

**The Coordination Chemistry of 1,10-Phenanthroline-2,9-dicarbaldehyde dioxime. 1.
Synthesis, Structures, Adsorption Behaviour and Magnetic Properties of a New
Family of Polynuclear Iron Clusters**

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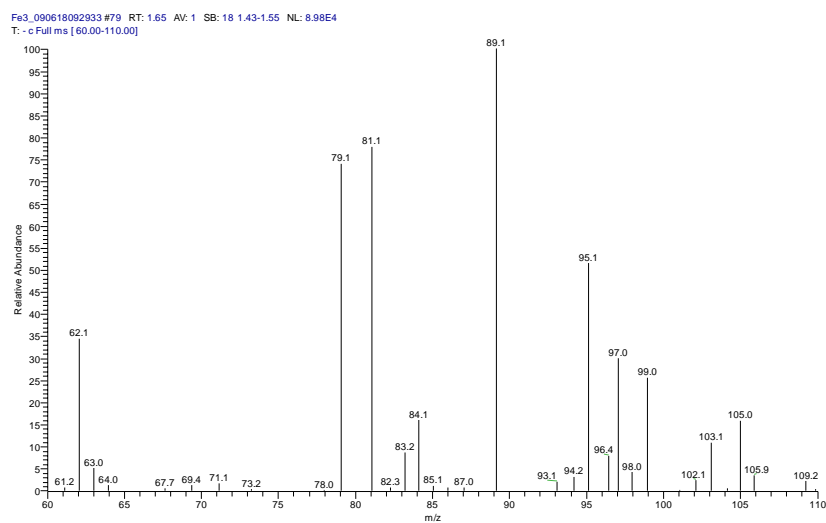
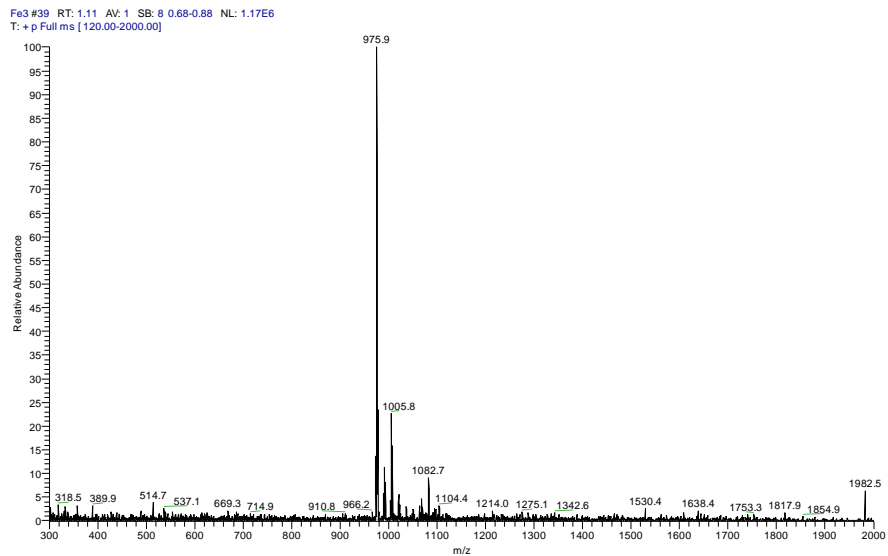


Figure S1. ESI-MS Spectra for 2.

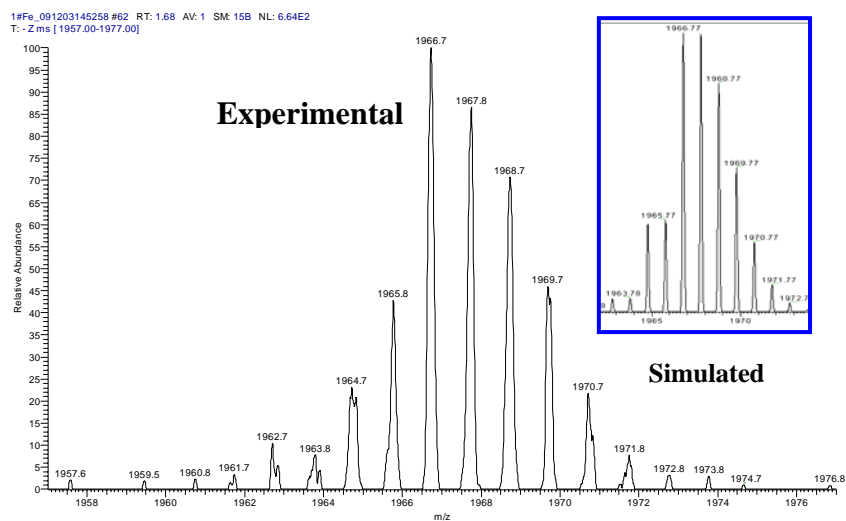


Figure S2. ESI-MS Spectra for 5.

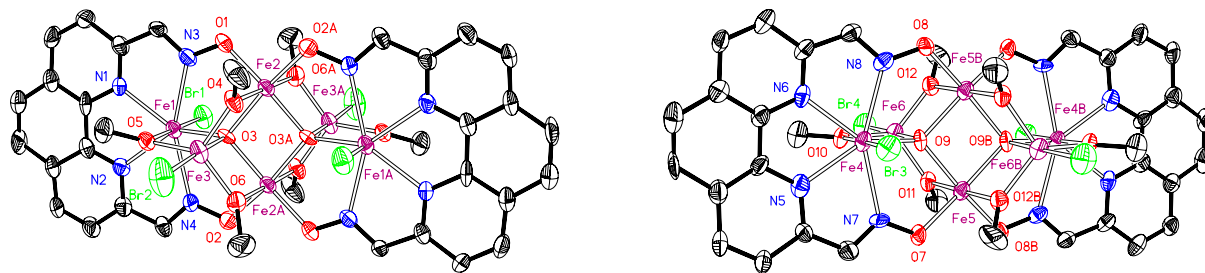


Figure S3. Perspective views of the molecular structures in **4** (H atoms and solvent molecules are omitted for clarity) with thermal ellipsoids at 30% probability.

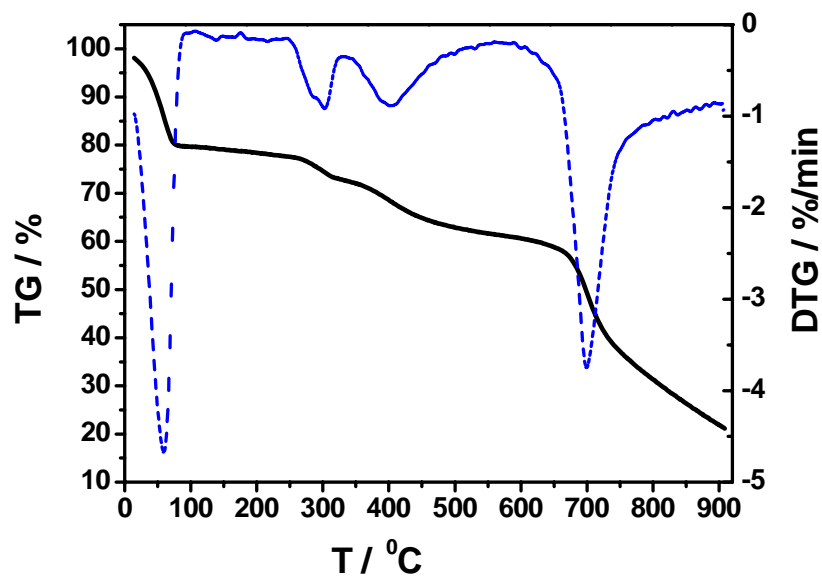


Figure S4. TG curve of **2** under N_2 .

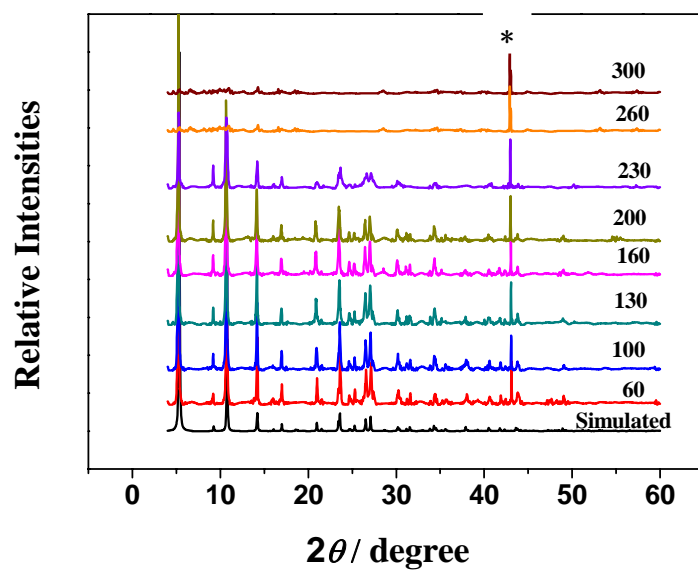


Figure S5. Variable-temperature X-ray powder diffraction (VTXRPD) of **2** under N₂ at standard atmospheric pressure from 60 °C to 300 °C. (* marks the diffraction peak of back ground)

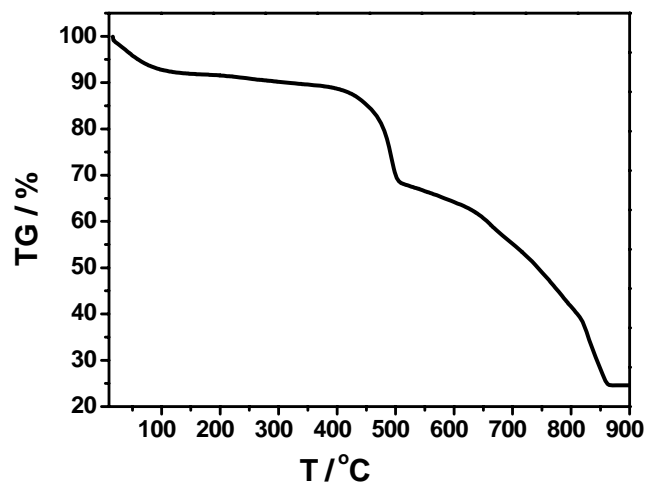


Figure S6. TG curve of **5** under N₂.

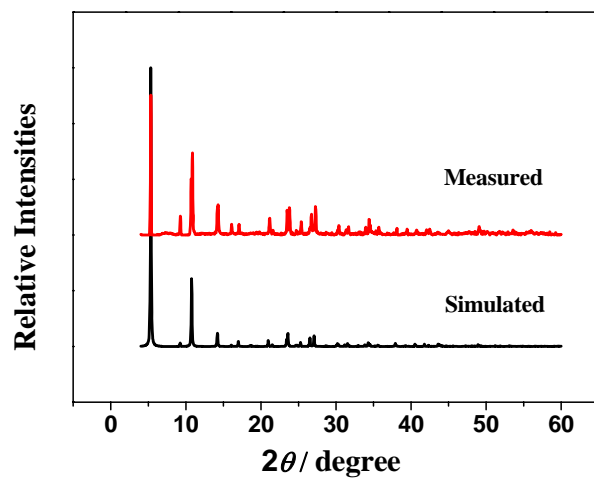


Figure S7. XRD patterns of 2

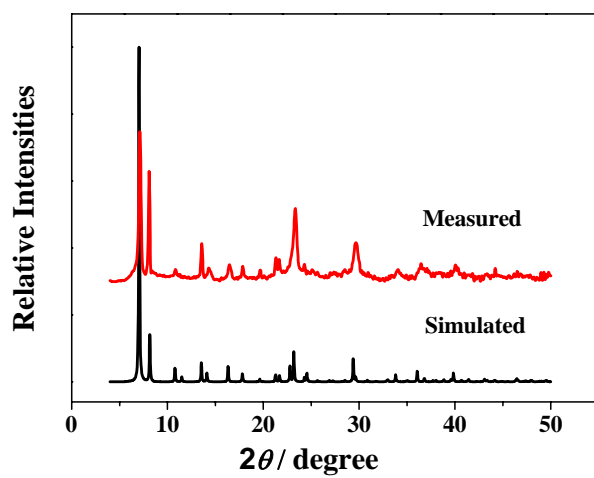


Figure S8. XRD patterns of 5

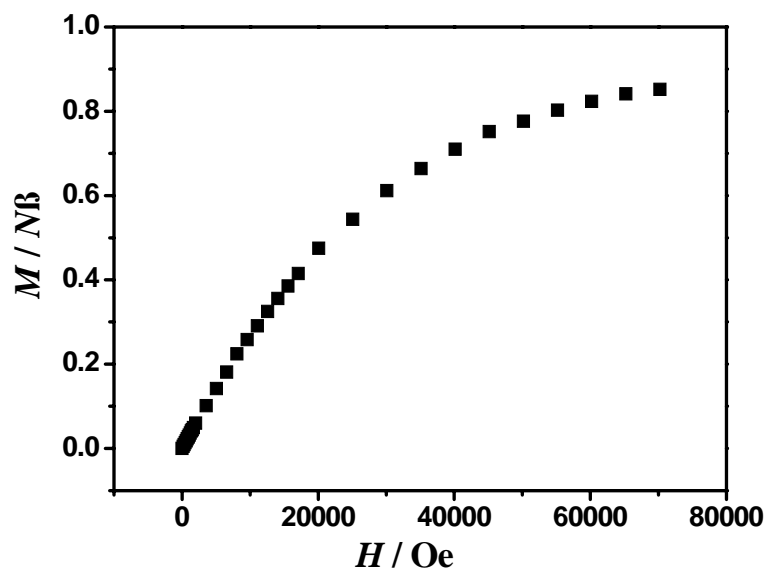


Figure S9. Field dependence of magnetization for **2** at $T = 2$ K.

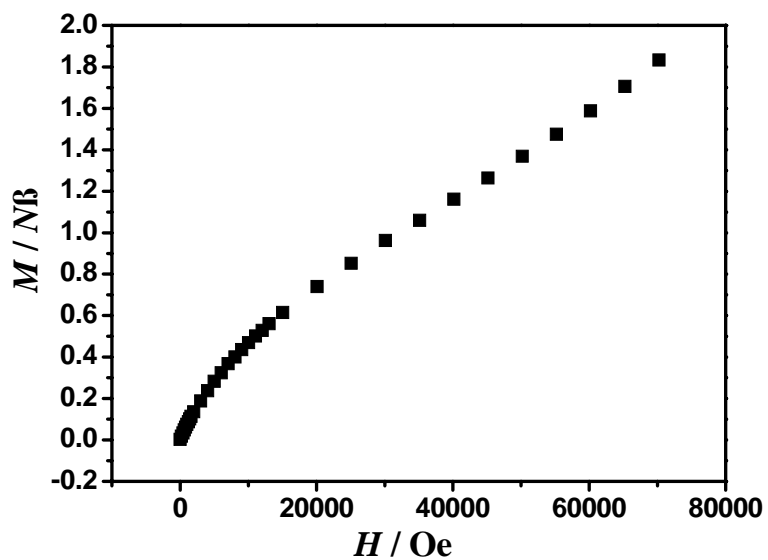


Figure S10. Field dependence of magnetization for **5** at $T = 2$ K.

Table S1. Selected bond lengths (Å) and angles (°) for **1** and **2**.

| | 1 | 2 | | 1 | 2 |
|-------------------|------------|------------|-------------------|------------|------------|
| Fe(1)-O(1) | 1.9064(9) | 1.9085(5) | Fe(1)-N(2c) | 2.353(3) | 2.366(2) |
| Fe(1)-O(2a) | 1.988(3) | 1.9993(18) | Fe(1)-N(2) | 2.353(3) | 2.366(2) |
| Fe(1)-O(2b) | 1.988(3) | 1.9993(19) | O(1)-Fe(1b) | 1.9064(9) | 1.9085(5) |
| Fe(1)-N(1c) | 2.243(4) | 2.250(2) | O(1)-Fe(1d) | 1.9064(9) | 1.9085(5) |
| Fe(1)-N(1) | 2.243(4) | 2.250(2) | O(2)-Fe(1d) | 1.988(3) | 1.9993(18) |
| O(1)-Fe(1)-O(2a) | 90.59(8) | 90.69(5) | O(2a)-Fe(1)-N(2c) | 93.29(12) | 93.07(8) |
| O(1)-Fe(1)-O(2b) | 90.59(8) | 90.69(5) | O(2b)-Fe(1)-N(2c) | 86.96(11) | 87.22(8) |
| O(2a)-Fe(1)-O(2b) | 178.83(17) | 178.62(11) | N(1c)-Fe(1)-N(2c) | 67.48(12) | 67.39(9) |
| O(1)-Fe(1)-N(1c) | 144.71(9) | 144.63(5) | N(1)-Fe(1)-N(2c) | 137.42(13) | 137.50(8) |
| O(2a)-Fe(1)-N(1c) | 87.28(11) | 87.14(8) | O(1)-Fe(1)-N(2) | 77.50(9) | 77.51(6) |
| O(2b)-Fe(1)-N(1c) | 91.77(12) | 91.74(8) | O(2a)-Fe(1)-N(2) | 86.96(11) | 87.22(8) |
| O(1)-Fe(1)-N(1) | 144.71(9) | 144.63(5) | O(2b)-Fe(1)-N(2) | 93.29(11) | 93.07(8) |
| O(2a)-Fe(1)-N(1) | 91.77(12) | 91.74(8) | N(1c)-Fe(1)-N(2) | 137.42(13) | 137.50(8) |
| O(2b)-Fe(1)-N(1) | 87.28(11) | 87.14(8) | N(1)-Fe(1)-N(2) | 67.48(12) | 67.38(8) |
| N(1c)-Fe(1)-N(1) | 70.57(17) | 70.74(11) | N(2c)-Fe(1)-N(2) | 155.00(17) | 155.02(11) |
| O(1)-Fe(1)-N(2c) | 77.50(9) | 77.51(6) | | | |

Symmetry codes for **1** and **2**: a) x, x-y+1, -z+3/2; b) -x+y, -x+1, z; c) -y+1, -x+1, -z+3/2; d) -y+1, x-y+1, z.

Table S2. Selected bond lengths (Å) and angles (°) for **3**.

| | | | |
|-------------|----------|-------------|----------|
| Fe(1)-O(3) | 1.950(4) | Fe(4)-O(9) | 1.956(4) |
| Fe(1)-O(5) | 2.050(4) | Fe(4)-O(10) | 2.037(4) |
| Fe(1)-N(2) | 2.270(5) | Fe(4)-N(6) | 2.246(5) |
| Fe(1)-N(1) | 2.231(6) | Fe(4)-Cl(3) | 2.270(2) |
| Fe(1)-Cl(1) | 2.260(2) | Fe(4)-N(5) | 2.242(6) |
| Fe(1)-N(4) | 2.426(6) | Fe(4)-N(8) | 2.385(6) |
| Fe(1)-N(3) | 2.352(6) | Fe(4)-N(7) | 2.372(6) |
| Fe(2)-O(1) | 1.966(5) | Fe(5)-O(8b) | 1.963(4) |
| Fe(2)-O(2a) | 1.979(5) | Fe(5)-O(7) | 1.967(4) |
| Fe(2)-O(3a) | 2.004(4) | Fe(5)-O(9) | 2.019(4) |
| Fe(2)-O(3) | 2.021(4) | Fe(5)-O(9b) | 2.020(4) |
| Fe(2)-O(4) | 2.055(5) | Fe(5)-O(11) | 2.068(4) |

| | | | |
|-------------------|------------|-------------------|------------|
| Fe(2)-O(6) | 2.046(5) | Fe(5)-O(12b) | 1.879(4) |
| Fe(3)-O(4) | 1.885(5) | Fe(6)-O(11) | 1.903(4) |
| Fe(3)-O(6a) | 1.880(5) | Fe(6)-O(12) | 1.879(4) |
| Fe(3)-O(5) | 1.935(4) | Fe(6)-O(10) | 1.938(4) |
| Fe(3)-O(3) | 2.119(4) | Fe(6)-O(9) | 2.125(4) |
| Fe(3)-Cl(2) | 2.252(2) | Fe(6)-Cl(4) | 2.272(2) |
| O(3)-Fe(1)-O(5) | 80.08(17) | O(9)-Fe(4)-O(10) | 79.95(16) |
| O(3)-Fe(1)-N(2) | 141.0(2) | O(9)-Fe(4)-N(6) | 141.6(2) |
| O(5)-Fe(1)-N(2) | 86.89(18) | O(10)-Fe(4)-N(6) | 87.17(18) |
| O(3)-Fe(1)-N(1) | 144.8(2) | O(9)-Fe(4)-Cl(3) | 103.12(12) |
| O(5)-Fe(1)-N(1) | 87.4(2) | O(10)-Fe(4)-Cl(3) | 176.83(13) |
| N(2)-Fe(1)-N(1) | 69.9(2) | N(6)-Fe(4)-Cl(3) | 90.79(15) |
| O(3)-Fe(1)-Cl(1) | 99.48(13) | O(9)-Fe(4)-N(5) | 142.9(2) |
| O(5)-Fe(1)-Cl(1) | 179.53(13) | O(10)-Fe(4)-N(5) | 88.88(19) |
| N(2)-Fe(1)-Cl(1) | 93.55(15) | N(6)-Fe(4)-N(5) | 70.2(2) |
| N(1)-Fe(1)-Cl(1) | 92.94(16) | Cl(3)-Fe(4)-N(5) | 93.65(14) |
| O(3)-Fe(1)-N(4) | 76.38(18) | O(9)-Fe(4)-N(8) | 78.31(17) |
| O(5)-Fe(1)-N(4) | 91.45(19) | O(10)-Fe(4)-N(8) | 88.89(18) |
| N(2)-Fe(1)-N(4) | 67.3(2) | N(6)-Fe(4)-N(8) | 67.3(2) |
| N(1)-Fe(1)-N(4) | 137.1(2) | Cl(3)-Fe(4)-N(8) | 90.93(14) |
| Cl(1)-Fe(1)-N(4) | 88.57(15) | N(5)-Fe(4)-N(8) | 139.02(19) |
| O(3)-Fe(1)-N(3) | 78.35(19) | O(9)-Fe(4)-N(7) | 77.35(17) |
| O(5)-Fe(1)-N(3) | 78.35(19) | O(10)-Fe(4)-N(7) | 90.53(18) |
| N(2)-Fe(1)-N(3) | 138.4(2) | N(6)-Fe(4)-N(7) | 139.2(2) |
| N(1)-Fe(1)-N(3) | 68.6(2) | Cl(3)-Fe(4)-N(7) | 89.43(14) |
| Cl(1)-Fe(1)-N(3) | 90.78(16) | N(5)-Fe(4)-N(7) | 67.4(2) |
| N(4)-Fe(1)-N(3) | 154.3(2) | N(8)-Fe(4)-N(7) | 153.55(18) |
| O(1)-Fe(2)-O(2a) | 97.0(2) | O(8b)-Fe(5)-O(7) | 97.42(19) |
| O(1)-Fe(2)-O(3a) | 164.31(19) | O(8b)-Fe(5)-O(9) | 165.57(18) |
| O(2a)-Fe(2)-O(3a) | 92.96(18) | O(7)-Fe(5)-O(9) | 91.21(17) |
| O(1)-Fe(2)-O(3) | 92.13(17) | O(8b)-Fe(5)-O(9b) | 92.17(17) |
| O(2a)-Fe(2)-O(3) | 165.31(19) | O(7)-Fe(5)-O(9b) | 165.32(17) |
| O(3a)-Fe(2)-O(3) | 80.71(17) | O(9)-Fe(5)-O(9b) | 81.99(16) |

| | | | |
|-------------------|------------|--------------------|------------|
| O(1)-Fe(2)-O(4) | 91.8(2) | O(8b)-Fe(5)-O(11) | 89.21(18) |
| O(2a)-Fe(2)-O(4) | 88.98(19) | O(7)-Fe(5)-O(11) | 91.19(19) |
| O(3a)-Fe(2)-O(4) | 100.49(19) | O(9)-Fe(5)-O(11) | 79.03(16) |
| O(3)-Fe(2)-O(4) | 79.26(17) | O(9b)-Fe(5)-O(11) | 100.86(18) |
| O(1)-Fe(2)-O(6) | 89.2(2) | O(8b)-Fe(5)-O(12b) | 89.92(19) |
| O(2a)-Fe(2)-O(6) | 89.8(2) | O(7)-Fe(5)-O(12b) | 89.26(19) |
| O(3a)-Fe(2)-O(6) | 78.70(18) | O(9)-Fe(5)-O(12b) | 101.77(17) |
| O(3)-Fe(2)-O(6) | 101.77(17) | O(9b)-Fe(5)-O(12b) | 78.83(17) |
| O(4)-Fe(2)-O(6) | 178.53(19) | O(11)-Fe(5)-O(12b) | 179.07(17) |
| O(4)-Fe(3)-O(6a) | 109.4(2) | O(11)-Fe(6)-O(12) | 108.0(2) |
| O(4)-Fe(3)-O(5) | 118.4(2) | O(11)-Fe(6)-O(10) | 119.9(2) |
| O(6a)-Fe(3)-O(5) | 122.6(2) | O(12)-Fe(6)-O(10) | 122.3(2) |
| O(4)-Fe(3)-O(3) | 80.74(17) | O(11)-Fe(6)-O(9) | 80.23(16) |
| O(6a)-Fe(3)-O(3) | 79.65(18) | O(12)-Fe(6)-O(9) | 80.25(17) |
| O(5)-Fe(3)-O(3) | 78.70(17) | O(10)-Fe(6)-O(9) | 78.18(16) |
| O(4)-Fe(3)-Cl(2) | 104.22(16) | O(11)-Fe(6)-Cl(4) | 101.45(14) |
| O(6a)-Fe(3)-Cl(2) | 101.55(13) | O(12)-Fe(6)-Cl(4) | 101.99(14) |
| O(5)-Fe(3)-Cl(2) | 97.94(14) | O(10)-Fe(6)-Cl(4) | 98.37(13) |
| O(3)-Fe(3)-Cl(2) | 174.97(13) | O(9)-Fe(6)-Cl(4) | 176.53(12) |

Symmetry codes for **3**: a) -x, -y, -z; b) -x-1, -y-1, -z-1.

Table S3. Selected bond lengths (Å) and angles (°) for **4**.

| | | | |
|-------------|-----------|-------------|-----------|
| Fe(1)-O(3) | 1.966(9) | Fe(2)-O(1) | 1.952(10) |
| Fe(1)-O(5) | 2.060(11) | Fe(2)-O(2a) | 1.960(10) |
| Fe(1)-N(1) | 2.257(11) | Fe(2)-O(3a) | 1.994(8) |
| Fe(1)-N(2) | 2.274(12) | Fe(2)-O(3) | 2.018(8) |
| Fe(1)-N(3) | 2.378(13) | Fe(2)-O(6a) | 2.035(10) |
| Fe(1)-N(4) | 2.418(11) | Fe(2)-O(4) | 2.073(11) |
| Fe(1)-Br(1) | 2.429(3) | Fe(3)-O(5) | 1.933(10) |
| Fe(3)-O(3) | 2.119(8) | Fe(3)-O(6) | 1.887(10) |
| Fe(3)-O(4) | 1.857(10) | Fe(3)-Br(2) | 2.366(3) |
| Fe(4)-O(9) | 1.954(9) | Fe(5)-O(8b) | 1.943(10) |
| Fe(4)-O(10) | 2.038(9) | Fe(5)-O(7) | 1.944(9) |
| Fe(4)-N(6) | 2.245(12) | Fe(5)-O(9b) | 2.028(10) |

| | | | |
|------------------|-----------|-------------------|-----------|
| Fe(4)-N(5) | 2.252(12) | Fe(5)-O(9) | 2.031(8) |
| Fe(4)-N(7) | 2.400(10) | Fe(5)-O(11) | 2.033(10) |
| Fe(4)-N(8) | 2.415(11) | Fe(5)-O(12b) | 2.054(10) |
| Fe(4)-Br(3) | 2.428(3) | Fe(6)-O(11) | 1.885(10) |
| Fe(6)-O(10) | 1.933(10) | Fe(6)-Br(4) | 2.408(3) |
| Fe(6)-O(9) | 2.106(9) | Fe(6)-O(12) | 1.886(9) |
| O(3)-Fe(1)-O(5) | 80.2(4) | O(2a)-Fe(2)-O(3a) | 93.2(4) |
| O(3)-Fe(1)-N(1) | 144.6(4) | O(1)-Fe(2)-O(3) | 92.6(4) |
| O(5)-Fe(1)-N(1) | 87.8(4) | O(2a)-Fe(2)-O(3) | 166.1(4) |
| O(3)-Fe(1)-N(2) | 140.9(4) | O(3a)-Fe(2)-O(3) | 80.3(4) |
| O(5)-Fe(1)-N(2) | 87.5(4) | O(1)-Fe(2)-O(6a) | 89.1(4) |
| N(1)-Fe(1)-N(2) | 70.6(4) | O(2a)-Fe(2)-O(6a) | 89.4(5) |
| O(3)-Fe(1)-N(3) | 78.4(4) | O(3a)-Fe(2)-O(6a) | 78.5(3) |
| O(5)-Fe(1)-N(3) | 89.1(4) | O(3)-Fe(2)-O(6a) | 101.1(4) |
| N(1)-Fe(1)-N(3) | 68.2(4) | O(1)-Fe(2)-O(4) | 91.3(5) |
| N(2)-Fe(1)-N(3) | 138.8(4) | O(2a)-Fe(2)-O(4) | 90.5(4) |
| O(3)-Fe(1)-N(4) | 76.3(4) | O(3a)-Fe(2)-O(4) | 101.0(4) |
| O(5)-Fe(1)-N(4) | 91.1(4) | O(3)-Fe(2)-O(4) | 78.9(4) |
| N(1)-Fe(1)-N(4) | 137.5(4) | O(6a)-Fe(2)-O(4) | 179.6(4) |
| N(2)-Fe(1)-N(4) | 66.9(4) | O(4)-Fe(3)-O(6) | 109.5(5) |
| N(3)-Fe(1)-N(4) | 154.2(4) | O(4)-Fe(3)-O(5) | 118.3(5) |
| O(3)-Fe(1)-Br(1) | 99.3(2) | O(6)-Fe(3)-O(5) | 123.0(4) |
| O(5)-Fe(1)-Br(1) | 179.5(3) | O(4)-Fe(3)-O(3) | 81.4(4) |
| N(1)-Fe(1)-Br(1) | 92.7(3) | O(6)-Fe(3)-O(3) | 78.9(4) |
| N(2)-Fe(1)-Br(1) | 92.7(3) | O(5)-Fe(3)-O(3) | 79.5(4) |
| N(3)-Fe(1)-Br(1) | 91.0(3) | O(4)-Fe(3)-Br(2) | 104.2(3) |
| N(4)-Fe(1)-Br(1) | 88.6(3) | O(6)-Fe(3)-Br(2) | 98.9(3) |
| O(1)-Fe(2)-O(2a) | 96.5(4) | O(5)-Fe(3)-Br(2) | 97.7(3) |
| O(1)-Fe(2)-O(3a) | 164.2(4) | O(3)-Fe(3)-Br(2) | 174.5(3) |
| O(9)-Fe(4)-O(10) | 79.4(4) | O(8b)-Fe(5)-O(7) | 96.6(4) |
| O(9)-Fe(4)-N(6) | 142.0(4) | O(8b)-Fe(5)-O(9b) | 92.7(4) |
| O(10)-Fe(4)-N(6) | 87.5(4) | O(7)-Fe(5)-O(9b) | 164.7(4) |
| O(9)-Fe(4)-N(5) | 143.9(4) | O(8b)-Fe(5)-O(9) | 165.8(4) |

| | | | |
|-------------------|----------|--------------------|----------|
| O(10)-Fe(4)-N(5) | 89.1(4) | O(7)-Fe(5)-O(9) | 91.5(4) |
| N(6)-Fe(4)-N(5) | 70.2(5) | O(9b)-Fe(5)-O(9) | 82.0(4) |
| O(9)-Fe(4)-N(7) | 77.1(4) | O(8b)-Fe(5)-O(11) | 90.2(4) |
| O(10)-Fe(4)-N(7) | 89.8(4) | O(7)-Fe(5)-O(11) | 90.8(4) |
| N(6)-Fe(4)-N(7) | 138.8(5) | O(9b)-Fe(5)-O(11) | 101.3(4) |
| N(5)-Fe(4)-N(7) | 68.6(5) | O(9)-Fe(5)-O(11) | 77.9(4) |
| O(9)-Fe(4)-N(8) | 76.9(4) | O(8b)-Fe(5)-O(12b) | 89.5(4) |
| O(10)-Fe(4)-N(8) | 91.6(4) | O(7)-Fe(5)-O(12b) | 89.6(4) |
| N(6)-Fe(4)-N(8) | 67.9(4) | O(9b)-Fe(5)-O(12b) | 78.4(4) |
| N(5)-Fe(4)-N(8) | 138.1(5) | O(9)-Fe(5)-O(12b) | 102.3(4) |
| N(7)-Fe(4)-N(8) | 153.3(4) | O(11)-Fe(5)-O(12b) | 179.5(4) |
| O(9)-Fe(4)-Br(3) | 103.2(3) | O(8b)-Fe(5)-O(7) | 96.6(4) |
| O(10)-Fe(4)-Br(3) | 177.2(3) | O(8b)-Fe(5)-O(9b) | 92.8(4) |
| N(6)-Fe(4)-Br(3) | 91.0(3) | O(7)-Fe(5)-O(9b) | 164.7(4) |
| N(5)-Fe(4)-Br(3) | 88.2(3) | O(8b)-Fe(5)-O(9) | 165.8(4) |
| N(7)-Fe(4)-Br(3) | 89.8(3) | O(7)-Fe(5)-O(9) | 91.5(4) |
| N(8)-Fe(4)-Br(3) | 89.9(3) | O(9b)-Fe(5)-O(9) | 82.0(4) |
| O(12)-Fe(6)-O(11) | 108.5(4) | O(10)-Fe(6)-O(9) | 78.2(4) |
| O(12)-Fe(6)-O(10) | 122.6(4) | O(12)-Fe(6)-Br(4) | 101.0(3) |
| O(11)-Fe(6)-O(10) | 118.7(4) | O(11)-Fe(6)-Br(4) | 102.0(3) |
| O(12)-Fe(6)-O(9) | 80.3(4) | O(10)-Fe(6)-Br(4) | 99.3(3) |
| O(11)-Fe(6)-O(9) | 79.4(4) | O(9)-Fe(6)-Br(4) | 177.6(3) |

Symmetry codes for **4**: a) $-x+1, -y+3, -z$; b) $-x, -y+4, -z-1$.

Table S4. Selected bond lengths (Å) and angles (°) for **5**

| | | | |
|--------------|------------|--------------|------------|
| Fe(1)-O(1a) | 2.1057(19) | Cl(1)-Fe(1d) | 2.7048(4) |
| Fe(1)-O(3b) | 2.1082(19) | Cl(1)-Fe(1e) | 2.7048(4) |
| Fe(1)-N(1) | 2.176(2) | Cl(1)-Fe(1a) | 2.7048(4) |
| Fe(1)-N(2) | 2.186(2) | O(1)-C(13) | 1.292(3) |
| Fe(1)-O(1) | 2.3713(19) | O(1)-Fe(1d) | 2.1057(19) |
| Fe(1)-O(3) | 2.3726(19) | O(2)-C(13) | 1.229(4) |
| Fe(1)-Cl(1) | 2.7048(4) | O(3)-C(14) | 1.282(4) |
| Cl(1)-Fe(1b) | 2.7048(4) | O(3)-Fe(1c) | 2.1078(19) |
| Cl(1)-Fe(1c) | 2.7048(4) | | |

| | | | |
|---------------------|------------|---------------------|------------|
| O(1a)-Fe(1)-O(3b) | 156.93(8) | Fe(1)-Cl(1)-Fe(1d) | 89.914(12) |
| O(1a)-Fe(1)-N(1) | 97.46(8) | Fe(1c)-Cl(1)-Fe(1d) | 180.0 |
| O(3b)-Fe(1)-N(1) | 100.72(8) | Fe(1b)-Cl(1)-Fe(1e) | 89.914(12) |
| O(1a)-Fe(1)-N(2) | 99.44(8) | Fe(1)-Cl(1)-Fe(1e) | 180.0 |
| O(3b)-Fe(1)-N(2) | 99.29(8) | Fe(1c)-Cl(1)-Fe(1e) | 89.914(12) |
| N(1)-Fe(1)-N(2) | 73.34(9) | Fe(1d)-Cl(1)-Fe(1e) | 90.086(12) |
| O(1a)-Fe(1)-O(1) | 86.03(10) | Fe(1b)-Cl(1)-Fe(1a) | 180.0 |
| O(3b)-Fe(1)-O(1) | 87.30(7) | Fe(1)-Cl(1)-Fe(1a) | 89.914(12) |
| N(1)-Fe(1)-O(1) | 69.11(8) | Fe(1c)-Cl(1)-Fe(1a) | 90.086(12) |
| N(2)-Fe(1)-O(1) | 142.45(8) | Fe(1d)-Cl(1)-Fe(1a) | 89.914(12) |
| O(1a)-Fe(1)-O(3) | 87.49(7) | Fe(1e)-Cl(1)-Fe(1a) | 90.086(12) |
| O(3b)-Fe(1)-O(3) | 86.79(2) | C(13)-O(1)-Fe(1d) | 124.45(17) |
| N(1)-Fe(1)-O(3) | 142.21(8) | C(13)-O(1)-Fe(1) | 118.31(17) |
| N(2)-Fe(1)-O(3) | 68.89(8) | Fe(1d)-O(1)-Fe(1) | 117.13(8) |
| O(1)-Fe(1)-O(3) | 148.66(7) | C(14)-O(3)-Fe(1c) | 123.96(18) |
| O(1a)-Fe(1)-Cl(1) | 78.55(5) | C(14)-O(3)-Fe(1) | 118.67(18) |
| O(3b)-Fe(1)-Cl(1) | 78.38(5) | Fe(1c)-O(3)-Fe(1) | 117.27(9) |
| N(1)-Fe(1)-Cl(1) | 143.49(7) | C(1)-N(1)-C(5) | 118.7(2) |
| N(2)-Fe(1)-Cl(1) | 143.15(6) | C(1)-N(1)-Fe(1) | 123.82(19) |
| O(1)-Fe(1)-Cl(1) | 74.40(5) | C(5)-N(1)-Fe(1) | 117.40(19) |
| O(3)-Fe(1)-Cl(1) | 74.26(5) | C(10)-N(2)-C(6) | 118.3(2) |
| Fe(1b)-Cl(1)-Fe(1) | 90.086(12) | C(10)-N(2)-Fe(1) | 123.97(19) |
| Fe(1b)-Cl(1)-Fe(1c) | 89.914(12) | C(6)-N(2)-Fe(1) | 117.76(19) |
| Fe(1)-Cl(1)-Fe(1c) | 90.086(12) | Fe(1)-Cl(1)-Fe(1d) | 89.914(12) |
| Fe(1b)-Cl(1)-Fe(1d) | 90.086(12) | Fe(1c)-Cl(1)-Fe(1d) | 180.0 |

Symmetry codes for **5**: a) $-y+1, x-y-1, z$; b) $y+1, -x+y+1, -z+2$; c) $x-y, x-1, -z+2$; d) $-x+y+2, -x+1, z$; e) $-x+2, -y, -z+2$.