Synthesis and Magnetochemistry of Heterometallic Triangular Fe\textsuperscript{III}_2Ln\textsuperscript{III} (Ln = La, Gd, Tb, Dy, and Ho) and Fe\textsuperscript{III}_2Y\textsuperscript{III} Complexes

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Figure S1. Structure of Fe\textsubscript{2}LnO core. Ln\textsuperscript{III} green, Fe\textsuperscript{III} orange, N blue, O, red and C grey.

Table S1. Some important bond distances in Angstroms (Å)

<table>
<thead>
<tr>
<th>Ln</th>
<th>Ln-O1/O2</th>
<th>Ln-O3</th>
<th>Ln-Fe1/Fe2</th>
<th>Fe1-O1</th>
<th>Fe2-O2</th>
<th>Fe1/Fe2-O3</th>
<th>Fe1-Fe2</th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
<td>2.499/2.475</td>
<td>2.534</td>
<td>3.483/3.471</td>
<td>1.950</td>
<td>1.965</td>
<td>1.837/1.836</td>
<td>3.191</td>
</tr>
<tr>
<td>Gd</td>
<td>2.408/2.377</td>
<td>2.446</td>
<td>3.412/3.401</td>
<td>1.956</td>
<td>1.964</td>
<td>1.834/1.838</td>
<td>3.188</td>
</tr>
<tr>
<td>Tb</td>
<td>2.348/2.385</td>
<td>2.432</td>
<td>3.381/3.398</td>
<td>1.965</td>
<td>1.949</td>
<td>1.828/1.832</td>
<td>3.174</td>
</tr>
<tr>
<td>Dy</td>
<td>2.376/2.338</td>
<td>2.416</td>
<td>3.389/3.376</td>
<td>1.941</td>
<td>1.965</td>
<td>1.836/1.832</td>
<td>3.177</td>
</tr>
<tr>
<td>Ho</td>
<td>2.376/2.340</td>
<td>2.412</td>
<td>3.390/3.374</td>
<td>1.949</td>
<td>1.967</td>
<td>1.836/1.830</td>
<td>3.177</td>
</tr>
</tbody>
</table>

Table S2. Some important bond angles in degrees (°)

<table>
<thead>
<tr>
<th>Ln</th>
<th>Ln-Fe1-Ln</th>
<th>Ln-Fe2-Ln</th>
<th>Ln-O3-Fe1</th>
<th>Ln-O3-Fe2</th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
<td>62.50</td>
<td>62.87</td>
<td>104.52</td>
<td>104.02</td>
</tr>
<tr>
<td>Gd</td>
<td>61.92</td>
<td>62.29</td>
<td>104.81</td>
<td>104.19</td>
</tr>
<tr>
<td>Tb</td>
<td>62.35</td>
<td>61.81</td>
<td>104.13</td>
<td>104.78</td>
</tr>
<tr>
<td>Dy</td>
<td>61.77</td>
<td>62.20</td>
<td>104.89</td>
<td>104.40</td>
</tr>
<tr>
<td>Ho</td>
<td>61.73</td>
<td>62.24</td>
<td>104.506</td>
<td>104.52</td>
</tr>
<tr>
<td>Y</td>
<td>62.14</td>
<td>61.81</td>
<td>104.74</td>
<td>105.07</td>
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</tbody>
</table>
Figure S2. Molecular packing in unit cell.

Table S3. N––H bond distance in Angstroms (Å). (Hydrogen bond between acetonitrile ‘N’ and dmem CH₂)

<table>
<thead>
<tr>
<th>Ln</th>
<th>N––H bond distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
<td>3.816</td>
</tr>
<tr>
<td>Gd</td>
<td>3.788</td>
</tr>
<tr>
<td>Tb</td>
<td>3.807</td>
</tr>
<tr>
<td>Dy</td>
<td>3.833</td>
</tr>
<tr>
<td>Ho</td>
<td>3.842</td>
</tr>
<tr>
<td>Y</td>
<td>3.841</td>
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</tbody>
</table>

Table S4. Coupling constant \( J \) values for Fe cluster with structural parameters.

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Molecular Formula</th>
<th>Fe-( \mu )-O (Å)</th>
<th>Fe-( \mu )-O-Fe (°)</th>
<th>( J ) (cm(^{-1}))</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>([\text{Fe}_3\text{O}(\text{O}_2\text{CBu})_2(\text{N}_3)_3(\text{dmem})_2])</td>
<td>1.8716(19)/1.8647(19)</td>
<td>162.82(11)</td>
<td>-45.9</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>([\text{Fe}_2\text{CaO}(\text{O}_2\text{CCl}_3)_6(\text{THF})_2]\cdot\text{THF}</td>
<td>1.827(1)</td>
<td>124.09</td>
<td>-58.9</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>([\text{Fe}_2\text{SrO}(\text{O}_2\text{CCl}_3)_6(\text{THF})_2]\cdot0.5\text{THF}</td>
<td>--</td>
<td>--</td>
<td>-75.4</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>([\text{Fe}_2\text{BaO}(\text{O}_2\text{CCl}_3)_6(\text{THF})_3]\cdot0.5\text{THF0.5H}_2\text{O}</td>
<td>1.816(3)</td>
<td>123.55</td>
<td>-60.40</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>([\text{Fe}_2\text{O}(\text{TeEO}_2\text{CPH})_2\text{Cl}]\ (\text{isosceles})</td>
<td>1.862(7)/1.867(7)</td>
<td>159.1(3)</td>
<td>-55.0(6)</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>([\text{Fe}_2\text{Gd}_2(\text{O})(\text{OH})(\text{TBCC})_2]\cdot(\text{dmf})_4(\text{MeOH})_2(\text{H}_2\text{O})_2\text{Cl}]</td>
<td>1.87</td>
<td>144.7</td>
<td>-85.0</td>
<td>4</td>
</tr>
<tr>
<td>7</td>
<td>([\text{Fe}_2\text{MgO}(\text{O}_2\text{CCCH}_3)_6(\text{Py})_3]</td>
<td>1.890(3)</td>
<td>120</td>
<td>-62(3)</td>
<td>5</td>
</tr>
<tr>
<td>8</td>
<td>([\text{Fe}_2\text{MnO}(\text{O}_2\text{CCCH}_3)_6(\text{Py})_3]</td>
<td>1.867(2)/1.862(2)</td>
<td>122.85</td>
<td>-64(3)</td>
<td>5</td>
</tr>
<tr>
<td>9</td>
<td>([\text{Fe}_2\text{NiO}(\text{O}_2\text{CCCH}_3)_6(\text{Py})_3]</td>
<td>--</td>
<td>--</td>
<td>-73(3)</td>
<td>5</td>
</tr>
<tr>
<td>10</td>
<td>([\text{Fe}_2\text{NiO}(\text{O}_2\text{CCCH}_3)_6]</td>
<td>1.875/1.891</td>
<td>119.8</td>
<td>-71(3)</td>
<td>5</td>
</tr>
<tr>
<td>11</td>
<td>([\text{Fe}_2\text{Gd}_2(\text{O})(\text{O}_2\text{CCCl}_3)(\text{H}_2\text{O})(\text{THF})_3]</td>
<td>~1.8</td>
<td>~125</td>
<td>-35</td>
<td>6</td>
</tr>
<tr>
<td>12</td>
<td>([\text{Fe}_3\text{Y}(\text{O}_2\text{O})_2(\text{CCl}_3\text{CO}_2)_6]</td>
<td>~1.8</td>
<td>~125</td>
<td>-35</td>
<td>6</td>
</tr>
<tr>
<td>13</td>
<td>([\text{Fe}_3\text{Lu}(\text{O}_2\text{O})_2(\text{CCl}_3\text{CO}_2)_6]</td>
<td>~1.8</td>
<td>~125</td>
<td>-35</td>
<td>6</td>
</tr>
<tr>
<td>14</td>
<td>([\text{Fe}_3\text{O}(\text{Etsao})(\text{benz})_2(\text{MeOH})_2]</td>
<td>1.887</td>
<td>120.65</td>
<td>-38</td>
<td>7</td>
</tr>
<tr>
<td>15</td>
<td>([\text{Fe}_3\text{O}(\text{Etsao})(\text{benz})_2(\text{MeOH})_2]</td>
<td>1.905</td>
<td>122.65</td>
<td>-29.3</td>
<td>7</td>
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References: