

SUPPLEMENTARY INFORMATION

A Mn₁₅ Single – Molecule Magnet Consisting of a Supertetrahedron Incorporated in a Loop

Eleni E. Moushi, Antonio Masello, Wolfgang Wernsdorfer, Vassilios Nastopoulos, George Christou, and Anastasios J. Tasiopoulos*

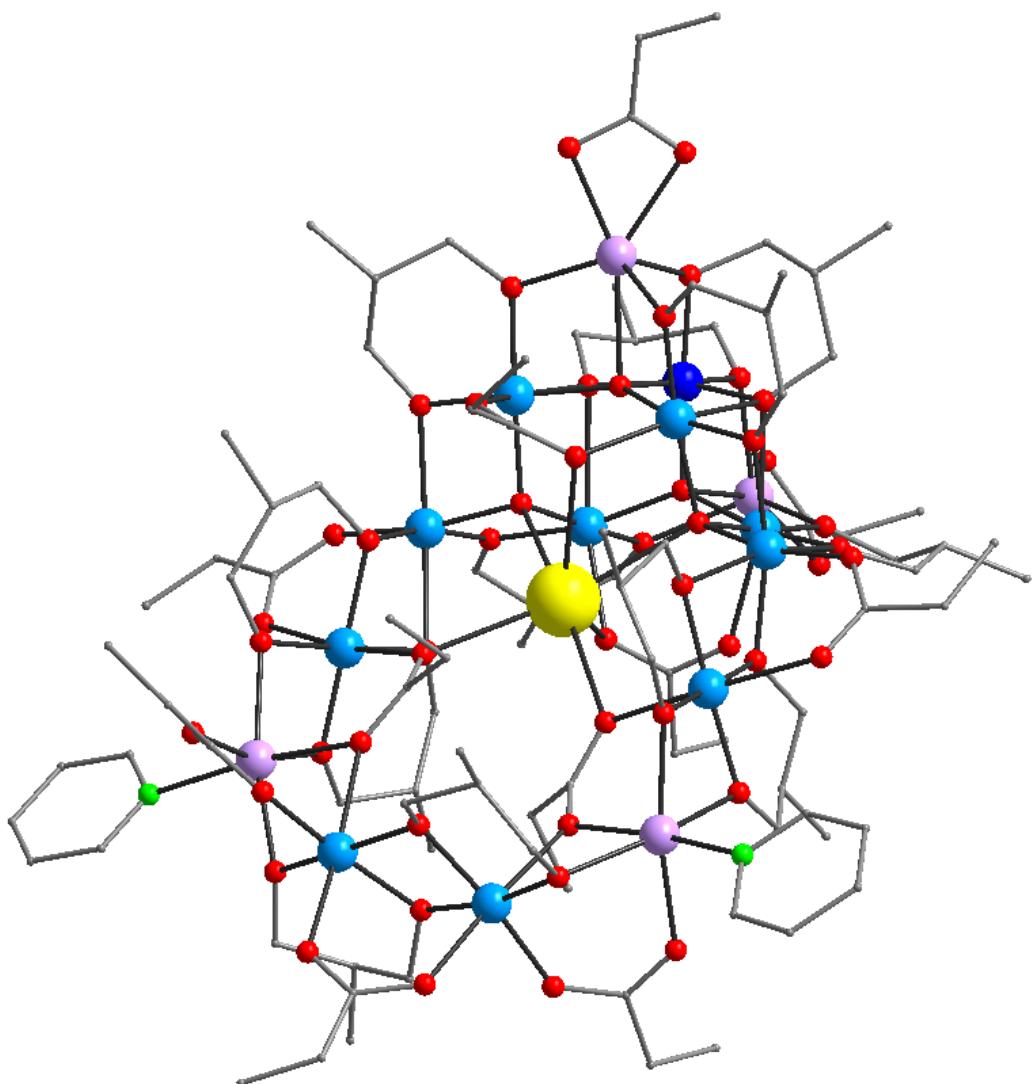


Figure S1. Molecular structure of complex **2**. Mn^{II} = purple, Mn^{III} = blue, Mn^{IV} = dark blue, K = yellow, O = red, N = green, C = grey. Hydrogen atoms have been omitted for clarity.

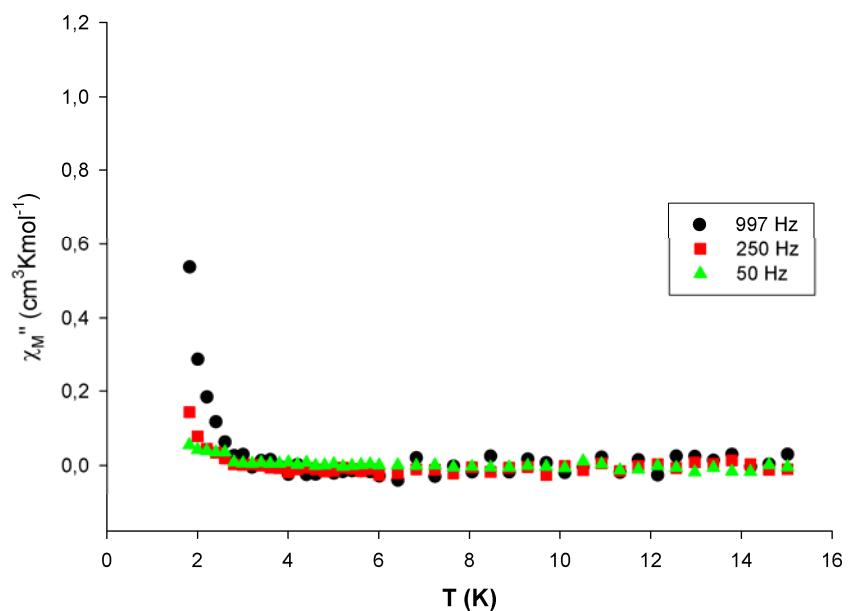


Fig. S2 Plot of the out-of-phase (χ''_M) ac magnetic susceptibility versus T for **1**·0.5py at the indicated frequencies.

Table S1. Selected interatomic distances (\AA) for complex **2**

$\text{K}^+ - \text{O}$	2.725(5) – 2.938(6)
$\text{Mn}^{2+} - \text{O}$	2.101(6) – 2.342(5)
$\text{Mn}^{3+} - \text{O}$	1.858(6) – 2.473(6)
$\text{Mn}^{4+} - \text{O}$	1.893(5) – 1.903(5)
$\text{Mn}^{2+} - \text{N}$	2.226(7) – 2.259(7)

Table S2. Bond valence sum (BVS) calculations for complex **2^a**

	Mn ^{II}	Mn ^{III}	Mn ^{IV}
Mn1	<u>1.96</u>	1.80	1.88
Mn2	4.21	3.85	<u>4.04</u>
Mn3	<u>1.90</u>	1.74	1.82
Mn4	3.27	<u>2.99</u>	3.14
Mn5	3.30	<u>3.02</u>	3.17
Mn6	3.24	<u>2.96</u>	3.11
Mn7	3.24	<u>2.96</u>	3.11
Mn8	3.19	<u>2.92</u>	3.06
Mn9	3.31	<u>3.03</u>	3.18
Mn10	<u>1.97</u>	1.82	1.89
Mn11	3.23	<u>2.95</u>	3.10
Mn12	3.23	<u>2.95</u>	3.10
Mn13	<u>2.04</u>	1.89	1.95
Mn14	3.29	<u>3.01</u>	3.16
Mn15	3.23	<u>2.96</u>	3.10

^a The underlined value is the one closest to the charge for which it was calculated.^b The oxidation state is the nearest whole number to the underlined value.