SUPPORTING INFORMATION

Binding of Higher Alcohols onto Mn_{12} Single-Molecule Magnets: Access to the Highest Barrier Mn_{12} SMM

Christos Lampropoulos[†], Gage Redler[‡], Saiti Data[‡], Khalil A. Abboud[†], Stephen O. Hill[*‡$], and George Christou *[,†]

Department of Chemistry, University of Florida, Gainesville, Florida 32611; Department of Physics, University of Florida, Gainesville, Florida 32611; Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310.

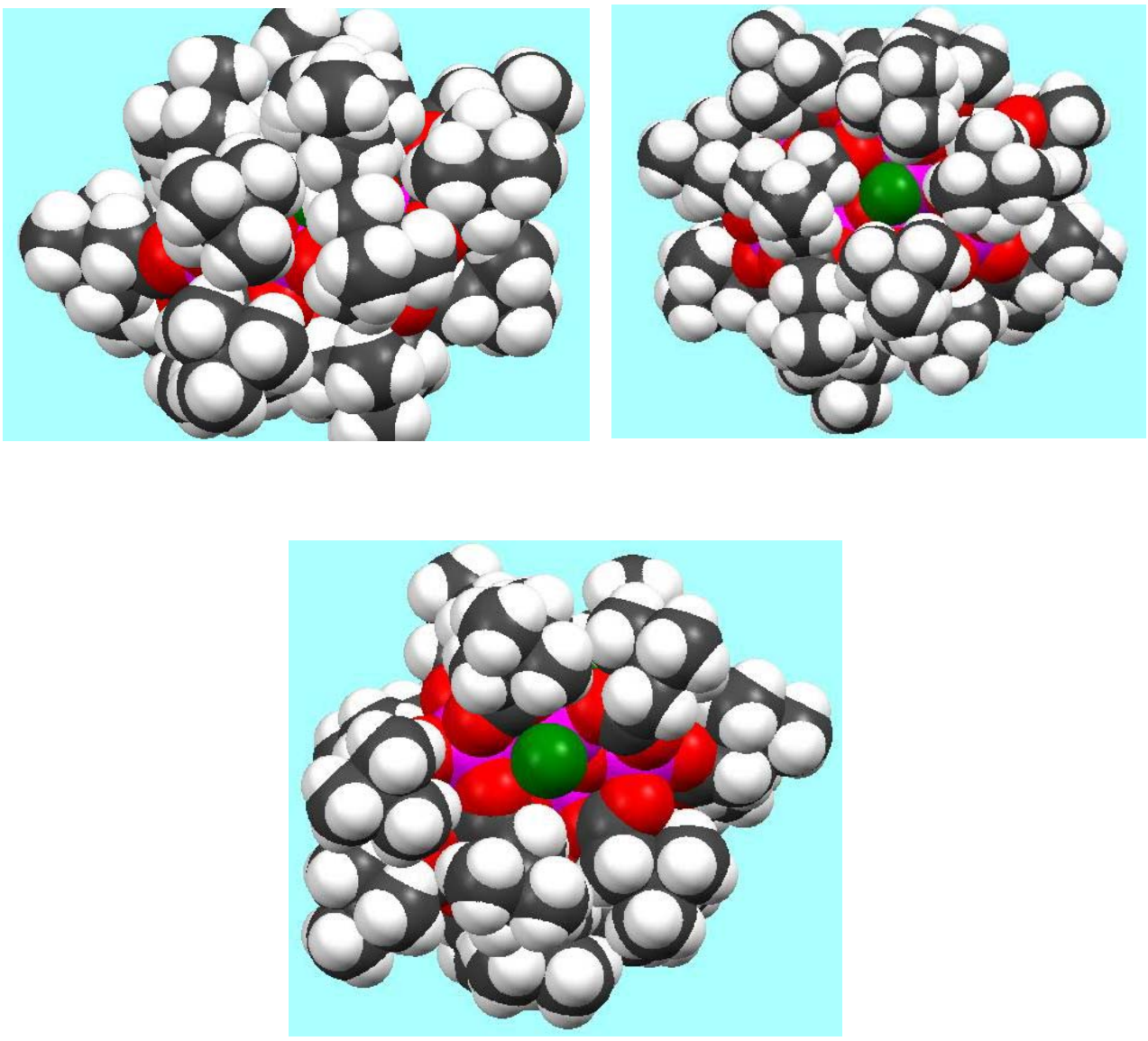

Figure S1. Space-filling diagrams of complex **3** showing the water ligand O atoms (in green) and their degree of envelopment by the carboxylates: (top left) the most buried water molecule (O50), barely visible; (top right) more visible water molecule O40, but still too enveloped to form H-bonds with lattice ButOH molecules; and (bottom) most exposed water molecule O37, that can form two H-bonds with lattive ButOH molecules (se text): Mn violet; O red; C black; H white.

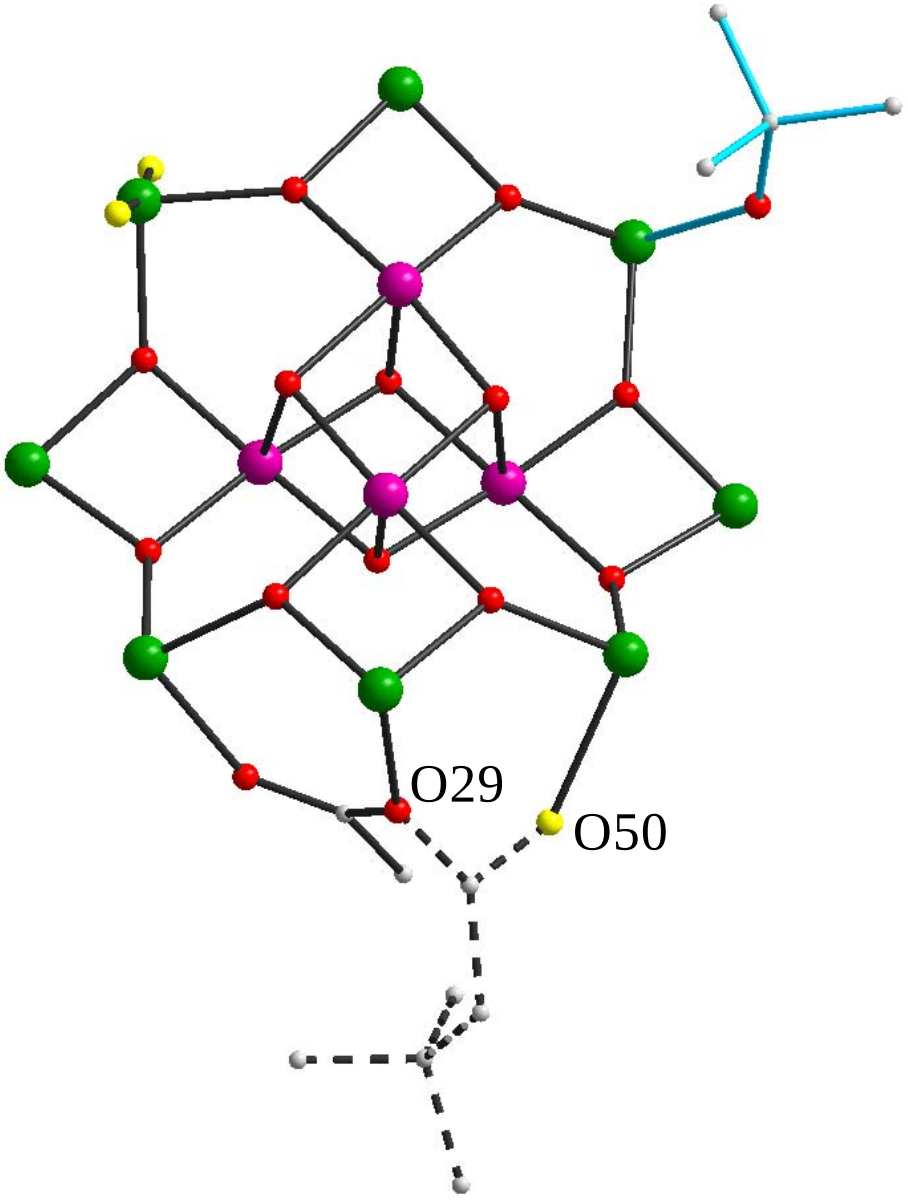

Figure S2. PovRay representation of the extended core of complex **3**, emphasizing the static disorder (80:20) between the water molecule (O50), and a tert-butyl acetate ligand. The tert-butyl acetate groups which are not involved in the static disorder, as well as all hydrogen atoms have been omitted for clarity. The water oxygens are shown in yellow; the bonds of the Bu^{t}OH ligand are denoted in sky-blue for emphasis. Color code: Mn^{IV} purple; Mn^{III} green; O red; C gray.

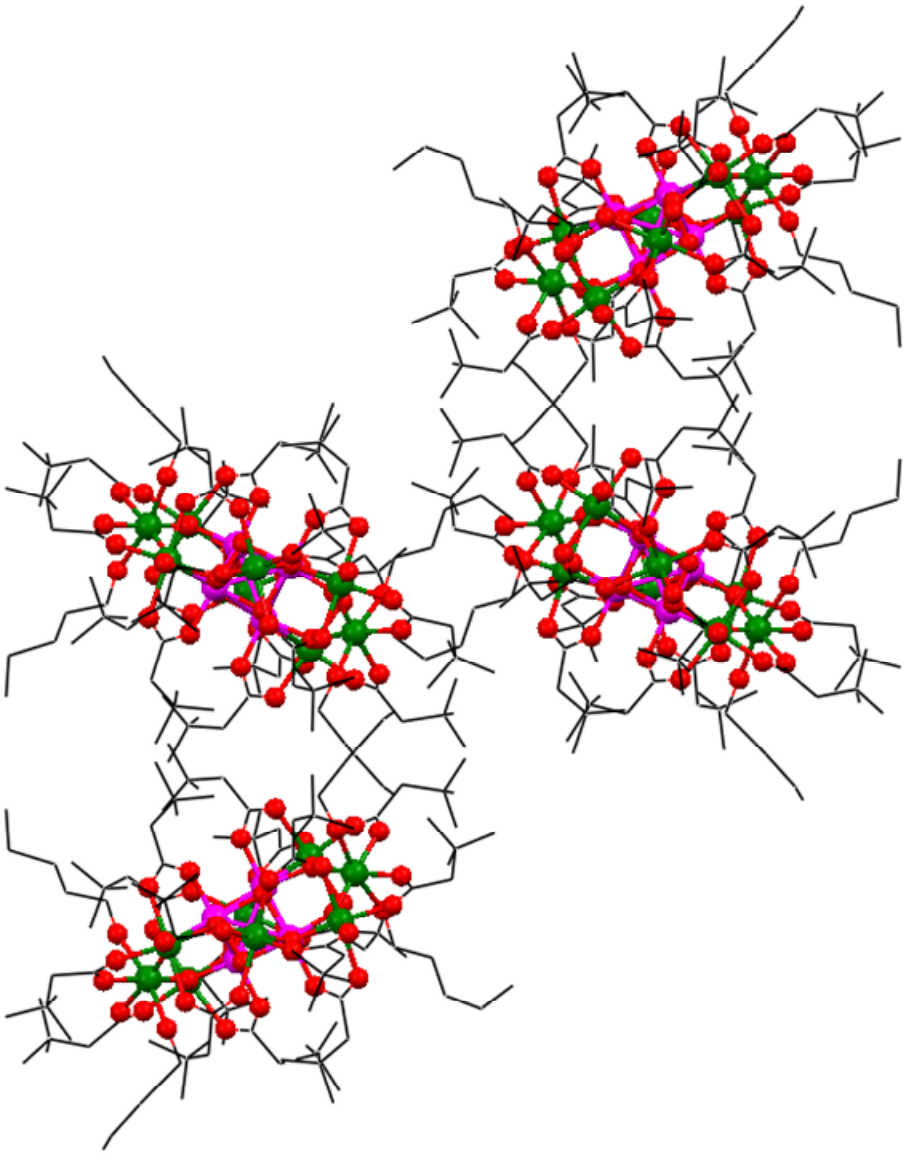

Figure S3. Packing diagram for complex **4**, showing the two orientations of symmetry-related Mn_{12} complexes. Color code: Mn^{IV} purple; Mn^{III} green; O red; C gray.

Table S1. BVS Calculations for the Mn[a] atoms of complexes **3** and **4**.

	3			**4**		
Atom	Mn^{II}	Mn^{III}	Mn^{IV}	Mn^{II}	Mn^{III}	Mn^{IV}
Mn1	3.23	<u>2.96</u>	3.10	3.28	<u>3.00</u>	3.15
Mn2	4.23	3.87	<u>4.06</u>	4.16	3.80	<u>3.99</u>
Mn3	4.19	3.83	<u>4.02</u>	4.18	3.83	<u>4.02</u>
Mn4	3.25	<u>2.97</u>	3.12	3.27	<u>3.00</u>	3.15
Mn5	3.24	<u>2.97</u>	3.12	3.24	<u>2.97</u>	3.12
Mn6	4.18	3.82	<u>4.01</u>	4.26	3.89	<u>4.09</u>
Mn7	4.15	3.80	<u>3.99</u>	4.25	3.88	<u>4.08</u>
Mn8	3.29	<u>3.01</u>	3.16	3.24	<u>2.97</u>	3.11
Mn9	3.24	<u>2.96</u>	3.11	3.21	<u>2.93</u>	3.08
Mn10	3.22	<u>2.95</u>	3.09	3.23	<u>2.95</u>	3.10
Mn11	3.25	<u>2.97</u>	3.12	3.31	<u>3.03</u>	3.18
Mn12	3.39	<u>3.10</u>	3.25	3.24	<u>2.96</u>	3.11

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