Supporting Information

Trigonal prismatic anionic iron (III) complex of a radical o-imino-benzo-semiquinonate derivative: Structural and spectral analysis


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**Fig. S1:** (a) Simulated and (b) powder X-ray diffraction pattern of complex 1.

**Fig. S2:** IR spectrum of complex 1.
**Fig. S3**: Plot of the three highest alpha SOMOs of complex 1.

Table S1. Selected bond lengths (Å) for 1.

<table>
<thead>
<tr>
<th>Atoms</th>
<th>distance</th>
<th>Atoms</th>
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<tbody>
<tr>
<td>Fe1-O6</td>
<td>2.006(2)</td>
<td>O2-C7</td>
<td>1.223(5)</td>
<td>C5-C6</td>
<td>1.360(6)</td>
<td>C23-C24</td>
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<td>Fe1-O3</td>
<td>2.008(3)</td>
<td>O3-C9</td>
<td>1.290(4)</td>
<td>C8-C13</td>
<td>1.419(5)</td>
<td>C24-C25</td>
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<td>Fe1-O1</td>
<td>2.018(3)</td>
<td>O4-C28</td>
<td>1.280(5)</td>
<td>C8-C9</td>
<td>1.443(5)</td>
<td>C25-C26</td>
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<td>Fe1-N1</td>
<td>2.045(3)</td>
<td>O5-C28</td>
<td>1.235(5)</td>
<td>C9-C10</td>
<td>1.417(5)</td>
<td>C26-C27</td>
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<tr>
<td>Fe1-O4</td>
<td>2.053(3)</td>
<td>O6-C30</td>
<td>1.281(4)</td>
<td>C10-C11</td>
<td>1.375(5)</td>
<td>C29-C34</td>
<td>1.413(5)</td>
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<td>Fe1-N2</td>
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<td>C1-C2</td>
<td>1.393(5)</td>
<td>C11-C12</td>
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<td>N1-C2</td>
<td>1.409(5)</td>
<td>C1-C7</td>
<td>1.498(6)</td>
<td>C22-C23</td>
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<td>C31-C32</td>
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<td>C3-C4</td>
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<td>1.505(6)</td>
<td>C33-C34</td>
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<tr>
<td>O1-C7</td>
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<td>C4-C5</td>
<td>1.380(6)</td>
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Table S2. Selected bond angles (°) for 1.

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<td>O1-Fe1-O3</td>
<td>135.17(11)</td>
<td>O3-Fe1-O4</td>
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<td>O4-Fe1-N1</td>
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<td>O1-Fe1-O4</td>
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<td>O1-Fe1-O6</td>
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<td>O3-Fe1-N1</td>
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<td>O6-Fe1-N1</td>
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<td>O3-Fe1-N2</td>
<td>87.39(12)</td>
<td>O6-Fe1-N2</td>
<td>76.25(13)</td>
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<td>O1-Fe1-N2</td>
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<td>O4-Fe1-O6</td>
<td>136.74(11)</td>
<td>N1-Fe1-N2</td>
<td>142.64(13)</td>
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