

## Supplementary material

### Hexanuclear manganese(III) single-molecule magnets from derivatized salicylamidoximes

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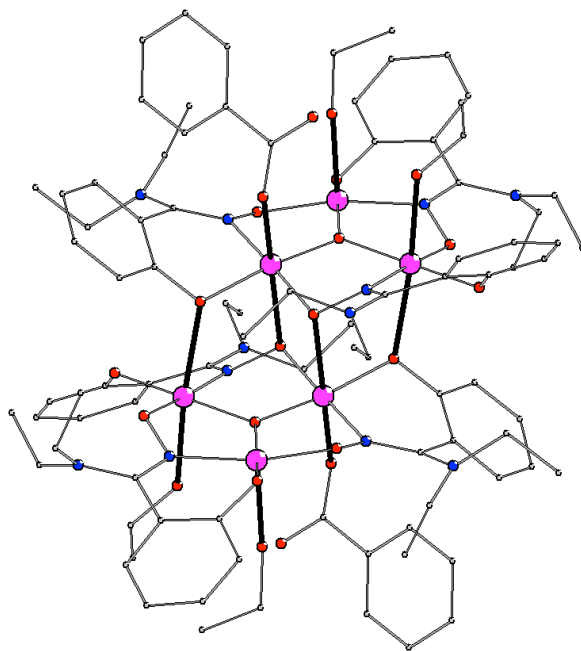
#### 1. Synthesis of derivatized salicylamidoximes

**1.1. Dimethylsalicylamidoxime (Me<sub>2</sub>N-saoH<sub>2</sub>):** A 2 M solution of dimethylamine in THF (5 mL) was added dropwise to a solution of Cl-saoH<sub>2</sub><sup>a</sup> (0.858 g, 5.0 mmol) in THF (20 mL), which resulted in the precipitation of dimethylammonium chloride. The latter was removed by filtration and the filtrate was concentrated under reduced pressure to afford a brown residue which was dissolved in a 1:4 acetone/H<sub>2</sub>O mixture (50 mL) upon heating at 80 °C. The resulting solution was left undisturbed for crystallization of Me<sub>2</sub>N-saoH<sub>2</sub>. Yield: 30%. Anal. calcd. (found) for C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>: C 59.9 (59.5), H 6.7 (7.2), N 15.6 (15.3)%. IR (KBr pellet/cm<sup>-1</sup>): 3189m, 3000w, 2954m, 2884m, 1623vs, 1608s, 1579m, 1483vs, 1378vs, 1217m, 1152m, 1074m, 1032m, 955s, 763s, 676m.

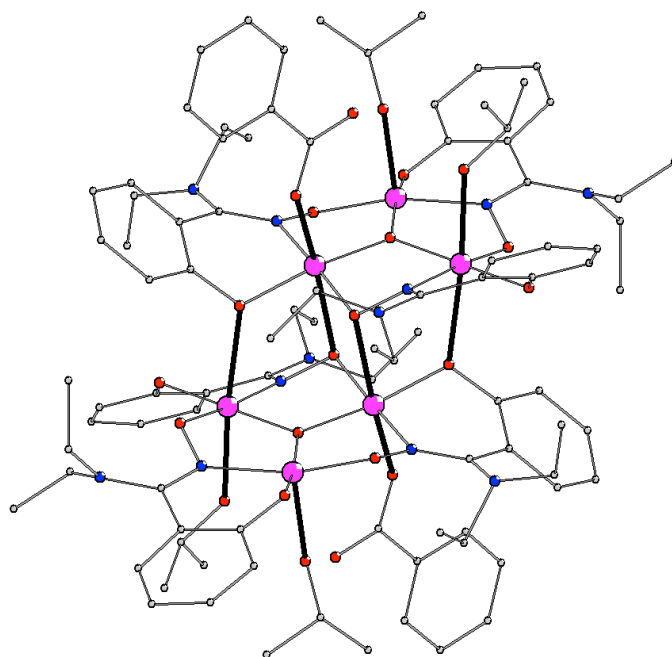
**1.2. Diethylsalicylamidoxime (Et<sub>2</sub>N-saoH<sub>2</sub>):** A solution of diethylamine (1.28 mL, 12.0 mmol) in THF (5 mL) was added dropwise to a solution of Cl-saoH<sub>2</sub><sup>a</sup> (1.0 g, 6.0 mmol) in THF (20 mL). A white precipitate of diethylammonium chloride was removed by filtration, then the filtrate was concentrated under reduced pressure to afford a brown-orange oil which was treated by a 1:2 acetone/H<sub>2</sub>O mixture (60 mL) mixture at 80 °C. A small amount of a not yet identified red solid was removed by hot filtration and the filtrate was left undisturbed for crystallization of Et<sub>2</sub>N-saoH<sub>2</sub> as light yellow needles. Yield: 65%. Anal. calcd. (found) for C<sub>11</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>: C 63.4 (62.7), H 7.7 (7.9), N 13.5 (13.5)%. IR (KBr pellet/cm<sup>-1</sup>): 3220m, 2974m, 2931m, 2872w, 1618s, 1599s, 1508m, 1434m, 1217m, 1156w, 915m, 753s.

<sup>a</sup> Hydroximoyl chloride was prepared according to: J. W. Bode, Y. Hachisu, T. Matura and K. Suzuki, Org. Lett. 5 (2003) 391.

## 2. Molecular structures of compounds **3** and **4**



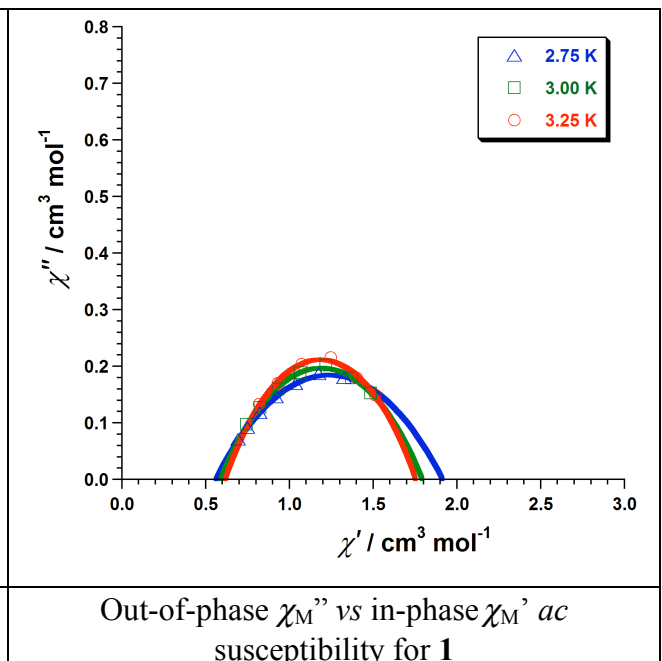
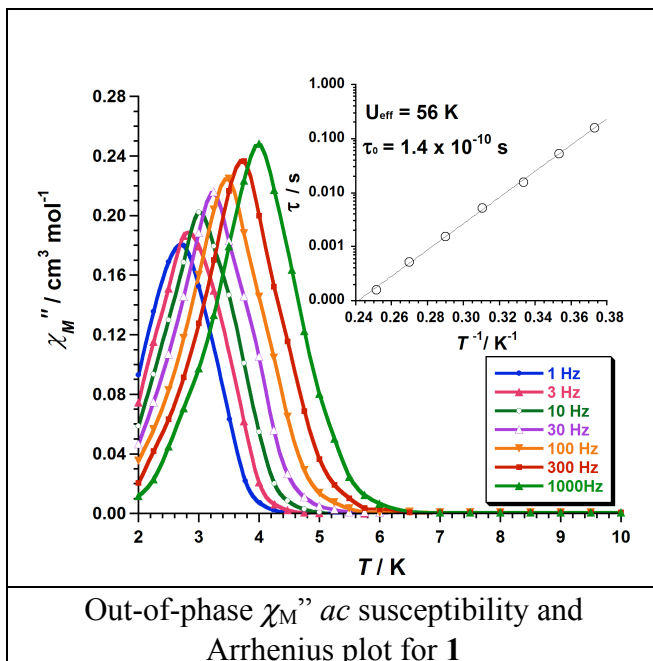
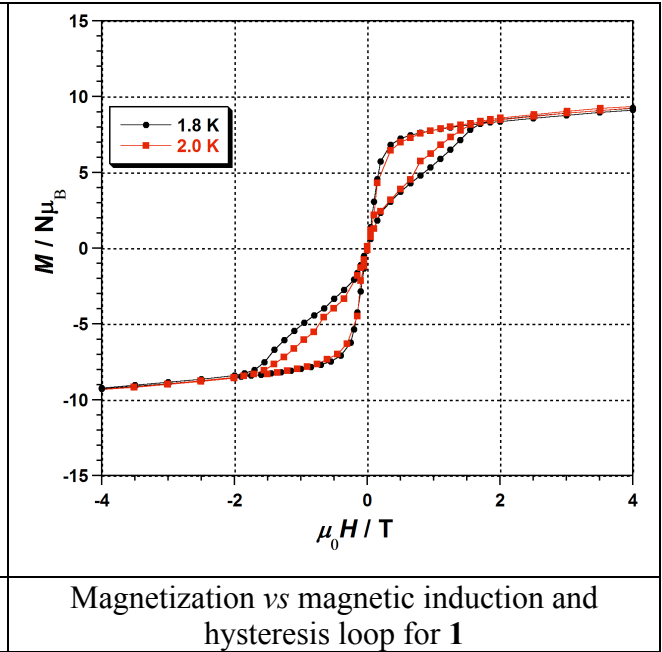
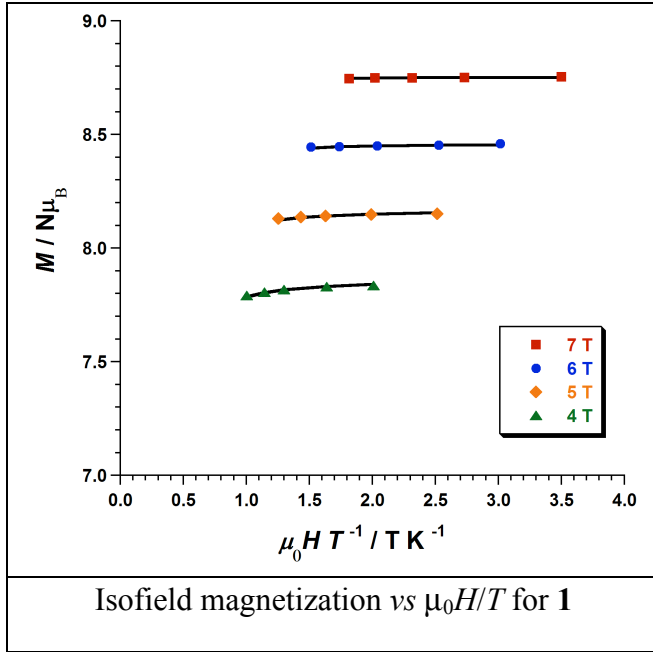
**Fig. S1.** Molecular structure of the  $\{\text{Mn}_6\}$  cluster in **3**, highlighting the elongated bonds as heavy lines. Colour code: Mn, purple; O, red; N, blue; C, black..



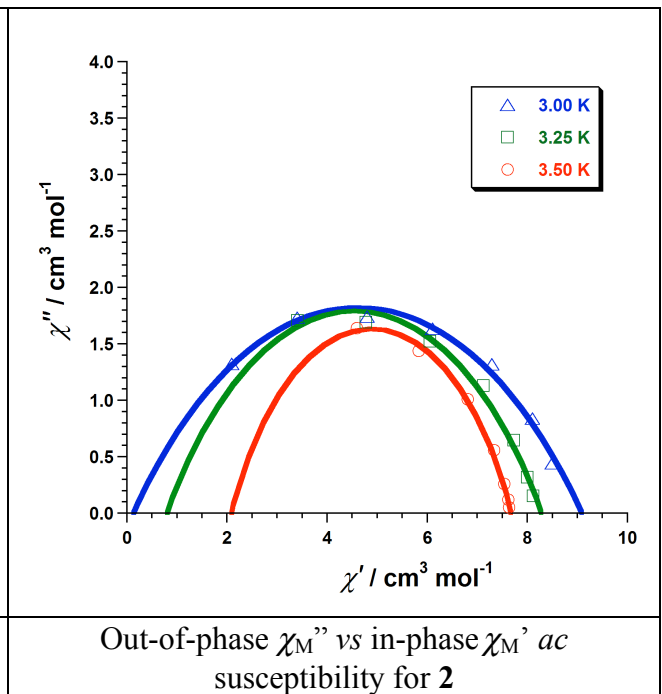
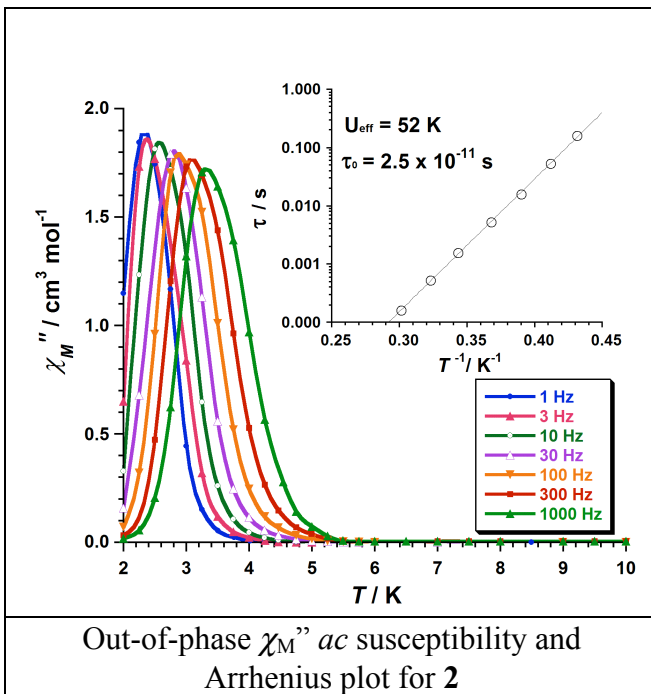
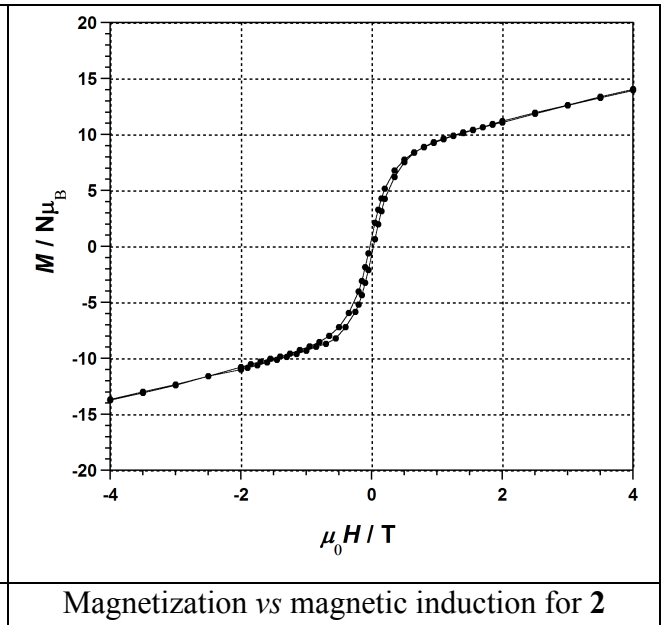
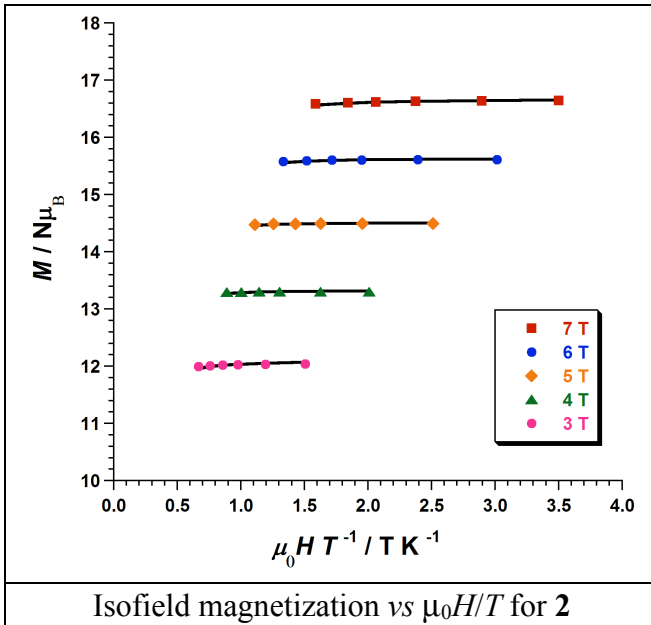
**Fig. S2.** Molecular structure of the  $\{\text{Mn}_6\}$  cluster in **4**. Colour code as in Fig. 1.

### 3. Magnetic data for compounds 1-4

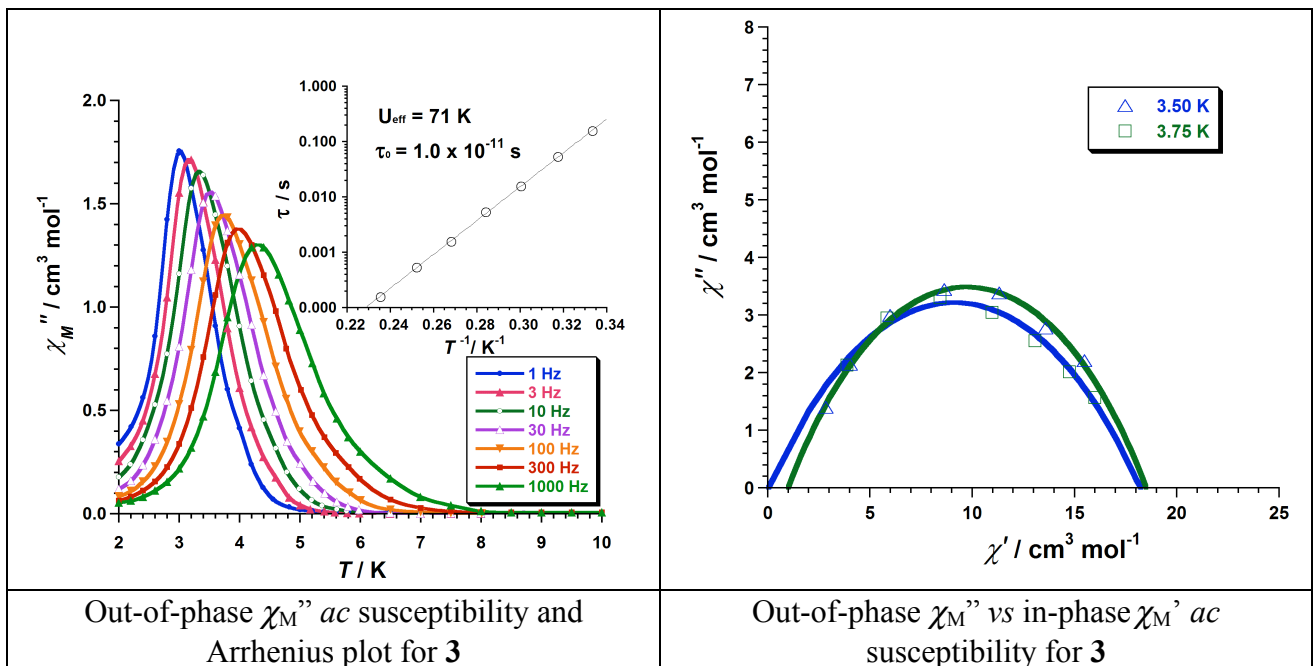
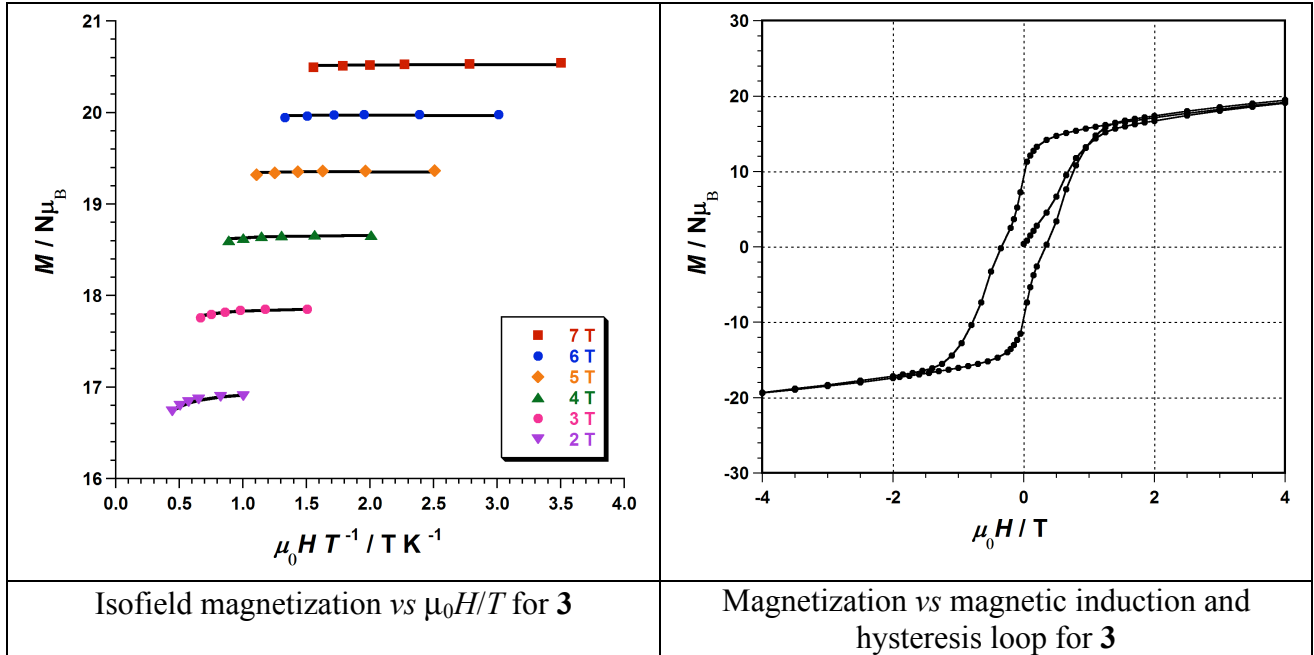
#### Compound 1



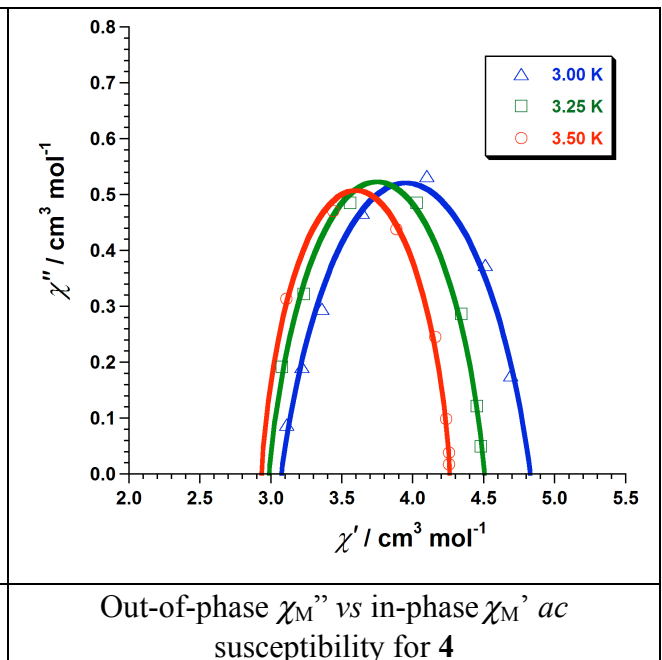
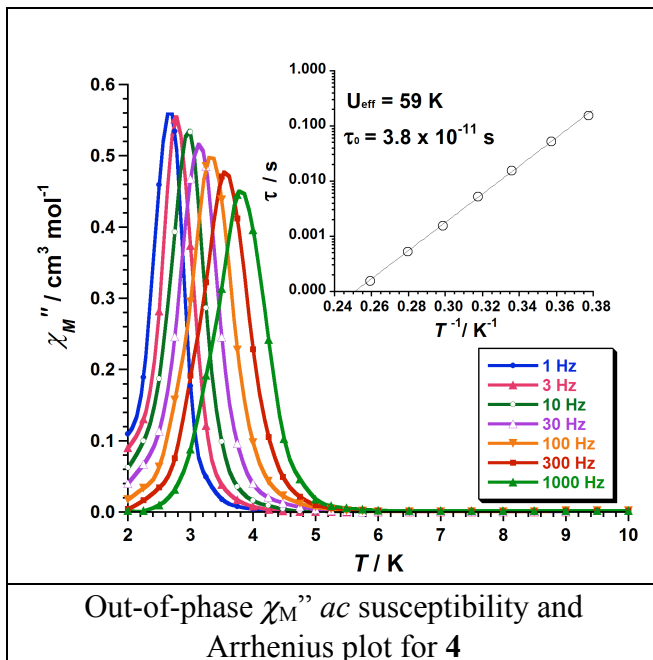
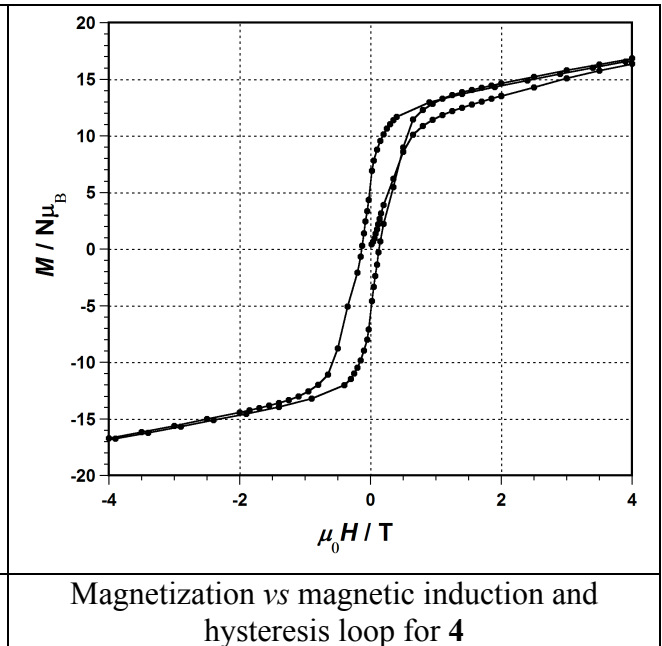
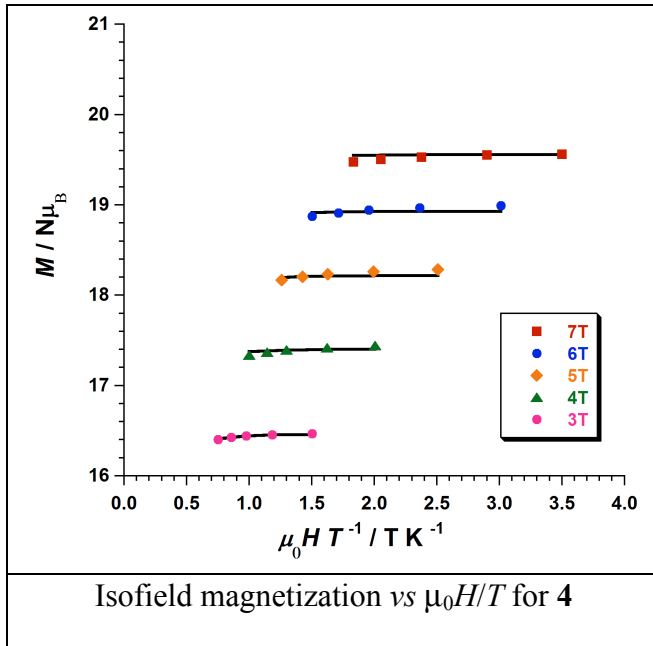
## Compound 2



## Compound 3



## Compound 4



**4. Tables of bond lengths and angles**Table S1. Bond lengths / Å and angles / ° for compound **1**.

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Mn(1)-O(2)	1.873(4)
Mn(1)-O(1)	1.885(4)
Mn(1)-O(7)	1.889(4)
Mn(1)-N(1)	1.973(4)
Mn(1)-O(8)	2.262(4)
Mn(1)-O(4)#1	2.333(4)
Mn(1)-Mn(2)	3.2343(11)
Mn(2)-O(1)	1.887(4)
Mn(2)-O(4)	1.893(4)
Mn(2)-O(3)	1.928(3)
Mn(2)-N(3)	1.993(4)
Mn(2)-O(9)	2.112(4)
Mn(2)-O(3)#1	2.354(4)
Mn(2)-Mn(3)	3.2220(12)
Mn(3)-O(1)	1.849(4)
Mn(3)-O(6)	1.850(4)
Mn(3)-O(5)	1.887(4)
Mn(3)-N(5)	2.006(5)
Mn(3)-O(11)	2.142(4)
N(1)-C(7)	1.310(6)
N(1)-O(3)	1.387(5)
N(2)-C(7)	1.354(7)
N(2)-C(8)	1.459(7)
N(2)-C(9)	1.464(7)
N(3)-C(16)	1.295(7)
N(3)-O(5)	1.370(5)
N(4)-C(16)	1.364(7)
N(4)-C(17)	1.444(8)
N(4)-C(18)	1.452(8)
N(5)-C(25)	1.306(7)
N(5)-O(7)	1.373(5)
N(6)-C(25)	1.368(7)
N(6)-C(27)	1.451(8)
N(6)-C(26)	1.467(8)
O(2)-C(1)	1.335(6)
O(3)-Mn(2)#1	2.354(4)
O(4)-C(10)	1.346(6)

O(4)-Mn(1)#1	2.333(4)
O(6)-C(19)	1.318(7)
O(8)-C(28)	1.438(9)
O(8)-H(8)	0.8774
O(9)-C(30)	1.242(7)
O(10)-C(30)	1.260(7)
O(11)-C(37)	1.399(8)
O(11)-H(11A)	0.9347
C(1)-C(6)	1.396(8)
C(1)-C(2)	1.400(8)
C(2)-C(3)	1.372(8)
C(2)-H(2)	0.9500
C(3)-C(4)	1.388(9)
C(3)-H(3)	0.9500
C(4)-C(5)	1.374(8)
C(4)-H(4)	0.9500
C(5)-C(6)	1.398(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.472(7)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(15)	1.395(8)
C(10)-C(11)	1.399(8)
C(11)-C(12)	1.372(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.391(9)
C(12)-H(12)	0.9500
C(13)-C(14)	1.392(8)
C(13)-H(13)	0.9500
C(14)-C(15)	1.394(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.478(8)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800



C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.398(8)
C(19)-C(24)	1.406(8)
C(20)-C(21)	1.375(9)
C(20)-H(20)	0.9500
C(21)-C(22)	1.376(9)
C(21)-H(21)	0.9500
C(22)-C(23)	1.360(9)
C(22)-H(22)	0.9500
C(23)-C(24)	1.407(8)
C(23)-H(23)	0.9500
C(24)-C(25)	1.463(8)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.424(11)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.500(8)
C(31)-C(36)	1.369(8)
C(31)-C(32)	1.381(9)
C(32)-C(33)	1.385(9)
C(32)-H(32)	0.9500
C(33)-C(34)	1.376(11)
C(33)-H(33)	0.9500
C(34)-C(35)	1.353(12)
C(34)-H(34)	0.9500
C(35)-C(36)	1.377(10)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.472(11)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900

C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-Cl(3)	1.715(9)
C(39)-Cl(1)	1.735(8)
C(39)-Cl(2)	1.736(9)
C(39)-H(39)	1.0000
O(2)-Mn(1)-O(1)	176.92(16)
O(2)-Mn(1)-O(7)	91.93(16)
O(1)-Mn(1)-O(7)	91.14(15)
O(2)-Mn(1)-N(1)	88.63(17)
O(1)-Mn(1)-N(1)	88.34(16)
O(7)-Mn(1)-N(1)	175.11(18)
O(2)-Mn(1)-O(8)	91.61(16)
O(1)-Mn(1)-O(8)	87.74(15)
O(7)-Mn(1)-O(8)	96.55(17)
N(1)-Mn(1)-O(8)	88.30(16)
O(2)-Mn(1)-O(4)#1	89.00(15)
O(1)-Mn(1)-O(4)#1	91.24(14)
O(7)-Mn(1)-O(4)#1	91.23(15)
N(1)-Mn(1)-O(4)#1	83.92(16)
O(8)-Mn(1)-O(4)#1	172.18(14)
O(2)-Mn(1)-Mn(2)	146.17(12)
O(1)-Mn(1)-Mn(2)	30.99(11)
O(7)-Mn(1)-Mn(2)	120.34(12)
N(1)-Mn(1)-Mn(2)	58.33(12)
O(8)-Mn(1)-Mn(2)	94.21(11)
O(4)#1-Mn(1)-Mn(2)	81.04(9)
O(1)-Mn(2)-O(4)	168.76(16)
O(1)-Mn(2)-O(3)	89.72(15)
O(4)-Mn(2)-O(3)	90.64(15)
O(1)-Mn(2)-N(3)	88.51(17)
O(4)-Mn(2)-N(3)	89.23(17)
O(3)-Mn(2)-N(3)	170.19(17)
O(1)-Mn(2)-O(9)	99.12(16)
O(4)-Mn(2)-O(9)	92.05(15)
O(3)-Mn(2)-O(9)	94.97(15)
N(3)-Mn(2)-O(9)	94.84(17)
O(1)-Mn(2)-O(3)#1	84.28(14)

O(4)-Mn(2)-O(3)#1	84.68(13)
O(3)-Mn(2)-O(3)#1	80.79(14)
N(3)-Mn(2)-O(3)#1	89.43(15)
O(9)-Mn(2)-O(3)#1	174.59(13)
O(1)-Mn(2)-Mn(3)	30.07(11)
O(4)-Mn(2)-Mn(3)	144.06(11)
O(3)-Mn(2)-Mn(3)	117.45(11)
N(3)-Mn(2)-Mn(3)	59.20(13)
O(9)-Mn(2)-Mn(3)	106.27(11)
O(3)#1-Mn(2)-Mn(3)	78.77(9)
O(1)-Mn(2)-Mn(1)	30.95(11)
O(4)-Mn(2)-Mn(1)	148.85(11)
O(3)-Mn(2)-Mn(1)	58.99(10)
N(3)-Mn(2)-Mn(1)	119.41(13)
O(9)-Mn(2)-Mn(1)	97.02(11)
O(3)#1-Mn(2)-Mn(1)	83.72(8)
Mn(3)-Mn(2)-Mn(1)	60.42(3)
O(1)-Mn(3)-O(6)	166.24(19)
O(1)-Mn(3)-O(5)	91.97(16)
O(6)-Mn(3)-O(5)	83.77(17)
O(1)-Mn(3)-N(5)	90.11(16)
O(6)-Mn(3)-N(5)	90.36(18)
O(5)-Mn(3)-N(5)	163.41(18)
O(1)-Mn(3)-O(11)	92.00(16)
O(6)-Mn(3)-O(11)	101.53(19)
O(5)-Mn(3)-O(11)	97.83(18)
N(5)-Mn(3)-O(11)	98.54(18)
O(1)-Mn(3)-Mn(2)	30.76(11)
O(6)-Mn(3)-Mn(2)	142.97(13)
O(5)-Mn(3)-Mn(2)	61.21(11)
N(5)-Mn(3)-Mn(2)	119.65(13)
O(11)-Mn(3)-Mn(2)	95.22(12)
C(7)-N(1)-O(3)	117.0(4)
C(7)-N(1)-Mn(1)	130.3(4)
O(3)-N(1)-Mn(1)	110.7(3)
C(7)-N(2)-C(8)	122.8(5)
C(7)-N(2)-C(9)	122.6(4)
C(8)-N(2)-C(9)	113.6(5)
C(16)-N(3)-O(5)	115.9(4)
C(16)-N(3)-Mn(2)	126.8(4)

O(5)-N(3)-Mn(2)	114.2(3)
C(16)-N(4)-C(17)	121.6(5)
C(16)-N(4)-C(18)	122.8(5)
C(17)-N(4)-C(18)	115.3(5)
C(25)-N(5)-O(7)	114.4(4)
C(25)-N(5)-Mn(3)	127.1(4)
O(7)-N(5)-Mn(3)	116.4(3)
C(25)-N(6)-C(27)	123.6(5)
C(25)-N(6)-C(26)	118.9(5)
C(27)-N(6)-C(26)	115.3(5)
Mn(3)-O(1)-Mn(1)	120.94(19)
Mn(3)-O(1)-Mn(2)	119.17(19)
Mn(1)-O(1)-Mn(2)	118.05(18)
C(1)-O(2)-Mn(1)	122.0(3)
N(1)-O(3)-Mn(2)	112.1(3)
N(1)-O(3)-Mn(2)#1	113.4(3)
Mn(2)-O(3)-Mn(2)#1	99.21(14)
C(10)-O(4)-Mn(2)	118.3(3)
C(10)-O(4)-Mn(1)#1	115.5(3)
Mn(2)-O(4)-Mn(1)#1	117.35(16)
N(3)-O(5)-Mn(3)	116.9(3)
C(19)-O(6)-Mn(3)	128.7(4)
N(5)-O(7)-Mn(1)	120.9(3)
C(28)-O(8)-Mn(1)	127.3(5)
C(28)-O(8)-H(8)	96.3
Mn(1)-O(8)-H(8)	106.1
C(30)-O(9)-Mn(2)	135.7(4)
C(37)-O(11)-Mn(3)	130.0(4)
C(37)-O(11)-H(11A)	105.8
Mn(3)-O(11)-H(11A)	117.8
O(2)-C(1)-C(6)	124.7(5)
O(2)-C(1)-C(2)	116.4(5)
C(6)-C(1)-C(2)	118.9(5)
C(3)-C(2)-C(1)	121.2(6)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	120.0(6)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	119.4(6)

C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	121.5(6)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(1)-C(6)-C(5)	118.9(5)
C(1)-C(6)-C(7)	122.7(5)
C(5)-C(6)-C(7)	118.4(5)
N(1)-C(7)-N(2)	123.3(5)
N(1)-C(7)-C(6)	116.9(5)
N(2)-C(7)-C(6)	119.8(5)
N(2)-C(8)-H(8A)	109.5
N(2)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
N(2)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(2)-C(9)-H(9A)	109.5
N(2)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(2)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(4)-C(10)-C(15)	122.2(5)
O(4)-C(10)-C(11)	118.2(5)
C(15)-C(10)-C(11)	119.6(5)
C(12)-C(11)-C(10)	120.3(6)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	121.4(6)
C(11)-C(12)-H(12)	119.3
C(13)-C(12)-H(12)	119.3
C(12)-C(13)-C(14)	118.1(6)
C(12)-C(13)-H(13)	121.0
C(14)-C(13)-H(13)	121.0
C(13)-C(14)-C(15)	121.7(6)
C(13)-C(14)-H(14)	119.1
C(15)-C(14)-H(14)	119.1
C(14)-C(15)-C(10)	118.9(5)
C(14)-C(15)-C(16)	118.7(5)

C(10)-C(15)-C(16)	122.4(5)
N(3)-C(16)-N(4)	123.5(5)
N(3)-C(16)-C(15)	118.0(5)
N(4)-C(16)-C(15)	118.5(5)
N(4)-C(17)-H(17A)	109.5
N(4)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(4)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-H(18A)	109.5
N(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(6)-C(19)-C(20)	117.4(5)
O(6)-C(19)-C(24)	123.1(5)
C(20)-C(19)-C(24)	119.5(5)
C(21)-C(20)-C(19)	120.8(6)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(20)-C(21)-C(22)	120.1(6)
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-H(21)	120.0
C(23)-C(22)-C(21)	120.0(6)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	122.1(6)
C(22)-C(23)-H(23)	118.9
C(24)-C(23)-H(23)	118.9
C(19)-C(24)-C(23)	117.4(5)
C(19)-C(24)-C(25)	122.8(5)
C(23)-C(24)-C(25)	119.8(5)
N(5)-C(25)-N(6)	123.6(5)
N(5)-C(25)-C(24)	120.6(5)
N(6)-C(25)-C(24)	115.8(5)
N(6)-C(26)-H(26A)	109.5
N(6)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5

N(6)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(6)-C(27)-H(27A)	109.5
N(6)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(6)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-O(8)	110.8(8)
C(29)-C(28)-H(28A)	109.5
O(8)-C(28)-H(28A)	109.5
C(29)-C(28)-H(28B)	109.5
O(8)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	108.1
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(9)-C(30)-O(10)	125.3(5)
O(9)-C(30)-C(31)	118.3(5)
O(10)-C(30)-C(31)	116.4(5)
C(36)-C(31)-C(32)	118.9(6)
C(36)-C(31)-C(30)	121.9(6)
C(32)-C(31)-C(30)	119.2(5)
C(31)-C(32)-C(33)	120.3(7)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(34)-C(33)-C(32)	119.2(8)
C(34)-C(33)-H(33)	120.4
C(32)-C(33)-H(33)	120.4
C(35)-C(34)-C(33)	120.7(7)
C(35)-C(34)-H(34)	119.6
C(33)-C(34)-H(34)	119.6
C(34)-C(35)-C(36)	119.8(8)
C(34)-C(35)-H(35)	120.1
C(36)-C(35)-H(35)	120.1
C(31)-C(36)-C(35)	120.9(7)

C(31)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6
O(11)-C(37)-C(38)	113.7(7)
O(11)-C(37)-H(37A)	108.8
C(38)-C(37)-H(37A)	108.8
O(11)-C(37)-H(37B)	108.8
C(38)-C(37)-H(37B)	108.8
H(37A)-C(37)-H(37B)	107.7
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
Cl(3)-C(39)-Cl(1)	109.7(4)
Cl(3)-C(39)-Cl(2)	111.2(5)
Cl(1)-C(39)-Cl(2)	111.5(5)
Cl(3)-C(39)-H(39)	108.1
Cl(1)-C(39)-H(39)	108.1
Cl(2)-C(39)-H(39)	108.1

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2



Table S2. Bond lengths / Å and angles / ° for compound **3**.

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Mn(1)-O(2)	1.8721(18)
Mn(1)-O(1)	1.8911(16)
Mn(1)-O(7)	1.8926(17)
Mn(1)-N(1)	1.9746(19)
Mn(1)-O(8)	2.2470(19)
Mn(1)-O(4)#1	2.3418(17)
Mn(1)-Mn(2)	3.2329(7)
Mn(2)-O(1)	1.8787(16)
Mn(2)-O(4)	1.8985(16)
Mn(2)-O(3)	1.9312(16)
Mn(2)-N(3)	1.980(2)
Mn(2)-O(9)	2.1516(17)
Mn(2)-O(3)#1	2.3941(16)
Mn(3)-O(6)	1.8597(19)
Mn(3)-O(1)	1.8595(16)
Mn(3)-O(5)	1.8892(19)
Mn(3)-N(5)	2.012(2)
Mn(3)-O(11)	2.1653(19)
O(2)-C(1)	1.326(3)
O(3)-N(1)	1.387(2)
O(3)-Mn(2)#1	2.3941(16)
O(4)-C(13)	1.354(3)
O(4)-Mn(1)#1	2.3418(17)
O(5)-N(3)	1.372(3)
O(6)-C(24)	1.330(3)
O(7)-N(5)	1.374(3)
O(8)-C(35)	1.411(4)
O(8)-H(8)	0.8516
O(9)-C(37)	1.255(3)
O(10)-C(37)	1.250(3)
O(11)-C(44B)	1.38(2)
O(11)-C(44A)	1.454(17)
O(11)-H(11)	0.8732
N(1)-C(7)	1.308(3)
N(2)-C(7)	1.360(3)
N(2)-C(10)	1.455(4)
N(2)-C(8)	1.487(4)
N(3)-C(19)	1.293(4)

N(4A)-C(19)	1.442(5)
N(4A)-C(22A)	1.456(8)
N(4A)-C(20A)	1.504(10)
N(4B)-C(19)	1.399(7)
N(4B)-C(22B)	1.468(17)
N(4B)-C(20B)	1.493(11)
N(5)-C(30)	1.308(3)
N(6)-C(30)	1.363(4)
N(6)-C(31)	1.461(4)
N(6)-C(33)	1.471(5)
C(1)-C(2)	1.394(4)
C(1)-C(6)	1.408(4)
C(2)-C(3)	1.356(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.368(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.395(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.477(3)
C(8)-C(9)	1.510(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.478(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(13)-C(14)	1.390(4)
C(13)-C(18)	1.393(4)
C(14)-C(15)	1.379(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.363(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.377(5)

C(16)-H(16)	0.9500
C(17)-C(18)	1.406(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.465(4)
C(20A)-C(21A)	1.528(11)
C(20A)-H(20A)	0.9900
C(20A)-H(20B)	0.9900
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(22A)-C(23A)	1.466(12)
C(22A)-H(22A)	0.9900
C(22A)-H(22B)	0.9900
C(23A)-H(23A)	0.9800
C(23A)-H(23B)	0.9800
C(23A)-H(23C)	0.9800
C(20B)-C(21B)	1.522(16)
C(20B)-H(20C)	0.9900
C(20B)-H(20D)	0.9900
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22B)-C(23B)	1.541(18)
C(22B)-H(22C)	0.9900
C(22B)-H(22D)	0.9900
C(23B)-H(23D)	0.9800
C(23B)-H(23E)	0.9800
C(23B)-H(23F)	0.9800
C(24)-C(29)	1.399(4)
C(24)-C(25)	1.411(4)
C(25)-C(26)	1.367(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.377(6)
C(26)-H(26)	0.9500
C(27)-C(28)	1.370(5)
C(27)-H(27)	0.9500
C(28)-C(29)	1.401(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.468(4)
C(31)-C(32)	1.501(6)

C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.406(6)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.444(6)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.497(4)
C(38)-C(39)	1.367(5)
C(38)-C(43)	1.384(5)
C(39)-C(40)	1.392(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.380(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.363(7)
C(41)-H(41)	0.9500
C(42)-C(43)	1.395(5)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44A)-C(45A)	1.515(15)
C(44A)-H(44A)	0.9900
C(44A)-H(44B)	0.9900
C(45A)-H(45A)	0.9800
C(45A)-H(45B)	0.9800
C(45A)-H(45C)	0.9800
C(44B)-C(45B)	1.433(14)
C(44B)-H(44C)	0.9900
C(44B)-H(44D)	0.9900
C(45B)-H(45D)	0.9800
C(45B)-H(45E)	0.9800

C(45B)-H(45F)	0.9800
O(2)-Mn(1)-O(1)	175.94(7)
O(2)-Mn(1)-O(7)	92.70(8)
O(1)-Mn(1)-O(7)	90.88(7)
O(2)-Mn(1)-N(1)	88.73(8)
O(1)-Mn(1)-N(1)	87.86(7)
O(7)-Mn(1)-N(1)	174.86(9)
O(2)-Mn(1)-O(8)	91.55(8)
O(1)-Mn(1)-O(8)	86.19(7)
O(7)-Mn(1)-O(8)	95.97(8)
N(1)-Mn(1)-O(8)	88.92(8)
O(2)-Mn(1)-O(4)#1	89.82(7)
O(1)-Mn(1)-O(4)#1	91.88(6)
O(7)-Mn(1)-O(4)#1	93.10(8)
N(1)-Mn(1)-O(4)#1	81.97(7)
O(8)-Mn(1)-O(4)#1	170.76(7)
O(2)-Mn(1)-Mn(2)	146.29(6)
O(1)-Mn(1)-Mn(2)	30.84(5)
O(7)-Mn(1)-Mn(2)	119.79(6)
N(1)-Mn(1)-Mn(2)	58.11(6)
O(8)-Mn(1)-Mn(2)	93.56(5)
O(4)#1-Mn(1)-Mn(2)	80.33(4)
O(1)-Mn(2)-O(4)	167.82(7)
O(1)-Mn(2)-O(3)	90.80(7)
O(4)-Mn(2)-O(3)	91.21(7)
O(1)-Mn(2)-N(3)	87.54(8)
O(4)-Mn(2)-N(3)	89.30(8)
O(3)-Mn(2)-N(3)	174.36(8)
O(1)-Mn(2)-O(9)	97.50(7)
O(4)-Mn(2)-O(9)	94.41(7)
O(3)-Mn(2)-O(9)	92.61(7)
N(3)-Mn(2)-O(9)	92.95(8)
O(1)-Mn(2)-O(3)#1	85.55(6)
O(4)-Mn(2)-O(3)#1	82.85(6)
O(3)-Mn(2)-O(3)#1	81.91(6)
N(3)-Mn(2)-O(3)#1	92.59(7)
O(9)-Mn(2)-O(3)#1	173.79(7)
O(1)-Mn(2)-Mn(1)	31.07(5)
O(4)-Mn(2)-Mn(1)	149.82(5)

O(3)-Mn(2)-Mn(1)	59.86(5)
N(3)-Mn(2)-Mn(1)	118.60(6)
O(9)-Mn(2)-Mn(1)	95.28(5)
O(3)#1-Mn(2)-Mn(1)	84.52(4)
O(6)-Mn(3)-O(1)	166.57(8)
O(6)-Mn(3)-O(5)	88.11(8)
O(1)-Mn(3)-O(5)	90.66(7)
O(6)-Mn(3)-N(5)	89.77(9)
O(1)-Mn(3)-N(5)	88.61(8)
O(5)-Mn(3)-N(5)	167.77(9)
O(6)-Mn(3)-O(11)	98.07(9)
O(1)-Mn(3)-O(11)	95.36(8)
O(5)-Mn(3)-O(11)	95.92(8)
N(5)-Mn(3)-O(11)	96.31(9)
Mn(3)-O(1)-Mn(2)	120.40(9)
Mn(3)-O(1)-Mn(1)	120.62(8)
Mn(2)-O(1)-Mn(1)	118.09(8)
C(1)-O(2)-Mn(1)	120.71(15)
N(1)-O(3)-Mn(2)	111.36(12)
N(1)-O(3)-Mn(2)#1	112.84(11)
Mn(2)-O(3)-Mn(2)#1	98.09(6)
C(13)-O(4)-Mn(2)	116.86(16)
C(13)-O(4)-Mn(1)#1	118.65(15)
Mn(2)-O(4)-Mn(1)#1	119.51(7)
N(3)-O(5)-Mn(3)	115.93(14)
C(24)-O(6)-Mn(3)	121.97(18)
N(5)-O(7)-Mn(1)	117.25(14)
C(35)-O(8)-Mn(1)	131.9(2)
C(35)-O(8)-H(8)	100.7
Mn(1)-O(8)-H(8)	125.5
C(37)-O(9)-Mn(2)	135.57(17)
C(44B)-O(11)-C(44A)	21.7(12)
C(44B)-O(11)-Mn(3)	131.2(7)
C(44A)-O(11)-Mn(3)	141.0(6)
C(44B)-O(11)-H(11)	114.3
C(44A)-O(11)-H(11)	106.0
Mn(3)-O(11)-H(11)	112.4
C(7)-N(1)-O(3)	117.70(19)
C(7)-N(1)-Mn(1)	128.94(16)
O(3)-N(1)-Mn(1)	112.40(13)

C(7)-N(2)-C(10)	121.1(2)
C(7)-N(2)-C(8)	120.2(2)
C(10)-N(2)-C(8)	118.3(2)
C(19)-N(3)-O(5)	117.5(2)
C(19)-N(3)-Mn(2)	125.5(2)
O(5)-N(3)-Mn(2)	115.09(14)
C(19)-N(4A)-C(22A)	120.2(5)
C(19)-N(4A)-C(20A)	123.1(5)
C(22A)-N(4A)-C(20A)	115.7(6)
C(19)-N(4B)-C(22B)	140.7(12)
C(19)-N(4B)-C(20B)	110.1(7)
C(22B)-N(4B)-C(20B)	107.4(12)
C(30)-N(5)-O(7)	115.6(2)
C(30)-N(5)-Mn(3)	126.3(2)
O(7)-N(5)-Mn(3)	116.17(14)
C(30)-N(6)-C(31)	118.2(3)
C(30)-N(6)-C(33)	121.4(3)
C(31)-N(6)-C(33)	120.3(3)
O(2)-C(1)-C(2)	118.1(2)
O(2)-C(1)-C(6)	123.7(2)
C(2)-C(1)-C(6)	118.1(2)
C(3)-C(2)-C(1)	122.1(3)
C(3)-C(2)-H(2)	119.0
C(1)-C(2)-H(2)	119.0
C(2)-C(3)-C(4)	120.1(3)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	119.1(3)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	121.9(3)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	118.6(2)
C(5)-C(6)-C(7)	118.7(2)
C(1)-C(6)-C(7)	122.7(2)
N(1)-C(7)-N(2)	123.4(2)
N(1)-C(7)-C(6)	117.0(2)
N(2)-C(7)-C(6)	119.6(2)
N(2)-C(8)-C(9)	115.3(3)

N(2)-C(8)-H(8A)	108.4
C(9)-C(8)-H(8A)	108.4
N(2)-C(8)-H(8B)	108.4
C(9)-C(8)-H(8B)	108.4
H(8A)-C(8)-H(8B)	107.5
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(2)-C(10)-C(11)	115.1(3)
N(2)-C(10)-H(10A)	108.5
C(11)-C(10)-H(10A)	108.5
N(2)-C(10)-H(10B)	108.5
C(11)-C(10)-H(10B)	108.5
H(10A)-C(10)-H(10B)	107.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(4)-C(13)-C(14)	118.5(3)
O(4)-C(13)-C(18)	121.3(2)
C(14)-C(13)-C(18)	120.2(2)
C(15)-C(14)-C(13)	120.2(3)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	120.5(3)
C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(15)-C(16)-C(17)	120.0(3)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.1(4)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(13)-C(18)-C(17)	117.8(3)
C(13)-C(18)-C(19)	123.0(2)



C(17)-C(18)-C(19)	119.2(3)
N(3)-C(19)-N(4B)	120.2(4)
N(3)-C(19)-N(4A)	122.6(3)
N(4B)-C(19)-N(4A)	37.0(3)
N(3)-C(19)-C(18)	118.1(3)
N(4B)-C(19)-C(18)	114.3(4)
N(4A)-C(19)-C(18)	118.2(3)
N(4A)-C(20A)-C(21A)	112.2(8)
N(4A)-C(20A)-H(20A)	109.2
C(21A)-C(20A)-H(20A)	109.2
N(4A)-C(20A)-H(20B)	109.2
C(21A)-C(20A)-H(20B)	109.2
H(20A)-C(20A)-H(20B)	107.9
C(20A)-C(21A)-H(21A)	109.5
C(20A)-C(21A)-H(21B)	109.5
H(21A)-C(21A)-H(21B)	109.5
C(20A)-C(21A)-H(21C)	109.5
H(21A)-C(21A)-H(21C)	109.5
H(21B)-C(21A)-H(21C)	109.5
N(4A)-C(22A)-C(23A)	106.5(7)
N(4A)-C(22A)-H(22A)	110.4
C(23A)-C(22A)-H(22A)	110.4
N(4A)-C(22A)-H(22B)	110.4
C(23A)-C(22A)-H(22B)	110.4
H(22A)-C(22A)-H(22B)	108.6
C(22A)-C(23A)-H(23A)	109.5
C(22A)-C(23A)-H(23B)	109.5
H(23A)-C(23A)-H(23B)	109.5
C(22A)-C(23A)-H(23C)	109.5
H(23A)-C(23A)-H(23C)	109.5
H(23B)-C(23A)-H(23C)	109.5
N(4B)-C(20B)-C(21B)	118.0(10)
N(4B)-C(20B)-H(20C)	107.8
C(21B)-C(20B)-H(20C)	107.8
N(4B)-C(20B)-H(20D)	107.8
C(21B)-C(20B)-H(20D)	107.8
H(20C)-C(20B)-H(20D)	107.2
C(20B)-C(21B)-H(21D)	109.5
C(20B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5

C(20B)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
N(4B)-C(22B)-C(23B)	114.3(16)
N(4B)-C(22B)-H(22C)	108.7
C(23B)-C(22B)-H(22C)	108.7
N(4B)-C(22B)-H(22D)	108.7
C(23B)-C(22B)-H(22D)	108.7
H(22C)-C(22B)-H(22D)	107.6
C(22B)-C(23B)-H(23D)	109.5
C(22B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(22B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
O(6)-C(24)-C(29)	122.7(3)
O(6)-C(24)-C(25)	118.0(3)
C(29)-C(24)-C(25)	119.2(3)
C(26)-C(25)-C(24)	120.3(4)
C(26)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	120.6(4)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(28)-C(27)-C(26)	119.7(3)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(29)	121.5(4)
C(27)-C(28)-H(28)	119.2
C(29)-C(28)-H(28)	119.2
C(24)-C(29)-C(28)	118.3(3)
C(24)-C(29)-C(30)	122.9(3)
C(28)-C(29)-C(30)	118.8(3)
N(5)-C(30)-N(6)	123.2(3)
N(5)-C(30)-C(29)	117.9(3)
N(6)-C(30)-C(29)	118.8(2)
N(6)-C(31)-C(32)	114.1(3)
N(6)-C(31)-H(31A)	108.7
C(32)-C(31)-H(31A)	108.7
N(6)-C(31)-H(31B)	108.7

C(32)-C(31)-H(31B)	108.7
H(31A)-C(31)-H(31B)	107.6
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-N(6)	117.3(5)
C(34)-C(33)-H(33A)	108.0
N(6)-C(33)-H(33A)	108.0
C(34)-C(33)-H(33B)	108.0
N(6)-C(33)-H(33B)	108.0
H(33A)-C(33)-H(33B)	107.2
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
O(8)-C(35)-C(36)	112.2(4)
O(8)-C(35)-H(35A)	109.2
C(36)-C(35)-H(35A)	109.2
O(8)-C(35)-H(35B)	109.2
C(36)-C(35)-H(35B)	109.2
H(35A)-C(35)-H(35B)	107.9
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(10)-C(37)-O(9)	124.9(2)
O(10)-C(37)-C(38)	117.9(3)
O(9)-C(37)-C(38)	117.2(3)
C(39)-C(38)-C(43)	120.8(3)
C(39)-C(38)-C(37)	119.8(3)
C(43)-C(38)-C(37)	119.4(3)
C(38)-C(39)-C(40)	120.0(5)
C(38)-C(39)-H(39)	120.0

C(40)-C(39)-H(39)	120.0
C(41)-C(40)-C(39)	118.9(5)
C(41)-C(40)-H(40)	120.6
C(39)-C(40)-H(40)	120.6
C(42)-C(41)-C(40)	121.5(4)
C(42)-C(41)-H(41)	119.2
C(40)-C(41)-H(41)	119.2
C(41)-C(42)-C(43)	119.4(5)
C(41)-C(42)-H(42)	120.3
C(43)-C(42)-H(42)	120.3
C(38)-C(43)-C(42)	119.3(4)
C(38)-C(43)-H(43)	120.3
C(42)-C(43)-H(43)	120.3
O(11)-C(44A)-C(45A)	105.4(10)
O(11)-C(44A)-H(44A)	110.7
C(45A)-C(44A)-H(44A)	110.7
O(11)-C(44A)-H(44B)	110.7
C(45A)-C(44A)-H(44B)	110.7
H(44A)-C(44A)-H(44B)	108.8
O(11)-C(44B)-C(45B)	119.1(15)
O(11)-C(44B)-H(44C)	107.5
C(45B)-C(44B)-H(44C)	107.5
O(11)-C(44B)-H(44D)	107.5
C(45B)-C(44B)-H(44D)	107.5
H(44C)-C(44B)-H(44D)	107.0
C(44B)-C(45B)-H(45D)	109.5
C(44B)-C(45B)-H(45E)	109.5
H(45D)-C(45B)-H(45E)	109.5
C(44B)-C(45B)-H(45F)	109.5
H(45D)-C(45B)-H(45F)	109.5
H(45E)-C(45B)-H(45F)	109.5

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Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+2

Table S3. Bond lengths / Å and angles / ° for compound 4.

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Mn(1)-O(2)	1.8918(18)
Mn(1)-O(1)	1.9154(17)
Mn(1)-O(7)	1.9154(19)
Mn(1)-N(1)	1.995(2)
Mn(1)-O(11)	2.279(2)
Mn(1)-O(4)#1	2.3673(19)
Mn(2)-O(1)	1.9010(17)
Mn(2)-O(4)	1.9244(18)
Mn(2)-O(3)	1.9599(19)
Mn(2)-N(3)	2.014(2)
Mn(2)-O(8)	2.156(2)
Mn(2)-O(3)#1	2.4293(18)
Mn(3)-O(6)	1.878(2)
Mn(3)-O(1)	1.8853(19)
Mn(3)-O(5)	1.9187(19)
Mn(3)-N(5)	2.035(2)
Mn(3)-O(10)	2.167(2)
O(2)-C(1)	1.335(3)
O(3)-N(1)	1.405(2)
O(3)-Mn(2)#1	2.4293(18)
O(4)-C(12)	1.370(3)
O(4)-Mn(1)#1	2.3673(19)
O(5)-N(3)	1.390(3)
O(6)-C(23)	1.338(4)
O(7)-N(5)	1.397(3)
O(8)-C(34)	1.270(4)
O(9)-C(34)	1.266(4)
O(10)-C(41)	1.450(4)
O(10)-H(10)	0.8505
O(11)-C(44)	1.443(4)
O(11)-H(11)	0.7260
N(1)-C(7)	1.317(3)
N(2)-C(7)	1.377(3)
N(2)-C(8)	1.473(4)
N(2)-C(10)	1.486(4)
N(3)-C(18)	1.322(3)
N(4)-C(19B)	1.179(18)
N(4)-C(18)	1.382(5)

N(4)-C(21A)	1.435(8)
N(4)-C(19A)	1.681(9)
N(4)-C(21B)	1.755(15)
N(5)-C(29)	1.316(3)
N(6)-C(29)	1.388(3)
N(6)-C(32)	1.473(4)
N(6)-C(30)	1.489(4)
C(1)-C(2)	1.414(4)
C(1)-C(6)	1.430(4)
C(2)-C(3)	1.380(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.398(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.405(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.501(3)
C(8)-C(9)	1.517(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.512(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.411(5)
C(12)-C(13)	1.410(4)
C(13)-C(14)	1.397(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.372(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.379(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.407(4)
C(16)-H(16)	0.9500

C(17)-C(18)	1.486(4)
C(19A)-C(20A)	1.541(12)
C(19A)-H(19A)	0.9900
C(19A)-H(19B)	0.9900
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(19B)-C(20B)	1.526(16)
C(19B)-H(19C)	0.9900
C(19B)-H(19D)	0.9900
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21A)-C(22)	1.552(10)
C(21A)-H(21A)	0.9900
C(21A)-H(21B)	0.9900
C(21B)-C(22)	1.380(14)
C(21B)-H(21C)	0.9900
C(21B)-H(21D)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(22)-H(22D)	0.9600
C(22)-H(22E)	0.9600
C(22)-H(22F)	0.9600
C(23)-C(24)	1.412(4)
C(23)-C(28)	1.421(4)
C(24)-C(25)	1.386(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.407(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.387(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.423(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.495(4)
C(30)-C(31)	1.518(5)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31A)	0.9800

C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.533(5)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.517(4)
C(35)-C(36)	1.391(5)
C(35)-C(40)	1.400(5)
C(36)-C(37)	1.408(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.376(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.360(8)
C(38)-H(38)	0.9500
C(39)-C(40)	1.398(6)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
C(41)-C(42)	1.477(6)
C(41)-C(43)	1.525(5)
C(41)-H(41)	1.0000
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(46)	1.468(6)
C(44)-C(45)	1.505(6)
C(44)-H(44)	1.0000
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
O(2)-Mn(1)-O(1)	176.44(8)



O(2)-Mn(1)-O(7)	93.20(8)
O(1)-Mn(1)-O(7)	90.07(8)
O(2)-Mn(1)-N(1)	89.15(8)
O(1)-Mn(1)-N(1)	87.77(8)
O(7)-Mn(1)-N(1)	172.66(9)
O(2)-Mn(1)-O(11)	91.80(8)
O(1)-Mn(1)-O(11)	86.37(8)
O(7)-Mn(1)-O(11)	97.46(9)
N(1)-Mn(1)-O(11)	89.41(8)
O(2)-Mn(1)-O(4)#1	87.56(8)
O(1)-Mn(1)-O(4)#1	93.74(7)
O(7)-Mn(1)-O(4)#1	91.93(8)
N(1)-Mn(1)-O(4)#1	81.22(8)
O(11)-Mn(1)-O(4)#1	170.61(7)
O(1)-Mn(2)-O(4)	168.19(8)
O(1)-Mn(2)-O(3)	90.19(7)
O(4)-Mn(2)-O(3)	91.21(8)
O(1)-Mn(2)-N(3)	88.22(8)
O(4)-Mn(2)-N(3)	89.15(9)
O(3)-Mn(2)-N(3)	173.85(8)
O(1)-Mn(2)-O(8)	98.84(8)
O(4)-Mn(2)-O(8)	92.79(8)
O(3)-Mn(2)-O(8)	93.11(8)
N(3)-Mn(2)-O(8)	93.00(9)
O(1)-Mn(2)-O(3)#1	86.67(7)
O(4)-Mn(2)-O(3)#1	82.02(7)
O(3)-Mn(2)-O(3)#1	80.22(7)
N(3)-Mn(2)-O(3)#1	93.75(8)
O(8)-Mn(2)-O(3)#1	171.41(8)
O(6)-Mn(3)-O(1)	167.86(9)
O(6)-Mn(3)-O(5)	87.25(9)
O(1)-Mn(3)-O(5)	91.41(8)
O(6)-Mn(3)-N(5)	89.26(9)
O(1)-Mn(3)-N(5)	88.78(8)
O(5)-Mn(3)-N(5)	164.28(9)
O(6)-Mn(3)-O(10)	98.13(9)
O(1)-Mn(3)-O(10)	94.02(8)
O(5)-Mn(3)-O(10)	95.85(9)
N(5)-Mn(3)-O(10)	99.81(9)
Mn(3)-O(1)-Mn(2)	119.82(9)

Mn(3)-O(1)-Mn(1)	120.73(9)
Mn(2)-O(1)-Mn(1)	118.47(10)
C(1)-O(2)-Mn(1)	121.67(15)
N(1)-O(3)-Mn(2)	112.07(14)
N(1)-O(3)-Mn(2)#1	112.31(12)
Mn(2)-O(3)-Mn(2)#1	99.78(7)
C(12)-O(4)-Mn(2)	116.11(17)
C(12)-O(4)-Mn(1)#1	119.28(15)
Mn(2)-O(4)-Mn(1)#1	120.13(8)
N(3)-O(5)-Mn(3)	115.69(15)
C(23)-O(6)-Mn(3)	125.62(18)
N(5)-O(7)-Mn(1)	117.72(14)
C(34)-O(8)-Mn(2)	140.4(2)
C(41)-O(10)-Mn(3)	130.3(2)
C(41)-O(10)-H(10)	114.1
Mn(3)-O(10)-H(10)	113.5
C(44)-O(11)-Mn(1)	138.8(2)
C(44)-O(11)-H(11)	112.3
Mn(1)-O(11)-H(11)	108.9
C(7)-N(1)-O(3)	117.6(2)
C(7)-N(1)-Mn(1)	129.30(17)
O(3)-N(1)-Mn(1)	111.87(15)
C(7)-N(2)-C(8)	120.4(2)
C(7)-N(2)-C(10)	120.6(2)
C(8)-N(2)-C(10)	118.1(2)
C(18)-N(3)-O(5)	117.3(2)
C(18)-N(3)-Mn(2)	125.6(2)
O(5)-N(3)-Mn(2)	115.27(15)
C(19B)-N(4)-C(18)	128.4(7)
C(19B)-N(4)-C(21A)	101.9(8)
C(18)-N(4)-C(21A)	129.7(5)
C(19B)-N(4)-C(19A)	22.5(8)
C(18)-N(4)-C(19A)	117.7(4)
C(21A)-N(4)-C(19A)	108.7(5)
C(19B)-N(4)-C(21B)	124.1(8)
C(18)-N(4)-C(21B)	105.6(5)
C(21A)-N(4)-C(21B)	28.2(4)
C(19A)-N(4)-C(21B)	136.0(5)
C(29)-N(5)-O(7)	115.2(2)
C(29)-N(5)-Mn(3)	128.1(2)

O(7)-N(5)-Mn(3)	115.18(15)
C(29)-N(6)-C(32)	118.0(2)
C(29)-N(6)-C(30)	121.9(3)
C(32)-N(6)-C(30)	116.5(3)
O(2)-C(1)-C(2)	117.8(2)
O(2)-C(1)-C(6)	124.4(2)
C(2)-C(1)-C(6)	117.7(2)
C(3)-C(2)-C(1)	121.9(3)
C(3)-C(2)-H(2)	119.1
C(1)-C(2)-H(2)	119.1
C(2)-C(3)-C(4)	120.4(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	119.0(3)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	121.9(3)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	119.0(2)
C(5)-C(6)-C(7)	118.8(2)
C(1)-C(6)-C(7)	122.3(2)
N(1)-C(7)-N(2)	123.9(2)
N(1)-C(7)-C(6)	117.2(2)
N(2)-C(7)-C(6)	118.8(2)
N(2)-C(8)-C(9)	114.4(3)
N(2)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8A)	108.7
N(2)-C(8)-H(8B)	108.7
C(9)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(2)-C(10)-C(11)	115.6(3)
N(2)-C(10)-H(10A)	108.4
C(11)-C(10)-H(10A)	108.4

N(2)-C(10)-H(10B)	108.4
C(11)-C(10)-H(10B)	108.4
H(10A)-C(10)-H(10B)	107.4
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(4)-C(12)-C(17)	122.1(3)
O(4)-C(12)-C(13)	118.4(3)
C(17)-C(12)-C(13)	119.4(3)
C(14)-C(13)-C(12)	119.8(4)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	121.3(3)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	118.7(3)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.6
C(15)-C(16)-C(17)	122.8(4)
C(15)-C(16)-H(16)	118.6
C(17)-C(16)-H(16)	118.6
C(16)-C(17)-C(12)	117.7(3)
C(16)-C(17)-C(18)	119.9(3)
C(12)-C(17)-C(18)	122.3(3)
N(3)-C(18)-N(4)	123.3(3)
N(3)-C(18)-C(17)	117.3(3)
N(4)-C(18)-C(17)	119.4(3)
C(20A)-C(19A)-N(4)	112.7(6)
C(20A)-C(19A)-H(19A)	109.0
N(4)-C(19A)-H(19A)	109.0
C(20A)-C(19A)-H(19B)	109.0
N(4)-C(19A)-H(19B)	109.0
H(19A)-C(19A)-H(19B)	107.8
N(4)-C(19B)-C(20B)	109.1(13)
N(4)-C(19B)-H(19C)	109.9
C(20B)-C(19B)-H(19C)	109.9
N(4)-C(19B)-H(19D)	109.9

C(20B)-C(19B)-H(19D)	109.9
H(19C)-C(19B)-H(19D)	108.3
C(19B)-C(20B)-H(20D)	109.5
C(19B)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(19B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
N(4)-C(21A)-C(22)	114.3(6)
N(4)-C(21A)-H(21A)	108.7
C(22)-C(21A)-H(21A)	108.7
N(4)-C(21A)-H(21B)	108.7
C(22)-C(21A)-H(21B)	108.7
H(21A)-C(21A)-H(21B)	107.6
C(22)-C(21B)-N(4)	105.8(9)
C(22)-C(21B)-H(21C)	110.6
N(4)-C(21B)-H(21C)	110.6
C(22)-C(21B)-H(21D)	110.6
N(4)-C(21B)-H(21D)	110.6
H(21C)-C(21B)-H(21D)	108.7
C(21B)-C(22)-C(21A)	32.5(5)
C(21B)-C(22)-H(22A)	109.1
C(21A)-C(22)-H(22A)	109.5
C(21B)-C(22)-H(22B)	79.7
C(21A)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21B)-C(22)-H(22C)	134.1
C(21A)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21B)-C(22)-H(22D)	108.9
C(21A)-C(22)-H(22D)	108.9
H(22A)-C(22)-H(22D)	0.8
H(22B)-C(22)-H(22D)	110.2
H(22C)-C(22)-H(22D)	109.3
C(21B)-C(22)-H(22E)	106.3
C(21A)-C(22)-H(22E)	131.8
H(22A)-C(22)-H(22E)	108.7
H(22B)-C(22)-H(22E)	28.4
H(22C)-C(22)-H(22E)	83.8

H(22D)-C(22)-H(22E)	109.5
C(21B)-C(22)-H(22F)	113.1
C(21A)-C(22)-H(22F)	83.6
H(22A)-C(22)-H(22F)	110.0
H(22B)-C(22)-H(22F)	130.7
H(22C)-C(22)-H(22F)	28.1
H(22D)-C(22)-H(22F)	109.5
H(22E)-C(22)-H(22F)	109.5
O(6)-C(23)-C(24)	117.8(3)
O(6)-C(23)-C(28)	123.4(3)
C(24)-C(23)-C(28)	118.7(3)
C(25)-C(24)-C(23)	121.7(3)
C(25)-C(24)-H(24)	119.2
C(23)-C(24)-H(24)	119.2
C(24)-C(25)-C(26)	120.1(3)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	119.1(3)
C(27)-C(26)-H(26)	120.5
C(25)-C(26)-H(26)	120.5
C(26)-C(27)-C(28)	121.9(3)
C(26)-C(27)-H(27)	119.1
C(28)-C(27)-H(27)	119.1
C(23)-C(28)-C(27)	118.4(3)
C(23)-C(28)-C(29)	122.8(3)
C(27)-C(28)-C(29)	118.7(3)
N(5)-C(29)-N(6)	123.2(3)
N(5)-C(29)-C(28)	119.1(2)
N(6)-C(29)-C(28)	117.7(2)
N(6)-C(30)-C(31)	111.6(3)
N(6)-C(30)-H(30A)	109.3
C(31)-C(30)-H(30A)	109.3
N(6)-C(30)-H(30B)	109.3
C(31)-C(30)-H(30B)	109.3
H(30A)-C(30)-H(30B)	108.0
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5

H(31B)-C(31)-H(31C)	109.5
N(6)-C(32)-C(33)	114.0(3)
N(6)-C(32)-H(32A)	108.8
C(33)-C(32)-H(32A)	108.8
N(6)-C(32)-H(32B)	108.8
C(33)-C(32)-H(32B)	108.8
H(32A)-C(32)-H(32B)	107.7
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(9)-C(34)-O(8)	125.7(3)
O(9)-C(34)-C(35)	118.2(3)
O(8)-C(34)-C(35)	116.1(3)
C(36)-C(35)-C(40)	119.6(3)
C(36)-C(35)-C(34)	120.2(3)
C(40)-C(35)-C(34)	120.1(3)
C(35)-C(36)-C(37)	119.1(5)
C(35)-C(36)-H(36)	120.4
C(37)-C(36)-H(36)	120.4
C(38)-C(37)-C(36)	120.5(5)
C(38)-C(37)-H(37)	119.8
C(36)-C(37)-H(37)	119.8
C(39)-C(38)-C(37)	120.6(4)
C(39)-C(38)-H(38)	119.7
C(37)-C(38)-H(38)	119.7
C(38)-C(39)-C(40)	120.4(5)
C(38)-C(39)-H(39)	119.8
C(40)-C(39)-H(39)	119.8
C(39)-C(40)-C(35)	119.8(5)
C(39)-C(40)-H(40)	120.1
C(35)-C(40)-H(40)	120.1
O(10)-C(41)-C(42)	110.7(3)
O(10)-C(41)-C(43)	109.7(3)
C(42)-C(41)-C(43)	112.6(4)
O(10)-C(41)-H(41)	107.9
C(42)-C(41)-H(41)	107.9
C(43)-C(41)-H(41)	107.9

C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
O(11)-C(44)-C(46)	110.3(4)
O(11)-C(44)-C(45)	110.2(4)
C(46)-C(44)-C(45)	115.0(4)
O(11)-C(44)-H(44)	107.0
C(46)-C(44)-H(44)	107.0
C(45)-C(44)-H(44)	107.0
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1