Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information

Triethylamine-templated nanocalix Ln_{12} clusters of diacylhydrazone: crystal structure and magnetic properties

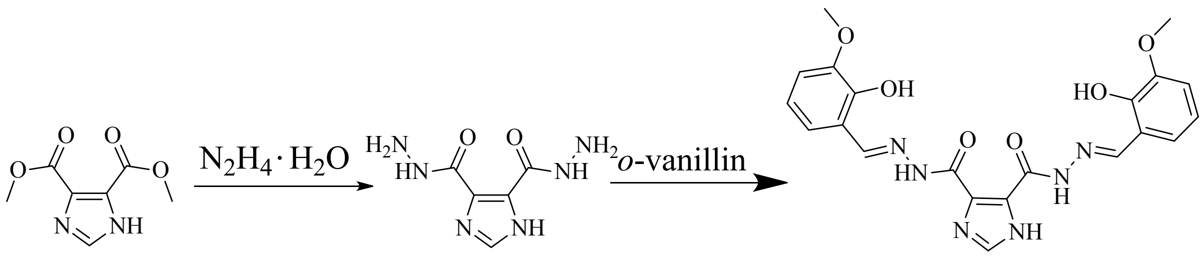
Zhi-Rong Luo,[a] Hua-Hong Zou,*[a] Zi-Lu Chen,[a] Bo Li,*[b] Kai Wang,[c] Fu-Pei Liang*[a,c]

[a]State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, P. R. China. E-mail: fliangoffice@yahoo.com
[b]College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, P. R. China.E-mail: libozzu0107@163.com
[c]Guangxi Key Laboratory of Electrochemical and Magnetochemical Functional Materials, College of Chemistry and Bioengineering, Guilin University of Technology, Guilin 541004, P. R. China.

Synthesis of H_5ovih

The synthetic route for H_5ovih is presented in Scheme S1. Subsequently, the dimethyl 1H-imidazole-4,5-dicarboxylate (3.68 g, 20 mmol) and $N_2H_4·H_2O$ (20 mL, 80%) was refluxed in MeOH (180 mL) at 85 °C for 12 h. The o-vanillin (7.6 g, 50 mmol) was then added slowly and the reaction was keep at 85 °C for another 12 h. Upon cooling and filtering, yellow solid of N,N'-bis(o-vanillidene)-1H-imidazole-4,5-dicarbohydrazide (H_5ovih) was obtained with a yield of 95% (based on 1H-imidazole-4,5-dicarboxylate). HRMS (ESI) m/z: 453.1528 $[M+H]^+$. Elemental analysis Calcd. (%): C, 55.75; H, 4.46; N, 18.58%. Found: C, 55.69; H, 4.40; N, 18.50%. IR spectrum (cm^{-1}): 3315 (s), 3175 (vs), 2990 (m), 2842 (m), 2712 (w), 1666 (vs), 1610 (m), 1580 (s), 1547 (s), 1514 (s), 1468 (s), 1438 (s), 1361 (s), 1280 (m), 1254 (vs), 1145 (m), 1063 (s), 939 (m), 892 (m), 836 (m), 781 (m), 732 (m), 633 (w), 594 (w), 561 (m), 520 (w), 494 (w), 455 (w). ^{1}H NMR:14.38 (s 1H), 13.81(s,1H), 12.51 (s, 1H), 10.90 (s, 1H), 10.77 (s, 1H), 8.91 (s, 1H), 8.10 (s, 1H), 7.29 (d, J = 6.0

Hz, 1H), 7.16 (d, J = 6.0 Hz, 1H), 7.08-7.06 (m, 2H), 6.91 (t, J = 8.0 Hz, 2H), 3.84 (s, 6H); ^{13}C NMR: 160.5, 154.7, 151.0, 148.8, 148.5, 147.9, 147.7, 138.1, 132.4, 128.9, 121.3, 121.2, 119.6, 119.4, 114.6, 56.4.



Scheme S1. Synthetic route of H_5ovih.

Crystallographic Analyses

The intensity data were recorded on a Bruker SMART CCD system with Mo-K_α radiation (λ = 0.71073 Å). The crystal structures were solved by Direct Methods and refined employing full-matrix least squares on F^2 (SHELXTL-2008).[1] The diffraction data of compounds **1-3** were treated by the 'SQUEEZE' method as implemented in PLATON.[2] All non-hydrogen atoms were refined anisotropically, and hydrogen atoms of the organic ligands were generated theoretically onto the specific atoms and refined isotropically with fixed thermal factors. The unidentified solvent molecules were not included for all the three structures. CCDC 1902974-1902977 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/data_request/cif.

SQUEEZE results for these three compounds are as follows:

(1) Compound **1**

```
loop_
   _platon_squeeze_void_nr
   _platon_squeeze_void_average_x
   _platon_squeeze_void_average_y
   _platon_squeeze_void_average_z
   _platon_squeeze_void_volume
   _platon_squeeze_void_count_electrons
   _platon_squeeze_void_content
```

1	-0.098	-0.120	-0.004	11303	1848"
2	0.000	0.000	0.250	973	120"
3	0.000	0.000	0.750	973	120"
4	0.667	0.333	0.083	973	120"
5	0.667	0.333	0.583	973	120"
6	0.333	0.667	0.417	970	120"
7	0.333	0.667	0.917	970	120"

That is, SQUEEZE gives 2568 electrons/unit cell for the voids, and each formula unit has 2531/12 = 214 electrons (since Z = 12). And 1 $(CH_3CH_2)_3N$ has been solved and exists in the crystal structure. Each $(CH_3CH_2)_3N$ has 58 electrons, 1 CH_3CN molecule has 22 electrons, and 1 H_2O has 10 electrons. Because of the disorder of the free $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules, parts of the $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules are difficult to locate in the final structural refinement. The number of free molecules is further confirmed by elemental analyses and TGA analysis. Therefore the chemical formula of complex is found to be $[Gd_{12}(H_2ovih)_3(\mu_3\text{-}O)_9(H_2O)_{24}(NO_3)_9]\cdot 2C_6H_{15}N\cdot 3C_2H_3N\cdot 9H_2O$. The total number of electrons of the guest molecule is the same as that of the calculation. Full details can be found in the CIF files. The CCDC number is 1902975.

(2) Compound **2**

loop_

_platon_squeeze_void_nr

_platon_squeeze_void_average_x

_platon_squeeze_void_average_y

_platon_squeeze_void_average_z

_platon_squeeze_void_volume

_platon_squeeze_void_count_electrons

_platon_squeeze_void_content

1	-0.089	-0.103	-0.004	10886	1935"
2	0.000	0.000	0.250	968	144"
3	0.000	0.000	0.750	968	144"
4	0.667	0.333	0.083	973	144"
5	0.667	0.333	0.583	973	144"

6	0.333	0.667	0.417	974	144"	
7	0.333	0.667	0.917	974	144"	

That is, SQUEEZE gives 2799 electrons/unit cell for the voids, and each formula unit has 2799/12 = 233 electrons (since Z = 12). And 1 $(CH_3CH_2)_3N$ has been solved and exists in the crystal structure. Each $(CH_3CH_2)_3N$ has 58 electrons, 1 CH_3CN molecule has 22 electrons, and 1 H_2O has 10 electrons. Because of the disorder of the free $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules, parts of the $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules are difficult to locate in the final structural refinement. The number of free molecules is further confirmed by elemental analyses and TGA analysis. Therefore the chemical formula of complex is found to be $[Tb_{12}(H_2ovih)_3(\mu_3\text{-}O)_9(H_2O)_{24}(NO_3)_9]\cdot 2C_6H_{15}N\cdot 4C_2H_3N\cdot 9H_2O$. The total number of electrons of the guest molecule is the same as that of the calculation. Full details can be found in the CIF files. The CCDC number is 1902976.

(3) Compound **3**

```
loop_
  _platon_squeeze_void_nr
  _platon_squeeze_void_average_x
  _platon_squeeze_void_average_y
  _platon_squeeze_void_average_z
  _platon_squeeze_void_volume
  _platon_squeeze_void_count_electrons
  _platon_squeeze_void_content
   1   -0.114 -0.125 -0.003     10312     1721''
   2    0.000  0.000  0.250       924      135''
   3    1.000  0.000  0.750       924      135''
   4    0.667  0.333  0.083       931      135''
   5    0.667  0.333  0.583       931      135''
   6    0.333  0.667  0.417       932      135''
   7    0.333  0.667  0.917       932      135''
```

That is, SQUEEZE gives 2531 electrons/unit cell for the voids, and each formula unit has 2531/12 = 211 electrons (since Z = 12). And 1 $(CH_3CH_2)_3N$ has been solved and exists in the crystal structure. Each $(CH_3CH_2)_3N$ has 58 electrons, 1 CH_3CN

molecule has 22 electrons, and 1 H_2O has 10 electrons. Because of the disorder of the free $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules, parts of the $(CH_3CH_2)_3N$, CH_3CN and H_2O molecules are difficult to locate in the final structural refinement. The number of free molecules is further confirmed by elemental analyses and TGA analysis. Therefore the chemical formula of complex is found to be $[Dy_{12}(H_2ovih)_3(\mu_3\text{-}O)_9(H_2O)_{24}(NO_3)_9]\cdot 2C_6H_{15}N\cdot 3C_2H_3N\cdot 9H_2O$. The total number of electrons of the guest molecule is the same as that of the calculation. Full details can be found in the CIF files. The CCDC number is 1902977.

Table S1 Crystal data and structure refinements for the ligand and the compounds 1-3.

Compound	ligand	**1**	**2**	**3**
CCDC No.	1902974	1902975	1902976	1902977
Empirical formula	$C_{23}H_{23}N_7O_6$	$C_{69}H_{114}Gd_{12}N_{28}O_{78}$	$C_{69}H_{114}Tb_{12}N_{28}O_{78}$	$C_{69}H_{114}Dy_{12}N_{28}O_{78}$
Formula weight	493.48	4470.88	4490.92	4533.88
Temperature (K)	150(2)	150(2)	150(2)	150(2)
Crystal system	Monoclinic	Trigonal	Trigonal	Trigonal
Space group	*P2₁/c*	*Rc*	*Rc*	*Rc*
Unit cell dimensions				
a (Å)	4.6284(2)	31.0997(3)	31.0269(10)	30.9262(8)
b (Å)	18.7941(10)	31.0997(3)	31.0269(10)	30.9262(8)
c (Å)	26.5269(14)	61.3340(12)	60.690(3)	60.130(3)
α (°)	90	90	90	90
β (°)	93.527(2)	90	90	90
γ (°)	90	120	120	120
Volume (Å^3), Z	2303.1(2), 4	51375.1(4), 12	50597(4), 12	49805(4), 12
Calculated density (g·cm^{-3})	1.423	1.734	1.769	1.814
Absorption coefficient (mm^{-1})	0.106	4.661	5.046	5.415
F(000)	1032	25392	25536	25680
θ range for data collection (°)	2.300-25.010	1.310-26.998	2.274-25.442	2.281-25.401
Data/restraints/parameters	4070 / 0 / 330	12448 / 2 / 565	10355 / 2 / 565	10171 / 3 / 565
Goodness-of-fit on F^2	1.041	1.048	1.057	1.024
Final R^a indices [$I > 2\sigma(I)$]	$R_1 = 0.0480$, $wR_2 = 0.1100$	$R_1 = 0.0291$, $wR_2 = 0.0922$	$R_1 = 0.0285$, $wR_2 = 0.0845$	$R_1 = 0.0370$, $wR_2 = 0.0753$
R indices (all data)	$R_1 = 0.0748$, $wR_2 = 0.1280$	$R_1 = 0.0356$, $wR_2 = 0.0955$	$R_1 = 0.0356$, $wR_2 = 0.0868$	$R_1 = 0.0644$, $wR_2 = 0.0797$

$^aR_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$. $^b\omega R_2 = [\Sigma[\omega(F_0^2 - F_c^2)^2]/\Sigma[\omega(F_0^2)^2]]^{1/2}$

Thermal analysis

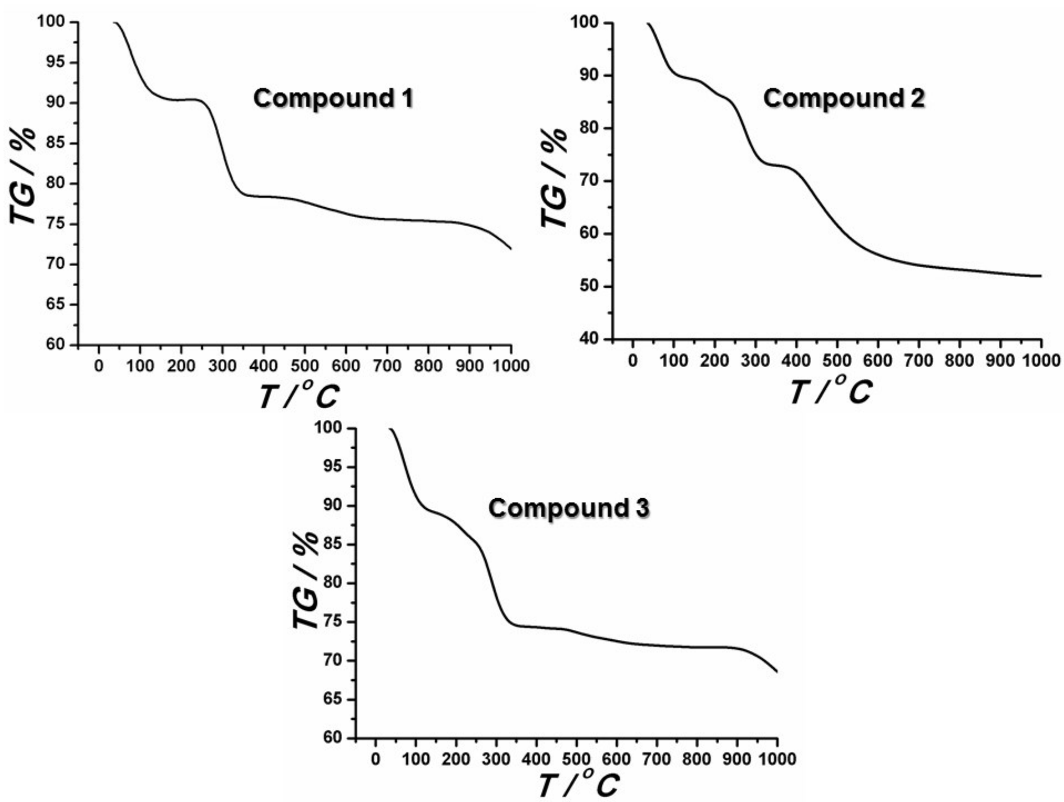


Figure S1 Complexes **1-3** TG curves.

PXRD analysis

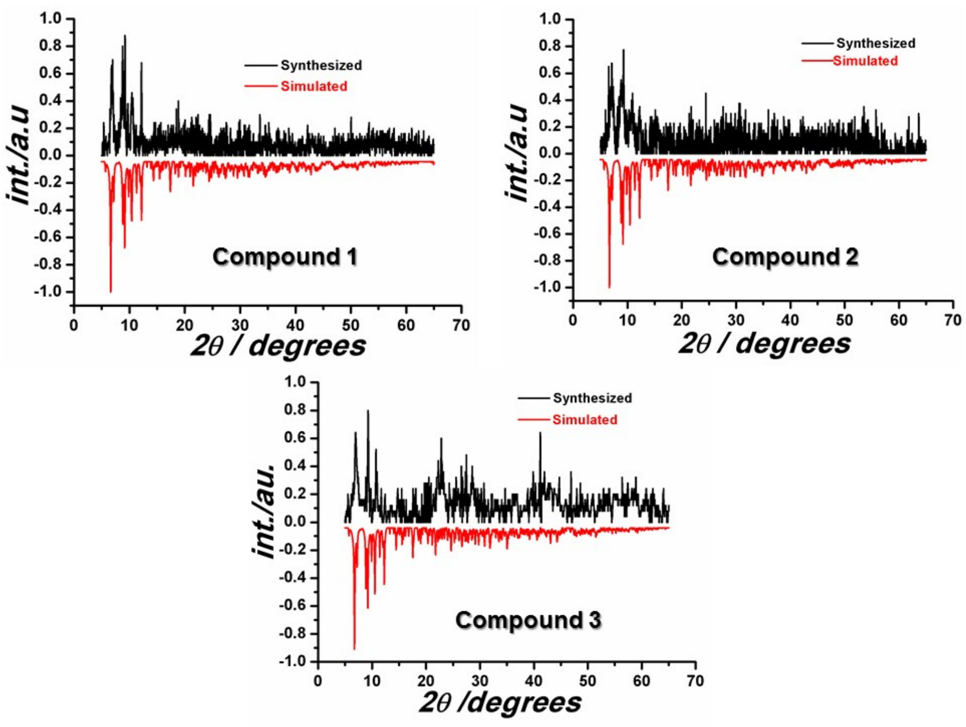


Figure S2 Experimental X-ray difraction and simulated X-ray difraction diagrams of **1**-**3**.

Structural Details

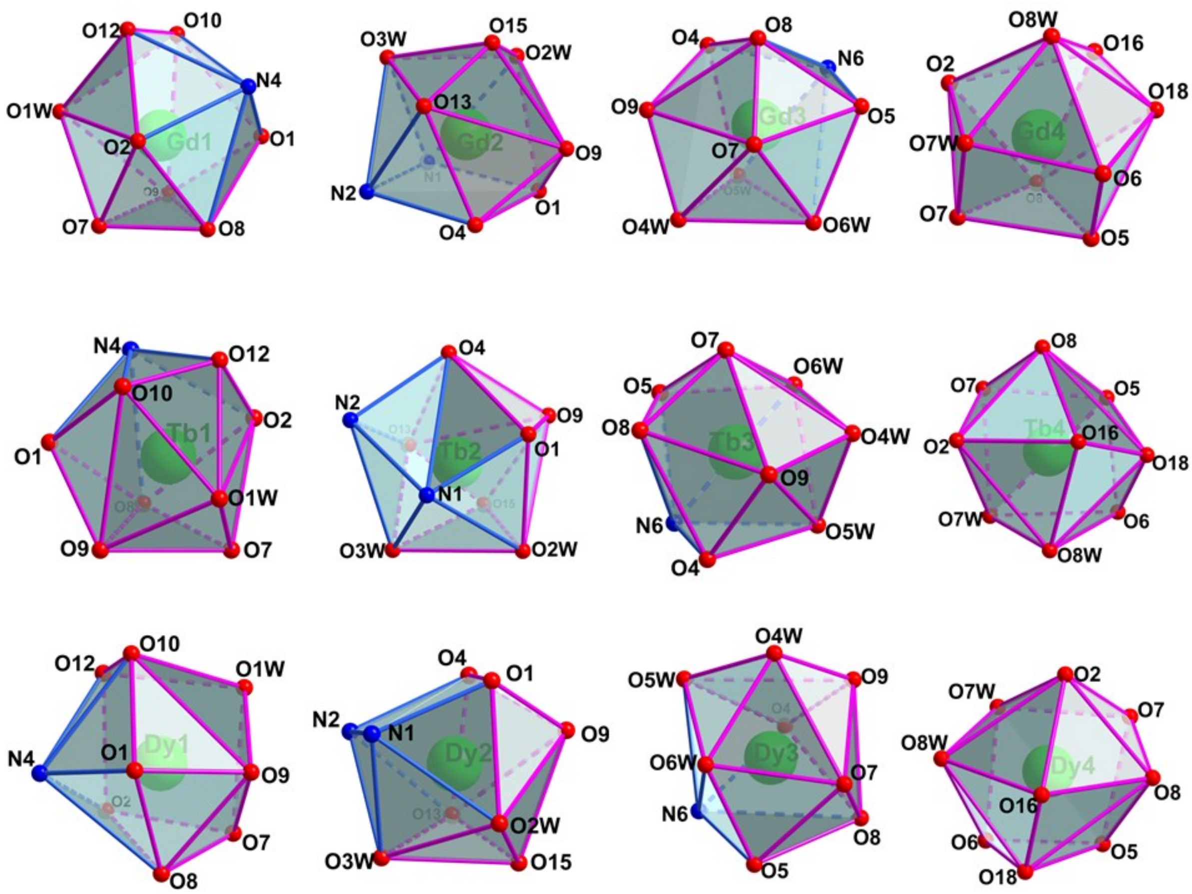


Figure S3 Coordination polyhedron surrounding of Ln(III) for **1**-**3**.

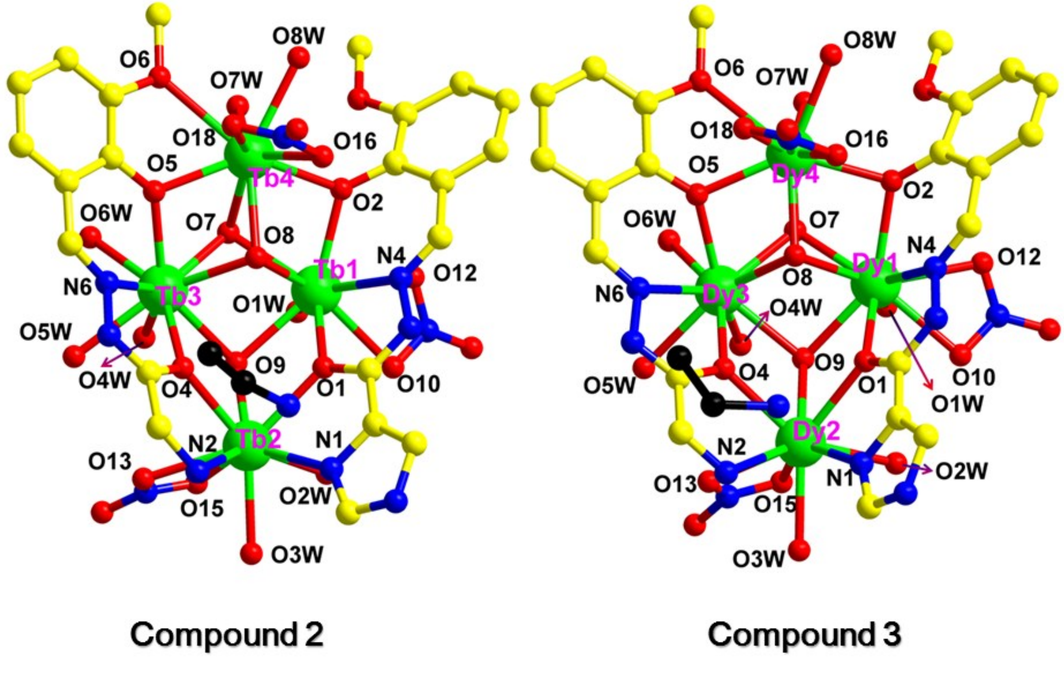


Figure S4 The asymmetry unit of **2-3**. Tb and Dy, green; C, yellow and black; N, blue; O, red.

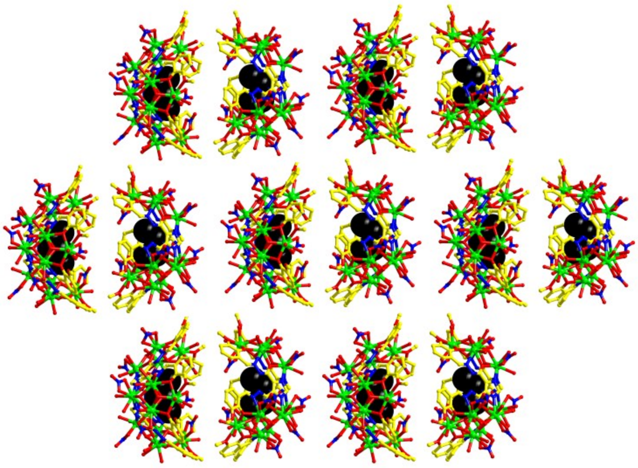


Figure S5 Packing diagram of **1**. Gd, green; C, yellow and black; N, blue; O, red.

Magnetic analysis

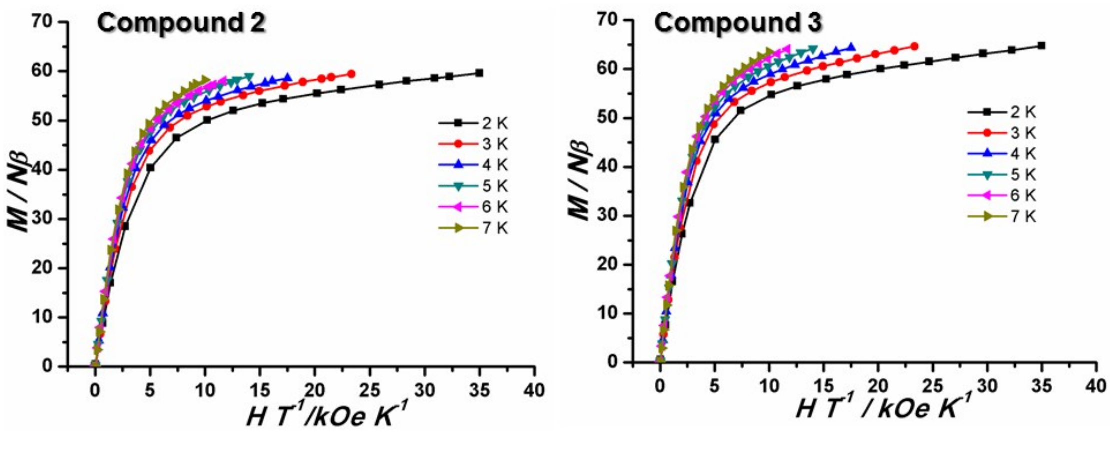


Fig. S6 Plots of M-HT^{-1} of **2-3** at 2-7 K.

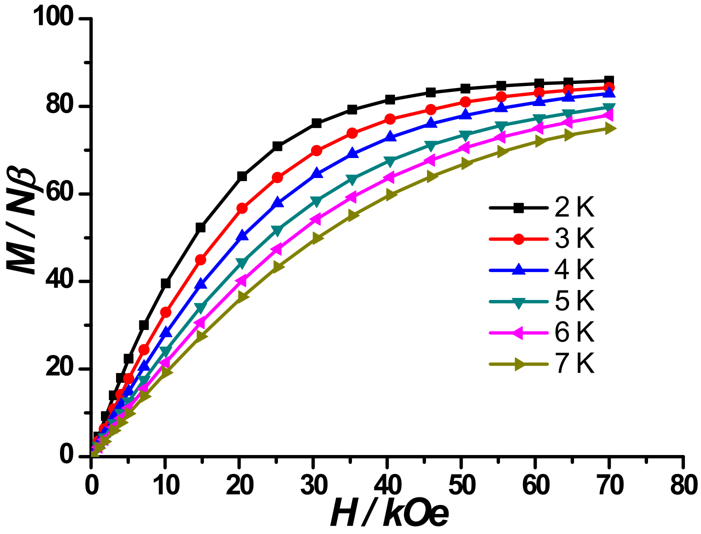


Fig. S7 Plots of M-H of **1** in the range of T = 2-7 K and H = 0-70 kOe.

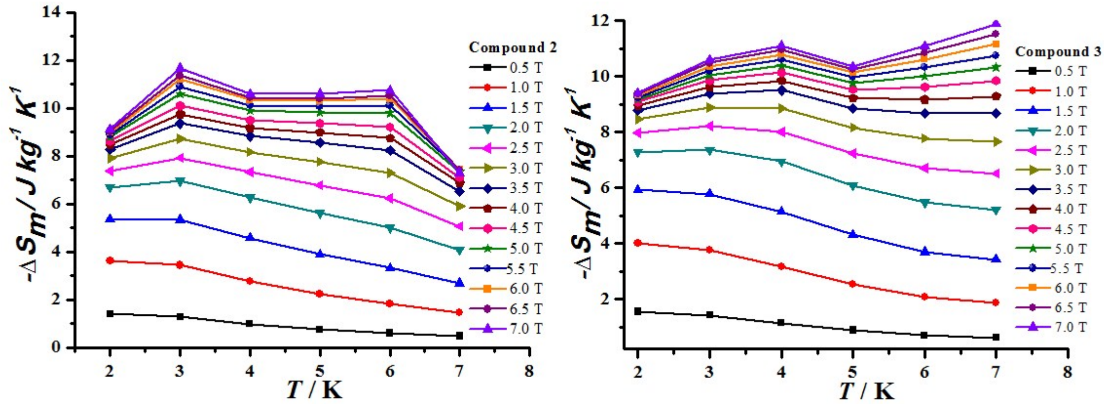


Figure S8 The plots of $-\Delta S_m$-T of **2-3** in the range of T = 2-7 K and H = 0.5-7 T.

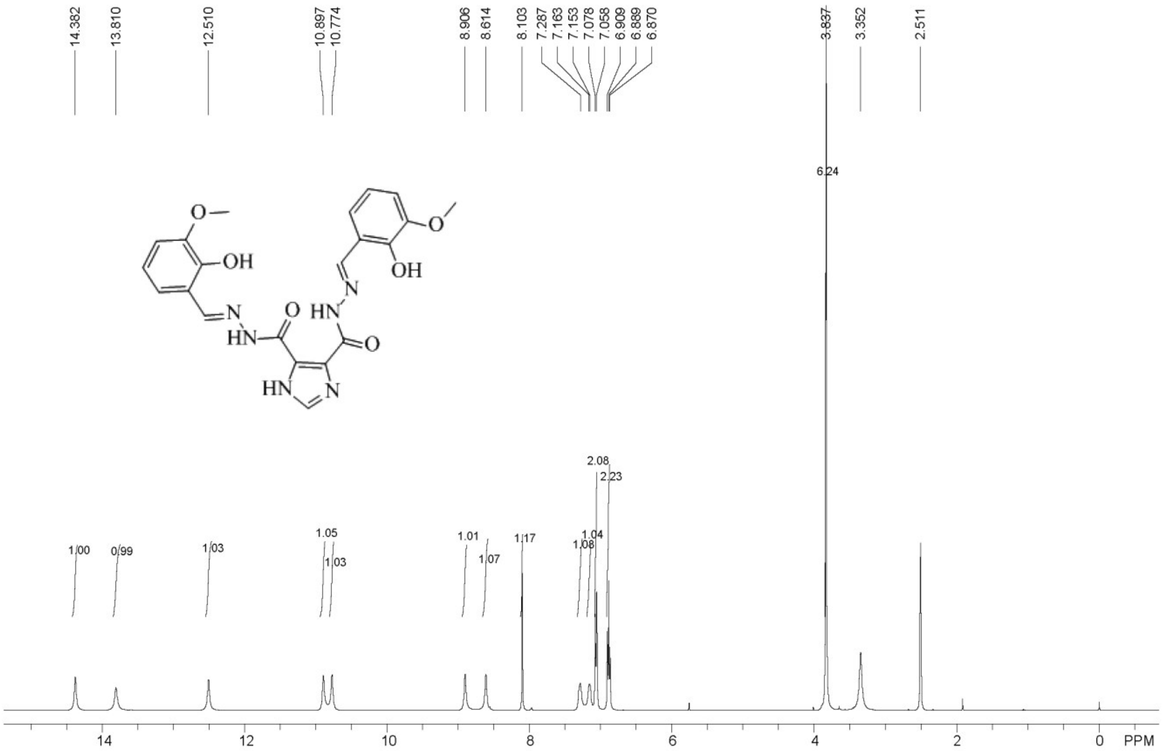


Figure S9 The ^{1}H NMR of H_5ovih.

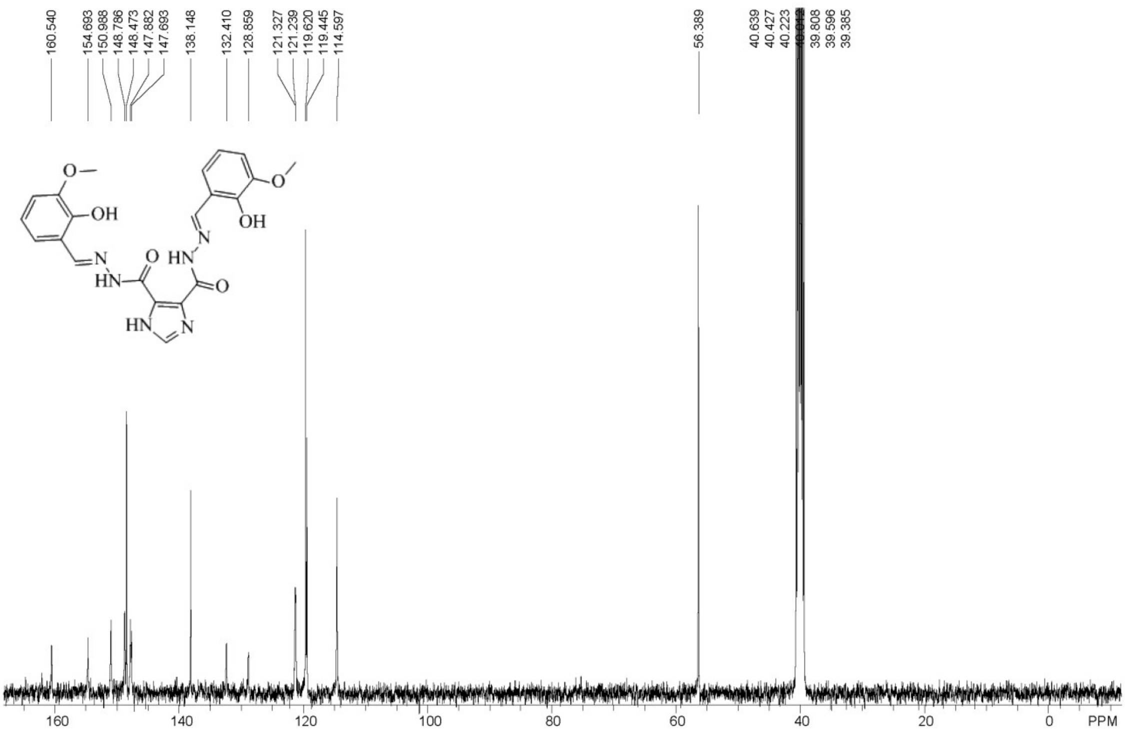


Figure S10 The ^{13}C NMR of H_5ovih.

Table S2 Selected bond lengths (Å) and angles (°) for **1-3**

1			
Gd(1)-O(2)	2.347(3)	Gd(1)-O(8)	2.375(3)
Gd(1)-O(7)	2.411(3)	Gd(1)-O(9)	2.421(3)
Gd(1)-O(1)	2.435(3)	Gd(1)-O(10)	2.512(3)
Gd(1)-O(1W)	2.503(3)	Gd(1)-O(12)	2.515(3)
Gd(1)-N(4)	2.556(4)	Gd(1)-N(7)	2.929(4)
Gd(2)-O(9)	2.401(3)	Gd(2)-O(3W)	2.426(3)
Gd(2)-O(2W)	2.438(3)	Gd(2)-O(4)	2.439(3)
Gd(2)-O(1)	2.455(3)	Gd(2)-O(13)	2.478(4)
Gd(2)-N(2)	2.529(3)	Gd(2)-N(1)	2.529(3)
Gd(2)-O(15)	2.614(3)	Gd(2)-N(8)	2.955(4)
Gd(3)-O(7)	2.342(3)	Gd(3)-O(6W)	2.362(3)
Gd(3)-O(5)	2.359(3)	Gd(3)-O(8)	2.380(3)
Gd(3)-O(4)	2.386(3)	Gd(3)-O(9)	2.434(3)
Gd(3)-O(5W)	2.510(3)	Gd(3)-N(6)	2.543(4)
Gd(3)-O(4W)	2.608(4)	Gd(4)-O(5)	2.328(3)
Gd(4)-O(8)	2.388(3)	Gd(4)-O(2)	2.385(3)
Gd(4)-O(7)	2.406(3)	Gd(4)-O(8W)	2.417(3)
Gd(4)-O(7W)	2.429(3)	Gd(4)-O(18)	2.463(3)
Gd(4)-O(16)	2.554(4)	Gd(4)-O(6)	2.667(3)
Gd(4)-N(9)	2.903(4)	O(2)-Gd(1)-O(8)	76.89(10)
O(2)-Gd(1)-O(7)	71.26(11)	O(8)-Gd(1)-O(7)	59.66(9)
O(2)-Gd(1)-O(9)	144.39(10)	O(8)-Gd(1)-O(9)	75.91(9)
O(7)-Gd(1)-O(9)	75.31(10)	O(2)-Gd(1)-O(1)	127.64(10)
O(8)-Gd(1)-O(1)	74.21(9)	O(7)-Gd(1)-O(1)	124.74(10)
O(9)-Gd(1)-O(1)	64.83(9)	O(2)-Gd(1)-O(10)	121.39(11)
O(8)-Gd(1)-O(10)	145.17(10)	O(7)-Gd(1)-O(10)	150.36(11)
O(9)-Gd(1)-O(10)	93.89(10)	O(1)-Gd(1)-O(10)	71.36(10)
O(2)-Gd(1)-O(1W)	104.69(11)	O(8)-Gd(1)-O(1W)	132.71(10)
O(7)-Gd(1)-O(1W)	75.85(11)	O(9)-Gd(1)-O(1W)	78.21(10)
O(1)-Gd(1)-O(1W)	126.99(10)	O(10)-Gd(1)-O(1W)	74.93(11)
O(2)-Gd(1)-O(12)	73.21(10)	O(8)-Gd(1)-O(12)	146.06(10)
O(7)-Gd(1)-O(12)	122.64(10)	O(9)-Gd(1)-O(12)	137.82(10)
O(1)-Gd(1)-O(12)	112.59(10)	O(10)-Gd(1)-O(12)	50.58(10)
O(1W)-Gd(1)-O(12)	71.49(11)	O(2)-Gd(1)-N(4)	71.12(11)
O(8)-Gd(1)-N(4)	83.68(10)	O(7)-Gd(1)-N(4)	132.09(11)
O(9)-Gd(1)-N(4)	127.44(10)	O(1)-Gd(1)-N(4)	63.12(10)
O(10)-Gd(1)-N(4)	76.37(11)	O(1W)-Gd(1)-N(4)	142.56(11)
O(12)-Gd(1)-N(4)	71.80(11)	O(2)-Gd(1)-N(7)	97.89(11)
O(8)-Gd(1)-N(7)	158.04(11)	O(7)-Gd(1)-N(7)	139.37(11)
O(9)-Gd(1)-N(7)	115.64(11)	O(1)-Gd(1)-N(7)	93.36(11)
O(10)-Gd(1)-N(7)	25.50(11)	O(1W)-Gd(1)-N(7)	69.22(11)

O(12)-Gd(1)-N(7)	25.25(10)	N(4)-Gd(1)-N(7)	74.50(11)
O(9)-Gd(2)-O(3W)	142.58(10)	O(9)-Gd(2)-O(2W)	84.08(10)
O(3W)-Gd(2)-O(2W)	75.41(10)	O(9)-Gd(2)-O(4)	65.96(9)
O(3W)-Gd(2)-O(4)	135.09(10)	O(2W)-Gd(2)-O(4)	148.38(10)
O(9)-Gd(2)-O(1)	64.81(9)	O(3W)-Gd(2)-O(1)	135.54(10)
O(2W)-Gd(2)-O(1)	75.39(9)	O(4)-Gd(2)-O(1)	82.54(10)
O(9)-Gd(2)-O(13)	91.00(11)	O(3W)-Gd(2)-O(13)	72.86(12)
O(2W)-Gd(2)-O(13)	118.88(11)	O(4)-Gd(2)-O(13)	73.51(11)
O(1)-Gd(2)-O(13)	151.53(11)	O(9)-Gd(2)-N(2)	130.53(10)
O(3W)-Gd(2)-N(2)	76.29(10)	O(2W)-Gd(2)-N(2)	145.24(11)
O(4)-Gd(2)-N(2)	64.86(10)	O(1)-Gd(2)-N(2)	113.13(10)
O(13)-Gd(2)-N(2)	70.37(11)	O(9)-Gd(2)-N(1)	129.27(11)
O(3W)-Gd(2)-N(1)	77.70(11)	O(2W)-Gd(2)-N(1)	79.72(11)
O(4)-Gd(2)-N(1)	110.94(10)	O(1)-Gd(2)-N(1)	64.64(10)
O(13)-Gd(2)-N(1)	138.59(12)	N(2)-Gd(2)-N(1)	74.87(11)
O(9)-Gd(2)-O(15)	70.40(10)	O(3W)-Gd(2)-O(15)	73.61(10)
O(2W)-Gd(2)-O(15)	72.11(11)	O(4)-Gd(2)-O(15)	104.93(10)
O(1)-Gd(2)-O(15)	126.39(10)	O(13)-Gd(2)-O(15)	49.45(11)
N(2)-Gd(2)-O(15)	118.01(11)	N(1)-Gd(2)-O(15)	143.81(10)
O(9)-Gd(2)-N(8)	82.38(10)	O(3W)-Gd(2)-N(8)	69.29(11)
O(2W)-Gd(2)-N(8)	95.93(11)	O(4)-Gd(2)-N(8)	90.11(11)
O(1)-Gd(2)-N(8)	146.57(10)	O(13)-Gd(2)-N(8)	23.69(11)
N(2)-Gd(2)-N(8)	92.56(11)	N(1)-Gd(2)-N(8)	146.67(11)
O(15)-Gd(2)-N(8)	25.93(11)	O(7)-Gd(3)-O(6W)	79.49(11)
O(7)-Gd(3)-O(5)	73.89(10)	O(6W)-Gd(3)-O(5)	71.03(11)
O(7)-Gd(3)-O(8)	60.55(10)	O(6W)-Gd(3)-O(8)	129.68(10)
O(5)-Gd(3)-O(8)	69.48(10)	O(7)-Gd(3)-O(4)	129.95(10)
O(6W)-Gd(3)-O(4)	149.85(11)	O(5)-Gd(3)-O(4)	118.70(10)
O(8)-Gd(3)-O(4)	78.31(10)	O(7)-Gd(3)-O(9)	76.31(10)
O(6W)-Gd(3)-O(9)	125.50(10)	O(5)-Gd(3)-O(9)	141.99(10)
O(8)-Gd(3)-O(9)	75.55(9)	O(4)-Gd(3)-O(9)	66.27(9)
O(7)-Gd(3)-O(5W)	142.78(12)	O(6W)-Gd(3)-O(5W)	76.45(11)
O(5)-Gd(3)-O(5W)	122.76(12)	O(8)-Gd(3)-O(5W)	152.96(10)
O(4)-Gd(3)-O(5W)	74.74(11)	O(9)-Gd(3)-O(5W)	95.21(11)
O(7)-Gd(3)-N(6)	139.10(11)	O(6W)-Gd(3)-N(6)	99.35(11)
O(5)-Gd(3)-N(6)	67.37(10)	O(8)-Gd(3)-N(6)	93.07(10)
O(4)-Gd(3)-N(6)	63.86(10)	O(9)-Gd(3)-N(6)	130.12(10)
O(5W)-Gd(3)-N(6)	73.29(12)	O(7)-Gd(3)-O(4W)	81.83(13)
O(6W)-Gd(3)-O(4W)	70.06(12)	O(5)-Gd(3)-O(4W)	137.06(12)
O(8)-Gd(3)-O(4W)	126.61(11)	O(4)-Gd(3)-O(4W)	104.09(12)
O(9)-Gd(3)-O(4W)	58.71(11)	O(5W)-Gd(3)-O(4W)	63.47(14)
N(6)-Gd(3)-O(4W)	136.73(13)	O(5)-Gd(4)-O(8)	69.86(10)
O(5)-Gd(4)-O(2)	139.29(10)	O(8)-Gd(4)-O(2)	75.91(9)
O(5)-Gd(4)-O(7)	73.26(10)	O(8)-Gd(4)-O(7)	59.56(9)

O(2)-Gd(4)-O(7)	70.70(10)	O(5)-Gd(4)-O(8W)	134.92(11)
O(8)-Gd(4)-O(8W)	144.71(11)	O(2)-Gd(4)-O(8W)	85.72(11)
O(7)-Gd(4)-O(8W)	140.77(11)	O(5)-Gd(4)-O(7W)	103.90(11)
O(8)-Gd(4)-O(7W)	132.86(10)	O(2)-Gd(4)-O(7W)	83.61(10)
O(7)-Gd(4)-O(7W)	73.72(10)	O(8W)-Gd(4)-O(7W)	72.84(11)
O(5)-Gd(4)-O(18)	75.88(11)	O(8)-Gd(4)-O(18)	89.26(10)
O(2)-Gd(4)-O(18)	125.68(11)	O(7)-Gd(4)-O(18)	141.99(10)
O(8W)-Gd(4)-O(18)	77.24(11)	O(7W)-Gd(4)-O(18)	135.98(11)
O(5)-Gd(4)-O(16)	113.58(12)	O(8)-Gd(4)-O(16)	74.97(11)
O(2)-Gd(4)-O(16)	76.72(12)	O(7)-Gd(4)-O(16)	128.74(11)
O(8W)-Gd(4)-O(16)	71.57(12)	O(7W)-Gd(4)-O(16)	140.27(12)
O(18)-Gd(4)-O(16)	48.97(12)	O(5)-Gd(4)-O(6)	61.75(10)
O(8)-Gd(4)-O(6)	130.98(9)	O(2)-Gd(4)-O(6)	150.83(9)
O(7)-Gd(4)-O(6)	110.36(10)	O(8W)-Gd(4)-O(6)	75.96(11)
O(7W)-Gd(4)-O(6)	69.48(10)	O(18)-Gd(4)-O(6)	72.46(11)
O(16)-Gd(4)-O(6)	117.22(12)	O(5)-Gd(4)-N(9)	94.59(12)
O(8)-Gd(4)-N(9)	81.24(11)	O(2)-Gd(4)-N(9)	101.43(12)
O(7)-Gd(4)-N(9)	140.80(11)	O(8W)-Gd(4)-N(9)	73.10(12)
O(7W)-Gd(4)-N(9)	145.05(11)	O(18)-Gd(4)-N(9)	24.26(11)
O(16)-Gd(4)-N(9)	24.71(12)	O(6)-Gd(4)-N(9)	94.81(12)

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Tb(1)-N(4)	2.553(4)	Tb(1)-O(1)	2.429(3)
Tb(1)-O(2)	2.327(3)	Tb(1)-O(7)	2.398(3)
Tb(1)-O(8)	2.345(3)	Tb(1)-O(9)	2.402(3)
Tb(1)-O(10)	2.499(3)	Tb(1)-O(12)	2.499(3)
Tb(1)-O(1W)	2.456(4)	Tb(2)-N(1)	2.498(3)
Tb(2)- N(2)	2.549(3)	Tb(2)-O(1)	2.428(3)
Tb(2)-O(4)	2.424(3)	Tb(2)-O(9)	2.370(3)
Tb(2)-O(13)	2.478(3)	Tb(2)-O(13)	2.478(3)
Tb(2)-O(2W)	2.423(3)	Tb(2)-O(3W)	2.396(3)
Tb(3)-N(6)	2.524(4)	Tb(3)-O(4)	2.381(3)
Tb(3)-O(5)	2.317(3)	Tb(3)-O(7)	2.335(3)
Tb(3)-O(8)	2.395(3)	Tb(3)-O(9)	2.430(3)
Tb(3)-O(6W)	2.411(3)	Tb(3)-O(4W)	2.4651(11)
Tb(3)-O(5W)	2.478(3)	Tb(4)-O(2)	2.379(3)
Tb(4)-O(5)	2.322(3)	Tb(4)-O(6)	2.644(3)
Tb(4)-O(7)	2.389(3)	Tb(4)-O(8)	2.384(3)
Tb(4)-O(16)	2.532(3)	Tb(4)-O(18)	2.431(4)
Tb(4)-O(7W)	2.413(3)	Tb(4)-O(8W)	2.422(4)
O(2)-Tb(1)-O(8)	77.29(10)	O(2)-Tb(1)-O(7)	71.67(10)
O(8)-Tb(1)-O(7)	60.89(10)	O(2)-Tb(1)-O(9)	145.19(10)
O(8)-Tb(1)-O(9)	76.28(10)	O(7)-Tb(1)-O(9)	75.83(10)
O(2)-Tb(1)-O(1)	128.19(10)	O(8)-Tb(1)-O(1)	73.76(9)

O(7)-Tb(1)-O(1)	124.88(10)	O(9)-Tb(1)-O(1)	63.83(9)
O(2)-Tb(1)-O(1W)	107.00(14)	O(8)-Tb(1)-O(1W)	133.72(11)
O(7)-Tb(1)-O(1W)	76.51(12)	O(9)-Tb(1)-O(1W)	76.58(13)
O(1)-Tb(1)-O(1W)	124.11(14)	O(2)-Tb(1)-O(10)	121.16(10)
O(8)-Tb(1)-O(10)	143.71(10)	O(7)-Tb(1)-O(10)	150.64(11)
O(9)-Tb(1)-O(10)	93.42(10)	O(1)-Tb(1)-O(10)	70.53(10)
O(1W)-Tb(1)-O(10)	74.42(13)	O(2)-Tb(1)-O(12)	73.40(11)
O(8)-Tb(1)-O(12)	146.03(11)	O(7)-Tb(1)-O(12)	122.95(10)
O(9)-Tb(1)-O(12)	137.25(11)	O(1)-Tb(1)-O(12)	112.17(10)
O(1W)-Tb(1)-O(12)	72.45(12)	O(10)-Tb(1)-O(12)	50.35(10)
O(2)-Tb(1)-N(4)	71.24(11)	O(8)-Tb(1)-N(4)	82.91(10)
O(7)-Tb(1)-N(4)	132.60(11)	O(9)-Tb(1)-N(4)	126.70(10)
O(1)-Tb(1)-N(4)	63.36(10)	O(1W)-Tb(1)-N(4)	142.96(12)
O(10)-Tb(1)-N(4)	75.67(11)	O(12)-Tb(1)-N(4)	71.75(11)
O(9)-Tb(2)-O(3W)	142.88(11)	O(9)-Tb(2)-O(4)	66.28(9)
O(3W)-Tb(2)-O(4)	136.46(11)	O(9)-Tb(2)-O(2W)	83.09(10)
O(3W)-Tb(2)-O(2W)	75.00(11)	O(4)-Tb(2)-O(2W)	147.64(10)
O(9)-Tb(2)-O(1)	64.33(9)	O(3W)-Tb(2)-O(1)	133.85(10)
O(4)-Tb(2)-O(1)	82.72(10)	O(2W)-Tb(2)-O(1)	74.42(10)
O(9)-Tb(2)-O(13)	91.19(10)	O(3W)-Tb(2)-O(13)	74.78(11)
O(4)-Tb(2)-O(13)	73.22(11)	O(2W)-Tb(2)-O(13)	119.55(11)
O(1)-Tb(2)-O(13)	151.26(10)	O(9)-Tb(2)-N(1)	129.38(10)
O(3W)-Tb(2)-N(1)	75.91(11)	O(4)-Tb(2)-N(1)	111.29(10)
O(2W)-Tb(2)-N(1)	79.67(11)	O(1)-Tb(2)-N(1)	65.26(10)
O(13)-Tb(2)-N(1)	138.37(11)	O(9)-Tb(2)-N(2)	131.38(10)
O(3W)-Tb(2)-N(2)	76.66(11)	O(4)-Tb(2)-N(2)	65.35(10)
O(2W)-Tb(2)-N(2)	145.29(11)	O(1)-Tb(2)-N(2)	113.41(10)
O(13)-Tb(2)-N(2)	70.63(11)	N(1)-Tb(2)-N(2)	74.32(10)
O(9)-Tb(2)-O(15)	71.32(10)	O(3W)-Tb(2)-O(15)	73.64(11)
O(4)-Tb(2)-O(15)	105.32(11)	O(2W)-Tb(2)-O(15)	72.45(12)
O(1)-Tb(2)-O(15)	126.79(10)	O(13)-Tb(2)-O(15)	49.25(11)
N(1)-Tb(2)-O(15)	142.92(11)	N(2)-Tb(2)-O(15)	117.66(11)
O(5)-Tb(3)-O(7)	73.99(10)	O(5)-Tb(3)-O(4)	119.08(10)
O(7)-Tb(3)-O(4)	130.41(10)	O(5)-Tb(3)-O(8)	70.24(10)
O(7)-Tb(3)-O(8)	61.08(10)	O(4)-Tb(3)-O(8)	78.16(10)
O(5)-Tb(3)-O(6W)	71.16(12)	O(7)-Tb(3)-O(6W)	80.82(11)
O(4)-Tb(3)-O(6W)	148.03(11)	O(8)-Tb(3)-O(6W)	131.47(11)
O(5)-Tb(3)-O(9)	142.05(10)	O(7)-Tb(3)-O(9)	76.48(10)
O(4)-Tb(3)-O(9)	66.01(9)	O(8)-Tb(3)-O(9)	74.85(9)
O(6W)-Tb(3)-O(9)	126.50(11)	O(5)-Tb(3)-O(4W)	133.05(15)
O(7)-Tb(3)-O(4W)	81.0(2)	O(4)-Tb(3)-O(4W)	107.47(16)
O(8)-Tb(3)-O(4W)	128.69(17)	O(6W)-Tb(3)-O(4W)	66.02(14)
O(9)-Tb(3)-O(4W)	62.98(13)	O(5)-Tb(3)-O(5W)	121.35(12)
O(7)-Tb(3)-O(5W)	142.05(13)	O(4)-Tb(3)-O(5W)	75.72(11)

O(8)-Tb(3)-O(5W)	153.75(11)	O(6W)-Tb(3)-O(5W)	73.67(12)
O(9)-Tb(3)-O(5W)	96.58(12)	O(4W)-Tb(3)-O(5W)	63.2(2)
O(5)-Tb(3)-N(6)	67.50(11)	O(7)-Tb(3)-N(6)	139.55(12)
O(4)-Tb(3)-N(6)	64.16(11)	O(8)-Tb(3)-N(6)	93.75(11)
O(6W)-Tb(3)-N(6)	97.65(12)	O(9)-Tb(3)-N(6)	130.16(10)
O(4W)-Tb(3)-N(6)	135.5(2)	O(5W)-Tb(3)-N(6)	72.59(14)
O(5)-Tb(4)-O(7)	72.89(10)	O(5)-Tb(4)-O(2)	139.06(10)
O(7)-Tb(4)-O(2)	70.94(10)	O(5)-Tb(4)-O(8)	70.34(10)
O(7)-Tb(4)-O(8)	60.47(10)	O(2)-Tb(4)-O(8)	75.54(9)
O(5)-Tb(4)-O(8W)	135.85(11)	O(7)-Tb(4)-O(8W)	139.26(11)
O(2)-Tb(4)-O(8W)	84.95(11)	O(8)-Tb(4)-O(8W)	144.48(11)
O(5)-Tb(4)-O(7W)	104.11(11)	O(7)-Tb(4)-O(7W)	73.25(11)
O(2)-Tb(4)-O(7W)	83.21(11)	O(8)-Tb(4)-O(7W)	133.12(11)
O(8W)-Tb(4)-O(7W)	71.64(13)	O(5)-Tb(4)-O(18)	76.00(12)
O(7)-Tb(4)-O(18)	142.61(11)	O(2)-Tb(4)-O(18)	126.38(12)
O(8)-Tb(4)-O(18)	89.85(11)	O(8W)-Tb(4)-O(18)	78.10(12)
O(7W)-Tb(4)-O(18)	135.31(12)	O(5)-Tb(4)-O(16)	114.74(11)
O(7)-Tb(4)-O(16)	128.58(10)	O(2)-Tb(4)-O(16)	75.54(11)
O(8)-Tb(4)-O(16)	74.23(10)	O(8W)-Tb(4)-O(16)	72.28(12)
O(7W)-Tb(4)-O(16)	139.33(12)	O(18)-Tb(4)-O(16)	50.86(12)
O(5)-Tb(4)-O(6)	62.15(10)	O(7)-Tb(4)-O(6)	109.76(11)
O(2)-Tb(4)-O(6)	150.38(10)	O(8)-Tb(4)-O(6)	131.81(9)
O(8W)-Tb(4)-O(6)	76.11(11)	O(7W)-Tb(4)-O(6)	69.40(12)
O(18)-Tb(4)-O(6)	71.97(13)	O(16)-Tb(4)-O(6)	118.51(12)

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Dy(1)-O(2)	2.328(4)	Dy(1)-O(8)	2.332(4)
Dy(1)-O(7)	2.366(4)	Dy(1)-O(9)	2.386(4)
Dy(1)-O(1)	2.426(4)	Dy(1)-O(10)	2.486(4)
Dy(1)-O(1W)	2.503(5)	Dy(1)-O(12)	2.500(4)
Dy(1)-N(4)	2.554(5)	Dy(2)-O(9)	2.377(4)
Dy(2)-O(2W)	2.402(4)	Dy(2)-O(1)	2.411(4)
Dy(2)-O(4)	2.417(4)	Dy(2)-O(3W)	2.411(4)
Dy(2)-O(13)	2.448(5)	Dy(2)-N(1)	2.509(5)
Dy(2)-N(2)	2.542(5)	Dy(2)-O(15)	2.556(4)
Dy(3)-O(7)	2.306(4)	Dy(3)-O(5)	2.315(4)
Dy(3)-O(4)	2.365(4)	Dy(3)-O(8)	2.376(4)
Dy(3)-O(6W)	2.415(4)	Dy(3)-O(9)	2.421(4)
Dy(3)-N(6)	2.522(5)	Dy(3)-O(5W)	2.522(4)
Dy(3)-O(4W)	2.555(6)	Dy(4)-O(5)	2.297(4)
Dy(4)-O(2)	2.350(4)	Dy(4)-O(8)	2.370(4)
Dy(4)-O(7)	2.387(4)	Dy(4)-O(7W)	2.408(4)
Dy(4)-O(8W)	2.421(4)	Dy(4)-O(18)	2.475(4)
Dy(4)-O(16)	2.498(5)	Dy(4)-O(6)	2.649(4)

O(2)-Dy(1)-O(8)	77.27(14)	O(2)-Dy(1)-O(7)	71.63(14)
O(8)-Dy(1)-O(7)	61.06(14)	O(2)-Dy(1)-O(9)	145.11(14)
O(8)-Dy(1)-O(9)	76.97(13)	O(7)-Dy(1)-O(9)	75.45(13)
O(2)-Dy(1)-O(1)	128.52(14)	O(8)-Dy(1)-O(1)	73.60(14)
O(7)-Dy(1)-O(1)	124.62(14)	O(9)-Dy(1)-O(1)	64.30(13)
O(2)-Dy(1)-O(10)	121.94(15)	O(8)-Dy(1)-O(10)	143.77(14)
O(7)-Dy(1)-O(10)	149.89(15)	O(9)-Dy(1)-O(10)	92.55(14)
O(1)-Dy(1)-O(10)	70.64(14)	O(2)-Dy(1)-O(1W)	108.56(16)
O(8)-Dy(1)-O(1W)	133.08(15)	O(7)-Dy(1)-O(1W)	76.40(15)
O(9)-Dy(1)-O(1W)	73.87(15)	O(1)-Dy(1)-O(1W)	122.41(16)
O(10)-Dy(1)-O(1W)	73.73(15)	O(2)-Dy(1)-O(12)	73.69(15)
O(8)-Dy(1)-O(12)	147.17(15)	O(7)-Dy(1)-O(12)	121.48(14)
O(9)-Dy(1)-O(12)	135.73(14)	O(1)-Dy(1)-O(12)	113.89(14)
O(10)-Dy(1)-O(12)	51.25(14)	O(1W)-Dy(1)-O(12)	71.96(15)
O(2)-Dy(1)-N(4)	71.28(16)	O(8)-Dy(1)-N(4)	83.16(15)
O(7)-Dy(1)-N(4)	132.87(16)	O(9)-Dy(1)-N(4)	127.84(15)
O(1)-Dy(1)-N(4)	63.92(15)	O(10)-Dy(1)-N(4)	76.21(16)
O(1W)-Dy(1)-N(4)	143.59(16)	O(12)-Dy(1)-N(4)	73.34(16)
O(9)-Dy(2)-O(2W)	82.61(13)	O(9)-Dy(2)-O(1)	64.67(13)
O(2W)-Dy(2)-O(1)	74.77(14)	O(9)-Dy(2)-O(4)	66.47(13)
O(2W)-Dy(2)-O(4)	147.22(13)	O(1)-Dy(2)-O(4)	82.08(14)
O(9)-Dy(2)-O(3W)	144.37(15)	O(2W)-Dy(2)-O(3W)	80.61(16)
O(1)-Dy(2)-O(3W)	138.17(16)	O(4)-Dy(2)-O(3W)	131.19(16)
O(9)-Dy(2)-O(13)	92.62(15)	O(2W)-Dy(2)-O(13)	119.93(16)
O(1)-Dy(2)-O(13)	152.32(15)	O(4)-Dy(2)-O(13)	73.99(15)
O(3W)-Dy(2)-O(13)	69.49(16)	O(9)-Dy(2)-N(1)	130.06(15)
O(2W)-Dy(2)-N(1)	80.09(15)	O(1)-Dy(2)-N(1)	65.65(15)
O(4)-Dy(2)-N(1)	111.15(14)	O(3W)-Dy(2)-N(1)	77.27(16)
O(13)-Dy(2)-N(1)	136.30(16)	O(9)-Dy(2)-N(2)	131.56(15)
O(2W)-Dy(2)-N(2)	145.63(15)	O(1)-Dy(2)-N(2)	113.05(14)
O(4)-Dy(2)-N(2)	65.40(15)	O(3W)-Dy(2)-N(2)	71.98(17)
O(13)-Dy(2)-N(2)	69.29(15)	N(1)-Dy(2)-N(2)	74.04(15)
O(9)-Dy(2)-O(15)	72.83(14)	O(2W)-Dy(2)-O(15)	72.11(16)
O(1)-Dy(2)-O(15)	128.48(15)	O(4)-Dy(2)-O(15)	106.76(16)
O(3W)-Dy(2)-O(15)	72.17(15)	O(13)-Dy(2)-O(15)	49.82(15)
N(1)-Dy(2)-O(15)	141.31(16)	N(2)-Dy(2)-O(15)	116.68(16)
O(7)-Dy(3)-O(5)	74.27(14)	O(7)-Dy(3)-O(4)	130.19(14)
O(5)-Dy(3)-O(4)	119.03(14)	O(7)-Dy(3)-O(8)	61.28(14)
O(5)-Dy(3)-O(8)	70.07(14)	O(4)-Dy(3)-O(8)	78.02(14)
O(7)-Dy(3)-O(6W)	78.58(15)	O(5)-Dy(3)-O(6W)	72.11(15)
O(4)-Dy(3)-O(6W)	150.07(15)	O(8)-Dy(3)-O(6W)	130.47(15)
O(7)-Dy(3)-O(9)	75.90(14)	O(5)-Dy(3)-O(9)	142.20(14)
O(4)-Dy(3)-O(9)	66.59(13)	O(8)-Dy(3)-O(9)	75.49(13)
O(6W)-Dy(3)-O(9)	123.43(15)	O(7)-Dy(3)-N(6)	139.87(16)

O(5)-Dy(3)-N(6)	67.40(15)	O(4)-Dy(3)-N(6)	64.57(16)
O(8)-Dy(3)-N(6)	93.91(15)	O(6W)-Dy(3)-N(6)	99.94(17)
O(9)-Dy(3)-N(6)	131.15(15)	O(7)-Dy(3)-O(5W)	141.84(16)
O(5)-Dy(3)-O(5W)	124.71(15)	O(4)-Dy(3)-O(5W)	73.50(15)
O(8)-Dy(3)-O(5W)	151.51(14)	O(6W)-Dy(3)-O(5W)	77.65(15)
O(9)-Dy(3)-O(5W)	93.07(15)	N(6)-Dy(3)-O(5W)	73.87(17)
O(7)-Dy(3)-O(4W)	80.4(2)	O(5)-Dy(3)-O(4W)	137.5(2)
O(4)-Dy(3)-O(4W)	103.4(2)	O(8)-Dy(3)-O(4W)	124.9(2)
O(6W)-Dy(3)-O(4W)	69.7(2)	O(9)-Dy(3)-O(4W)	56.80(19)
N(6)-Dy(3)-O(4W)	137.3(2)	O(5W)-Dy(3)-O(4W)	63.5(2)
O(5)-Dy(4)-O(2)	139.56(15)	O(5)-Dy(4)-O(8)	70.47(13)
O(2)-Dy(4)-O(8)	76.09(13)	O(5)-Dy(4)-O(7)	73.07(14)
O(2)-Dy(4)-O(7)	70.87(14)	O(8)-Dy(4)-O(7)	60.22(13)
O(5)-Dy(4)-O(7W)	104.53(15)	O(2)-Dy(4)-O(7W)	82.72(15)
O(8)-Dy(4)-O(7W)	133.83(14)	O(7)-Dy(4)-O(7W)	74.23(14)
O(5)-Dy(4)-O(8W)	135.14(15)	O(2)-Dy(4)-O(8W)	85.23(15)
O(8)-Dy(4)-O(8W)	143.31(15)	O(7)-Dy(4)-O(8W)	141.21(15)
O(7W)-Dy(4)-O(8W)	72.74(16)	O(5)-Dy(4)-O(18)	75.57(16)
O(2)-Dy(4)-O(18)	126.67(17)	O(8)-Dy(4)-O(18)	89.31(15)
O(7)-Dy(4)-O(18)	141.96(15)	O(7W)-Dy(4)-O(18)	135.22(16)
O(8W)-Dy(4)-O(18)	76.83(16)	O(5)-Dy(4)-O(16)	114.45(15)
O(2)-Dy(4)-O(16)	75.63(15)	O(8)-Dy(4)-O(16)	73.51(14)
O(7)-Dy(4)-O(16)	127.62(14)	O(7W)-Dy(4)-O(16)	139.19(16)
O(8W)-Dy(4)-O(16)	71.36(16)	O(18)-Dy(4)-O(16)	51.09(16)
O(5)-Dy(4)-O(6)	61.91(14)	O(2)-Dy(4)-O(6)	149.68(14)
O(8)-Dy(4)-O(6)	131.77(14)	O(7)-Dy(4)-O(6)	109.68(15)
O(7W)-Dy(4)-O(6)	68.96(15)	O(8W)-Dy(4)-O(6)	76.42(15)
O(18)-Dy(4)-O(6)	72.53(17)	O(16)-Dy(4)-O(6)	119.37(15)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y, -z+1

Table S3 Hydrogen-bonding geometries for the ligand.

D–H···A	Symmetry code	D–H(Å)	H···A(Å)	D···A(Å)	D–H···A(°)
N(2)-H(2A)...O(4)		0.88	1.82	2.669(2)	161.4
N(3)-H(3)...O(3)	-x+1,-y,-z+1	0.88	1.94	2.771(2)	157.7
O(2)-H(2)...N(1)		0.84	1.88	2.616(2)	145.0
O(5)-H(5)...N(6)		0.84	1.88	2.609(3)	144.5

Table S4 Coordination sphere of peripheral Ln atoms indicated by the SHAPE program[3].

Metal ions	Coordination Number	Coordination sphere	CShM value	Shape	Symmetry
Gd(1)	9 (NO_8 mode)	MFF-9	22.09008	Muffin	C_s
		CSAPR-9	22.11056	Spherical capped square antiprism	C_{4v}
		TCTPR-9	22.91991	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	23.93726	Capped square antiprism J10	C_{4v}
		JTCTPR-9	25.54826	Tricapped trigonal prism J51	D_{3h}
		HH-9	26.74937	Hula-hoop	C_{2v}
		CCU-9	27.10824	Spherical-relaxed capped cube	C_{4v}
		JCCU-9	28.07256	Capped cube J8	C_{4v}
		JTC-9	28.12732	Johnson triangular cupola J3	C_{3v}
		JTDIC-9	30.89386	Tridiminished icosahedron J63	C_{3v}
		HBPY-9	30.92638	Heptagonal bipyramid	D_{7h}
		OPY-9	35.70801	Octagonal pyramid	C_{8v}
		EP-9	40.37884	Enneagon	D_{9h}
Gd(2)	9 (N_2O_7 mode)	JCSAPR-9	22.53433	Capped square antiprism J10	C_{4v}
		MFF-9	22.82765	Muffin	C_s
		JTCTPR-9	23.11447	Tricapped trigonal prism J51	D_{3h}
		CSAPR-9	23.12328	Spherical capped square antiprism	C_{4v}
		TCTPR-9	23.58377	Spherical tricapped trigonal prism	D_{3h}
		JCCU-9	25.57449	Capped cube J8	C_{4v}
		CCU-9	25.7775	Spherical-relaxed capped cube	C_{4v}
		HH-9	26.48263	Hula-hoop	C_{2v}
		JTC-9	28.54664	Johnson triangular cupola J3	C_{3v}
		JTDIC-9	29.62449	Tridiminished icosahedron J63	C_{3v}
		HBPY-9	34.1006	Heptagonal bipyramid	D_{7h}
		OPY-9	36.09615	Octagonal pyramid	C_{8v}
		EP-9	43.70385	Enneagon	D_{9h}
Gd(3)	9 (NO_8 mode)	MFF-9	21.82866	Muffin	C_s
		CSAPR-9	22.35077	Spherical capped square antiprism	C_{4v}
		JCSAPR-9	22.64098	Capped square antiprism J10	C_{4v}
		JTCTPR-9	22.71645	Tricapped trigonal prism J51	D_{3h}
		TCTPR-9	22.9588	Spherical tricapped trigonal prism	D_{3h}
		JTC-9	23.05172	Johnson triangular cupola J3	C_{3v}
		CCU-9	25.01687	Spherical-relaxed capped cube	C_{4v}
		JCCU-9	25.76126	Capped cube J8	C_{4v}
		HH-9	27.12729	Hula-hoop	C_{2v}
		JTDIC-9	30.33794	Tridiminished icosahedron J63	C_{3v}
		OPY-9	30.73049	Octagonal pyramid	C_{8v}
		HBPY-9	33.68158	Heptagonal bipyramid	D_{7h}
		EP-9	42.91052	Enneagon	D_{9h}
Gd(4)	9 (O_9 mode)	JTCTPR-9	21.40367	Tricapped trigonal prism J51	D_{3h}
		MFF-9	21.49983	Muffin	C_s

		JCSAPR-9	21.59685	Capped square antiprism J10	C_{4v}
		CSAPR-9	21.62744	Spherical capped square antiprism	C_{4v}
		TCTPR-9	22.41307	Spherical tricapped trigonal prism	D_{3h}
		JTC-9	23.50101	Johnson triangular cupola J3	C_{3v}
		JCCU-9	27.46689	Capped cube J8	C_{4v}
		JTDIC-9	27.66357	Tridiminished icosahedron J63	C_{3v}
		CCU-9	27.73131	Spherical-relaxed capped cube	C_{4v}
		HH-9	28.1476	Hula-hoop	C_{2v}
		OPY-9	33.9598	Octagonal pyramid	C_{8v}
		HBPY-9	34.61125	Heptagonal bipyramid	D_{7h}
		EP-9	43.44815	Enneagon	D_{9h}
Tb(1)	9 (NO_8 mode)	CSAPR-9	1.44256	Spherical capped square antiprism	*C4v*
		MFF-9	2.11992	Muffin	C_s
		TCTPR-9	2.40717	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	2.47767	Capped square antiprism J10	C_{4v}
		JTCTPR-9	3.38707	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.90089	Spherical-relaxed capped cube	C_{4v}
		JCCU-9	9.39317	Capped cube J8	C_{4v}
		HH-9	11.05493	Hula-hoop	C_{2v}
		JTDIC-9	12.71984	Tridiminished icosahedron J63	C_{3v}
		JTC-9	14.51745	Johnson triangular cupola J3	C_{3v}
		HBPY-9	15.80814	Heptagonal bipyramid	D_{7h}
		OPY-9	20.20395	Octagonal pyramid	C_{8v}
		EP-9	34.29652	Enneagon	D_{9h}
Tb(2)	9 (N_2O_7 mode)	MFF-9	1.70587	Muffin	C_s
		CSAPR-9	1.96993	Spherical capped square antiprism	C_{4v}
		JCSAPR-9	2.51328	Capped square antiprism J10	C_{4v}
		TCTPR-9	2.95089	Spherical tricapped trigonal prism	D_{3h}
		JTCTPR-9	4.26509	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.40098	Spherical-relaxed capped cube	C_{4v}
		HH-9	8.79849	Hula-hoop	C_{2v}
		JCCU-9	8.85546	Capped cube J8	C_{4v}
		JTDIC-9	11.14905	Tridiminished icosahedron J63	C_{3v}
		JTC-9	16.35569	Johnson triangular cupola J3	C_{3v}
		HBPY-9	17.33882	Heptagonal bipyramid	D_{7h}
		OPY-9	22.89401	Octagonal pyramid	C_{8v}
		EP-9	35.95851	Enneagon	D_{9h}
Tb(3)	9 (NO_8 mode)	MFF-9	1.24294	Muffin	C_s
		CSAPR-9	1.88147	Spherical capped square antiprism	C_{4v}
		TCTPR-9	2.31792	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	3.13503	Capped square antiprism J10	C_{4v}
		JTCTPR-9	4.19352	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.20012	Spherical-relaxed capped cube	C_{4v}

		JCCU-9	8.51408	Capped cube J8	C_{4v}
		HH-9	8.72231	Hula-hoop	C_{2v}
		JTDIC-9	12.11484	Tridiminished icosahedron J63	C_{3v}
		JTC-9	15.71514	Johnson triangular cupola J3	C_{3v}
		HBPY-9	16.14691	Heptagonal bipyramid	D_{7h}
		OPY-9	23.46466	Octagonal pyramid	C_{8v}
		EP-9	35.65003	Enneagon	D_{9h}
Tb(4)	9 (O_9 mode)	MFF-9	1.16671	Muffin	C_s
		CSAPR-9	1.29212	Spherical capped square antiprism	C_{4v}
		JCSAPR-9	2.10467	Capped square antiprism J10	C_{4v}
		TCTPR-9	2.15706	Spherical tricapped trigonal prism	D_{3h}
		JTCTPR-9	3.22025	Tricapped trigonal prism J51	D_{3h}
		CCU-9	9.62056	Spherical-relaxed capped cube	C_{4v}
		HH-9	10.33293	Hula-hoop	C_{2v}
		JCCU-9	10.62396	Capped cube J8	C_{4v}
		JTDIC-9	11.09969	Tridiminished icosahedron J63	C_{3v}
		JTC-9	15.47868	Johnson triangular cupola J3	C_{3v}
		HBPY-9	19.56801	Heptagonal bipyramid	D_{7h}
		OPY-9	22.81858	Octagonal pyramid	C_{8v}
		EP-9	33.97814	Enneagon	D_{9h}
Dy(1)	9 (NO_8 mode)	CSAPR-9	1.3436	Spherical capped square antiprism	C_{4v}
		MFF-9	2.04008	Muffin	C_s
		TCTPR-9	2.23976	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	2.36062	Capped square antiprism J10	C_{4v}
		JTCTPR-9	3.5522	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.68433	Spherical-relaxed capped cube	C_{4v}
		JCCU-9	9.16827	Capped cube J8	C_{4v}
		HH-9	11.21442	Hula-hoop	C_{2v}
		JTDIC-9	12.63875	Tridiminished icosahedron J63	C_{3v}
		JTC-9	15.04718	Johnson triangular cupola J3	C_{3v}
		HBPY-9	15.95916	Heptagonal bipyramid	D_{7h}
		OPY-9	19.98125	Octagonal pyramid	C_{8v}
		EP-9	35.08856	Enneagon	D_{9h}
Dy(2)	9 (N_2O_7 mode)	MFF-9	1.72382	Muffin	C_s
		CSAPR-9	1.83269	Spherical capped square antiprism	C_{4v}
		JCSAPR-9	2.43645	Capped square antiprism J10	C_{4v}
		TCTPR-9	2.48893	Spherical tricapped trigonal prism	D_{3h}
		JTCTPR-9	4.2165	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.87988	Spherical-relaxed capped cube	C_{4v}
		HH-9	8.95358	Hula-hoop	C_{2v}
		JCCU-9	9.20937	Capped cube J8	C_{4v}
		JTDIC-9	10.5208	Tridiminished icosahedron J63	C_{3v}
		JTC-9	16.21003	Johnson triangular cupola J3	C_{3v}

		HBPY-9	16.75571	Heptagonal bipyramid	D_{7h}
		OPY-9	22.34561	Octagonal pyramid	C_{8v}
		EP-9	35.78242	Enneagon	D_{9h}
Dy(3)	9 (NO_8 mode)	MFF-9	1.46539	Muffin	C_s
		CSAPR-9	2.09559	Spherical capped square antiprism	C_{4v}
		TCTPR-9	2.75335	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	3.30091	Capped square antiprism J10	C_{4v}
		JTCTPR-9	4.28724	Tricapped trigonal prism J51	D_{3h}
		CCU-9	7.42348	Spherical-relaxed capped cube	C_{4v}
		JCCU-9	8.57101	Capped cube J8	C_{4v}
		HH-9	8.57839	Hula-hoop	C_{2v}
		JTDIC-9	11.83282	Tridiminished icosahedron J63	C_{3v}
		JTC-9	15.44273	Johnson triangular cupola J3	C_{3v}
		HBPY-9	15.55447	Heptagonal bipyramid	D_{7h}
		OPY-9	22.71552	Octagonal pyramid	C_{8v}
		EP-9	34.81173	Enneagon	D_{9h}
Dy(4)	9 (O_9 mode)	MFF-9	1.19948	Muffin	C_s
		CSAPR-9	1.23661	Spherical capped square antiprism	C_{4v}
		TCTPR-9	2.0785	Spherical tricapped trigonal prism	D_{3h}
		JCSAPR-9	2.10146	Capped square antiprism J10	C_{4v}
		JTCTPR-9	3.20984	Tricapped trigonal prism J51	D_{3h}
		CCU-9	9.77244	Spherical-relaxed capped cube	C_{4v}
		HH-9	10.67888	Hula-hoop	C_{2v}
		JCCU-9	10.81779	Capped cube J8	C_{4v}
		JTDIC-9	11.28638	Tridiminished icosahedron J63	C_{3v}
		JTC-9	15.57416	Johnson triangular cupola J3	C_{3v}
		HBPY-9	19.52953	Heptagonal bipyramid	D_{7h}
		OPY-9	22.72358	Octagonal pyramid	C_{8v}
		EP-9	34.08958	Enneagon	D_{9h}

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