Single chain magnet based on 1D polymeric selenite-bridged Mn(III) complex with a N2O2 donor

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Supporting Information

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

Complex **1**			
Mn(1)-O(3)	1.864(9)	Mn(2)-O(6)	1.856(9)
Mn(1)-O(4)	1.827(9)	Mn(2)-O(5)	1.825(10)
Mn(1)-N(1)	1.916(12)	Mn(2)-N(4)	1.900(13)
Mn(1)-N(2)	1.925(12)	Mn(2)-N(3)	1.948(12)
Mn(1)-O(1)	2.060(8)	Mn(2)-O(2)	2.051(10)
Mn(1)-O(3)#1	2.470(8)	Mn(2)-O(6)#2	
Se(1)-O(1)	1.675(8)	Se(1)-O(2)	1.622(9)
O(3)-Mn(1)-O(4)	95.5(4)	O(6)-Mn(2)-O(5)	92.8(4)
O(3)-Mn(1)-N(1)	89.6(4)	O(6)-Mn(2)-N(4)	92.0(4)
O(4)-Mn(1)-N(1)	172.9(5)	O(5)-Mn(2)-N(4)	166.6(5)
O(3)-Mn(1)-N(2)	167.3(4)	O(6)-Mn(2)-N(3)	163.9(4)
O(4)-Mn(1)-N(2)	91.3(5)	O(5)-Mn(2)-N(3)	90.4(5)
N(1)-Mn(1)-N(2)	82.8(5)	N(4)-Mn(2)-N(3)	81.7(5)
O(3)-Mn(1)-O(1)	92.8(4)	O(6)-Mn(2)-O(2)	97.4(4)
O(4)-Mn(1)-O(1)	96.5(4)	O(5)-Mn(2)-O(2)	96.7(4)
N(1)-Mn(1)-O(1)	88.2(4)	N(4)-Mn(2)-O(2)	95.1(4)
N(2)-Mn(1)-O(1)	97.2(4)	N(3)-Mn(2)-O(2)	97.9(4)
O(1)-Mn(1)-O(3)#1	171.9(3)	O(2)-Mn(2)-O(6)#2	97.4(4)

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

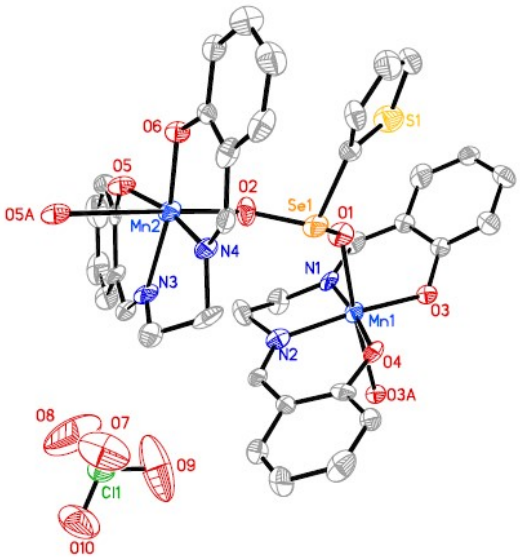


Figure S1. The asymmetric unit of complex **1**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

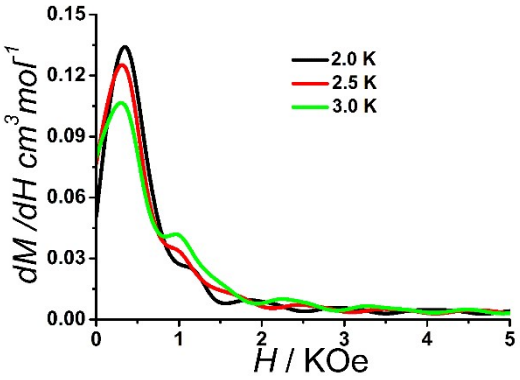


Figure S2. The derivative of field-dependent magnetization of **1** measured at different temperatures.

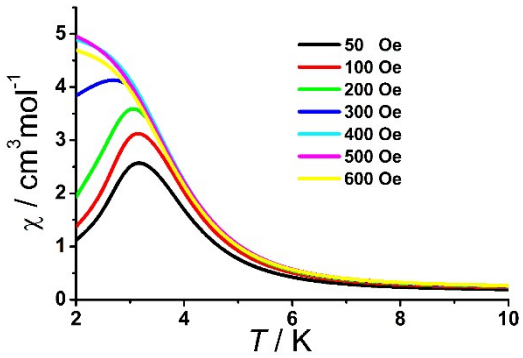


Figure S3 The χ_M *versus T* plots measured at different external fields of **1**.

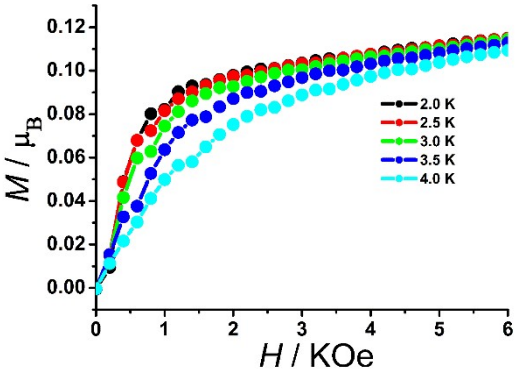


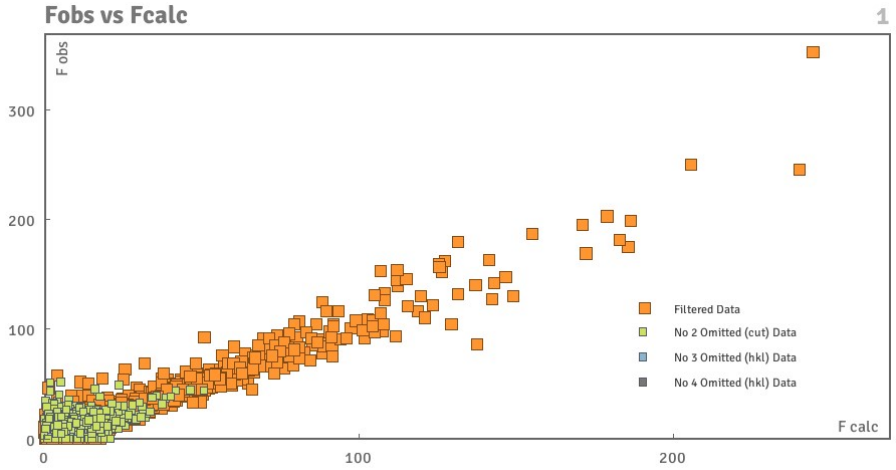
Figure S4 The *M versus H* plots measured at different temperature of complex **1**.

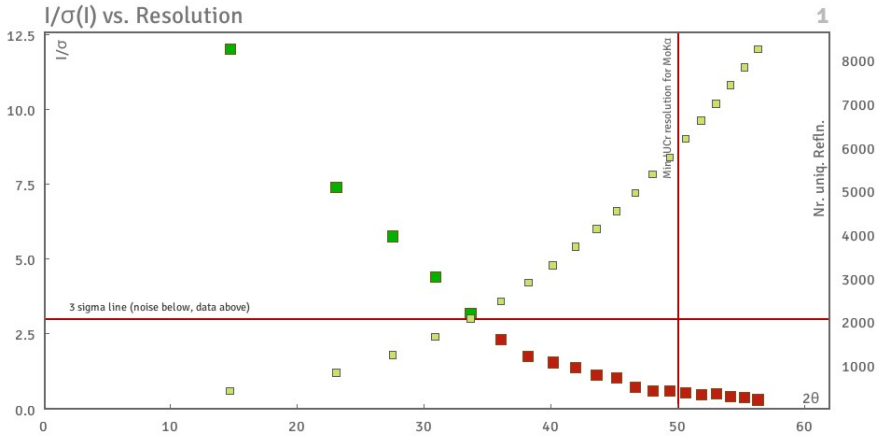
This structure is based on extremely weak data; the minimum require resolution of 50° in 2Θ has not meaningfully been reached. Only data up to around 40° contain information, the rest is noise.

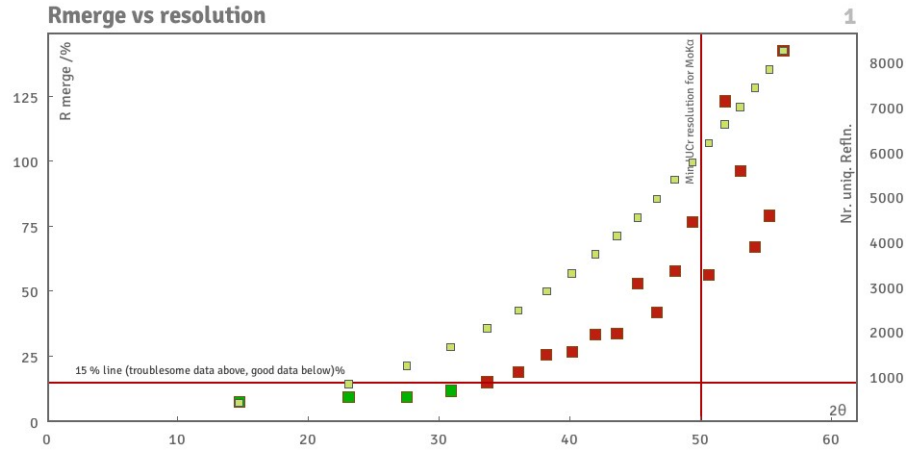
Please recollect new data on this material, making sure to reach 50° resolution.

If you can not do this, please add the attached images to your SI, and provide a credible reason as to why it was impossible to obtain data to the minimum required resolution. Your answer must contain the exposure time and scan width of the frames.

Thank you.







Response:

We appreciate your valuable comments. Yes, the data of the structure in this paper is indeed not strong. We realized that in the very beginning. The crystal grows so small and thin, that its diffraction was very weak. To improve the data, we have tried many times to cultivate bigger crystal in size in different solvents, but failed. Then, we tried to set longer exposure time. The frustration is that even when we set exposure time as 100s, its diffraction was still very weak. It looks like the weakness came from crystal itself, and it was impossible to obtain data to the minimum required resolution.

The exposure time per frame was 100s, and the scan width was 0.9° in this study.