*Electronic Supplementary Information (ESI)*

# Step-by-step synthesis of one $Fe_6$ wheel and two $Fe_{10}$ clusters derived from multidentate triethanoamine ligand

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## Experimental Section

**Materials and methods.** All chemicals were of reagent grade and were used as purchased without further purification. Elemental analysis (C and H) was performed on a Perkin-Elmer 240C analyzer (Perkin-Elmer, USA). $[Fe_3O(HCO_2)_6(H_2O)_3]\cdot NO_3$ and $[Fe_3O(HCOO)_6(H_2O)_3]\cdot Cl$ were prepared using the procedures reported previously with small modification.[S1] The XRPD spectrum was recorded on a Rigaku D/Max-2500 diffractometer at 40 kV, 100 mA for a Cu-target tube and a graphite monochromator. Simulation of the XRPD spectrum was carried out by the single-crystal data and diffraction-crystal module of the Mercury (Hg) program available free of charge *via* the Internet at http://www.iucr.org. IR spectra were measured in the range of 400-4000 $cm^{-1}$ on a Tensor 27 OPUS FT-IR spectrometer using KBr pellets (Bruker, German). Magnetic susceptibility was measured by a Quantum Design MPMS superconducting quantum interference device (SQUID). Diamagnetic corrections were estimated by using Pascal constants and background corrections by experimental measurement on sample holders.

**X-ray Crystallography.**

X-ray single-crystal diffraction data were collected on a SCX-Mini diffractometer at 293(2) K (for **1**) and a Rigaku RAXIS-RAPID diffractometer at 113(2) K (for **2** and **3**) with Mo-Kα radiation (λ = 0.71073 Å) by ω scan mode. The program *Crystalclear*[S2] was used for the integration of the diffraction profiles. The structures were solved by direct method using the SHELXS program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL (semi-empirical absorption corrections were applied by using the SADABS program).[S3] The non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on $F^2$. All hydrogen atoms of were generated theoretically at the specific atoms and refined isotropically with fixed thermal factors. The selected bond lengths and angles are given in Tables S1-S3 (ESI).

**References**


S1. (a) M. K. Johnson, D. B. Powell and R. D. Cannon, *Spectrochim. Acta*., 1981, **37**, 995; (b) A. M. Bond, R. J. H. Clark, D. G. Humphrey, P. Panayiotopoulos, B. W. Skelton and A. H. White, *J. Chem. Soc., Dalton Trans.,* 1998, 1845.

S2. Rigaku, Process-Auto; Rigaku Americas Corporation: The Woodlands, Texas, 1998.

S3. G. M. Sheldrick, *SHELXL97, Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, 1997.

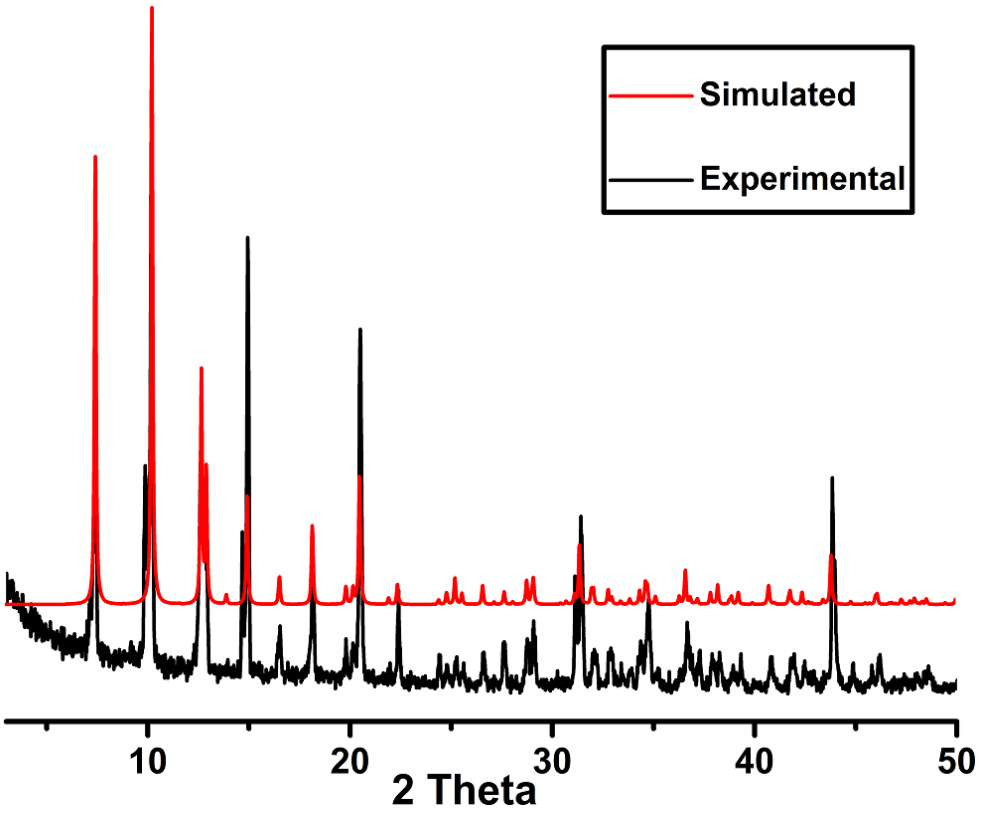
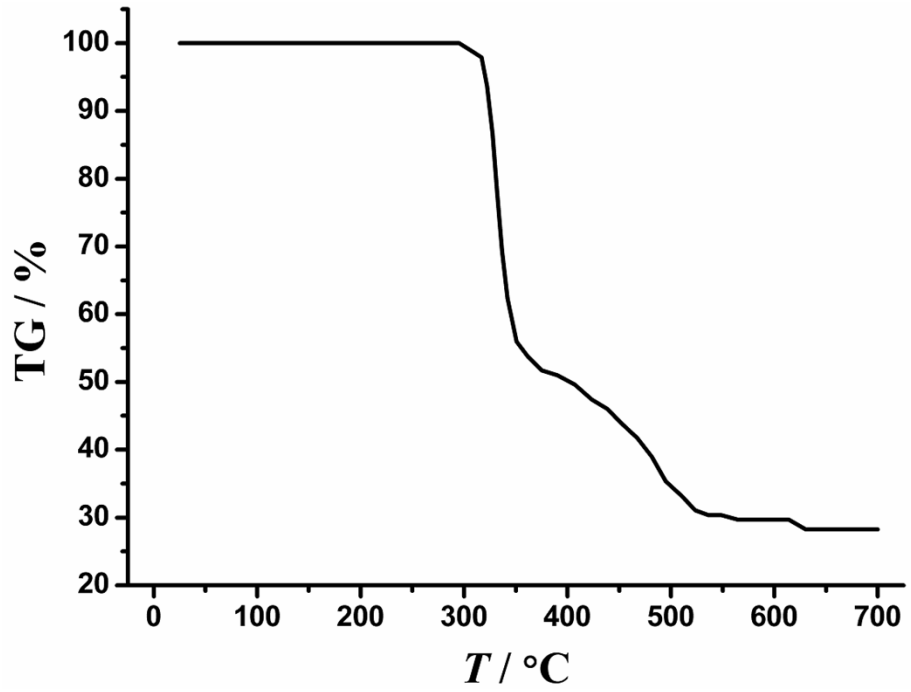
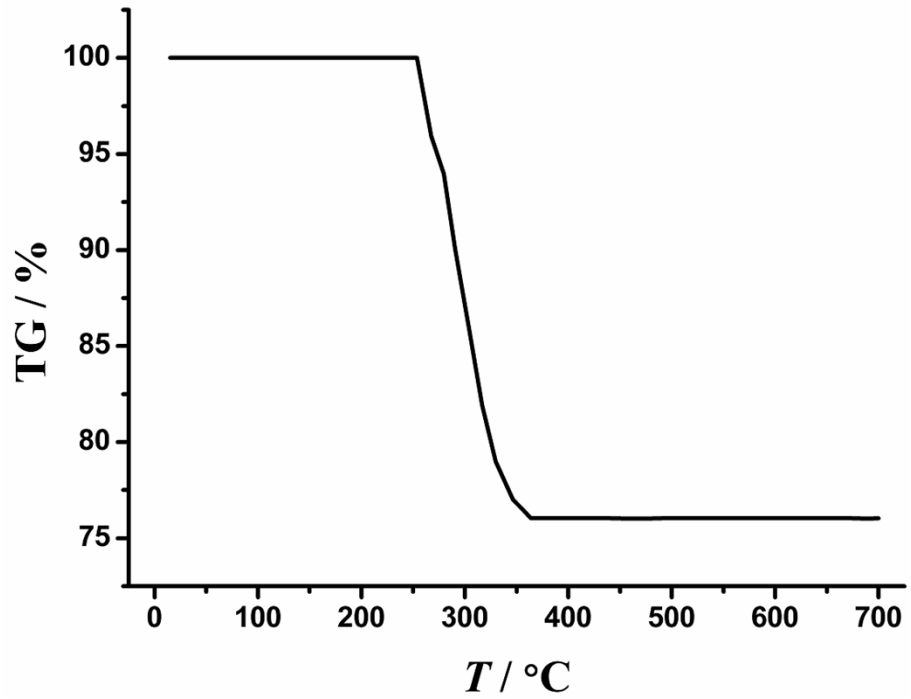



**Fig. S1** X-ray powder diffraction patterns of **1**.




**(a)**




**(b)**

**Fig. S2** TGA curves for **2** and **3**.

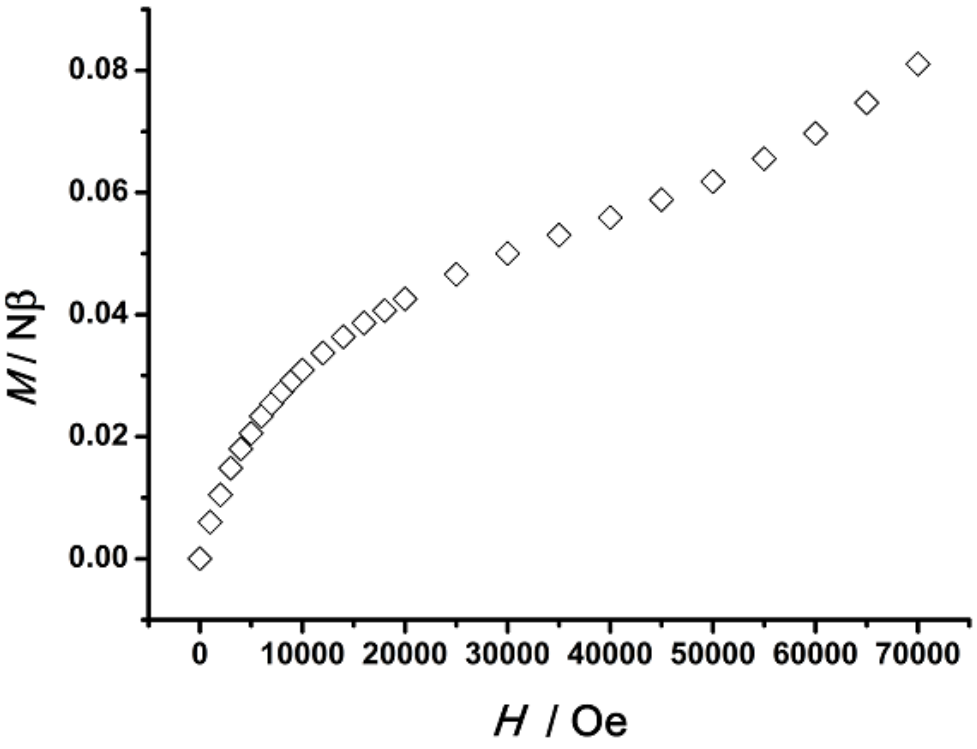



**Fig. S3** The *M vs. H* curve of **1**.

**Table S1.** Selected bond lengths (Å) and angles (°) for complex **1**[a]

| | | | |
|---|---|---|---|
| Fe1—O1 | 1.923(4) | Fe1—O3$^{\#1}$ | 2.033(3) |
| Fe1—O3 | 1.990(3) | Fe1—O2$^{\#2}$ | 2.068(3) |
| Fe1—O2 | 1.993(3) | Fe1—N1 | 2.211(4) |
| | | | |
| O1—Fe1—O3 | 93.27(15) | O2—Fe1—O2$^{\#2}$ | 100.9(2) |
| O1—Fe1—O2 | 106.56(15) | O3$^{\#1}$—Fe1—O2$^{\#2}$ | 92.88(14) |
| O3—Fe1—O2 | 96.43(14) | O1—Fe1—N1 | 80.17(16) |
| O1—Fe1—O3$^{\#1}$ | 102.91(16) | O3—Fe1—N1 | 109.25(15) |
| O3—Fe1—O3$^{\#1}$ | 163.26(19) | O2—Fe1—N1 | 153.20(14) |
| O2—Fe1—O3$^{\#1}$ | 75.05(13) | O3$^{\#1}$—Fe1—N1 | 78.16(14) |
| O1—Fe1—O2$^{\#2}$ | 151.05(15) | O2$^{\#2}$—Fe1—N1 | 79.54(15) |
| O3—Fe1—O2$^{\#2}$ | 74.34(13) | | |

[a]Symmetry codes: #1: x−y, x, −z+1; #2: y, −x+y, −z+1.

**Table S2.** Selected bond lengths (Å) and angles (°) for complex **2**

| | | | |
|---|---|---|---|
| Fe1—O4 | 1.884(11) | Fe8—O18 | 2.041(11) |
| Fe1—O6 | 1.920(10) | Fe8—O20 | 2.040(10) |
| Fe1—O7 | 1.929(10) | Fe8—O25 | 2.057(11) |
| Fe1—O5 | 1.966(11) | Fe9—O3 | 1.922(10) |
| Fe1—N1 | 2.269(12) | Fe9—O16 | 2.005(11) |
| Fe2—O1 | 1.984(11) | Fe9—O17 | 2.020(10) |
| Fe2—O8 | 2.014(11) | Fe9—O18 | 2.029(10) |
| Fe2—O9 | 2.029(10) | Fe9—O2 | 2.146(10) |
| Fe2—O7 | 2.037(10) | Fe9—N5 | 2.264(14) |
| Fe2—O2 | 2.180(11) | Fe10—O21 | 1.908(11) |
| Fe2—N2 | 2.256(13) | Fe10—O17 | 1.931(11) |
| Fe3—O1 | 1.905(10) | Fe10—O20 | 1.981(12) |
| Fe3—O26 | 1.957(11) | Fe10—O19 | 1.989(10) |
| Fe3—O13 | 2.000(10) | Fe10—N6 | 2.254(13) |
| Fe3—O6 | 2.049(10) | Fe7—O3 | 1.938(10) |
| Fe3—O8 | 2.091(11) | Fe7—O30 | 1.996(11) |
| Fe3—O22 | 2.120(10) | Fe7—O11 | 2.012(10) |
| Fe4—O1 | 1.895(11) | Fe7—O15 | 2.020(10) |
| Fe4—O28 | 1.951(12) | Fe7—O24 | 2.073(10) |
| Fe4—O14 | 2.026(9) | Fe7—O19 | 2.099(10) |
| Fe4—O10 | 2.075(10) | Fe8—O3 | 1.945(10) |
| Fe4—O23 | 2.098(10) | Fe8—O32 | 1.996(12) |
| Fe4—O5 | 2.131(10) | Fe8—O12 | 2.024(10) |
| Fe5—O11 | 1.984(10) | Fe5—N3 | 2.177(11) |
| Fe5—O2 | 1.989(10) | Fe6—O13 | 1.983(11) |
| Fe5—O12 | 2.000(10) | Fe6—O14 | 1.990(10) |
| Fe5—O9 | 2.022(10) | Fe6—O2 | 2.023(11) |
| Fe5—O10 | 2.055(10) | Fe6—O16 | 2.060(10) |

| | | | |
|---|---|---|---|
| Fe6—N4 | 2.231(12) | Fe6—O15 | 2.068(10) |
| | | | |
| O4—Fe1—O6 | 108.9(5) | O32—Fe8—O12 | 96.4(5) |
| O4—Fe1—O7 | 92.6(5) | O3—Fe8—O18 | 76.8(4) |
| O6—Fe1—O7 | 104.9(5) | O32—Fe8—O18 | 100.5(5) |
| O4—Fe1—O5 | 124.1(5) | O12—Fe8—O18 | 92.2(4) |
| O6—Fe1—O5 | 118.7(5) | O3—Fe8—O20 | 83.9(4) |
| O7—Fe1—O5 | 101.3(5) | O32—Fe8—O20 | 90.6(5) |
| O4—Fe1—N1 | 81.9(5) | O12—Fe8—O20 | 170.2(5) |
| O6—Fe1—N1 | 81.3(5) | O18—Fe8—O20 | 93.3(5) |
| O7—Fe1—N1 | 172.9(4) | O3—Fe8—O25 | 94.6(4) |
| O5—Fe1—N1 | 78.3(5) | O32—Fe8—O25 | 88.3(5) |
| O1—Fe2—O8 | 77.9(4) | O12—Fe8—O25 | 85.8(4) |
| O1—Fe2—O9 | 133.3(4) | O18—Fe8—O25 | 171.2(4) |
| O8—Fe2—O9 | 148.0(4) | O20—Fe8—O25 | 87.6(5) |
| O1—Fe2—O7 | 80.4(4) | O3—Fe9—O16 | 134.0(5) |
| O8—Fe2—O7 | 102.6(4) | O3—Fe9—O17 | 79.9(4) |
| O9—Fe2—O7 | 91.9(4) | O16—Fe9—O17 | 90.6(4) |
| O1—Fe2—O2 | 90.2(4) | O3—Fe9—O18 | 77.6(4) |
| O8—Fe2—O2 | 97.6(4) | O16—Fe9—O18 | 147.8(4) |
| O9—Fe2—O2 | 77.9(4) | O17—Fe9—O18 | 103.7(4) |
| O7—Fe2—O2 | 155.3(4) | O3—Fe9—O2 | 91.6(4) |
| O1—Fe2—N2 | 144.9(5) | O16—Fe9—O2 | 78.7(4) |
| O8—Fe2—N2 | 79.4(5) | O17—Fe9—O2 | 155.3(4) |
| O9—Fe2—N2 | 75.6(5) | O18—Fe9—O2 | 96.9(4) |
| O7—Fe2—N2 | 78.8(4) | O3—Fe9—N5 | 141.6(5) |
| O2—Fe2—N2 | 119.2(4) | O16—Fe9—N5 | 77.1(5) |
| O1—Fe3—O26 | 175.1(5) | O17—Fe9—N5 | 77.8(4) |
| O1—Fe3—O13 | 88.9(4) | O18—Fe9—N5 | 77.9(5) |
| O26—Fe3—O13 | 95.4(4) | O2—Fe9—N5 | 120.3(4) |
| O1—Fe3—O6 | 84.8(4) | O21—Fe10—O17 | 90.9(5) |
| O26—Fe3—O6 | 91.3(4) | O21—Fe10—O20 | 107.9(6) |
| O13—Fe3—O6 | 170.7(5) | O17—Fe10—O20 | 105.2(5) |
| O1—Fe3—O8 | 77.8(4) | O21—Fe10—O19 | 121.7(5) |
| O26—Fe3—O8 | 99.5(5) | O17—Fe10—O19 | 102.9(5) |
| O13—Fe3—O8 | 92.3(4) | O20—Fe10—O19 | 121.7(5) |
| O6—Fe3—O8 | 93.1(4) | O21—Fe10—N6 | 80.2(4) |
| O1—Fe3—O22 | 94.0(4) | O17—Fe10—N6 | 170.8(4) |
| O26—Fe3—O22 | 88.7(5) | O20—Fe10—N6 | 79.8(5) |
| O13—Fe3—O22 | 87.5(4) | O19—Fe10—N6 | 80.3(5) |
| O6—Fe3—O22 | 86.1(5) | O13—Fe6—O14 | 96.6(4) |
| O8—Fe3—O22 | 171.8(4) | O13—Fe6—O2 | 115.4(4) |
| O1—Fe4—O28 | 168.6(5) | O14—Fe6—O2 | 97.2(4) |
| O1—Fe4—O14 | 88.3(4) | O13—Fe6—O16 | 86.7(4) |
| O28—Fe4—O14 | 98.2(5) | O14—Fe6—O16 | 176.5(4) |

| | | | |
|---|---|---|---|
| O1—Fe4—O10 | 82.0(4) | O2—Fe6—O16 | 80.3(4) |
| O28—Fe4—O10 | 88.5(5) | O13—Fe6—O15 | 148.3(4) |
| O14—Fe4—O10 | 90.8(4) | O14—Fe6—O15 | 100.7(4) |
| O1—Fe4—O23 | 98.9(4) | O2—Fe6—O15 | 88.7(4) |
| O28—Fe4—O23 | 90.8(5) | O16—Fe6—O15 | 76.9(4) |
| O14—Fe4—O23 | 86.7(4) | O13—Fe6—N4 | 78.6(4) |
| O10—Fe4—O23 | 177.4(4) | O14—Fe6—N4 | 81.2(4) |
| O1—Fe4—O5 | 84.1(4) | O2—Fe6—N4 | 166.0(5) |
| O28—Fe4—O5 | 90.4(5) | O16—Fe6—N4 | 100.5(5) |
| O14—Fe4—O5 | 169.8(4) | O15—Fe6—N4 | 78.0(4) |
| O10—Fe4—O5 | 94.9(4) | O3—Fe7—O30 | 173.1(5) |
| O23—Fe4—O5 | 87.6(4) | O3—Fe7—O11 | 90.5(4) |
| O11—Fe5—O2 | 94.4(4) | O30—Fe7—O11 | 93.0(4) |
| O11—Fe5—O12 | 97.0(5) | O3—Fe7—O15 | 81.9(4) |
| O2—Fe5—O12 | 113.7(4) | O30—Fe7—O15 | 92.1(5) |
| O11—Fe5—O9 | 176.6(5) | O11—Fe7—O15 | 91.2(4) |
| O2—Fe5—O9 | 82.6(4) | O3—Fe7—O24 | 95.5(4) |
| O12—Fe5—O9 | 85.7(4) | O30—Fe7—O24 | 90.6(5) |
| O11—Fe5—O10 | 98.7(4) | O11—Fe7—O24 | 87.5(4) |
| O2—Fe5—O10 | 91.8(4) | O15—Fe7—O24 | 177.1(4) |
| O12—Fe5—O10 | 148.7(4) | O3—Fe7—O19 | 82.8(4) |
| O9—Fe5—O10 | 79.7(4) | O30—Fe7—O19 | 94.6(4) |
| O11—Fe5—N3 | 82.6(4) | O11—Fe7—O19 | 169.4(4) |
| O2—Fe5—N3 | 167.9(5) | O15—Fe7—O19 | 95.9(4) |
| O12—Fe5—N3 | 78.4(4) | O24—Fe7—O19 | 85.1(4) |
| O9—Fe5—N3 | 99.9(4) | O3—Fe8—O32 | 173.7(5) |
| O10—Fe5—N3 | 77.1(4) | O3—Fe8—O12 | 89.4(4) |

**Table S3.** Selected bond lengths (Å) and angles (°) for complex **3**

| | | | |
|---|---|---|---|
| O18—Fe2 | 2.061(6) | Fe8—O25 | 1.940(7) |
| Fe1—O4 | 1.989(6) | Fe8—O24 | 1.956(6) |
| Fe1—O2 | 1.991(6) | Fe8—N5 | 2.257(7) |
| Fe1—O1 | 2.000(6) | Fe9—O5 | 1.982(6) |
| Fe1—O3 | 2.007(6) | Fe9—O11 | 1.986(6) |
| Fe1—O5 | 2.143(6) | Fe9—O12 | 1.993(6) |
| Fe1—N1 | 2.277(8) | Fe9—O22 | 2.048(6) |
| Fe2—O19 | 1.914(6) | Fe9—O13 | 2.066(6) |
| Fe2—O15 | 2.003(6) | Fe9—N6 | 2.201(7) |
| Fe2—O24 | 2.047(6) | Fe10—O19 | 1.913(6) |
| Fe2—O20 | 2.088(6) | Fe10—O16 | 1.993(6) |
| Fe2—Cl1 | 2.326(3) | Fe10—O13 | 2.057(6) |
| Fe3—O19 | 1.969(6) | Fe10—O25 | 2.059(6) |
| Fe3—O20 | 1.992(6) | Fe10—O17 | 2.091(6) |
| Fe3—O21 | 1.996(6) | Fe10—Cl4 | 2.342(3) |
| Fe3—O22 | 1.999(6) | Fe5—Cl2 | 2.324(3) |
| Fe3—O5 | 2.164(6) | Fe6—O4 | 1.887(6) |
| Fe3—N2 | 2.293(8) | Fe6—O12 | 1.999(6) |
| Fe3—Fe9 | 2.9270(18) | Fe6—O14 | 2.056(6) |
| Fe4—O5 | 1.992(6) | Fe6—O10 | 2.072(6) |
| Fe4—O16 | 1.992(6) | Fe6—O7 | 2.073(6) |
| Fe4—O15 | 2.012(6) | Fe6—Cl3 | 2.359(3) |
| Fe4—O1 | 2.026(6) | Fe7—O6 | 1.884(6) |
| Fe4—O14 | 2.064(6) | Fe7—O2 | 1.945(6) |
| Fe4—N3 | 2.203(7) | Fe7—O7 | 1.949(7) |
| Fe5—O4 | 1.937(6) | Fe7—O8 | 1.961(6) |
| Fe5—O11 | 2.002(6) | Fe7—N4 | 2.267(8) |
| Fe5—O8 | 2.029(6) | Fe8—O23 | 1.879(6) |
| Fe5—O3 | 2.073(6) | Fe8—O21 | 1.935(6) |
| Fe5—O9 | 2.081(6) | | |
| | | | |
| O18—Fe2—O20 | 171.8(3) | O16—Fe10—Cl4 | 95.96(19) |
| O4—Fe1—O2 | 80.8(2) | O13—Fe10—Cl4 | 91.53(18) |
| O4—Fe1—O1 | 133.8(3) | O25—Fe10—Cl4 | 90.49(19) |
| O2—Fe1—O1 | 90.7(2) | O17—Fe10—Cl4 | 91.76(19) |
| O4—Fe1—O3 | 78.3(2) | O3—Fe1—N1 | 77.8(3) |
| O2—Fe1—O3 | 104.5(2) | O5—Fe1—N1 | 120.4(2) |
| O1—Fe1—O3 | 146.9(3) | O19—Fe2—O15 | 86.8(3) |
| O4—Fe1—O5 | 90.2(2) | O19—Fe2—O24 | 84.3(3) |
| O2—Fe1—O5 | 153.9(3) | O15—Fe2—O24 | 168.5(3) |
| O1—Fe1—O5 | 77.9(2) | O19—Fe2—O18 | 94.7(3) |
| O3—Fe1—O5 | 97.6(2) | O15—Fe2—O18 | 85.5(3) |
| O4—Fe1—N1 | 143.1(3) | O24—Fe2—O18 | 87.9(3) |
| O2—Fe1—N1 | 78.5(3) | O19—Fe2—O20 | 77.1(2) |

| | | | |
|---|---|---|---|
| O1—Fe1—N1 | 76.7(3) | O15—Fe2—O20 | 94.5(2) |
| O24—Fe2—O20 | 90.7(2) | O4—Fe5—O11 | 87.8(2) |
| O21—Fe3—O5 | 154.0(3) | O19—Fe3—O20 | 78.2(3) |
| O22—Fe3—O5 | 78.1(2) | O19—Fe3—O21 | 81.6(2) |
| O19—Fe3—N2 | 142.9(3) | O20—Fe3—O21 | 103.8(3) |
| O20—Fe3—N2 | 77.2(3) | O19—Fe3—O22 | 135.3(3) |
| O21—Fe3—N2 | 77.8(3) | O20—Fe3—O22 | 145.6(3) |
| O22—Fe3—N2 | 76.1(3) | O21—Fe3—O22 | 91.3(2) |
| O5—Fe3—N2 | 121.4(3) | O19—Fe3—O5 | 89.3(2) |
| O5—Fe4—O16 | 96.8(2) | O20—Fe3—O5 | 98.0(2) |
| O5—Fe4—O15 | 115.0(3) | O11—Fe5—O8 | 170.2(3) |
| O16—Fe4—O15 | 97.0(3) | O4—Fe5—O3 | 77.9(2) |
| O5—Fe4—O1 | 80.9(2) | O11—Fe5—O3 | 93.5(2) |
| O16—Fe4—O1 | 176.7(2) | O8—Fe5—O3 | 90.8(2) |
| O15—Fe4—O1 | 86.1(2) | O4—Fe5—O9 | 93.9(3) |
| O5—Fe4—O14 | 89.4(2) | O11—Fe5—O9 | 86.1(2) |
| O16—Fe4—O14 | 98.2(2) | O8—Fe5—O9 | 88.3(2) |
| O15—Fe4—O14 | 149.3(2) | O3—Fe5—O9 | 171.8(2) |
| O1—Fe4—O14 | 79.5(2) | O4—Fe5—Cl2 | 172.1(2) |
| O5—Fe4—N3 | 166.6(3) | O11—Fe5—Cl2 | 94.68(19) |
| O16—Fe4—N3 | 82.0(3) | O8—Fe5—Cl2 | 93.73(19) |
| O15—Fe4—N3 | 78.3(3) | O3—Fe5—Cl2 | 94.40(18) |
| O1—Fe4—N3 | 99.7(3) | O9—Fe5—Cl2 | 93.80(19) |
| O14—Fe4—N3 | 77.6(3) | O4—Fe5—O8 | 84.6(2) |
| O4—Fe6—O12 | 89.5(3) | O2—Fe7—O7 | 101.7(3) |
| O4—Fe6—O14 | 82.6(3) | O6—Fe7—O8 | 109.4(3) |
| O12—Fe6—O14 | 89.6(2) | O2—Fe7—O8 | 104.6(3) |
| O4—Fe6—O10 | 95.6(3) | O7—Fe7—O8 | 122.3(3) |
| O12—Fe6—O10 | 86.7(2) | O6—Fe7—N4 | 80.1(3) |
| O14—Fe6—O10 | 175.9(2) | O2—Fe7—N4 | 170.8(3) |
| O4—Fe6—O7 | 83.0(3) | O7—Fe7—N4 | 81.0(3) |
| O12—Fe6—O7 | 170.1(2) | O8—Fe7—N4 | 80.8(3) |
| O14—Fe6—O7 | 95.9(2) | O23—Fe8—O21 | 91.9(3) |
| O10—Fe6—O7 | 87.5(2) | O23—Fe8—O25 | 118.5(3) |
| O4—Fe6—Cl3 | 172.29(19) | O21—Fe8—O25 | 103.6(3) |
| O12—Fe6—Cl3 | 96.36(19) | O7—Fe6—Cl3 | 91.63(19) |
| O14—Fe6—Cl3 | 92.43(19) | O6—Fe7—O2 | 91.0(3) |
| O10—Fe6—Cl3 | 89.71(19) | O6—Fe7—O7 | 120.5(3) |
| O23—Fe8—O24 | 113.1(3) | O19—Fe10—O16 | 90.6(3) |
| O21—Fe8—O24 | 102.1(3) | O19—Fe10—O13 | 82.1(2) |
| O25—Fe8—O24 | 120.6(3) | O16—Fe10—O13 | 90.7(2) |
| O23—Fe8—N5 | 80.4(3) | O19—Fe10—O25 | 83.8(3) |
| O21—Fe8—N5 | 172.2(3) | O16—Fe10—O25 | 170.9(3) |
| O25—Fe8—N5 | 80.9(3) | O13—Fe10—O25 | 95.5(2) |
| O24—Fe8—N5 | 80.5(3) | O19—Fe10—O17 | 94.9(3) |

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| O5—Fe9—O11 | 115.6(3) | O16—Fe10—O17 | 86.5(2) |
| O5—Fe9—O12 | 96.7(2) | O13—Fe10—O17 | 175.9(2) |
| O11—Fe9—O12 | 96.1(2) | O25—Fe10—O17 | 86.9(2) |
| O5—Fe9—O22 | 81.3(2) | O19—Fe10—Cl4 | 170.9(2) |
| O11—Fe9—O22 | 85.6(2) | O22—Fe9—O13 | 79.4(2) |
| O12—Fe9—O22 | 177.8(2) | O5—Fe9—N6 | 166.6(3) |
| O5—Fe9—O13 | 89.6(2) | O11—Fe9—N6 | 77.8(3) |
| O11—Fe9—O13 | 148.3(2) | O12—Fe9—N6 | 81.4(3) |
| O12—Fe9—O13 | 99.7(2) | O22—Fe9—N6 | 100.4(3) |