

Electronic Supplementary Material (ESI)

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Single chain magnet behaviour in selenite-bridged out-of-plane Mn₂O₂ dimer motif

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Supporting Information

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

Complex 1			
Mn(1)-O(3)	1.875(5)	Mn(3)-O(10)	1.864(6)
Mn(1)-O(4)	1.879(5)	Mn(3)-O(9)	1.894(5)
Mn(1)-N(2)	1.982(6)	Mn(3)-N(6)	1.963(7)
Mn(1)-N(1)	1.983(7)	Mn(3)-N(5)	1.988(8)
Mn(1)-O(1)	2.062(5)	Mn(3)-O(7)	2.033(5)
Mn(2)-O(5)	1.865(5)	Mn(4)-O(11)	1.856(6)
Mn(2)-O(6)	1.906(4)	Mn(4)-O(12)	1.916(5)
Mn(2)-N(3)	1.986(6)	Mn(4)-N(8)	1.983(7)
Mn(2)-N(4)	1.986(7)	Mn(4)-N(7)	1.985(6)
Mn(2)-O(2)	2.105(5)	Mn(4)-O(8)	2.042(5)
Mn(2)-O(6)#1	2.519(5)	O(10)-Mn(3)-O(9)	91.8(3)
O(3)-Mn(1)-O(4)	93.3(2)	O(10)-Mn(3)-N(6)	90.7(3)
O(3)-Mn(1)-N(2)	165.7(3)	O(9)-Mn(3)-N(6)	160.1(3)
O(4)-Mn(1)-N(2)	89.5(3)	O(10)-Mn(3)-N(5)	164.6(3)
O(3)-Mn(1)-N(1)	91.7(3)	O(9)-Mn(3)-N(5)	90.6(3)
O(4)-Mn(1)-N(1)	164.2(3)	N(6)-Mn(3)-N(5)	82.0(3)
N(2)-Mn(1)-N(1)	82.1(3)	O(10)-Mn(3)-O(7)	99.6(2)
O(3)-Mn(1)-O(1)	101.1(2)	O(9)-Mn(3)-O(7)	99.4(2)
O(4)-Mn(1)-O(1)	95.2(2)	N(6)-Mn(3)-O(7)	99.7(3)
N(2)-Mn(1)-O(1)	92.6(2)	N(5)-Mn(3)-O(7)	95.0(3)
N(1)-Mn(1)-O(1)	98.5(2)	O(11)-Mn(4)-O(12)	95.6(2)
O(5)-Mn(2)-O(6)	95.9(2)	O(11)-Mn(4)-N(8)	170.0(2)
O(5)-Mn(2)-N(3)	91.2(2)	O(12)-Mn(4)-N(8)	89.3(2)
O(6)-Mn(2)-N(3)	166.5(2)	O(11)-Mn(4)-N(7)	91.5(3)
O(5)-Mn(2)-N(4)	171.8(2)	O(12)-Mn(4)-N(7)	166.6(2)
O(6)-Mn(2)-N(4)	89.7(2)	N(8)-Mn(4)-N(7)	82.1(3)
N(3)-Mn(2)-N(4)	82.1(3)	O(11)-Mn(4)-O(8)	97.2(3)

O(5)-Mn(2)-O(2)	96.5(2)	O(12)-Mn(4)-O(8)	93.4(2)
O(6)-Mn(2)-O(2)	94.2(2)	N(8)-Mn(4)-O(8)	91.3(3)
N(3)-Mn(2)-O(2)	96.3(2)	N(7)-Mn(4)-O(8)	97.0(2)
N(4)-Mn(2)-O(2)	89.0(2)	Se(1)-O(1)-Mn(1)	134.7(3)
O(5)-Mn(2)-O(6)#1	91.57(19)	Se(1)-O(2)-Mn(2)	121.3(3)
O(6)-Mn(2)-O(6)#1	80.42(19)	Se(2)-O(7)-Mn(3)	122.9(3)
N(3)-Mn(2)-O(6)#1	88.0(2)	Se(2)-O(8)-Mn(4)	152.0(3)
N(4)-Mn(2)-O(6)#1	83.5(2)	O(2)-Se(1)-O(1)	103.8(3)
O(2)-Mn(2)-O(6)#1	170.79(19)	O(8)-Se(2)-O(7)	108.4(3)

Symmetry code for complex **1**: -x+1, -y+2, -z+1;

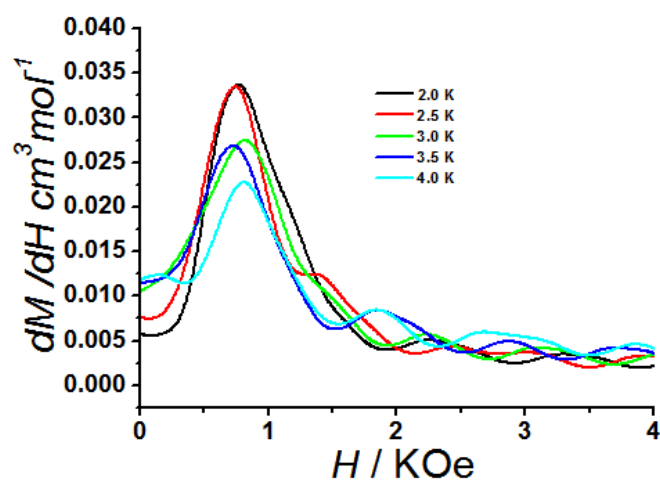


Figure S1. The derivative of field-dependent magnetization of **1** measured at different temperatures.

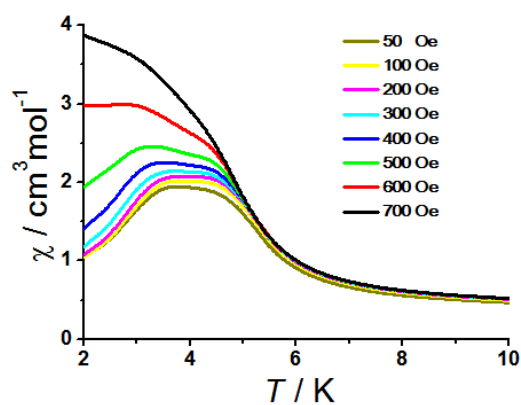


Figure S2 The χ_M versus T plots measured at different external fields of **1**.

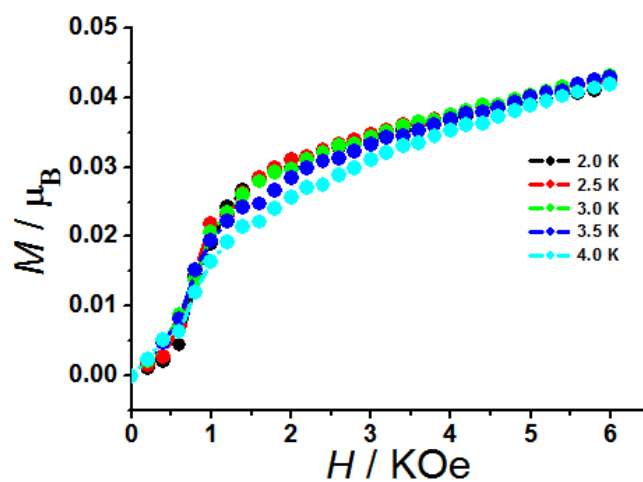


Figure S3 The M versus H plots measured at different temperature of complex **1**.

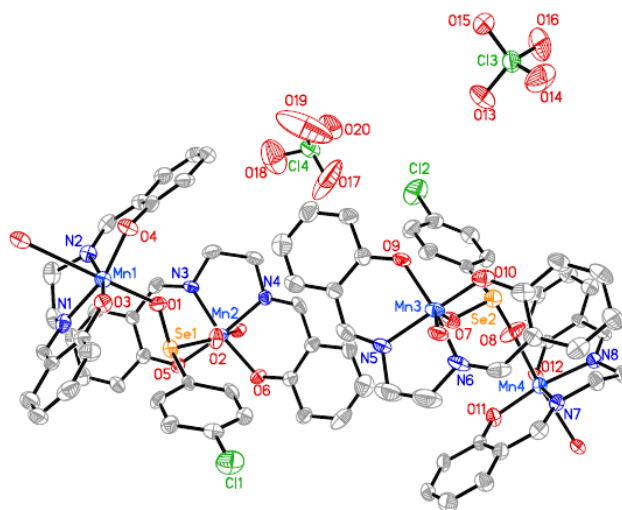


Figure S4 The asymmetric unit of complex **1**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

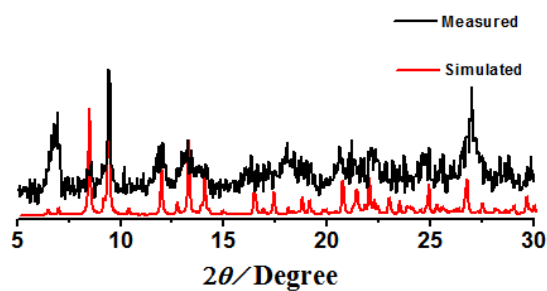


Figure S5. The powder XRD pattern of complex **1** in black and its simulation in red.

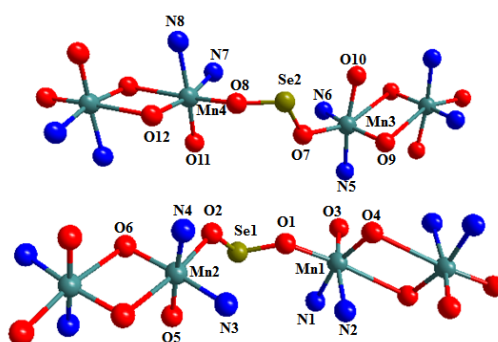


Figure S6. A plot of each Mn-dimer with its atom labels.