## **Supporting Information**

## **Steric Hindrances Create a Discrete Linear Dy**<sub>4</sub> **Complex Exhibiting SMM Behaviour**

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Fig. S1 The experimental XRD pattern of samples (red) and the calculated XRD pattern of single crystal X-ray diffraction data (black) for 1 (left) and 2 (right), respectively.



**Fig. S2** Coordination polyhedra observed in **1** showing distorted bicapped trigonal-prismatic geometry for Dy1 and Dy2. (Symmetry codes: A, 1 -x+1,-y-1,-z).



Fig. S3 Packing arrangement of the molecules along *a* (top), *b* (middle), *c* (bottom) axis, respectively. Violet (Dy), Red (O), Blue (N).



Fig. S4 Temperature (top) and frequency (bottom) dependence of the in-phase ( $\chi'$ ) ac susceptibility of 1, under zero dc field. Solid lines are eye guides.

Table S1 Selected bold lengths (A) and bold angles ( ) of 1.								
Dy(1)-O(11)	2.273(5)	O(17)-Dy(1)-O(13)	80.08(19)	O(7)-Dy(2)-O(5)	127.82(17)			
Dy(1)-O(14)	2.278(5)	O(12)-Dy(1)-O(13)	53.19(18)	O(10)-Dy(2)-O(1)	153.0(2)			
Dy(1)-O(9)	2.300(5)	O(16)-Dy(1)-O(13)	146.63(19)	O(10)-Dy(2)-O(8)	90.28(19)			
Dy(1)-O(17)	2.307(5)	O(15)-Dy(1)-O(13)	129.17(17)	O(1)-Dy(2)-O(8)	92.89(19)			
Dy(1)-O(12)	2.417(6)	O(14)-Dy(1)-O(15)	69.0(2)	O(10)-Dy(2)-O(4)	82.99(18)			
Dy(1)-O(16)	2.421(5)	O(9)-Dy(1)-O(15)	82.1(2)	O(1)-Dy(2)-O(4)	105.22(17)			
Dy(1)-O(15)	2.495(6)	O(17)-Dy(1)-O(15)	77.4(2)	O(8)-Dy(2)-O(4)	152.37(19)			
Dy(1)-O(13)	2.502(5)	O(12)-Dy(1)-O(15)	142.2(2)	O(10)-Dy(2)-O(6)	136.60(18)			
Dy(2)-O(10)	2.238(5)	O(16)-Dy(1)-O(15)	68.57(19)	O(1)-Dy(2)-O(6)	70.40(17)			
Dy(2)-O(1)	2.252(5)	O(11)-Dy(1)-O(13)	78.43(19)	O(8)-Dy(2)-O(6)	84.32(18)			
Dy(2)-O(8)	2.284(5)	O(14)-Dy(1)-O(13)	73.7(2)	O(4)-Dy(2)-O(6)	82.41(18)			
Dy(2)-O(4)	2.396(5)	O(9)-Dy(1)-O(17)	149.3(2)	O(10)-Dy(2)-O(7)	83.09(18)			
Dy(2)-O(6)	2.435(5)	O(11)-Dy(1)-O(12)	75.31(19)	O(1)-Dy(2)-O(7)	123.77(18)			
Dy(2)-O(7)	2.438(5)	O(14)-Dy(1)-O(12)	78.5(2)	O(8)-Dy(2)-O(7)	77.48(18)			
Dy(2)-O(5)	2.450(5)	O(9)-Dy(1)-O(12)	78.4(2)	O(4)-Dy(2)-O(7)	75.12(18)			
Dy(2)-N(1)	2.533(6)	O(17)-Dy(1)-O(12)	130.8(2)	O(6)-Dy(2)-O(7)	53.67(16)			
O(9)-Dy(1)-O(13)	130.56(19)	O(11)-Dy(1)-O(16)	74.4(2)	O(10)-Dy(2)-O(5)	81.47(18)			
O(11)-Dy(1)-O(14)	149.6(2)	O(14)-Dy(1)-O(16)	135.9(2)	O(1)-Dy(2)-O(5)	83.06(18)			
O(11)-Dy(1)-O(9)	100.68(19)	O(9)-Dy(1)-O(16)	74.09(19)	O(8)-Dy(2)-O(5)	151.53(19)			
O(14)-Dy(1)-O(9)	88.7(2)	O(17)-Dy(1)-O(16)	77.22(18)	O(4)-Dy(2)-O(5)	53.71(18)			
O(11)-Dy(1)-O(17)	81.7(2)	O(12)-Dy(1)-O(16)	133.94(17)	O(6)-Dy(2)-O(5)	120.05(17)			
O(14)-Dy(1)-O(17)	104.7(2)	O(11)-Dy(1)-O(15)	140.6(2)					

Gd(1)-O(14)2.297(5)O(11)-Gd(1)-O(16)82.20(18)O(8)-Gd(2)-O(1)152.30(16)Gd(1)-O(9)2.301(5)O(12)-Gd(1)-O(16)142.20(18)O(8)-Gd(2)-O(10)92.35(18)Gd(1)-O(15)2.327(5)O(13)-Gd(1)-O(16)129.07(17)O(8)-Gd(2)-O(5)83.35(17)Gd(1)-O(11)2.327(5)O(13)-Gd(1)-O(13)80.10(17)O(1)-Gd(2)-O(5)152.07(17)Gd(1)-O(12)2.431(5)O(12)-Gd(1)-O(13)130.27(17)O(10)-Gd(2)-O(5)152.07(17)Gd(1)-O(13)2.505(5)O(12)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)84.07(17)Gd(1)-O(16)2.512(5)O(17)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)123.33(15)Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)73.30(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(1)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)83.50(16)Gd(2)-O(1)2.48(4)O(15)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.02(15)Gd(2)-O(4)2.470(5)O(11)-Gd(1)-O(12)78.30(18)O(1)-Gd(2)-O(4)83.45(15)Gd(2)-O(4)2.560(5)O(11)-Gd(1)-O(17)78.30(18)O(1)-Gd(2)-O(4)83.45(15)Gd(2)-O(4)2.560(5)O(1)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)83.45(15)Gd(2)-O(1)-150.54(1)-O(17)74.31(14)O(1)-Gd(2)-O(4)152.44(16)Gd(2)-O(1)150.54(1)-O(17)74.31(17)O(1		Tuble 52 beleteted bond lengths (1) and bond angles ( ) of 2.							
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Gd(1)-O(15) 2.327(5) O(17)-Gd(1)-O(16) 69.07(17) O(1)-Gd(2)-O(10) 92.35(18)   Gd(1)-O(11) 2.327(5) O(13)-Gd(1)-O(16) 129.07(17) O(8)-Gd(2)-O(5) 83.35(17)   Gd(1)-O(12) 2.431(5) O(15)-Gd(1)-O(13) 80.10(17) O(1)-Gd(2)-O(5) 152.07(17)   Gd(1)-O(13) 2.451(5) O(11)-Gd(1)-O(13) 130.27(17) O(10)-Gd(2)-O(5) 152.07(17)   Gd(1)-O(13) 2.509(5) O(12)-Gd(1)-O(13) 52.95(16) O(8)-Gd(2)-O(7) 84.07(17)   Gd(1)-O(16) 2.512(5) O(17)-Gd(1)-O(13) 146.67(16) O(1)-Gd(2)-O(7) 123.33(15)   Gd(2)-O(8) 2.263(5) O(14)-Gd(1)-O(16) 48.90(18) O(10)-Gd(2)-O(7) 75.30(16)   Gd(2)-O(1) 2.268(4) O(9)-Gd(1)-O(16) 140.71(18) O(5)-Gd(2)-O(6) 137.11(16)   Gd(2)-O(10) 2.312(5) O(15)-Gd(1)-O(11) 149.53(18) O(1)-Gd(2)-O(6) 83.02(15)   Gd(2)-O(7) 2.460(4) O(14)-Gd(1)-O(12) 78.30(18) O(10)-Gd(2)-O(6) 83.02(15)   Gd(2)-O(4) 2.462(4) <tho< td=""><td>Gd(1)-O(9)</td><td>2.301(5)</td><td>O(12)-Gd(1)-O(16)</td><td>142.20(18)</td><td>O(8)-Gd(2)-O(10)</td><td>90.11(18)</td></tho<>	Gd(1)-O(9)	2.301(5)	O(12)-Gd(1)-O(16)	142.20(18)	O(8)-Gd(2)-O(10)	90.11(18)			
Gd(1)-O(11) 2.327(5) O(13)-Gd(1)-O(16) 129.07(17) O(8)-Gd(2)-O(5) 83.35(17)   Gd(1)-O(12) 2.431(5) O(15)-Gd(1)-O(13) 80.10(17) O(1)-Gd(2)-O(5) 152.07(17)   Gd(1)-O(13) 2.451(5) O(11)-Gd(1)-O(13) 130.27(17) O(10)-Gd(2)-O(5) 152.07(17)   Gd(1)-O(13) 2.509(5) O(12)-Gd(1)-O(13) 52.95(16) O(8)-Gd(2)-O(7) 84.07(17)   Gd(1)-O(16) 2.512(5) O(17)-Gd(1)-O(13) 146.67(16) O(1)-Gd(2)-O(7) 123.33(15)   Gd(2)-O(8) 2.263(5) O(14)-Gd(1)-O(16) 68.90(18) O(10)-Gd(2)-O(7) 75.30(16)   Gd(2)-O(1) 2.268(4) O(9)-Gd(1)-O(16) 140.71(18) O(5)-Gd(2)-O(7) 75.30(16)   Gd(2)-O(1) 2.312(5) O(15)-Gd(1)-O(11) 149.53(18) O(1)-Gd(2)-O(6) 83.02(15)   Gd(2)-O(7) 2.460(4) O(1)-Gd(1)-O(12) 78.31(17) O(5)-Gd(2)-O(6) 83.02(15)   Gd(2)-O(6) 2.462(4) O(9)-Gd(1)-O(12) 78.31(17) O(1)-Gd(2)-O(4) 83.12(17)   Gd(2)-N(1) 2.460(5) O(11)-G	Gd(1)-O(15)	2.327(5)	O(17)-Gd(1)-O(16)	69.07(17)	O(1)-Gd(2)-O(10)	92.35(18)			
Gd(1)-O(12)2.431(5)O(15)-Gd(1)-O(13)80.10(17)O(1)-Gd(2)-O(5)105.96(16)Gd(1)-O(17)2.451(5)O(11)-Gd(1)-O(13)130.27(17)O(10)-Gd(2)-O(5)152.07(17)Gd(1)-O(13)2.509(5)O(12)-Gd(1)-O(13)52.95(16)O(8)-Gd(2)-O(7)123.33(15)Gd(1)-O(16)2.512(5)O(17)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)123.33(15)Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)77.03(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(7)2.48(4)O(15)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(1)-Gd(1)-O(12)78.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.462(4)O(9)-Gd(1)-O(12)78.40(18)O(7)-Gd(2)-O(6)83.12(17)Gd(2)-O(1)2.560(5)O(11)-Gd(1)-O(12)78.40(18)O(1)-Gd(2)-O(4)81.72(17)O(14)-Gd(1)-O(15)158.20O(9)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.31(17)O(5)-Gd(2)-O(4)127.64(15)O(14)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)180.02O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(14)-Gd(1)-O(11) <td< td=""><td>Gd(1)-O(11)</td><td>2.327(5)</td><td>O(13)-Gd(1)-O(16)</td><td>129.07(17)</td><td>O(8)-Gd(2)-O(5)</td><td>83.35(17)</td></td<>	Gd(1)-O(11)	2.327(5)	O(13)-Gd(1)-O(16)	129.07(17)	O(8)-Gd(2)-O(5)	83.35(17)			
Gd(1)-O(17)2.451(5)O(11)-Gd(1)-O(13)130.27(17)O(10)-Gd(2)-O(5)152.07(17)Gd(1)-O(13)2.509(5)O(12)-Gd(1)-O(13)52.95(16)O(8)-Gd(2)-O(7)84.07(17)Gd(1)-O(16)2.512(5)O(17)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)123.33(15)Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)77.03(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(5)2.428(4)O(15)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(14)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.422(4)O(9)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.13(15)Gd(2)-O(4)2.479(5)O(11)-Gd(1)-O(12)78.40(18)O(7)-Gd(2)-O(4)81.72(17)O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.30(18)O(1)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.31(17)O(10)-Gd(2)-O(4)152.44(16)O(9)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.31(17)O(10)-Gd(2)-O(4)152.44(16)O(9)-Gd(1)-O(11)80.02O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(14)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)73.92(18)O(6)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(11)<	Gd(1)-O(12)	2.431(5)	O(15)-Gd(1)-O(13)	80.10(17)	O(1)-Gd(2)-O(5)	105.96(16)			
Gd(1)-O(13)2.509(5)O(12)-Gd(1)-O(13)52.95(16)O(8)-Gd(2)-O(7)84.07(17)Gd(1)-O(16)2.512(5)O(17)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)123.33(15)Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)77.03(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(5)2.428(4)O(15)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(14)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.479(5)O(15)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.13(15)Gd(2)-N(1)2.560(5)O(11)-Gd(1)-O(12)78.40(18)O(7)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)149.61(19)O(14)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.31(7)O(10)-Gd(2)-O(4)152.44(16)O(9)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.31(7)O(10)-Gd(2)-O(4)152.44(15)O(14)-Gd(1)-O(11)88.0(2)O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)73.92(18)I27.64(15)O(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)I27.64(15)	Gd(1)-O(17)	2.451(5)	O(11)-Gd(1)-O(13)	130.27(17)	O(10)-Gd(2)-O(5)	152.07(17)			
Gd(1)-O(16)2.512(5)O(17)-Gd(1)-O(13)146.67(16)O(1)-Gd(2)-O(7)123.33(15)Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)77.03(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(5)2.428(4)O(15)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(9)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.479(5)O(15)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.13(15)Gd(2)-O(4)2.479(5)O(11)-Gd(1)-O(12)78.40(18)O(7)-Gd(2)-O(4)81.72(17)O(14)-Gd(1)-O(1)149.61(19)O(14)-Gd(1)-O(17)74.30(18)O(1)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.30(17)O(7)-Gd(2)-O(4)152.44(16)O(9)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.37(17)O(7)-Gd(2)-O(4)127.64(15)O(14)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)73.92(18)VVVVO(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)VVVVVO(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)VVVVV <td>Gd(1)-O(13)</td> <td>2.509(5)</td> <td>O(12)-Gd(1)-O(13)</td> <td>52.95(16)</td> <td>O(8)-Gd(2)-O(7)</td> <td>84.07(17)</td>	Gd(1)-O(13)	2.509(5)	O(12)-Gd(1)-O(13)	52.95(16)	O(8)-Gd(2)-O(7)	84.07(17)			
Gd(2)-O(8)2.263(5)O(14)-Gd(1)-O(16)68.90(18)O(10)-Gd(2)-O(7)77.03(16)Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(5)2.428(4)O(15)-Gd(1)-O(11)149.53(18)O(1)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(14)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.462(4)O(9)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(4)2.479(5)O(15)-Gd(1)-O(12)78.40(18)O(7)-Gd(2)-O(6)83.13(15)Gd(2)-N(1)2.560(5)O(11)-Gd(1)-O(17)78.40(18)O(10)-Gd(2)-O(4)81.72(17)O(14)-Gd(1)-O(19)149.61(19)O(14)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)74.31(7)O(10)-Gd(2)-O(4)53.16(15)O(14)-Gd(1)-O(11)88.0(2)O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)73.30(17)O(5)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)II	Gd(1)-O(16)	2.512(5)	O(17)-Gd(1)-O(13)	146.67(16)	O(1)-Gd(2)-O(7)	123.33(15)			
Gd(2)-O(1)2.268(4)O(9)-Gd(1)-O(16)140.71(18)O(5)-Gd(2)-O(7)75.30(16)Gd(2)-O(10)2.312(5)O(15)-Gd(1)-O(16)77.94(19)O(8)-Gd(2)-O(6)137.11(16)Gd(2)-O(5)2.428(4)O(15)-Gd(1)-O(11)149.53(18)O(1)-Gd(2)-O(6)83.50(16)Gd(2)-O(7)2.460(4)O(14)-Gd(1)-O(12)78.25(18)O(10)-Gd(2)-O(6)83.02(15)Gd(2)-O(6)2.462(4)O(9)-Gd(1)-O(12)75.31(17)O(5)-Gd(2)-O(6)83.02(15)Gd(2)-O(4)2.479(5)O(15)-Gd(1)-O(12)130.43(18)O(7)-Gd(2)-O(6)83.13(15)Gd(2)-N(1)2.560(5)O(11)-Gd(1)-O(17)78.40(18)O(8)-Gd(2)-O(4)81.72(17)O(14)-Gd(1)-O(19)149.61(19)O(14)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)83.45(15)O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.31(7)O(5)-Gd(2)-O(4)53.16(15)O(14)-Gd(1)-O(15)88.0(2)O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)73.92(18)120.01(16)	Gd(2)-O(8)	2.263(5)	O(14)-Gd(1)-O(16)	68.90(18)	O(10)-Gd(2)-O(7)	77.03(16)			
Gd(2)-O(10) $2.312(5)$ $O(15)-Gd(1)-O(16)$ $77.94(19)$ $O(8)-Gd(2)-O(6)$ $137.11(16)$ $Gd(2)-O(5)$ $2.428(4)$ $O(15)-Gd(1)-O(11)$ $149.53(18)$ $O(1)-Gd(2)-O(6)$ $70.54(15)$ $Gd(2)-O(7)$ $2.460(4)$ $O(14)-Gd(1)-O(12)$ $78.25(18)$ $O(10)-Gd(2)-O(6)$ $83.50(16)$ $Gd(2)-O(6)$ $2.462(4)$ $O(9)-Gd(1)-O(12)$ $75.31(17)$ $O(5)-Gd(2)-O(6)$ $83.02(15)$ $Gd(2)-O(4)$ $2.479(5)$ $O(15)-Gd(1)-O(12)$ $130.43(18)$ $O(7)-Gd(2)-O(6)$ $53.13(15)$ $Gd(2)-N(1)$ $2.560(5)$ $O(11)-Gd(1)-O(12)$ $78.40(18)$ $O(8)-Gd(2)-O(4)$ $81.72(17)$ $O(14)-Gd(1)-O(9)$ $149.61(19)$ $O(14)-Gd(1)-O(17)$ $136.03(18)$ $O(1)-Gd(2)-O(4)$ $83.45(15)$ $O(14)-Gd(1)-O(15)$ $105.8(2)$ $O(9)-Gd(1)-O(17)$ $74.21(17)$ $O(10)-Gd(2)-O(4)$ $152.44(16)$ $O(9)-Gd(1)-O(15)$ $80.93(19)$ $O(15)-Gd(1)-O(17)$ $74.37(17)$ $O(5)-Gd(2)-O(4)$ $127.64(15)$ $O(14)-Gd(1)-O(11)$ $88.0(2)$ $O(11)-Gd(1)-O(17)$ $74.07(17)$ $O(7)-Gd(2)-O(4)$ $127.64(15)$ $O(9)-Gd(1)-O(11)$ $100.96(18)$ $O(12)-Gd(1)-O(17)$ $73.92(18)$ $V$ $V$	Gd(2)-O(1)	2.268(4)	O(9)-Gd(1)-O(16)	140.71(18)	O(5)-Gd(2)-O(7)	75.30(16)			
Gd(2)-O(5) $2.428(4)$ $O(15)-Gd(1)-O(11)$ $149.53(18)$ $O(1)-Gd(2)-O(6)$ $70.54(15)$ $Gd(2)-O(7)$ $2.460(4)$ $O(14)-Gd(1)-O(12)$ $78.25(18)$ $O(10)-Gd(2)-O(6)$ $83.50(16)$ $Gd(2)-O(6)$ $2.462(4)$ $O(9)-Gd(1)-O(12)$ $75.31(17)$ $O(5)-Gd(2)-O(6)$ $83.02(15)$ $Gd(2)-O(4)$ $2.479(5)$ $O(15)-Gd(1)-O(12)$ $130.43(18)$ $O(7)-Gd(2)-O(6)$ $83.02(15)$ $Gd(2)-N(1)$ $2.560(5)$ $O(11)-Gd(1)-O(12)$ $78.40(18)$ $O(8)-Gd(2)-O(4)$ $81.72(17)$ $O(14)-Gd(1)-O(9)$ $149.61(19)$ $O(14)-Gd(1)-O(17)$ $74.21(17)$ $O(10)-Gd(2)-O(4)$ $83.45(15)$ $O(14)-Gd(1)-O(15)$ $80.93(19)$ $O(15)-Gd(1)-O(17)$ $74.21(17)$ $O(10)-Gd(2)-O(4)$ $152.44(16)$ $O(9)-Gd(1)-O(15)$ $80.93(19)$ $O(15)-Gd(1)-O(17)$ $77.33(17)$ $O(5)-Gd(2)-O(4)$ $127.64(15)$ $O(14)-Gd(1)-O(11)$ $88.0(2)$ $O(11)-Gd(1)-O(17)$ $74.07(17)$ $O(7)-Gd(2)-O(4)$ $127.64(15)$ $O(9)-Gd(1)-O(11)$ $100.96(18)$ $O(12)-Gd(1)-O(17)$ $133.60(17)$ $O(6)-Gd(2)-O(4)$ $120.01(16)$ $O(9)-Gd(1)-O(13)$ $78.28(17)$ $O(14)-Gd(1)-O(13)$ $73.92(18)$ $V(1)-V(1)$ $V(1)-V(1)$	Gd(2)-O(10)	2.312(5)	O(15)-Gd(1)-O(16)	77.94(19)	O(8)-Gd(2)-O(6)	137.11(16)			
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Gd(2)-O(5)	2.428(4)	O(15)-Gd(1)-O(11)	149.53(18)	O(1)-Gd(2)-O(6)	70.54(15)			
$Gd(2)-O(6)$ $2.462(4)$ $O(9)-Gd(1)-O(12)$ $75.31(17)$ $O(5)-Gd(2)-O(6)$ $83.02(15)$ $Gd(2)-O(4)$ $2.479(5)$ $O(15)-Gd(1)-O(12)$ $130.43(18)$ $O(7)-Gd(2)-O(6)$ $53.13(15)$ $Gd(2)-N(1)$ $2.560(5)$ $O(11)-Gd(1)-O(12)$ $78.40(18)$ $O(8)-Gd(2)-O(4)$ $81.72(17)$ $O(14)-Gd(1)-O(9)$ $149.61(19)$ $O(14)-Gd(1)-O(17)$ $136.03(18)$ $O(1)-Gd(2)-O(4)$ $83.45(15)$ $O(14)-Gd(1)-O(15)$ $105.8(2)$ $O(9)-Gd(1)-O(17)$ $74.21(17)$ $O(10)-Gd(2)-O(4)$ $152.44(16)$ $O(9)-Gd(1)-O(15)$ $80.93(19)$ $O(15)-Gd(1)-O(17)$ $77.33(17)$ $O(5)-Gd(2)-O(4)$ $53.16(15)$ $O(14)-Gd(1)-O(11)$ $88.0(2)$ $O(11)-Gd(1)-O(17)$ $74.07(17)$ $O(7)-Gd(2)-O(4)$ $127.64(15)$ $O(9)-Gd(1)-O(11)$ $100.96(18)$ $O(12)-Gd(1)-O(17)$ $133.60(17)$ $O(6)-Gd(2)-O(4)$ $120.01(16)$ $O(9)-Gd(1)-O(13)$ $78.28(17)$ $O(14)-Gd(1)-O(13)$ $73.92(18)$ $V_{11}$ $V_{11}$	Gd(2)-O(7)	2.460(4)	O(14)-Gd(1)-O(12)	78.25(18)	O(10)-Gd(2)-O(6)	83.50(16)			
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Gd(2)-O(6)	2.462(4)	O(9)-Gd(1)-O(12)	75.31(17)	O(5)-Gd(2)-O(6)	83.02(15)			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Gd(2)-O(4)	2.479(5)	O(15)-Gd(1)-O(12)	130.43(18)	O(7)-Gd(2)-O(6)	53.13(15)			
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Gd(2)-N(1)	2.560(5)	O(11)-Gd(1)-O(12)	78.40(18)	O(8)-Gd(2)-O(4)	81.72(17)			
O(14)-Gd(1)-O(15)105.8(2)O(9)-Gd(1)-O(17)74.21(17)O(10)-Gd(2)-O(4)152.44(16)O(9)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)77.33(17)O(5)-Gd(2)-O(4)53.16(15)O(14)-Gd(1)-O(11)88.0(2)O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)133.60(17)O(6)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)	O(14)-Gd(1)-O(9)	149.61(19)	O(14)-Gd(1)-O(17)	136.03(18)	O(1)-Gd(2)-O(4)	83.45(15)			
O(9)-Gd(1)-O(15)80.93(19)O(15)-Gd(1)-O(17)77.33(17)O(5)-Gd(2)-O(4)53.16(15)O(14)-Gd(1)-O(11)88.0(2)O(11)-Gd(1)-O(17)74.07(17)O(7)-Gd(2)-O(4)127.64(15)O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)133.60(17)O(6)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)	O(14)-Gd(1)-O(15)	105.8(2)	O(9)-Gd(1)-O(17)	74.21(17)	O(10)-Gd(2)-O(4)	152.44(16)			
O(14)-Gd(1)-O(11) 88.0(2) O(11)-Gd(1)-O(17) 74.07(17) O(7)-Gd(2)-O(4) 127.64(15)   O(9)-Gd(1)-O(11) 100.96(18) O(12)-Gd(1)-O(17) 133.60(17) O(6)-Gd(2)-O(4) 120.01(16)   O(9)-Gd(1)-O(13) 78.28(17) O(14)-Gd(1)-O(13) 73.92(18)	O(9)-Gd(1)-O(15)	80.93(19)	O(15)-Gd(1)-O(17)	77.33(17)	O(5)-Gd(2)-O(4)	53.16(15)			
O(9)-Gd(1)-O(11)100.96(18)O(12)-Gd(1)-O(17)133.60(17)O(6)-Gd(2)-O(4)120.01(16)O(9)-Gd(1)-O(13)78.28(17)O(14)-Gd(1)-O(13)73.92(18)	O(14)-Gd(1)-O(11)	88.0(2)	O(11)-Gd(1)-O(17)	74.07(17)	O(7)-Gd(2)-O(4)	127.64(15)			
O(9)-Gd(1)-O(13) 78.28(17) O(14)-Gd(1)-O(13) 73.92(18)	O(9)-Gd(1)-O(11)	100.96(18)	O(12)-Gd(1)-O(17)	133.60(17)	O(6)-Gd(2)-O(4)	120.01(16)			
	O(9)-Gd(1)-O(13)	78.28(17)	O(14)-Gd(1)-O(13)	73.92(18)					

Table S2 Selected bond lengths (Å) and bond angles (°) of **2**.