Spectroscopic and Magnetic Properties of a Series of mu-Cyano Bridged Bimetallic Compounds of the Type M-II-NC-Fe-III (M = Mn, Co, and Zn) Using the Building Block [Fe-III(CN)(5)imidazole](2-)

Tchouka, Heloise; Meetsma, Auke; Browne, Wesley R.

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Spectroscopic and magnetic properties of a series of \( \mu \)-cyano bridged bimetallic compounds of the type M\(^{\text{II}}\)-NC-Fe\(^{\text{III}}\) (M = Mn, Co and Zn) using the building-block [Fe\(^{\text{III}}\)(CN)\(_5\)imidazole]\(^{2-}\)

*Heloïse Tchouka, Auke Meetsma, Wesley Browne*

Supporting information

Table S1 Selected bond lengths (Å) and angles (deg)\(^{a,b}\) for 1

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<th>Value (Å)</th>
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C1-Fe1-C1_a   174.88(13)  N4-C4-C3   111.6(6)
C1-Fe1-C1_f  88.69(12)  N3-C5-N4   113.0(6)
C1-Fe1-C1_h  91.08(12)

*a*Estimated standard deviations in the last significant digits are given in parentheses.

*b*Symmetry code: [-a] -1-x, 1/2-y, z; [-b] x, -y, -z; [-c] -x, 1/2+y, -z; [-d] -x, -y, -z; [-e] x, 1/2+y, -z; [-f] -1-x, y, z; [-g] -x, y, z; [-h] x, 1/2-y, z; [-i] -1/2-x, y, -1/2-z.

Table S2  selected bond lengths (Å) and angles (deg)\(^{a,b}\) for 2

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\( ^a \text{Estimated standard deviations in the last significant digits are given in parentheses.} \)

\( ^b \text{Symmetry code: [}_a[ ] \text{-1}+x, y, z; [}_b[ ] 1+x, y, z; [}_c[ ] 2-x, -1/2+y, 1/2-z; [}_d[ ] 2-x, 1/2+y, 1/2-z; [}_e[ ] 3-x, -1/2+y, 1/2-z; [}_f[ ] 3-x, 1/2 +y, 1/2 -z} \)
Estimated standard deviations in the last significant digits are given in parentheses.

Symmetry code: [a] 3/2-x, 1-y, -1/2+z; [b] -1/2+x, 3/2-y, 1/2-z; [c] 1/2+x, 3/2-y, 1/2-z; [d] 1-x, -1/2+y, 1-z; [e] 1-x, 1/2+y, 1-z; [f] 1-x, 1-y, 1-z; [g] -1/2+x, y, 1/2-z; [h] 1/2+x, y, 1/2-z; [i] 3/2-x, 1/2+y, 1/2+z; [j] x, 1/2-y, z; [k] x, 3/2-y, z.
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<td>N5-C6-C5</td>
<td>106.3(5)</td>
</tr>
<tr>
<td>N2-Mn-N3_b</td>
<td>138.52(11)</td>
<td>N6-C7-C8</td>
<td>122.2(5)</td>
</tr>
<tr>
<td>N2-Mn-N3_d</td>
<td>81.19(10)</td>
<td>C7-C8-C9</td>
<td>119.4(5)</td>
</tr>
<tr>
<td>N2-Mn-N2_g</td>
<td>84.85(11)</td>
<td>C8-C9-C10</td>
<td>118.2(5)</td>
</tr>
<tr>
<td>N6-Mn-N7</td>
<td>70.23(14)</td>
<td>C9-C10-C11</td>
<td>120.5(5)</td>
</tr>
<tr>
<td>N6-Mn-N3_b</td>
<td>87.36(11)</td>
<td>N6-C11-C10</td>
<td>121.0(5)</td>
</tr>
<tr>
<td>N6-Mn-N3_d</td>
<td>87.36(11)</td>
<td>N6-C11-C12</td>
<td>115.2(4)</td>
</tr>
<tr>
<td>N6-Mn-N2_g</td>
<td>130.05(9)</td>
<td>C10-C11-C12</td>
<td>123.9(5)</td>
</tr>
<tr>
<td>N7-Mn-N3_b</td>
<td>133.05(8)</td>
<td>N7-C12-C11</td>
<td>116.1(4)</td>
</tr>
<tr>
<td>Bond</td>
<td>Angle (°) (σ)</td>
<td>Bond</td>
<td>Angle (°) (σ)</td>
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<tr>
<td>N7-Mn-N3_d</td>
<td>133.05(8)</td>
<td>N7-C12-C13</td>
<td>121.1(5)</td>
</tr>
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<td>C11-C12-C13</td>
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<td>N3_b-Mn-N3_d</td>
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<td>C12-C13-C14</td>
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<td>C13-C14-C15</td>
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<td>C14-C15-C16</td>
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<td>157.6(3)</td>
<td>N7-C16-C15</td>
<td>122.7(6)</td>
</tr>
</tbody>
</table>

*a* Estimated standard deviations in the last significant digits are given in parentheses.

*b* Symmetry code: [a] x, -1/2-y, z; [b] -1/2+x, 1/2-y, 1/2-z; [c] 1/2+x, 1/2-y, 1/2-z; [d] -1/2+x, y, 1/2-z; [e] 1/2+x, y, 1/2-z; [f] x, -1/2-y, z; [g] x, 1/2-y, z;