Spin crossover in discrete polynuclear iron(II) complexes

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Electronic Supporting Information
Figure S1. Distribution of octahedral distortion parameter, $\Sigma (^\circ)$, for the Fe(II) centres in the 68 dinuclear complexes reviewed herein, presented by type 2A triply bridged, 2B doubly bridged, 2C single bridged, and 2D anion bridged.
Figure S2. Distribution of continuous shape measured value, CShM, of octahedral distortion, for the Fe(II) centres in the 68 dinuclear complexes reviewed herein, presented by type 2A triply bridged, 2B doubly bridged, 2C single bridged, and 2D anion bridged.
Figure S3. $\Sigma^v$ vs CShM for the 2A dinuclear complexes reviewed herein. Colour code: green 2A triply triazole bridged; violet 2A triply stranded helicates.
Figure S4. Σ (°) vs CShM for tetranuclear complexes reviewed herein. Colour code: blue 4A square; green 4B grids; red 4C cages.
Table S1. Formula, CCDC deposition number, selected parameters, and references, for the structurally characterised complexes out of the 127 complexes reviewed.

<table>
<thead>
<tr>
<th>2A</th>
<th>T (K)</th>
<th>CCDC</th>
<th>Fe-Fe (Å)</th>
<th>Octahedral Distortion from ideal</th>
<th>Σ (°)</th>
<th>Spin state</th>
<th>T_s (K)</th>
<th>SCO</th>
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S6
<p>| Compound | Formula | ΔH/kJ mol⁻¹ | | | | | | | |
|----------|---------|-------------|-------------|-------------|------------|-------------|-------------|-------------|-------------|-------------|
| Fe₂(L11)(BF₄)₂·4MeCN | 100 | 1568783 | 11.623 | 1.494, 1.082 | 84.9, 74.5 | HS-(mixed) | LS/LS | ↓150 | Gradual, 15 k hysteresis | N6 |
| Fe₂(L12)(ClO₄)₂·2MeCN | 150 | 702672 | 11.452 | 1.058, 1.001 | 65.2, 61.8 | LS-S | 140 | Complete, very narrow hysteresis, one-step | N6 |
| Fe₂(L12)(ClO₄)₂·1.5H₂O | 150 | 836247 | 11.45 | 1.837, 0.960 | 62.3, 85.3 | LS-HS | 210-265 | Gradual, incomplete, hysteresis, one step | N6 |
| Fe₂(L13)(BF₄)₂·4MeCN·0.5H₂O | 150 | 1540558 | 11.33 | 0.735, 0.708 | 54.4, 65 | LS-LS | 348 | Complete, One-step, abrupt | N6 |
| Fe₂(L13)(BF₄)₂·2MeCN | 298 | 1540559 | 11.36 | 0.720, 1.000 | 58.3, 70 | LS-LS/HS(mixed) | - | Abrupt, 7K wide hysteresis | N6 |
| Fe₂(L14)(BF₄)₂·2MeNO₂·1H₂O | 173 | 738553 | 3.8695 | 1.293, 6.084 | 66.4, 158.5 | LS-HS | ↑190 - 183 | Abrupt, incomplete, one-step | N6 |
| Fe₂(L14)(ClO₄)₂·5MeNO₂ | 103 | 647353 | 3.8507 | 1.360, 6.154 | 63.8, 152.5 | LS-HS | 240 | Abrupt, incomplete, one-step | N6 |
| Fe₂(L14)(ClO₄)₂·5MeNO₂ | 293 | 647354 | 4.0362 | 3.698, 5.005 | 116.0, 124.2 | HS-HS | - | - | - | - |
| Fe₂(L15)(ClO₄)₂·2MeCN·0.5H₂O | 163 | 738562 | 3.8450 | 3.656, 1.057 | 137.6, 64.6 | HS-LS | 120 | Incomplete, abrupt, one step | N6 |
| Fe₂(L15)(ClO₄)₂·2MeCN | 113 | 738561 | 4.178 | 2.815, 2.886 | 132.16, 135.29 | HS-HS | - | HS | N6 |
| Cl[Fe₂(L16)]Cl(PF₆)₂·5.7MeOH | 100 | 1455576 | 9.731 | 3.522, 0.755 | 115.8, 58.8 | HS-LS | 302 | Gradual Incomplete, one step | N6 |
| Cl[Fe₂(L16)]Cl(PF₆)₂·5.7MeOH | 280 | 1455581 | 9.730 | 3.337, 0.874 | 113.2, 62.4 | HS-LS | - | - | - |
| Cl[Fe₂(L16)]Cl(PF₆)₂·3MeOH·H₂O | 90 | 1455315 | 9.675 | 0.943 | 62.1 | LS | 160, 265 | Gradual Complete, two step, hysteresis | N6 |
| Cl[Fe₂(L16)]Cl(PF₆)₂·3MeOH·H₂O | 300 | 1455317 | 9.799 | 2.424 | 95.1 | HS | - | - | - |
| Br[Fe₂(L16)]Br(PF₆)₂·4MeO·H | 100 | 1455591 | 9.670 | 3.275, 0.810 | 113.7, 61.2 | HS-LS | 258 | Gradual Incomplete, one step | N6 |
| Br[Fe₂(L16)]Br(PF₆)₂·4MeO·H | 280 | 1455597 | 9.705 | 3.020, 1.615 | 109.8, 84.1 | HS-HS | - | - | - |
| Br[Fe₂(L16)]Br(PF₆)₂·MeO·H·H₂O | 90 | 1455322 | 9.694 | 1.005 | 64.5 | LS | 200 | Gradual Complete, one step | N6 |
| Br[Fe₂(L16)]Br(PF₆)₂·MeO·H·H₂O | 296 | 1455320 | 9.786 | 2.468 | 96.7 | HS | - | - | - |</p>
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<tr>
<th>2B</th>
<th>T (K)</th>
<th>CCDC</th>
<th>Fe-Fe (Å)</th>
<th>Octahedral Distortion from ideal</th>
<th>Σ (°)</th>
<th>Spin state</th>
<th>T_h (K)</th>
<th>SCO</th>
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<td>N6</td>
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### Table 2C

| Ref. | [Fe\(_2\)L\(_{22}\)\(_3\)(OTf)\(_3\)(MeCN)] | 133 | 1023524 | 4.19 | 3.065, 3.239 | 75.7 | 2LS-LS/HS (mix) | 210, 130 | Gradual, incomplete, one step | N6 | 29 |
| Ref. | [Fe\(_2\)L\(_{22}\)\(_3\)(OTf)\(_3\)(MeCN)] | 133 | 1023524 | 4.19 | 3.065, 3.239 | 75.7 | 2LS-LS/HS (mix) | 210, 130 | Gradual, incomplete, one step | N6 | 29 |
| Ref. | [Fe\(_2\)L\(_{23}\)\(_3\)]\(_3\)DMF-H\(_2\)O | 123 | 899998 | 6.94 | 0.877 | 52, 76.1 | HS | - | - | N6 | 30 |
| Ref. | [Fe\(_2\)L\(_{24}\)\(_3\)]\(_3\)DMF-H\(_2\)O | 123 | 899999 | 6.75 | 0.444, 0.884 | 52, 76.1 | HS | - | - | N6 | 30 |
| Ref. | [Fe\(_2\)L\(_{25}\)\(_3\)]\(_3\)BPh\(_4\)\(_4\)·2MeOH | 110 | 899159 | 7.17 | 1.521 | 72.69 | 2LS | - | - | N6 | 31 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{27}\))·2MeOH | 293 | 807893 | 13.79 | 0.769 | 2\times 65.9 | 2 LS | 159 | Abrupt, complete, one step | N6 | 32 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{29}\)) | 293 | 807895 | 13.85 | 1.774, 1.005 | 88.1, 65.2 | HS-HS | - | - | N6 | 32 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{29}\)) | 90 | 807893 | 13.38 | 0.224 | 2\times 38.2 | LS | 182 | Gradual, complete, two step | N6 | 32 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{29}\)) | 183 | 807892 | 13.55 | 0.418 | 2\times 82 | 2LS/LS | 182 | Gradual, complete, two step | N6 | 32 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{29}\)) | 300 | 807894 | 13.74 | 0.875 | 105.8 | HS | 182 | Gradual, complete, two step | N6 | 32 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{30}\))·2MeOH | 110 | 864188 | 11.13 | 0.422 | 37 | LS | 210 | Abrupt, complete, two step | N6 | 33 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{30}\))·2MeOH | 290 | 864186 | 11.45 | 1.220 | 67.4 | HS | - | - | N6 | 33 |
| Ref. | [Fe\(_2\)L\(_{26}\)\(_3\)]\(_3\)(NCS)\(_4\)(L\(_{30}\))·2MeOH | 293 | 846878 | 14.03 | 0.901 | 80.3 | HS | - | - | N6 | 34 |

The table provides data on a series of compounds with their respective Fe-Fe distances, octahedral distortions from ideal, spin states, and SCO (Spectral Change on Oxidation) values.
<table>
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<th>2D</th>
<th>T (K)</th>
<th>CCDC</th>
<th>Fe-Fe (Å)</th>
<th>Octahedral Distortion from ideal</th>
<th>Σ (°)</th>
<th>Spin state</th>
<th>T&lt;sub&gt;x&lt;/sub&gt; (K)</th>
<th>SCO</th>
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<td>263318</td>
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<td>0.451, 0.430</td>
<td>2x 47, 2x 49.4</td>
<td>4x LS</td>
<td>342, 157K</td>
<td>two step, gradual, complete</td>
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<td>1413422</td>
<td>7.075</td>
<td>0.409</td>
<td>2x 51</td>
<td>2x LS</td>
<td>365</td>
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<td>O3N3-N6-N3O3</td>
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<td>Σ (*)</td>
<td>Spin state</td>
<td>Tᵢ (K)</td>
<td>SCO</td>
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<td>HS-(mix)LS/HS-HS</td>
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<td>gradual, incomplete, one step</td>
<td>O₃N₃-N₆-N₃O₂ O₁</td>
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<td>3.79,3.80</td>
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<td>24.24,23</td>
<td>HS-LS-HS</td>
<td>400/310</td>
<td>gradual, incomplete, one step, 90 K wide hysteresis</td>
<td>O₃N₃-N₆-N₃O₃</td>
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<td>O₂O₁-N₃-N₆-N₃O₂ O₁</td>
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<td>HS-HS-HS</td>
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**4A**

<p>| Fe₃L₄₅₃(L₄₈)₃(μ-NC)₆(PF₆)₄ | 100   | 274456    | 5.00,4.95,4.99,4.99 | 0.468, 0.583, 0.442, 0.311 | 52.3,61.4,47.1,45.08 | LS-LS-LS-LS | 160,380 | Gradual, Two step, | N₄C₂⁻N₆ |
|                            | 200   | 274455    | 5.04,5.02,4.99,4.99 | 0.482, 1.794, 0.493, 0.300 | 50.3,108.1,47.6,44.6 | LS-HS-LS-LS |        |                               |                       |</p>
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<th>Octahedral Distortion from ideal</th>
<th>Σ (°)</th>
<th>Spin state</th>
<th>T½ (K)</th>
<th>SCO</th>
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**Note:** The table above contains data on various compounds, including their formulae, crystallographic data, and phase transitions. The entries include the temperature (T), crystallographic data (CCDC), Fe-Fe distance (Å), octahedral distortion from ideal, Σ (°), spin state, T½ (K), and SCO (S). The references (ref) are indicated in the last column.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Experimental Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Fe^{II}L53]_4^2(ClO_4)_6·3MeCN·5H_2O</td>
<td>120</td>
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<tr>
<td>[Fe^{II}L54]_4^2(ClO_4)_7(CH_3NO)_2·6H_2O</td>
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<td>[Fe^{II}L65]_4^2Cl·9H_2O</td>
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<td>[Fe^{II}L66]_4^2(BF_4)_4·7MeOH·2H_2O</td>
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<tr>
<td>[Fe^{II}L66]_4^2(BF_4)_4·MeOH·2H_2O</td>
<td>283</td>
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<tr>
<td>[Fe^{II}L67]_4^2(BF_4)_4·4DMF</td>
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<tr>
<td>[Fe^{II}L67]_4^2(BF_4)_4·4DMF</td>
<td>233</td>
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<tr>
<td>[Fe^{II}L67]_4^2(BF_4)_6·3CH_3CN</td>
<td>133</td>
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<tr>
<td>[Fe^{II}(HL67)·(L67)]_4[BF_4]_4·2CH_3CN <strong>trinuclear</strong></td>
<td>133</td>
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<tr>
<td>[Fe^{II}L68]_4^2(PF_6)_6·DMF·THF</td>
<td>133</td>
</tr>
<tr>
<td>[Fe^{II}L68]_4^2(PF_6)_6·4DMF</td>
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<tr>
<td>Complex</td>
<td>T (K)</td>
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<tr>
<td>----------------------------------------------</td>
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<tr>
<td><a href="ClO4">FeII(68)4</a>4·0.25DMF·D ME</td>
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<tr>
<td><a href="BF4">FeII(68)4</a>4·THF·4H2O</td>
<td>293</td>
</tr>
<tr>
<td>[FeII(68)4]Br·4DMF·2H2O</td>
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<tr>
<td><a href="BF4">FeII(68)4</a>2·2MeCN</td>
<td>293</td>
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<td><a href="CF3SO3">FeII(70)4</a>8·12MeNO2·C6H14·4H2O</td>
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<td><a href="CF3SO3">FeII(70)4</a>3(F)3·2MeNO2·H2O</td>
<td>180</td>
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</table>

4C
<table>
<thead>
<tr>
<th>Compound</th>
<th>Form</th>
<th>Raman Shifts</th>
<th>Spin State</th>
<th>Optical Activity</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td><a href="BF%3Csub%3E4%3C/sub%3E">Fe&lt;sup&gt;II&lt;/sup&gt;(L71)&lt;sub&gt;4&lt;/sub&gt;</a>&lt;sub&gt;8&lt;/sub&gt;·14.75CH&lt;sub&gt;3&lt;/sub&gt;CN·4.5C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;6&lt;/sub&gt;·3H&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>293</td>
<td>907706</td>
<td>14.46, 14.29, 14.11, 14.52, 14.46, 14.11</td>
<td>1.125, 1.181</td>
<td>66.9, 69.5</td>
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<tr>
<td>Fe&lt;sup&gt;II&lt;/sup&gt;(L73)&lt;sub&gt;4&lt;/sub&gt;(CF&lt;sub&gt;3&lt;/sub&gt;SO&lt;sub&gt;3&lt;/sub&gt;)&lt;sub&gt;8&lt;/sub&gt;</td>
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<td>908546</td>
<td>6×11.8 5</td>
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<td>65.1</td>
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<td><a href="BF%3Csub%3E4%3C/sub%3E">Fe&lt;sup&gt;II&lt;/sup&gt;(L74)&lt;sub&gt;4&lt;/sub&gt;</a>&lt;sub&gt;8&lt;/sub&gt;·16CH&lt;sub&gt;3&lt;/sub&gt;CN</td>
<td>100</td>
<td>1057843</td>
<td>3×14.61, 3×14.78, 3×14.54, 3×14.94, 3×14.56, 3×15.14</td>
<td>1.643, 0.911, 0.997, 2.111, 1.543, 1.035</td>
<td>82.0, 66.8, 69.6, 121.5, 86.1, 74.7</td>
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<tr>
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<td>1025013</td>
<td>3×9.56, 3×9.67</td>
<td>0.878, 0.595</td>
<td>61.1, 49.5</td>
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<tr>
<td><a href="ClO%3Csub%3E4%3C/sub%3E">Fe&lt;sup&gt;II&lt;/sup&gt;(L75)&lt;sub&gt;4&lt;/sub&gt;</a>&lt;sub&gt;8&lt;/sub&gt; (S)</td>
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<td>1025014</td>
<td>3×9.66, 3×9.48</td>
<td>0.999, 0.433</td>
<td>60.2, 42.0</td>
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<tr>
<td><a href="ClO%3Csub%3E4%3C/sub%3E">Fe&lt;sup&gt;II&lt;/sup&gt;(L76)&lt;sub&gt;4&lt;/sub&gt;</a>&lt;sub&gt;8&lt;/sub&gt;·11.59MeCN·2C&lt;sub&gt;6&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt;·H&lt;sub&gt;2&lt;/sub&gt;O (R)</td>
<td>123</td>
<td>1025015</td>
<td>9.66, 9.45, 9.70, 9.59, 9.64, 9.79</td>
<td>0.739, 0.828, 0.761, 0.995</td>
<td>55.8, 57.8, 55.8, 63.8</td>
</tr>
<tr>
<td><a href="ClO%3Csub%3E4%3C/sub%3E">Fe&lt;sup&gt;II&lt;/sup&gt;(L76)&lt;sub&gt;4&lt;/sub&gt;</a>&lt;sub&gt;8&lt;/sub&gt;·3MeCN (S)</td>
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<td>1025016</td>
<td>9.74, 9.70, 9.68, 9.41</td>
<td>0.763, 0.749, 0.868, 0.968</td>
<td>56.4, 54.6, 60.3, 63.1</td>
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<tr>
<td>Complex</td>
<td>T (K)</td>
<td>CCDC</td>
<td>Fe-Fe (Å)</td>
<td>Octahedral Distortion from ideal</td>
<td>Σ (°)</td>
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<tr>
<td>[{FeIl(L77)}3][ClO4]3·2MeCN (S)</td>
<td>123</td>
<td>1025017</td>
<td>9.77, 9.76</td>
<td>3x9.53, 3x9.81</td>
<td>0.818, 0.791</td>
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<tr>
<td>[{FeII(L78)}6][ClO4]6·2MeCN</td>
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<td>1447306</td>
<td>11.35, 11.04, 11.90, 11.73, 11.95, 11.18, 3x11.9, 3x11.7, 8</td>
<td>0.443, 0.525, 0.540, 0.482, 0.799, 0.540</td>
<td>42.9, 45.3, 48.6, 42.7, 52.9, 49.9</td>
</tr>
</tbody>
</table>

References