SUPPLEMENTARY MATERIAL

Assessment of a Computational Protocol for Predicting Co-59 NMR Chemical Shift

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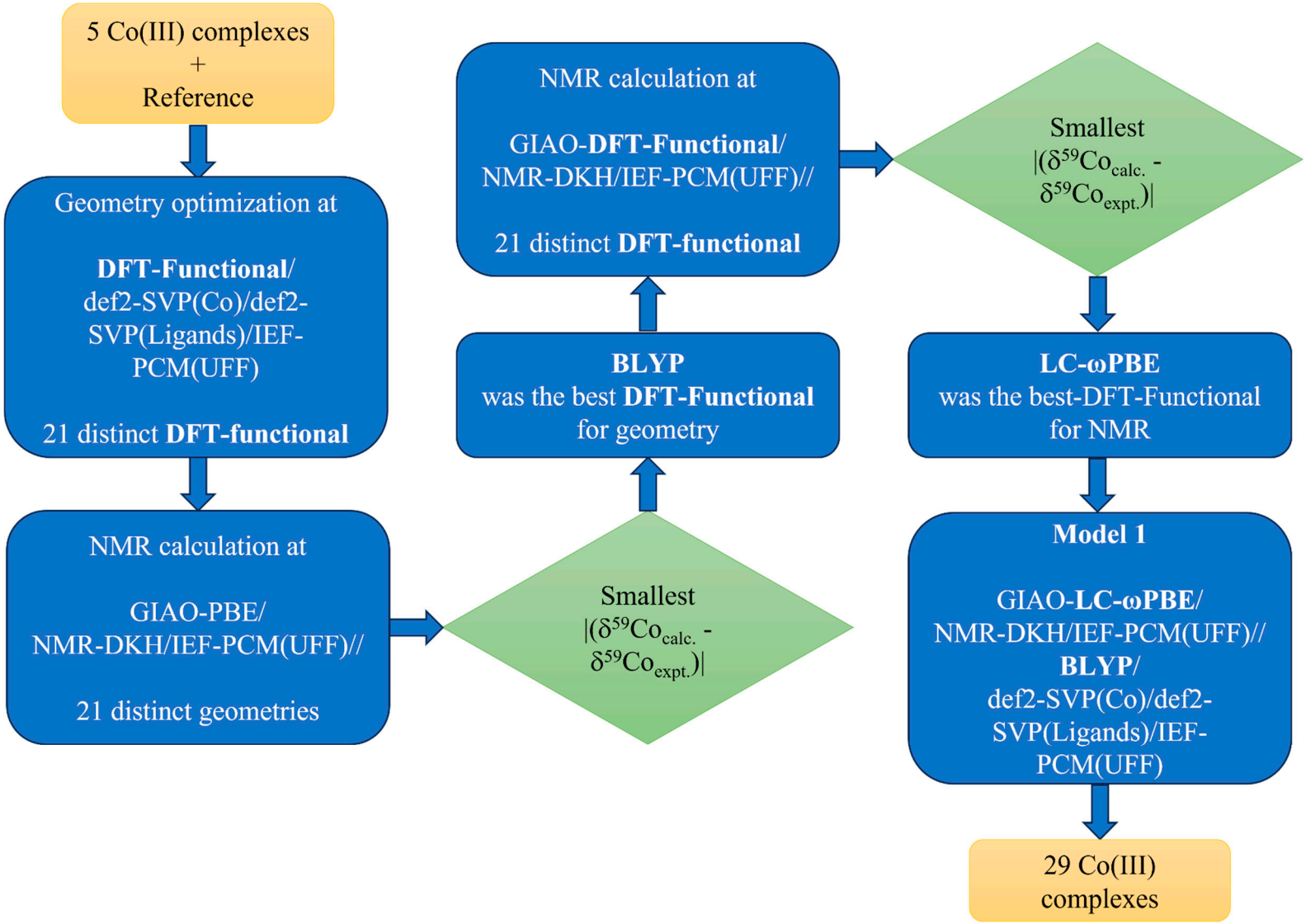

Figure S1. Benchmarking flowchart applied to obtain Model 1.

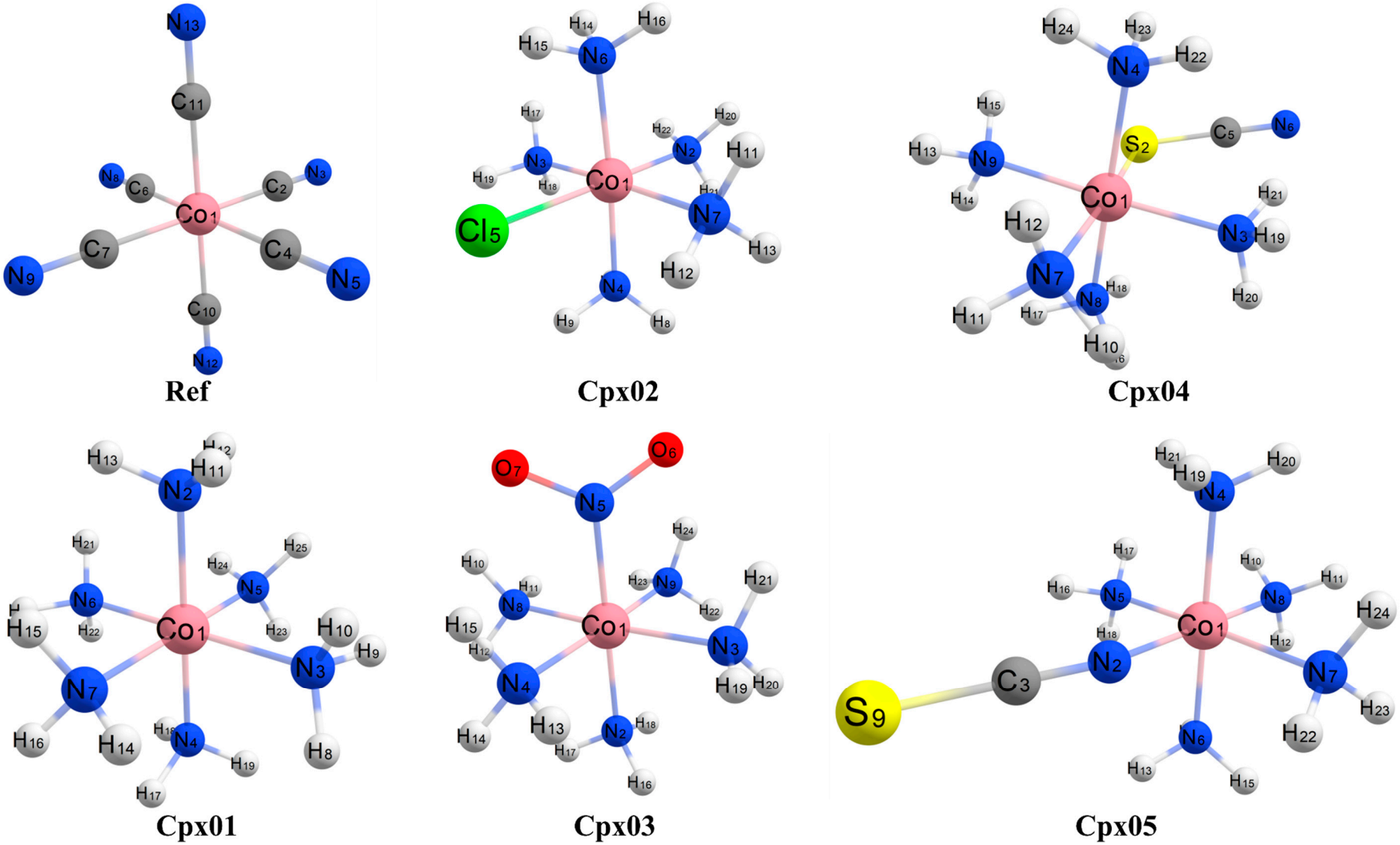

Figure S2. 3D structure (with labels) of Co(III) complexes considered in the initial set of the benchmarking. Ref - $[Co(CN)_6]^{3-}$, Cpx01 - $[Co(NH_3)_6]^{3+}$, Cpx02 - $[Co(NH_3)_5Cl]^{2+}$, Cpx03 - $[Co(NH_3)_5(NO_2)]^{2+}$, Cpx04 - $[Co(NH_3)_5(SCN)]^{2+}$, and Cpx05 - $[Co(NH_3)_5(NCS)]^{2+}$.

Table S1. Calculated bond lengths (Å) and bond angles (º) for Ref – $[Co(CN)_6]^{3-}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-C**	**C2-Co-C6**	**C2-Co-C7**	**Co-C2-N3**	**MRD**
GGA	BP86	1.902	90.0	180.0	180.0	0.35%
	BLYP	1.931	90.0	180.0	179.9	0.72%
	PBE	1.898	90.0	180.0	179.9	0.34%
	PW91	1.898	90.1	180.0	179.9	0.36%
meta-GGA	M06-L	1.923	90.0	180.0	179.9	0.61%
	TPSS	1.909	90.0	180.0	180.0	0.44%
	BB95	1.901	90.0	180.0	180.0	0.34%
Hybrid	B3PW91	1.906	90.0	180.0	179.9	0.39%
	B3LYP	1.928	90.0	180.0	179.8	0.66%
	PBE0	1.913	90.0	180.0	180.0	0.49%
	BHandHLYP	1.949	90.0	180.0	179.8	0.94%
Hybrid meta-GGA	TPSSh	1.910	90.0	180.0	179.8	0.43%
	B1B95	1.906	90.0	180.0	179.9	0.39%
	BMK	1.951	90.0	180.0	179.9	0.98%
	M06	1.912	90.0	180.0	179.9	0.47%
	M06-2X	1.977	89.9	180.0	179.8	1.28%
LR corrected	CAM-B3LYP	1.918	90.0	180.0	180.0	0.56%
	LC-BLYP	1.890	90.0	180.0	180.0	0.45%
	LC-wPBE	1.893	90.0	180.0	179.9	0.40%
	B97D3	1.914	90.0	180.0	180.0	0.51%
	wB97xD	1.921	90.0	180.0	179.9	0.59%
	Experimental	**1.900**	**89.9**	**180.0**	**177.9**	

Experimental X-ray values obtained from [a]Iwata and Saito [56]. MRD = mean relative deviation, eq. (4).

Table S2. Calculated bond lengths (Å) and bond angles (º) for Cpx01 – $[Co(NH_3)_6]^{3+}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-N**	**N3-Co-N7**	**N4-Co-N2**	**Co-N3-H8**	**MRD**
GGA	BP86	1.986	89.9	180.0	113.5	1.54%
	BLYP	2.010	90.1	180.0	114.0	2.02%
	PBE	1.984	90.1	180.0	114.1	1.71%
	PW91	1.982	90.1	180.0	114.1	1.68%
meta-GGA	M06-L	1.998	90.0	180.0	113.8	1.79%
	TPSS	1.987	90.1	180.0	113.9	1.70%
	BB95	1.989	90.1	180.0	114.1	1.77%
Hybrid	B3PW91	1.980	90.1	180.0	114.0	1.64%
	B3LYP	1.993	90.1	180.0	113.9	1.78%
	PBE0	1.972	90.1	180.0	114.0	1.53%
	BHandHLYP	1.984	90.1	180.0	114.0	1.69%
Hybrid meta-GGA	TPSSh	1.982	90.0	180.0	113.5	1.52%
	B1B95	1.976	90.1	180.0	113.3	1.42%
	BMK	1.995	90.0	180.0	114.1	1.82%
	M06	1.974	89.9	180.0	113.5	1.39%
	M06-2X	1.999	89.6	180.0	113.5	1.62%
LR corrected	CAM-B3LYP	1.974	90.0	180.0	113.9	1.51%
	LC-BLYP	1.946	89.9	180.0	113.3	1.37%
	LC-wPBE	1.961	90.0	180.0	113.2	1.18%
	B97D3	1.992	90.0	180.0	113.4	1.62%
	wB97xD	1.984	89.5	180.0	114.2	1.56%
	Experimental	1.961	88.8	180.0	109.5	

Experimental X-ray values obtained from Kruger and Reynhardt [51]. MRD = mean relative deviation, eq. (4).

Table S3. Calculated bond lengths (Å) and bond angles (º) for Cpx02 – $[Co(NH_3)_5Cl]^{2+}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-N**	**Co-Cl**	**N4-Co-Cl**	**N2-Co-Cl**	**N2-Co-N4**	**N2-Co-N6**	**Co-N4-H9**	**MRD**
GGA	BP86	1.984	2.277	88.0	179.6	91.9	92.1	106.5	1.69%
	BLYP	2.000	2.305	87.8	179.6	92.6	91.3	106.8	1.96%
	PBE	1.975	2.273	87.7	179.7	92.5	91.6	106.4	1.67%
	PW91	1.978	2.267	87.7	179.3	92.6	91.8	107.1	1.68%
meta-GGA	M06-L	1.995	2.281	88.3	179.3	91.6	91.6	107.0	1.58%
	TPSS	1.978	2.271	87.9	179.6	91.9	92.0	106.5	1.61%
	BB95	1.982	2.274	88.5	179.6	91.2	92.0	108.2	1.23%
Hybrid	B3PW91	1.972	2.257	89.0	179.4	90.5	91.7	107.0	1.14%
	B3LYP	1.988	2.274	88.8	179.4	91.0	91.6	107.2	1.27%
	PBE0	1.969	2.252	88.9	179.5	91.3	91.0	107.0	1.18%
	BHandHLYP	1.980	2.265	87.9	179.4	91.6	91.7	108.6	1.29%
Hybrid meta-GGA	TPSSh	1.973	2.262	88.6	179.1	92.0	90.9	106.9	1.33%
	B1B95	1.966	2.252	88.1	179.6	92.1	91.4	106.7	1.51%
	BMK	1.991	2.280	88.8	179.4	91.4	91.4	106.9	1.41%
	M06	1.967	2.253	88.8	179.7	91.4	90.7	107.3	1.09%
	M06-2X	1.993	2.275	89.0	179.1	91.9	90.4	106.7	1.39%
LR corrected	CAM-B3LYP	1.970	2.247	88.7	179.6	91.8	91.8	106.3	1.54%
	LC-BLYP	1.940	2.224	88.4	179.5	91.1	92.0	107.8	1.40%
	LC-wPBE	1.956	2.235	88.6	179.4	91.6	91.5	106.7	1.41%
	B97D3	1.979	2.273	88.7	179.2	90.7	92.1	107.3	1.25%
	wB97xD	1.979	2.265	88.2	179.7	92.0	92.3	106.3	1.67%
	Experimental	1.951	2.270	90.3	179.7	89.4	90.6	109.5	

Experimental X-ray values obtained from Messmer and Amma [53]. MRD = mean relative deviation, eq. (4).

Table S4. Calculated bond lengths (Å) and bond angles (º) for Cpx03 – $[Co(NH_3)_5(NO_2)]^{2+}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-N**	**Co-NO2**	**N3-Co-N4**	**N3-Co-N8**	**N3-Co-N5**	**N2-Co-N5**	**Co-N5-O6**	**Co-N3-H21**	**MRD**
GGA	BP86	2.031	1.914	92.2	177.0	88.7	179.3	118.7	107.6	1.27%
	BLYP	2.003	1.946	92.2	177.0	88.7	179.3	118.7	108.0	1.12%
	PBE	1.975	1.912	92.0	177.4	89.0	179.3	118.6	107.7	0.83%
	PW91	1.973	1.910	92.0	177.3	89.0	179.3	118.7	107.6	0.85%
meta-GGA	M06-L	1.992	1.942	92.6	176.8	88.6	179.2	118.4	108.9	1.04%
	TPSS	1.977	1.916	92.1	177.1	88.8	179.2	118.8	107.7	0.86%
	BB95	1.975	1.916	92.1	177.4	89.0	179.2	118.6	107.7	0.82%
Hybrid	B3PW91	1.971	1.934	92.3	176.0	88.2	179.4	118.8	107.9	1.02%
	B3LYP	1.986	1.952	92.4	176.1	88.2	179.3	118.8	108.0	1.20%
	PBE0	1.963	1.930	92.4	176.0	88.1	179.4	118.8	107.9	1.08%
	BHandHLYP	1.973	1.956	92.3	175.6	88.0	179.6	119.0	108.4	1.12%
Hybrid meta-GGA	TPSSh	1.972	1.925	92.1	176.8	88.7	179.2	118.8	107.9	0.82%
	B1B95	1.963	1.931	92.4	176.3	88.5	179.2	118.7	107.9	1.03%
	BMK	1.989	1.973	92.6	175.1	87.8	179.2	119.0	107.9	1.51%
	M06	1.967	1.939	91.9	176.9	88.5	179.2	118.7	108.5	0.88%
	M06-2X	1.992	1.970	92.7	175.1	87.8	179.2	118.8	107.9	1.54%
LR corrected	CAM-B3LYP	1.966	1.934	92.5	175.8	88.1	179.4	119.0	107.7	1.11%
	LC-BLYP	1.936	1.907	92.8	175.8	87.9	179.4	119.0	107.2	1.47%
	LC-wPBE	2.008	2.011	92.3	175.0	87.7	179.1	119.2	108.9	1.72%
	B97D3	1.986	1.930	91.4	177.4	88.7	179.1	118.5	108.6	0.87%
	wB97xD	1.976	1.943	91.7	176.5	88.3	179.0	119.0	108.4	0.95%
	Experimental	1.974	1.924	91.9	179.9	90.0	180.0	120.2	109.5	

Experimental X-ray values obtained from Cotton and Edwards [54]. MRD = mean relative deviation, eq. (4).

Table S5. Calculated bond lengths (Å) and bond angles (º) for Cpx04 – $[Co(NH_3)_5(SCN)]^{2+}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-N**	**Co-SCN**	**N3-Co-N4**	**N4-Co-N8**	**N4-Co-S**	**N7-Co-S**	**Co-S-C**	**MRD**
GGA	BP86	2.009	2.338	89.5	178.3	90.0	175.2	104.7	1.50%
	BLYP	2.007	2.382	89.6	178.8	90.5	175.4	105.2	1.71%
	PBE	1.980	2.328	90.5	177.7	89.6	175.9	103.0	1.35%
	PW91	1.980	2.325	89.8	177.0	89.5	175.7	102.0	1.67%
meta-GGA	M06-L	1.998	2.360	88.9	177.5	90.2	175.7	99.9	2.30%
	TPSS	1.983	2.382	90.4	177.6	90.0	175.7	103.6	1.61%
	BB95	1.984	2.333	88.4	177.1	90.8	175.0	101.4	1.89%
Hybrid	B3PW91	1.975	2.335	90.4	178.4	90.6	175.7	104.0	1.06%
	B3LYP	1.990	2.362	89.6	179.4	90.9	175.2	104.0	1.54%
	PBE0	1.968	2.328	90.2	178.5	90.7	175.8	103.2	1.09%
	BHandHLYP	1.981	2.354	90.1	178.3	90.6	175.8	102.7	1.43%
Hybrid meta-GGA	TPSSh	1.977	2.334	90.4	178.3	90.5	175.8	103.8	1.09%
	B1B95	1.971	2.324	88.9	177.1	90.1	175.5	100.5	1.85%
	BMK	1.996	2.364	89.0	176.9	90.1	175.5	100.7	2.26%
	M06	1.972	2.333	89.5	177.1	89.7	175.4	100.6	1.88%
	M06-2X	2.000	2.374	88.9	177.1	90.0	175.7	99.1	2.57%
LR corrected	CAM-B3LYP	1.974	2.324	89.7	177.3	89.7	175.6	101.7	1.62%
	LC-BLYP	1.946	2.284	89.0	177.9	90.8	175.4	101.0	1.17%
	LC-wPBE	1.961	2.287	89.4	177.6	90.4	175.6	101.9	1.18%
	B97D3	1.991	2.355	89.0	177.3	90.3	175.3	101.3	2.04%
	wB97xD	1.985	2.332	89.2	177.5	90.5	175.2	101.1	1.81%
	Experimental	1.932	2.272	90.6	178.3	91.6	176.0	104.9	

Experimental X-ray values obtained from Snow and Boomsma [55]. MRD = mean relative deviation, eq. (4).

Table S6. Calculated bond lengths (Å) and bond angles (º) for Cpx05 – $[Co(NH_3)_5(NCS)]^{2+}$ at **DFT-Functional**/def2-SVP/def2-SVP/IEF-PCM(UFF) level. The mean relative deviation (MRD) in relation to the experimental X-ray values considering all structural parameters evaluated is also presented.

	DFT-Functional	**Co-N**	**Co-NCS**	**N4-Co-N7**	**N4-Co-N6**	**N4-Co-NCS**	**N8-Co-NCS**	**Co-N2-C**	**MRD**
GGA	BP86	1.985	1.889	90.0	177.3	88.8	179.4	159.4	2.79%
	BLYP	2.004	1.917	89.4	178.1	89.4	179.6	158.5	2.72%
	PBE	1.978	1.889	89.9	177.4	88.7	179.0	157.7	2.93%
	PW91	1.973	1.889	90.0	177.4	88.9	179.3	155.3	3.01%
meta-GGA	M06-L	1.990	1.912	89.8	177.7	89.0	179.8	152.8	3.12%
	TPSS	1.976	1.891	89.9	177.1	89.0	179.8	161.7	2.49%
	BB95	1.978	1.894	90.5	177.2	89.4	179.1	158.0	2.83%
Hybrid	B3PW91	1.974	1.888	90.0	177.4	88.7	179.5	178.7	1.18%
	B3LYP	1.986	1.902	89.7	177.6	88.9	179.4	176.9	1.32%
	PBE0	1.964	1.887	90.0	177.7	88.5	179.4	177.9	1.20%
	BHandHLYP	1.975	1.908	90.2	177.7	88.9	179.1	179.8	0.97%
Hybrid meta-GGA	TPSSh	1.972	1.885	90.0	177.4	88.8	179.6	176.3	1.36%
	B1B95	1.964	1.889	89.8	177.3	88.6	179.4	177.7	1.25%
	BMK	1.992	1.914	90.2	177.9	89.9	179.0	172.5	1.46%
	M06	1.965	1.889	90.7	177.7	89.6	179.4	167.5	1.95%
	M06-2X	1.991	1.923	90.1	177.5	88.6	179.4	179.3	1.04%
LR corrected	CAM-B3LYP	1.967	1.894	90.3	177.4	88.6	179.4	178.3	1.19%
	LC-BLYP	1.939	1.873	90.3	177.4	88.9	179.5	178.8	1.07%
	LC-wPBE	1.954	1.883	90.1	177.4	88.6	179.2	179.2	1.09%
	B97D3	1.988	1.904	89.8	178.1	88.2	178.1	148.0	3.77%
	wB97xD	1.973	1.895	90.1	177.9	89.2	179.0	178.8	1.05%
	Experimental	1.941	1.941	90.0	180.0	90.0	180.0	180.0	

Experimental X-ray values obtained from Snow and Boomsma [55]. MRD = mean relative deviation, eq. (4).

NMR-DKH basis set for the Co atom (GAUSSIAN PROGRAM FORMAT)

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Model 1: Optimized structures at BLYP/def2-SVP/def2-SVP/IEF-PCM(UFF) level

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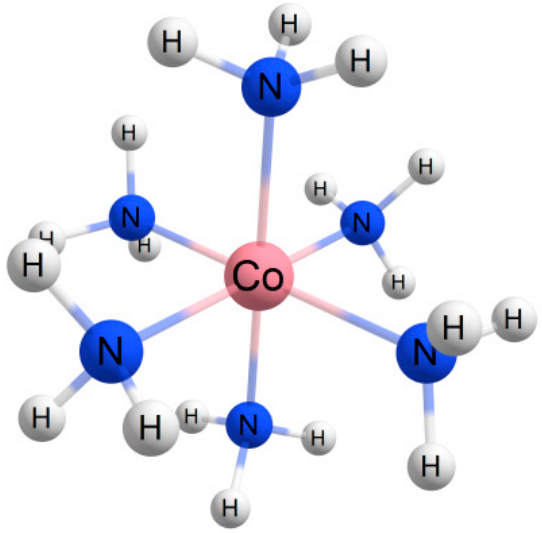

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N	0.142158	0.030008	-2.004169
N	-1.436080	1.404098	-0.102069
N	-1.396605	-1.441557	-0.114420
N	1.436080	-1.404098	0.102069
H	2.116671	1.388762	-0.625234
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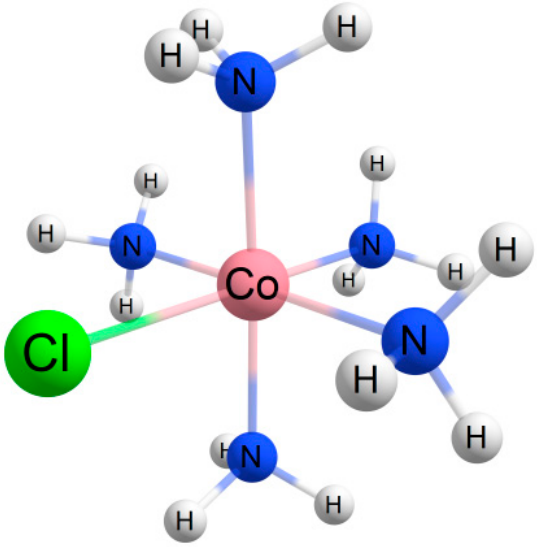
H	0.736364	0.217532	2.489311
H	-0.844128	0.630915	2.376419
H	-0.412151	-0.949000	2.392904
H	2.392599	-1.017185	0.037055
H	1.424208	-1.935845	0.988102
H	1.389762	-2.122911	-0.639978
H	0.844128	-0.630915	-2.376419
H	-0.736364	-0.217532	-2.489311
H	0.412151	0.949000	-2.392904
H	-1.005914	-2.395775	-0.036598
H	-2.116671	-1.388762	0.625234
H	-1.925723	-1.444932	-1.002649
H	-1.424208	1.935845	-0.988102
H	-2.392599	1.017185	-0.037055
H	-1.389762	2.122911	0.639978

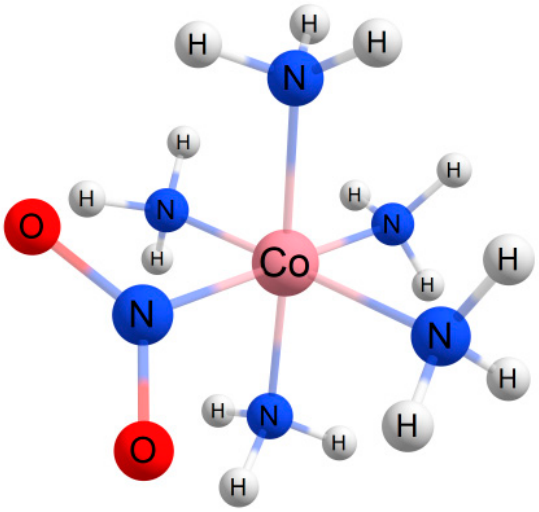
Cpx02: $[Co(NH_3)_5Cl]^{2+}$



22

Co	0.225589	0.001049	-0.002071
N	2.237893	0.016642	-0.016040
N	0.136750	1.816863	0.832429
N	0.114990	0.858054	-1.808381
Cl	-2.079218	-0.031554	0.024121
N	0.197951	-0.833401	1.813842
N	0.177050	-1.808986	-0.858002
H	0.364403	0.244547	-2.600136
H	-0.874679	1.119503	-1.954298
H	0.674474	1.717301	-1.936008
H	0.335897	-2.595579	-0.208128
H	-0.776654	-1.948425	-1.231767
H	0.837741	-1.962836	-1.637503
H	0.665388	-0.294030	2.559849
H	-0.796910	-0.911903	2.085015
H	0.594063	-1.784603	1.878102
H	0.479569	1.878008	1.804859
H	0.622402	2.571817	0.321238
H	-0.864877	2.073577	0.863822
H	2.653627	-0.860108	0.338276
H	2.646252	0.152447	-0.954869
H	2.642656	0.764161	0.570470

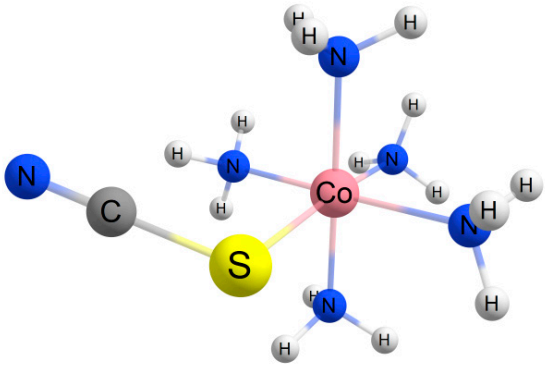
Cpx03: $[Co(NH_3)_5(NO_2)]^{2+}$



24

Co	-0.346508	0.000149	-0.002612
N	-2.403053	0.008276	0.003527
N	-0.308061	-1.409778	1.419930
N	-0.322651	1.475481	1.352727
N	1.599580	0.003428	0.012521
O	2.198946	-1.087371	0.011158
O	2.193427	1.097293	0.021225
N	-0.283598	1.391334	-1.442213
N	-0.299237	-1.473413	-1.360925
H	0.617552	1.895149	-1.364157
H	-0.322283	1.022087	-2.405763
H	-1.025456	2.107644	-1.398641
H	-0.388445	1.165740	2.335418
H	-1.067215	2.182656	1.243336
H	0.580356	1.975561	1.267957
H	-2.804382	-0.162451	0.939865
H	-2.823476	0.897722	-0.309836
H	-2.820467	-0.710316	-0.609557
H	-0.315315	-1.059526	2.391480
H	-1.079114	-2.095392	1.370705
H	0.573281	-1.943494	1.316662
H	-0.925295	-2.268985	-1.157069
H	-0.523656	-1.193466	-2.329111
H	0.659775	-1.863636	-1.378798

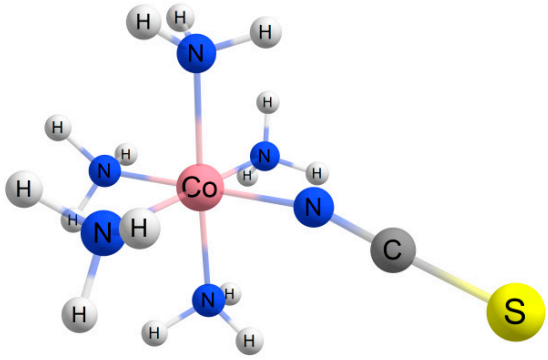
Cpx04: $[Co(NH_3)_5(SCN)]^{2+}$



24

Co	-0.590081	0.053986	-0.001070
S	1.443860	-1.183705	0.084850
N	0.289866	1.790465	0.469287
N	-0.291337	0.445322	-1.946555
C	2.668593	-0.026303	0.007598
N	3.520112	0.795891	-0.041633
N	-2.406465	0.972513	-0.036020
N	-0.849175	-0.351807	1.947229
N	-1.431666	-1.696918	-0.535228
H	-2.444351	1.849173	0.509144
H	-3.167766	0.388705	0.348016
H	-2.713771	1.235955	-0.986751
H	-2.335218	-1.598341	-1.027967
H	-1.628255	-2.332736	0.255062
H	-0.830282	-2.243747	-1.174088
H	-1.169657	0.449019	2.516287
H	-1.529434	-1.103785	2.145171
H	0.042268	-0.667144	2.365391
H	-0.132577	2.609669	0.002127
H	0.264991	2.013255	1.477862
H	1.295481	1.810975	0.218666
H	-0.132465	1.442391	-2.166062
H	0.545843	-0.053049	-2.292150
H	-1.065283	0.150885	-2.564575

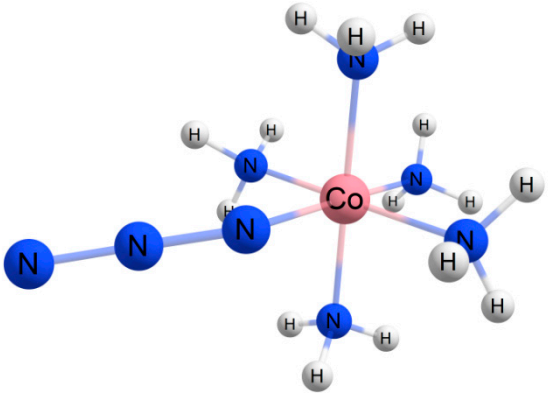
Cpx05: $[Co(NH_3)_5(NCS)]^{2+}$



24

Co	0.82252	0.00181	0.00391
N	-1.05366	-0.10998	-0.37284
C	-2.23976	-0.04853	-0.18138
N	0.86106	-1.98046	0.29797
N	0.39037	0.30944	1.93083
N	0.74431	1.97557	-0.34063
N	1.15721	-0.30302	-1.95659
N	2.78968	0.10418	0.39589
S	-3.85135	-0.00683	0.01261
H	3.04317	-0.19760	1.35115
H	3.36953	-0.47511	-0.23219
H	3.17061	1.05941	0.30592
H	-0.23980	2.28235	-0.28411
H	1.27658	2.57450	0.31158
H	1.06493	2.24550	-1.28432
H	-0.59329	0.04851	2.10683
H	0.96049	-0.22739	2.60430
H	0.47545	1.29571	2.22406
H	0.04949	-2.40331	-0.18006
H	1.70272	-2.46040	-0.05912
H	0.78280	-2.26636	1.28734
H	0.29288	-0.05279	-2.46426
H	1.92517	0.24428	-2.37779
H	1.34867	-1.28588	-2.21068

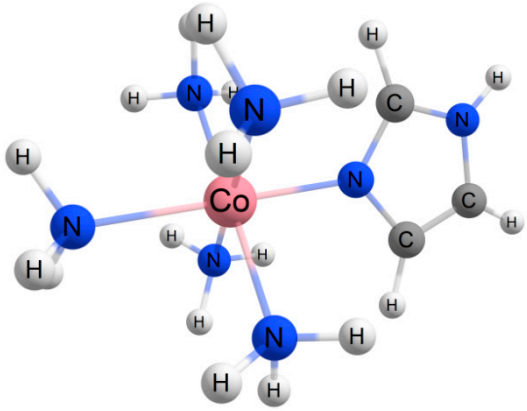
Cpx06: $[Co(NH_3)_5(N_3)]^{2+}$



24

Co	-0.42014	-0.01221	-0.00147
N	0.36872	-1.79500	-0.47720
N	-0.60285	-0.59632	1.90940
N	-0.17515	0.68368	-1.86612
N	-1.15294	1.78430	0.52817
N	-2.27940	-0.68739	-0.48739
N	1.32340	0.73870	0.51157
N	2.40767	0.28820	0.17503
N	3.48776	-0.07139	-0.09332
H	-1.89307	1.76937	1.24945
H	-1.53048	2.36025	-0.24183
H	-1.04157	1.02242	-2.31581
H	0.23264	0.01500	-2.53951
H	-2.97938	0.06504	-0.58819
H	-2.68973	-1.34045	0.19956
H	-1.56492	-0.67868	2.27727
H	-0.11224	0.08844	2.50748
H	-0.28035	-2.59004	-0.34805
H	1.19772	-2.02274	0.09594
H	0.69453	-1.87527	-1.45422
H	-0.14851	-1.50171	2.11014
H	-2.29923	-1.19596	-1.38603
H	0.47680	1.48463	-1.84945
H	-0.35877	2.31599	0.92195

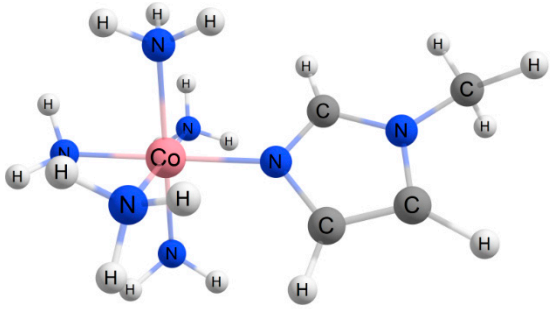
Cpx07: $[Co(NH_3)_5(HIm)]^{3+}$ – HIm = imidazole



30

Co	0.835421	-0.001024	0.000377
N	2.853050	-0.014785	-0.012086
N	0.843055	1.586256	1.232479
N	0.831427	-1.572484	-1.251780
N	-1.148477	0.007982	0.009778
C	-1.955966	-1.072902	0.038801
C	-1.982476	1.129689	-0.027781
C	-3.297261	0.704936	-0.019764
N	-3.250100	-0.674949	0.022710
H	-1.658070	-2.124142	0.069783
H	-1.614470	2.158037	-0.056859
H	-4.236427	1.262913	-0.039859
H	-4.055983	-1.308077	0.039382
H	1.682083	1.653902	1.832135
H	0.040464	1.572686	1.883451
H	3.284897	0.240981	0.891378
H	3.266484	0.640806	-0.696690
H	1.658547	-1.607567	-1.871141
H	0.016845	-1.555472	-1.887422
N	0.854852	-1.176201	1.630598
H	1.423390	-0.791361	2.402759
H	1.222026	-2.131807	1.486405
N	0.820937	1.187492	-1.617054
H	1.239655	2.121284	-1.472689
H	-0.140354	1.360770	-1.956196
H	-0.090552	-1.297824	2.031100
H	3.258296	-0.937692	-0.242600
H	1.324269	0.796145	-2.430270
H	0.807959	-2.501911	-0.800374
H	0.795578	2.502449	0.757494

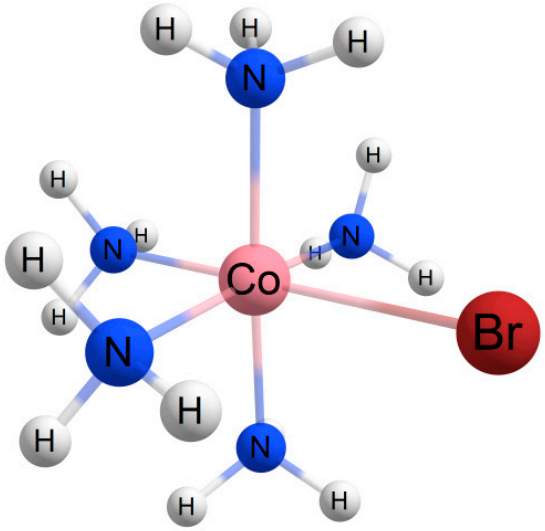
Cpx08: $[Co(NH_3)_5(MeIm)]^{3+}$ – MeIm = methylimidazole



33

H	2.112330	1.917525	-1.428908
H	0.480566	1.816925	-1.644940
N	1.332657	1.245066	-1.523204
H	1.685203	2.330614	0.920456
H	-3.685555	1.932481	-0.018817
C	-2.840412	1.239225	-0.011989
H	1.475429	0.797698	-2.443401
H	-0.967717	2.436344	-0.007710
C	-1.478644	1.470099	-0.008568
N	-3.009577	-0.135634	-0.002133
N	1.373706	1.434596	1.330666
H	2.063555	1.232124	2.072944
C	-4.299532	-0.848791	-0.001986
N	-0.817271	0.241153	0.000784
C	-1.778641	-0.708504	0.005119
Co	1.143917	-0.054366	0.000994
H	0.493553	1.647436	1.829106
H	3.551964	-0.369918	-0.963048
H	-1.634743	-1.792153	0.015305
H	3.677409	0.335284	0.509099
N	3.135648	-0.370292	-0.016946
H	0.078054	-1.446306	-1.895578
N	0.939839	-1.540508	-1.332833
H	1.712345	-1.590707	-2.017772
N	0.947198	-1.320981	1.551968
H	3.410751	-1.279429	0.391290
H	0.018519	-1.227720	1.996200
H	0.903973	-2.487563	-0.921169
H	1.627012	-1.164696	2.314849
H	1.040435	-2.323516	1.316384
H	-4.861457	-0.599022	-0.920764
H	-4.887549	-0.548215	0.884467
H	-4.111844	-1.935289	0.031603

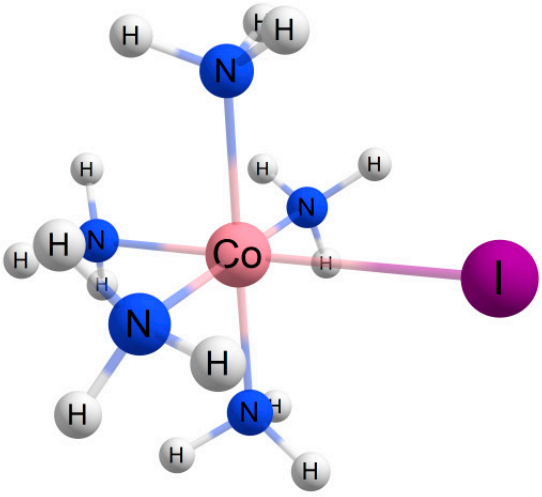
Cpx09: $[CoBr(NH_3)_6]^{2+}$



22

Co	0.600800	-0.000133	0.004603
N	0.521146	-1.800935	0.885431
N	2.622719	0.009738	0.001994
N	0.560929	1.784333	-0.908426
N	0.559433	0.885538	1.801830
N	0.564625	-0.914644	-1.773706
H	3.027490	0.191207	-0.930651
H	3.031299	0.730731	0.618281
H	3.045583	-0.880625	0.311378
H	1.300226	-2.447257	0.676318
H	0.468207	-1.760341	1.916071
H	-0.345795	-2.280368	0.592433
H	1.027224	-1.837636	-1.789846
H	-0.420302	-1.076042	-2.043392
H	0.989362	-0.383652	-2.551107
H	1.068474	1.842576	-1.806331
H	-0.426501	2.008669	-1.117910
H	0.918665	2.574183	-0.347211
H	0.866109	1.871954	1.819003
H	-0.417097	0.892351	2.141388
H	1.121080	0.414918	2.530472
Br	-1.865074	0.011278	-0.005516

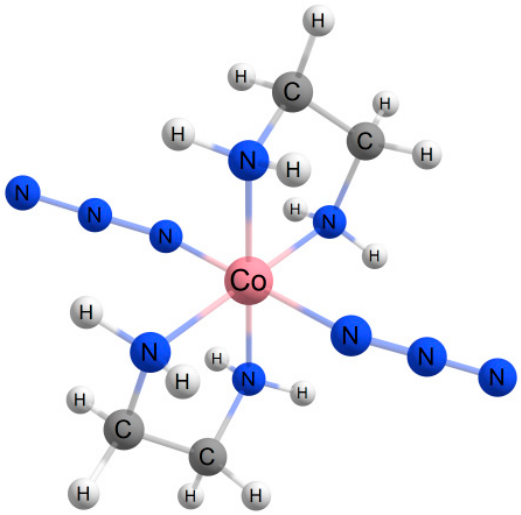
Cpx10: $[Co(NH_3)_5I]^{2+}$



22

Co	0.943971	-0.000072	-0.004005
N	0.918882	-1.220436	1.587089
N	2.977483	-0.027237	-0.027767
N	0.911345	1.268132	-1.556892
N	0.931119	1.577577	1.237773
N	0.898787	-1.592564	-1.228781
H	3.380164	0.111889	-0.969157
H	3.404164	0.708698	0.558689
H	3.384895	-0.913234	0.312716
H	1.716521	-1.097699	2.233253
H	0.064197	-1.077357	2.149909
H	0.916675	-2.224738	1.346003
H	1.732326	-2.201918	-1.176324
H	0.083851	-2.195867	-1.030055
H	0.807027	-1.351518	-2.228827
H	1.005750	0.814175	-2.479850
H	0.008139	1.768813	-1.594577
H	1.645458	1.995793	-1.540068
H	1.425131	2.413399	0.884965
H	-0.042681	1.878143	1.412556
H	1.338824	1.395079	2.169675
I	-1.751339	-0.001132	-0.000391

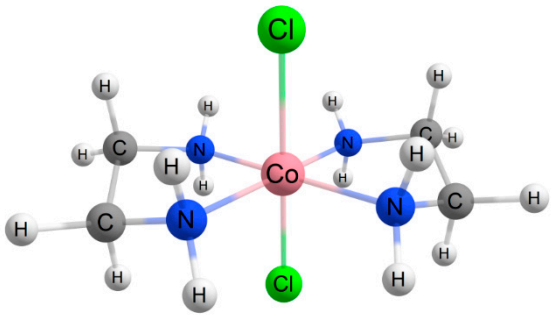
Cpx11: *trans*-$[Co(en)_2(N_3)_2]^+$ – en = ethylenediamine



31

Co	0.000012	-0.000053	-0.000027
N	1.091041	1.148262	-1.229455
H	1.880468	0.674273	-1.694849
H	0.437080	1.434936	-1.975776
N	0.037506	1.575783	1.236890
H	-0.845581	1.768860	1.733388
H	0.733681	1.333358	1.961052
N	-1.091146	-1.148389	1.229304
H	-0.437265	-1.435246	1.975629
H	-1.880566	-0.674355	1.694678
N	-0.037523	-1.575922	-1.237003
H	-0.733764	-1.333414	-1.961077
H	0.845477	-1.769066	-1.733628
C	1.584668	2.352147	-0.483376
H	1.860903	3.169069	-1.178807
H	2.493992	2.057890	0.074200
C	0.477967	2.788690	0.475201
H	0.828548	3.587506	1.158474
H	-0.395483	3.171344	-0.085425
C	-1.584855	-2.352151	0.483109
H	-2.494037	-2.057704	-0.074592
H	-1.861342	-3.169057	1.178453
C	-0.478053	-2.788777	-0.475311
H	0.395319	-3.171394	0.085469
H	-0.828539	-3.587662	-1.158556
N	1.600257	-0.688498	0.960388
N	-1.600366	0.688200	-0.960434
N	2.670945	-0.898652	0.416527
N	-2.670690	0.899218	-0.416187
N	3.726050	-1.117768	-0.043958
N	-3.725728	1.118144	0.044549

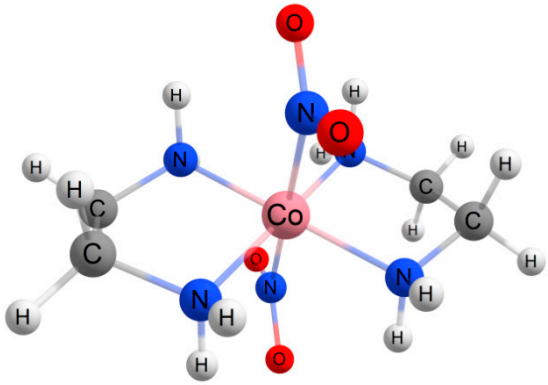
Cpx12: *trans*-$[Co(en)_2Cl_2]^+$ – en = ethylenediamine



27

Co	0.000000	-0.000029	-0.000020
N	-1.465704	0.085932	-1.354248
H	-1.293715	0.785458	-2.091540
H	-1.503924	-0.841263	-1.808642
N	-1.465976	-0.081443	1.354324
H	-1.294771	-0.777476	2.095092
H	-1.504387	0.847742	1.804708
N	1.465713	-0.086652	1.354202
H	1.503601	0.839717	1.810286
H	1.293832	-0.787627	2.090159
N	1.465970	0.081486	-1.354420
H	1.504904	-0.847974	-1.804207
H	1.294570	0.776945	-2.095682
C	-2.760549	0.385327	-0.660138
H	-3.628532	0.109172	-1.291076
H	-2.790558	1.475802	-0.477311
C	-2.760172	-0.383283	0.660261
H	-3.628766	-0.108332	1.290905
H	-2.788252	-1.473832	0.477628
C	2.760829	-0.384626	0.659890
H	2.791764	-1.475022	0.476710
H	3.628579	-0.107980	1.290925
C	2.759860	0.384330	-0.660292
H	2.786934	1.474858	-0.477400
H	3.628737	0.110282	-1.290951
Cl	-0.002530	-2.300695	-0.167292
Cl	0.002538	2.300375	0.167505

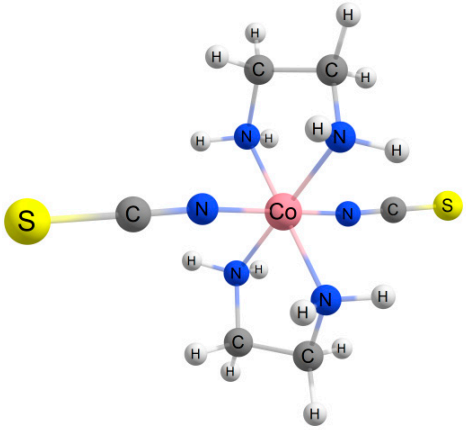
Cpx13: *trans*-$[Co(en)_2(NO_2)_2]^+$ – en = ethylenediamine



31

Co	0.000125	0.000081	0.000042
N	-1.458457	0.106743	-1.351463
H	-1.258215	0.857557	-2.031498
H	-1.471569	-0.787394	-1.871903
N	-1.458430	-0.107980	1.351441
H	-1.257591	-0.859042	2.031024
H	-1.472154	0.785881	1.872326
N	1.458552	-0.107183	1.351563
H	1.472997	0.785514	1.874296
H	1.257539	-0.859553	2.029720
N	1.458451	0.108683	-1.351467
H	1.472781	-0.783403	-1.875247
H	1.257091	0.861923	-2.028566
C	-2.767114	0.375878	-0.665366
H	-3.622095	0.072704	-1.300840
H	-2.838618	1.467334	-0.499131
C	-2.766940	-0.377729	0.665282
H	-3.622077	-0.075001	1.300754
H	-2.837891	-1.469217	0.499041
C	2.767199	-0.376477	0.665281
H	2.838264	-1.467934	0.498983
H	3.622225	-0.073652	1.300841
C	2.767284	0.377356	-0.665231
H	2.838849	1.468779	-0.498884
H	3.622122	0.074183	-1.300867
N	-0.000834	1.962006	0.124204
N	0.000669	-1.961857	-0.124236
O	0.004207	2.640917	-0.924967
O	-0.006587	2.494751	1.256883
O	-0.004600	-2.494556	-1.256935
O	0.006072	-2.640853	0.924858

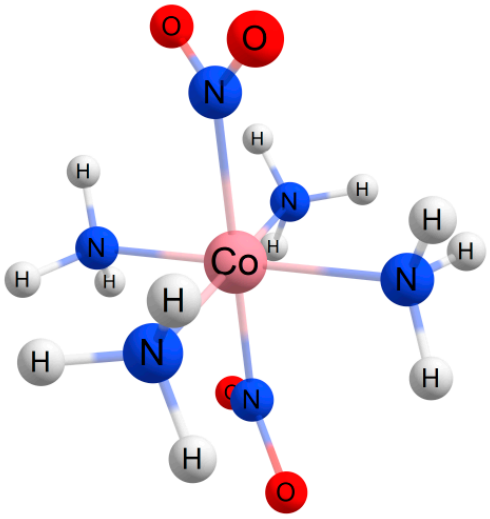
Cpx14: *trans*-$[Co(en)_2(NCS)_2]^+$ – en = ethylenediamine



31

Co	-0.000152	0.000713	-0.000315
N	-0.364334	-1.445178	-1.342955
H	-1.113627	-1.206184	-2.009383
H	0.501279	-1.562657	-1.893201
N	0.085487	-1.491495	1.338172
H	0.867521	-1.389735	2.002045
H	-0.784675	-1.458504	1.892466
N	0.364221	1.446696	1.342356
H	-0.501733	1.564998	1.891887
H	1.112869	1.207232	2.009341
N	-0.085849	1.493136	-1.338975
H	0.783892	1.459472	-1.893881
H	-0.868495	1.392064	-2.002234
C	-0.701239	-2.716846	-0.622909
H	-0.560009	-3.594758	-1.283614
H	-1.767919	-2.671172	-0.334047
C	0.196467	-2.797841	0.609302
H	-0.089915	-3.643621	1.264972
H	1.254634	-2.928293	0.315483
C	0.702480	2.717807	0.622059
H	1.769056	2.670909	0.333062
H	0.562275	3.596014	1.282599
C	-0.195363	2.799541	-0.609986
H	-1.253351	2.930930	-0.315866
H	0.091572	3.645106	-1.265691
N	-1.873929	0.187810	0.325853
N	1.873635	-0.186019	-0.326391
C	-3.065829	0.151898	0.180178
C	3.065492	-0.153001	-0.179590
S	-4.685895	0.125488	0.042538
S	4.685524	-0.130179	-0.040423

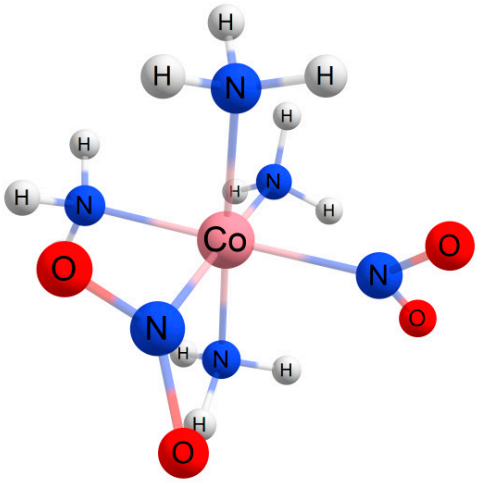
Cpx15: *trans*-$[Co(NH_3)_4(NO_2)]^+$



23

Co	0.000012	0.000008	-0.000015
N	-1.971805	0.000016	0.000047
N	0.000495	-1.437402	1.375155
N	-0.000306	1.437870	1.374701
N	1.971786	-0.000004	-0.000077
O	2.579823	-1.089650	-0.068427
O	2.579772	1.089715	0.068311
N	0.000273	1.437449	-1.375158
N	-0.000496	-1.437976	-1.374632
H	0.805654	2.069102	-1.230140
H	0.052904	1.127208	-2.357746
H	-0.873309	1.984500	-1.284100
H	-0.053840	1.127712	2.357261
H	-0.805084	2.070140	1.229127
H	0.873804	1.984172	1.284141
H	0.052261	-1.127064	2.357754
H	-0.872631	-1.985106	1.283644
H	0.806403	-2.068477	1.230577
H	-0.807064	-2.068322	-1.230526
H	-0.051093	-1.127912	-2.357379
H	0.872115	-1.986342	-1.282226
O	-2.579814	1.089684	-0.068281
O	-2.579790	-1.089686	0.068369

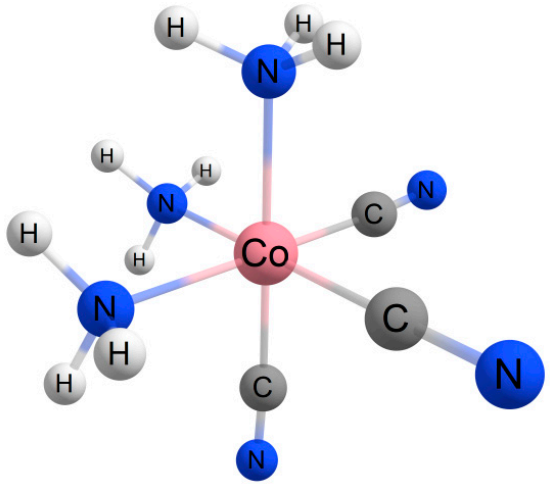
Cpx16: *cis*-$[Co(NH_3)_4(NO_2)_2]^+$



23

Co	0.000065	0.422331	-0.000040
N	1.461304	1.837893	0.230986
N	0.387136	0.364337	-1.956500
N	-1.460898	1.838169	-0.231218
N	-1.369007	-0.943479	-0.255334
O	-1.231871	-1.795226	-1.150363
O	-2.379590	-0.917587	0.481396
N	-0.386981	0.364871	1.956452
N	1.368778	-0.943763	0.255454
H	-1.376226	0.076321	2.054799
H	0.184320	-0.391650	2.370981
H	-0.244670	1.221326	2.512923
H	-1.595931	2.166866	-1.199890
H	-1.330683	2.689602	0.336785
H	-2.364394	1.430005	0.060615
H	1.330667	2.689651	-0.336433
H	1.597097	2.166052	1.199739
H	2.364594	1.429894	-0.061717
H	0.244933	1.220591	-2.513319
H	1.376336	0.075610	-2.054797
H	-0.184306	-0.392264	-2.370716
O	1.231169	-1.795547	1.150368
O	2.379565	-0.918035	-0.480996

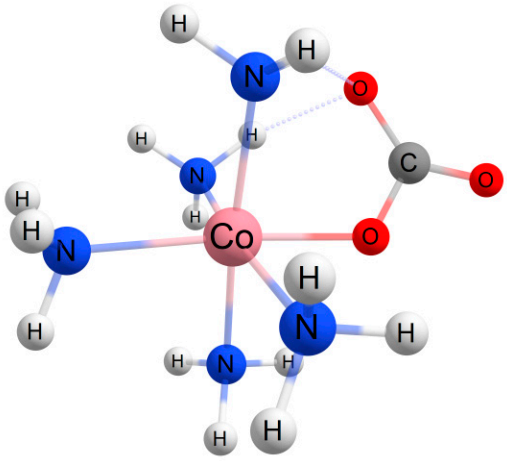
Cpx17: *fac*-$[Co(CN)_3(NH_3)_3]$



19

Co	0.001679	-0.000312	-0.180775
N	1.142874	1.244038	-1.362404
N	0.543328	-1.599770	-1.361637
N	-1.624936	0.328238	-1.401379
H	2.146163	1.015058	-1.296223
H	0.912192	1.244367	-2.368118
H	1.053083	2.221708	-1.047570
H	1.488255	-1.932152	-1.117455
H	-0.086469	-2.402511	-1.212957
H	0.552341	-1.421502	-2.377699
H	-1.418228	0.388066	-2.410503
H	-2.334536	-0.412568	-1.296137
H	-2.096445	1.210743	-1.152301
C	-1.037164	-1.141942	0.891629
C	1.494379	-0.307267	0.919948
C	-0.496935	1.466537	0.882738
N	2.470923	-0.511291	1.551399
N	-1.712741	-1.886645	1.510579
N	-0.822786	2.424464	1.491157

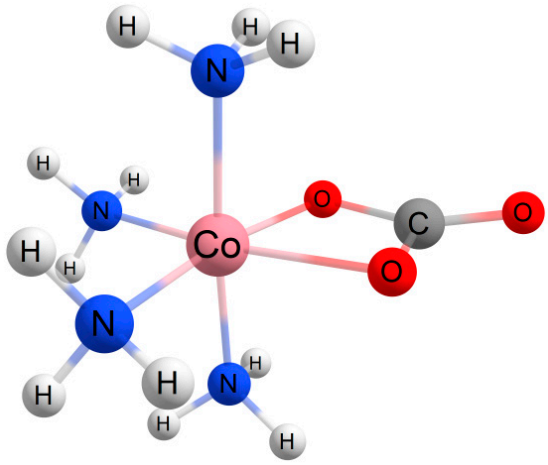
Cpx18: $[Co(NH_3)_5(CO_3)]^+$



25

Co	0.672029	0.012133	-0.003319
N	2.597559	-0.673012	0.007218
N	1.084134	1.356154	1.428511
N	0.077975	-1.315037	1.350254
N	0.063047	-1.280271	-1.385554
N	1.065558	1.379153	-1.419656
H	-0.934193	-1.453339	-1.063862
H	0.029758	-0.917192	-2.349674
H	0.560879	-2.182119	-1.433819
H	0.050649	-0.976245	2.323311
H	0.590994	-2.209429	1.368444
H	-0.920185	-1.488483	1.033977
H	2.986021	-0.757528	0.959812
H	2.722236	-1.603675	-0.421516
H	3.251436	-0.055415	-0.498935
H	1.302589	0.971225	2.361066
H	1.834519	2.036980	1.231062
H	0.201885	1.887488	1.521568
H	1.695610	2.155760	-1.163420
H	1.424397	1.016259	-2.316843
H	0.138041	1.798672	-1.601744
O	-1.092610	0.812888	0.006310
C	-2.296496	0.149668	0.009666
O	-3.315393	0.873820	0.026451
O	-2.281789	-1.151392	-0.005664

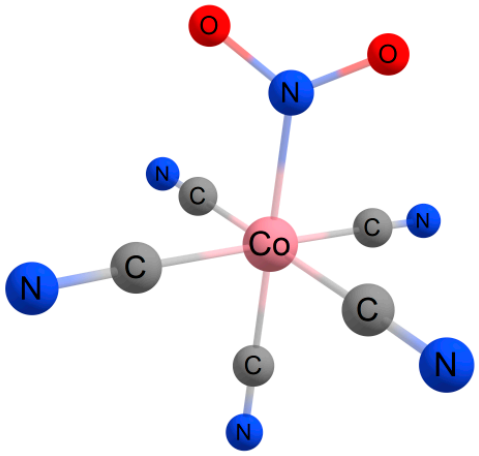
Cpx19: *cis*-$[Co(NH_3)_4(CO_3)]^+$



21

Co	-0.432368	0.000020	-0.000032
N	-1.779057	0.019592	-1.505438
N	-0.359055	-1.986440	-0.019417
N	-1.779075	-0.019671	1.505420
O	1.157140	-0.011337	1.093048
N	-0.359164	1.986423	0.019453
O	1.157157	0.011439	-1.093047
H	0.174815	2.288933	0.849663
H	0.179258	2.304970	-0.801754
H	-1.245959	2.514221	0.021786
H	-2.471300	-0.784638	1.475909
H	-2.334062	0.844491	1.605651
H	-1.269412	-0.130729	2.396845
H	-2.333823	-0.844734	-1.605440
H	-2.471498	0.784354	-1.475811
H	-1.269590	0.130681	-2.396966
H	-1.245766	-2.514384	-0.021637
H	0.175005	-2.289116	-0.849514
H	0.179376	-2.304731	0.801888
C	1.941394	0.000023	0.000001
O	3.172327	-0.000018	0.000011

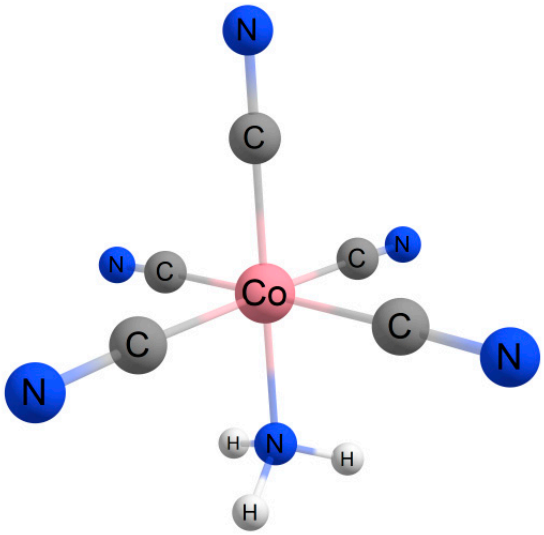
Cpx20: $[Co(CN)_5(NO_2)]^{3-}$



14

Co	0.193982	-0.000020	0.000002
C	0.199291	-1.321716	-1.407474
N	0.222367	-2.126084	-2.273643
C	2.115448	-0.000119	0.000015
C	0.199456	1.321781	1.407397
N	3.298047	-0.000224	0.000107
N	0.222568	2.126320	2.273406
C	0.207737	1.398530	-1.331172
C	0.207661	-1.398557	1.331169
N	0.240663	2.247795	-2.153039
N	0.240449	-2.247830	2.153034
N	-1.838587	0.000028	0.000037
O	-2.469550	1.081563	0.005622
O	-2.469652	-1.081441	-0.005496

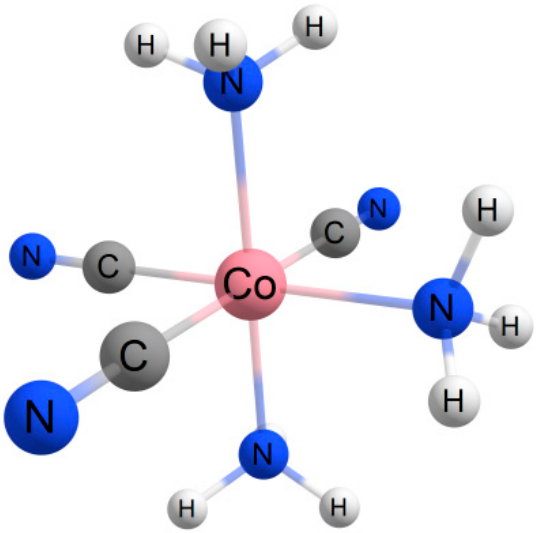
Cpx21: $[Co(NH_3)(CN)_5]^{2-}$



15

Co	-0.000216	-0.002431	-0.076383
C	-1.413444	1.310938	-0.103117
N	-2.274297	2.118199	-0.161428
C	0.001351	0.000489	1.804639
C	1.412613	-1.314591	-0.100847
N	0.002352	0.001621	2.986485
N	2.278687	-2.115760	-0.167182
C	-1.313660	-1.413840	-0.099461
C	1.312896	1.411072	-0.105579
N	-2.121251	-2.273809	-0.167770
N	2.115212	2.276515	-0.163764
H	-0.089460	0.957934	-2.525535
H	0.869578	-0.394327	-2.525516
H	-0.779783	-0.549421	-2.524556
N	0.000290	0.005668	-2.145749

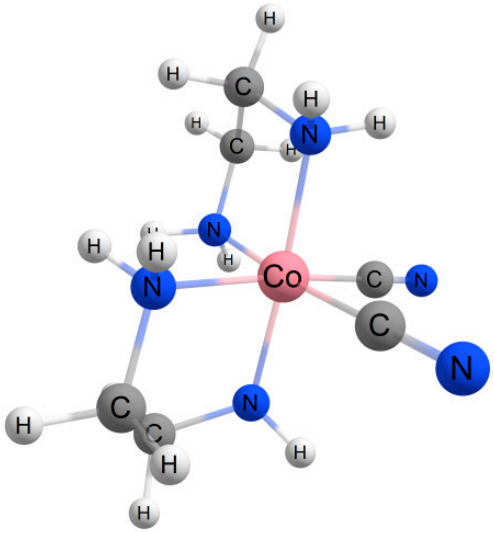
Cpx22: *mer*-$[Co(CN)_3(NH_3)_3]$



19

Co	-0.000002	-0.105912	-0.001264
C	-0.000472	1.777919	-0.001963
N	-0.000260	2.958062	0.016976
C	1.931187	-0.119898	0.000109
C	-1.931238	-0.122359	0.001373
N	3.110452	-0.167181	-0.002228
N	-3.110515	-0.168901	0.001172
H	-0.040224	-1.022608	-2.435742
H	-0.813365	0.436336	-2.377697
H	0.842824	0.373578	-2.381505
H	-0.018868	-2.574099	0.940955
H	-0.815601	-2.567912	-0.492994
H	0.843616	-2.563871	-0.455349
H	0.005121	0.860513	2.364310
H	-0.834213	-0.560751	2.410338
H	0.832696	-0.567686	2.409790
N	-0.002965	-0.083413	-2.010920
N	0.002452	-2.169273	-0.007596
N	0.001009	-0.107560	2.010441

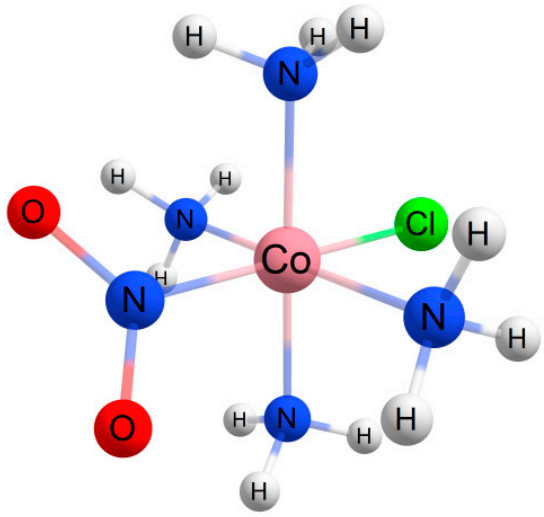
Cpx23: *cis*-$[Co(CN)_2(en)_2]^+$ – en = ethylenediamine



29

C	-2.370964	-1.045243	1.104441
H	-3.358177	-0.909191	1.588612
H	-1.894758	-1.935684	1.557536
N	-1.483511	0.138839	1.356092
H	-1.134354	0.138007	2.326478
H	-2.022562	1.013190	1.262142
Co	0.000054	0.197798	-0.000046
C	-2.509056	-1.210946	-0.406958
H	-3.061862	-2.136650	-0.660154
H	-3.053302	-0.352687	-0.843947
N	-1.127260	-1.220071	-0.997413
H	-1.188040	-1.015237	-2.006001
H	-0.737806	-2.174543	-0.941784
C	2.509527	-1.210245	0.407453
H	3.062370	-2.135758	0.661245
H	3.054193	-0.351645	0.843257
N	1.128084	-1.218567	0.998761
H	1.189432	-1.011320	2.006811
H	0.738757	-2.173227	0.945616
C	2.370701	-1.045932	-1.104022
H	3.357701	-0.910516	-1.588809
H	1.894045	-1.936660	-1.556082
N	1.483363	0.138117	-1.356268
H	1.133884	0.136555	-2.326537
H	2.022541	1.012492	-1.263226
C	0.887994	1.541496	0.979627
C	-0.888464	1.540353	-0.980734
N	1.455505	2.366426	1.603679
N	-1.456462	2.364602	-1.605245

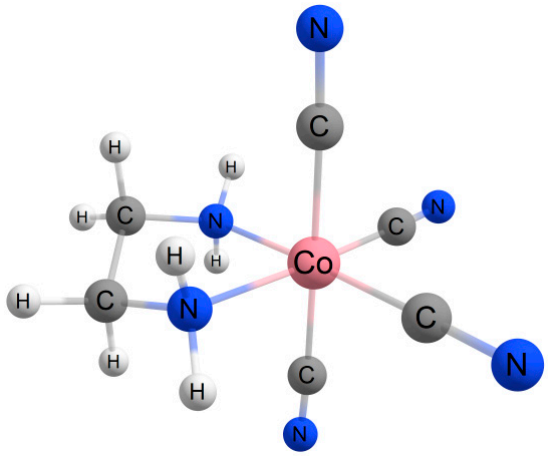
Cpx24: *trans*-$[Co(NH_3)_4(NO_2)Cl]^+$



21

Co	-0.126129	-0.000080	0.000002
N	-0.148343	1.469724	-1.344734
N	-0.136899	1.393115	1.424621
N	-0.149376	-1.469808	1.344441
N	-0.136672	-1.393228	-1.424587
H	-0.160636	1.160824	-2.328934
H	-0.994925	2.048122	-1.227048
H	0.686601	2.070436	-1.236287
H	-0.008056	-1.039075	-2.385255
H	0.619707	-2.080889	-1.271941
H	-1.044242	-1.884928	-1.422792
H	0.683455	-2.073207	1.234658
H	-0.158968	-1.161416	2.328850
H	-0.997907	-2.045578	1.227820
H	-1.045266	1.883300	1.422493
H	-0.007615	1.039349	2.385310
H	0.618499	2.081657	1.271273
Cl	-2.461346	0.000293	-0.000137
N	1.801786	-0.000054	0.000163
O	2.402842	-1.093164	0.010481
O	2.402689	1.093209	-0.009883

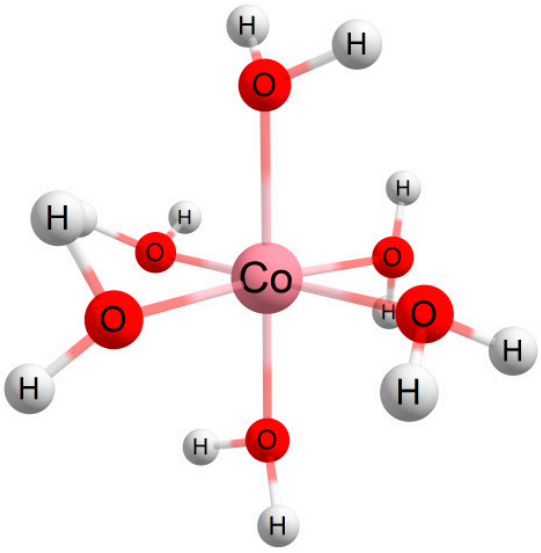
Cpx25: $[Co(en)(CN)_4]^-$ – en = ethylenediamine



15

Co	-0.000216	-0.002431	-0.076383
C	-1.413444	1.310938	-0.103117
N	-2.274297	2.118199	-0.161428
C	0.001351	0.000489	1.804639
C	1.412613	-1.314591	-0.100847
N	0.002352	0.001621	2.986485
N	2.278687	-2.115760	-0.167182
C	-1.313660	-1.413840	-0.099461
C	1.312896	1.411072	-0.105579
N	-2.121251	-2.273809	-0.167770
N	2.115212	2.276515	-0.163764
H	-0.089460	0.957934	-2.525535
H	0.869578	-0.394327	-2.525516
H	-0.779783	-0.549421	-2.524556
N	0.000290	0.005668	-2.145749

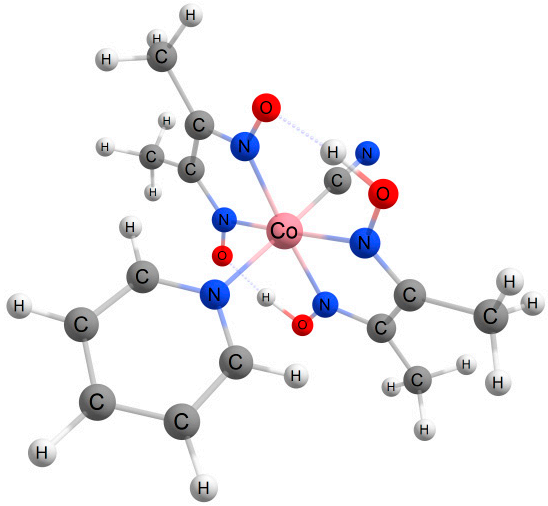
Cpx26: $[Co(OH_2)_6]^{3+}$



19

Co	-0.006932	-0.012323	0.011026
O	1.466242	-0.086803	1.272801
H	1.309820	-0.316840	2.219975
H	2.022605	0.730082	1.257243
O	-0.949466	1.436672	0.893458
H	-0.885378	1.582517	1.866454
H	-1.901224	1.510609	0.641739
O	1.057624	-1.240240	-1.047452
H	0.639097	-1.980528	-1.547534
H	1.816797	-1.620174	-0.541947
O	-1.029370	-1.426189	0.865889
H	-1.501907	-1.208997	1.705431
H	-0.587727	-2.295720	1.019296
O	-1.481420	0.051332	-1.252458
H	-2.051157	-0.755198	-1.205462
H	-1.307369	0.220169	-2.209585
O	1.017699	1.394527	-0.839621
H	0.553922	2.260910	-0.934663
H	1.429207	1.171495	-1.709595

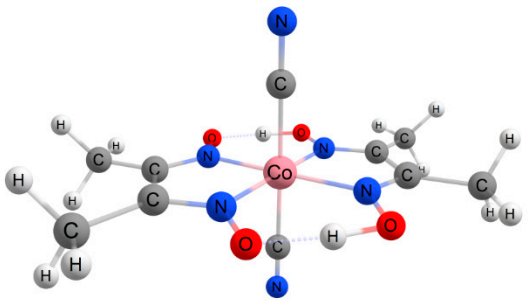
Cpx27: *trans*-[Co(DH)$_2$(CN)(py)] – py = pyridine, DH = dimethylglyoximato



44

Co	-0.00114	-0.47665	0.00279
H	3.71924	-0.59648	-2.63481
H	0.22031	-0.51510	-2.69136
O	1.29837	-0.52005	-2.59694
C	3.95480	-0.67367	-1.56002
H	4.66836	0.12991	-1.28757
H	4.46845	-1.64067	-1.37766
O	-1.21571	-0.53287	-2.56439
N	1.48525	-0.50288	-1.26408
C	2.69511	-0.57816	-0.74243
H	-3.60623	-1.23926	-2.57484
H	4.56987	-1.51787	1.26614
N	-1.43606	-0.57617	-1.27495
C	2.69794	-0.56785	0.73970
N	-0.08003	1.60349	-0.00513
C	3.96141	-0.63690	1.55425
C	-3.88103	-0.85727	-1.57433
C	-2.64114	-0.72685	-0.72849
H	-4.38253	0.12490	-1.71669
N	1.48994	-0.48599	1.26459
H	4.59042	0.26206	1.38683
H	-4.61762	-1.53977	-1.10958
H	3.71925	-0.70311	2.62839
C	-2.64197	-0.71747	0.74084
N	-1.43507	-0.57069	1.28596
O	1.30818	-0.47071	2.59809
C	-3.88882	-0.84993	1.57661
O	-1.20393	-0.53106	2.57353
H	-4.65174	-0.09741	1.29067
H	0.23013	-0.48258	2.69500
H	-4.35331	-1.85068	1.44865
H	-3.63339	-0.71666	2.64234
C	0.03766	-2.37154	0.01058
N	0.07709	-3.54967	0.01523
C	1.05794	2.34638	-0.00664
C	-1.26732	2.26509	-0.00845
C	1.05156	3.74883	-0.01103
C	-0.17778	4.42912	-0.01413
C	-1.35666	3.66508	-0.01291
H	2.00927	1.80413	-0.00418
H	2.00794	4.28869	-0.01187
H	-0.21591	5.52754	-0.01741
H	-2.34786	4.13803	-0.01521
H	-2.17723	1.65533	-0.00682

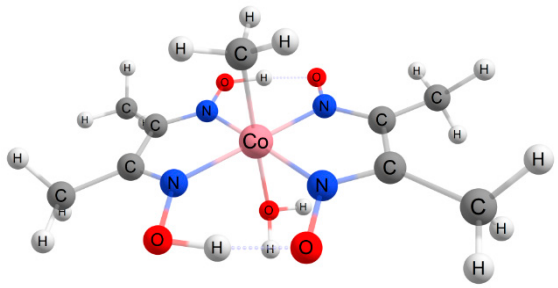
Cpx28: *trans*-[Co(DH)$_2$(CN)$_2$]$^-$ – DH = dimethylglyoximato



35

Co	-0.017577	-0.000017	-0.000019
H	3.696815	2.633145	0.047992
H	0.185829	2.682649	0.001614
O	1.274111	2.593638	-0.004678
C	3.940011	1.558289	-0.005693
H	4.590184	1.294227	0.853292
H	4.529732	1.373751	-0.927826
O	-1.230498	2.572915	0.009534
N	1.464755	1.261173	-0.000252
C	2.676016	0.738848	-0.000433
H	-3.665118	2.634297	-0.051397
H	4.590865	-1.293364	-0.852673
N	-1.459111	1.280285	0.003434
C	2.676030	-0.738802	0.000125
C	3.940036	-1.558224	0.005553
C	-3.930077	1.563822	0.006071
C	-2.671363	0.733323	0.001501
H	-4.524339	1.395753	0.929208
N	1.464784	-1.261150	-0.000025
H	4.529039	-1.374527	0.928324
H	-4.586838	1.310318	-0.851832
H	3.696908	-2.633039	-0.049257
C	-2.671384	-0.733333	-0.001275
N	-1.459137	-1.280327	-0.003170
O	1.274220	-2.593666	0.004531
C	-3.930140	-1.563777	-0.005922
O	-1.230533	-2.572925	-0.009298
H	-4.587373	-1.309618	0.851418
H	0.186104	-2.682723	-0.001601
H	-4.523881	-1.396288	-0.929516
H	-3.665264	-2.634224	0.052379
C	-0.034903	0.003010	-1.935126
N	-0.037236	0.004851	-3.115039
C	-0.034348	-0.003043	1.935138
N	-0.036307	-0.004873	3.115058

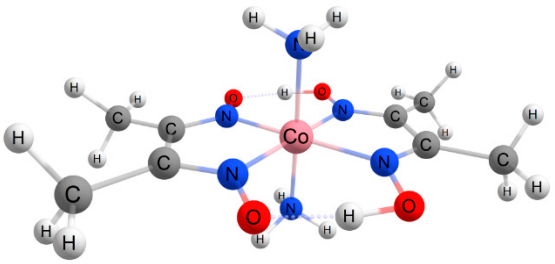
Cpx29: *trans*-[Co(DH)$_2$(CH$_3$)(OH$_2$)] – DH = dimethylglyoximato



38

Co	-0.01074	-0.00130	0.05513
H	3.66364	2.65039	-0.08734
H	0.18385	2.69016	0.11732
O	1.27258	2.59886	0.10220
C	3.92487	1.57942	-0.04253
H	4.54644	1.40607	0.86087
H	4.55022	1.32595	-0.92270
O	-1.22866	2.57415	0.09266
N	1.45482	1.25820	0.06279
C	2.67128	0.74537	-0.00664
H	-0.90422	0.35787	2.45859
H	-3.64870	2.62451	-0.08999
H	4.82749	-1.00820	-0.01481
N	-1.44300	1.26984	0.08866
C	2.66926	-0.73348	-0.03690
C	-0.00749	-0.13973	2.04195
C	3.89945	-1.60006	-0.09124
H	0.90690	0.33252	2.45057
C	-3.91527	1.55435	-0.03355
C	-2.65637	0.72741	0.01738
H	-4.54397	1.39371	0.86808
N	1.45343	-1.24672	-0.00486
H	3.87923	-2.34380	0.73149
H	-4.53963	1.29175	-0.91252
H	-0.02143	-1.21790	2.29351
H	3.92790	-2.17968	-1.03807
C	-2.65164	-0.74281	-0.00706
N	-1.43265	-1.28005	0.02026
O	1.29292	-2.58886	-0.01578
C	-3.90551	-1.57742	-0.05321
O	-1.21154	-2.58201	0.01503
H	-4.59756	-1.31511	0.77360
H	0.20449	-2.69408	0.00837
H	-4.46358	-1.42399	-1.00137
H	-3.63765	-2.64569	0.02737
O	-0.05098	0.13826	-2.08734
H	-0.18378	1.08146	-2.32236
H	-0.85391	-0.30121	-2.44025

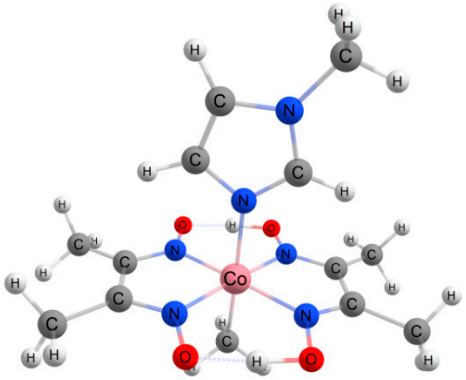
Cpx30: *trans*-[Co(DH)$_2$(CH$_3$)(OH$_2$)] – DH = dimethylglyoximato



39

Co	-0.027067	-0.000016	0.000006
H	3.709218	2.628863	-0.044986
H	0.225588	2.707178	0.057729
O	1.294193	2.603308	0.079196
C	3.942852	1.554240	0.038323
H	4.504378	1.384824	0.980703
H	4.611561	1.261687	-0.795700
O	-1.225233	2.569754	-0.008222
N	1.467385	1.265374	0.041282
C	2.677559	0.741528	0.019957
H	-3.670586	2.634529	0.037139
H	4.504359	-1.384686	-0.980753
N	-1.460049	1.281832	0.020750
C	2.677560	-0.741496	-0.019932
C	3.942894	-1.554145	-0.038345
C	-3.931309	1.563515	-0.020289
C	-2.674174	0.734709	0.004101
H	-4.598033	1.307650	0.828394
N	1.467407	-1.265361	-0.041181
H	4.611622	-1.261506	0.795633
H	-4.508491	1.387150	-0.952060
H	3.709353	-2.628782	0.044996
C	-2.674210	-0.734663	-0.004172
N	-1.460105	-1.281854	-0.020836
O	1.294306	-2.603373	-0.079036
C	-3.931375	-1.563427	0.020250
O	-1.225331	-2.569736	0.008123
H	-4.508428	-1.387191	0.952128
H	0.225906	-2.707277	-0.057704
H	-4.598205	-1.307424	-0.828305
H	-3.670683	-2.634441	-0.037353
H	-0.106604	1.099810	-2.301288
H	0.779504	-0.292592	-2.438043
H	-0.872189	-0.364545	-2.405755
H	-0.105354	-1.100026	2.301214
H	0.778404	0.293852	2.438317
H	-0.873386	0.363047	2.405554
N	-0.057417	-0.115964	1.993544
N	-0.057133	0.115849	-1.993542

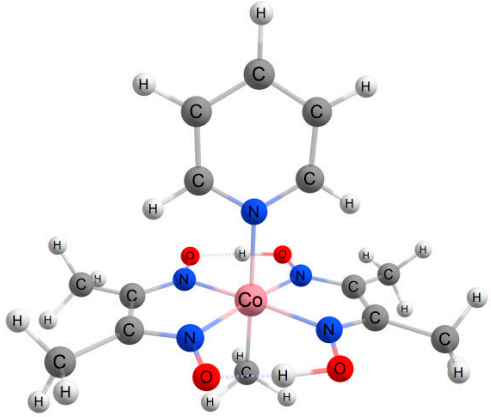
Cpx31: *trans*-[Co(DH)$_2$(CH$_3$)(MeIm)] – DH = dimethylglyoximato; MeIm = methylimidazole



47

Co	-0.202991	-0.627711	0.038665
H	3.278819	-1.907890	-2.575109
H	-0.103812	-0.952363	-2.628794
O	0.973093	-1.157870	-2.547818
C	3.584165	-1.711277	-1.532858
H	4.346195	-0.903050	-1.538380
H	4.075728	-2.616656	-1.123596
O	-1.477675	-0.662910	-2.508276
N	1.191161	-1.070142	-1.217363
C	2.384494	-1.324072	-0.707656
H	-3.969804	-0.775928	-2.414305
H	3.943562	-2.520274	1.564285
N	-1.649032	-0.510071	-1.207163
C	2.420962	-1.197676	0.763374
C	3.660243	-1.446256	1.583439
C	-4.091470	-0.177792	-1.491520
C	-2.839947	-0.283085	-0.657382
H	-4.290946	0.871031	-1.804814
N	1.250540	-0.862019	1.282662
H	4.525824	-0.876670	1.189145
H	-4.982352	-0.532087	-0.939151
H	3.484226	-1.153349	2.632861
C	-2.799552	-0.140553	0.804325
N	-1.582466	-0.292590	1.323201
O	1.101067	-0.718947	2.615113
C	-4.012360	0.138948	1.656077
O	-1.333120	-0.211079	2.618296
H	-4.588890	1.006336	1.274623
H	0.022720	-0.477497	2.712125
H	-4.706907	-0.728629	1.677089
H	-3.691072	0.347771	2.691950
C	-0.607451	-2.602862	0.137281
H	-0.705873	-2.969690	-0.902866
H	0.218265	-3.137854	0.645677
H	-1.552600	-2.774586	0.687140
N	0.177521	1.423957	-0.121356
C	1.372388	2.021865	-0.021688
C	-0.744257	2.439804	-0.338346
H	2.330060	1.523906	0.154066
C	-0.086714	3.657515	-0.369073
H	-1.811510	2.237536	-0.458128
H	-0.449717	4.678646	-0.514462
N	1.258741	3.376061	-0.165503
C	2.353793	4.352371	-0.116795
H	2.445852	4.876042	-1.087719
H	2.166071	5.097413	0.679727
H	3.298973	3.824519	0.099728

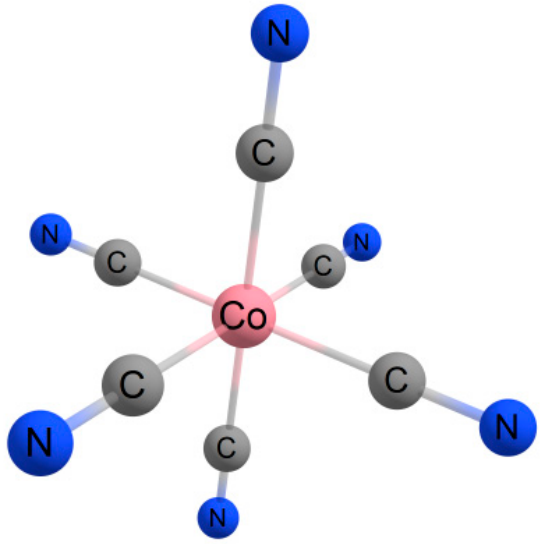
Cpx32: *trans*-[Co(DH)$_2$(CH$_3$)(py)] – DH = dimethylglyoximato; py = pyridine



46

Co	0.001710	-0.557350	0.017223
H	3.700878	-0.804971	-2.606543
H	0.190079	-0.725555	-2.662730
O	1.283748	-0.726439	-2.570673
C	3.942314	-0.827412	-1.530166
H	4.650116	-0.004011	-1.303261
H	4.470042	-1.778022	-1.305556
O	-1.216681	-0.728831	-2.550445
N	1.468048	-0.649480	-1.234697
C	2.682762	-0.702391	-0.713819
H	-3.604754	-1.359126	-2.538886
H	4.538749	-1.592181	1.356477
N	-1.427494	-0.699160	-1.247945
C	2.681025	-0.644215	0.762376
N	-0.057011	1.571143	-0.039356
C	3.939720	-0.687716	1.588642
C	-3.881118	-0.954461	-1.547669
C	-2.639898	-0.803410	-0.705820
H	-4.386716	0.022117	-1.714693
N	1.463949	-0.559295	1.276046
H	4.586560	0.190380	1.381588
H	-4.618501	-1.627192	-1.068734
H	3.686825	-0.693603	2.662626
C	-2.638883	-0.749113	0.762193
N	-1.422924	-0.621760	1.294044
O	1.280352	-0.509379	2.610653
C	-3.885456	-0.840211	1.605378
O	-1.206745	-0.564264	2.595025
H	-4.640154	-0.084971	1.303583
H	0.179387	-0.523322	2.703453
H	-4.368403	-1.836430	1.510854
H	-3.621740	-0.680929	2.665782
C	1.085255	2.304989	-0.068214
C	-1.237162	2.243398	-0.052184
C	1.092566	3.707861	-0.110097
C	-0.131812	4.398309	-0.123148
C	-1.317531	3.644284	-0.093673
H	2.031160	1.749874	-0.057992
H	2.052628	4.241396	-0.132010
H	-0.160966	5.496762	-0.155554
H	-2.304335	4.127041	-0.102166
H	-2.150233	1.636102	-0.027925
C	0.028738	-2.580133	0.001427
H	0.036406	-2.896434	-1.059026
H	0.937566	-2.949786	0.513429
H	-0.871250	-2.976191	0.507786

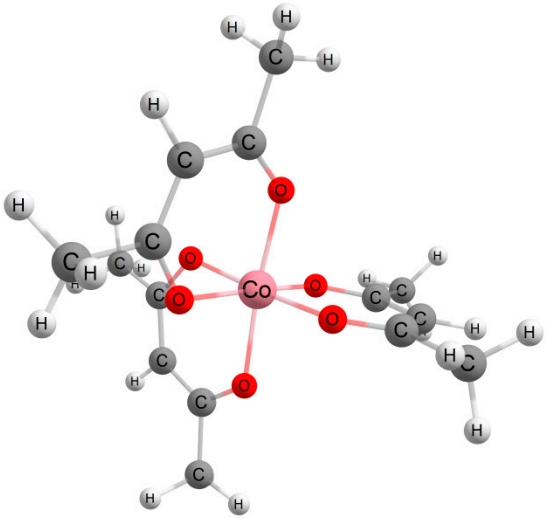
Reference: $[Co(CN)_6]^{3-}$



13

Co	0.000006	-0.000007	0.000042
C	0.933371	1.275542	-1.107699
N	1.504445	2.055748	-1.787844
C	1.166417	-1.402286	-0.632734
N	1.881207	-2.260770	-1.019574
C	-1.166408	1.402261	0.632831
C	-0.933320	-1.275596	1.107769
N	-1.881336	2.260922	1.019023
N	-1.504326	-2.055872	1.787890
C	-1.224169	-0.363970	-1.447333
C	1.224161	0.363983	1.447426
N	-1.975217	-0.587317	-2.332549
N	1.975164	0.587374	2.332670

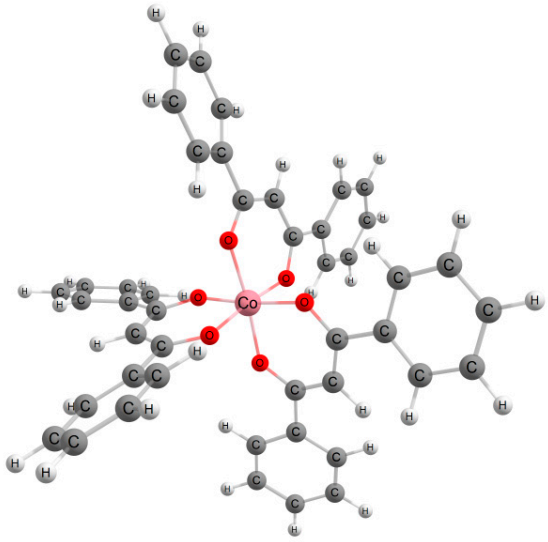
Cpx33: $[Co(acac)_3]$ – acac = acetylacetonato



43

Co	-0.005619	-0.003410	-0.004814
O	-0.395817	1.498004	1.144166
O	1.470975	-0.404824	1.161472
O	1.226065	0.919671	-1.157906
O	-1.424134	0.574933	-1.169651
O	0.196726	-1.544143	-1.147638
O	-1.108188	-1.076515	1.148164
C	1.131104	-2.416260	-1.003245
C	2.125374	-2.408345	0.005134
C	2.230596	-1.432681	1.025141
C	1.140414	-3.531489	-2.046105
C	3.311430	-1.584344	2.091603
H	0.179879	-3.546560	-2.591999
H	1.318484	-4.518235	-1.575357
H	1.958031	-3.357469	-2.776377
H	3.473936	-0.620412	2.607911
H	4.263507	-1.939495	1.651471
H	2.988745	-2.333961	2.844180
C	-2.654039	0.228860	-1.027087
C	-2.381886	-1.196311	1.015948
C	-3.165612	-0.603721	-0.002987
C	-3.611876	0.782073	-2.078338
C	-3.066330	-2.045016	2.083459
H	-3.066694	1.431677	-2.786309
H	-4.424493	1.363711	-1.597435
H	-4.087368	-0.048555	-2.638707
H	-2.319033	-2.663289	2.613483
H	-3.844771	-2.696147	1.640551
H	-3.563306	-1.384913	2.824954
C	1.545563	2.157175	-1.016063
C	0.143435	2.656776	1.003136
C	1.065263	3.025753	-0.005725
C	2.514988	2.704002	-2.060728
C	-0.270360	3.697432	2.041450
H	2.945410	1.875247	-2.651167
H	3.329023	3.281925	-1.580363
H	1.979898	3.391394	-2.748341
H	-1.081551	3.298052	2.676274
H	-0.609075	4.630086	1.547894
H	0.594465	3.958293	2.685972
H	-4.244966	-0.803626	0.000557
H	1.431671	4.060537	-0.004881
H	2.856496	-3.226630	0.005229

Cpx34: [Co(dbzm)$_3$] – dbzm = dibenzoylmethanato



85

Co	-0.006200	0.006023	-0.001525
O	-1.033979	1.141991	-1.156032
O	-1.449356	-0.440927	1.179451
O	-0.525244	-1.464394	-1.115460
O	1.151046	-1.008687	1.141054
O	1.488591	0.280691	-1.169736
O	0.333240	1.528406	1.113774
C	-2.293577	1.381246	-1.011450
C	-3.106118	0.869852	0.032512
C	-2.654439	0.005142	1.061098
C	-2.881180	2.292579	-2.057808
C	-2.010857	3.117880	-2.814769
C	-2.516455	3.980460	-3.801312
C	-3.900615	4.026983	-4.061216
C	-4.774303	3.202266	-3.325816
C	-4.271315	2.344432	-2.331940
C	-3.609671	-0.483026	2.119419
C	-3.279560	-1.649942	2.855292
C	-4.145379	-2.143412	3.845165
C	-5.352152	-1.473971	4.130067
C	-5.684375	-0.305554	3.416900
C	-4.823691	0.185172	2.419339
C	-0.114591	-2.678172	-0.965157
C	0.800696	-3.110012	0.028130
C	1.386239	-2.270354	1.009533
C	-0.673749	-3.655041	-1.967710
C	-0.664892	-5.057385	-1.757811
C	-1.200086	-5.929972	-2.721523
C	-1.751261	-5.420061	-3.913261
C	-1.772286	-4.027898	-4.130337
C	-1.245179	-3.153526	-3.165520
C	2.348598	-2.835421	2.023035
C	2.600362	-2.100386	3.209875
C	3.488644	-2.589120	4.182017
C	4.153188	-3.815745	3.983198
C	3.921951	-4.548931	2.802893
C	3.027471	-4.065416	1.831908
C	2.351280	1.232397	-1.045606
C	2.308997	2.245798	-0.053908
C	1.317341	2.348001	0.954936
C	3.450426	1.219426	-2.076594
C	4.683727	1.892377	-1.885963
C	5.684375	1.847431	-2.872419
C	5.471198	1.133281	-4.067858
C	4.251512	0.456086	-4.266392
C	3.253457	0.492216	-3.278599
C	1.368187	3.464894	1.965501
C	2.081615	4.669239	1.739869
C	2.094795	5.686404	2.710420
C	1.400028	5.518655	3.924413
C	0.682458	4.328424	4.157289
C	0.661048	3.314070	3.185906
H	-4.158273	1.163569	0.044508
H	-0.933270	3.070257	-2.612237
H	-1.826611	4.620074	-4.371916
H	-4.296857	4.698781	-4.837248
H	-5.855099	3.222022	-3.530575
H	-4.968055	1.693254	-1.787255
H	-2.335343	-2.162955	2.631790
H	-3.877216	-3.055734	4.398656
H	-6.029127	-1.858612	4.907383
H	-6.617930	0.231476	3.641428
H	-5.092964	1.109754	1.891130
H	1.077122	-4.166721	0.036451
H	-0.260341	-5.476354	-0.826794
H	-1.191695	-7.014570	-2.537259
H	-2.167158	-6.105001	-4.667222
H	-2.202873	-3.621305	-5.057645
H	-1.262907	-2.067586	-3.325370
H	2.082633	-1.143472	3.353996
H	3.664557	-2.009535	5.100568
H	4.852681	-4.196436	4.742360
H	4.446079	-5.501218	2.633262
H	2.879906	-4.643151	0.909601
H	3.096653	3.002686	-0.067896
H	4.879418	2.436087	-0.952063
H	6.638688	2.367916	-2.702949
H	6.254189	1.101921	-4.840151
H	4.078089	-0.105495	-5.196547
H	2.303140	-0.037834	-3.422528
H	2.610737	4.829913	0.790917
H	2.646489	6.617868	2.514416
H	1.414756	6.314731	4.683790
H	0.134614	4.190971	5.101523
H	0.097830	2.387239	3.356160