Supporting Information for:

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

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Crystallography

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

<table>
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<th>Empirical formula</th>
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<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_{39}H_{54}CoN_{10}O_{3}Cl</td>
<td>805.30</td>
<td>849.76</td>
<td>896.75</td>
<td>968.75</td>
</tr>
<tr>
<td>Color</td>
<td>Orange</td>
<td>Orange</td>
<td>Orange</td>
<td>Yellow</td>
</tr>
<tr>
<td>Habit</td>
<td>Parallelepiped</td>
<td>Block</td>
<td>Block</td>
<td>Block</td>
</tr>
<tr>
<td>T (K)</td>
<td>120(2)</td>
<td>120(2)</td>
<td>120(2)</td>
<td>120(2)</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Trigonal</td>
<td>Trigonal</td>
<td>Trigonal</td>
<td>Triclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>P\textoverline{3}</td>
<td>P\textoverline{3}</td>
<td>P\textoverline{3}</td>
<td>P\textoverline{1}</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>a (Å)</td>
<td>15.2335(1)</td>
<td>15.5579(15)</td>
<td>15.8091(7)</td>
<td>12.7632(10)</td>
</tr>
<tr>
<td>b (Å)</td>
<td>15.2335(1)</td>
<td>15.5579(15)</td>
<td>15.8091(7)</td>
<td>12.8064(10)</td>
</tr>
<tr>
<td>c (Å)</td>
<td>12.5157(2)</td>
<td>12.1716(17)</td>
<td>12.0675(10)</td>
<td>14.9046(11)</td>
</tr>
<tr>
<td>α (°)</td>
<td>90</td>
<td>90</td>
<td>90</td>
<td>75.900(4)</td>
</tr>
<tr>
<td>β (°)</td>
<td>90</td>
<td>90</td>
<td>90</td>
<td>83.780(4)</td>
</tr>
<tr>
<td>γ (°)</td>
<td>120</td>
<td>120</td>
<td>120</td>
<td>74.500(4)</td>
</tr>
<tr>
<td>Volume (Å³)</td>
<td>2515.27(5)</td>
<td>2551.4(6)</td>
<td>2611.9(3)</td>
<td>2274.4(3)</td>
</tr>
<tr>
<td>(\rho_{\text{calc}}) (g cm⁻³)</td>
<td>1.063</td>
<td>1.106</td>
<td>1.140</td>
<td>1.415</td>
</tr>
<tr>
<td>GooF</td>
<td>1.073</td>
<td>1.157</td>
<td>1.086</td>
<td>1.023</td>
</tr>
<tr>
<td>(R_1) ((wR_2)^b) (%)</td>
<td>6.67 (22.37)</td>
<td>5.56 (20.06)</td>
<td>3.48 (10.26)</td>
<td>4.25 (9.40)</td>
</tr>
</tbody>
</table>

\(^{a}\)Obtained with graphite-monochromated Mo Kα (\(λ = 0.71073\) Å) radiation.

\(^{b}\)\(R_1 = \sum||F_o| - |F_c||/\sum|F_o|; \ wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)]\}^{1/2}\)

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

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co–N_{\text{imine}} (Å)</td>
<td>2.120(6)</td>
<td>2.106(6)</td>
<td>2.105(3)</td>
<td>2.100(5)(^a)</td>
</tr>
<tr>
<td>Co–N_{\text{pyridine}} (Å)</td>
<td>2.262(3)</td>
<td>2.253(3)</td>
<td>2.258(3)</td>
<td>2.246(5)(^a)</td>
</tr>
<tr>
<td>Co–N_{\text{bridge}} (Å)</td>
<td>2.574(5)</td>
<td>2.592(6)</td>
<td>2.633(2)</td>
<td>2.706(2)</td>
</tr>
<tr>
<td>N_{\text{imine}} plane···N_{\text{pyridine}} plane (Å)</td>
<td>2.099(2)</td>
<td>2.092(3)</td>
<td>2.068(4)</td>
<td>2.075(2)</td>
</tr>
<tr>
<td>Twist angle (°)</td>
<td>49.8(4)</td>
<td>50.5(3)</td>
<td>51.3(6)</td>
<td>51.2(9)</td>
</tr>
<tr>
<td>Θ (°)</td>
<td>200</td>
<td>189</td>
<td>193</td>
<td>187</td>
</tr>
<tr>
<td>Σ (°)</td>
<td>125.9(3)</td>
<td>120.4(4)</td>
<td>117.9(5)</td>
<td>113.3(2)</td>
</tr>
<tr>
<td>Area of Binding Pocket (Å²)(^b)</td>
<td>19.03(1)</td>
<td>20.32(1)</td>
<td>21.89(6)</td>
<td>21.12(5)</td>
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<tr>
<td>H_{\text{amide}}···X (Å)</td>
<td>2.483(3)</td>
<td>2.706(4)</td>
<td>2.924(2)</td>
<td>2.541(4)(^c)</td>
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<tr>
<td>Co···X (Å)</td>
<td>5.161(2)</td>
<td>5.238(1)</td>
<td>5.2116(6)</td>
<td>5.3027(7)(^d)</td>
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<tr>
<td>Shortest Co···Co (Å)</td>
<td>9.292(2)</td>
<td>9.392(1)</td>
<td>9.4798(9)</td>
<td>8.0030(8)</td>
</tr>
</tbody>
</table>

\(^{a}\)Averaged values of three arms

\(^{b}\)Calculated using amide carbonyl carbons as corners of triangle.

\(^{c}\)Defined using the closest O···H distance

\(^{d}\)Defined as Co···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: $y = 4.12 \times 10^{-6}(x) + 7.09 \times 10^{-5}$ ($R^2 = 0.99999$).

**Figure S7.** Field dependence of magnetization for 2 collected at 100 K. Fit: $y = 4.58 \times 10^{-6}(x) - 1.54 \times 10^{-6}$ ($R^2 = 1$).
Figure S8. Field dependence of magnetization for 3 collected at 100 K. Fit: $y = 4.28 \times 10^{-6}(x) + 2.42 \times 10^{-4}$ ($R^2 = 0.99993$).

Figure S9. Field dependence of magnetization for 4 collected at 100 K. Fit: $y = 2.99 \times 10^{-6}(x) + 8.59 \times 10^{-5}$ ($R^2 = 0.99997$).
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

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.\textsuperscript{1}

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

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.\textsuperscript{2}
Table S4. Parameters acquired from fitting reduced magnetization data in ANISOFIT 2.0.2,a

<table>
<thead>
<tr>
<th>Salt</th>
<th>(g_{\text{initial}})</th>
<th>(g_{\text{fit}})</th>
<th>(D_{\text{initial}}) ((\text{cm}^{-1}))</th>
<th>(D_{\text{fit}}) ((\text{cm}^{-1}))</th>
<th>(D_{\text{red}}) ((\text{cm}^{-1}))</th>
<th>(E_{\text{initial}}) ((\text{cm}^{-1}))</th>
<th>(E_{\text{fit}}) ((\text{cm}^{-1}))</th>
<th>(E_{\text{red}}) ((\text{cm}^{-1}))</th>
<th>(f_{\text{sum}})</th>
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<tbody>
<tr>
<td>1</td>
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<td>2.32</td>
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<td>3</td>
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<td>–</td>
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<td>1</td>
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<td>2.30</td>
<td>5</td>
<td>2.530</td>
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<td>0.146</td>
<td>–</td>
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<tr>
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<td>0.004421</td>
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<tr>
<td>4</td>
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<tr>
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<td>2.22</td>
<td>–10</td>
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<td>2.349</td>
<td>0.053</td>
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<tr>
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<tr>
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<td>2.22</td>
<td>–100</td>
<td>2.217</td>
<td>4.769</td>
<td>3</td>
<td>2.440</td>
<td>0.112</td>
<td>0.04126</td>
</tr>
</tbody>
</table>

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:

\[
|D_{zz}| \geq |D_{yy}| \geq |D_{xx}|
\]  (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:

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

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:

\[
D = 3/2D_{zz} = -3/2(D_{xx} + D_{yy}) \quad (3)
\]
\[
E = \sqrt{2}(D_{xx} - D_{yy}) \quad (4)
\]
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 $\chi'$ (left) and $\chi''$ (right) for 1 at various applied fields. Lines are guides for the eye. $T = 1.9$ K, $H_{ac} = 4$ Oe.

![Graph showing frequency dependence of $\chi'$ and $\chi''$ for 1.]()

**Figure S17.** Determination of optimal field for 1. Plot of $\chi''$ 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.

![Graph showing plot of $\chi''$ maxima vs. applied field for 1.](image)

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

![Graph showing frequency dependence of $\chi'$ and $\chi''$ for 2.](image)
Figure S19. Field scan for 3. Frequency dependence of $\chi'$ (left) and $\chi''$ (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 $\chi'$ (left) and $\chi''$ (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 $\chi''$ maxima as a function of temperature. The black line represents the fit for an Orbach-only process according to: $\tau^{-1} = \tau_0^{-1} \exp(-U_{\text{eff}}/k_B T)$, giving $\tau_0 = 1.33 \times 10^{-6}$, $U_{\text{eff}} = 13.2$ 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)

<table>
<thead>
<tr>
<th>(T) (K)</th>
<th>(\chi_T) (cm(^3) mol(^{-1}))</th>
<th>(\chi_s) (cm(^3) mol(^{-1}))</th>
<th>(\tau) (s)</th>
<th>(\alpha)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.8</td>
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<td>0.00101355</td>
<td>0.223774</td>
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<tr>
<td>1.9</td>
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<td>0.000872805</td>
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<td>0.0383541</td>
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<tr>
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<td>0.183466</td>
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These parameters were fit for an Orbach only process according to \(\tau^{-1} = \tau_0^{-1} \exp(-U_{\text{eff}}/k_B T)\), giving \(\tau_0 = 8.25 \times 10^{-7}\), \(U_{\text{eff}} = 10.1\) K (R\(^2\) = 0.99559).

Figure S23. Field scan for [CoL\(^{5-OOMe}\)](ClO\(_4\))\(_2\). Frequency dependence of \(\chi''\) 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 utilized the LANL2 basis and effective core potential for Cl, Br, and Cr; the Stoll basis and potential were used for I and H, C, and N were described with a 6-31g* model. Restricted and unrestricted B3LYP and APFD hybrid density functionals were used in geometry optimizations. All CASSCF, CASCI, and NEVPT2 computations utilized the ORCA suite of electronic structure codes, and the Ahlrichs basis and Stuttgart pseudopotential for I.

For the $[\text{Co(NH}_3)_7]^{2+}$ 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 $[\text{CoL}^{5-\text{ONH}}\text{Bu}]X_2$.

<table>
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<th>X</th>
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<th>B3LYP</th>
<th>APFD</th>
<th>APFD (constrained)$^a$</th>
</tr>
</thead>
<tbody>
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</tbody>
</table>

$^a$Co-N$_{\text{bridge}}$ distance constrained to that found experimentally

### Table S7. Co-N bond distances (Å) for $[\text{CoL}^{5-\text{ONH}}\text{Bu}]X_2$ computed structures.

<table>
<thead>
<tr>
<th>X</th>
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<th>APFD (constrained)$^a$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Co-N$_{\text{bridge}}$</td>
<td>Co-N$_{\text{im}}$</td>
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<td>Br</td>
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<tr>
<td>ClO$_4$</td>
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$^a$Co-N$_{\text{bridge}}$ distance constrained to that found experimentally
Table S8. Computed $g$ matrices for [CoL$_5$–ONHtBu]X$_2$.

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<th>X</th>
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<th>$g_{yy}$</th>
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<th>$g_{iso}$</th>
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Table S9. Computed $D$ (cm$^{-1}$) and $E/D$ for [CoL$_5$–ONHtBu]X$_2$.

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Figure S24. Calculated $E/D$ (a), $g_{sml}$ (b), $g_{med}$ (c), and $g_{lg}$ (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\(^{5-}\text{ONHtBu}\)]\(_2\).

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<td>D</td>
<td>E/D</td>
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<tr>
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<td>5(Q)</td>
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<td>1.257</td>
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<tr>
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<td>6(D)</td>
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<tr>
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<td>7(D)</td>
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<tr>
<td>Br</td>
<td>1(Q)</td>
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<tr>
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\(^a\) Q = quartet; D = doublet

For comparison, the computed D, E/D and g data for the bis-trispyrazolylborate Co(II) complex compares well to the experimental results of 1.0 and 8.5

Table S11. Atomic coordinates for the B3LYP structure [CoL\textsuperscript{5-ONHtBu}]Cl\textsubscript{2}.

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**Table S24.** Atomic coordinates for the APFD Co(NH$_3$)$_6$•NH$_3$ $\phi = 15^\circ$ model.
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**Table S25.** Atomic coordinates for the APFD Co(NH$_3$)$_6$·NH$_3$ φ = 30° model.

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Table S26. Atomic coordinates for the APFD Co(NH\(_3\))\(_6\)•NH\(_3\) \(\phi = 37.5^\circ\) model.

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Table S27. Atomic coordinates for the APFD Co(NH\(_3\))\(_6\)•NH\(_3\) \(\phi = 45^\circ\) model.

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**Table S28.** Atomic coordinates for the APFD Co(NH₃)₆•NH₃ φ = 52.5° model.
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Table S29. Atomic coordinates for the APFD Co(NH$_3$)$_6$•NH$_3$ $\phi = 60^\circ$ model.

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