Supporting Information

A Mn(II)-cluster-based coordination framework derived from a $C_3$ symmetric ligand: Synthesis, structure and magnetic properties

Yong-Jun Bian, Yuan Tian, Ai-Hua Zhang and Yong-Qiang Chen*

College of Chemistry and Chemical Engineering, Jinzhong University, Jinzhong, Shanxi 030619, P. R. of China. E-mail: chenyongqiang@jzxy.edu.cn
Table S1. Selected bond distances (Å) and angles (°) for complex 1

| Bond/Angle | Distance/Angle |
|------------|---------------|
| Mn(1)-O(1) | 2.145(3)      |
| Mn(1)-O(5) | 2.202(3)      |
| Mn(1)-O(7)#1 | 2.302(3)      |
| Mn(2)-O(2)#2 | 2.168(3)      |
| Mn(2)-O(9) | 2.140(3)      |
| Mn(2)-O(12) | 2.235(4)      |
| Mn(3)-O(6)#1 | 2.161(3)      |
| Mn(3)-O(10)#4 | 2.100(3)      |
| Mn(3)-O(24)#5 | 2.171(3)      |
| Mn(4)-O(17) | 2.086(4)      |
| Mn(4)-O(19) | 2.146(3)      |
| Mn(5)-O(18) | 2.128(3)      |
| Mn(5)-O(23)#2 | 2.147(3)      |
| Mn(5)-O(13)#7 | 2.171(3)      |
| Mn(6)-O(15) | 2.085(3)      |
| Mn(6)-O(22)#1 | 2.119(3)      |
| Mn(6)-O(14)#2 | 2.183(3)      |
| Mn(7)-O(31) | 2.183(4)      |
| Mn(7)-O(26) | 2.198(4)      |
| Mn(7)-O(34) | 2.146(4)      |
| O(3)-Mn(1)-O(1) | 97.95(13) |
| O(3)-Mn(1)-O(5) | 97.99(12) |
| O(1)-Mn(1)-O(5) | 84.88(12) |
| O(11)-Mn(1)-O(7) | 93.26(11) |
| O(5)-Mn(1)-O(7) | 85.95(12) |
| O(11)-Mn(1)-O(7)#1 | 81.64(11) |
| O(5)-Mn(1)-O(7)#1 | 89.37(11) |
| O(9)-Mn(2)-O(2)#2 | 164.81(13) |
| O(9)-Mn(2)-O(12) | 83.53(14) |
| O(2)#2-Mn(2)-O(12) | 82.52(14) |
| O(11)#2-Mn(2)-O(4)#2 | 93.98(12) |
| O(12)-Mn(2)-O(4)#2 | 94.96(14) |
| O(11)#2-Mn(2)-O(25)#3 | 83.91(12) |
| O(12)-Mn(2)-O(25)#3 | 88.14(14) |
| O(11)-Mn(3)-O(10)#4 | 108.08(13) |
| O(10)#4-Mn(3)-O(6)#1 | 122.41(13) |
| O(10)#4-Mn(3)-O(8) | 88.00(12) |
| O(11)-Mn(3)-O(24)#5 | 88.57(12) |
| O(6)#1-Mn(3)-O(24)#5 | 83.68(13) |
| Bond                  | Distance | Bond                  | Distance | Bond                  | Distance |
|-----------------------|----------|-----------------------|----------|-----------------------|----------|
| O(16)#6-Mn(4)-O(17)   | 120.23(16)| O(16)#6-Mn(4)-O(21)#3 | 111.66(16)| O(17)-Mn(4)-O(21)#3  | 126.93(15)|
| O(16)#6-Mn(4)-O(19)   | 94.21(13) | O(21)#3-Mn(4)-O(19)  | 93.37(13) | O(16)#6-Mn(4)-O(28)   | 91.06(17) |
| O(17)-Mn(4)-O(21)#3  | 83.48(16) | O(19)-Mn(4)-O(28)    | 175.49(15)| O(17)-Mn(4)-O(28)    | 85.15(15) |
| O(18)-Mn(5)-O(21)#3  | 95.34(13) | O(18)-Mn(5)-O(23)#2  | 84.57(13) | O(18)-Mn(5)-O(29)    | 101.15(15)|
| O(18)-Mn(5)-O(23)#2  | 94.99(14) | O(19)-Mn(5)-O(29)    | 99.46(15) | O(19)-Mn(5)-O(29)    | 93.97(14) |
| O(19)-Mn(5)-O(29)    | 126.93(15)| O(19)-Mn(5)-O(13)#7  | 92.21(12) | O(19)-Mn(5)-O(13)#7  | 93.97(14) |
| O(19)-Mn(5)-O(13)#1  | 90.40(12) | O(19)-Mn(5)-O(13)#1  | 75.81(12) | O(19)-Mn(5)-O(13)#1  | 75.81(12) |
| O(19)-Mn(5)-O(13)#1  | 89.50(13) | O(19)-Mn(5)-O(13)#1  | 165.95(13)| O(19)-Mn(5)-O(13)#1  | 165.95(13)|
| O(19)-Mn(5)-O(13)#1  | 76.08(12) | O(19)-Mn(5)-O(13)#1  | 106.31(13)| O(19)-Mn(5)-O(13)#1  | 106.31(13)|
| O(19)-Mn(5)-O(13)#1  | 124.88(14)| O(19)-Mn(5)-O(13)#1  | 128.78(13)| O(19)-Mn(5)-O(13)#1  | 128.78(13)|
| O(19)-Mn(5)-O(13)#1  | 96.33(14) | O(19)-Mn(5)-O(13)#1  | 91.25(12) | O(19)-Mn(5)-O(13)#1  | 91.25(12) |
| O(19)-Mn(5)-O(13)#1  | 82.16(14) | O(19)-Mn(5)-O(13)#1  | 86.65(14) | O(19)-Mn(5)-O(13)#1  | 86.65(14) |
| O(19)-Mn(5)-O(13)#1  | 102.37(12)| O(19)-Mn(5)-O(13)#1  | 83.82(14) | O(19)-Mn(5)-O(13)#1  | 83.82(14) |
| O(19)-Mn(5)-O(13)#1  | 164.68(13)| O(19)-Mn(5)-O(13)#1  | 178.04(18)| O(19)-Mn(5)-O(13)#1  | 178.04(18)|
| O(19)-Mn(5)-O(13)#1  | 86.74(17) | O(19)-Mn(5)-O(13)#1  | 94.78(15) | O(19)-Mn(5)-O(13)#1  | 94.78(15) |
| O(19)-Mn(5)-O(13)#1  | 88.84(17) | O(19)-Mn(5)-O(13)#1  | 89.38(14) | O(19)-Mn(5)-O(13)#1  | 89.38(14) |
| O(19)-Mn(5)-O(13)#1  | 175.06(14)| O(19)-Mn(5)-O(13)#1  | 88.45(14) | O(19)-Mn(5)-O(13)#1  | 88.45(14) |
| O(19)-Mn(5)-O(13)#1  | 89.48(13) | O(19)-Mn(5)-O(13)#1  | 89.3(2)   | O(19)-Mn(5)-O(13)#1  | 89.3(2)   |
| O(19)-Mn(5)-O(13)#1  | 89.47(18) | O(19)-Mn(5)-O(13)#1  | 91.58(15) | O(19)-Mn(5)-O(13)#1  | 91.58(15) |

Symmetry transformations used to generate the equivalent atoms: #1: -x+1, -y+1, -z+1; #2: x-1, y, z; #3: x-1, y, z-1; #4: x+1, y, z; #5: x, y, z-1; #6: x, y-1, z-1; #7: x-1, y-1, z-1; #8: x, y+1, z+1; #9: x-1, y+1, z.
Figure S1. The IR spectra of 1.

Figure S2. The TGA curve of 1.
Figure S3. The simulated (red line) and experimental (black line) powder X-ray diffraction patterns for complex 1.

Figure S4. The plots of $M$ vs. $H$ curve at 2K of 1.