with a pseudo-VoigtA function; for all fits, the shape parameter is fixed to 0.5, and the active range is set to 7680 – 7725 eV. V2C XES spectra of cobalt complexes **1** to **6** are well fitted by four or five peak. For complexes **7** to **10**, while a four-peak fit model improves the goodness-of-fit with a significantly reduced WSSR value compared to a three-peak fit, one of the individual peaks (~7708 eV) has a very large uncertainty in peak area. We therefore consider the three-peak fit as the best curve-fitting model.

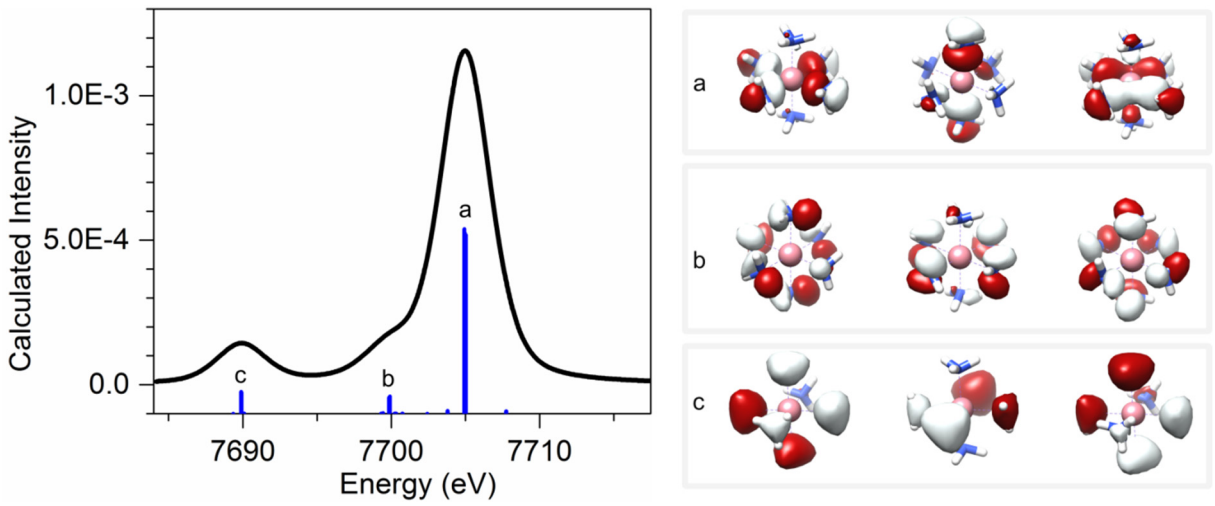

Figure S4. Calculated cobalt Kβ V2C X-ray Emission spectra of $[Co^{III}(NH_3)_6]Cl_3$ (**1**) and molecular orbitals (labeled as MOs a to c) that contribute significantly to the calculated V2C X-ray emission spectrum. MOs are visualized with a contour level of 0.05.

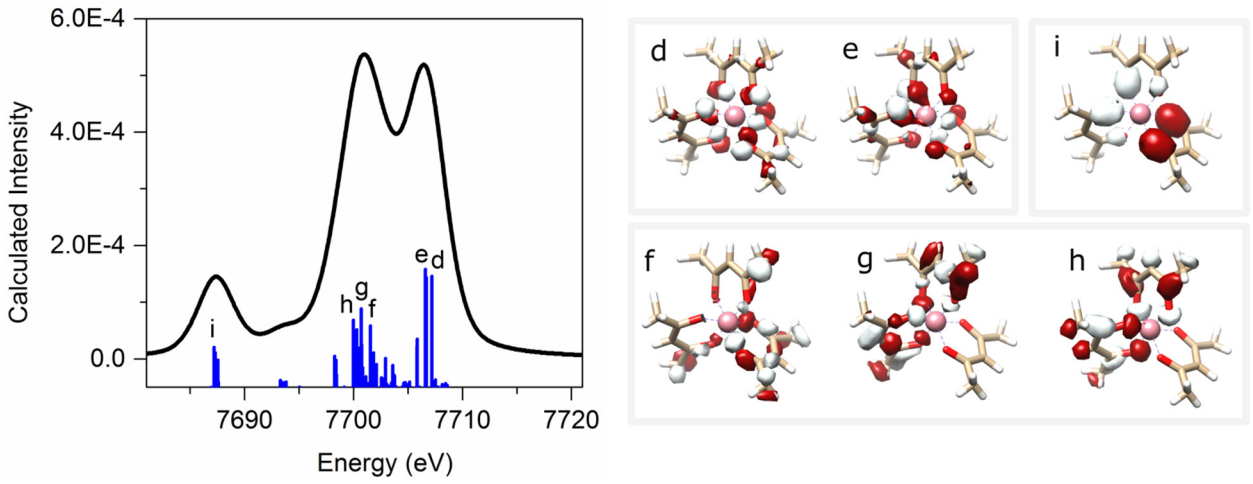

Figure S5. Calculated cobalt Kβ V2C X-ray Emission spectra of $[Co^{III}(acac)_3]$ (**5**) and molecular orbitals (labeled as MOs d to i) that contribute significantly to the calculated V2C X-ray emission spectrum. MOs are visualized with contour level of 0.05.

Table S2. Löwdin population analq qysis results for molecular orbitals that contribute significantly to the cobalt Kβ V2C X-ray emission spectrum of $[Co^{III}(NH_3)_6]Cl_3$ (**1**) based on crystal structure coordinates (CSD Refcode: ADIYES)

MO label	Co s	Co p	Co d	N s	N p	H s
	0%	9.3%	0%	3.2%	76.6%	4.2%
a	0%	9.2%	0%	3.3%	76.5%	4.3%
	0%	9.3%	0%	3.5%	76.6%	4.4%
	0%	1.3%	0%	0%	61.9%	32.5%
b	0%	1.4%	0%	0.2%	61.8%	32.7%
	0%	1.5%	0%	0%	61.8%	32.6%
	0%	3.4%	0%	46.5%	0.9%	41.5%
c	0%	3.3%	0%	46.6%	0.9%	41.5%
	0%	3.2%	0%	46.6%	1.2%	41.5%

Table S3. Fits to experimental vs DFT-calculated-and-width-modulated spectra of complex **1**.

Experimental spectrum of **1** (eV)[a]	[b]Calculated spectrum of **1** (eV)
7705.7	7705.7
7701.1	7700.6
7691.3	7690.6
7715.1	

[a] Peak centers of pseudo-Voigt functions fitted to the experimental spectrum of **1**; [b] Scalar-corrected peak energies of MOs a-c that contribute intensely to calculated V2C X-ray emission spectrum of **1**.

Table S4. Löwdin population analysis results for molecular orbitals that contribute significantly to the cobalt Kβ V2C X-ray emission spectrum of [$Co^{III}(acac)_3$] (**5**) based on crystal structure coordinates (CSD Refcode: ACOSEU).

MO label	Co s	Co p	Co d	C s	C p	O s	O p	H s
d	0%	1.2%	0.9%	1.2%	26.7%	0.4%	63.2%	0.4%
e	0%	1.9%	5.8%	1.4%	25.5%	1.4%	57.5%	1.6%
f	0%	2.1%	1.4%	0.8%	50.3%	1.4%	25.0%	16.9%
g	0%	2.3%	1.1%	0.6%	53.1%	2.8%	23.7%	13.6%
h	0%	2.1%	3.3%	9.6%	32.2%	9.2%	30.0%	10.9%
i	0.1%	2.7%	0.3%	21.1%	14.8%	52.2%	5.8%	0.7%

Table S5. Löwdin population analysis results of molecular orbitals that contribute significantly to the cobalt Kβ V2C X-ray emission spectrum of geometry-optimized [$Co^{III}(dmgH)(dmgH_2)Cl_2$] (**6**).

MO label	Co s	Co p	Co d	Cl s	Cl p	O s	O p	N s	N p	C s	C p	H s
j	0%	4.1%	3.0%	0.1%	20.1%	0.4%	46.7%	1.4%	12.9%	0.7%	6.2%	1.5%
k	0%	3.2%	8.4%	0.2%	11.7%	1.8%	35.2%	1.1%	19.7%	0.2%	10.8%	4.8%
l	0.1%	2.8%	0.3%	0.1%	0.6%	2.3%	19.8%	4.1%	34.8%	1.5%	26.5%	6.0%
m	0.2%	5.4%	0.4%	67.9%	0%	0.4%	0.7%	1.8%	1.3%	9.0%	6.1%	5.2%

Table S6. Löwdin population analysis results for molecular orbitals that have >20% Löwdin population from the two chloride ligands *and* contribute significantly to the intensity of the Kβ V2C X-ray emission spectra of geometry-optimized $[Co^{III}(dmgH)(dmgH_2)(Cl)_2]$.

MO label	Co s	Co p	Co d	Cl s	Cl p	O s	O p	N s	N p	C s	C p	H s
α	0.2%	5.4%	0.4%	67.9%	0%	0.4%	0.7%	1.8%	1.3%	9.0%	6.1%	5.2%
β	0%	2.5%	8.6%	0.4%	29.9%	0%	43.0%	0%	2.2%	0%	9.2%	1.8%
	0%	4.1%	3.0%	0.1%	20.1%	0.4%	46.7%	1.4%	12.9%	0.7%	6.2%	1.5%
	0%	1.4%	21.7%	0%	56.6%	0%	15.8%	0%	1.5%	0%	1.3%	0.4%
	0%	1.9%	4.9%	0.2%	40.0%	0%	17.5%	0%	4.2%	0%	23.9%	5.2%

Table S7. Löwdin population analysis results for molecular orbitals that have >20% Löwdin population from the two pyridine ligands *and* contribute significantly to the intensity of the Kβ V2C X-ray emission spectra of geometry-optimized $[Co^{III}(dmgH)_2(py)_2]^+$.

MO	cobalt			Pyridine					dmg ligands						
label	Co s	Co p	Co d	C s	C p	N s	N p	H s	O s	O p	N s	N p	C s	C p	H s
γ	0%	1.9%	0%	4.6%	47.8%	0.8%	11.2%	22.6%	0%	2.0%	0%	5.0%	0%	1.2%	0%
δ	0%	2.1%	0%	2.4%	29.0%	1.0%	15.8%	13.2%	0%	1.4%	0%	2.0%	0%	21.5%	9.2%
ε	0%	4.7%	0%	0%	32.4%	2.4%	27.8%	12.2%	0%	12.2%	0%	0.6%	0%	2.6%	0.8%
ζ	0%	1.7%	0%	0%	44.6%	0%	16.6%	0%	0.8%	10.0%	2.0%	14.6%	0%	4.8%	1.2%

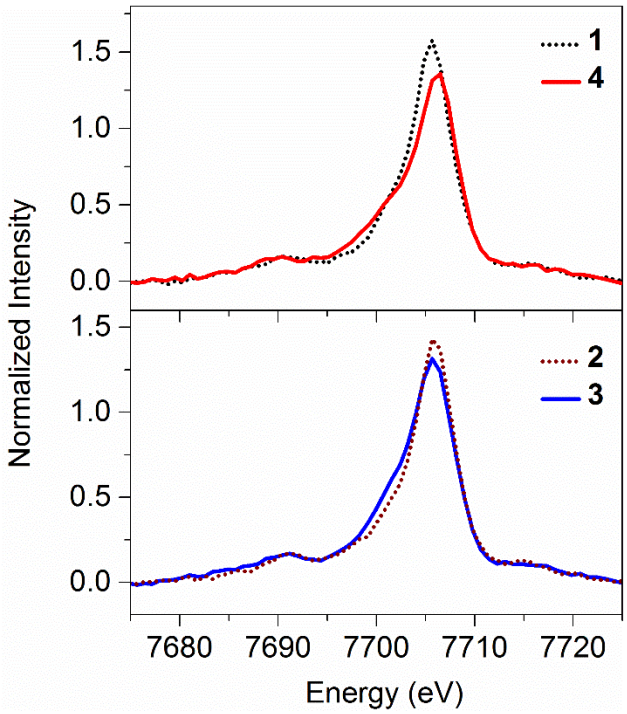

Figure S6. Energy-calibrated background-subtracted normalized experimental cobalt Kβ X-ray emission spectra of cobalt complexes **1** and **4** (Panel A), and complexes **2** and **3** (Panel B).

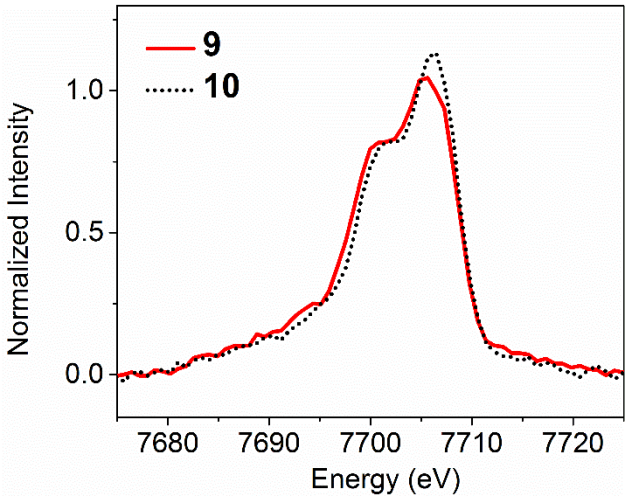

Figure S7. Energy-calibrated background-subtracted normalized experimental cobalt Kβ X-ray emission spectra of cobalt complexes **9** and **10**.

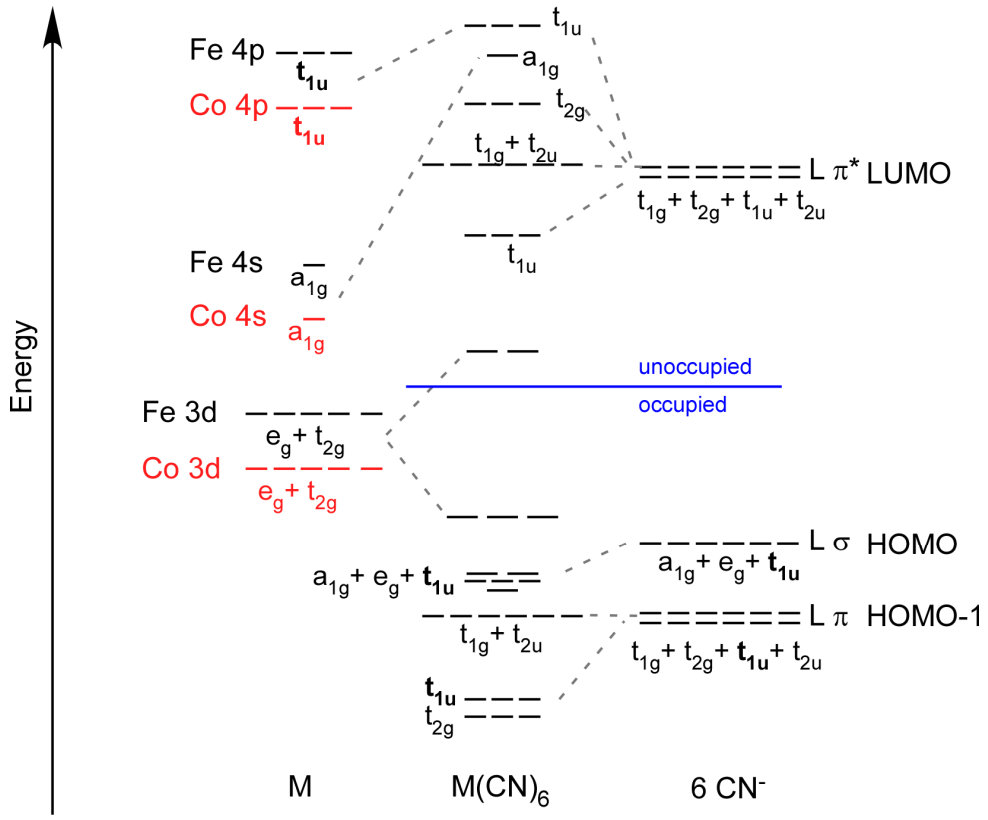

Figure S8. Qualitative MO diagram for octahedral ML_6 complexes with L being a π-acceptor like CN^-, and M being Fe^{3+} or Co^{3+}.

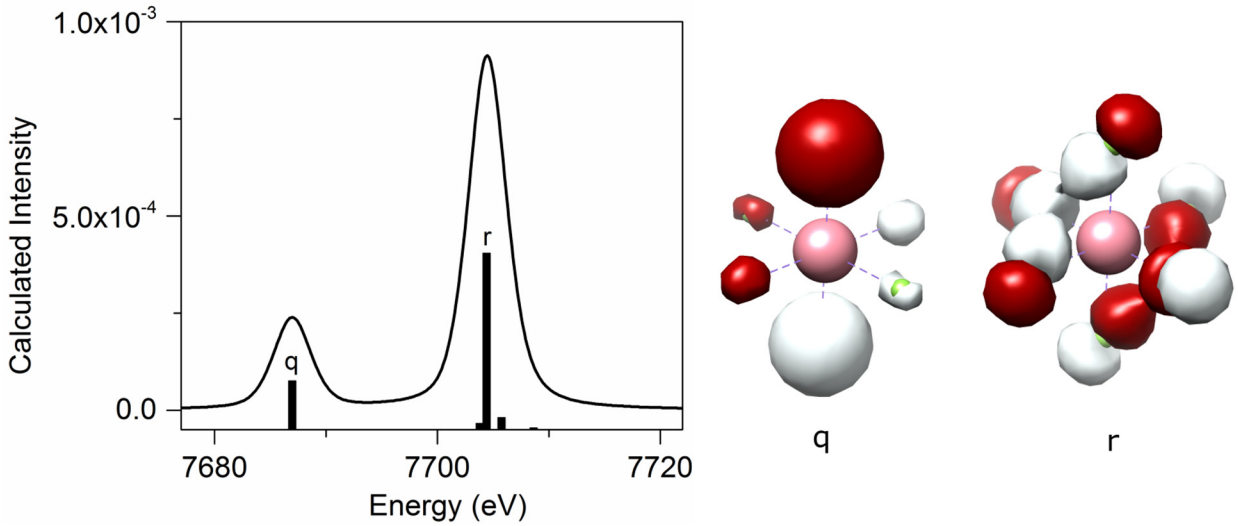

Figure S9. Calculated cobalt Kβ V2C X-ray Emission spectra of the *hypothetical low-spin* $[Co^{III}F_6]^{3-}$ complex and key molecular orbitals (labeled as MOs q and r) that contribute significantly to the calculated V2C X-ray emission spectrum. MOs are visualized with a contour level of 0.05.

Sample Gaussian Geometry Optimization Input File

%chk=Cbl_1chloroethyl_pyr.chk
%nprocshared=16
%mem=30GB
#p opt=maxcycles=512 freq ub3lyp/6-31g(d) geom=connectivity scf(MaxCycle=512)

Title line

0 1
Molecular specification (xyz coordinates and connectivity table)

Sample ORCA XES Calculation Input File

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! RKS BP86 TZVP def2-TZV/J TightSCF SlowConv SCFConv7 COSMO
! Grid4 NoFinalGrid Normalprint

%scf
MaxIter 500
end

%maxcore 1024

%xes CoreOrb 0
OrbOp 0
end

* xyz 3 1
Co      0       0       0
N       ……
*
```

Optimized xyz coordinates for $[Co^{III}(NH_3)_6]^{3+}$

Co	0.00000000	0.00000000	0.00000000
N	0.01746854	2.01337005	0.00006083
H	-0.88337570	2.45501533	0.22333774
H	0.28089412	2.43772205	-0.89830351
H	0.67107943	2.43663772	0.67119213
N	-2.01396500	-0.00232762	0.00034433
H	-2.43788041	-0.89667510	0.27842047
H	-2.44853373	0.20101326	-0.90864594
H	-2.44513780	0.68053285	0.63650649
N	0.01360191	0.01414944	-2.01366628
H	-0.22369579	-0.88316013	-2.45493786
H	0.91912151	0.25959919	-2.43358636
H	-0.64301096	0.67922302	-2.44217971
N	-0.01279266	-0.01295699	2.01384848
H	-0.92061535	-0.24745556	2.43489417
H	0.23522587	0.88206538	2.45386599
H	0.63664420	-0.68494309	2.44247148
N	2.01357306	0.00000000	0.00000000
H	2.44753490	-0.21830409	0.90571855
H	2.43963261	0.89740602	-0.26431177
H	2.44303377	-0.67418160	-0.64650073
N	-0.01687569	-2.01348257	-0.00064037
H	-0.28348579	-2.43824332	0.89665078
H	0.88495077	-2.45479651	-0.22073364
H	-0.66800801	-2.43625791	-0.67442201

Reoriented xyz coordinates for $[Co^{III}(NH_3)_6]^{3+}$ based on a crystal structure (CSD Refcode: ADIYES)

Co	0	0	0
N	0.0238582	1.95391172	-0.0001242
H	0.07427808	2.25722192	0.85722268
H	-0.73720266	2.26668043	-0.38780807
H	0.74716322	2.24880789	-0.46877715
N	1.95398989	0	0
H	2.25740659	0.36711916	-0.77555531
H	2.2557564	-0.85544044	0.06795865
H	2.257153	0.48653087	0.70671022
N	0.01143826	0.01637733	1.95174094
H	0.68354436	0.55277122	2.24740195
H	0.14016533	-0.83103939	2.26106359
H	-0.78652549	0.33262409	2.25756484
N	-0.0531984	-1.95957205	-0.05665515
H	-0.69442862	-2.2292464	-0.64301894
H	-0.24450913	-2.28201983	0.77174359
H	0.75693856	-2.275913	-0.32604769
N	-1.95600068	-0.02155335	0.01391186
H	-2.26282013	0.72930379	0.4256498
H	-2.24829369	-0.75567141	0.46405699
H	-2.26524781	-0.04692647	-0.84180637
N	0.00685159	0.03519519	-1.97083845
H	-0.84163736	0.15741618	-2.2745531
H	0.33095614	-0.75300854	-2.28691246
H	0.5349085	0.71785305	-2.25997971

Optimized xyz coordinates for $[Co^{III}(NH_3)_5Cl]^{2+}$

Co	0.00000000	0.00000000	0.00000000
Cl	0.08424536	0.0846196	2.21934842
N	0.00982108	-1.99097996	0.1543627
H	0.58894058	-2.51447106	-0.51004626
H	0.35714077	-2.22700697	1.09177213
N	-1.99026117	-0.00129379	0.16052186
H	-2.52296006	-0.57011438	-0.50545632
H	-2.22894403	-0.34497562	1.09835747
N	0.00490878	1.99774362	-0.00005772
H	-0.67320311	2.47544744	-0.60218537
H	-0.19655736	2.30272585	0.96017208
N	1.99770331	0.00000000	0.00000000
H	2.30014365	0.26334462	0.94600341
H	2.43777847	-0.90982185	-0.16904373
N	-0.09894903	-0.08500686	-2.02731224
H	-0.64432196	0.67184272	-2.4514423
H	0.81031228	-0.04006835	-2.4978757
H	-2.42295667	0.92653686	0.11976882
H	0.90415155	2.43378016	-0.22565169
H	2.47267949	0.64341323	-0.64126395
H	-0.91273598	-2.43454278	0.10691055
H	-0.53000349	-0.94292225	-2.38584249

Optimized xyz coordinates for $[Co^{III}(NH_3)_4(CO_3)]^+$

Co	0	0	0
O	-1.78233133	-0.47560419	0.00117976
O	-0.10643988	-1.84164289	0.00324376
O	-2.22342272	-2.72784368	0.00538959
N	-0.08678728	-0.10347783	1.97689683
N	-0.41055613	1.99003417	-0.00331243
N	2.03173341	0	0
N	-0.08759712	-0.1103227	-1.97639784
C	-1.46565655	-1.79826981	0.00355515
H	-1.07787588	-0.02774918	2.22252944
H	0.4319926	0.53179172	2.58651159
H	0.18489921	-1.05953651	2.22320844
H	-1.43426293	2.03035361	-0.00301162
H	-0.10845879	2.52975649	-0.81683216
H	-0.10803903	2.5324466	0.80836575
H	2.5011936	0.41420994	0.80784371
H	2.49952016	0.39731898	-0.81723433
H	2.27868561	-0.9941361	0.00967837
H	-1.07902577	-0.03639369	-2.22156312
H	0.18482393	-1.06686206	-2.21998658
H	0.43001348	0.52362046	-2.5884819

Optimized xyz coordinates for $[Co^{III}(en)_3]^{3+}$

Co	0.0008	0.0004	0.0002
N	0.4329	-1.6001	-1.1275
N	-1.0109	-1.3168	1.1263
N	-1.6024	0.4278	-1.1317
N	-0.6389	1.5330	1.1270
N	1.1736	1.1757	-1.1279
N	1.6462	-0.2143	1.1296
C	-0.4570	-2.7660	-0.7526
C	-0.6264	-2.7323	0.7526
C	-2.1707	1.7784	-0.7514
C	-2.0585	1.9023	0.7543
C	2.6275	0.9858	-0.7518
C	2.6820	0.8238	0.7537
H	1.4068	-1.9026	-1.0237
H	0.3416	-1.4432	-2.1365
H	-2.0263	-1.2280	1.0169
H	-0.8725	-1.2068	2.1362
H	-2.3499	-0.2666	-1.0325
H	-1.4192	0.4339	-2.1405
H	-0.0582	2.3710	1.0182
H	-0.6113	1.3574	2.1367
H	0.9500	2.1707	-1.0231
H	1.0840	1.0196	-2.1373
H	2.0770	-1.1391	1.0282
H	1.4787	-0.1424	2.1386
H	-0.0188	-3.7091	-1.0934
H	-1.4133	-2.6446	-1.2705
H	-1.3875	-3.4405	1.0940
H	0.3055	-2.9795	1.2703
H	-3.2063	1.8697	-1.0929

H	-1.5882	2.5491	-1.2651
H	-2.2962	2.9132	1.0995
H	-2.7355	1.2139	1.2694
H	3.2270	1.8353	-1.0930
H	2.9991	0.0957	-1.2685
H	3.6752	0.5170	1.0956
H	2.4324	1.7555	1.2705

Optimized xyz coordinates for $[Co^{III}(acac)_3]$

Co	0.00000000	-0.00000000	0.00000000
C	0.14803054	2.11344104	-2.38177062
C	0.09897761	2.60007702	-1.06769095
O	0.04341273	1.88792250	-0.01100948
C	0.10857631	4.09175436	-0.81680480
O	-0.20149501	0.09088373	1.87519998
C	0.76892688	0.13146282	2.70220149
C	2.13080119	0.10763017	2.36887991
C	2.60817219	0.04235099	1.05198556
O	1.88835358	-0.00000000	0.00000000
C	0.35139335	0.21463929	4.15365876
C	4.09789574	0.01539919	0.79147290
H	0.16727710	4.66878047	-1.74286081
H	-0.80032443	4.37328384	-0.27366427
H	0.95982475	4.34931605	-0.17690747
H	-0.24120672	1.12315185	4.30855275
H	1.20790810	0.22444262	4.83203085
H	-0.29330964	-0.63672925	4.39812521
H	4.37042201	0.85488794	0.14243449
H	4.68255462	0.06870344	1.71307331
H	4.35478600	-0.90449760	0.25452894
H	2.85437605	0.14314818	3.17393462
H	0.19817086	2.83140478	-3.19086653
O	0.07529898	-0.21456974	-1.87440478
O	0.07377340	-1.88171265	0.14364822
O	-1.87986952	0.11802632	-0.13412740
C	0.13655873	0.74962260	-2.70720500
C	-0.94818993	-2.64496116	0.13253184
C	-2.66795204	-0.88441361	-0.10433973

C	0.20399180	0.32126930	-4.15636458
C	-2.28166192	-2.22650330	0.01966806
C	-0.62937394	-4.11873397	0.25177391
C	-4.13453102	-0.53092961	-0.21599944
H	0.23007379	1.17266098	-4.84073112
H	1.09855062	-0.29232882	-4.31111568
H	-0.66250762	-0.30591205	-4.39290402
H	-3.05704248	-2.98255426	0.02760614
H	0.01118053	-4.41950715	-0.58464929
H	-1.52858695	-4.73944578	0.25669442
H	-0.06282925	-4.29679418	1.17248451
H	-4.30614224	0.02712167	-1.14309054
H	-4.77710982	-1.41457426	-0.20371009
H	-4.41240098	0.12835709	0.61380007

Reoriented xyz coordinates for [$Co^{III}(acac)_3$] based on a crystal structure (CSD Refcode: ACOSEU)

Co	0.00000000	0.00000000	0.00000000
C	2.12638951	-2.33341306	-0.15180081
C	2.60626983	-1.03380125	-0.09611691
O	1.88664849	0.00000000	0.00000000
C	4.09721837	-0.80023862	-0.16178862
O	0.06949427	1.87813936	0.00121805
C	-0.12367003	2.59291801	1.03256927
C	-0.25451743	2.08141312	2.32143613
C	-0.14006803	0.76358049	2.69060794
O	0.00981852	-0.21113365	1.88597720
C	-0.19699162	4.04138796	0.75756631
C	-0.20789343	0.34473276	4.12923514
H	4.54454891	-1.52097356	0.15802960
H	4.16106322	-0.27086648	-0.80456946
H	4.41647066	-0.17116659	0.38068059
H	0.42296367	4.32454690	0.09843830
H	-0.06238131	4.49466959	1.30543499
H	-1.31473723	4.23263316	0.32470205
H	0.44581848	0.52242214	4.45444854
H	-0.58212079	1.03788177	4.64950268
H	-0.62081482	-0.48996222	4.27153716
H	-0.30818844	2.69128787	2.98211563
H	2.85218494	-3.12987134	-0.20361461
O	-0.17878728	-1.87425926	-0.12186986
O	-1.87246993	0.10025046	0.12754722
O	0.08682363	0.10487593	-1.89290907
C	0.78623333	-2.68911533	-0.14601784
C	-2.63087192	0.42971942	-0.83601061
C	-0.91915733	0.39877019	-2.61499090
C	0.41716855	-4.15387189	-0.16052161

C	-2.19365458	0.60498884	-2.14661094
C	-4.04508185	0.61356825	-0.45467631
C	-0.58972403	0.53033350	-4.07232672
H	1.07014768	-4.64048740	-0.55880451
H	-0.07317431	-4.21513803	0.51279180
H	-0.27301010	-4.37582000	-0.67642545
H	-2.83716326	0.76008616	-2.75760481
H	-4.34250626	-0.02352292	0.18142655
H	-4.54353176	0.55954936	-0.97657085
H	-4.10120335	1.71047693	0.06198915
H	-0.84908300	-0.07989610	-4.42565988
H	-1.27636759	1.00154753	-4.51682706
H	0.26943000	0.87543552	-4.24639952

Optimized xyz coordinates for $[Co^{III}(dmgH)(dmgH_2)(Cl)_2]$

Co	0	0	0
Cl	0	0	2.26031009
O	-2.4997946	1.26803826	0.12376632
O	0.50304941	-2.79574941	-0.51880901
O	2.6927615	-1.22089921	0.14893664
N	1.94296539	-0.08270649	0.05185473
O	-0.49848344	2.85603696	-0.08574805
N	-0.42423508	-1.83584546	-0.06434259
N	-1.9008625	0.14658053	0.05292171
N	0.41172475	1.87034308	-0.03028913
C	1.66330737	2.2057116	-0.02858389
C	-1.69081766	-2.14666513	-0.06260808
C	-2.21697632	-3.53117306	-0.27151913
H	-1.40338382	-4.25325391	-0.33276044
H	-2.80707428	-3.57422962	-1.19475103
H	-2.88367359	-3.80408137	0.55381591
C	2.10284428	3.63520368	-0.08015666
H	1.7756557	4.09579916	-1.01957054
H	3.18679246	3.72916817	0.00028754
H	1.63265201	4.19927072	0.73258336
C	2.57099648	1.04804689	0.03876045
C	-2.55810718	-1.00551829	0.11072303
C	4.05975435	1.18769217	0.10668475
H	4.53543168	0.20788173	0.1270454
H	4.35083228	1.73938493	1.00831756
H	4.43224948	1.74564835	-0.75987658
C	-4.04287727	-1.08189876	0.28635019
H	-4.44554127	-0.06931255	0.33424044
H	-4.30802119	-1.60608787	1.21299135
H	-4.52344223	-1.60989755	-0.54619287

H	-1.38970975	2.35297636	-0.00745523
Cl	0.08824767	-0.14877052	-2.28833914
H	0.64526636	-2.49923608	-1.44969768
H	2.02545391	-1.94616585	0.10570557

Optimized xyz coordinates for [$Co^{III}(dmgH)_2(Cl)(py)$]

Co	0	0	0
Cl	0	0	2.23074763
O	0.75630137	2.72286983	0.04904231
O	-2.58225212	-1.1382261	0.12247194
O	-0.73274386	-2.76999053	0.02244672
N	0.28861192	-1.88367721	0.03254783
O	2.66706131	1.10250933	0.03373534
N	-1.88309411	-0.00407784	0.04061957
N	-0.27340441	1.86752815	0.01861798
N	-0.05592722	0.03022417	-1.96548051
N	1.90957231	-0.03239038	0.01903756
C	2.47882124	-1.18564132	0.12397548
C	-2.46596307	1.15308908	-0.03262988
C	-3.94591768	1.31474621	-0.09259093
H	-4.36262752	0.45123549	-0.07624709
H	-4.18536787	1.76959585	-0.90413231
H	-4.24321219	1.82848804	0.66200585
C	3.94173372	-1.38163006	0.33002524
H	4.38438367	-0.5291648	0.31335191
H	4.29313981	-1.93817228	-0.36869611
H	4.09185203	-1.80242113	1.17959064
C	1.51225382	-2.29785734	0.09389408
C	-1.50925781	2.26327803	-0.04636204
C	1.91264206	-3.7426223	0.15830253
H	1.1277163	-4.29442326	0.12444617
H	2.38531093	-3.90820308	0.97775426
H	2.48073687	-3.95041215	-0.58656838
C	-1.91015308	3.70154457	-0.10280096
H	-1.12559468	4.2532816	-0.09875837

H	-2.45378348	3.91147496	0.66017822
H	-2.40981374	3.86298918	-0.90550942
C	-0.92709129	-0.85061946	-4.01338227
H	-1.47508687	-1.4672457	-4.44476947
C	-0.8308945	-0.84446223	-2.63139448
H	-1.32104244	-1.46739142	-2.14561654
C	0.59179081	0.98539624	-4.0610219
H	1.08720866	1.62106699	-4.52566029
C	0.63853447	0.94436343	-2.67473465
H	1.16367919	1.56236607	-2.22197119
C	-0.19566776	0.07430718	-4.74800281
H	-0.24830848	0.090229	-5.86905118
H	-1.70590437	-2.01642608	0.05777704
H	1.7404439	1.94451728	0.05216906

Optimized xyz coordinates for $[Co^{III}(dmgH)_2(py)_2]^+$

C	-1.55422061	-2.28808159	0.00010202
C	-2.49497937	-1.16296829	0.00020792
C	1.55422458	2.2880998	-0.00018301
C	2.49498387	1.16298297	-0.00040091
C	-1.96532487	-3.72801165	0.0000953
C	-3.98524397	-1.3029078	0.00041414
C	1.96534139	3.72802627	-0.00022729
C	3.98525142	1.30289971	-0.00082814
N	-0.296732	-1.90695784	-0.00007236
N	-1.91551225	0.00001611	-0.00004399
N	0.29673669	1.90697671	0.00000137
N	1.91551536	0	0
O	0.69685618	-2.74672295	-0.00026463
O	-2.70177222	1.11147092	-0.00003929
O	-0.69685443	2.7467392	0.00008064
O	2.7017934	-1.11144815	0.0001363
Co	0	0	0
H	-1.07356416	-4.35578801	-0.00016459
H	-2.56681062	-3.97097515	-0.88386758
H	-2.56636994	-3.97113522	0.88431577
H	-4.41048709	-0.80751322	-0.87959331
H	-4.41064753	-0.80271195	0.87757843
H	-4.29133244	-2.34932098	0.00312066
H	2.56313999	3.97203149	-0.88643174
H	2.57006948	3.97009775	0.88173856
H	1.07359386	4.35580905	0.0037456
H	4.41068868	0.80026587	-0.87656219
H	4.41042681	0.80990096	0.88057707
H	4.29136869	2.34929157	-0.00629966

H	-2.01970642	1.87440668	0.0000524
H	2.01973454	-1.87438712	-0.00011138
C	0.6185847	-0.98273739	2.67376821
C	0.63907361	-1.01325486	4.06280544
C	0.00005311	-0.00007982	4.77537861
C	-0.63902308	1.01310078	4.06286859
C	-0.61863129	0.98260314	2.67382842
N	-0.00005205	-0.00006069	1.98441722
H	1.09304229	-1.76166466	2.09022324
H	1.15053235	-1.82605741	4.567011
H	0.00009106	-0.00009039	5.86109776
H	-1.15045796	1.82588945	4.56711916
H	-1.09313918	1.76152977	2.09032221
N	0.00006282	0.00008627	-1.98446921
C	-0.61845491	0.98282167	-2.67383714
C	0.61867297	-0.98257021	-2.67387239
C	-0.63879587	1.01341947	-4.06287828
C	0.63920927	-1.01299725	-4.06291148
C	0.00025345	0.00025261	-4.77544044
H	0.00032853	0.00031658	-5.86115853
H	1.15062086	-1.82580789	-4.56715006
H	1.09306557	-1.76156427	-2.09036326
H	-1.09295446	1.76173448	-2.09030319
H	-1.15018189	1.8262651	-4.56708579

Optimized xyz coordinates for [$Co^{III}(dmgH)_2(^iPr)(py)$]

Co	0	0	0
O	0.72900869	-2.73000165	0.10641484
O	-2.56552903	1.18679503	0.06250298
O	-0.65116061	2.8217772	0.04506319
N	0.32007325	1.88706744	0.00186305
O	2.65968873	-1.12770695	0.04026288
N	-1.88934491	0.05248189	0.02479256
N	-0.26748551	-1.86807916	0.04297885
N	-0.01379664	0.00612904	2.09813492
N	1.91883473	0	0
C	2.51195113	1.15860414	0.01291063
C	-2.46843268	-1.12315717	0.07673728
C	-3.95703859	-1.2869213	0.13776219
H	-4.4179503	-0.30842078	0.28250221
H	-4.25390601	-1.95142535	0.9577844
H	-4.35016663	-1.72019052	-0.79151615
C	4.00009803	1.33507037	0.03101983
H	4.48888707	0.3620743	-0.02472288
H	4.32833801	1.84160138	0.94712698
H	4.33181702	1.94545124	-0.81723558
C	1.55903041	2.28049634	0.01822362
C	-1.52321787	-2.24173491	0.07920317
C	1.9382792	3.7295802	0.05219607
H	1.47849128	4.25843063	-0.79020606
H	3.02049598	3.86616522	0.00907456
H	1.55922866	4.20430588	0.96496884
C	-1.91984689	-3.68516282	0.15027019
H	-1.14274519	-4.29700203	-0.3144202
H	-2.8745727	-3.86188615	-0.35427177

H	-2.02487625	-4.02362947	1.19038922
C	-0.89995556	0.84305391	4.16624353
H	-1.59812948	1.50924285	4.66272207
C	-0.85589887	0.80878207	2.77549369
H	-1.51965834	1.41943539	2.17253706
C	0.81612902	-0.82896689	4.19038751
H	1.49228111	-1.5033126	4.70592272
C	0.80100556	-0.80381042	2.7988768
H	1.44263781	-1.45544853	2.21728785
C	-0.04613999	0.01297527	4.89050667
H	-1.53305268	2.2274202	0.0119376
H	1.91328504	-1.89340777	0.01834044
C	-0.11989637	-0.12037573	-2.03317387
H	-0.99844664	-0.7630465	-2.15483456
C	-0.42101471	1.20384539	-2.73418087
H	0.43224778	1.89338492	-2.70375387
H	-0.63889997	1.01753764	-3.79773139
H	-1.28813794	1.71635042	-2.30919524
C	1.06007842	-0.82837009	-2.69854919
H	0.83219234	-1.00191516	-3.76219343
H	1.97865093	-0.22950751	-2.6666012
H	1.27387901	-1.80131113	-2.2481636
H	-0.0574706	0.01692827	5.97689271

Optimized xyz coordinates for [$Co^{III}(dmgH)_2$(*cis*-1,2-dichlorovinyl)(py)]

C	-0.09455000	-2.66615200	-0.63579800
C	-0.00032600	-2.61433200	0.82318500
C	0.14910800	2.68755000	0.66909200
C	0.00276500	2.63220700	-0.78365300
C	-0.19450200	-3.93287000	-1.42949700
C	-0.00011300	-3.81483500	1.71956900
C	0.24937800	3.95426600	1.46290000
C	-0.09903800	3.83275200	-1.67429700
C	-1.91774500	0.04803500	0.15943700
C	-2.72228900	-0.07712600	-0.89830100
N	-0.08990800	-1.47755900	-1.19626000
N	0.09353200	-1.40795400	1.29502300
N	0.19711100	1.49704400	1.22879500
N	-0.03537200	1.42381700	-1.25800800
O	-0.13458000	-1.31622100	-2.49061000
O	0.22911200	-1.24808500	2.63787300
O	0.39787200	1.33313100	2.50073700
O	-0.16425700	1.26314900	-2.60634100
Cl	-2.63992000	0.24233600	1.75965700
Co	0.03700400	0.00895200	0.01858100
H	-0.11728200	-3.69058100	-2.49047500
H	-1.15560600	-4.43532300	-1.26007700
H	0.59984900	-4.64061500	-1.16489900
H	-0.72550400	-3.67255100	2.52706800
H	0.98092100	-3.94369100	2.19271900
H	-0.24634000	-4.72475800	1.16971700
H	-0.59679700	4.62066700	1.25855600
H	1.16978000	4.50850600	1.23698800
H	0.24979500	3.70180900	2.52438700

H	-1.08932100	3.86728600	-2.14381000
H	0.63365200	3.76793100	-2.48540800
H	0.06001700	4.75849100	-1.11902200
Cl	-4.48101100	-0.05861100	-0.88517400
H	-2.33006800	-0.21615800	-1.89677800
H	0.22439400	-0.22792300	2.74111300
H	-0.18145700	0.24188900	-2.70495300
C	2.67014300	-0.30771400	-1.33282700
C	4.05156100	-0.36140800	-1.48702900
C	4.86587900	-0.14375800	-0.37708900
C	4.26147700	0.12204100	0.84994100
C	2.87266700	0.16193300	0.92606500
N	2.08573400	-0.04971900	-0.14662100
H	2.00096300	-0.48651600	-2.16759200
H	4.47102000	-0.57286500	-2.46514100
H	5.94787900	-0.18042300	-0.46672700
H	4.84917600	0.29952900	1.74462400
H	2.36229900	0.38153700	1.85786500

Optimized xyz coordinates for $[Co^{III}(CN)_6]^{3-}$

Co	1.965812	0.512821	-1.460000
C	1.965812	0.512821	0.470000
N	1.965812	0.512821	1.630000
C	3.895812	0.512821	-1.460000
N	5.055812	0.512821	-1.460000
C	1.965812	-1.417179	-1.460000
N	1.965812	-2.577179	-1.460000
C	1.965812	0.512821	-3.390000
N	1.965812	0.512821	-4.550000
C	1.965812	2.442821	-1.460000
N	1.965812	3.602821	-1.460000
C	0.035812	0.512821	-1.460000
N	-1.124188	0.512821	-1.460000

Optimized xyz coordinates for $[Co^{III}(ox)_3]^{3-}$

Co	1.603175000	2.574668000	1.953809000
O	1.982157000	4.418113000	2.291195000
O	-0.133873000	3.191234000	1.444995000
O	2.199320000	2.707223000	0.141728000
O	1.172615000	0.765277000	1.510816000
O	3.333387000	2.032508000	2.561081000
O	1.066089000	2.333292000	3.772855000
O	1.008510000	6.445588000	2.186388000
O	-1.326551000	5.093087000	1.270646000
O	2.393762000	1.462538000	-1.724529000
O	1.246320000	-0.669849000	-0.222568000
O	4.402790000	1.402678000	4.439787000
O	1.901833000	1.712641000	5.769366000
C	0.992090000	5.216127000	2.048004000
C	-0.290223000	4.472987000	1.539927000
C	2.070014000	1.614080000	-0.539924000
C	1.444064000	0.440072000	0.287368000
C	3.390684000	1.763671000	3.826272000
C	2.017038000	1.940263000	4.558582000

Optimized xyz coordinates for low-spin $[Co^{III}F_6]^{3-}$

Co	0.000000000	0.000000000	0.000000000
F	0.000335290	1.875475825	0.000164089
F	-1.875824334	0.000000000	-0.000398150
F	0.000000000	0.000000000	-1.875876086
F	-0.000335290	-1.875475825	-0.000164089
F	1.875824334	0.000000000	0.000398150
F	0.000000000	0.000000000	1.875876086

Optimized xyz coordinates for low-spin $[Co^{III}(OH)_6]^{3-}$

Co	0.0181	-0.0066	0.0946
O	-1.5116	0.3449	-1.1870
H	-0.8592	0.9120	-1.6393
O	1.5150	-0.1046	1.3252
H	1.9422	0.6116	0.8220
O	1.0391	1.3477	-0.9481
H	1.4094	0.6034	-1.4544
O	-0.9768	-1.5876	0.7556
H	-1.6860	-1.3860	0.1215
O	0.8570	-1.3203	-1.1407
H	0.3411	-1.9738	-0.6302
O	-0.9328	1.3218	1.1707
H	-1.5553	1.3950	0.4204

Optimized xyz coordinates for low-spin $[Co^{III}(dtc)_3]$

Co	-0.001737000	0.002597000	-0.000054000
C	0.713219000	-2.670976000	-0.001042000
C	1.897073000	-4.542019000	-1.064892000
C	1.076237000	-5.104339000	-2.228313000
C	1.959775000	1.954044000	0.000825000
C	3.926065000	2.971952000	1.063277000
C	2.995564000	3.909661000	-1.064738000
C	3.501197000	3.867616000	2.229717000
C	3.887524000	3.473844000	-2.230014000
N	1.060464000	-3.967308000	-0.000714000
N	2.912624000	2.898991000	0.000271000
S	0.758259000	1.810934000	-1.229031000
S	1.184745000	-1.557464000	-1.231762000
S	1.807090000	0.755366000	1.232272000
S	-1.561199000	1.190076000	1.231265000
S	-0.252544000	-1.942625000	1.229187000
S	-1.945176000	-0.242655000	-1.232744000
C	0.623577000	-4.881928000	1.064663000
C	-2.674198000	0.719768000	-0.000253000
C	1.615572000	-4.955959000	2.228179000
N	-3.970691000	1.066287000	0.000286000
C	-4.886227000	0.628426000	-1.064004000
C	-4.545365000	1.900861000	1.065995000
C	-4.964955000	1.621337000	-2.226461000
C	-5.105832000	1.077471000	2.228533000
H	-5.871347000	0.491562000	-0.604526000
H	-4.553563000	-0.350203000	-1.418886000
H	-5.300780000	2.608221000	-1.888566000
H	-3.986366000	1.732118000	-2.702166000

H	-5.676114000	1.260830000	-2.978390000
H	-4.311779000	0.492197000	2.700933000
H	-5.890366000	0.390633000	1.891371000
H	-5.540083000	1.743312000	2.982969000
H	-3.769597000	2.584249000	1.420445000
H	-5.332723000	2.510032000	0.608523000
H	-0.356412000	-4.551367000	1.417854000
H	0.490145000	-5.868445000	0.607336000
H	1.254707000	-5.664918000	2.981981000
H	2.602859000	-5.292350000	1.892038000
H	1.725249000	-3.975759000	2.700787000
H	2.579345000	-3.765236000	-1.418899000
H	2.507001000	-5.328106000	-0.606198000
H	0.389194000	-5.888942000	-1.891726000
H	0.491432000	-4.311108000	-2.702621000
H	1.743894000	-5.538912000	-2.980939000
H	4.125949000	1.956390000	1.414122000
H	4.847656000	3.346185000	0.604057000
H	2.597735000	3.474880000	2.704831000
H	3.300982000	4.892056000	1.895980000
H	4.298281000	3.905968000	2.980923000
H	1.982150000	4.119050000	-1.416262000
H	3.378855000	4.828246000	-0.607066000
H	4.909581000	3.264066000	-1.894966000
H	3.934157000	4.269191000	-2.982553000
H	3.485913000	2.573581000	-2.703659000

Optimized xyz coordinates for low-spin $[Co^{III}(SCN)_6]^{3-}$

Co	0.0000	-0.0001	0.0003
S	-1.2443	0.0307	2.0375
S	-1.2430	1.7503	-1.0446
S	1.2458	1.7785	0.9931
S	1.2448	-0.0305	-2.0366
S	1.2440	-1.7502	1.0449
S	-1.2460	-1.7781	-0.9920
C	-2.3094	-1.2661	2.2435
C	2.3084	1.2674	-2.2431
C	-2.3106	-1.3065	-2.2179
C	2.3130	1.3070	2.2167
N	-3.0748	-2.1130	2.5222
N	-3.0760	-1.1234	-3.0906
N	3.0730	2.1150	-2.5219
N	3.0800	1.1236	3.0878
C	-2.3023	2.5827	-0.0229
C	2.3001	-2.5848	0.0217
N	-3.0638	3.2509	0.5724
N	3.0595	-3.2547	-0.5745

Optimized xyz coordinates for low-spin $[Co^{III}Cl_6]^{3-}$

Co	0.0003	0.0001	-0.0004
Cl	-0.0653	-2.2019	-0.9350
Cl	1.8702	-0.6319	1.3553
Cl	0.0657	2.2024	0.9355
Cl	1.4960	0.6930	-1.7347
Cl	-1.4970	-0.6935	1.7358
Cl	-1.8701	0.6318	-1.3562

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