Supporting Information for

Series anionic host coordination polymers based on azoxybenzene carboxylate: structures, luminescence and magnetic properties†

Xun Feng,*[a] Nan Guo[c], Haipeng Chen[a], Helin Wang[a], Lingyun Yue[a], Xin Chen[a], Seik Weng Ng[d], Xinfang Liu[a], Lufang Ma[a], Liya Wang*[b]

[a] College of Chemistry and Chemical Engineering and Henan Key Laboratory of Function Oriented Porous Materials, Luoyang Normal University, Luoyang 471934, China,

[b] School of Life Science and Technology, Nanyang Normal University, Nanyang, 473601, China,

[c] College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou,450001, China

[d] The University of Nottingham Malaysia Campus, 43500, Semenyih, Selangor, Malaysia

1. Reagents, general procedures and physical measurements.

All reagents used in the syntheses were of obtained from commercial sources, and starting materials and reagents were analytical grade. The elemental microanalysis was performed by the North-West University of China, Department of Chemistry. Fourier transform infrared (FT-IR) spectra (4000 ~ 400 cm^{-1}) were measured on a Nicolet Avatar 360 FT-IR spectrometer using KBr pellet samples. Absorptions are described as very strong (vs), strong (s), medium (m), weak (w), shoulder (sh), and broad (br) and stretches (st) are labeled symmetric (s) or asymmetric (as). Magnetic measurements were performed in the temperature range 2-300 K, using a Quantum Design MPMS-XL SQUID magnetometer equipped with a 0.1 T magnet. The diamagnetic corrections for the compounds were estimated using Pascal's constants, and magnetic data were corrected for diamagnetic contributions of the sample holder.

Materials

The lanthanide oxides (Sm, Eu, Gd, Tb, Dy and Er) are 99.9% purity, H_4aobtc acid and bipy ligands are analytical grade and used as received. The solvents used in this study were either AR or spectroscopic grade.

Methods

Thermogravimetry and differential thermal analysis were recorded using a SDT 2960 simultaneous thermal analyzer (DTA Instruments, New Castle, DE) in N_2 atmosphere. The powder X-ray diffraction (PXRD) patterns were measured using a Bruker D8 Advance powder diffractometer at 40 kV, 40 mA for Cu Kα radiation (λ = 1.5418 Å), with a scan speed of 0.2 s/step and a step size of 0.02 (2θ). UV-visible spectra were recorded at 25 °C by a Shimadzu Model 1601 spectrophotometer, in quartz cells of 1 cm, using DMF as a solvent. Luminescence spectra of the polymers in a 1 cm quartz spectrophotometer fluorescence cell (Starna) in methanol were run on a Cary Eclipse fluorescence spectrophotometer. Steady state emission and excitation spectra were recorded on a F7000 spectrofluorimeter equipped with a 450 W xenon lamp as the excitation source.

Syntheses of polymers 2-6

The same procedure for polymer **1** was employed in preparation coordination polymers **2-6**. Ligand bipy (0.1 mmol, 0.016 g) and 0.1 mmol of lanthanide(III) nitrate hexahydrate, (**2**) = $Eu(NO_3)_3{\cdot}6H_2O$, 0.044 g; (**3**)= $Gd(NO_3)_3{\cdot}5H_2O$, 0.044 g; (**4**) = $Tb(NO_3)_3{\cdot}6H_2O$, 0.047 g; (**5**)= $Dy(NO_3)_3{\cdot}6H_2O$ g; (**6**)= $Er(NO_3)_3{\cdot}6H_2O$, 0.047, 0.045g) were mixed in an ethanol-water solution (10 mL) of H_4aobtc acid (0.05 mmol, 0.020 g). After stirring for 30 min in air, the aqueous mixture was placed into 25 mL Teflon-lined autoclave under autogenous pressure being heated at 150 °C for 90 h, and then the autoclave was cooled over a period of 24 h at a rate 5 °C/h. Light brown crystals of (**2**) were obtained suitable for X-ray diffraction analysis. For (**2**), yield: 0.0395 g (50%). Elemental analysis (%): calcd for $C_{26}H_{25}N_4O_{14}Eu$: C 40.58, H 3.27, N 7.28, found: C 40.96, H 3.29, N 7.30. IR: 3046br, 2418m, 1618s, 1446vs, 1379m, 1078s, 824m. For (**3**), yield: 0.0341 g (43%). Elemental analysis (%): calcd for $C_{26}H_{25}N_4O_{14}Gd$: C 40.27, H 3.12, N 7.22, found: C 40.29, H 3.14, N 7.21. IR: 3325s, 3036br, 2158m, 1656m, 1613sh, 1475vs, 1127m, 1009s, 802s, For (**4**), yield: 0.0298 g (38%). Elemental analysis (%): calcd for $C_{26}H_{25}N_4O_{14}Tb$, C 40.27, H 3.19, N 7.23, found: C 40.22, H 3.21, N 7.19. IR: 3432s, 3327br, 1603s, 1562s, 1374s, 1017s, 929s, 508s. For (**5**), yield: 0.0341 g (43%). Elemental analysis (%): calcd for $C_{26}H_{25}N_4O_{14}Dy$: C 40.27, H 3.19, N 7.23, found: C 39.97, H 3.19, N 7.21. IR: 3215br, 1756s, 1613s, 1572vs, 1009s, 832s, For (**6**), yield: 0.0341 g (43%). Elemental analysis (%): calcd for $C_{26}H_{25}N_4O_{14}Er$: C 39.80, H 3.21, N 7.14, found: C 39.48, H 3.19, N 7.17. IR: 3325s, 3036br, 1756m, 1613vs, 1372s, 1009s, 764sh, 737s.

2 Additional figures

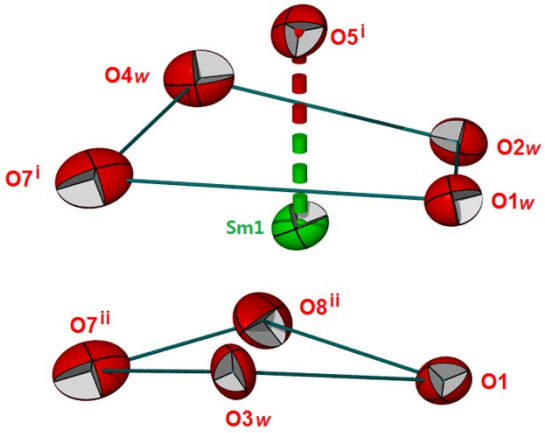


Fig. S1. Coordination environment in **1**

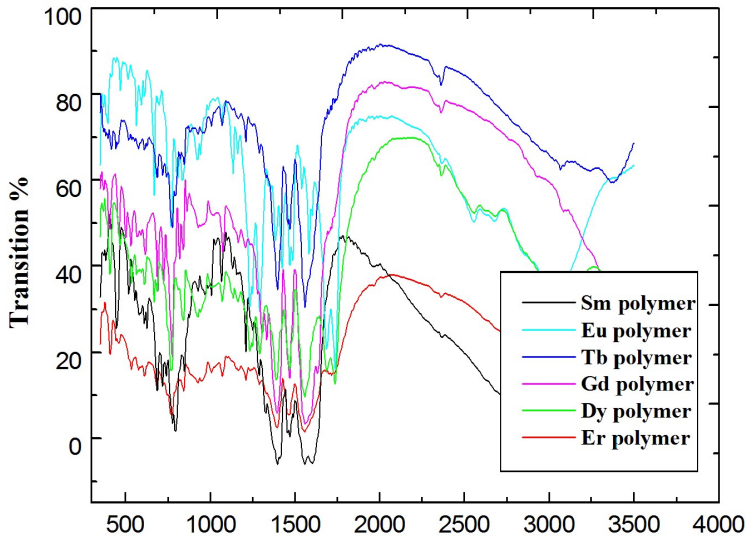


Fig. S2 Fourier transforms infrared spectra of polymers **1- 6**.

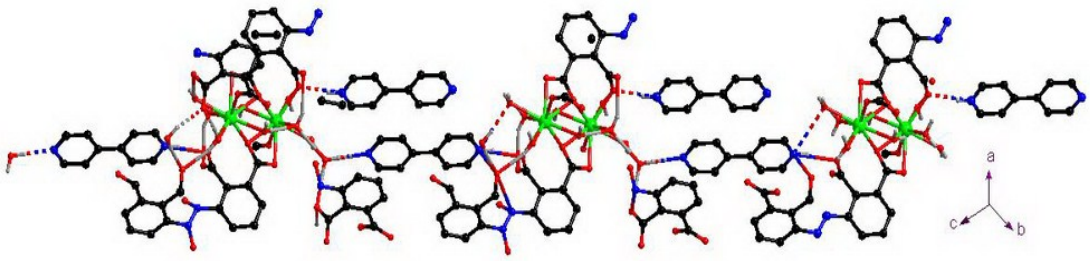


Fig. S3 Illustration of $Hbipy^{+}$ propagating the $\{Sm_2\}$ binuclear units into 1D chain through hydrogen bonding.

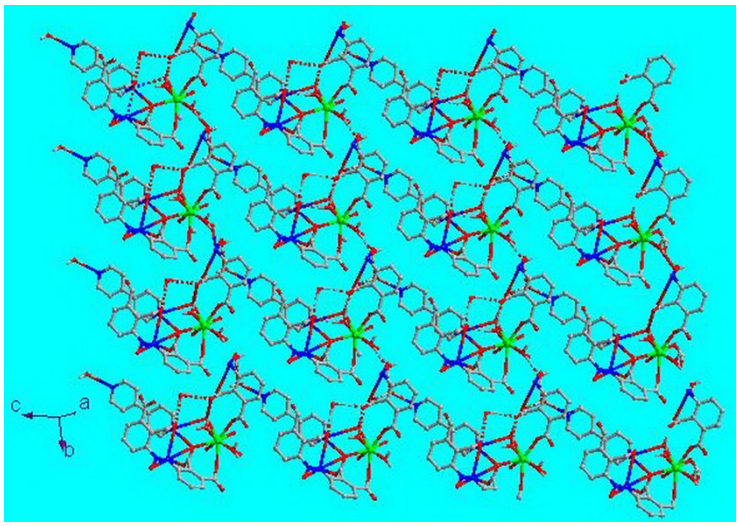


Fig. S4 2D array through the through hydrogen bonding along approximatelyite *bc* plane.

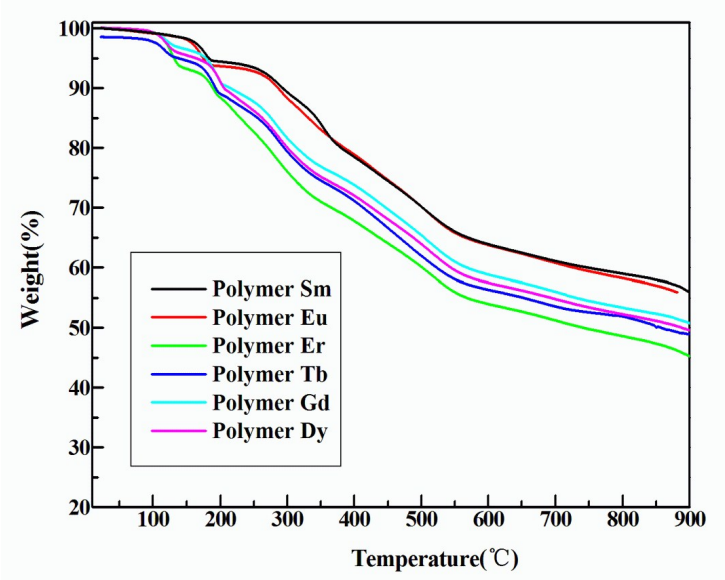


Fig. S5. The TG diagrams of polymers **1-6**

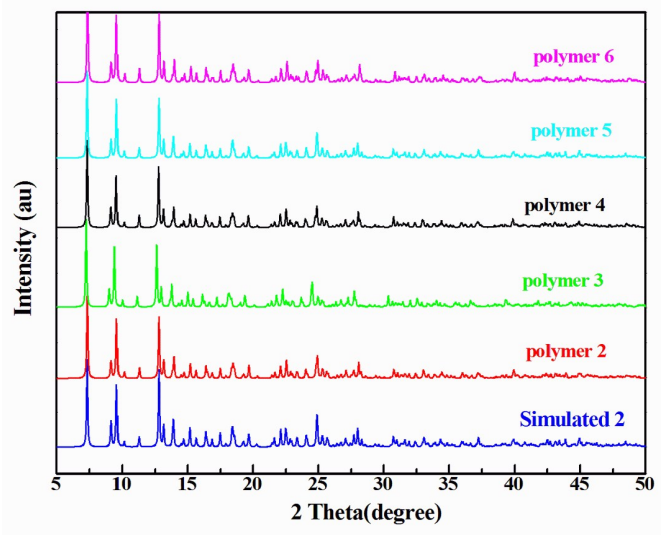


Fig. S6. The simulated (a) and experimental (b) powders XRD patterns of polymers **2-6**.

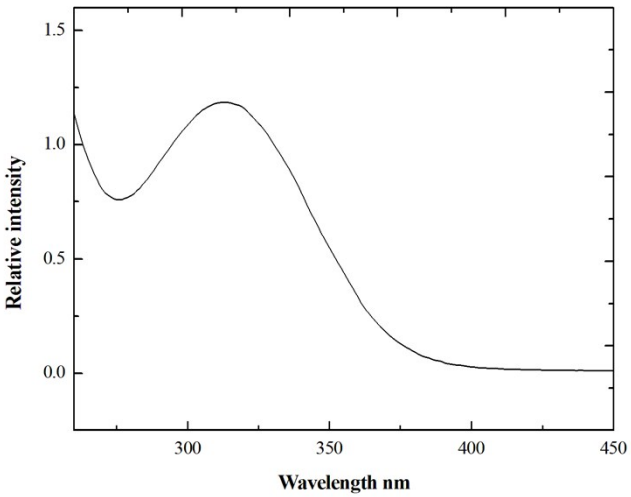


Fig. S7 Uv –vis absorption of the H_4aobtc acid ligand in CH_3OH solution.

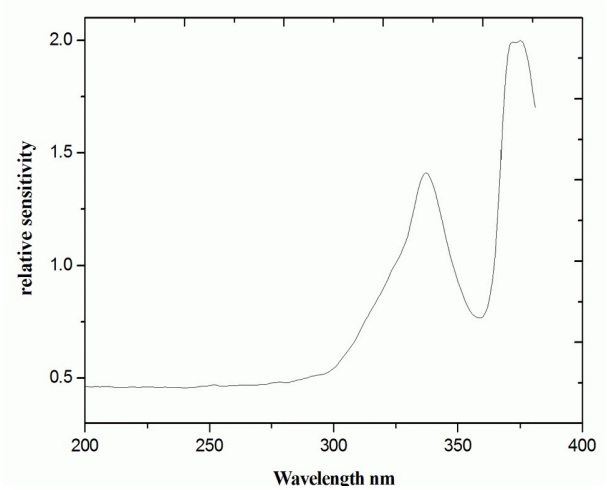


Fig. S8 Uv –vis absorption of the Gd polymer **3**

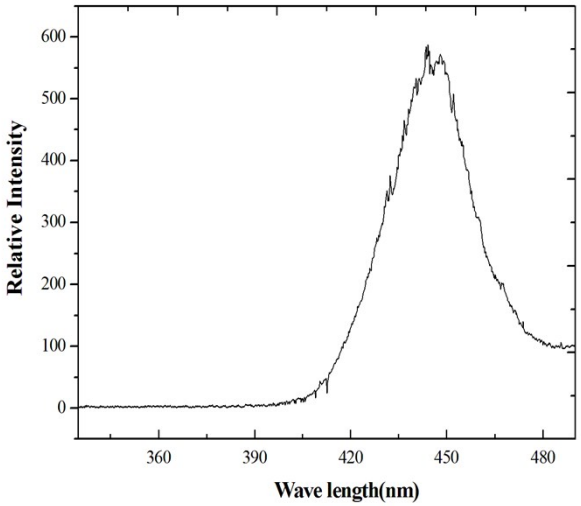


Fig. S9 Phosphorescence spectrum of Gd polymer **3** measured at 77 K in a methanol suspension.

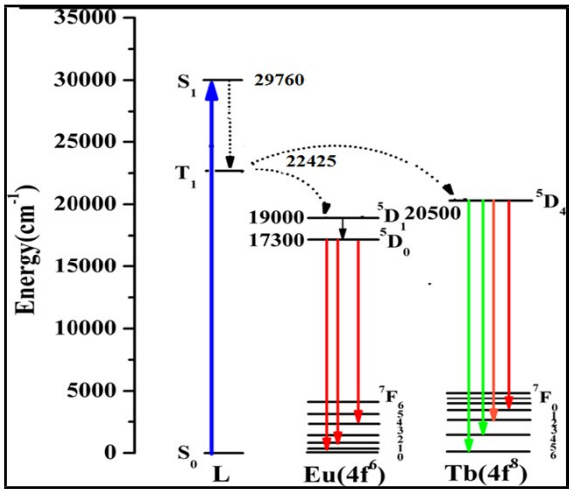
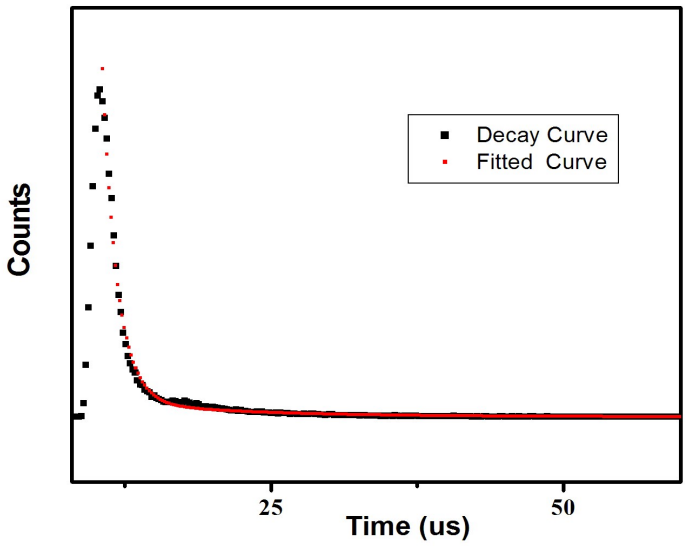
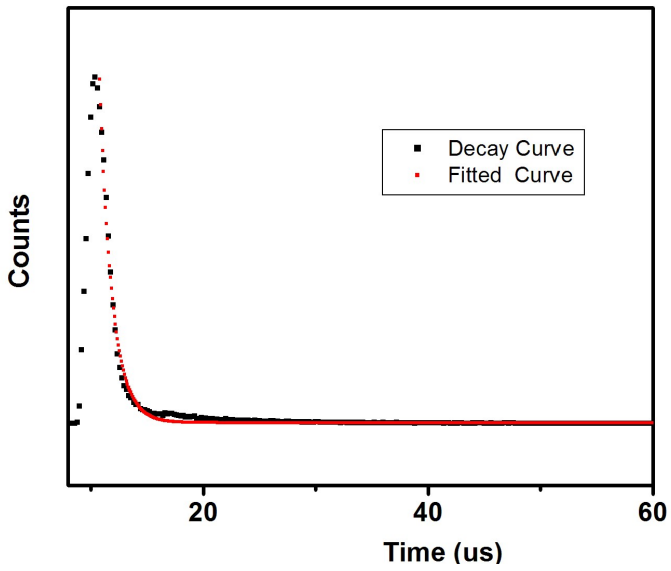


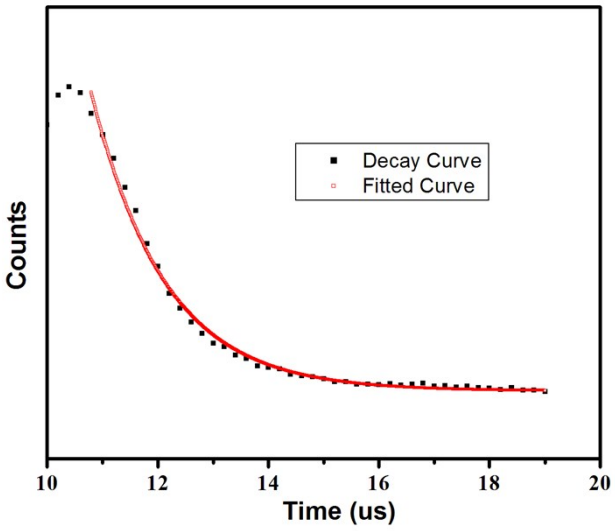
Fig. S10. Energy level scheme showing energy transfer processes in polymers **2** and **4**.



(a)



(b)



(c)

Fig. S11. The decay curves of luminescence intensity for **2** (a), **3** (b) and **4** (c).

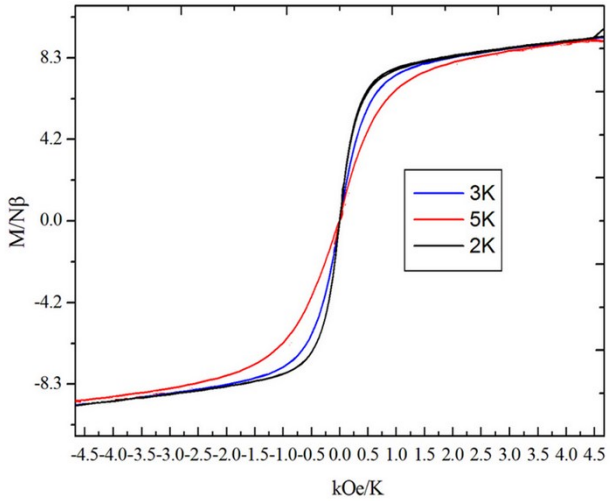


Fig. S12. M versus H data of polymer **5** at 2 K, 3 K and 5 K.

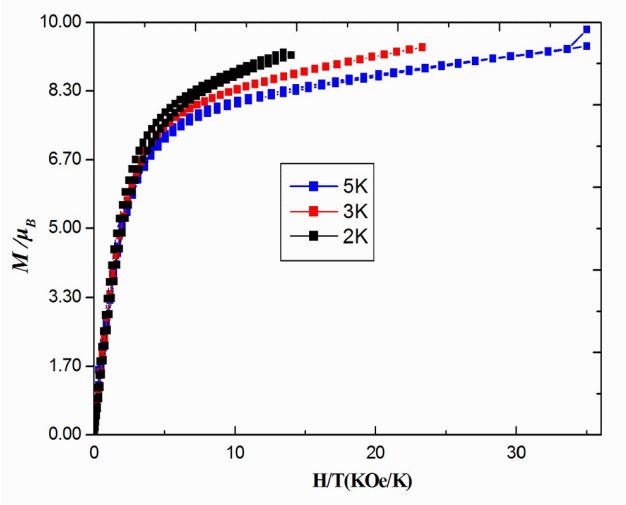


Fig. S13 *M* versus *H* data of **5** at 2, 3 and 5 K.

3 Additional Tables

Table S1 Selected bond distances (Å) and angles (degree) for polymers **1-6**

Polymer 1					
Bond	Å	Bond	Å	Bond	Å
Sm(1)-O(1w)	2.472(4)	Sm(1)-O(2w)	2.401(4)	Sm(1)-O(3w)	2.586(5)
Sm(1)-O(4w)	2.449(4)	Sm(1)-O(4) #1	2.529(4)	Sm(1)-O(4)	2.601(4)
Sm(1)-O(5)	2.465(4)	Sm(1)-O(7)	2.393(4)	Sm(1)-O(8)	2.375(4)
O(4)-Sm(1)#1	2.529(4)				
angle	deg	angle	deg	angle	deg
O(1w)-Sm(1)-O(3w)	129.73(14)	O(1w)-Sm(1)-O(4)#1	116.81(12)	O(1w)-Sm(1)-O(4)	152.01(13)
O(2w)-Sm(1)-O(1w)	78.20(14)	O(2w)-Sm(1)-O(3w)	139.41(14)	O(2w)-Sm(1)-O(4w)	145.72(14)
O(2w)-Sm(1)-O(4)#1	71.82(14)	O(2w)-Sm(1)-O(4)	75.44(13)	O(2w)-Sm(1)-O(5)	113.16(15)
O(3w)-Sm(1)-O(4)	77.68(13)	O(4w)-Sm(1)-O(1w)	75.58(13)	O(4w)-Sm(1)-O(3w)	74.87(13)
O(4w)-Sm(1)-O(4)#1	140.63(14)	O(4w)-Sm(1)-O(4)	123.83(12)	O(4w)-Sm(1)-O(5)	73.59(13)
O(4)#1-Sm(1)-O(3w)	69.04(13)	O(4)#1-Sm(1)-O(4)	62.98(13)	O(5)-Sm(1)-O(1w)	136.18(13)
O(5)-Sm(1)-O(3w)	69.55(16)	O(5)-Sm(1)-O(4)	51.00(12)	O(5)-Sm(1)-O(4)#1	106.79(13)
O(7)-Sm(1)-O(1w)	66.38(14)	O(7)-Sm(1)-O(2w)	107.77(14)	O(7)-Sm(1)-O(3w)	69.66(15)
O(7)-Sm(1)-O(4w)	81.34(13)	O(7)-Sm(1)-O(4)#1	71.95(12)	O(7)-Sm(1)-O(4)	131.32(13)
O(7)-Sm(1)-O(5)	136.31(14)	O(8)-Sm(1)-O(1w)	69.45(14)	O(8)-Sm(1)-O(2w)	74.10(14)
O(8)-Sm(1)-O(3w)	138.2(14)	O(8)-Sm(1)-O(4w)	76.24(13)	O(8)-Sm(1)-O(4)#1	142.72(12)
O(8)-Sm(1)-O(4)	74.19(13)	O(8)-Sm(1)-O(7)	134.10(14)		
Polymer 2					
Bond	Å	Bond	Å	Bond	Å
Eu(1)-O(7)#1	2.355(3)	Eu(1)-O(3)	2.363(3)	Eu(1)-O(2w)	2.384(4)
Eu(1)-O(1w)	2.421(3)	Eu(1)-O(2)#2	2.437(4)	Eu(1)-O(3w)	2.462(4)
Eu(1)-O(1)	2.521(3)	Eu(1)-O(4w)	2.567(4)	Eu(1)-O(1)#2	2.596(4)
Eu(1)-Eu(1)#2	4.3763(7)	O(1)-Eu(1)#2	2.596(4)	O(2)-Eu(1)#2	2.437(4)
O(7)-Eu(1)#2	2.355(3)				
angle	deg	angle	deg	angle	deg
O(7)#1-Eu(1)-O(3)	133.54(13)	O(7)#1-Eu(1)-O(2w)	74.60(12)	O(3)-Eu(1)-O(2w)	107.24(12)
O(7)#1-Eu(1)-O(1w)	76.44(12)	O(3)-Eu(1)-O(1w)	80.78(12)	O(2w)-Eu(1)-O(1w)	146.09(13)
O(7)#1-Eu(1)-O(2)#2	73.99(13)	O(3)-Eu(1)-O(2)#2	136.15(13)	O(2w)-Eu(1)-O(2)#2	113.83(13)
O(1w)-Eu(1)-O(2)#2	73.89(12)	O(7)#1-Eu(1)-O(3w)	69.05(13)	O(3)-Eu(1)-O(3w)	66.30(12)
O(3)-Eu(1)-O(3w)	66.30(12)	O(2w)-Eu(1)-O(3w)	77.85(13)	O(1w)-Eu(1)-O(3w)	75.59(13)
O(2)#2-Eu(1)-O(3w)	136.36(12)	O(7)#1-Eu(1)-O(1)	142.81(11)	O(3)-Eu(1)-O(1)	72.43(11)
O(2w)-Eu(1)-O(1)	71.54(12)	O(1w)-Eu(1)-O(1)	140.34(12)	O(2)#2-Eu(1)-O(1)	106.32(12)
O(3w)-Eu(1)-O(1)	117.10(12)	O(7)#1-Eu(1)-O(4w)	137.98(12)	O(3)-Eu(1)-O(4w)	70.18(13)
O(2w) -Eu(1)-O(4w)	139.04(12)	O(1w)-Eu(1)-O(4w)	74.87(12)	O(2)#2-Eu(1)-O(4w)	68.97(13)
O(3w)-Eu(1)-O(4w)	130.29(12)	O(1)-Eu(1)-O(4w)	68.87(11)	O(7)#1-Eu(1)-O(1)#2	94.55(12)
O(3)-Eu(1)-O(1)#2	131.47(11)	O(2w) -Eu(1)-O(1)#2	75.39(12)	O(1w) -Eu(1)-O(1)#2	124.44(12)

O(2)#2-Eu(1)-O(1)#2	51.31(11)	O(3w)-Eu(1)-O(1)#2	151.59(12)	O(1)-Eu(1)-O(1)#2	62.46(13)

Polymer 3

Bond	Å	Bond	Å	Bond	Å
Gd(1)-O(7)#1	2.385(3)	Gd(1)-O(1)	2.400(3)	Gd(1)-O(4w)	2.416(3)
Gd(1)-O(2w)	2.458(3)	Gd(1)-O(4)#2	2.484(3)	Gd(1)-O(3w)	2.494(3)
Gd(1)-O(3)	2.552(3)	Gd(1)-O(1w)	2.601(3)	Gd(1)-O(3)#2	2.631(3)
O(3)-Gd(1)#2	2.631(3)	O(4)-Gd(1)#2	2.484(3)	O(7)-Gd(1)#1	2.385(3)
angle	deg	angle	deg	angle	deg
O(7)#1-Gd(1)-O(1)	133.84(10)	O(7)#1-Gd(1)-O(4w)	74.88(10)	O(1)-Gd(1)-O(4w)	107.05(11)
O(7)#1-Gd(1)-O(2w)	76.17(10)	O(1)-Gd(1)-O(2w)	81.10(10)	O(4w)-Gd(1)-O(2w)	146.06(10)
O(7)#1-Gd(1)-O(4)#2	73.63(11)	O(1)-Gd(1)-O(4)#2	136.21(11)	O(4w)-Gd(1)-O(4)#2	113.92(11)
O(2w)-Gd(1)-O(4)#2	73.69(10)	O(7)#1-Gd(1)-O(3w)	69.51(11)	O(1)-Gd(1)-O(3w)	66.14(10)
O(4w)-Gd(1)-O(3w)	77.98(11)	O(2w)-Gd(1)-O(3w)	75.58(10)	O(4)#2-Gd(1)-O(3w)	75.58(10)
O(7)#1-Gd(1)-O(3)	142.60(9)	O(1)-Gd(1)-O(3)	72.53(9)	O(4w)-Gd(1)-O(3)	71.22(10)
O(2w)-Gd(1)-O(3)	140.76(10)	O(4)#2-Gd(1)-O(3)	106.34(10)	O(3w)-Gd(1)-O(3)	117.04(10)
O(7)#1-Gd(1)-O(1w)	137.46(10)	O(1)-Gd(1)-O(1w)	70.19(11)	O(4w)-Gd(1)-O(1w)	139.29(10)
O(2w)-Gd(1)-O(1w)	74.64(10)	O(4)#2-Gd(1)-O(1w)	68.91(11)	O(3w)-Gd(1)-O(1w)	129.93(11)
O(3)-Gd(1)-O(1w)	69.38(9)	O(7)#1-Gd(1)-O(3)#2	94.42(10)	O(1)-Gd(1)-O(3)#2	131.35(9)
O(4w)-Gd(1)-O(3)#2	75.61(10)	O(2w)-Gd(1)-O(3)#2	124.14(9)	O(4)#2-Gd(1)-O(3)#2	51.21(9)
O(3w)-Gd(1)-O(3)#2	151.96(10)	O(3)-Gd(1)-O(3)#2	62.36(11)	O(1w)-Gd(1)-O(3)#2	77.51(10)
Gd(1)-O(3)-Gd(1)#2	117.64(10)				

Polymer 4

Bond	Å	Bond	Å	Bond	Å
Tb(1)-O(1)	2.346(2)	Tb(1)-O(1w)	2.450(3)	Tb(1)-O(2w)	2.410(2)
Tb(1)-O(3w)	2.566(3)	Tb(1)-O(4w)	2.370(2)	Tb(1)-O(6)#1	2.353(2)
Tb(1)-O(7)#1	2.522(2)	Tb(1)-O(7)#2	2.598(3)	Tb(1)-O(8)#2	2.434(3)
O(6)-Tb(1)#1	2.353(2)	O(7)-Tb(1)#3	2.598(2)	O(7)-Tb(1)#1	2.522(2)
O(8)-Tb(1)#3	2.435(3)				
angle	deg	angle	deg	angle	deg
O(1)-Tb(1)-O(1w)	69.46(9)	O(1)-Tb(1)-O(2w)	76.50(8)	O(1)-Tb(1)-O(3w)	137.68(9)
O(1)-Tb(1)-O(4w)	75. 01(9)	O(1)-Tb(1)-O(6)#1	134.00(9)	O(1)-Tb(1)-O(7)#1	142.86(8)
O(1)-Tb(1)-O(7)#2	93.98(8)	O(1)-Tb(1)-O(8)#2	73.36(10)	O(1w)-Tb(1)-O(3w)	130.44(9)
O(1w)-Tb(1)-O(7)#2	151.08(9)	O(1w)-Tb(1)-O(7)#1	117.21(9)	O(2w)-Tb(1)-O(1w)	75.71(9)
O(2w)-Tb(1)-O(3w)	74.90(8)	O(2w)-Tb(1)-O(7)#2	124.73(8)	O(2w)-Tb(1)-O(7)#1	140.15(8)
O(2w)-Tb(1)-O(8)#2	73.85(8)	O(3w)-Tb(1)-O(7)#2	77.82(8)	O(4w)-Tb(1)-O(1w)	78.01(9)
O(4w)-Tb(1)-O(2w)	146.46(9)	O(4w)-Tb(1)-O(3w)	138.64(8)	O(4w)-Tb(1)-O(7)#1	71.39(8)
O(4w)-Tb(1)-O(7)#2	74.77(9)	O(4w)-Tb(1)-O(8)#2	113.72(9)	O(6)#1-Tb(1)-O(1w)	66.41(9)
O(6)#1-Tb(1)-O(2w)	80.73(9)	O(6)#1-Tb(1)-O(3w)	70.13(9)	O(6)#1-Tb(1)-O(4w)	107.24(9)
O(6)#1-Tb(1)-O(7)#2	131.58(8)	O(6)#1-Tb(1)-O(7)#1	72.41(8)	O(6)#1-Tb(1)-O(8)#2	136.22(10)
O(7)#1-Tb(1)-O(3w)	68.61(8)	O(7)#1-Tb(1)-O(7)#2	62.38(9)	O(8)#2-Tb(1)-O(1w)	136.22(9)
O(8)#2-Tb(1)-O(3w)	69.15(9)	O(8)#2-Tb(1)-O(7)#2	51.63(8)	O(8)#2-Tb(1)-O(7)#1	106.33(9)

Polymer **5**

Bond	Å	Bond	Å	Bond	Å
Dy(1)-O(1)	2.393(4)	Dy(1)-O(3)	2.526(3)	Dy(1)-O(3)#1	2.606(4)

Dy(1)-O(4)#1	2.463(4)	Dy(1)-O(7)#2	2.376(4)	Dy(1)-O(1w)	2.448(3)
Dy(1)-O(2w)	2.476(4)	Dy(1)-O(3w)	2.403(4)	Dy(1)-O(4w)	2.591(4)
O(3)-Dy(1)#1	2.606(3)	O(4)-Dy(1)#1	2.463(4)	O(7)-Dy(1)#2	2.376(4)
angle	deg	angle	deg	angle	deg
O(7)#2-Dy(1)-O(1)	133.96(13)	O(7)#2-Dy(1)-O(3w)	74.14(12)	O(1)-Dy(1)-O(3w)	107.79(13)
O(7)#2-Dy(1)-O(1w)	76.32(12)	O(1)-Dy(1)-O(1w)	81.26(12)	O(3w)-Dy(1)-O(1w)	145.90(13)
O(7)#2-Dy(1)-O(4)#1	73.80(14)	O(1)-Dy(1)-O(4)#1	136.00(13)	O(3w)-Dy(1)-O(4)#1	113.42(14)
O(1w)-Dy(1)-O(4)#1	73.41(12)	O(7)#2-Dy(1)-O(2w)	69.34(13)	O(1)-Dy(1)-O(2w)	66.36(12)
O(1w)-Dy(1)-O(2w)	75.67(12)	O(4)#1-Dy(1)-O(2w)	136.25(12)	O(1)-Dy(1)-O(3)	71.92(11)
O(3w)-Dy(1)-O(2w)	78.25(13)	O(7)#2-Dy(1)-O(3)	142.84(12)	O(3w)-Dy(1)-O(3)	71.83(13)
O(1w)-Dy(1)-O(3)	140.44(13)	O(4)#1-Dy(1)-O(3)	106.77(12)	O(2w)-Dy(1)-O(3)	116.79(11)
O(7)#2-Dy(1)-O(4w)	137.95(12)	O(1)-Dy(1)-O(4w)	69.77(13)	O(3w)-Dy(1)-O(4w)	139.42(12)
O(1w)-Dy(1)-O(4w)	74.68(12)	O(4)#1-Dy(1)-O(4w)	69.15(14)	O(2w)-Dy(1)-O(4w)	129.78(12)
O(3)-Dy(1)-O(4w)	69.08(11)	O(7)#2-Dy(1)-O(3)#1	94.32(13)	O(1)-Dy(1)-O(3)#1	131.34(12)
O(3w)-Dy(1)-O(3)#1	75.50(12)	O(1w)-Dy(1)-O(3)#1	123.68(12)	O(4)#1-Dy(1)-O(3)#1	51.03(11)
O(2w)-Dy(1)-O(3)#1	152.11(12)	O(3)-Dy(1)-O(3)#1	63.06(14)	O(4w)-Dy(1)-O(3)#1	77.54(12)
Polymer **6**					
Bond	Å	Bond	Å	Bond	Å
Er(1)-O(1)	2.325(2)	Er(1)-O(3)	2.511(2)	Er(1)-O(3)#1	2.590(2)
Er(1)-O(4)#1	2.398(2)	Er(1)-O(7)#2	2.318(2)	Er(1)-O(1w)	2.369(2)
Er(1)-O(2w)	2.424(2)	Er(1)-O(3w)	2.328(2)	Er(1)-O(4w)	2.532(2)
O(3)-Er(1)#1	2.591(2)	O(4)-Er(1)#1	2.398(2)	O(7)-Er(1)#2	2.318(2)
angle	deg	angle	deg	angle	deg
O(7)#2-Er(1)-O(1)	134.33(8)	O(7)#2-Er(1)-O(3w)	75.81(7)	O(1)-Er(1)-O(3w)	106.30(8)
O(7)#2-Er(1)-O(1w)	76.43(7)	O(3w)-Er(1)-O(4)#1	114.43(8)	O(3w)-Er(1)-O(1w)	146.71(8)
O(7)#2-Er(1)-O(4)#1	73.33(8)	O(1)-Er(1)-O(4)#1	136.19(8)	O(1)-Er(1)-O(1w)	80.87(7)
O(1w)-Er(1)-O(4)#1	74.09(7)	O(7)#2-Er(1)-O(2w)	69.44(8)	O(1)-Er(1)-O(2w)	66.84(8)
O(4)#1-Er(1)-O(2w)	136.48(8)	O(1w)-Er(1)-O(2w)	75.96(8)	O(3w)-Er(1)-O(2w)	77.34(8)
O(7)#2-Er(1)-O(3)	143.14(7)	O(1)-Er(1)-O(3)	72.27(7)	O(3w)-Er(1)-O(3)	71.31(7)
O(1w)-Er(1)-O(3)	139.82(7)	O(4)#1-Er(1)-O(3)	105.68(7)	O(2w)-Er(1)-O(3)	117.57(7)
O(7)#2-Er(1)-O(4w)	137.33(8)	O(1)-Er(1)-O(4w)	70.34(8)	O(3w)-Er(1)-O(4w)	138.26(7)
O(1w)-Er(1)-O(4w)	75.01(7)	O(4)#1-Er(1)-O(4w)	68.77(8)	O(2w)-Er(1)-O(4w)	131.10(7)
O(3)-Er(1)-O(4w)	68.15(7)	O(7)#2-Er(1)-O(3)#1	94.06(7)	O(1)-Er(1)-O(3)#1	131.13(7)
O(3w)-Er(1)-O(3)#1	74.90(7)	O(1w)-Er(1)-O(3)#1	125.20(7)	O(4)#1-Er(1)-O(3)#1	51.84(7)
O(2w)-Er(1)-O(3)#1	150.51(7)	O(3)-Er(1)-O(3)#1	61.81(8)	O(4w)-Er(1)-O(3)#1	77.65(7)

Symmetry codes : for 1 #1 -x+1, -y, -z; #2 x+1, y+1, z; #3 x-1, y-1, z; for **2**: #1 1-x, 2-y, 1-z; #2 –x, 1-y, 1-z; #3 1+x, +y, +z; #4 –x, 2-y, -z; for **3** #1 -x+1,-y+2,-z+1; #2 -x,-y+1,-z+1; #3 x-1,y,z; #4 -x+1,-y+3,-z+2; for **4** #1 1-x, 1-y, 1-z; #2 -1+x, -1+y, +z; #3 1+x, 1+y, +z; for **5**, #1 -x,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 x-1, y, z; #4 -x,-y+2,-z; for **6** #1 -x,-y+1,-z+1,#2 -x+1,-y+2,-z+1,#3 x-1,y,z, #4 -x,-y+2,-z.

Table S2. Hydrogen bonds parameters for polymers 1-6 [Å and ^{0}]

Polymer **1**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C2 -- H2... O14	0.9300	2.2900	3.2060	168.00
C5 -- H5...O8	0.9300	2.5200	3.1447	125.00
C19 -- H19... O2	0.9300	2.2100	2.7652	118.00
C19 -- H19...O9	0.9300	2.5600	3.2697	133.00
C21 -- H21.... O4	0.9300	2.5500	3.4674	171.00
O(1w)-H(1wa)...O(3)	0.82	1.90	2.715(7)	176
O(3w)-H(3wb)...O(5w)	0.71(9)	2.06(9)	2.689(7)	149(10)
O(4w)-H(4wb)...O(5w)	0.82	1.87	2.693(7)	175
O(1w)-H(1wb)...O(3)	0.86(1)	2.06(8)	2.838(7)	150(7)
O(2w)-H(2wa)...O(3w)	0.81(8)	1.97(8)	2.772(7)	171(7)
Polymer **2**				
D-H...A	D-H...A	D-H...A	D-H...A	D-H...A
O(1w)-H(11)...O(6)#1	0.842(10)	1.943(11)	2.784(5)	178(3)
O(1w)-H(12)...O(5w)	0.846(10)	1.866(14)	2.687(6)	163(3)
O(2w)-H(21)...O(8)#1	0.842(10)	1.799(17)	2.622(5)	165(5)
O(2w)-H(22)...O(4w)#2	0.840(10)	1.942(13)	2.774(5)	171(5)
O(3w)-H(31)...O(5)	0.836(10)	2.045(15)	2.851(5)	162(3)
O(3w)-H(32)...O(5)#1	0.840(10)	1.889(17)	2.714(5)	167(5)
O(4w)-H(41)...O(4)	0.838(10)	2.209(18)	2.984(6)	154(3)
O(4w)-H(42)...O(5w)	0.839(10)	1.843(13)	2.675(5)	170(4)
O(5w)-H(51)...O(6)#3	0.843(10)	1.871(12)	2.703(6)	169(2)
O(5w)-H(52)...N(3)	0.837(10)	1.954(14)	2.778(6)	167(3)
N(4)-H(4)...O(3)#4	0.879(10)	1.95(2)	2.803(5)	164(6)
Polymer **3**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1w)-H(11)...O(2)	0.84(1)	2.28(3)	3.026(5)	147(5)
O(1w)-H(12)...O(5w)	0.85(1)	1.90(2)	2.711(4)	160(6)
O(2w)-H(21)...O(6)#1	0.85(1)	1.98(1)	2.819(5)	170(6)
O(2w)-H(22)...O(5w)	0.84(1)	1.89(1)	2.716(5)	168(5)
O(3w)-H(31)...O(5)	0.84(1)	2.08(2)	2.880(5)	160(4)
O(3w)-H(32)...O(5)#1	0.84(1)	1.92(2)	2.746(4)	169(6)
O(4w)-H(41)...O(8)#1	0.84(1)	1.84(2)	2.658(5)	167(6)
O(4w)-H(42)...O(1w)#2	0.84(1)	1.99(1)	2.824(4)	171(5)
O(5w)-H(51)...O(6)#3	0.84(1)	1.92(2)	2.741(5)	166(6)
O(5w)-H(52)...N(4)#4	0.84(1)	1.97(1)	2.810(5)	173(5)
N(3)-H(3)...O(1)	0.88(1)	1.97(2)	2.831(5)	168(6)
Polymer **4**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1w)-H(1wa)...O(3)#2	0.89	2.01	2.8595(1)	161

O(1w)-H(1wb)...O(6)	0.89	2.32	2.6394(1)	101
O(2w)-H(2wa)...O(5w)	0.94	1.80	2.6867(1)	157
O(2w)-H(3wa)...O(5w)	0.89	1.81	2.6821(1)	164
O(3w)-H(3wb)...O(5)	0.89	2.16	2.9765(1)	152
O(3w)-H(5wa)...N(3)	0.85	1.95	2.7662(1)	162
O(4w)-H(5wb)...O(4)	0.85	1.88	2.7234(1)	175
O(1w)-H(1wa)...O(3)#2	0.89	2.01	2.8595(1)	161
O(1w)-H(1wa)...O(3)	0.82(4)	2.07(4)	2.866(4)	165(5)
O(2w)-H(2wa)...O(5w)	0.94	1.78	2.683(4)	160
O(3w)-H(3wa)...O(5w)	0.89	1.80	2.679(5)	166
O(3w)-H(3wb)...O(5)	0.90	2.17	2.974(5)	149
O(3w)-H(3wa)...O(6)	0.90	2.52	2.832(5)	101
Polymer **5**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1w)-H(11)...O(6)#2	0.84(1)	1.93(1)	2.763(6)	170(6)
O(1w)-H(12)...O(5w)	0.84(1)	1.85(2)	2.677(6)	167(7)
O(2w)-H(21)...O(5)	0.84(1)	2.03(2)	2.831(5)	159(5)
O(2w)-H(22)...O(5)#2	0.83(1)	1.89(2)	2.714(5)	173(6)
O(3w)-H(31)...O(8)#2	0.84(1)	1.80(1)	2.632(6)	174(6)
O(3w)-H(32)...O(4w)#1	0.84(1)	1.93(1)	2.768(5)	174(7)
O(4w)-H(41)...O(2)	0.84(1)	2.22(3)	2.975(7)	150(5)
O(4w)-H(42)...O(5w)	0.83(1)	1.84(2)	2.667(5)	171(6)
O(5w)-H(51)...O(6)#3	0.83(1)	1.92(3)	2.719(6)	159(8)
O(5w)-H(52)...N(4)#4	0.84(1)	1.92(1)	2.760(6)	178(7)
Polymer **6**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1w)-H(11)...O(6)#2	0.85(1)	1.96(1)	2.797(3)	175(4)
O(1w)-H(12)...O(5w)	0.84(1)	1.85(1)	2.675(3)	168(3)
O(2w)-H(21)...O(5)	0.84(1)	2.03(1)	2.853(3)	166(3)
O(2w)-H(22)...O(5)#2	0.84(1)	1.89(1)	2.711(3)	165(3)
O(3w)-H(31)...O(8)#2	0.84(1)	1.80(1)	2.625(3)	168(4)
O(3w)-H(32)...O(4w)#1	0.84(1)	1.96(1)	2.788(3)	171(4)
O(4w)-H(41)...O(2)	0.84(1)	2.18(2)	2.973(4)	157(3)
O(4w)-H(42)...O(5w)	0.84(1)	1.87(2)	2.683(3)	161(4)
O(5w)-H(51)...O(6)#3	0.83(1)	1.89(1)	2.715(3)	171(4)
O(5w)-H(52)...N(4)#4	0.84(1)	1.95(1)	2.774(4)	168(4)
O(1w)-H(1wa)...O(3)	0.82(4)	2.07(4)	2.866(4)	165(5)
O(3w)-H(3wa)...O(5w)	0.89	1.80	2.679(5)	166
O(5w)-H(5wa)...N(3)	0.85	1.93	2.775(5)	175

Symmetry transformations used to generate equivalent atoms: for **2**: #1 1-x, 2-y, 1-z; #2 –x, 1-y, 1-z; #3 1+x, +y, +z; #4 –x, 2-y, -z; for **3** #1 -x+1,-y+2,-z+1; #2 -x,-y+1,-z+1; #3 x-1,y,z; #4 -x+1,-y+3,-z+2; for **4** #1 1-x, 1-y, 1-z; #2 -1+x, -1+y, +z; #3 1+x, 1+y, +z; for **5**, #1 -x,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 x-1, y, z; #4 -x,-y+2,-z; for **6** #1 -x,-y+1,-z+1,#2 -x+1,-y+2,-z+1,#3 x-1,y,z, #4 -x,-y+2,-z.