ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Title:
Indirect effect of the hydrogen bonds on the magnetic coupling on Mn(III) dinuclear compounds

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Content:
Figure S1. Arrangement of the nitrate ions on compound 2................................................................. 2
Table TS1. Magneto-structural parameters for Mn(III) dinuclear compounds........................................... 3
Table TS2. Results of the DFT calculations for compound 1 and the models derived from it............... 4
Table TS3. Results of the DFT calculations for compound 2 and the models derived from it............. 5
Table TS4. X-ray crystallographic data details for compounds 1 and 2 ......................................................... 6
Bibliography.................................................................................................................................................. 7
Figure S1. View of the disposition of the planes containing coordinated and non-coordinated nitrate ions for compound 2.
Table TS1. Magnetic coupling constants $J$ and selected structural parameters for $[\text{Mn}(L)(NN)]_2(\mu-O)(\mu-n-\text{RC}_{6}H_{4}\text{COO})_2]X_2$ compounds ($n = 4$ for monosubstituted carboxylates and $n = 3$ for 1 and 2).

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* This work; $^a$ $H = -J\{S_1, S_2\}$; $^b$ average Elongation (Eq. 1): $\Delta = (z - \bar{xy}) / \sqrt{\bar{xy} \bar{xy} = (x+y)/2}$; $^c$ average ronbicity: $\rho = (y - x) / x$; $^d$ average O-Carboxy-Carboxy-Carboxy; $^e$ relative orientation of the O₃; L-Mn···Mn-L angle; $^f$ angle between the equatorial plane of the octahedron N₂O₂ and the NO₃ plane; abbreviations: bpy = 2,2’-bipyridine, phen = 1,10-phenantroline.
Table TS2. Magnetic interaction ($J_{\text{cal}}$), charge ($Q$) and charge loss ($\Delta Q$) on the perchlorate anions (X), the water ligands (Lw) and in the two manganese ions of the complex (Mn\textsubscript{w} and Mn\textsubscript{Cl}), for different models based on the crystallographic data of $[^{[\text{Mn(bpy)(H}_2\text{O})]}(\mu-2,6\text{-Cl}_2\text{C}_6\text{H}_3\text{COO})_2(\mu-O)[\text{Mn(bpy)}(\text{ClO}_4)]\text{ClO}_4]$ (1) (Mn\textsubscript{w}···(ClO\textsubscript{4})\textsubscript{1/2}···w'···Mn'). A scheme for the frame work units in each model is shown in Table 5. ($H = -JS_1S_2$)

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<th>$J_{\text{cal}}$ /cm$^{-1}$</th>
<th>$Q$ (X) /me</th>
<th>$Q$ (Lw) /me</th>
<th>$\Delta Q$ (2X+w) /me</th>
<th>$Q$ (w') /me</th>
<th>$\Delta Q$ (2X+2w) /me</th>
<th>$Q$ (Mn\textsubscript{w}) /me</th>
<th>$Q$ (Mn\textsubscript{Cl}) /me</th>
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Table TS3. Magnetic exchange ($J_{\text{cal}}$), charge ($Q$) and charge loss ($\Delta Q$) and spin density ($\rho$) on the extra bridge, and charge in the two manganese ions of the complex and the monodentate ligands, for different models based on the crystallographic data of [(Mn(bpy)(H$_2$O))(μ-2,6-Cl$_2$C$_6$H$_3$COO)$_2$]μ-O)(Mn(bpy)(NO$_3$)]NO$_3$·H$_2$O·CH$_3$CN (2·H$_2$O·CH$_3$CN) (Mn-L···W···X···L···W-Mn). A scheme for the frame work units in each model is shown in Table 6. ($H = -JS_1\cdot S_2$)

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<th>$\rho$ (X) /me</th>
<th>$\rho$ (W) /me</th>
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Table TS4. X-ray crystallographic data collection and structure refinement details for compounds [(Mn(bpy)(H₂O))(µ-2,6-Cl₂C₆H₃COO)](µ-O)(Mn(bpy)(ClO₄))ClO₄ (1) and [(Mn(bpy)(H₂O))(µ-2,6-Cl₂C₆H₃COO)](µ-O)(Mn(bpy)(NO₃))NO₃·H₂O·CH₃CN (2·H₂O·CH₃CN).

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<td>1016.32</td>
</tr>
<tr>
<td>T / K</td>
<td>293</td>
<td>100</td>
</tr>
<tr>
<td>λ (Mo Kα) / Å</td>
<td>0.71073</td>
<td>0.71073</td>
</tr>
<tr>
<td>crystal system</td>
<td>P2₁/c (No. 14)</td>
<td>Pca2₁(Nº21)</td>
</tr>
<tr>
<td>space group</td>
<td>Monoclinic</td>
<td>Orthorhombic</td>
</tr>
<tr>
<td>a / Å</td>
<td>11.693(2)</td>
<td>18.6545(12)</td>
</tr>
<tr>
<td>b / Å</td>
<td>39.642(8)</td>
<td>14.0357(8)</td>
</tr>
<tr>
<td>c / Å</td>
<td>9.7135(18)</td>
<td>15.6154(10)</td>
</tr>
<tr>
<td>β / deg.</td>
<td>111.005(7)</td>
<td></td>
</tr>
<tr>
<td>V / Å³</td>
<td>4203.3(14)</td>
<td>4088.6(4)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>ρ&lt;sub&gt;calc&lt;/sub&gt; / g cm⁻³</td>
<td>1.636</td>
<td>1.651</td>
</tr>
<tr>
<td>μ / mm⁻¹</td>
<td>1.051</td>
<td>0.934</td>
</tr>
<tr>
<td>Absorption coefficient / mm⁻¹</td>
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<td>0.934</td>
</tr>
<tr>
<td>F(000)</td>
<td>2080</td>
<td>2052</td>
</tr>
<tr>
<td>Crystal size / mm</td>
<td>0.344 x 0.090 x 0.056</td>
<td>0.534 x 0.248 x 0.153</td>
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<tr>
<td>Θ range / deg.</td>
<td>1.9 to 28.4</td>
<td>2.5 to 27.2</td>
</tr>
<tr>
<td>limiting indices</td>
<td>-14 ≤ h ≤ 15, -52 ≤ k ≤ 52, -12 ≤ l ≤ 12</td>
<td>-23 ≤ h ≤ 23, -18 ≤ k ≤ 17, -20 ≤ l ≤ 16</td>
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<tr>
<td>Independent reflections</td>
<td>88576 / 10480 [R(int) = 0.0573]</td>
<td>17365/7592 [R(int) = 0.0517]</td>
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<tr>
<td>Completeness to theta / %</td>
<td>99.7</td>
<td>98.5</td>
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<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
<td>Semi-empirical from equivalents</td>
</tr>
<tr>
<td>Max. and min. transmission</td>
<td>0.7457 and 0.6807</td>
<td>0.7455 and 0.5728</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
<td>Full-matrix least-squares on F²</td>
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<td>data / restraints / parameters</td>
<td>10480 / 95 / 649</td>
<td>7592 / 14 / 530</td>
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<tr>
<td>goodness-of-fit on F²</td>
<td>1.057</td>
<td>1.084</td>
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<tr>
<td>final R indices [I&gt;2σ(I)]</td>
<td>R₁ = 0.0497, wR₂ = 0.1198</td>
<td>R₁ = 0.0700, wR₂ = 0.1856</td>
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<tr>
<td>R indices (all data)</td>
<td>R₁ = 0.0637, wR₂ = 0.1266</td>
<td>R₁ = 0.0753, wR₂ = 0.1907</td>
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</tbody>
</table>

<sup>a</sup> R₁ = Σ(|F₀| - |F₁|) / Σ|F₀|.  <sup>b</sup> wR² = Σ[ω(F₀² - F₁²)²] / Σ[ω(F₀²)²]²/2, ω = 1/[σ²(F₀²) + (0.0675P)² + 1.4805P], where P = (F₀² + 2F₁²) / 3.
Gómez, V.; Corbella, M.; Aullón, G. Two Temperature-Independent Spinomers of the Dinuclear Mn(III) Compound \([\text{Mn}(\text{H}_2\text{O})(\text{Phen})]_2[\mu-2-\text{ClC}_6\text{H}_4\text{COO}]_2[\mu-\text{O}][\text{ClO}_4]_2\). Inorg. Chem. 2010, 49 (4), 1471–1480 DOI: 10.1021/ic901719t.

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Escrive-Tur, L.; Font-Bardia, M.; Albela, B.; Corbella, M. New Insights into the Comprehension of the Magnetic Properties of Dinuclear MnIII Compounds with the General Formula \([\text{Mn}(\text{L})(\text{NN})][\mu-\text{O}][\mu-\text{n}-\text{RC}_6\text{H}_4\text{COO}]_2]_2X_2\). Dalton Trans. 2016, 45 (29), 11753–11764 DOI: 10.1039/C6DT01097K.


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