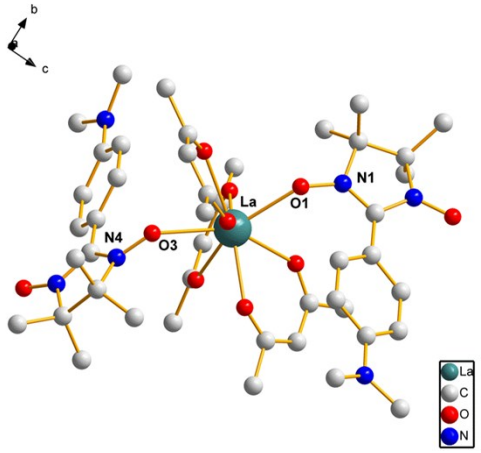


Fig. S1 The molecular structure of complex **1**. Fluorine and hydrogen atoms are not shown for the sake of clarity.

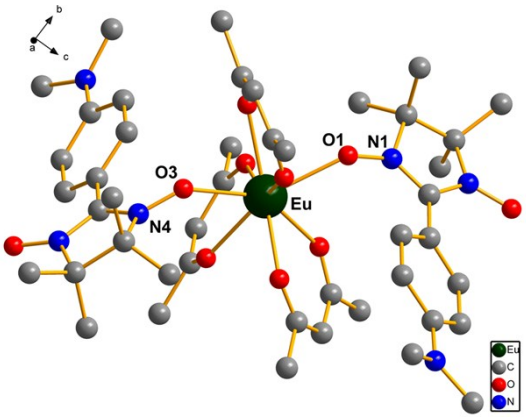


Fig. S2 The molecular structure of complex **2**. Fluorine and hydrogen atoms are not shown for the sake of clarity.

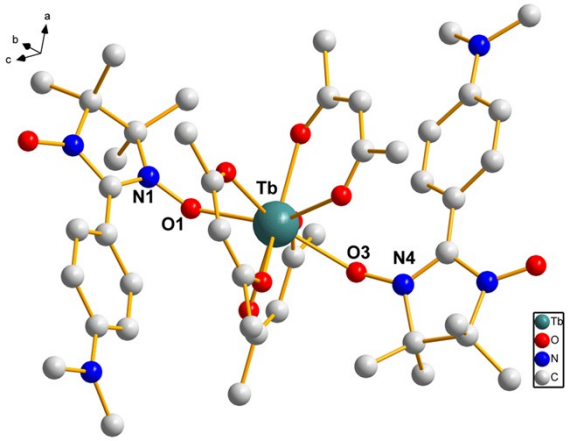


Fig. S3 The molecular structure of complex **4**. Fluorine and hydrogen atoms are not shown for the sake of clarity.

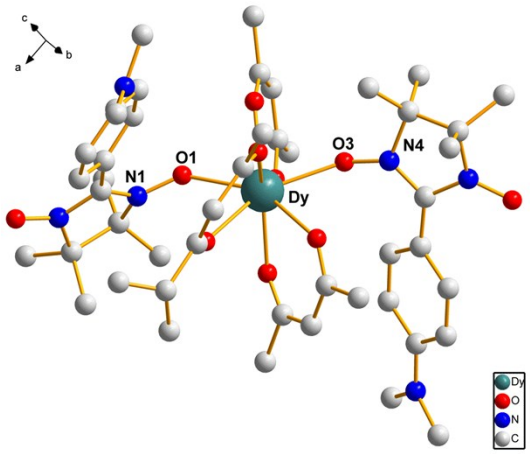


Fig. S4 The molecular structure of complex **5**. Fluorine and hydrogen atoms are not shown for the sake of clarity.

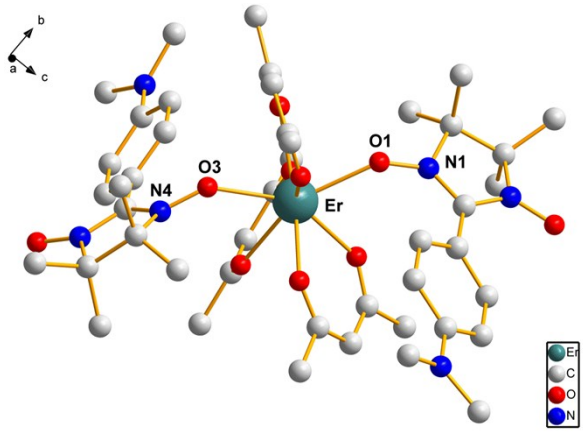


Fig. S5 The molecular structure of complex **6**. Fluorine and hydrogen atoms are not shown for the sake of clarity.

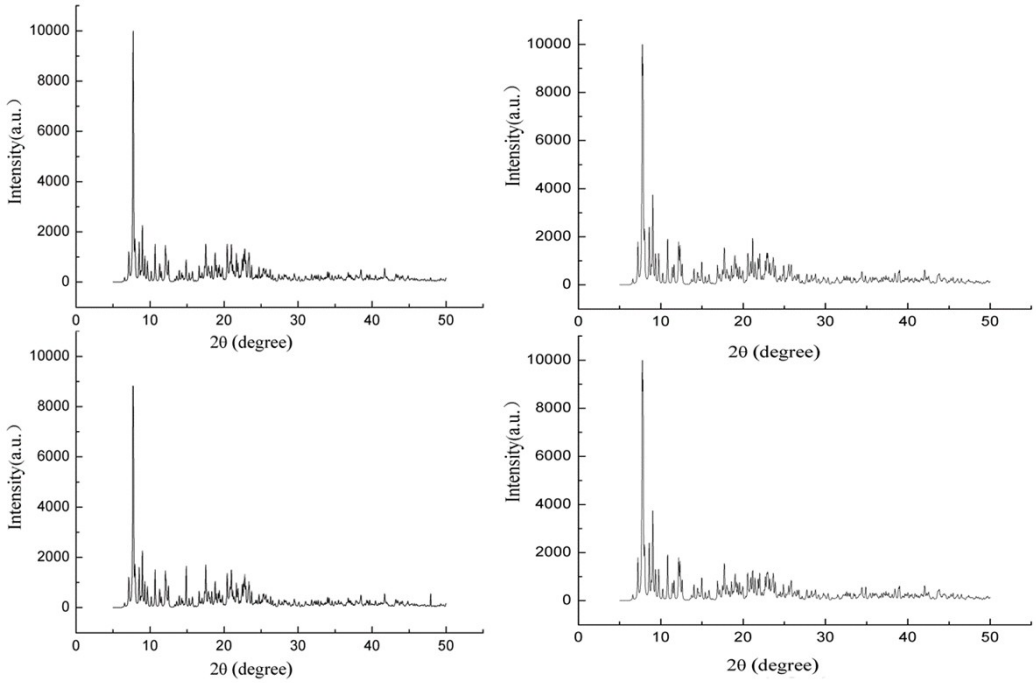


Fig. S6 X-ray powder diffraction patterns of complexes **1**(left), **3**(right). Calculated pattern from single-crystal X-ray data (upper); experimental data (lower).

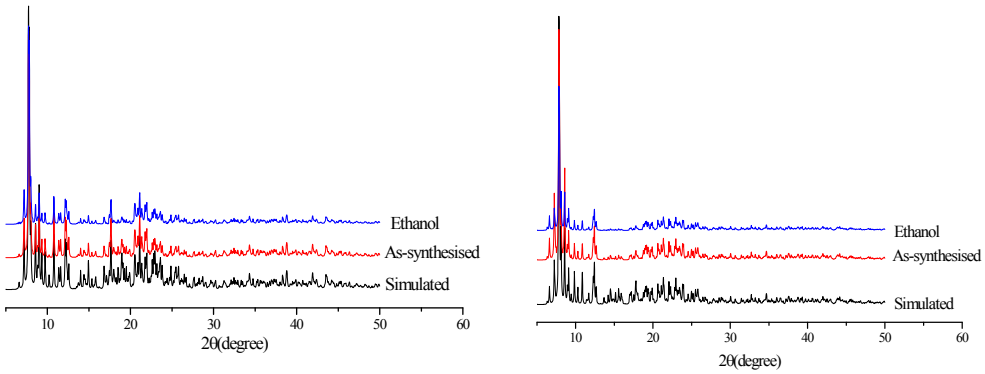


Fig. S7 X-ray powder diffraction patterns of complexes **2**(left) and **4**(right), the samples after the luminescence experiment are labled as "Ethanol".

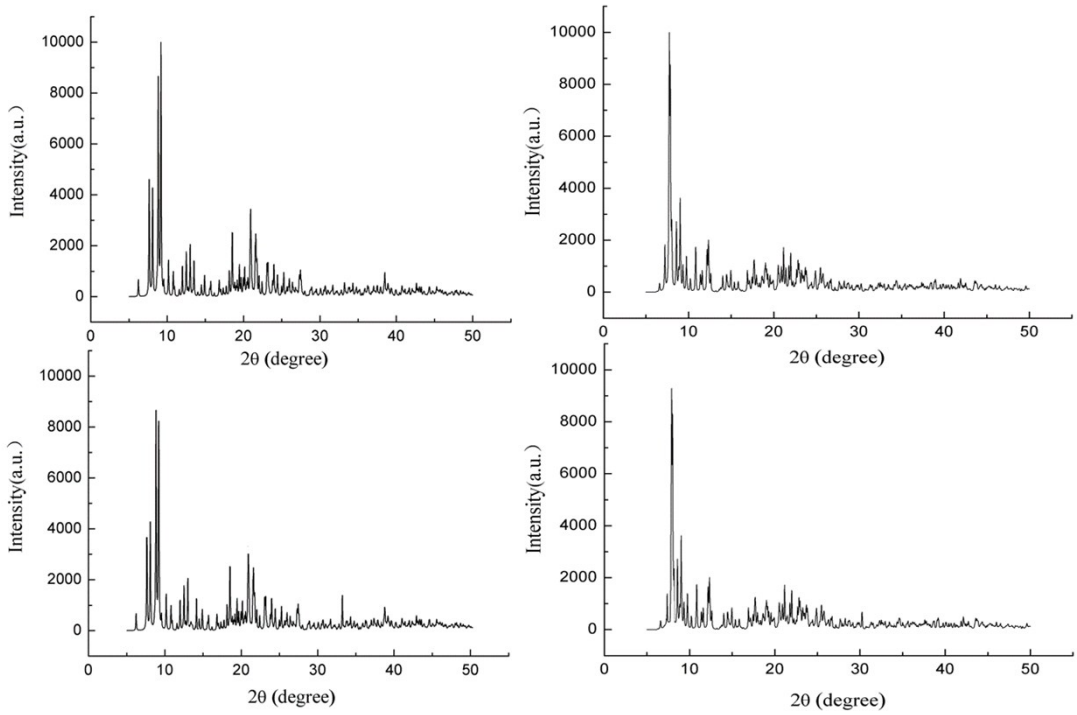


Fig. S8 X-ray powder diffraction patterns of complexes **5**(left), **6**(right). Calculated pattern from single-crystal X-ray data (upper); experimental data (lower).

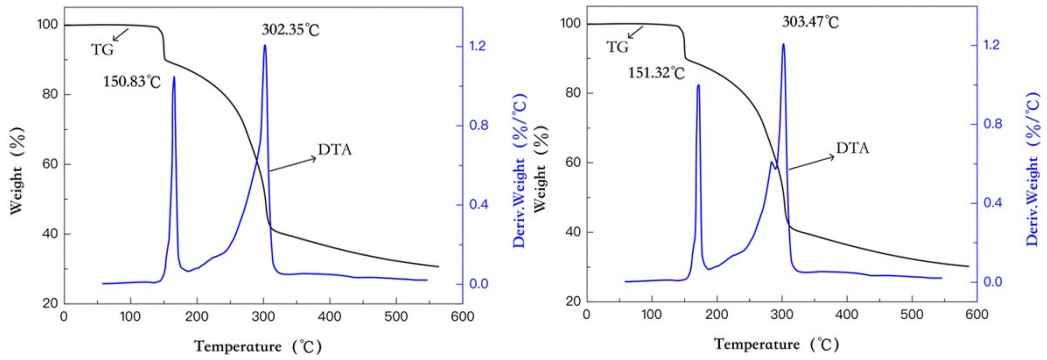


Fig. S9 Thermal analysis curve of the complexes **1** and **2**.

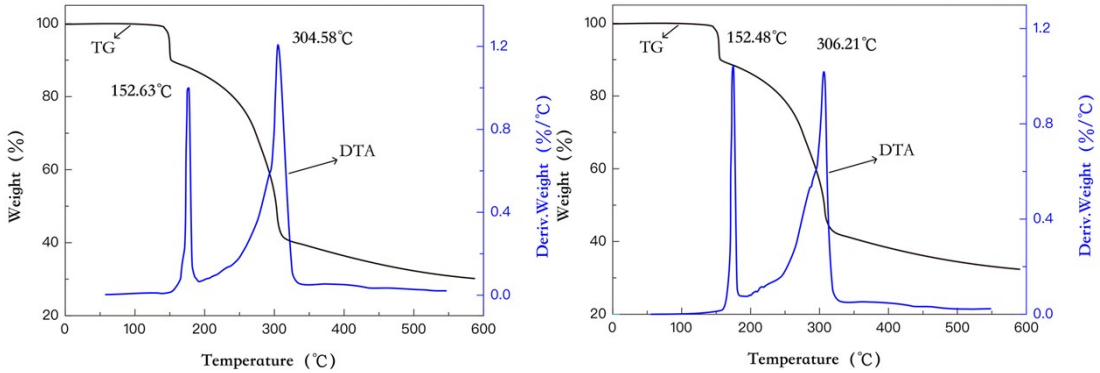


Fig. S10 Thermal analysis curve of the complexes **3** and **4**.

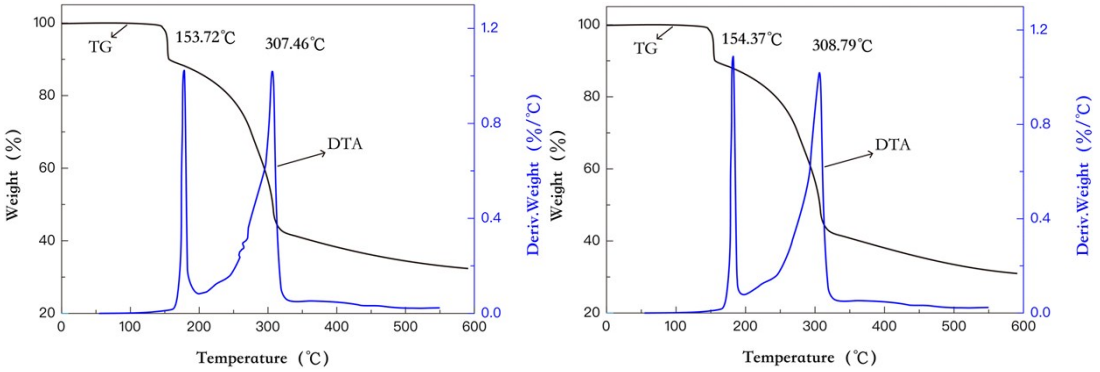


Fig. S11 Thermal analysis curve of the complexes **5** and **6**.

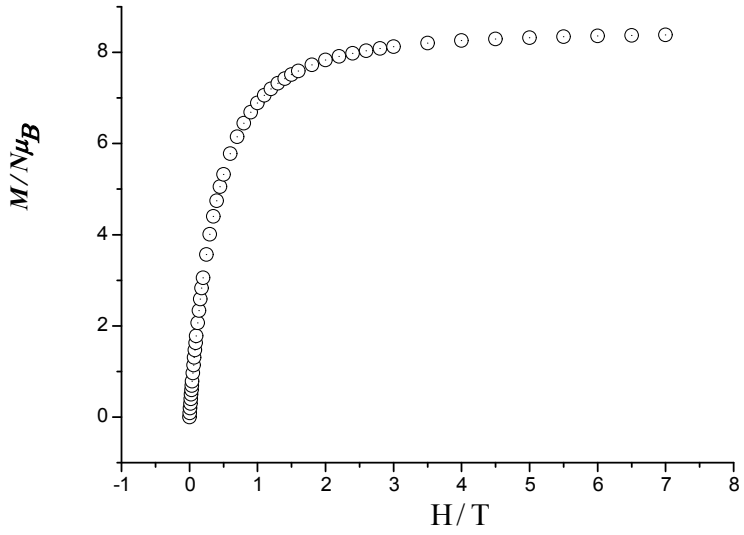


Fig. S12 Field dependence of the magnetization performed at 2 K for complex 3.

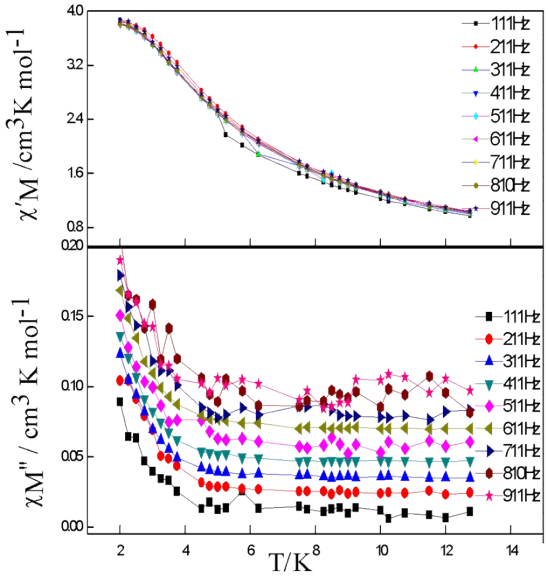


Fig.S13 Frequency dependence of real (top) and imaginary (down) components of the ac magnetic susceptibility for **4** under zero applied dc field.

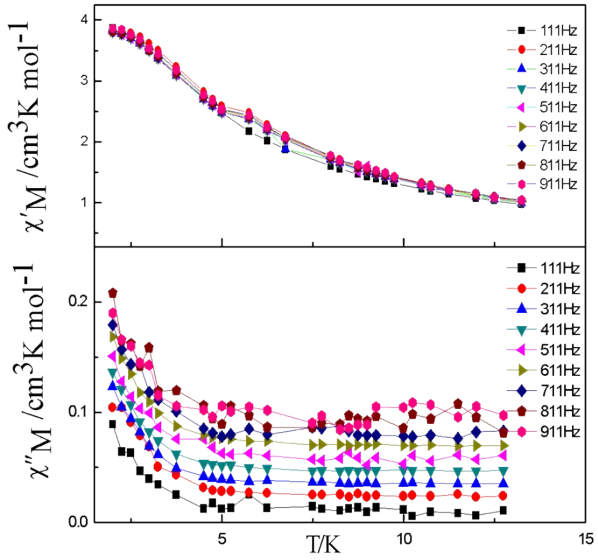


Fig. S14 Frequency dependence of real (top) and imaginary (down) components of the ac magnetic susceptibility for **4** under 2000 Oe applied dc field.

Table S1 The Important Bond Lengths(Å) and Angles(°) for **1-6**

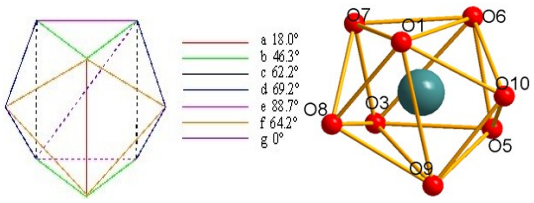
		1	
Bond lengths			
La(1)-O(1)	2.439(3)	La(1)-O(3)	2.454(3)
La(1)-O(6)	2.472(2)	La(1)-O(9)	2.478(3)
La(1)-O(8)	2.517(2)	La(1)-O(10)	2.517(3)
La(1)-O(7)	2.523(3)	La(1)-O(5)	2.541(3)
La(2)-O(11)#1	2.466(2)	La(2)-O(11)	2.466(2)
La(2)-O(14)	2.491(3)	La(2)-O(14)#1	2.491(3)
La(2)-O(15)	2.520(3)	La(2)-O(13)	2.520(2)
La(2)-O(15)#1	2.520(3)	La(2)-O(13)#1	2.520(3)
Bond angles			
O(1)-La(1)-O(3)	141.44(9)	O(1)-La(1)-O(6)	90.76(9)
O(3)-La(1)-O(6)	101.34(9)	O(1)-La(1)-O(9)	106.68(9)
O(3)-La(1)-O(9)	91.05(10)	O(6)-La(1)-O(9)	133.80(9)
O(1)-La(1)-O(8)	76.92(9)	O(3)-La(1)-O(8)	73.67(9)
O(6)-La(1)-O(8)	148.20(9)	O(9)-La(1)-O(8)	77.99(9)
O(1)-La(1)-O(10)	73.46(9)	O(3)-La(1)-O(10)	144.98(9)
O(6)-La(1)-O(10)	75.25(9)	O(9)-La(1)-O(10)	69.77(10)
O(8)-La(1)-O(10)	126.76(9)	O(1)-La(1)-O(7)	76.08(9)
O(3)-La(1)-O(7)	70.58(9)	O(6)-La(1)-O(7)	79.28(8)
O(9)-La(1)-O(7)	145.82(9)	O(8)-La(1)-O(7)	69.39(8)
O(10)-La(1)-O(7)	139.58(9)	O(1)-La(1)-O(5)	144.97(9)
O(3)-La(1)-O(5)	72.68(9)	O(6)-La(1)-O(5)	69.51(9)
O(9)-La(1)-O(5)	72.33(9)	O(8)-La(1)-O(5)	134.06(9)
O(10)-La(1)-O(5)	73.63(9)	O(7)-La(1)-O(5)	125.00(9)
		2	
Bond lengths			
Eu(1)-O(1)	2.344(2)	Eu(1)-O(3)	2.356(2)
Eu(1)-O(6)	2.367(2)	Eu(1)-O(9)	2.369(2)
Eu(1)-O(10)	2.409(3)	Eu(1)-O(8)	2.413(2)
Eu(1)-O(7)	2.417(2)	Eu(1)-O(5)	2.437(2)
Eu(2)-O(11)#1	2.378(2)	Eu(2)-O(11)	2.378(2)
Eu(2)-O(14)#1	2.382(2)	Eu(2)-O(14)	2.382(2)
Eu(2)-O(15)#1	2.415(2)	Eu(2)-O(15)	2.415(2)
Eu(2)-O(13)#1	2.416(2)	Eu(2)-O(13)	2.416(2)
Bond angles			
O(1)-Eu(1)-O(3)	139.59(8)	O(1)-Eu(1)-O(6)	91.42(8)
O(3)-Eu(1)-O(6)	101.43(8)	O(1)-Eu(1)-O(9)	105.42(9)
O(3)-Eu(1)-O(9)	90.52(9)	O(6)-Eu(1)-O(9)	137.61(8)
O(1)-Eu(1)-O(10)	73.76(8)	O(3)-Eu(1)-O(10)	146.51(8)
O(6)-Eu(1)-O(10)	75.21(9)	O(9)-Eu(1)-O(10)	72.86(9)
O(1)-Eu(1)-O(8)	75.25(8)	O(3)-Eu(1)-O(8)	73.64(8)

O(6)-Eu(1)-O(8)	147.72(8)	O(9)-Eu(1)-O(8)	74.66(8)
O(10)-Eu(1)-O(8)	126.33(8)	O(1)-Eu(1)-O(7)	75.02(8)
O(3)-Eu(1)-O(7)	71.37(8)	O(6)-Eu(1)-O(7)	75.99(8)
O(9)-Eu(1)-O(7)	145.55(8)	O(10)-Eu(1)-O(7)	136.44(8)
O(8)-Eu(1)-O(7)	72.22(8)	O(1)-Eu(1)-O(5)	146.83(8)
O(3)-Eu(1)-O(5)	73.09(8)	O(6)-Eu(1)-O(5)	71.98(8)
O(9)-Eu(1)-O(5)	73.05(8)	O(10)-Eu(1)-O(5)	74.28(9)
O(8)-Eu(1)-O(5)	132.73(8)	O(7)-Eu(1)-O(5)	125.35(8)
O(11)#1-Eu(2)-O(11)	146.48(12)	O(11)#1-Eu(2)-O(14)#1	91.99(8)
O(11)-Eu(2)-O(14)#1	99.03(8)	O(11)#1-Eu(2)-O(14)	99.03(8)
		3	
Bond lengths			
Gd(1)-O(1)	2.3329(19)	Gd(1)-O(3)	2.3411(19)
Gd(1)-O(6)	2.3482(19)	Gd(1)-O(9)	2.348(2)
Gd(1)-O(10)	2.392(2)	Gd(1)-O(8)	2.3942(19)
Gd(1)-O(7)	2.4004(19)	Gd(2)-O(11)	2.3621(19)
Gd(2)-O(11)#1	2.3622(19)	Gd(2)-O(14)	2.3640(19)
Gd(2)-O(14)#1	2.3641(19)	Gd(2)-O(13)#1	2.3990(19)
Gd(2)-O(13)	2.3991(19)	Gd(2)-O(15)	2.3991(19)
Gd(2)-O(15)#1	2.3992(19)	Gd(1)-O(3)	2.3411(19)
Gd(1)-O(1)	2.3329(19)		
Bond angles			
O(1)-Gd(1)-O(3)	139.42(7)	O(1)-Gd(1)-O(6)	91.61(7)
O(3)-Gd(1)-O(6)	101.19(7)	O(1)-Gd(1)-O(9)	105.10(7)
O(3)-Gd(1)-O(9)	90.77(7)	O(6)-Gd(1)-O(9)	137.97(7)
O(1)-Gd(1)-O(10)	73.67(7)	O(3)-Gd(1)-O(10)	146.79(7)
O(6)-Gd(1)-O(10)	75.32(7)	O(9)-Gd(1)-O(10)	73.04(7)
O(1)-Gd(1)-O(8)	75.13(7)	O(3)-Gd(1)-O(8)	73.63(7)
O(6)-Gd(1)-O(8)	147.59(7)	O(9)-Gd(1)-O(8)	74.44(7)
O(10)-Gd(1)-O(8)	126.33(7)	O(1)-Gd(1)-O(7)	74.90(7)
O(3)-Gd(1)-O(7)	71.43(7)	O(6)-Gd(1)-O(7)	75.62(7)
O(9)-Gd(1)-O(7)	145.63(7)	O(10)-Gd(1)-O(7)	136.02(7)
O(8)-Gd(1)-O(7)	72.42(7)	O(1)-Gd(1)-O(5)	146.96(7)
O(3)-Gd(1)-O(5)	73.18(7)	O(6)-Gd(1)-O(5)	72.23(7)
O(9)-Gd(1)-O(5)	73.11(7)	O(10)-Gd(1)-O(5)	74.40(7)
O(8)-Gd(1)-O(5)	132.56(7)	O(7)-Gd(1)-O(5)	125.52(7)
		4	
Bond lengths			
Tb(1)-O(1)	2.324(3)	Tb(1)-O(6)	2.330(3)
Tb(1)-O(3)	2.333(3)	Tb(1)-O(9)	2.340(3)
Tb(1)-O(8)	2.377(3)	Tb(1)-O(10)	2.381(3)
Tb(1)-O(7)	2.390(3)	Tb(1)-O(5)	2.396(3)
Tb(2)-O(14)#1	2.351(3)	Tb(2)-O(14)	2.351(3)
Tb(2)-O(11)#1	2.355(3)	Tb(2)-O(11)	2.356(3)

Tb(2)-O(13)#1	2.377(3)	Tb(2)-O(13)	2.377(3)
Tb(2)-O(15)	2.384(3)	Tb(2)-O(15)#1	2.385(3)
O(1)-N(1)	1.309(4)	O(2)-N(2)	1.294(5)
O(3)-N(4)	1.314(4)	O(4)-N(5)	1.273(4)
O(11)-N(7)	1.314(4)	O(12)-N(8)	1.272(4)
Bond angles			
O(1)-Tb(1)-O(6)	89.28(10)	O(1)-Tb(1)-O(3)	138.73(9)
O(6)-Tb(1)-O(3)	102.42(9)	O(1)-Tb(1)-O(9)	107.10(10)
O(6)-Tb(1)-O(9)	140.33(10)	O(3)-Tb(1)-O(9)	88.84(11)
O(1)-Tb(1)-O(8)	74.85(9)	O(6)-Tb(1)-O(8)	145.81(9)
O(3)-Tb(1)-O(8)	73.59(9)	O(9)-Tb(1)-O(8)	73.84(10)
O(1)-Tb(1)-O(10)	74.61(9)	O(6)-Tb(1)-O(10)	76.81(10)
O(3)-Tb(1)-O(10)	146.44(10)	O(9)-Tb(1)-O(10)	73.41(11)
O(8)-Tb(1)-O(10)	125.35(10)	O(1)-Tb(1)-O(7)	74.56(9)
O(6)-Tb(1)-O(7)	73.91(9)	O(3)-Tb(1)-O(7)	71.16(10)
O(9)-Tb(1)-O(7)	144.71(10)	O(8)-Tb(1)-O(7)	72.74(9)
O(10)-Tb(1)-O(7)	137.25(10)	O(1)-Tb(1)-O(5)	146.57(10)
O(6)-Tb(1)-O(5)	72.46(10)	O(3)-Tb(1)-O(5)	73.82(10)
O(9)-Tb(1)-O(5)	74.58(10)	O(8)-Tb(1)-O(5)	134.47(10)
O(10)-Tb(1)-O(5)	74.07(10)	O(7)-Tb(1)-O(5)	123.81(10)
		5	
Bond lengths			
Dy(1)-O(3)	Dy(1)-O(3)	Dy(1)-O(3)	Dy(1)-O(3)
Dy(1)-O(5)	Dy(1)-O(5)	Dy(1)-O(5)	Dy(1)-O(5)
Dy(1)-O(8)	Dy(1)-O(8)	Dy(1)-O(8)	Dy(1)-O(8)
Dy(1)-O(7)	Dy(1)-O(7)	Dy(1)-O(7)	Dy(1)-O(7)
O(1)-N(1)	O(1)-N(1)	O(1)-N(1)	O(1)-N(1)
O(4)-N(5)	O(4)-N(5)	O(4)-N(5)	O(4)-N(5)
Bond angles			
O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)
O(1)-Dy(1)-O(5)	O(1)-Dy(1)-O(5)	O(1)-Dy(1)-O(5)	O(1)-Dy(1)-O(5)
O(1)-Dy(1)-O(9)	O(1)-Dy(1)-O(9)	O(1)-Dy(1)-O(9)	O(1)-Dy(1)-O(9)
O(3)-Dy(1)-O(8)	O(3)-Dy(1)-O(8)	O(3)-Dy(1)-O(8)	O(3)-Dy(1)-O(8)
O(5)-Dy(1)-O(8)	O(5)-Dy(1)-O(8)	O(5)-Dy(1)-O(8)	O(5)-Dy(1)-O(8)
O(3)-Dy(1)-O(10)	O(3)-Dy(1)-O(10)	O(3)-Dy(1)-O(10)	O(3)-Dy(1)-O(10)
O(5)-Dy(1)-O(10)	O(5)-Dy(1)-O(10)	O(5)-Dy(1)-O(10)	O(5)-Dy(1)-O(10)
O(8)-Dy(1)-O(10)	O(8)-Dy(1)-O(10)	O(8)-Dy(1)-O(10)	O(8)-Dy(1)-O(10)
O(1)-Dy(1)-O(7)	O(1)-Dy(1)-O(7)	O(1)-Dy(1)-O(7)	O(1)-Dy(1)-O(7)
O(9)-Dy(1)-O(7)	O(9)-Dy(1)-O(7)	O(9)-Dy(1)-O(7)	O(9)-Dy(1)-O(7)
O(10)-Dy(1)-O(7)	O(10)-Dy(1)-O(7)	O(10)-Dy(1)-O(7)	O(10)-Dy(1)-O(7)
O(1)-Dy(1)-O(6)	O(1)-Dy(1)-O(6)	O(1)-Dy(1)-O(6)	O(1)-Dy(1)-O(6)
O(9)-Dy(1)-O(6)	O(9)-Dy(1)-O(6)	O(9)-Dy(1)-O(6)	O(9)-Dy(1)-O(6)
O(10)-Dy(1)-O(6)	O(10)-Dy(1)-O(6)	O(10)-Dy(1)-O(6)	O(10)-Dy(1)-O(6)
Bond angles	Bond angles	Bond angles	Bond angles

O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)	O(3)-Dy(1)-O(1)
		6	
Bond lengths			
Er(1)-O(1)	Er(1)-O(1)	Er(1)-O(1)	Er(1)-O(1)
Er(1)-O(6)	Er(1)-O(6)	Er(1)-O(6)	Er(1)-O(6)
Er(1)-O(10)	Er(1)-O(10)	Er(1)-O(10)	Er(1)-O(10)
Er(1)-O(7)	Er(1)-O(7)	Er(1)-O(7)	Er(1)-O(7)
Er(2)-O(14)	Er(2)-O(14)	Er(2)-O(14)	Er(2)-O(14)
Er(2)-O(11)#1	Er(2)-O(11)#1	Er(2)-O(11)#1	Er(2)-O(11)#1
Er(2)-O(15)#1	Er(2)-O(15)#1	Er(2)-O(15)#1	Er(2)-O(15)#1
Er(2)-O(13)#1	Er(2)-O(13)#1	Er(2)-O(13)#1	Er(2)-O(13)#1
Bond angles			
O(1)-Er(1)-O(3)	139(4)	O(1)-Er(1)-O(6)	91(4)
O(3)-Er(1)-O(6)	102(4)	O(1)-Er(1)-O(9)	105(4)
O(3)-Er(1)-O(9)	90(4)	O(6)-Er(1)-O(9)	140(4)
O(1)-Er(1)-O(10)	74(4)	O(3)-Er(1)-O(10)	147(4)
O(6)-Er(1)-O(10)	75(4)	O(9)-Er(1)-O(10)	74(4)
O(1)-Er(1)-O(8)	75(4)	O(3)-Er(1)-O(8)	74(4)
O(6)-Er(1)-O(8)	147(4)	O(9)-Er(1)-O(8)	73(4)
O(10)-Er(1)-O(8)	126(4)	O(1)-Er(1)-O(7)	75(4)
O(3)-Er(1)-O(7)	72(4)	O(6)-Er(1)-O(7)	74(4)
O(9)-Er(1)-O(7)	146(4)	O(10)-Er(1)-O(7)	135(4)
O(8)-Er(1)-O(7)	74(4)	O(1)-Er(1)-O(5)	147(4)
O(3)-Er(1)-O(5)	73(4)	O(6)-Er(1)-O(5)	74(4)
O(9)-Er(1)-O(5)	73(4)	O(10)-Er(1)-O(5)	75(4)
O(8)-Er(1)-O(5)	132(4)	O(7)-Er(1)-O(5)	125(4)

Table S2 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **1**

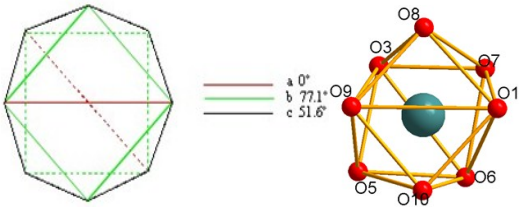


Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O9	16.963	-1.037	1.075369
46.3	O1-O7	58.849	12.549	157.477401
46.3	O1-O6	39.799	-6.501	42.263001
46.3	O9-O3	35.323	-10.977	120.494529
46.3	O9-O5	59.008	12.708	161.493264
62.2	O7-O3	66.033	3.833	14.691889
62.2	O6-O5	68.659	6.459	41.718681
69.2	O8-O7	57.495	-11.705	137.007025

69.2	O8-O3	56.951	-12.249	150.038001
69.2	O10-O6	56.347	-12.853	165.199609
69.2	O10-O5	49.828	-19.372	375.274384
88.7	O7-O6	71.307	-17.393	302.516449
88.7	O3-O5	73.687	-15.013	225.390169
64.2	O1-O8	65.613	1.413	1.996569
64.2	O1-O10	76.773	12.573	158.080329
64.2	O9-O8	75.731	11.531	132.963961
64.2	O9-O10	70.055	5.855	34.281025
0	O3-O6	19.848	19.848	393.943104

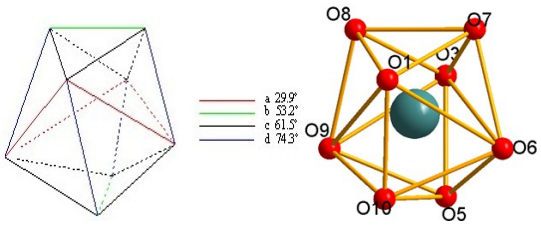
S=12.0552



Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O1-O9	16.963	16.963	287.743369
0	O6-O3	19.848	19.848	393.943104
51.6	O10-O6	56.347	4.747	22.534009
51.6	O6-O1	39.799	-11.801	139.263601
51.6	O1-O7	58.849	7.249	52.548001
51.6	O7-O8	57.495	5.895	34.751025
51.6	O8-O3	56.951	5.351	28.633201
51.6	O3-O9	35.323	-16.277	264.940729
51.6	O9-O5	59.008	7.408	54.878464
51.6	O5-O10	49.828	-1.772	3.139984
77.1	O10-O1	76.773	-0.327	0.106929
77.1	O1-O8	65.613	-11.487	131.951169
77.1	O8-O9	75.731	-1.369	1.874161
77.1	O9-O10	70.055	-7.045	49.632025
77.1	O6-O7	71.307	-5.793	33.558849
77.1	O7-O3	66.033	-11.067	122.478489
77.1	O3-O5	73.687	-3.413	11.648569
77.1	O5-O6	68.659	-8.441	71.250481

S=9.7322



Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O1-O9	16.963	-12.937	167.365969
29.9	O1-O6	39.799	9.899	97.990201
29.9	O3-O9	35.323	5.423	29.408929
29.9	O3-O6	19.848	-10.052	101.042704
74.3	O8-O9	75.731	1.431	2.047761
74.3	O1-O10	76.773	2.473	6.115729
74.3	O7-O6	71.307	-2.993	8.958049
74.3	O5-O3	73.687	-0.613	0.375769
61.5	O10-O9	70.055	8.555	73.188025
61.5	O10-O6	56.347	-5.153	26.553409
61.5	O5-O9	59.008	-2.492	6.210064
61.5	O5-O6	68.659	7.159	51.251281
61.5	O1-O8	65.613	4.113	16.916769
61.5	O1-O7	58.849	-2.651	7.027801
61.5	O3-O8	56.951	-4.549	20.693401
61.5	O3-O7	66.033	4.533	20.548089
53.2	O8-O7	57.495	4.295	18.447025
53.2	O10-O5	49.828	-3.372	11.370384
S=6.0805				

Table S3 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **2**

Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O9	17.911	0.089	0.007921
46.3	O1-O6	37.008	9.292	86.341264
46.3	O1-O7	59.261	-12.961	167.987521
46.3	O9-O3	34.525	11.775	138.650625
46.3	O9-O5	59.91	-13.61	185.2321
62.2	O7-O3	66.142	-3.942	15.539364
62.2	O6-O5	67.505	-5.305	28.143025
69.2	O8-O7	54.677	14.523	210.917529
69.2	O8-O3	57.522	11.678	136.375684
69.2	O10-O6	57.968	11.232	126.157824
69.2	O10-O5	52.049	17.151	294.156801
88.7	O7-O6	73.267	15.433	238.177489
88.7	O3-O5	73.903	14.797	218.951209
64.2	O1-O8	66.175	-1.975	3.900625

64.2	O1-O10	76.485	-12.285	150.921225
64.2	O9-O8	76.089	-11.889	141.348321
64.2	O9-O10	67.7	-3.5	12.25
0	O3-O6	20.087	-20.087	403.487569

S=12.6513

Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O9-O1	17.911	-17.911	320.803921
0	O3-O6	20.087	-20.087	403.487569
77.1	O3-O7	66.142	10.958	120.077764
77.1	O3-O5	73.903	3.197	10.220809
77.1	O6-O7	73.267	3.833	14.691889
77.1	O6-O5	67.505	9.595	92.064025
77.1	O8-O9	76.089	1.011	1.022121
77.1	O8-O1	66.175	10.925	119.355625
77.1	O10-O9	67.7	9.4	88.36
77.1	O10-O1	76.485	0.615	0.378225
51.5	O8-O3	57.522	-5.922	35.070084
51.6	O8-O7	54.677	-3.077	9.467929
51.6	O9-O3	34.525	17.075	291.555625
51.6	O9-O5	59.91	-8.31	69.0561
51.6	O1-O7	59.261	-7.661	58.690921
51.6	O1-O6	37.008	14.592	212.926464
51.6	O10-O6	57.968	-6.368	40.551424
51.6	O10-O5	52.049	-0.449	0.201601

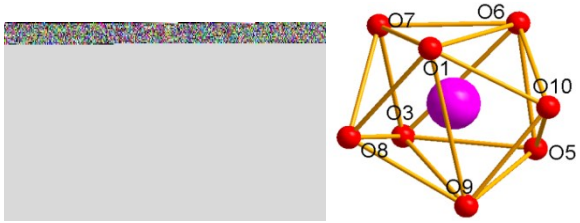
S=10.24101

Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O1-O9	17.911	11.989	143.736121
29.9	O1-O6	37.008	-7.108	50.523664
29.9	O3-O9	34.525	-4.625	21.390625
29.9	O3-O6	20.087	9.813	96.294969

53.2	O8-O7	54.677	-1.477	2.181529
53.2	O10-O5	52.094	1.106	1.223236
61.5	O3-O8	57.522	3.978	15.824484
61.5	O3-O7	66.142	-4.642	21.548164
61.5	O5-O6	67.505	-6.005	36.060025
61.5	O5-O9	59.91	1.59	2.5281
61.5	O1-O8	66.175	-4.675	21.855625
61.5	O1-O7	59.261	2.239	5.013121
61.5	O10-O9	67.4	-5.9	34.81
61.5	O10-O6	57.968	3.532	12.475024
74.3	O8-O9	76.089	-1.789	3.200521
74.3	O7-06	73.267	1.033	1.067089
74.3	O5-O3	73.903	0.397	0.157609
74.3	O1-O10	76.485	-2.185	4.774225
S=5.154793				

Table S4 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **3**

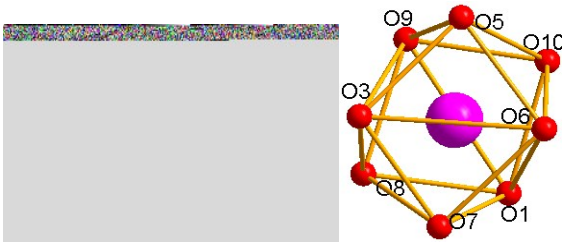


Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O9	18.239	0.239	0.057121
46.3	O1-O6	36.604	-9.696	94.012416
46.3	O1-O7	59.48	13.18	173.7124
46.3	O9-O5	60.011	13.711	187.991521
46.3	O9-O3	34.291	-12.009	144.216081
62.2	O7-O3	66.08	3.88	15.0544
62.2	O6-O5	44.738	-17.462	304.921444
69.2	O8-O7	54.325	-14.875	221.265625
69.2	O8-O3	57.737	-11.463	131.400369
69.2	O10-O6	58.09	-11.11	123.4321
69.2	O10-O5	52.227	-16.973	288.082729
88.7	O7-O6	73.316	-15.384	236.667456
88.7	O3-O5	73.893	-14.807	219.247249
64.2	O1-O10	76.574	12.374	153.115876
64.2	O1-O8	66.108	1.908	3.640464
64.2	O9-08	75.983	11.783	138.839089
64.2	09-O10	67.408	3.208	10.291264

0	O3-O6	20.493	20.493	419.963049

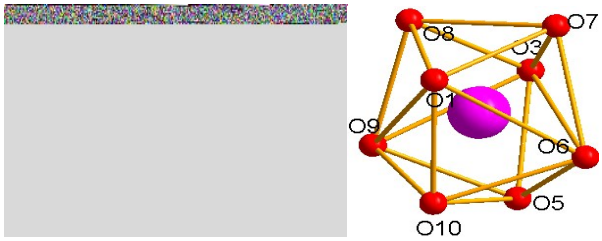
S=12.61813



Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O3-O6	20.493	20.493	419.963049
0	O9-O1	18.239	18.239	332.661121
77.1	O5-O3	73.893	-3.207	10.284849
77.1	O5-O6	67.206	-9.894	97.891236
77.1	O7-O3	66.08	-11.02	121.4404
77.1	O7-O6	73.316	-3.784	14.318656
77.1	O9-O10	67.408	-9.692	93.934864
77.1	O9-O8	75.983	-1.117	1.247689
77.1	O1-O10	76.574	-0.526	0.276676
77.1	O1-O8	66.108	-10.992	120.824064
51.5	O5-O9	60.011	8.411	70.744921
51.6	O5-O10	52.227	0.627	0.393129
51.6	O3-O9	34.291	-17.309	299.601481
51.6	O3-O8	57.737	6.137	37.662769
51.6	O6-O1	36.604	-14.996	224.880016
51.6	O6-O10	58.09	6.49	42.1201
51.6	O7-O1	59.48	7.88	62.0944
51.6	O7-O8	54.325	2.725	7.425625

S=10.42903



Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O1-O9	18.239	-11.661	135.978921
29.9	O1-O6	36.604	6.704	44.943616
29.9	O3-O9	34.291	4.391	19.280881
29.9	O3-O6	20.493	-9.407	88.491649
53.2	O8-O7	54.325	1.125	1.265625
53.2	O10-O5	52.227	-0.973	0.946729
61.5	O1-O8	66.108	4.608	21.233664

61.5	O1-O7	59.48	-2.02	4.0804
61.5	03-O8	57.737	-3.763	14.160169
61.5	03-O7	66.08	4.58	20.9764
61.5	O5-O9	60.011	-1.489	2.217121
61.5	O5-O6	67.206	5.706	32.558436
61.5	O10-O9	67.408	5.908	34.904464
61.5	O10-O6	58.09	-3.41	11.6281
74.3	O8-O9	75.983	1.683	2.832489
74.3	O7-O6	73.316	-0.984	0.968256
74.3	O1-O10	76.574	2.274	5.171076
74.3	O3-O5	73.893	-0.407	0.165649
S=4.954255				

Table S5 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **4**

Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O9	15.818	-2.182	4.761124
46.3	O1-O6	38.983	-7.317	53.538489
46.3	O1-O7	58.266	11.966	143.185156
46.3	O9-O3	37.425	-8.875	78.765625
46.3	O9-O5	31.002	-15.298	234.028804
62.2	O7-O3	67.029	4.829	23.319241
62.2	O6-O5	68.131	5.931	35.176761
69.2	O8-O7	53.566	-15.634	244.421956
69.2	O8-O3	56.535	-12.665	160.402225
69.2	O10-O6	56.178	-13.022	169.572484
69.2	O10-O5	53.92	-15.28	233.4784
88.7	O7-O6	73.653	-15.047	226.412209
88.7	O3-O5	73.631	-15.069	227.074761
64.2	O1-O8	67.256	3.056	9.339136
64.2	O1-O10	76.707	12.507	156.425049
64.2	O9-O8	76.315	12.115	146.773225
64.2	O9-O10	69.164	4.964	24.641296
0	O3-O6	17.973	17.973	323.028729
S=11.77178				

Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O9-O1	15.818	15.818	250.209124
0	O3-O6	17.973	17.973	323.028729
77.1	O3-O7	67.029	-10.071	101.425041
77.1	O3-O5	73.631	-3.469	12.033961
77.1	O6-O7	73.653	-3.447	11.881809
77.1	O6-O5	68.131	-8.969	80.442961
77.1	O8-O9	76.315	-0.785	0.616225
77.1	O8-O1	67.256	-9.844	96.904336
77.1	O10-O9	69.164	-7.936	62.980096
77.1	O10-O1	76.707	-0.393	0.154449
51.5	O8-O3	56.535	4.935	24.354225
51.6	O8-O7	53.566	1.966	3.865156
51.6	O9-O3	37.425	-14.175	200.930625
51.6	O9-O5	31.002	-20.598	424.277604
51.6	O1-O7	58.266	6.666	44.435556
51.6	O1-O6	38.983	-12.617	159.188689
51.6	O10-O6	56.178	4.578	20.958084
51.6	O10-O5	53.92	2.32	5.3824

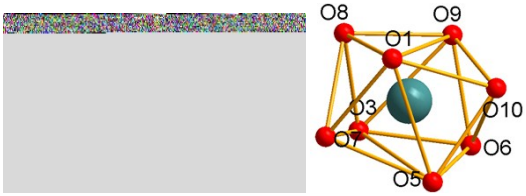
S=10.06388

Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O1-O9	15.818	-14.082	198.302724
29.9	O1-O6	38.983	9.083	82.500889
29.9	O3-O9	37.425	7.525	56.625625
29.9	O3-O6	17.973	-11.927	142.253329
53.2	O8-O7	53.566	0.366	0.133956
53.2	O10-O5	53.92	0.72	0.5184
61.5	O3-O8	56.535	-4.965	24.651225
61.5	O3-O7	67.029	5.529	30.569841
61.5	O5-O6	68.131	6.631	43.970161
61.5	O5-O9	31.002	-30.498	930.128004

61.5	O1-O8	67.256	5.756	33.131536
61.5	O1-O7	58.266	-3.234	10.458756
61.5	O10-O9	69.164	7.664	58.736896
61.5	O10-O6	56.178	-5.322	28.323684
74.3	O8-O9	76.315	2.015	4.060225
74.3	O7-06	73.653	-0.647	0.418609
74.3	O5-O3	73.631	-0.669	0.447561
74.3	O1-O10	76.707	2.407	5.793649
S=9.577245				

Table S6 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **5**



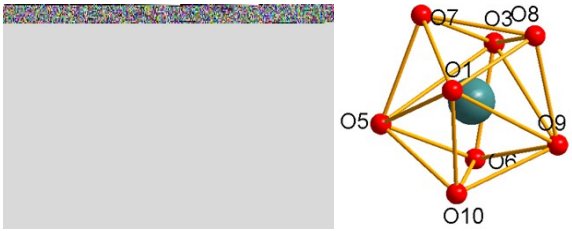
Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O5	32.933	14.933	222.994489
46.3	O1-O8	67.187	20.887	436.266769
46.3	O1-O9	19.086	-27.214	740.601796
46.3	O5-O3	20.476	-25.824	666.878976
46.3	O5-O6	66.185	19.885	395.413225
62.2	O3-O8	57.922	-4.278	18.301284
62.2	O6-O9	62.204	0.004	1.6E-05
69.2	O10-O9	66.589	-2.611	6.817321
69.2	O10-O6	51.596	-17.604	309.900816
69.2	O7-O8	51.615	-17.585	309.232225
69.2	O7-O3	67.784	-1.416	2.005056
88.7	O8-O9	76.352	-12.348	152.473104
88.7	O3-O6	74.737	-13.963	194.965369
64.2	O1-O7	60.905	-3.295	10.857025
64.2	O1-O10	75.965	11.765	138.415225
64.2	O5-O7	74.257	10.057	101.143249
64.2	O5-O10	61.429	-2.771	7.678441
0	O3-O9	64.861	64.861	4206.949321
S=20.97736				

Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O9-O3	31.794	31.794	1010.85844
0	O1-O5	32.933	32.933	1084.58249
77.1	O9-O8	76.352	-0.748	0.559504
77.1	O3-O8	57.922	-19.178	367.795684
77.1	O1-O7	60.905	-16.195	262.278025
77.1	O1-O10	75.965	-1.135	1.288225
77.1	O5-O7	74.257	-2.843	8.082649
77.1	O5-O10	61.429	-15.671	245.580241
77.1	O6-O9	62.204	-14.896	221.890816
77.1	O6-O3	74.737	-2.363	5.583769
51.5	O8-O1	67.187	15.587	242.954569
51.6	O8-O7	51.615	0.015	0.000225
51.6	O9-O1	19.086	-32.514	1057.1602
51.6	O9-O10	66.589	14.989	224.670121
51.6	O3-O7	67.784	16.184	261.921856
51.6	O3-O5	20.476	-31.124	968.703376
51.6	O6-O5	66.185	14.585	212.722225
51.6	O6-O10	51.596	-0.004	1.6E-05

S=18.5242

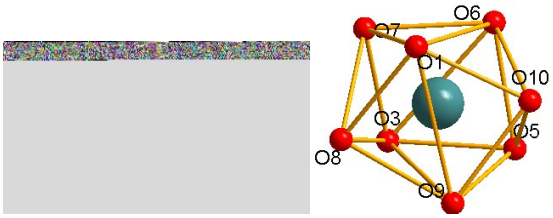


Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O3-O6	20.047	-9.853	97.081609
29.9	O1-O5	32.933	3.033	9.199089
29.9	O1-O9	19.086	-10.814	116.942596
29.9	O3-O5	20.476	-9.424	88.811776
53.2	O3-O9	31.794	1.894	3.587236
53.2	O7-O8	51.615	-1.585	2.512225
61.5	O10-O6	66.589	13.389	179.265321
61.5	O3-O8	57.922	-3.578	12.802084
61.5	O3-O7	67.784	6.284	39.488656
61.5	O1-O8	67.187	5.687	32.341969
61.5	O1-O7	60.905	-0.595	0.354025
61.5	O6-O9	62.204	0.704	0.495616
61.5	O6-O5	66.185	4.685	21.949225
61.5	O5-O10	61.429	-0.071	0.005041
74.3	O1-O8	67.187	5.687	32.341969
74.3	O8-O9	76.352	2.052	4.210704

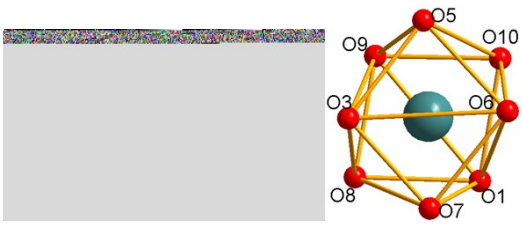
74.3	O6-O3	74.737	0.437	0.190969
74.3	O1-O10	75.965	1.665	2.772225
S=5.513985				

Table S7 The observed dihedral angle between planes along the *i*th edge(θ_i), the dihedral angle for the ideal structure(δ_i) and the estimated S values of complex **6**



Distorted bicapped trigonal prismatic

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
18	O1-O9	18.331	0.331	0.109561
46.3	O1-O7	59.319	13.019	169.494361
46.3	O1-O6	35.76	-10.54	111.0916
46.3	O9-O3	34.186	-12.114	146.748996
46.3	O9-O5	60.344	14.044	197.233936
62.2	O6-O5	66.667	4.467	19.954089
62.2	O7-O3	66.302	4.102	16.826404
69.2	O8-O7	53.233	-15.967	254.945089
69.2	O8-O3	57.958	-11.242	126.382564
69.2	O10-O6	46.656	-22.544	508.231936
69.2	O10-O5	53.444	-15.756	248.251536
88.7	O7-O6	74.158	-14.542	211.469764
88.7	O3-O5	19.013	-69.687	4856.277969
64.2	O1-O8	66.653	2.453	6.017209
64.2	O1-O10	76.406	12.206	148.986436
64.2	O9-O8	76.21	12.01	144.2401
64.2	O9-O5	60.344	-3.856	14.868736
0	O6-O3	20.047	20.047	401.882209
S=20.52507				

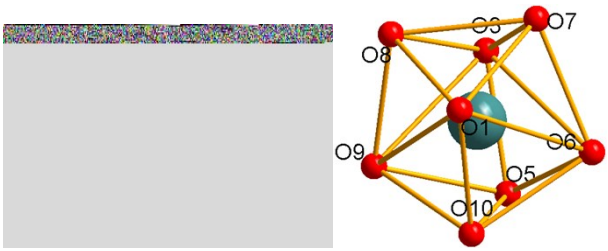


Square antiprism

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
0	O9-O1	18.331	18.331	336.025561
0	O3-O6	20.047	20.047	401.882209
77.1	O5-O3	74.277	-2.823	7.969329

77.1	O5-O6	66.667	-10.433	108.847489
77.1	O7-O3	66.302	-10.798	116.596804
77.1	O7-O6	74.158	-2.942	8.655364
77.1	O9-O10	66.441	-10.659	113.614281
77.1	O9-O8	76.21	-0.89	0.7921
77.1	O1-O10	76.406	-0.694	0.481636
77.1	O1-O8	66.653	-10.447	109.139809
51.5	O5-O10	46.154	-5.446	29.658916
51.6	O5-O9	60.344	8.744	76.457536
51.6	O6-O10	58.545	6.945	48.233025
51.6	O6-O1	35.76	-15.84	250.9056
51.6	O3-O9	34.186	-17.414	303.247396
51.6	O3-O8	57.958	6.358	40.424164
51.6	O7-O1	59.319	7.719	59.582961
51.6	O7-O8	53.233	1.633	2.666689

S=10.58086



Distorted dodecahedron geometry

θ_i(°)	Edge	δ_i(°)	δ_i-θ_i(°)	(δ_i-θ_i)^2
29.9	O3-O6	20.047	-9.853	97.081609
29.9	O3-O9	34.186	4.286	18.369796
29.9	O1-O9	18.331	-11.569	133.841761
29.9	O1-O6	35.76	5.86	34.3396
53.2	O8-O7	53.233	0.033	0.001089
53.2	O10-O5	53.444	0.244	0.059536
61.5	O3-O8	57.958	-3.542	12.545764
61.5	O3-O7	66.302	4.802	23.059204
61.5	O5-O6	66.667	5.167	26.697889
61.5	O5-O9	60.344	-1.156	1.336336
61.5	O1-O7	59.319	-2.181	4.756761
61.5	O1-O8	66.653	5.153	26.553409
61.5	O10-O9	66.441	4.941	24.413481
61.5	O10-O6	58.545	-2.955	8.732025
74.3	O1-O10	76.406	2.106	4.435236
74.3	O8-O9	76.21	1.91	3.6481
74.3	O7-O6	74.158	-0.142	0.020164
74.3	O5-O3	74.277	-0.023	0.000529

S=4.82983