Supporting Information for:

Anionic Guest-Dependent Tuning of Slow Magnetic Relaxation in Co(II) Tripodal Iminopyridine Complexes

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Contents

Crystallography

Table S1. Crystallographic and structural refinement data for **1**–**4**.[a]

	1	**2**	**3**	**4**
Empirical formula	$C_{39}H_{54}CoN_{10}O_3Cl$	$C_{39}H_{54}CoN_{10}O_3Br$	$C_{39}H_{54}CoN_{10}O_3I$	$C_{39}H_{54}CoN_{10}O_{11}Cl_2$
Formula mass (g mol^{-1})	805.30	849.76	896.75	968.75
Color	Orange	Orange	Orange	Yellow
Habit	Parallelepiped	Block	Block	Block
T (K)	120(2)	120(2)	120(2)	120(2)
Crystal system	Trigonal	Trigonal	Trigonal	Triclinic
Space group	$P\bar{3}$	$P\bar{3}$	$P\bar{3}$	$P\bar{1}$
Z	2	2	2	2
a (Å)	15.2335(1)	15.5579(15)	15.8091(7)	12.7632(10)
b (Å)	15.2335(1)	15.5579(15)	15.8091(7)	12.8064(10)
c (Å)	12.5157(2)	12.1716(17)	12.0675(10)	14.9046(11)
α (°)	90	90	90	75.900(4)
β (°)	90	90	90	83.780(4)
γ (°)	120	120	120	74.500(4)
Volume (Å^3)	2515.27(5)	2551.4(6)	2611.9(3)	2274.4(3)
ρ_{calc} (g cm^{-3})	1.063	1.106	1.140	1.415
GooF	1.073	1.157	1.086	1.023
R_1 (wR_2)[b] (%)	6.67 (22.37)	5.56 (20.06)	3.48 (10.26)	4.25 (9.40)

[a]Obtained with graphite-monochromated Mo Kα (λ = 0.71073 Å) radiation.
[b]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$; $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

Table S2. Selected bond lengths and angles for **1–4**.

	1	**2**	**3**	**4**
Co–N_{imine} (Å)	2.120(6)	2.106(6)	2.105(3)	2.100(5)[a]
Co–$N_{pyridine}$ (Å)	2.262(3)	2.253(3)	2.258(3)	2.246(5)[a]
Co–N_{bridge} (Å)	2.574(5)	2.592(6)	2.633(2)	2.706(2)
$N_{imine\ plane}\cdots N_{pyridine\ plane}$ (Å)	2.099(2)	2.092(3)	2.068(4)	2.075(2)
Twist angle (°)	49.8(4)	50.5(3)	51.3(6)	51.2(9)
Θ (°)	200	189	193	187
Σ (°)	125.9(3)	120.4(4)	117.9(5)	113.3(2)
Area of Binding Pocket (Å^2)[b]	19.03(1)	20.32(1)	21.89(6)	21.12(5)
$H_{amide}\cdots X$ (Å)	2.483(3)	2.706(4)	2.924(2)	2.541(4)[c]
Co$\cdots$X (Å)	5.161(2)	5.238(1)	5.2116(6)	5.3027(7)[d]
Shortest Co$\cdots$Co (Å)	9.292(2)	9.392(1)	9.4798(9)	8.0030(8)

[a]Averaged values of three arms
[b]Calculated using amide carbonyl carbons as corners of triangle.
[c]Defined using the closest O$\cdots$H distance
[d]Defined as Co$\cdots$Cl distance

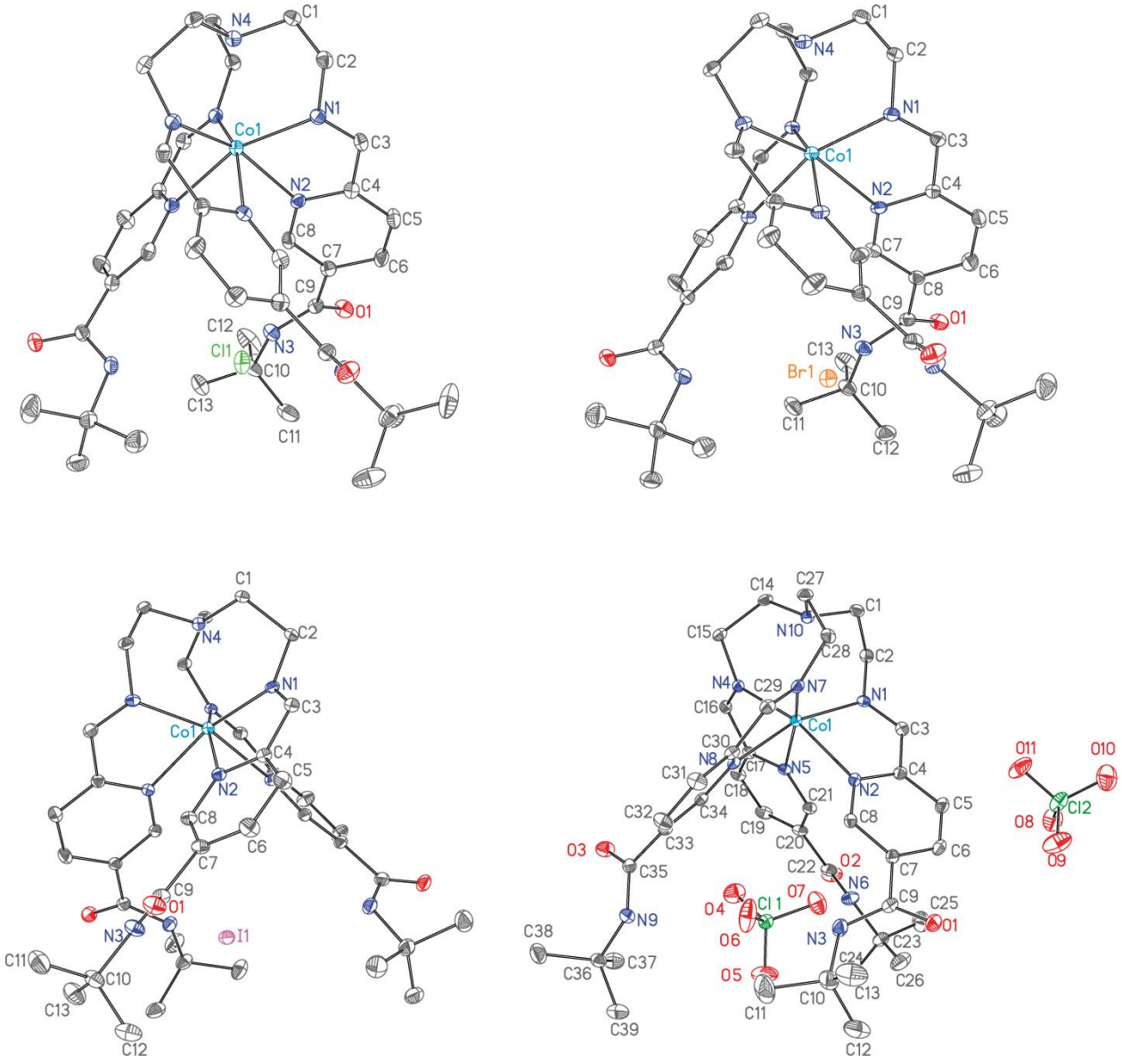


Figure S1. Crystal structures of **1**–**4**. Structures are rendered with 40% thermal ellipsoids, and hydrogen atoms are omitted for clarity. Atoms labels are shown for the asymmetric unit of **1**–**3** for clarity.

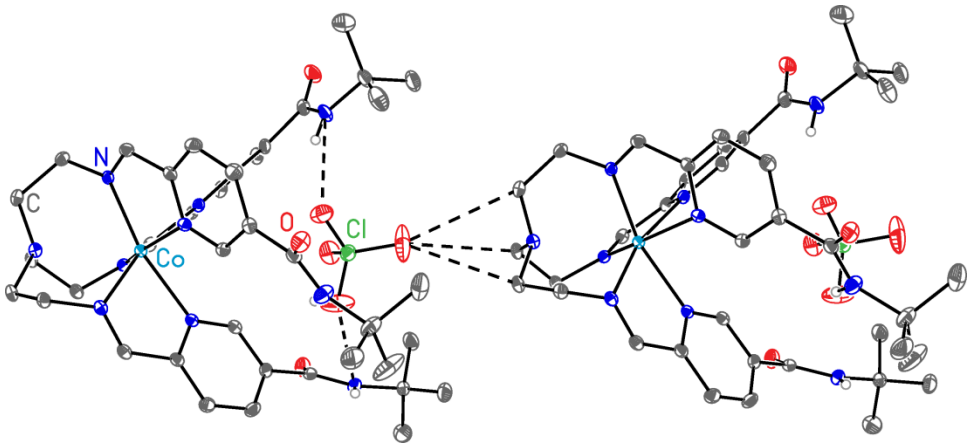


Figure S2. Intermolecular interactions in **4**. Atoms are rendered with 40% thermal ellipsoids. Hydrogen atoms, except those of the amides, are omitted for clarity.

Other Spectroscopic Results

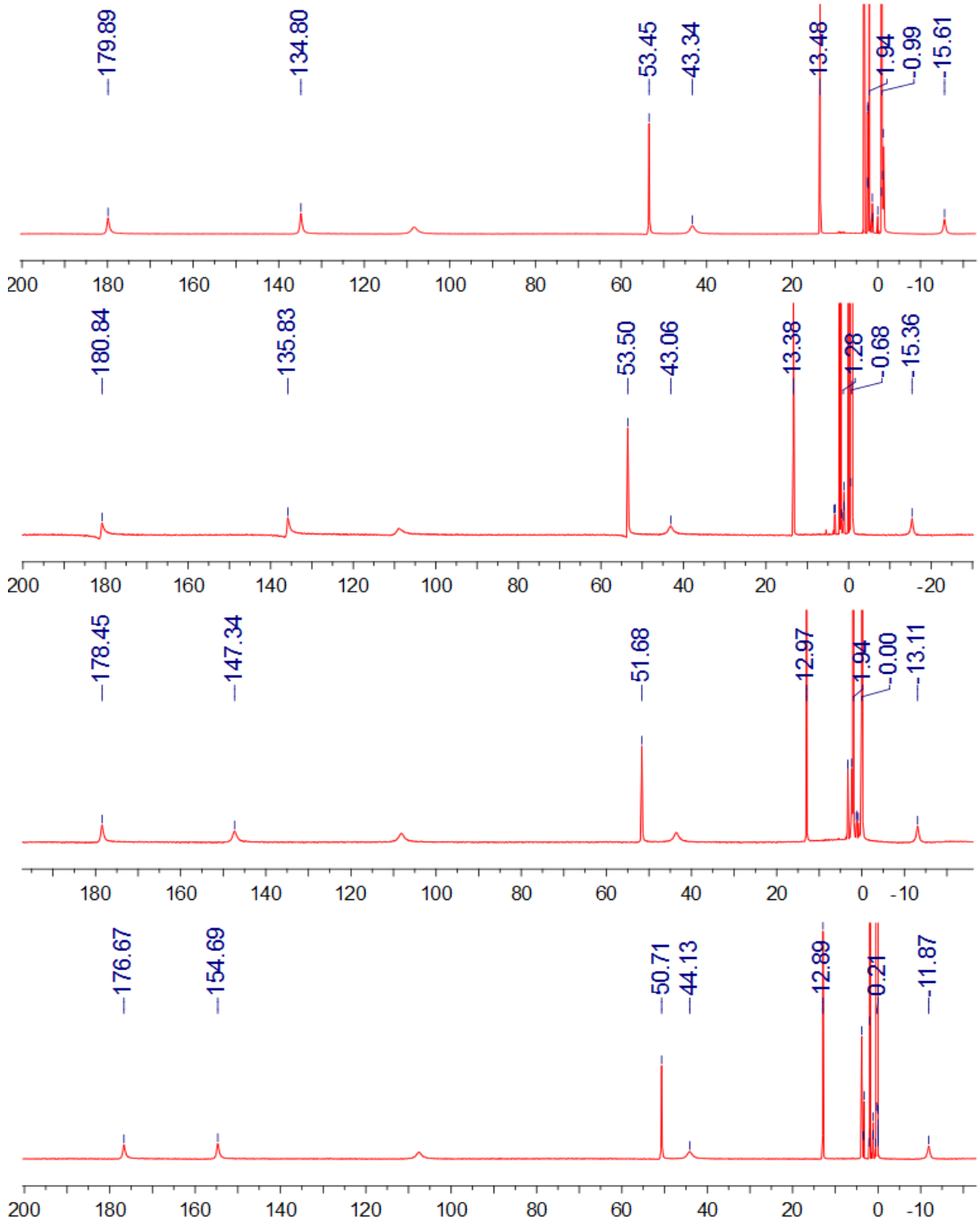


Figure S3. Paramagnetic NMR spectra of **1**–**4**. Spectra for **1** (top), **2** (second), **3** (third), **4** (bottom) obtained in d_3-acetonitrile at 23°C.

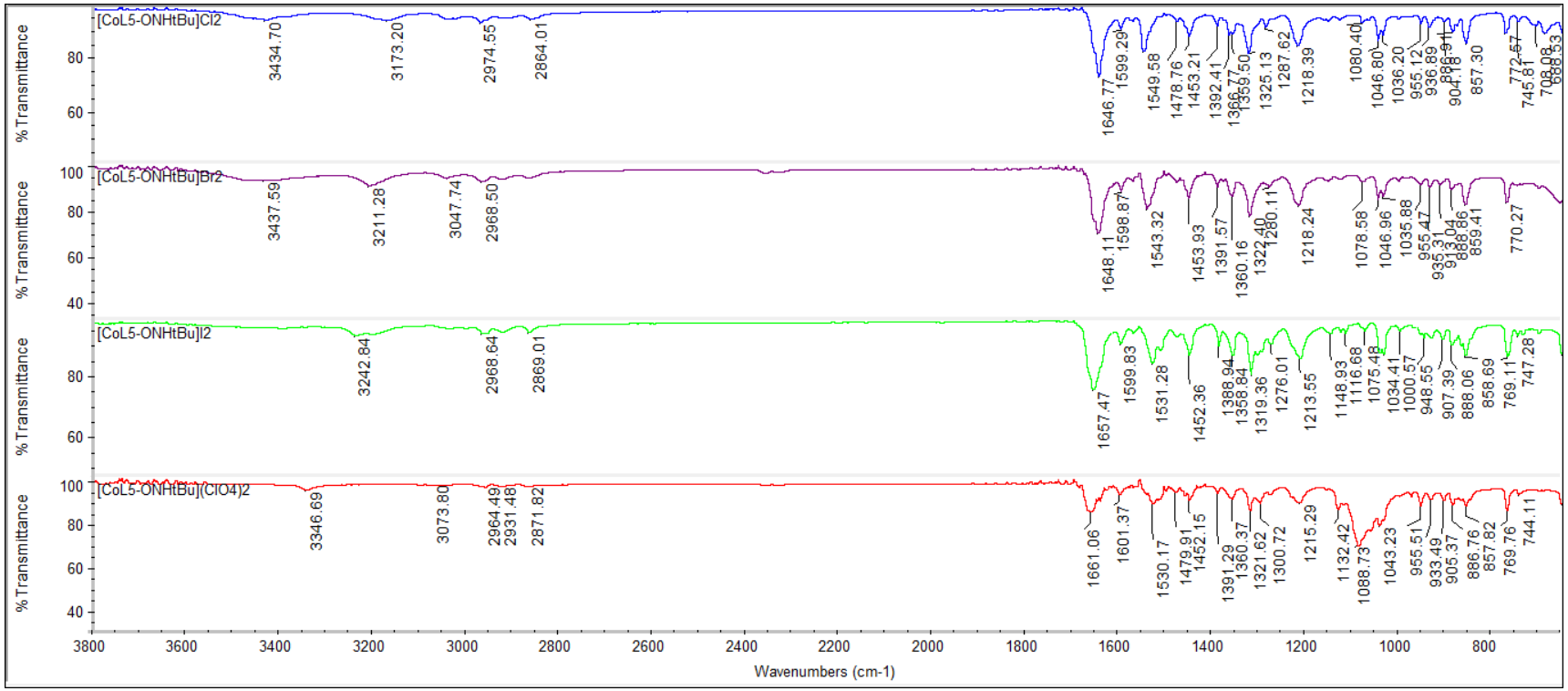


Figure S4. Stacked FT-IR spectra of **1–4**. Spectra collected by pressing crystalline samples onto a ZnSe ATR crystal.

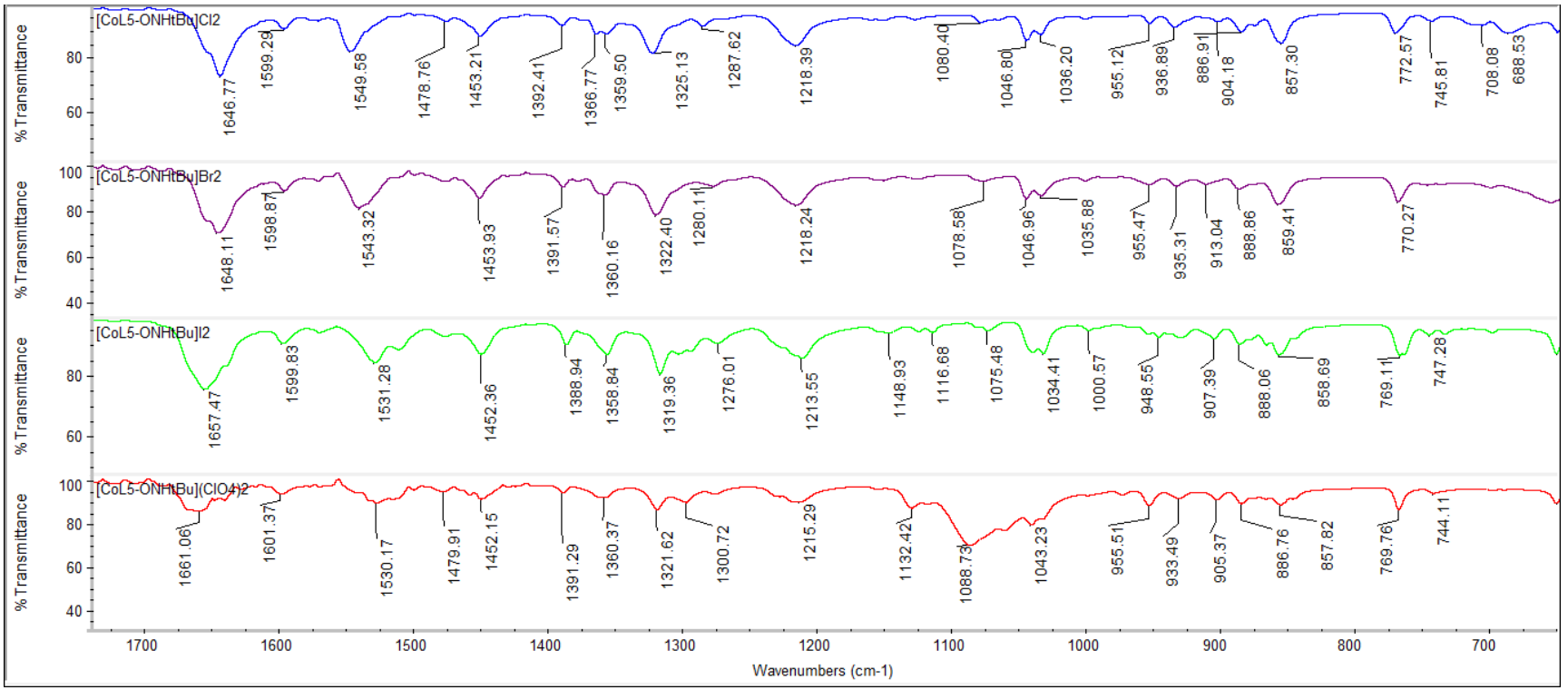


Figure S5. Zoom of 1740 cm^{-1} to 650 cm^{-1} region in stacked FT-IR spectra of **1–4**.

DC Magnetic Measurements and Magnetic Fits

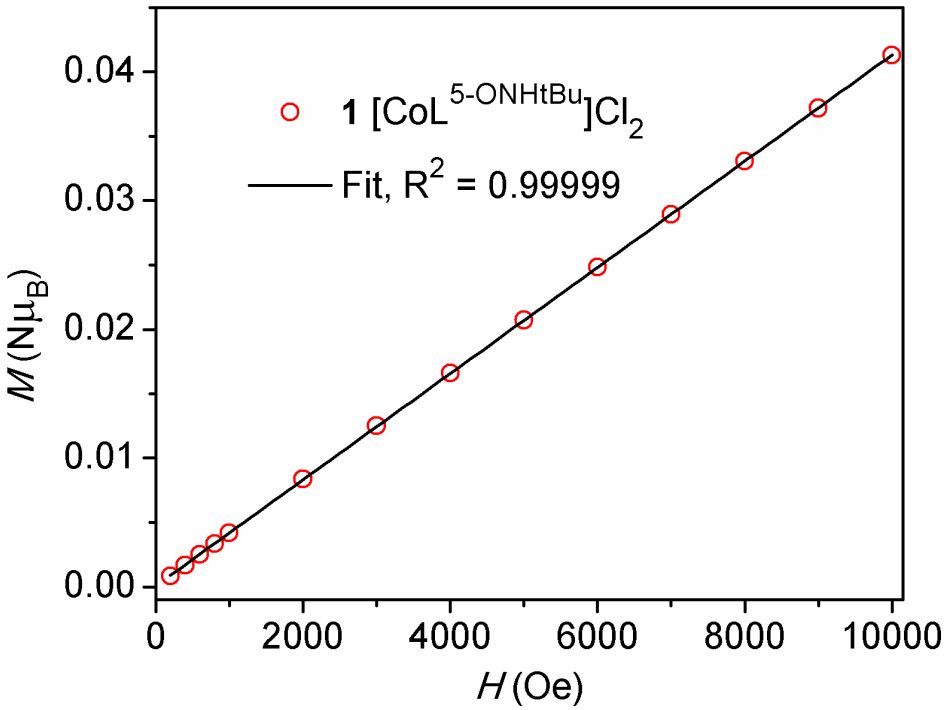


Figure S6. Field dependence of magnetization for **1** collected at 100 K. Fit: $y = 4.12\times10^{-6}(x) + 7.09\times10^{-5}$ ($R^2 = 0.99999$).

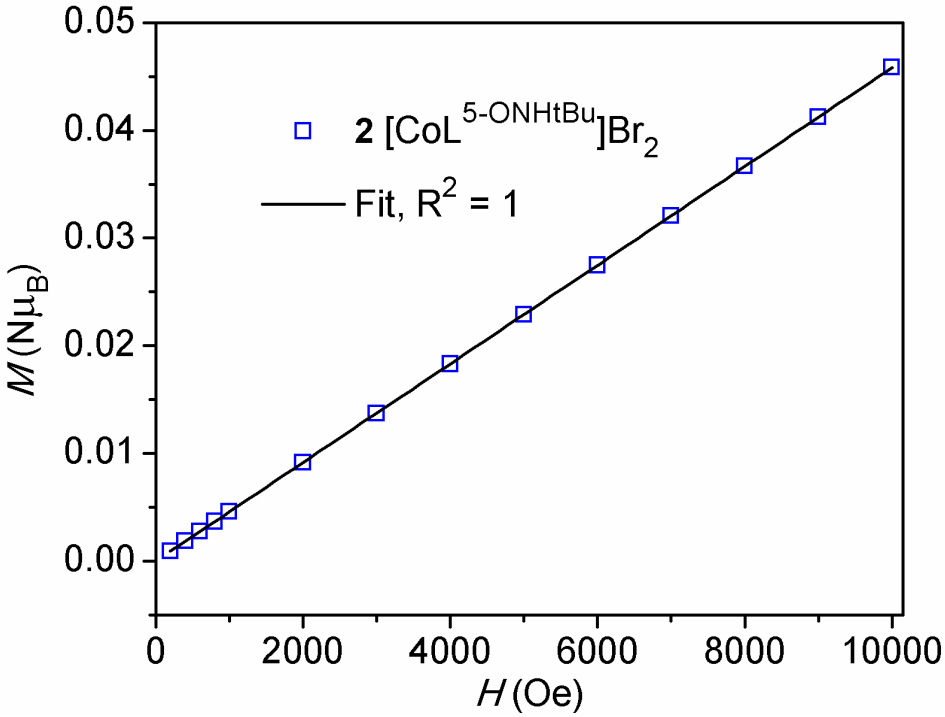


Figure S7. Field dependence of magnetization for **2** collected at 100 K. Fit: $y = 4.58\times10^{-6}(x) - 1.54\times10^{-6}$ ($R^2 = 1$).

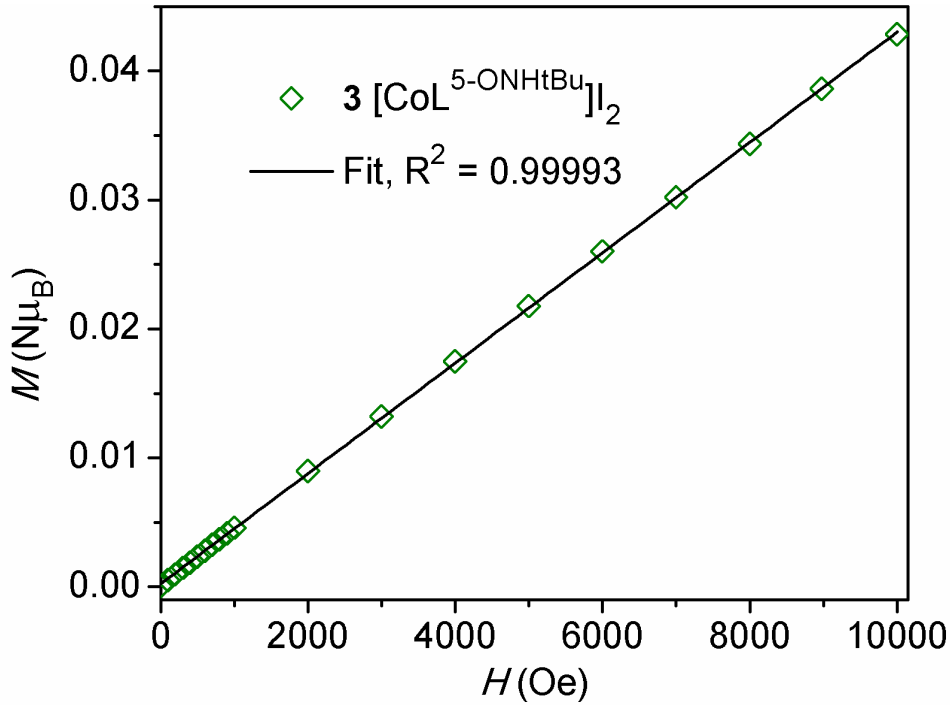


Figure S8. Field dependence of magnetization for **3** collected at 100 K. Fit: $y = 4.28\times10^{-6}(x) + 2.42\times10^{-4}$ ($R^2 = 0.99993$).

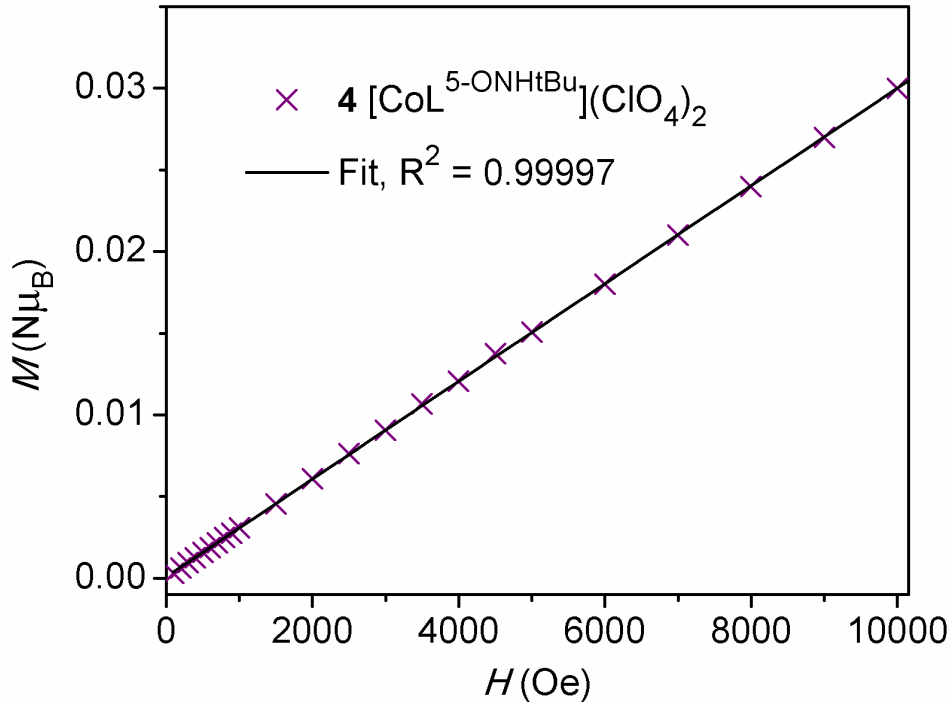


Figure S9. Field dependence of magnetization for **4** collected at 100 K. Fit: $y = 2.99\times10^{-6}(x) + 8.59\times10^{-5}$ ($R^2 = 0.99997$).

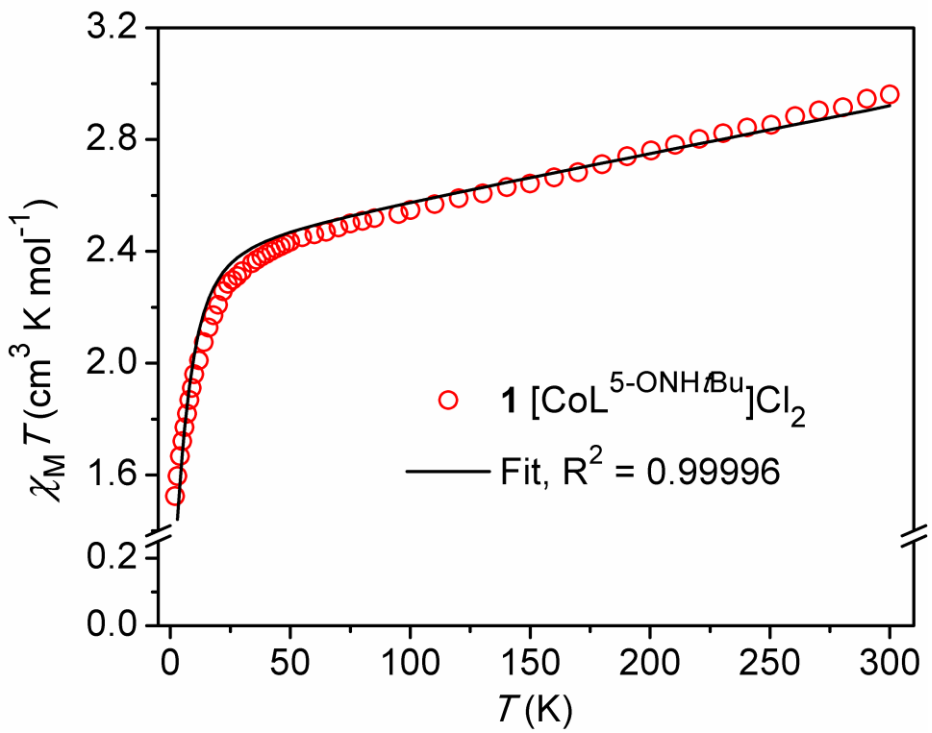


Figure S10. Magnetic susceptibility of **1**. Data collected from 1.8 K to 300 K under an applied dc field of 1000 Oe. Best fit acquired using PHI.[1]

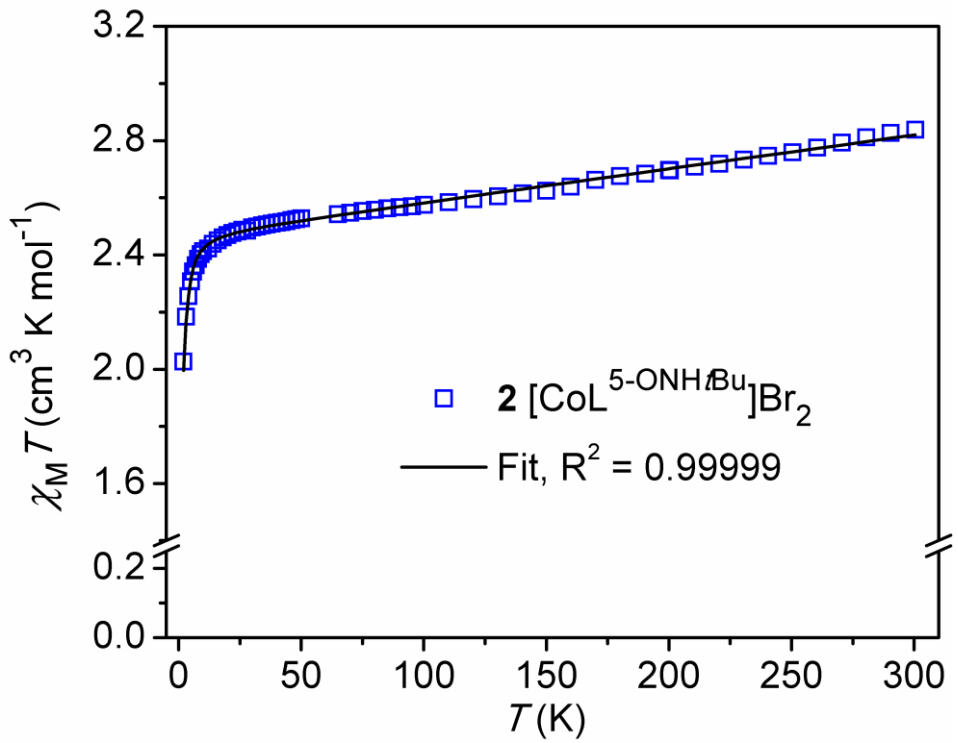


Figure S11. Magnetic susceptibility of **2**. Data collected from 1.8 K to 300 K under an applied dc field of 1000 Oe. Best fit acquired using PHI.[1]

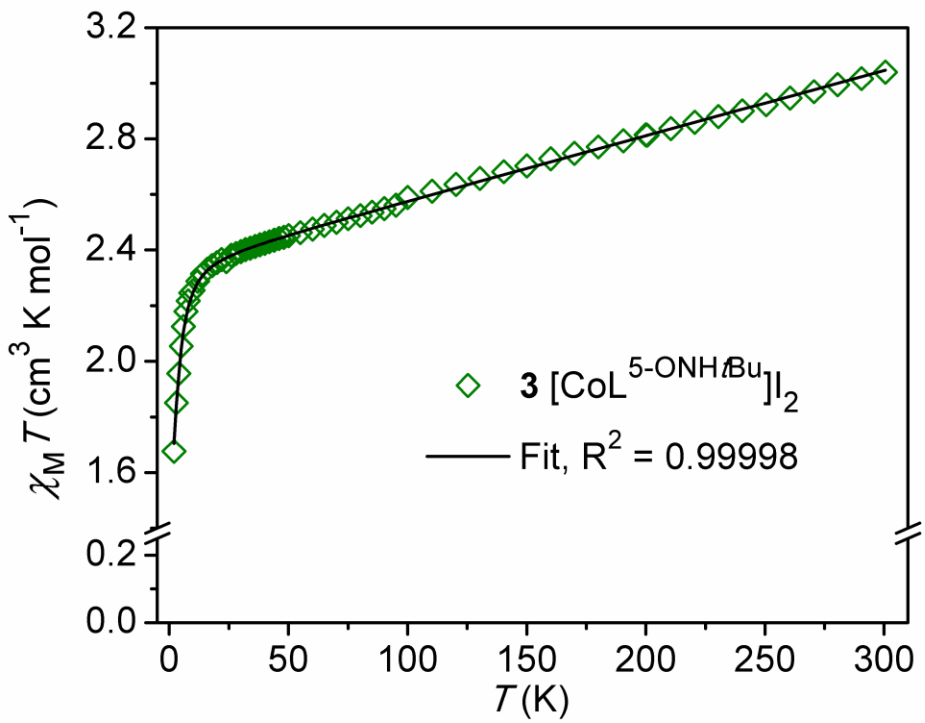
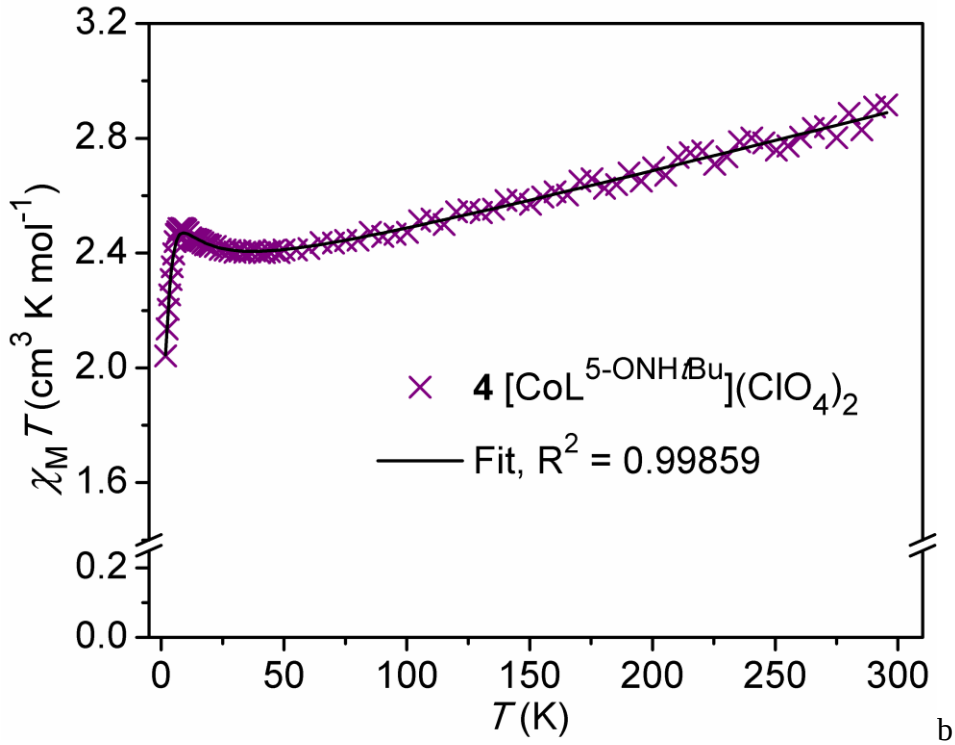


Figure S12. Magnetic susceptibility of **3**. Data collected from 1.8 K to 300 K under an applied dc field of 1000 Oe. Best fit acquired using PHI.[1]



b

Figure S13. Magnetic susceptibility of **4**. Data collected from 1.8 K to 300 K under an applied dc field of 1000 Oe. The line represents the best fit using PHI.[1]

Table S3. Anisotropy parameters acquired from fitting magnetic susceptibility data using PHI.[1]

Compound	g_x, g_y, g_z	D (cm^{-1})	E (cm^{-1})	TIP ($cm^3\ mol^{-1}$)	zJ (cm^{-1})	R^2
1	2.31, 2.39, 2.10	9.20	0.0173	0.00170	-0.099	0.99996
2	1.87, 2.56, 2.39	2.19	0.0011	0.00118	-	0.99999
3	2.14, 2.25, 2.32	3.61	1.44	0.00234	-	0.99998
4	3.55, 0.755, 1.04	4.21	0.253	0.00218	0.0281	0.99859

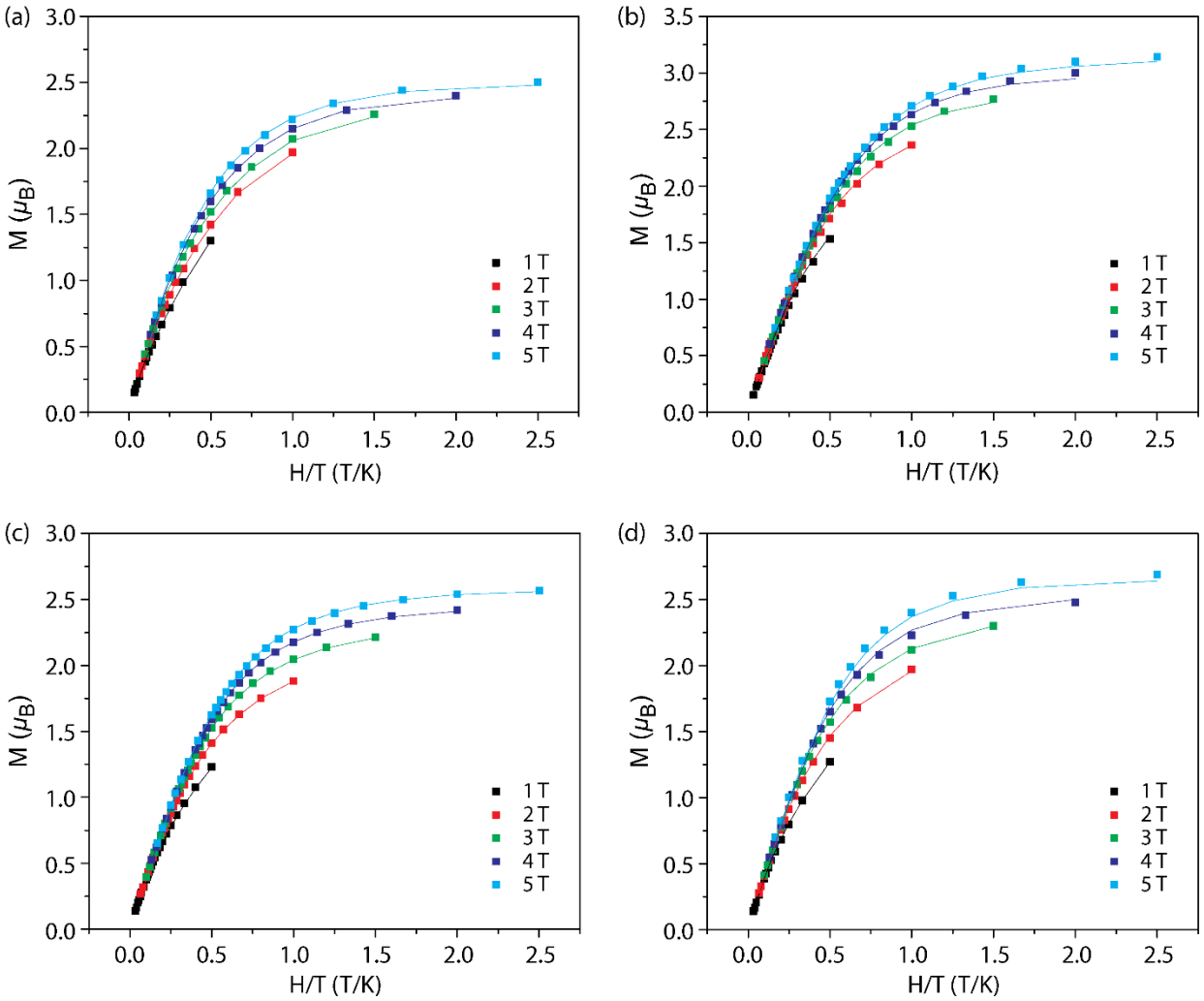


Figure S14. Reduced magnetization of **1**–**4**. Curves are presented for **1** (a), **2** (b), **3** (c), **4** (d), with best fit lines determined using ANISOFIT 2.0.[2]

Table S4. Parameters acquired from fitting reduced magnetization data in ANISOFIT 2.0.[2,a]

Salt	$g_{initial}$	g_{fit}	$D_{initial}$ (cm^{-1})	D_{fit}[b] (cm^{-1})	D_{red}[b] (cm^{-1})	$E_{initial}$ (cm^{-1})	E_{fit}[b] (cm^{-1})	E_{red}[b] (cm^{-1})	f_{sum}
1	2.30	2.32	10	9.490	–	3	-0.039	–	0.005031
1	2	2.307	–10	5.384	7.829	3	3.425	0.9792	0.02729
2	2.20	2.30	5	2.530	–	0.100	0.146	–	0.034279
2	2.20	2.30	–5	1.516	2.495	0.100	1.158	0.1793	0.023729
3	2.20	2.30	10	4.502	–	3	1.3488	–	0.007271
3	2.20	2.17	–10	3.770	4.218	3	1.571	1.414	0.004421
3	2.20	2.17	100	0.5015	4.248	3	2.665	1.082	0.003642
3	2.20	2.17	–100	3.770	4.218	3	1.571	1.414	0.004421
4	2.30	2.22	10	2.226	4.628	3	2.349	0.053	0.02462
4	2.22	2.22	–10	-2.226	4.628	3	2.349	0.053	0.02464
4	2.22	2.22	100	2.217	4.769	3	2.440	0.112	0.04126
4	2.22	2.22	–100	2.217	4.769	3	2.440	0.112	0.04126

[a] Subscript definitions: "initial" refers to the value put into the program; "fit" refers to the final value; "red" refers to the re-determined value according to the procedure described below.
[b] For completeness, the fit and re-determined values are quoted out to the .001, but the actual value is best described to the nearest 0.1.

Details of re-determination of *D* and *E* values obtained from ANISOFIT 2.0.

In cases where the initial fits from ANISOFIT 2.0 produced values $|E| \geq |1/3D|$, the principal values of the *D*-tensor were reassigned to fulfill the following relationship[3]:

$$|D_{zz}| \geq |D_{yy}| \geq |D_{xx}| \qquad (1)$$

The values of D_{zz}, D_{yy}, and D_{xx} were determined by the following equations, using the output *D* and *E* values obtained from ANISOFIT2.0:

$$D_{zz} = 2/3D \qquad (2a)$$
$$D_{yy} = 1/3D - E \qquad (2b)$$
$$D_{xx} = 1/3D + E \qquad (2c)$$

Cyclic permutations were performed in order to transform the largest value determined from the equations above to satisfy (1). Upon reorientation of the *D*-tensors the following equations are employed to calculate the new *D* and *E* values:

$$D = 3/2D_{zz} = -3/2(D_{xx} + D_{yy}) \qquad (3)$$
$$E = ½(D_{xx} - D_{yy}) \qquad (4)$$

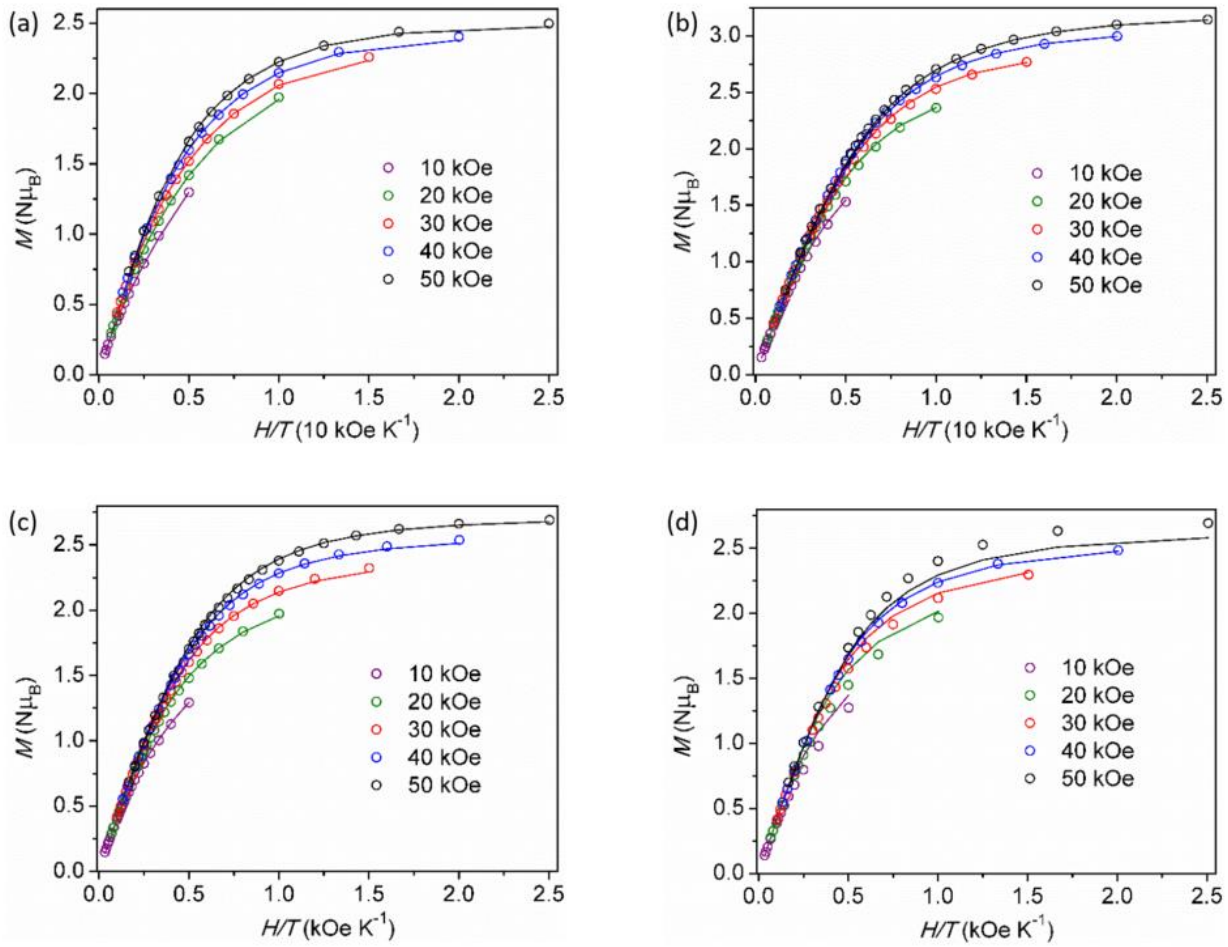


Figure S15. Reduced magnetization of **1–4**. Curves are presented for **1** (a), **2** (b), **3** (c), **4** (d), with lines representing fits obtained from PHI**.**[1]

AC Magnetic Data

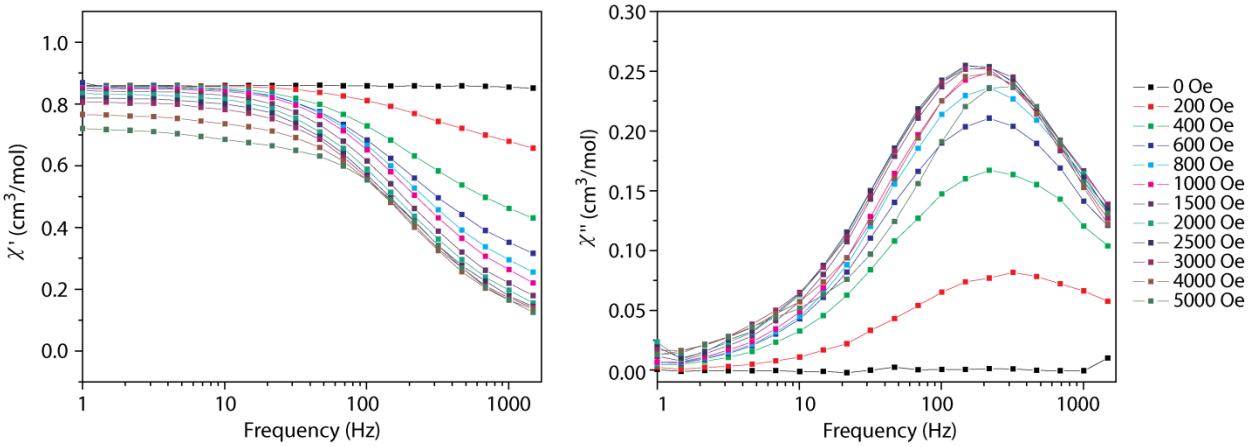


Figure S16. Field scan of **1**. Frequency dependence of χ' (left) and χ'' (right) for **1** at various applied fields. Lines are guides for the eye. T = 1.9 K, H_{ac} = 4 Oe.

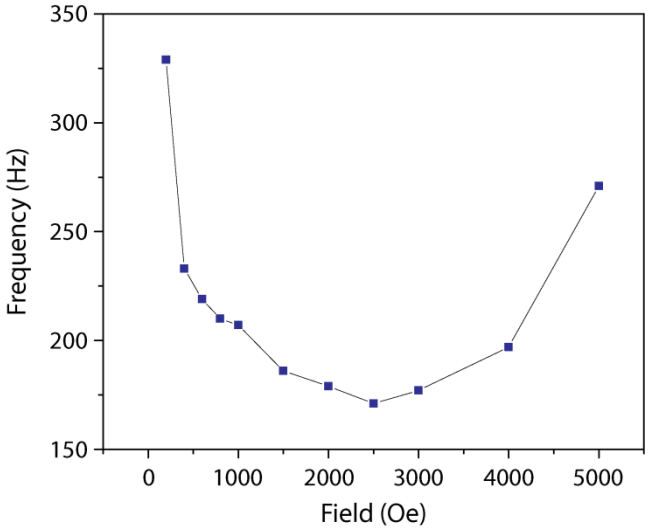


Figure S17. Determination of optimal field for **1**. Plot of χ'' maxima as a function of applied dc field for **1**. Line is a guide for the eye. 2500 Oe was selected as the optimal field for data collection.

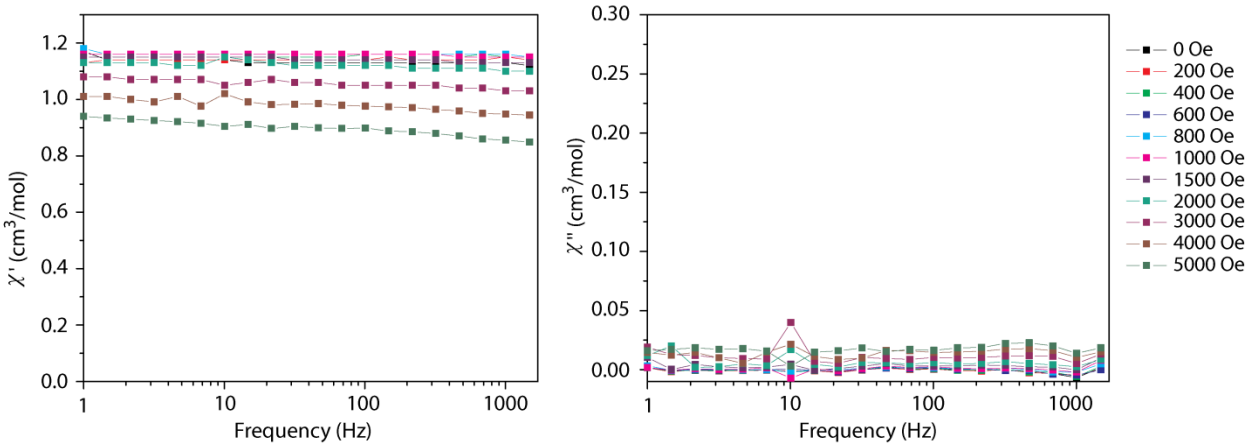


Figure S18. Field scan for **2**. Frequency dependence of χ' (left) and χ'' (right) for **2** at applied fields. Lines are guides for the eye. T = 1.9 K, H_{ac} = 4 Oe.

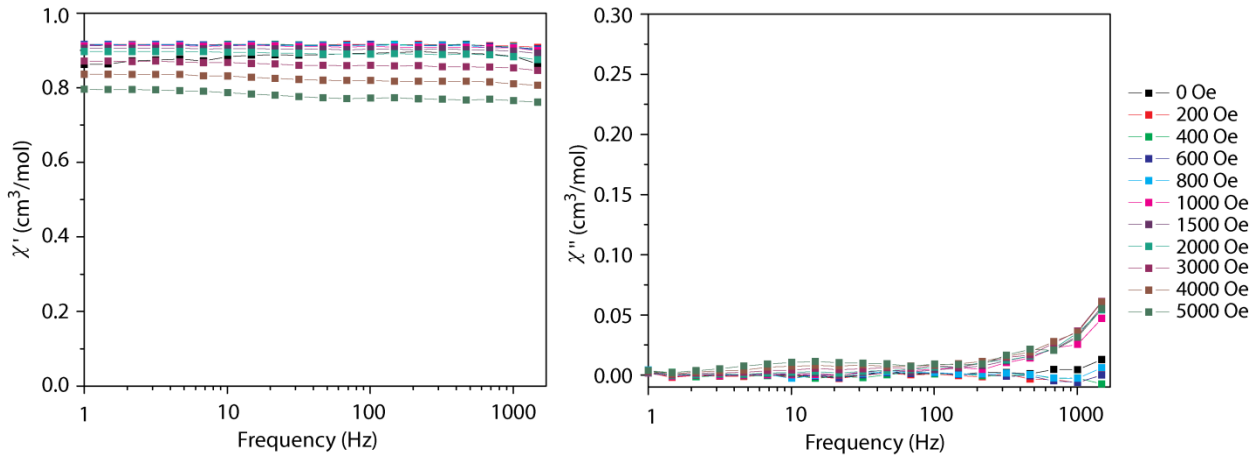


Figure S19. Field scan for **3**. Frequency dependence of χ' (left) and χ'' (right) for **3** at applied fields. Lines are guides for the eye. T = 1.9 K, H_{ac} = 4 Oe.

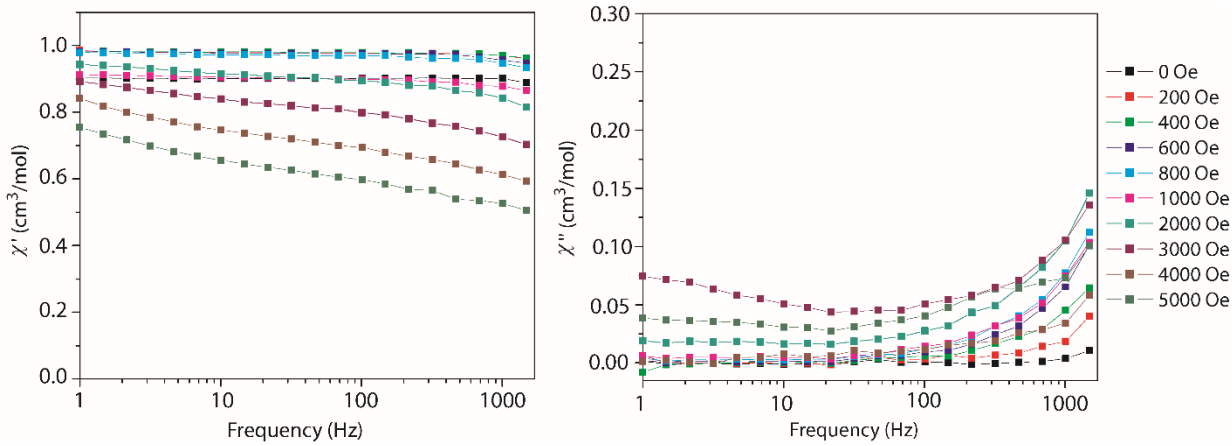


Figure S20. Field scan for **4**. Frequency dependence of χ' (left) and χ'' (right) for **4** at applied fields. Lines are guides for the eye. T = 1.9 K, H_{ac} = 4 Oe.

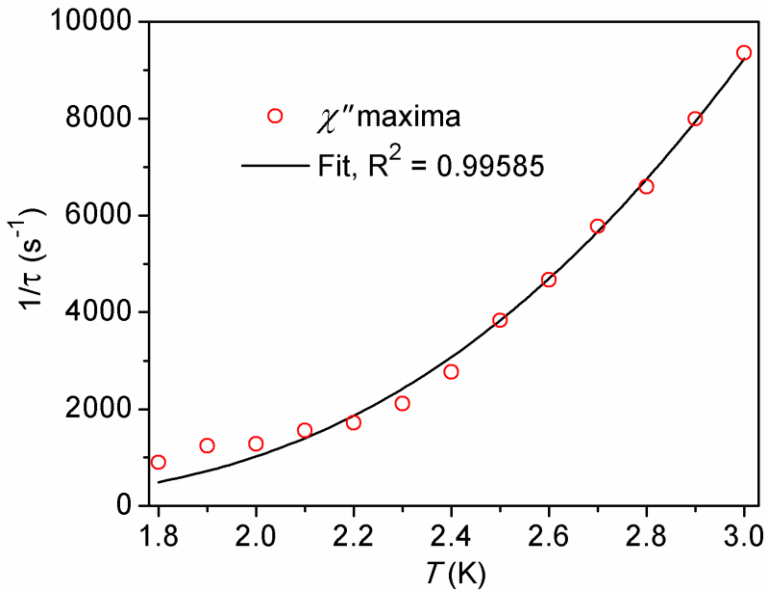


Figure S21. Arrhenius plot for **1**. Plot of frequency of χ'' maxima as a function of temperature. The black line represents the fit for an Orbach-only process according to: $\tau^{-1} = \tau_0^{-1} \exp(-U_{eff}/k_B T)$, giving $\tau_0 = 1.33\times10^{-6}$, $U_{eff} = 13.2$ K ($R^2 = 0.99585$). Inclusion of a term for a Raman process gave a better overall fit, but the values obtained were unreasonable.

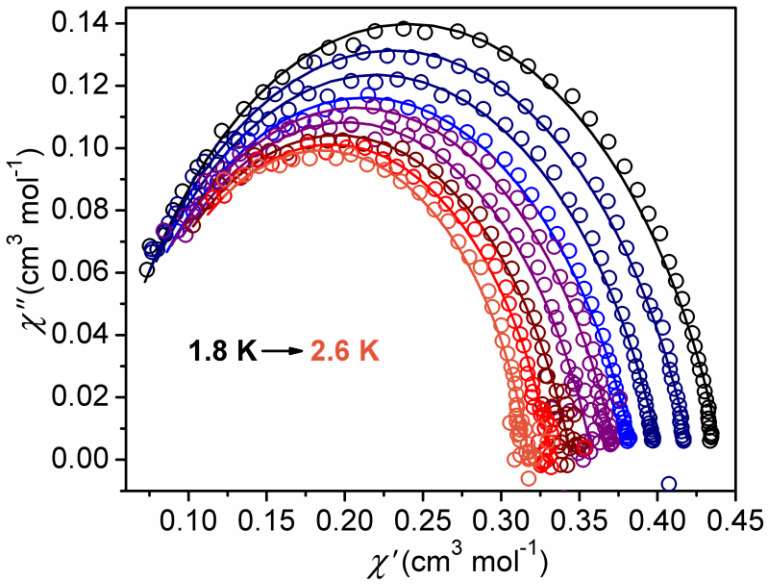


Figure S22. Cole-Cole plot for 1. The solid lines represent the fits obtained using CC-FIT.[4]

Table 5. Cole-Cole fitting parameters for **1** obtained from CC-FIT.[4] (R^2 = 0.999994 – 0.998939)

T (K)	χT (cm^3 mol^{-1})	χ_S (cm^3 mol^{-1})	τ (s)	α
1.8	0.440992	0.0405351	0.00101355	0.223774
1.9	0.421695	0.0386417	0.000872805	0.234623
2.0	0.402011	0.0383541	0.000739255	0.240319
2.1	0.385489	0.0398789	0.000625119	0.246331
2.2	0.374114	0.0401691	0.000555120	0.242854
2.3	0.358760	0.0433569	0.000460015	0.233843
2.4	0.345062	0.0453503	0.000383200	0.226611
2.5	0.332303	0.0500297	0.000310977	0.208008
2.6	0.317976	0.0519745	0.000240475	0.183466

These parameters were fit for an Orbach only process according to $\tau^{-1} = \tau_0^{-1} \exp(-U_{eff}/k_B T)$, giving $\tau_0 = 8.25\times10^{-7}$, U_{eff} = 10.1 K (R^2 = 0.99559).

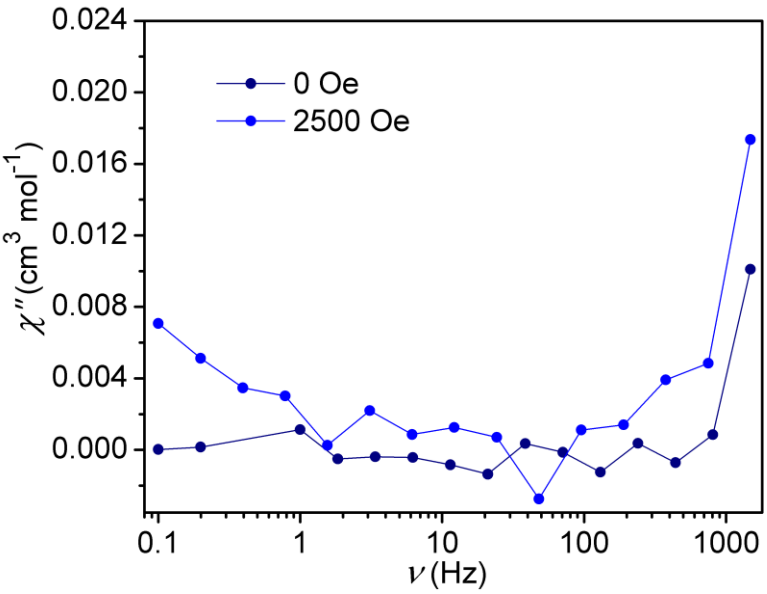


Figure S23. Field scan for $[CoL^{5\text{-}OOMe}](ClO_4)_2$. Frequency dependence of χ'' for the perchlorate salt of the ester-containing Co(II) complex at applied fields. Lines are guides for the eye. T = 1.9 K, H_{ac} = 4 Oe.

Electronic Structure Calculations

Electronic structure computations were started from the X-ray coordinates of **1**, with sp^3 C-H bond distances adjusted to 1.096 Å and sp^2 C-H bond distances adjusted to 1.090 Å prior to optimization. To maintain consistency, halide and perchlorate ions were placed along the three-fold axis, even for the anions that are disordered in the experimentally determined crystal structures. Geometry optimizations were carried out for each complex and Co-N metric parameters are collected in Table 1 in the main manuscript; computed total energies are collected in Table S7; atomic coordinates are provided as supplemental material (Tables S12-S23). Geometry optimizations in the G09 suite of electronic structure codes[5] utilized the LANL2[6] basis and effective core potential for Cl, Br, and Cr; the Stoll basis and potential were used for I[7] and H, C, and N were described with a 6-31g* model.[8–10] Restricted and unrestricted B3LYP and APFD hybrid density functionals were used in geometry optimizations.[11] All CASSCF, CASCI, and NEVPT2[12] computations utilized the ORCA suite of electronic structure codes,[13] and the Ahlrichs basis and Stuttgart pseudopotential for I.[14–17]

For the $[Co(NH_3)_7]^{2+}$ model calculations, optimized trigonal prismatic and octahedral structures were used to determine the rotational interpolation coordinate. Following a rotation about the centroid of facial plane, the Co-centroid-nitrogen angle was adjusted to maintain the Co-N distance.

Table S6. Total energies (in Hartrees) for computed structures $[CoL^{5–ONHtBu}]X_2$.

X	Related to	B3LYP	APFD	APFD (constrained)[a]
Cl	(**1**)	-2467.00834602	-2465.41606693	-2465.41514016
Br	(**2**)	-2463.44634974	-2461.86356267	-2461.86250858
I	(**3**)	-3028.72939569	-3027.06745301	-3027.06612363
ClO_4	(**4**)	-3067.64838012	-3065.61813113	-3065.61606927

[a] $Co\text{-}N_{bridge}$ distance constrained to that found experimentally

Table S7. Co-N bond distances (Å) for $[CoL^{5–ONHtBu}]X_2$ computed structures.

	B3LYP			APFD			APFD (constrained)[a]		
X	$Co\text{-}N_{bridge}$	$Co\text{-}N_{im}$	$Co\text{-}N_{py}$	$Co\text{-}N_{bridge}$	$Co\text{-}N_{im}$	$Co\text{-}N_{py}$	$Co\text{-}N_{bridge}$	$Co\text{-}N_{im}$	$Co\text{-}N_{py}$
Cl	2.711	2.169	2.310	2.378	2.159	2.266	2.574	2.154	2.238
Br	2.767	2.166	2.298	2.435	2.156	2.255	2.592	2.152	2.232
I	2.806	2.164	2.289	2.446	2.153	2.254	2.633	2.150	2.226
ClO_4	2.82	2.155	2.304	2.458	2.146	2.259	2.706	2.143	2.224

[a] $Co\text{-}N_{bridge}$ distance constrained to that found experimentally

Table S8. Computed *g* matrices for $[CoL^{5-ONHtBu}]X_2$.

X	Theory	g_{xx}	g_{yy}	g_{zz}	g_{iso}
Cl	B3LYP	2.068542	2.0814247	2.0817106	2.0772257
	CASSCF	2.177436	2.29738	2.298286	2.257701
	NEVPT2	2.152467	2.23867	2.239258	2.210132
	CASCI	2.181483	2.300091	2.301655	2.261076
Br	B3LYP	2.0526756	2.0643781	2.0646598	2.0605712
	CASSCF	2.172846	2.300113	2.302075	2.258345
	NEVPT2	2.148605	2.241192	2.242514	2.21077
	CASCI	2.176595	2.303329	2.304911	2.261612
I	B3LYP	2.0683886	2.0862396	2.0869088	2.0805123
	CASSCF	2.166893	2.314089	2.315256	2.265413
	NEVPT2	2.143905	2.252294	2.252877	2.216359
	CASCI	2.170405	2.314814	2.318342	2.267854
ClO_4	B3LYP	2.0691314	2.0890993	2.089304	2.0825116
	CASSCF	2.157189	2.338906	2.340017	2.278704
	NEVPT2	2.156937	2.338928	2.340034	2.278633
	CASCI	2.160941	2.340566	2.343033	2.281514

Table S9. Computed *D* (cm^{-1}) and *E/D* for $[CoL^{5-ONHtBu}]X_2$.

	CASSCF		NEVPT2		CASCI	
X	*D*	*E/D*	*D*	*E/D*	*D*	*E/D*
Cl	9.145237	0.003495	5.41296	0.006063	9.771335	0.030578
Br	9.815953	0.008753	5.939889	0.010532	10.544559	0.018662
I	11.631674	0.005952	7.235317	0.007068	12.378117	0.006461
ClO_4	14.844217	0.00345	8.204523	0.005878	15.866687	0.001770

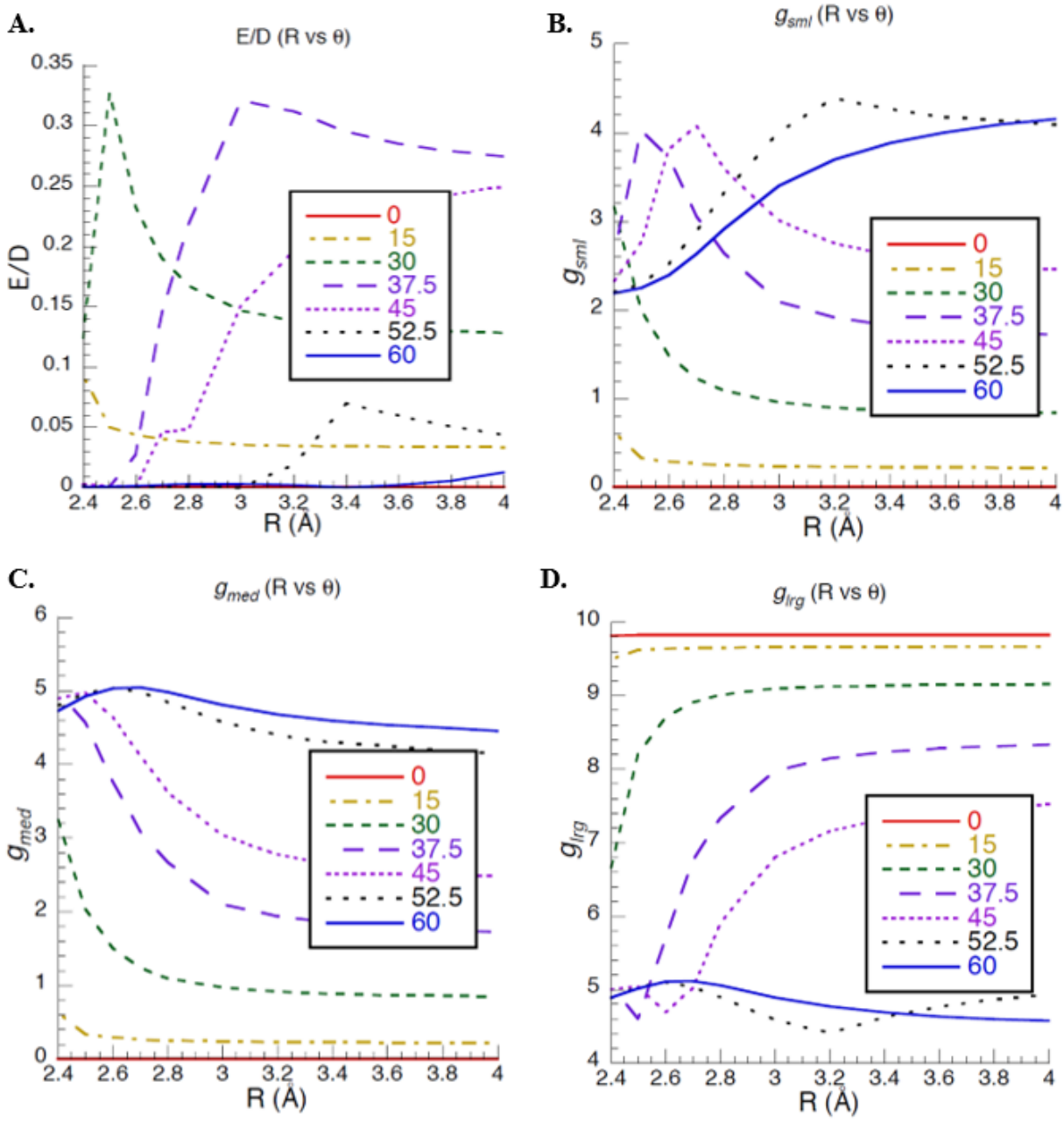


Figure S24. Calculated *E/D* (a), g_{sml} (b), g_{med} (c), and g_{lrg} (d) as a function of the seventh Co-N distance (R) at given distortion angles calculated using CASCI**.**

Table S10. Computed excitation energies (EE in eV), D (cm^{-1}), and E/D contributions per state for $[CoL^{5–ONHtBu}]X_2$.

		CASSCF			NEVPT2			APFD TD-DFT
X	State[a]	EE	*D*	*E/D*	EE	*D*	*E/D*	EE
Cl	1(Q)	0.409	12.917	4.451	0.52	10.219	-2.553	1.0021
	2(Q)	0.411	12.829	-4.454	0.523	10.153	2.509	1.0132
	3(Q)	0.913	-18.447	0.001	1.099	-15.348	0.002	1.6651
	4(Q)	1.055	1.345	0.633	1.287	1.103	0.981	2.1865
	5(Q)	1.063	1.257	-0.595	1.298	1.029	-0.918	2.2023
	6(D)	2.188	-1.244	-0.918	1.9	-1.431	-1.419	
	7(D)	2.193	-1.268	0.924	1.908	-1.457	1.441	
Br	1(Q)	0.401	13.037	11.82	0.51	10.325	8.62	0.9881
	2(Q)	0.403	12.979	-11.773	0.513	10.29	-8.598	0.997
	3(Q)	0.93	-18.085	0.001	1.121	-15.042	0.001	1.6846
	4(Q)	1.065	1.346	1.143	1.302	1.102	1.012	2.2037
	5(Q)	1.072	1.289	-1.096	1.308	1.057	-0.972	2.212
	6(D)	2.163	-1.289	-1.245	2.163	-1.494	-1.484	
	7(D)	2.168	-1.301	1.254	2.168	-1.506	1.494	
I	1(Q)	0.375	13.62	-1.471	0.478	10.771	-10.757	0.9526
	2(Q)	0.375	13.59	1.484	0.478	10.763	10.748	0.9583
	3(Q)	0.948	-17.808	0	1.144	-14.786	0	1.7096
	4(Q)	1.067	1.427	0.837	1.306	1.163	0.872	2.2189
	5(Q)	1.071	1.376	-0.79	1.311	1.126	-0.831	2.2273
	6(D)	2.124	-1.374	0.574	1.806	-1.619	0.273	
	7(D)	2.127	-1.371	-0.55	1.81	-1.614	-0.245	
ClO_4	1(Q)	0.334	14.737	9.303	0.424	11.928	5.748	0.9007
	2(Q)	0.335	14.712	-9.281	0.425	11.917	-5.742	0.9094
	3(Q)	0.975	-17.382	-0.001	1.175	-14.513	-0.001	1.7464
	4(Q)	1.068	1.516	1.506	1.306	1.245	1.235	2.2409
	5(Q)	1.071	1.479	-1.474	1.309	1.212	-1.205	2.2452
	6(D)	2.048	-1.498	-1.401	1.716	-1.787	-1.664	
	7(D)	2.05	-1.505	1.411	1.719	-1.797	1.677	

[a] Q = quartet; D = doublet

For comparison, the computed D, E/D and g data for the bis-trispyrazolylborate Co(II) complex g 1.377180 1.381479 8.541500, iso = 3.766720 D = -110.885342, E/D = 0.210239 compares well to the experimental results of 1.0 and 8.5
Marts, A. R.; Greer, S.M.Whitehead, D. R.; Woodruff, T. M.; Breece, R. M.; Shim, S. W.; Oseback, S. N.; Papish, E. T.; Jacobsen, F. E.; Cohen, S. M.; Tierney, D. L. "Dual Mode EPR Studies of a Kramers ion: High-Spin Co(II) in 4-, 5- and 6-Coordination" Appl. Magn. Räson. 2011, 40, 501-511

Table S11. Atomic coordinates for the B3LYP structure $[CoL^{5-ONHtBu}]Cl_2$.

atom	*x*	*y*	*z*
Co	2.292053	0.001273	-0.002163
N	0.946536	-0.929712	1.629185
N	3.09149	0.677524	1.896426
N	5.003348	-0.00029	-0.002733
N	3.091229	-1.982462	-0.36833
N	0.943605	-0.945061	-1.622142
N	3.09175	1.305953	-1.538931
N	0.946974	1.878719	-0.012453
C	-0.129451	-1.709224	1.490451
C	-0.835052	-2.243411	2.581502
C	-0.37938	-1.945572	3.866094
C	0.715246	-1.098739	4.022429
C	1.353227	-0.609958	2.881133
C	2.536108	0.251456	2.966357
C	4.368967	1.373911	1.945614
C	5.425282	0.435368	1.343487
C	5.425947	-1.38372	-0.298997
C	4.368714	-2.375354	0.209148
C	2.534288	-2.694259	-1.272643
C	1.349735	-2.188854	-1.972926
C	0.708557	-2.932864	-2.964886
C	-0.38921	-2.374848	-3.615583
C	-0.84443	-1.113889	-3.229102
C	-0.135419	-0.436062	-2.223409
C	5.426129	0.947596	-1.052848
C	4.369497	1.000648	-2.16652
C	2.534071	2.444101	-1.707354
C	1.350576	2.800516	-0.919364
C	0.70863	4.030674	-1.071506
C	-0.386858	4.318571	-0.260992
C	-0.839011	3.357625	0.643935
C	-0.129388	2.148374	0.731584
H	-0.435919	-1.924799	0.475287
C	-2.0058	-3.195227	2.444349
H	-0.888413	-2.387963	4.716055
H	1.082014	-0.828486	5.008279
H	2.934801	0.486264	3.95915
H	4.644205	1.653225	2.971801
H	4.281125	2.289822	1.350514
H	6.43068	0.880006	1.311868
H	5.497849	-0.448165	1.985923
H	6.430514	-1.579427	0.103515

atom	*x*	*y*	*z*
H	5.501147	-1.497219	-1.385331
H	4.64402	-3.402979	-0.0649
H	4.280887	-2.32129	1.300048
H	2.931875	-3.67135	-1.567459
H	1.074731	-3.921669	-3.224966
H	-0.901236	-2.890141	-4.421537
C	-2.019027	-0.520243	-3.980191
H	-0.442516	0.550092	-1.900778
H	6.431409	0.697066	-1.42201
H	5.499953	1.945465	-0.60857
H	4.645088	1.749656	-2.921436
H	4.281741	0.027352	-2.662321
H	2.931023	3.185759	-2.408838
H	1.072694	4.74723	-1.801883
H	-0.899272	5.27385	-0.307143
C	-2.010568	3.715408	1.535831
H	-0.433608	1.378862	1.428783
O	-2.196428	-0.861647	-5.151552
O	-2.17904	-4.040072	3.325417
O	-2.188407	4.902142	1.81884
C	-3.993966	1.020324	-3.813884
C	-3.978287	-3.828277	1.025951
C	-3.977526	2.804973	2.802962
N	-2.75947	-3.034281	1.331043
H	-2.685835	-2.132796	0.847133
N	-2.771122	0.363477	-3.282421
H	-2.693466	0.334626	-2.260001
N	-2.759122	2.670803	1.962526
H	-2.68568	1.797843	1.428842
C	-5.056353	-3.572502	2.097502
H	-5.964656	-4.139774	1.863038
H	-4.698585	-3.880854	3.083027
H	-5.317702	-2.508825	2.133436
C	-4.474419	-3.348171	-0.347749
H	-4.686583	-2.273813	-0.340871
H	-3.724157	-3.539278	-1.123887
H	-5.390245	-3.883457	-0.619382
C	-3.625179	-5.324853	0.957467
H	-4.515394	-5.901118	0.680626
H	-2.854695	-5.50253	0.198241
H	-3.25794	-5.685894	1.919912
C	-4.490827	1.968075	-2.709992
H	-3.743411	2.739279	-2.48995

atom	*x*	*y*	*z*
H	-5.409908	2.466729	-3.035104
H	-4.697913	1.424333	-1.782177
C	-5.069045	-0.039568	-4.124912
H	-5.979627	0.443512	-4.498098
H	-4.710341	-0.73904	-4.884082
H	-5.326844	-0.601853	-3.220268
C	-3.646976	1.829126	-5.076752
H	-2.879773	2.579314	-4.852631
H	-3.277955	1.177735	-5.871173
H	-4.540152	2.352781	-5.436195
C	-5.060176	3.593696	2.040197
H	-5.968049	3.675606	2.649125
H	-4.707241	4.600852	1.804838
H	-5.320198	3.083102	1.106033
C	-3.626936	3.506142	4.127704
H	-3.266597	4.521368	3.951608
H	-4.516754	3.553183	4.765812
H	-2.852296	2.946536	4.66476
C	-4.466709	1.375128	3.086028
H	-4.677666	0.835311	2.156754
H	-3.713148	0.806463	3.64336
H	-5.381977	1.408137	3.686231
Cl	8.396536	0.00309	0.001224
Cl	-2.627763	0.000687	0.007476

Table S12. Atomic coordinates for the B3LYP structure [$CoL^{5–ONHtBu}$]Br_2.

atom	*x*	*y*	*z*
Co	1.971376	-0.000084	-0.001506
N	0.667258	1.847444	-0.407728
N	2.796374	0.924446	-1.778195
N	4.738019	-0.000684	-0.002075
N	2.796541	1.074445	1.688199
N	0.666287	-0.572506	1.80149
N	2.796766	-2.001713	0.082802
N	0.663568	-1.274624	-1.395904
C	-0.379972	2.307919	0.283476
C	-1.049553	3.499072	-0.042569
C	-0.596077	4.224718	-1.145021
C	0.466515	3.731389	-1.897612
C	1.078438	2.542854	-1.495407
C	2.246366	2.001025	-2.195901
C	4.063078	0.469828	-2.331855

atom	*x*	*y*	*z*
C	5.140301	0.667907	-1.25257
C	5.140497	0.748045	1.202101
C	4.063121	1.781565	1.570539
C	2.247355	0.896568	2.829608
C	1.079099	0.019199	2.948256
C	0.468511	-0.229231	4.178949
C	-0.594101	-1.127778	4.22905
C	-1.049272	-1.716605	3.048424
C	-0.381254	-1.400767	1.853868
C	5.141157	-1.417601	0.044089
C	4.063551	-2.254674	0.753167
C	2.246453	-2.900355	-0.641794
C	1.077141	-2.563457	-1.459032
C	0.46557	-3.50483	-2.288961
C	-0.599244	-3.099458	-3.089369
C	-1.055176	-1.783012	-3.00699
C	-0.386288	-0.9066	-2.136551
H	-0.685838	1.716665	1.137361
C	-2.168888	4.096737	0.785754
H	-1.078753	5.166695	-1.383354
H	0.832791	4.263087	-2.770831
H	2.642775	2.560726	-3.049812
H	4.332609	1.01842	-3.244668
H	3.963035	-0.591693	-2.584371
H	6.130896	0.327286	-1.586587
H	5.233213	1.741074	-1.057828
H	6.131117	1.207435	1.073844
H	5.233166	0.042879	2.034162
H	4.332892	2.297868	2.501943
H	3.96268	2.530819	0.777364
H	2.644472	1.355101	3.741503
H	0.83643	0.258751	5.076671
H	-1.07539	-1.39479	5.164052
C	-2.167922	-2.733511	3.150225
H	-0.688379	-1.842568	0.914297
H	6.130884	-1.536012	0.507971
H	5.236425	-1.785076	-0.982655
H	4.333369	-3.319388	0.732155
H	3.963782	-1.945053	1.799666
H	2.642746	-3.919635	-0.701667

atom	*x*	*y*	*z*
H	0.833976	-4.52605	-2.316605
H	-1.081601	-3.775485	-3.787526
C	-2.176005	-1.363574	-3.936424
H	-0.695438	0.127052	-2.046996
O	-2.289733	-3.361851	4.203431
O	-2.29136	5.323	0.79971
O	-2.299087	-1.962339	-5.006591
C	-4.105539	-3.791041	1.951086
C	-4.102562	3.591214	2.307424
C	-4.114291	0.203447	-4.251221
N	-2.93211	3.211846	1.471307
H	-2.920879	2.241734	1.144382
N	-2.933534	-2.879194	2.042044
H	-2.922268	-2.108356	1.368183
N	-2.940962	-0.330368	-3.508636
H	-2.927523	-0.130278	-2.504799
C	-5.193518	4.232618	1.427684
H	-6.065698	4.493385	2.038369
H	-4.818233	5.141867	0.951494
H	-5.518374	3.533525	0.649057
C	-4.62748	2.289236	2.933589
H	-4.918397	1.565242	2.164932
H	-3.8639	1.823019	3.567223
H	-5.502157	2.504168	3.556406
C	-3.659119	4.559851	3.418307
H	-4.513436	4.794763	4.063201
H	-2.880405	4.101518	4.038971
H	-3.270066	5.489114	2.99825
C	-4.636324	-3.673646	0.513279
H	-3.876861	-3.988043	-0.212161
H	-5.51341	-4.317252	0.388672
H	-4.925153	-2.643917	0.276926
C	-5.192074	-3.355556	2.953838
H	-6.065185	-4.013612	2.873816
H	-4.812199	-3.405331	3.977315
H	-5.517186	-2.329867	2.746628
C	-3.661978	-5.239182	2.224347
H	-2.886763	-5.543757	1.51167
H	-3.268398	-5.346023	3.236852
H	-4.517586	-5.913613	2.10551

atom	*x*	*y*	*z*
C	-5.201017	-0.882878	-4.370626
H	-6.076192	-0.484806	-4.897195
H	-4.823658	-1.74499	-4.926174
H	-5.522172	-1.215115	-3.37706
C	-3.674123	0.689042	-5.643979
H	-3.283844	-0.135467	-6.243245
H	-4.530552	1.130218	-6.166387
H	-2.897402	1.457412	-5.554591
C	-4.642881	1.391317	-3.431212
H	-4.928622	1.083031	-2.41979
H	-3.883425	2.177187	-3.34467
H	-5.521589	1.819715	-3.924528
Br	8.350041	0.000492	-0.000481
Br	-3.063996	-0.000326	0.00448

Table S13. Atomic coordinates for the B3LYP structure $[CoL^{5–ONHtBu}]I_2$.

atom	*x*	*y*	*z*
Co	-1.691952	0.000069	0.001714
N	-0.416911	1.877014	0.304285
N	-2.533917	1.004051	1.724793
N	-4.498391	0.00011	0.002359
N	-2.534143	0.988258	-1.729609
N	-0.41643	-0.677808	-1.774537
N	-2.534157	-1.993723	0.011778
N	-0.414857	-1.199657	1.475197
C	0.602883	2.328743	-0.432717
C	1.243995	3.553978	-0.184191
C	0.80129	4.316929	0.897492
C	-0.230567	3.834007	1.698401
C	-0.825338	2.616402	1.363315
C	-1.983383	2.096263	2.097676
C	-3.793672	0.56467	2.306605
C	-4.884864	0.711554	1.231734
C	-4.8851	0.708904	-1.228545
C	-3.793602	1.71238	-1.639936
C	-1.984669	0.763085	-2.862077
C	-0.826701	-0.133142	-2.945036
C	-0.233693	-0.454485	-4.167198
C	0.798312	-1.389424	-4.184355
C	1.243081	-1.94161	-2.982113

atom	*x*	*y*	*z*
C	0.603733	-1.541569	-1.796746
C	-4.88517	-1.420241	0.004284
C	-3.794002	-2.27845	-0.659299
C	-1.983648	-2.862002	0.772133
C	-0.824494	-2.485928	1.588216
C	-0.229272	-3.384385	2.475403
C	0.804526	-2.932331	3.291683
C	1.248706	-1.614825	3.169132
C	0.606899	-0.787431	2.23241
H	0.901291	1.704711	-1.266156
C	2.305288	4.157602	-1.082409
H	1.262561	5.282119	1.077893
H	-0.591389	4.398851	2.552831
H	-2.374519	2.687655	2.932341
H	-4.059197	1.147757	3.19885
H	-3.685453	-0.485259	2.600863
H	-5.862007	0.374612	1.604822
H	-4.993908	1.775387	0.998555
H	-5.861889	1.201146	-1.123039
H	-4.995145	-0.025224	-2.032884
H	-4.0594	2.19288	-2.591291
H	-3.684646	2.492803	-0.878521
H	-2.376631	1.188762	-3.791891
H	-0.595967	0.000797	-5.084134
H	1.258174	-1.717873	-5.110403
C	2.304815	-3.02091	-3.054287
H	0.903949	-1.949197	-0.839315
H	-5.862188	-1.574895	-0.474278
H	-4.994806	-1.749623	1.042318
H	-4.059668	-3.342601	-0.599256
H	-3.685771	-2.009665	-1.716025
H	-2.375209	-3.880237	0.868394
H	-0.591063	-4.406303	2.53932
H	1.266316	-3.570714	4.037429
C	2.3126	-1.138641	4.138083
H	0.906261	0.245869	2.106931
O	2.371952	-3.697091	-4.081827
O	2.375405	5.385706	-1.148671
O	2.383208	-1.692647	5.236098
C	4.184744	-4.164131	-1.8413

atom	*x*	*y*	*z*
C	4.181731	3.681945	-2.683936
C	4.192203	0.484279	4.52005
N	3.075104	3.280368	-1.772241
H	3.124282	2.324614	-1.411684
N	3.078091	-3.174114	-1.951296
H	3.129153	-2.380887	-1.30772
N	3.083857	-0.105239	3.71944
H	3.131771	0.058179	2.711028
C	5.282125	4.41226	-1.889826
H	6.105076	4.692154	-2.55764
H	4.885826	5.319864	-1.428051
H	5.685381	3.762569	-1.104854
C	4.740394	2.384676	-3.289754
H	5.111246	1.706088	-2.513822
H	3.971254	1.856489	-3.865612
H	5.569324	2.619702	-3.965435
C	3.63038	4.580787	-3.805452
H	4.436084	4.82835	-4.505723
H	2.843267	4.059931	-4.36303
H	3.219484	5.507856	-3.401836
C	4.746543	-4.03388	-0.416703
H	3.978452	-4.263305	0.33136
H	5.574527	-4.737299	-0.280523
H	5.119583	-3.022284	-0.222826
C	5.282837	-3.846323	-2.874761
H	6.10619	-4.563953	-2.781676
H	4.884239	-3.905224	-3.890484
H	5.686134	-2.840738	-2.710301
C	3.632782	-5.585735	-2.051341
H	2.847442	-5.804929	-1.318579
H	3.219397	-5.704211	-3.054471
H	4.438798	-6.315368	-1.914287
C	5.29175	-0.569271	4.756591
H	6.115935	-0.13059	5.330909
H	4.895124	-1.42125	5.314154
H	5.693405	-0.926838	3.801771
C	3.643399	1.010057	5.858717
H	3.232646	0.198928	6.462498
H	4.450442	1.493444	6.420712
H	2.856706	1.753643	5.685744

atom	*x*	*y*	*z*
C	4.750919	1.654799	3.695609
H	5.119885	1.319093	2.720266
H	3.98232	2.417964	3.525224
H	5.581173	2.122987	4.234484
I	-8.405622	0.000291	0.000137
I	3.518257	0.001544	-0.005958

Table S14. Atomic coordinates for the B3LYP structure $[CoL^{5–ONHtBu}](ClO_4)_2$.

atom	x	y	z
Co	-1.748585	0.007244	0.000397
N	-0.4768	1.821473	-0.622801
N	-2.597262	1.689959	1.045909
N	-4.568438	0.004153	-0.001944
N	-2.593239	0.070306	-1.981157
N	-0.478373	-1.448558	-1.259372
N	-2.593186	-1.742369	0.933449
N	-0.481087	-0.35652	1.889109
C	0.541018	1.892773	-1.486857
C	1.157641	3.102528	-1.847618
C	0.683801	4.276562	-1.260226
C	-0.350474	4.20938	-0.330965
C	-0.913398	2.965988	-0.044864
C	-2.065797	2.834982	0.85477
C	-3.848256	1.559706	1.782488
C	-4.955454	1.192215	0.781195
C	-4.951726	0.088711	-1.423495
C	-3.842985	0.775117	-2.238009
C	-2.064086	-0.670377	-2.876403
C	-0.914813	-1.518826	-2.539555
C	-0.355614	-2.39069	-3.473366
C	0.674653	-3.23375	-3.066762
C	1.148002	-3.157636	-1.756075
C	0.535595	-2.237428	-0.888971
C	-4.951411	-1.269713	0.634711
C	-3.841816	-2.317426	0.448992
C	-2.064104	-2.148281	2.022154
C	-0.914879	-1.432086	2.588482
C	-0.351728	-1.807804	3.807807
C	0.681681	-1.036682	4.332239
C	1.154484	0.060508	3.610704

atom	x	y	z
C	0.536349	0.355872	2.384282
H	0.870824	0.949595	-1.905883
C	2.253869	3.256506	-2.888063
H	1.131208	5.219336	-1.555934
H	-0.733273	5.104178	0.150887
H	-2.46848	3.745014	1.312225
H	-4.10718	2.486382	2.312379
H	-3.722465	0.762987	2.524098
H	-5.912423	1.043831	1.296422
H	-5.095504	2.031913	0.094463
H	-5.909829	0.606481	-1.555326
H	-5.087625	-0.925821	-1.809038
H	-4.0993	0.773309	-3.306098
H	-3.717065	1.814792	-1.9158
H	-2.467417	-0.729065	-3.892992
H	-0.738462	-2.419112	-4.489238
H	1.118618	-3.963351	-3.735375
C	2.238372	-4.141046	-1.367462
H	0.86527	-2.132141	0.13774
H	-5.90827	-1.644231	0.250678
H	-5.089319	-1.096619	1.705857
H	-4.098854	-3.242248	0.983035
H	-3.714062	-2.556655	-0.6126
H	-2.466163	-3.000753	2.579877
H	-0.733527	-2.674332	4.339518
H	1.129327	-1.2537	5.29608
C	2.251164	0.884091	4.263382
H	0.86483	1.194057	1.78131
O	2.34552	-5.171747	-2.034966
O	2.371468	4.353158	-3.438469
O	2.363231	0.82058	5.489249
C	4.168859	-4.621772	0.164588
C	4.180477	2.16506	-4.071517
C	4.188603	2.440893	3.906025
N	3.019156	2.16966	-3.137887
H	2.957725	1.373762	-2.505047
N	3.01106	-3.81134	-0.307415
H	2.955885	-2.863088	0.060589
N	3.023611	1.634328	3.444636
H	2.96377	1.479069	2.439663

atom	x	y	z
C	5.243549	3.172772	-3.592213
H	6.109857	3.148902	-4.2632
H	4.839694	4.187611	-3.581326
H	5.586651	2.91702	-2.58343
C	4.76355	0.743213	-4.044855
H	5.103493	0.465136	-3.042118
H	4.021803	0.004065	-4.369034
H	5.619427	0.68657	-4.725125
C	3.703899	2.507358	-5.49474
H	4.552517	2.470767	-6.187165
H	2.955872	1.781687	-5.834478
H	3.265689	3.506579	-5.531035
C	4.766785	-3.87773	1.36931
H	4.032063	-3.773488	2.176135
H	5.621248	-4.44068	1.758353
H	5.11232	-2.875968	1.094065
C	5.223461	-4.734001	-0.953605
H	6.087706	-5.304851	-0.595005
H	4.809452	-5.241297	-1.827804
H	5.572363	-3.739385	-1.253026
C	3.683196	-6.016127	0.600152
H	2.938796	-5.931455	1.40035
H	3.237622	-6.554874	-0.238341
H	4.528861	-6.598801	0.982575
C	5.242427	1.520312	4.551826
H	6.109834	2.110712	4.868532
H	4.82976	1.012058	5.426152
H	5.586416	0.767648	3.83355
C	3.714944	3.513742	4.903237
H	3.270214	3.055666	5.788789
H	4.566441	4.128651	5.215972
H	2.973155	4.171898	4.436166
C	4.781846	3.114105	2.658143
H	5.119725	2.375702	1.923889
H	4.046844	3.765465	2.171225
H	5.640577	3.728152	2.947875
Cl	3.547985	-0.006583	-0.007431
O	2.958663	-1.122208	1.0365
O	2.968594	1.458277	0.439519
O	2.961451	-0.348474	-1.498144

atom	x	y	z
O	5.150926	-0.013808	-0.007697
Cl	-8.40099	-0.002869	0.002479
O	-7.818336	-0.117682	1.527192
O	-10.004912	-0.007469	0.008585
O	-7.830397	1.378677	-0.662032
O	-7.823953	-1.265017	-0.86367

Table S15. Atomic coordinates for the APFD structure $[CoL^{5–ONHtBu}]Cl_2$.

atom	*x*	*y*	*z*
Co	2.324544	-0.012439	0.03104
N	0.964641	1.750447	-0.391334
N	2.962918	0.846568	-1.847713
N	4.702855	-0.032835	0.05614
N	2.93482	1.16211	1.739806
N	0.928729	-0.542105	1.741189
N	2.911718	-2.077929	0.218383
N	0.946449	-1.220779	-1.295293
C	-0.061935	2.151767	0.344101
C	-0.883689	3.224486	-0.019858
C	-0.608379	3.88757	-1.210134
C	0.448667	3.450602	-2.003916
C	1.214668	2.379376	-1.554678
C	2.372725	1.87497	-2.29925
C	4.228947	0.367686	-2.329862
C	5.192871	0.617528	-1.172123
C	5.178658	0.701581	1.238031
C	4.204032	1.819749	1.604524
C	2.311791	1.047941	2.838419
C	1.148947	0.154802	2.872285
C	0.349767	0.013876	4.002664
C	-0.709908	-0.889666	3.958999
C	-0.948621	-1.598919	2.787999
C	-0.092363	-1.384219	1.701532
C	5.153059	-1.42907	0.11255
C	4.159679	-2.286523	0.890522
C	2.284547	-2.97369	-0.42086
C	1.14185	-2.551221	-1.232676
C	0.340285	-3.459739	-1.914303
C	-0.70434	-2.967241	-2.691522
C	-0.928885	-1.59542	-2.736508

atom	*x*	*y*	*z*
C	-0.063631	-0.76129	-2.017907
H	-0.226178	1.621907	1.272008
C	-1.990045	3.719368	0.865478
H	-1.220694	4.734771	-1.502569
H	0.687031	3.936236	-2.944877
H	2.707739	2.412319	-3.190655
H	4.565542	0.87879	-3.240486
H	4.126168	-0.702462	-2.547367
H	6.229053	0.309853	-1.381005
H	5.224227	1.698952	-0.99956
H	6.203252	1.069097	1.074194
H	5.223546	0.009668	2.085431
H	4.519173	2.340841	2.516542
H	4.119021	2.555618	0.795513
H	2.626689	1.550177	3.756866
H	0.560647	0.592526	4.896447
H	-1.350015	-1.048381	4.821032
C	-2.054637	-2.617067	2.7319
H	-0.229526	-1.930886	0.779353
H	6.162834	-1.49814	0.520159
H	5.200782	-1.82181	-0.908109
H	4.468392	-3.338478	0.911828
H	4.051525	-1.934005	1.92367
H	2.571096	-4.028837	-0.410223
H	0.536147	-4.525181	-1.840677
H	-1.347824	-3.631346	-3.260116
C	-2.040193	-1.062772	-3.596639
H	-0.18199	0.313233	-2.045359
O	-2.396347	-3.213461	3.757046
O	-2.261291	4.924458	0.882247
O	-2.391733	-1.693632	-4.596153
C	-3.664883	-3.701001	1.151148
C	-3.717371	2.948581	2.503713
C	-3.720731	0.785115	-3.762135
N	-2.584082	2.749732	1.589169
H	-2.482395	1.793176	1.229231
N	-2.558898	-2.797232	1.495987
H	-2.423606	-2.012217	0.850332
N	-2.561119	0.103661	-3.165994
H	-2.396547	0.318	-2.178224
C	-4.945072	3.422207	1.7165
H	-5.808489	3.529065	2.382996

atom	*x*	*y*	*z*
H	-4.745161	4.388306	1.245239
H	-5.200244	2.696661	0.934793
C	-3.994002	1.586845	3.145778
H	-4.256993	0.838635	2.389273
H	-3.112543	1.22718	3.689606
H	-4.825111	1.66958	3.853537
C	-3.343884	3.959261	3.590733
H	-4.175844	4.067221	4.295554
H	-2.464364	3.615063	4.146936
H	-3.122668	4.936322	3.156792
C	-3.821858	-3.621973	-0.369709
H	-2.903224	-3.947207	-0.871386
H	-4.64094	-4.270219	-0.696548
H	-4.043118	-2.597916	-0.689841
C	-4.951786	-3.233482	1.838674
H	-5.790839	-3.885463	1.570218
H	-4.828549	-3.25263	2.925303
H	-5.196606	-2.210333	1.532059
C	-3.317381	-5.134297	1.558774
H	-2.386858	-5.452884	1.075776
H	-3.19354	-5.216369	2.640925
H	-4.117582	-5.812789	1.242328
C	-4.972361	-0.090765	-3.626284
H	-5.848606	0.427543	-4.032596
H	-4.841662	-1.032106	-4.167206
H	-5.162485	-0.316939	-2.571068
C	-3.442028	1.111549	-5.229603
H	-3.303946	0.199251	-5.814852
H	-4.284059	1.67438	-5.647772
H	-2.539359	1.726233	-5.3194
C	-3.904455	2.083494	-2.973948
H	-4.080165	1.873808	-1.913146
H	-3.014262	2.717935	-3.056467
H	-4.76112	2.642644	-3.363899
Cl	8.682654	0.061454	-0.237932
Cl	-2.639597	-0.002214	0.012017

Table S16. Atomic coordinates for the APFD structure $[CoL^{5–ONHtBu}]Br_2$.

atom	*x*	*y*	*z*
Co	-2.000665	-0.011255	0.012086
N	-0.652577	1.596784	0.841332
N	-2.637878	0.346653	2.039265

atom	*x*	*y*	*z*
N	-4.43597	-0.009197	0.012013
N	-2.637201	1.561347	-1.318401
N	-0.648308	-0.098368	-1.789312
N	-2.642756	-1.947486	-0.686675
N	-0.645205	-1.530942	0.981746
C	0.329449	2.21615	0.204472
C	1.119344	3.203911	0.804421
C	0.867077	3.528076	2.133701
C	-0.142199	2.855636	2.818429
C	-0.888952	1.903649	2.130235
C	-2.023985	1.206059	2.742324
C	-3.886264	-0.255262	2.403569
C	-4.889971	0.276784	1.381799
C	-4.890104	1.034487	-0.920323
C	-3.883101	2.181828	-0.977524
C	-2.027862	1.73087	-2.418461
C	-0.889785	0.852874	-2.710269
C	-0.140885	0.964389	-3.878609
C	0.876906	0.040615	-4.105448
C	1.135708	-0.933872	-3.14712
C	0.34174	-0.952784	-1.994904
C	-4.895196	-1.337033	-0.423906
C	-3.891512	-1.964648	-1.389631
C	-2.032422	-2.985428	-0.286545
C	-0.885807	-2.801496	0.608827
C	-0.122487	-3.869982	1.070994
C	0.911015	-3.608704	1.967567
C	1.16854	-2.293987	2.343136
C	0.357406	-1.284938	1.810861
H	0.476865	1.940158	-0.831833
C	2.158612	3.971063	0.038232
H	1.4554	4.304403	2.613473
H	-0.36212	3.075336	3.858673
H	-2.32804	1.471581	3.75863
H	-4.203243	-0.010173	3.425185
H	-3.77883	-1.342875	2.318816
H	-5.898501	-0.122084	1.551652
H	-4.948148	1.362754	1.505735
H	-5.896795	1.384563	-0.657307
H	-4.953998	0.597345	-1.921875
H	-4.200695	2.942331	-1.702088
H	-3.771199	2.655438	0.004906

atom	*x*	*y*	*z*
H	-2.335259	2.470839	-3.162615
H	-0.364636	1.745568	-4.598522
H	1.467054	0.062508	-5.01665
C	2.185541	-1.975913	-3.406532
H	0.494788	-1.703994	-1.230809
H	-5.902835	-1.281171	-0.856343
H	-4.959363	-1.985214	0.455576
H	-4.209745	-2.973923	-1.680299
H	-3.782213	-1.35523	-2.294251
H	-2.343726	-3.999337	-0.553071
H	-0.345474	-4.881568	0.745997
H	1.514771	-4.410009	2.382717
C	2.235552	-2.00507	3.360134
H	0.506986	-0.249714	2.089798
O	2.436707	-2.311905	-4.565643
O	2.404941	5.138266	0.349136
O	2.510711	-2.852783	4.211676
C	3.806468	-3.502848	-2.25962
C	3.767118	3.791125	-1.873035
C	3.85118	-0.241507	4.107131
N	2.715516	3.283358	-0.979614
H	2.661518	2.265923	-0.908605
N	2.744728	-2.485795	-2.289648
H	2.685997	-1.896235	-1.4572
N	2.780582	-0.775746	3.252719
H	2.704571	-0.33729	2.33294
C	5.046287	4.062619	-1.073526
H	5.842745	4.415549	-1.738345
H	4.865417	4.824351	-0.309946
H	5.389324	3.146145	-0.580124
C	4.014779	2.690233	-2.90649
H	4.349695	1.76369	-2.425638
H	3.100197	2.472583	-3.470766
H	4.78767	3.009512	-3.612902
C	3.285328	5.06021	-2.579434
H	4.051039	5.401782	-3.284559
H	2.365803	4.859882	-3.141099
H	3.088986	5.858642	-1.86041
C	4.062305	-3.805409	-0.781635
H	3.151649	-4.175744	-0.296221
H	4.838845	-4.571056	-0.686332
H	4.395918	-2.909002	-0.245765

atom	*x*	*y*	*z*
C	5.078067	-2.95219	-2.913846
H	5.882177	-3.695194	-2.86725
H	4.891151	-2.70422	-3.962363
H	5.412645	-2.047674	-2.39337
C	3.331851	-4.772533	-2.969981
H	2.419384	-5.155993	-2.499326
H	3.125984	-4.577322	-4.024826
H	4.105626	-5.544896	-2.899607
C	5.134312	-1.055129	3.90745
H	5.94382	-0.647167	4.523309
H	4.97228	-2.099102	4.190304
H	5.448155	-1.020315	2.857866
C	3.412022	-0.263523	5.572857
H	3.242872	-1.286023	5.917434
H	4.189071	0.193397	6.195478
H	2.486511	0.308864	5.702826
C	4.068314	1.205722	3.65954
H	4.372029	1.254009	2.607287
H	3.149183	1.791697	3.778426
H	4.853072	1.669405	4.265748
Br	-8.467854	0.004954	0.007238
Br	3.073049	0.028789	-0.034014

Table S17. Atomic coordinates for the APFD structure $[CoL^{5–ONHtBu}]I_2$.

atom	*x*	*y*	*z*
Co	1.722914	0.003698	-0.004165
N	0.385391	-1.458492	1.071958
N	2.366275	-0.023277	2.050531
N	4.168821	0.00116	-0.00428
N	2.361559	-1.761588	-1.058829
N	0.386193	-0.189515	-1.808449
N	2.368337	1.79741	-1.007644
N	0.384881	1.665535	0.719202
C	-0.576127	-2.197822	0.539785
C	-1.341762	-3.100757	1.28686
C	-1.093271	-3.198001	2.652584
C	-0.107778	-2.396696	3.22368
C	0.623647	-1.55192	2.393081
C	1.751281	-0.753972	2.885776
C	3.608809	0.639742	2.312738
C	4.619519	-0.047313	1.394458
C	4.615834	-1.186932	-0.747261

atom	*x*	*y*	*z*
C	3.602556	-2.323572	-0.614479
C	1.747043	-2.114249	-2.11147
C	0.620531	-1.285458	-2.553135
C	-0.11406	-1.578416	-3.698862
C	-1.100536	-0.681627	-4.101191
C	-1.345471	0.450793	-3.330257
C	-0.574811	0.643796	-2.177415
C	4.620184	1.236543	-0.662597
C	3.609352	1.690087	-1.714928
C	1.753335	2.886222	-0.793322
C	0.623228	2.85729	0.14151
C	-0.112557	3.99676	0.455299
C	-1.103803	3.898698	1.428728
C	-1.351548	2.666202	2.025572
C	-0.579517	1.570587	1.62154
H	-0.720414	-2.101967	-0.529266
C	-2.331712	-4.029608	0.644319
H	-1.661521	-3.905245	3.249032
H	0.111189	-2.441824	4.286065
H	2.051091	-0.844016	3.933486
H	3.92381	0.56916	3.361344
H	3.494037	1.697421	2.048772
H	5.622177	0.388114	1.503651
H	4.689373	-1.096537	1.698444
H	5.617019	-1.503098	-0.424764
H	4.68754	-0.924547	-1.807492
H	3.917725	-3.196841	-1.199163
H	3.485827	-2.623775	0.433315
H	2.044773	-2.975056	-2.716153
H	0.101978	-2.474594	-4.272522
H	-1.673817	-0.843	-5.009043
C	-2.345395	1.467097	-3.800955
H	-0.713109	1.51947	-1.555722
H	5.621674	1.112031	-1.096473
H	4.692887	2.024843	0.093412
H	3.926894	2.631903	-2.179532
H	3.491756	0.932481	-2.498553
H	2.051261	3.838515	-1.240331
H	0.106338	4.940435	-0.034784
H	-1.67665	4.766687	1.740673
C	-2.346543	2.573051	3.146368
H	-0.722275	0.594887	2.069608

atom	*x*	*y*	*z*
O	-2.542467	1.608939	-5.008964
O	-2.514846	-5.147924	1.128062
O	-2.545402	3.556804	3.861304
C	-3.918366	3.249122	-3.006226
C	-3.8976	-4.261081	-1.297602
C	-3.899965	1.00117	4.328058
N	-2.915003	-3.542757	-0.471137
H	-2.915648	-2.527554	-0.57061
N	-2.923754	2.182375	-2.813219
H	-2.908673	1.759918	-1.884571
N	-2.914992	1.357828	3.294016
H	-2.901474	0.75192	2.473438
C	-5.172929	-4.521815	-0.489654
H	-5.917216	-5.034355	-1.109483
H	-4.953418	-5.146019	0.380917
H	-5.605461	-3.576059	-0.142955
C	-4.204268	-3.349505	-2.487067
H	-4.640408	-2.399173	-2.156537
H	-3.293514	-3.130684	-3.057006
H	-4.919501	-3.838242	-3.156291
C	-3.29164	-5.573726	-1.800176
H	-4.006619	-6.080646	-2.457235
H	-2.37713	-5.379287	-2.371958
H	-3.049384	-6.238316	-0.967852
C	-4.216977	3.808696	-1.614222
H	-3.308054	4.212489	-1.152293
H	-4.953019	4.615728	-1.686719
H	-4.622936	3.033056	-0.953648
C	-5.194028	2.672745	-3.629875
H	-5.944696	3.460988	-3.755674
H	-4.977804	2.236737	-4.609079
H	-5.616828	1.89402	-2.984541
C	-3.332189	4.354668	-3.888312
H	-2.414566	4.754736	-3.442307
H	-3.101011	3.978788	-4.887476
H	-4.054888	5.172802	-3.979871
C	-5.182208	1.818588	4.141707
H	-5.925486	1.533691	4.894892
H	-4.973618	2.886967	4.242586
H	-5.610701	1.635896	3.149502
C	-3.299989	1.234227	5.717106
H	-3.068643	2.290357	5.872713

atom	*x*	*y*	*z*
H	-4.013743	0.915163	6.484356
H	-2.380311	0.650815	5.838313
C	-4.194199	-0.488069	4.140556
H	-4.617114	-0.68746	3.148556
H	-3.280693	-1.084245	4.251872
H	-4.915845	-0.822044	4.892858
I	8.537909	-0.000576	0.006729
I	-3.48071	-0.014931	0.003497

Table S18. Atomic coordinates for the APFD structure $[CoL^{5–ONHtBu}](ClO_4)_2$.

atom	*x*	*y*	*z*
Co	1.88308	0.003785	-0.016611
N	0.54649	1.63483	-0.820678
N	2.52821	0.374073	-2.030081
N	4.341141	0.004049	-0.017363
N	2.529146	1.560354	1.31344
N	0.547492	-0.117581	1.802627
N	2.52913	-1.925139	0.666464
N	0.53595	-1.50629	-1.021633
C	-0.427832	2.264624	-0.182341
C	-1.225755	3.242131	-0.788086
C	-0.979545	3.550138	-2.122331
C	0.034104	2.882509	-2.802959
C	0.7826	1.93539	-2.112126
C	1.91215	1.234184	-2.729428
C	3.764491	-0.246273	-2.401738
C	4.788537	0.272256	-1.393373
C	4.788515	1.062136	0.902342
C	3.763718	2.193603	0.958594
C	1.918156	1.731949	2.411545
C	0.789447	0.845819	2.712153
C	0.047059	0.96567	3.88249
C	-0.96456	0.040946	4.122312
C	-1.216427	-0.956086	3.185332
C	-0.42617	-0.985959	2.030485
C	4.789877	-1.321469	0.437854
C	3.765969	-1.939333	1.388311
C	1.913312	-2.959922	0.268745
C	0.777379	-2.775058	-0.639125
C	0.023867	-3.847539	-1.1046
C	-1.000013	-3.592937	-2.011598
C	-1.251507	-2.283714	-2.409697

atom	*x*	*y*	*z*
C	-0.448169	-1.269315	-1.875911
H	-0.572322	1.98616	0.854698
C	-2.319303	3.990577	-0.078483
H	-1.583735	4.310149	-2.607461
H	0.250754	3.096383	-3.845148
H	2.207763	1.496025	-3.749201
H	4.07431	-0.012407	-3.428233
H	3.641269	-1.331796	-2.308503
H	5.781074	-0.154271	-1.57951
H	4.871971	1.355401	-1.524344
H	5.780514	1.437367	0.62534
H	4.873605	0.634405	1.905951
H	4.074676	2.96637	1.673075
H	3.637554	2.654841	-0.028249
H	2.217552	2.480918	3.14995
H	0.267315	1.758411	4.590851
H	-1.563399	0.076973	5.026821
C	-2.309284	-1.944784	3.481438
H	-0.57707	-1.740138	1.267385
H	5.781718	-1.268705	0.901471
H	4.876169	-1.975486	-0.43492
H	4.075769	-2.946799	1.694172
H	3.642852	-1.320496	2.285049
H	2.2127	-3.97465	0.545677
H	0.243797	-4.856533	-0.769435
H	-1.608752	-4.393525	-2.419552
C	-2.358886	-2.048322	-3.398411
H	-0.596953	-0.232552	-2.153489
O	-2.682431	-2.089061	4.647818
O	-2.704287	5.065203	-0.544487
O	-2.735281	-2.987323	-4.103703
C	-3.924062	-3.56076	2.468728
C	-3.910919	3.936699	1.847291
C	-4.002832	-0.381299	-4.265715
N	-2.784321	3.416693	1.051061
H	-2.608751	2.422187	1.175199
N	-2.790222	-2.620148	2.41695
H	-2.618851	-2.221688	1.496412
N	-2.851631	-0.793113	-3.44139
H	-2.666935	-0.188555	-2.643972
C	-5.199122	3.866274	1.019284
H	-6.05266	4.211236	1.613843

atom	*x*	*y*	*z*
H	-5.117196	4.497173	0.129673
H	-5.392706	2.835194	0.70194
C	-4.030849	3.03557	3.078555
H	-4.270819	2.005207	2.798804
H	-3.094979	3.028814	3.650103
H	-4.827222	3.408775	3.730458
C	-3.62416	5.370359	2.299836
H	-4.440002	5.719697	2.942137
H	-2.693165	5.409775	2.876835
H	-3.53536	6.04419	1.445842
C	-4.066729	-4.154072	1.065122
H	-3.137414	-4.645245	0.752464
H	-4.86652	-4.901635	1.062647
H	-4.313811	-3.384015	0.327876
C	-5.20091	-2.802151	2.848394
H	-6.061396	-3.480728	2.84673
H	-5.103973	-2.364894	3.846174
H	-5.393093	-1.997561	2.129301
C	-3.634389	-4.687194	3.463421
H	-2.714159	-5.214194	3.18643
H	-3.524525	-4.300087	4.477982
H	-4.459426	-5.407797	3.447677
C	-5.261339	-1.119389	-3.794678
H	-6.132991	-0.789663	-4.371326
H	-5.144658	-2.198794	-3.925839
H	-5.449718	-0.912201	-2.734934
C	-3.720607	-0.658335	-5.744311
H	-3.589031	-1.726213	-5.928105
H	-4.558765	-0.296548	-6.349977
H	-2.814229	-0.13192	-6.064677
C	-4.176157	1.125177	-4.059946
H	-4.421857	1.361397	-3.020133
H	-3.260133	1.664608	-4.329123
H	-4.988098	1.490495	-4.696923
Cl	-3.49556	0.01025	0.024308
O	-2.923014	-1.462952	-0.260012
O	-2.928428	0.9908	-1.113506
O	-2.925145	0.507357	1.44009
O	-5.082882	0.005351	0.026493
Cl	8.383323	-0.015509	-0.002705
O	7.840107	-1.224493	-0.898255
O	9.977397	-0.029705	0.002623

atom	*x*	*y*	*z*
O	7.861255	1.369399	-0.60895
O	7.841529	-0.177396	1.493802

Table S19. Coordinates for the APFD (Co-N_{bridge} constrained) structure $[CoL^{5–ONHtBu}]Cl_2$.

atom	*x*	*y*	*z*
Co	2.260001	0.00911	-0.007207
N	0.927251	-0.926853	-1.544096
N	2.979227	-2.004355	-0.262487
N	4.833992	0.01469	-0.003761
N	2.976086	1.22069	-1.638168
N	0.931352	1.809945	-0.058976
N	2.971491	0.816537	1.859663
N	0.948403	-0.863914	1.579295
C	-0.110078	-0.366753	-2.147488
C	-0.927292	-1.058876	-3.048963
C	-0.627931	-2.390971	-3.316058
C	0.444956	-2.992369	-2.661963
C	1.201892	-2.22279	-1.783119
C	2.36898	-2.761959	-1.07818
C	4.226028	-2.342694	0.363435
C	5.260141	-1.371813	-0.207437
C	5.255384	0.885005	-1.103862
C	4.228274	0.853766	-2.235934
C	2.361539	2.30076	-1.89697
C	1.197072	2.648503	-1.077875
C	0.436742	3.788925	-1.319355
C	-0.62822	4.068882	-0.466578
C	-0.916524	3.190545	0.573316
C	-0.098272	2.065559	0.733946
C	5.252125	0.53487	1.299966
C	4.219295	1.525215	1.839625
C	2.358585	0.498125	2.924884
C	1.204152	-0.398962	2.81614
C	0.448434	-0.777653	3.92203
C	-0.599647	-1.675818	3.733511
C	-0.876448	-2.139636	2.451548
C	-0.064187	-1.698066	1.400415
H	-0.290888	0.676943	-1.925341
C	-2.064414	-0.392225	-3.769889
H	-1.234929	-2.940524	-4.029261
H	0.698266	-4.03421	-2.832816
H	2.690581	-3.785046	-1.292301

atom	*x*	*y*	*z*
H	4.526435	-3.382309	0.180014
H	4.11043	-2.196388	1.443935
H	6.259541	-1.542765	0.21313
H	5.332489	-1.555946	-1.284305
H	6.261306	0.619196	-1.454357
H	5.308876	1.912887	-0.730322
H	4.525776	1.527662	-3.049555
H	4.125111	-0.160136	-2.640162
H	2.680342	2.991959	-2.682168
H	0.682632	4.4437	-2.149759
H	-1.236669	4.959025	-0.595162
C	-2.039574	3.50797	1.519741
H	-0.269355	1.365325	1.541618
H	6.255275	0.977637	1.245189
H	5.310727	-0.302417	2.003132
H	4.515356	1.894554	2.829891
H	4.110514	2.381241	1.16355
H	2.674373	0.838143	3.915264
H	0.685382	-0.385413	4.906231
H	-1.203029	-2.022283	4.567213
C	-1.981405	-3.13578	2.242282
H	-0.224269	-2.049661	0.389214
O	-2.334701	4.685178	1.7399
O	-2.368185	-0.765679	-4.905341
O	-2.256742	-3.937848	3.137663
C	-3.760546	2.445226	2.992902
C	-3.803146	1.39007	-3.520917
C	-3.702667	-3.870757	0.580231
N	-2.642529	0.607075	-3.073651
H	-2.509957	0.574257	-2.05744
N	-2.61562	2.421548	2.071024
H	-2.489265	1.542829	1.558132
N	-2.564674	-3.055999	1.029325
H	-2.461948	-2.155463	0.549795
C	-5.027364	0.476682	-3.649766
H	-5.906795	1.05599	-3.952991
H	-4.846791	-0.3012	-4.39713
H	-5.24529	-0.004479	-2.689251
C	-4.04571	2.446818	-2.440404
H	-4.255824	1.980905	-1.47096
H	-3.167892	3.093797	-2.325316
H	-4.900769	3.07242	-2.715931

atom	*x*	*y*	*z*
C	-3.492854	2.078766	-4.851678
H	-4.341438	2.704686	-5.149047
H	-2.610138	2.720799	-4.752792
H	-3.304928	1.344922	-5.638522
C	-4.00838	0.991219	3.401279
H	-3.126835	0.571318	3.900263
H	-4.854135	0.93759	4.094284
H	-4.235472	0.368258	2.528783
C	-4.993104	3.009916	2.277575
H	-5.860582	3.001622	2.947215
H	-4.809628	4.039078	1.956154
H	-5.232816	2.404982	1.395478
C	-3.421236	3.275929	4.232294
H	-2.533599	2.871355	4.731784
H	-3.228386	4.31726	3.965393
H	-4.258271	3.242353	4.938369
C	-4.93734	-3.555854	1.432193
H	-5.799577	-4.13576	1.084024
H	-4.750711	-3.802945	2.481112
H	-5.187092	-2.490875	1.362173
C	-3.350173	-5.357694	0.659291
H	-3.155876	-5.660024	1.690684
H	-4.181818	-5.954044	0.267989
H	-2.460195	-5.572195	0.056718
C	-3.955486	-3.480615	-0.878147
H	-4.19946	-2.415909	-0.967583
H	-3.070326	-3.681017	-1.493479
H	-4.792369	-4.06097	-1.279773
Cl	8.620225	0.022225	-0.002403
Cl	-2.576905	-0.031887	0.043963

Table S20. Coordinates for the APFD (Co-N_{bridge} constrained) structure $[CoL^{5–ONHtBu}]Br_2$.

atom	*x*	*y*	*z*
Co	1.949545	0.018503	0.009623
N	0.657728	-1.59564	0.850013
N	2.675827	-0.335762	2.003343
N	4.541531	0.024087	0.002719
N	2.66818	-1.520438	-1.311422
N	0.637761	0.098869	-1.793616
N	2.665601	1.930386	-0.671359
N	0.629589	1.539492	0.97452
C	-0.328903	-2.225531	0.23041

atom	*x*	*y*	*z*
C	-1.093873	-3.222398	0.847034
C	-0.809024	-3.542267	2.171164
C	0.207189	-2.859914	2.835421
C	0.928829	-1.899311	2.132556
C	2.071697	-1.192501	2.719448
C	3.915576	0.285305	2.372068
C	4.957385	-0.238854	1.381769
C	4.952933	-1.038007	-0.917524
C	3.907354	-2.153852	-0.962592
C	2.060004	-1.70385	-2.410768
C	0.910166	-0.844583	-2.71361
C	0.178891	-0.962095	-3.892468
C	-0.850307	-0.053151	-4.128713
C	-1.137832	0.914644	-3.171286
C	-0.360371	0.941506	-2.008154
C	4.953305	1.351295	-0.45807
C	3.904035	1.951121	-1.395867
C	2.055241	2.972747	-0.280628
C	0.89879	2.805361	0.60575
C	0.14942	3.885609	1.06316
C	-0.897544	3.639168	1.948077
C	-1.182452	2.328601	2.320002
C	-0.384024	1.305997	1.794455
H	-0.497695	-1.948819	-0.802779
C	-2.141085	-4.005009	0.107339
H	-1.378191	-4.325568	2.662518
H	0.451481	-3.078842	3.870356
H	2.389504	-1.449249	3.733779
H	4.215013	0.061168	3.403883
H	3.793996	1.370062	2.269141
H	5.950935	0.182224	1.585688
H	5.035345	-1.322218	1.518936
H	5.94526	-1.429823	-0.656927
H	5.032077	-0.612795	-1.923382
H	4.204247	-2.933747	-1.675393
H	3.78482	-2.609797	0.027031
H	2.376102	-2.446485	-3.148549
H	0.424711	-1.735589	-4.613452
H	-1.427741	-0.080808	-5.047873
C	-2.20081	1.940615	-3.442222
H	-0.531907	1.687182	-1.24223
H	5.943087	1.320116	-0.933016

atom	*x*	*y*	*z*
H	5.038602	2.009454	0.412395
H	4.197444	2.961024	-1.709855
H	3.781287	1.327261	-2.288922
H	2.371045	3.983492	-0.553795
H	0.392765	4.894207	0.743542
H	-1.492099	4.449467	2.35894
C	-2.267468	2.065026	3.325154
H	-0.551563	0.271228	2.066462
O	-2.44602	2.270915	-4.604169
O	-2.37238	-5.170474	0.435832
O	-2.541252	2.927317	4.162402
C	-3.853195	3.446532	-2.311261
C	-3.78908	-3.860681	-1.772378
C	-3.929725	0.344269	4.065828
N	-2.72296	-3.333672	-0.907318
H	-2.67357	-2.315015	-0.853263
N	-2.777703	2.443639	-2.33128
H	-2.717988	1.856864	-1.496947
N	-2.831658	0.844042	3.224736
H	-2.746665	0.388853	2.313905
C	-5.048797	-4.131099	-0.942259
H	-5.856515	-4.499119	-1.584937
H	-4.845554	-4.881075	-0.172747
H	-5.388335	-3.210645	-0.453859
C	-4.06683	-2.77497	-2.814096
H	-4.397867	-1.844695	-2.337816
H	-3.166269	-2.558072	-3.400878
H	-4.852185	-3.108743	-3.499816
C	-3.312548	-5.135148	-2.472629
H	-4.090928	-5.492104	-3.155914
H	-2.407429	-4.934977	-3.057255
H	-3.093745	-5.922276	-1.747698
C	-4.120766	3.751996	-0.835863
H	-3.218397	4.139079	-0.34795
H	-4.909711	4.505768	-0.748093
H	-4.442758	2.853172	-0.296983
C	-5.113425	2.875415	-2.969889
H	-5.928026	3.607341	-2.931213
H	-4.917319	2.625296	-4.016264
H	-5.438289	1.9687	-2.447127
C	-3.3927	4.719847	-3.024345
H	-2.487423	5.117355	-2.551489

atom	*x*	*y*	*z*
H	-3.180105	4.523994	-4.077672
H	-4.177179	5.481817	-2.959511
C	-5.1933	1.176688	3.822821
H	-6.023512	0.793952	4.427166
H	-5.019128	2.222476	4.091348
H	-5.484431	1.129229	2.767195
C	-3.523216	0.385875	5.540563
H	-3.344268	1.41142	5.870581
H	-4.322268	-0.046491	6.152808
H	-2.611163	-0.199822	5.70244
C	-4.163192	-1.10715	3.640698
H	-4.444663	-1.170295	2.583126
H	-3.257648	-1.706959	3.79102
H	-4.969095	-1.545032	4.238315
Br	8.533086	-0.003631	0.036328
Br	-3.080113	-0.051891	-0.046221

Table S21. Coordinates for the APFD (Co-N_{bridge} constrained) structure $[CoL^{5–ONHtBu}]I_2$.

atom	*x*	*y*	*z*
Co	1.664263	-0.016963	0.017701
N	0.373656	-1.772349	0.478238
N	2.400569	-0.806712	1.876757
N	4.297239	-0.02788	0.015958
N	2.396033	-1.228455	-1.600903
N	0.377634	0.472469	-1.729676
N	2.408034	1.984364	-0.228609
N	0.375205	1.266054	1.301569
C	-0.600152	-2.261077	-0.275126
C	-1.353566	-3.380666	0.096942
C	-1.077692	-3.977156	1.324223
C	-0.076159	-3.445772	2.13298
C	0.642879	-2.350237	1.66299
C	1.786449	-1.791211	2.392397
C	3.637563	-0.280859	2.379768
C	4.692145	-0.579488	1.31103
C	4.690498	-0.875373	-1.108856
C	3.626199	-1.938333	-1.395641
C	1.784787	-1.173223	-2.712683
C	0.650876	-0.249832	-2.831044
C	-0.051777	-0.0793	-4.020772
C	-1.038918	0.902526	-4.073237
C	-1.318575	1.650742	-2.933204

C	-0.582973	1.382338	-1.773307
C	4.696593	1.36842	-0.153556
C	3.642018	2.148603	-0.942018
C	1.797341	2.926648	0.364029
C	0.648223	2.580112	1.207694
C	-0.080147	3.539214	1.905958
C	-1.100893	3.110696	2.751326
C	-1.383289	1.750837	2.84653
C	-0.614205	0.86372	2.08454
H	-0.762622	-1.768436	-1.22635
C	-2.360233	-4.015094	-0.819887
H	-1.637904	-4.857298	1.624699
H	0.164592	-3.885265	3.096002
H	2.096643	-2.260345	3.330025
H	3.92795	-0.721097	3.342115
H	3.515819	0.800806	2.510819
H	5.679135	-0.210533	1.624457
H	4.773128	-1.666937	1.21504
H	5.669866	-1.344737	-0.939161
H	4.787825	-0.247272	-2.000122
H	3.915326	-2.549581	-2.260043
H	3.494762	-2.59593	-0.528447
H	2.092269	-1.749853	-3.589116
H	0.191328	-0.682203	-4.890347
H	-1.584051	1.105598	-4.990013
C	-2.305871	2.780112	-3.007221
H	-0.746309	1.947467	-0.86409
H	5.68221	1.452667	-0.632449
H	4.782504	1.82726	0.836578
H	3.937443	3.200164	-1.048119
H	3.510693	1.717166	-1.941334
H	2.109725	3.97222	0.298169
H	0.164842	4.592069	1.805423
H	-1.672569	3.814979	3.347978
C	-2.419578	1.278185	3.825691
H	-0.775721	-0.206117	2.137565
O	-2.479279	3.363031	-4.078712
O	-2.554955	-5.229885	-0.752402
O	-2.651147	1.949471	4.832391
C	-3.86214	4.176818	-1.625728
C	-3.941887	-3.548982	-2.704512
C	-4.013907	-0.591174	4.317146
N	-2.94259	-3.166909	-1.693545

H	-2.93748	-2.179542	-1.434757
N	-2.893279	3.089145	-1.831755
H	-2.905214	2.351396	-1.12711
N	-2.986403	0.092774	3.515599
H	-2.947174	-0.179218	2.533352
C	-5.217042	-4.050997	-2.01933
H	-5.970549	-4.31768	-2.769008
H	-5.002186	-4.933641	-1.410679
H	-5.635895	-3.271464	-1.372374
C	-4.239529	-2.283513	-3.511026
H	-4.651213	-1.492935	-2.872399
H	-3.329564	-1.90108	-3.988625
H	-4.971251	-2.505476	-4.294417
C	-3.361689	-4.619974	-3.631555
H	-4.085808	-4.852199	-4.419995
H	-2.4421	-4.257861	-4.104985
H	-3.135758	-5.536392	-3.082159
C	-4.174035	4.19193	-0.128156
H	-3.263836	4.36138	0.459532
H	-4.882612	4.995485	0.096485
H	-4.620072	3.243271	0.193982
C	-5.138204	3.904925	-2.428945
H	-5.872413	4.699671	-2.255768
H	-4.914984	3.862011	-3.498448
H	-5.584216	2.951065	-2.12442
C	-3.234963	5.512813	-2.031914
H	-2.318265	5.694786	-1.459511
H	-2.991227	5.524482	-3.096601
H	-3.937618	6.326996	-1.823639
C	-5.294243	0.24951	4.358097
H	-6.068136	-0.265555	4.93816
H	-5.09897	1.22085	4.820731
H	-5.676108	0.413483	3.343853
C	-3.48486	-0.848206	5.730215
H	-3.281538	0.090784	6.249809
H	-4.228334	-1.413097	6.30303
H	-2.560708	-1.435901	5.692445
C	-4.280564	-1.925595	3.618306
H	-4.650048	-1.77133	2.59726
H	-3.366721	-2.529424	3.56607
H	-5.035635	-2.49176	4.172846
I	8.605253	0.000432	0.021684
I	-3.533118	0.001098	-0.066937

Table S22. Coordinates for the APFD (Co-N_{bridge} constrained) $[CoL^{5–ONHtBu}](ClO_4)_2$.

atom	*x*	*y*	*z*
Co	1.796423	0.007111	0.001524
N	0.532136	0.852508	-1.622316
N	2.570924	-0.844883	-1.806896
N	4.502416	0.009892	-0.003612
N	2.571637	1.998142	0.167831
N	0.532881	0.986988	1.545526
N	2.578685	-1.127807	1.64221
N	0.535727	-1.824708	0.084408
C	-0.453531	1.72965	-1.503572
C	-1.210086	2.167592	-2.596839
C	-0.902558	1.64941	-3.8514
C	0.125114	0.720075	-3.978551
C	0.828094	0.351154	-2.836522
C	1.968991	-0.568118	-2.889666
C	3.794123	-1.592113	-1.738746
C	4.878895	-0.619846	-1.266994
C	4.880248	1.41843	0.0815
C	3.792239	2.31371	-0.517453
C	1.969567	2.796153	0.950321
C	0.827129	2.289978	1.717508
C	0.117198	3.096172	2.600847
C	-0.91654	2.522495	3.33464
C	-1.221892	1.176233	3.157665
C	-0.458149	0.446808	2.238833
C	4.883794	-0.767766	1.172907
C	3.80134	-0.690424	2.252789
C	1.985003	-2.209266	1.940684
C	0.842948	-2.626407	1.122217
C	0.146433	-3.802397	1.377938
C	-0.887171	-4.159039	0.517627
C	-1.206337	-3.331878	-0.555236
C	-0.455988	-2.162083	-0.726617
H	-0.640851	2.097375	-0.501342
C	-2.326809	3.170356	-2.505989
H	-1.472943	1.984344	-4.711986
H	0.386834	0.295793	-4.943013
H	2.284514	-0.960129	-3.86061
H	4.070413	-2.03993	-2.702153
H	3.654165	-2.39494	-1.00496
H	5.846956	-1.130758	-1.193782
H	4.987213	0.161886	-2.025636

atom	*x*	*y*	*z*
H	5.844623	1.610749	-0.404829
H	4.997558	1.683783	1.136957
H	4.068466	3.37207	-0.424811
H	3.648126	2.079512	-1.578995
H	2.28442	3.832911	1.097906
H	0.376544	4.144342	2.714428
H	-1.494123	3.101482	4.048177
C	-2.348173	0.601695	3.971921
H	-0.644545	-0.605198	2.056439
H	5.851887	-0.446319	1.575884
H	4.993462	-1.815618	0.876477
H	4.080479	-1.2977	3.123657
H	3.659112	0.346887	2.578383
H	2.307736	-2.856072	2.761169
H	0.416489	-4.42571	2.224927
H	-1.453993	-5.073443	0.660911
C	-2.331105	-3.761012	-1.457118
H	-0.65343	-1.474676	-1.541181
O	-2.704541	1.194535	4.993002
O	-2.661805	3.781574	-3.523653
O	-2.679345	-4.944292	-1.448934
C	-4.068267	-1.203153	4.096366
C	-4.054275	4.171398	-1.007088
C	-4.058709	-2.988265	-3.08377
N	-2.879468	3.325312	-1.286146
H	-2.692721	2.610378	-0.586705
N	-2.884674	-0.546582	3.510811
H	-2.69022	-0.80682	2.54677
N	-2.875709	-2.795419	-2.224559
H	-2.684995	-1.827556	-1.975927
C	-5.266668	3.635848	-1.777411
H	-6.157702	4.228157	-1.540416
H	-5.091121	3.685919	-2.855393
H	-5.459827	2.5932	-1.499929
C	-4.318182	4.080543	0.497203
H	-4.579263	3.060963	0.796035
H	-3.436738	4.392497	1.070218
H	-5.149621	4.74118	0.76281
C	-3.757263	5.624897	-1.383363
H	-4.619794	6.252329	-1.133053
H	-2.890439	5.994245	-0.823604
H	-3.551584	5.720315	-2.451255

atom	*x*	*y*	*z*
C	-4.299481	-2.490247	3.301603
H	-3.412464	-3.134467	3.330644
H	-5.137594	-3.042829	3.738104
H	-4.535605	-2.277418	2.254642
C	-5.286387	-0.282969	3.956745
H	-6.183629	-0.781797	4.340203
H	-5.135397	0.643223	4.517974
H	-5.453369	-0.032962	2.902763
C	-3.807602	-1.555866	5.562823
H	-2.930778	-2.207773	5.649
H	-3.637079	-0.658569	6.160628
H	-4.673158	-2.090813	5.969011
C	-5.270448	-3.344717	-2.215047
H	-6.165851	-3.448176	-2.838324
H	-5.101761	-4.287548	-1.687714
H	-5.452005	-2.555629	-1.476259
C	-3.784499	-4.077039	-4.124265
H	-3.592492	-5.039778	-3.646814
H	-4.652431	-4.178001	-4.785192
H	-2.916442	-3.808941	-4.737259
C	-4.308957	-1.658462	-3.797972
H	-4.553394	-0.86297	-3.087717
H	-3.427306	-1.349071	-4.371949
H	-5.147537	-1.768944	-4.492877
Cl	-3.438398	-0.005859	-0.017423
O	-2.884712	-1.339739	0.684455
O	-2.86527	0.044691	-1.516817
O	-2.853715	1.256753	0.784326
O	-5.02594	0.014095	-0.019242
Cl	8.443658	-0.015679	0.006815
O	7.896326	-1.517767	0.054721
O	10.038444	-0.031786	0.011966
O	7.922055	0.700124	-1.324637
O	7.915539	0.786548	1.285669

Table S23. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ $\varphi = 0°$ model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.41500000	-0.81700000	-1.39700000
H	-1.54707312	-1.82538539	-1.31271128
H	-2.35423266	-0.42721854	-1.31265300
H	-1.16400000	-0.67200000	-2.37500000

atom	*x*	*y*	*z*
N	1.41500000	-0.81700000	-1.39700000
H	2.35423266	-0.42721854	-1.31265300
H	1.54707312	-1.82538539	-1.31271128
H	1.16400000	-0.67200000	-2.37500000
N	0.00000000	1.63400000	-1.39700000
H	-0.80714254	2.25253613	-1.31272080
H	0.80714254	2.25253613	-1.31272080
H	0.00000000	1.34400000	-2.37500000
N	0.00000000	1.76081910	1.23293881
H	0.00000000	2.63540158	0.70794882
H	-0.80686486	1.83375061	1.85269609
H	0.80726573	1.83426950	1.85334196
N	1.52473063	-0.88072721	1.23293881
H	1.18361456	-1.61629762	1.85291462
H	2.28205016	-1.31817622	0.70794882
H	1.99158604	-0.21815875	1.85291063
N	-1.52484684	-0.88015897	1.23281032
H	-2.28233423	-1.31738932	0.70785652
H	-1.18486612	-1.61595542	1.85313096
H	-1.99193691	-0.21773149	1.85313096
N	0.00000000	0.00000000	2.30000000
H	0.00000000	0.91354546	2.70673664
H	0.79105840	-0.45693754	2.70673664
H	-0.79120115	-0.45669032	2.70673664

Table S24. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ φ = 15° model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.41500000	-0.81700000	-1.39700000
H	-1.48200000	-1.83500000	-1.37300000
H	-2.33000000	-0.36600000	-1.37300000
H	-1.16400000	-0.67200000	-2.37500000
N	1.41500000	-0.81700000	-1.39700000
H	2.33000000	-0.36600000	-1.37300000
H	1.48200000	-1.83500000	-1.37300000
H	1.16400000	-0.67200000	-2.37500000
N	0.00000000	1.63400000	-1.39700000
H	-0.84800000	2.20100000	-1.37300000
H	0.84800000	2.20100000	-1.37300000
H	0.00000000	1.34400000	-2.37500000
N	-0.45591068	1.70077316	1.23293881
H	-0.68235727	2.54553138	0.70794882
H	-1.30529637	1.59559817	1.78785426
H	0.33235006	2.03491728	1.78878565
N	1.70077316	-0.45591068	1.23293881

atom	*x*	*y*	*z*
H	1.59528557	-1.30621259	1.78760360
H	2.54553138	-0.68235727	0.70794882
H	2.03475126	0.33266259	1.78785036
N	-1.24495737	-1.24495737	1.23281032
H	-1.86340604	-1.86340604	0.70785652
H	-0.72928655	-1.92828655	1.78862129
H	-1.92828655	-0.72928655	1.78862129
H	0.71333341	0.71333341	2.65666635
H	-0.97443163	0.26109790	2.65666635
H	0.26109823	-0.97443136	2.65666686
N	0.00000000	0.00000000	2.30000000

Table S25. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ $\varphi = 30°$ model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.53210331	-0.88461372	-1.23877024
H	-2.05870571	-0.20938262	-1.79387552
H	-1.21059789	-1.67832035	-1.79362702
H	-2.28947265	-1.32190753	-0.71372186
N	1.52500670	-0.88051624	-1.23303233
H	1.20350128	-1.67422287	-1.78788911
H	2.05160910	-0.20528514	-1.78813761
H	2.28237604	-1.31781005	-0.70798395
N	0.00000000	1.76099877	-1.23306461
H	0.84800000	1.87944755	-1.78807352
H	-0.84800000	1.87944755	-1.78807352
H	0.00000000	2.63550312	-0.70787309
N	-0.81700000	1.41500000	1.39700000
H	-0.67200000	1.16400000	2.37500000
H	-0.36600000	2.33000000	1.37300000
H	-1.83500000	1.48200000	1.37300000
N	1.63400000	0.00000000	1.39700000
H	2.20100000	0.84800000	1.37300000
H	1.34400000	0.00000000	2.37500000
H	2.20100000	-0.84800000	1.37300000
N	-0.81700000	-1.41500000	1.39700000
H	-0.67200000	-1.16400000	2.37500000
H	-1.83500000	-1.48200000	1.37300000
H	-0.36600000	-2.33000000	1.37300000
H	0.87363824	0.50442575	-2.65666635
H	0.00002614	-1.00880579	-2.65666635
H	-0.87366442	0.50438006	-2.65666686
N	0.00000000	0.00000000	-2.30000000

Table S26. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ φ = 37.5° model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.69700000	-0.22300000	-1.30200000
H	-2.14300000	-1.13700000	-1.22200000
H	-2.36400000	0.54400000	-1.22200000
H	-1.50600000	-0.19800000	-2.30300000
N	1.04200000	-1.35800000	-1.30200000
H	2.05600000	-1.28700000	-1.22200000
H	0.71100000	-2.32000000	-1.22200000
H	0.92400000	-1.20500000	-2.30300000
N	0.65500000	1.58100000	-1.30200000
H	0.08700000	2.42500000	-1.22200000
H	1.65300000	1.77500000	-1.22200000
H	0.58100000	1.40300000	-2.30300000
N	-0.45597008	1.70139627	1.23337100
H	-0.68758796	2.56564990	0.74499019
H	-1.29906323	1.57382641	1.79273929
H	0.33865756	2.01286782	1.79386487
N	1.70139627	-0.45597008	1.23337100
H	1.57350030	-1.29997580	1.79249260
H	2.56564990	-0.68758796	0.74499019
H	2.01265062	0.33898386	1.79294490
N	-1.24546189	-1.24546189	1.23330992
H	-1.87889181	-1.87889181	0.74491553
H	-0.71315632	-1.91215632	1.79311552
H	-1.91215632	-0.71315632	1.79311552
N	0.00000000	0.00000000	2.30000000
H	0.71508151	0.71158102	2.65666635
H	-0.97378806	0.26348799	2.65666635
H	0.25870656	-0.97506906	2.65666686

Table S27. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ φ = 45° model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.41500000	-0.81700000	-1.39700000
H	-1.48200000	-1.83500000	-1.37300000
H	-2.33000000	-0.36600000	-1.37300000
H	-1.16400000	-0.67200000	-2.37500000
N	1.41500000	-0.81700000	-1.39700000
H	2.33000000	-0.36600000	-1.37300000
H	1.48200000	-1.83500000	-1.37300000
H	1.16400000	-0.67200000	-2.37500000
N	0.00000000	1.63400000	-1.39700000
H	-0.84800000	2.20100000	-1.37300000
H	0.84800000	2.20100000	-1.37300000

atom	*x*	*y*	*z*
H	0.00000000	1.34400000	-2.37500000
N	-1.24495737	1.24495737	1.23281032
H	-1.86340604	1.86340604	0.70785652
H	-1.92828655	0.72928655	1.78862129
H	-0.72928655	1.92828655	1.78862129
N	1.70077316	0.45591068	1.23293881
H	2.03475126	-0.33266259	1.78785036
H	2.54553138	0.68235727	0.70794882
H	1.59528557	1.30621259	1.78760360
N	-0.45591068	-1.70077316	1.23293881
H	-0.68235727	-2.54553138	0.70794882
H	0.33266259	-2.03475126	1.78785036
H	-1.30621259	-1.59528557	1.78760360
H	0.26119965	0.97440436	2.65666635
H	-0.97445869	-0.26099690	2.65666635
H	0.71325907	-0.71340749	2.65666686
N	0.00000000	0.00000000	2.30000000

Table S28. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ φ = 52.5° model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	-1.72600000	0.22700000	-1.26200000
H	-2.39000000	-0.54100000	-1.16000000
H	-2.16900000	1.14100000	-1.16000000
H	-1.57400000	0.20700000	-2.27000000
N	0.66600000	-1.60800000	-1.26200000
H	1.66300000	-1.80000000	-1.16000000
H	0.09600000	-2.44900000	-1.16000000
H	0.60700000	-1.46700000	-2.27000000
N	1.06000000	1.38100000	-1.26200000
H	0.72700000	2.34000000	-1.16000000
H	2.07300000	1.30800000	-1.16000000
H	0.96700000	1.25900000	-2.27000000
N	-0.45100000	1.68100000	1.26200000
H	-0.68691689	2.56032660	0.80298372
H	-1.29063257	1.53513670	1.82400627
H	0.34696748	1.97462614	1.82577797
N	1.68100000	-0.45100000	1.26200000
H	1.53480882	-1.29154455	1.82375974
H	2.56032660	-0.68691689	0.80298372
H	1.97440334	0.34729573	1.82486003
N	-1.23100000	-1.23100000	1.26200000
H	-1.87517502	-1.87517502	0.80165222
H	-0.68664346	-1.88564346	1.82499192
H	-1.88564346	-0.68664346	1.82499192

atom	*x*	*y*	*z*
N	0.00000000	0.00000000	2.30000000
H	0.71414198	0.71252393	2.65666635
H	-0.97413488	0.26220288	2.65666635
H	0.25999291	-0.97472685	2.65666686

Table S29. Atomic coordinates for the APFD $Co(NH_3)_6 \bullet NH_3$ $\varphi = 60°$ model.

atom	*x*	*y*	*z*
Co	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.15000000
N	2.15000000	0.00000000	0.00000000
N	-2.15000000	0.00000000	0.00000000
N	0.00000000	-2.15000000	0.00000000
N	0.00000000	2.15000000	0.00000000
N	0.00000000	0.00000000	-2.15000000
H	-0.89900000	-0.24100000	2.56900000
H	0.65800000	-0.65800000	2.56900000
H	0.24100000	0.89900000	2.56900000
H	2.56900000	0.89900000	0.24100000
H	2.56900000	-0.65800000	0.65800000
H	2.56900000	-0.24100000	-0.89900000
H	-2.56900000	-0.65813448	0.65813448
H	-2.56900000	0.89881630	0.24095075
H	-2.56900000	-0.24068181	-0.89908524
H	0.24100000	-2.56900000	-0.89900000
H	0.65800000	-2.56900000	0.65800000
H	-0.89900000	-2.56900000	0.24100000
H	0.24068181	2.56900000	-0.89908524
H	-0.89881630	2.56900000	0.24095075
H	0.65813448	2.56900000	0.65813448
H	-0.89908524	-0.24068181	-2.56900000
H	0.24095075	0.89881630	-2.56900000
H	0.65813448	-0.65813448	-2.56900000
H	-1.18011318	2.37729341	-1.18011300
H	-1.18011318	1.18011300	-2.37729341
H	-2.37729341	1.18011309	-1.18011309
N	-1.32790562	1.32790562	-1.32790562

References

1 N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini and K. S. Murray, *J. Comput. Chem.*, 2013, **34**, 1164–1175.

2 M. P. Shores, J. J. Sokol and J. R. Long, *J. Am. Chem. Soc.*, 2002, **124**, 2279–2292.

3 R. Boča, *Theoretical foundations of molecular magnetism*, Elsevier, 1999.

4 N. F. Chilton, CCFIT Program; The Chilton Group: Manchester, U.K. 2014.

5 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision E.01*, Gaussian, Inc.: Wallingford CT, 2009

6 P. J. Hay and T. H. Dunning, *J. Chem. Phys.*, 1976, **64**, 5077–5087.

7 K. A. Peterson, B. C. Shepler, D. Figgen and H. Stoll, *J. Phys. Chem. A*, 2006, **110**, 13877–13883.

8 R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724–+.

9 W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257–+.

10 J. S. Binkley, J. A. Pople and W. J. Hehre, *J. Am. Chem. Soc.*, 1980, **102**, 939–947.

11 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.

12 D. Ganyushin and F. Neese, *J. Chem. Phys.*, , DOI:Artn 11411710.1063/1.2894297.

13 F. Neese, *Wiley Interdiscip. Rev. Mol. Sci.*, 2012, **2**, 73–78.

14 A. Schafer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571–2577.

15 A. Schafer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829–5835.

16 K. A. Peterson, D. Figgen, E. Goll, H. Stoll and M. Dolg, *J. Chem. Phys.*, 2003, **119**, 11113–11123.

17 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.