

Two- and Three-Dimensional Networks of Lanthanide with Mixed Dicarboxylate Ligands: Syntheses, Crystal Structures and Photoluminescent Properties

Qing-Feng Yang,^a Yang Yu,^a Tian-You Song,^a Jie-Hui Yu,^a Xiao Zhang,^b Ji-Qing Xu^{*a} and Tie-Gang Wang^a

^a College of Chemistry and State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, Jilin, 130021, China. Fax: +86-431-85168624; Tel: +86-431-88499132; E-mail: xjq@mail.jlu.edu.cn

^b Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute Technology, Harbin, Heilongjiang, 150080, China.

Table S1 Selected bond lengths (Å) for **1–10**.

1					
Ce(1)–O(1)	2.4771(16)	Ce(1)–O(3)#4	2.5677(15)	Ce(1)–O(6)#3	2.5268(15)
Ce(1)–O(1)#1	2.6573(13)	Ce(1)–O(4)#4	2.5474(15)	Ce(1)–O(7)	2.4772(16)
Ce(1)–O(2)#1	2.5660(14)	Ce(1)–O(5)	2.5008(16)	Ce(1)–O(8)	2.5070(15)
2					
Pr(1)–O(1)	2.516(2)	Pr(1)–O(4)#1	2.633(2)	Pr(1)–O(6)#2	2.481(2)
Pr(1)–O(2)	2.546(2)	Pr(1)–O(4)#4	2.459(2)	Pr(1)–O(7)	2.489(3)
Pr(1)–O(3)#1	2.543(2)	Pr(1)–O(5)	2.506(2)	Pr(1)–O(8)	2.465(3)
3					
Nd(1)–O(1)	2.5252(19)	Nd(1)–O(4)#1	2.615(2)	Nd(1)–O(6)#2	2.493(2)
Nd(1)–O(2)	2.503(2)	Nd(1)–O(4)#3	2.443(2)	Nd(1)–O(7)	2.439(2)
Nd(1)–O(3)#1	2.5249(19)	Nd(1)–O(5)	2.464(2)	Nd(1)–O(8)	2.465(2)
4					
Sm(1)–O(1)	2.492(3)	Sm(1)–O(3)#1	2.496(3)	Sm(1)–O(6)#2	2.470(3)
Sm(1)–O(2)	2.612(3)	Sm(1)–O(4)#1	2.479(3)	Sm(1)–O(7)	2.413(3)
Sm(1)–O(2)#3	2.417(3)	Sm(1)–O(5)	2.441(3)	Sm(1)–O(8)	2.439(4)
5					
Eu(1)–O(1)	2.487(4)	Eu(1)–O(3)#1	2.480(4)	Eu(1)–O(6)#2	2.457(4)
Eu(1)–O(2)	2.599(4)	Eu(1)–O(4)#1	2.463(4)	Eu(1)–O(7)	2.401(4)
Eu(1)–O(2)#3	2.409(4)	Eu(1)–O(5)	2.432(4)	Eu(1)–O(8)	2.432(4)
6					
Gd(1)–O(1)	2.471(3)	Gd(1)–O(4)	2.423(3)	Gd(1)–O(7)	2.592(3)
Gd(1)–O(2)#1	2.456(3)	Gd(1)–O(5)#2	2.451(3)	Gd(1)–O(7)#3	2.391(3)
Gd(1)–O(3)#1	2.471(3)	Gd(1)–O(6)	2.385(3)	Gd(1)–O(8)	2.408(3)
7					
Tb(1)–O(2)	2.366(3)	Tb(1)–O(8)	2.397(4)	K(1)–O(6)	2.932(4)
Tb(1)–O(3)	2.388(4)	Tb(1)–O(9)	2.372(4)	K(1)–O(7)#5	2.718(4)

Tb(1)–O(4)#9	2.366(3)	K(1)–O(1)#2	3.079(4)	K(1)–O(8)	2.865(4)
Tb(1)–O(5)	2.406(3)	K(1)–O(2)	3.092(4)	K(1)–O(9)#5	2.985(4)
Tb(1)–O(6)	2.429(3)	K(1)–O(2)#2	3.057(4)		
Tb(1)–O(7)	2.359(3)	K(1)–O(3)#5	3.112(4)		
8					
Dy(1)–O(2)	2.356(3)	Dy(1)–O(8)	2.383(3)	K(1)–O(6)	2.930(3)
Dy(1)–O(3)	2.382(3)	Dy(1)–O(9)	2.359(3)	K(1)–O(7)#5	2.713(3)
Dy(1)–O(4)#8	2.350(3)	K(1)–O(1)#2	3.079(4)	K(1)–O(8)	2.864(4)
Dy(1)–O(5)	2.396(3)	K(1)–O(2)	3.082(4)	K(1)–O(9)#5	2.972(4)
Dy(1)–O(6)	2.424(3)	K(1)–O(2)#2	3.059(3)		
Dy(1)–O(7)	2.336(3)	K(1)–O(3)#5	3.092(4)		
9					
Ce(1)–O(1)	2.395(3)	Ce(2)–O(3)#6	2.362(3)	Ce(2)–O(14)	2.540(3)
Ce(1)–O(2)#5	2.472(3)	Ce(2)–O(4)#7	2.451(3)	K(1)–O(2)#5	2.655(3)
Ce(1)–O(7)#1	2.505(3)	Ce(2)–O(5)	2.472(3)	K(1)–O(6)#8	2.698(3)
Ce(1)–O(10)	2.499(3)	Ce(2)–O(7)#1	2.771(3)	K(1)–O(14)#2	2.906(3)
Ce(1)–O(11)#3	2.424(3)	Ce(2)–O(8)#1	2.583(3)	K(1)–O(1W)	2.806(3)
Ce(1)–O(12)#4	2.441(3)	Ce(2)–O(9)	2.616(3)	K(1)–O(2W)	2.761(4)
Ce(1)–O(13)	2.656(3)	Ce(2)–O(10)	2.686(3)	K(1)–O(3W)	2.632(4)
Ce(1)–O(1W)	2.577(3)	Ce(2)–O(13)	2.626(3)		
10					
Pr(1)–O(2)	2.474(3)	Pr(2)–O(1)	2.520(3)	Pr(2)–O(14)#2	2.560(3)
Pr(1)–O(7)	2.489(3)	Pr(2)–O(2)	2.787(4)	K(1)–O(4)#3	2.436(4)
Pr(1)–O(9)#3	2.465(3)	Pr(2)–O(3)#5	2.484(4)	K(1)–O(9)#3	2.397(4)
Pr(1)–O(10)#7	2.400(3)	Pr(2)–O(5)	2.434(3)	K(1)–O(13)#2	2.861(4)
Pr(1)–O(11)#8	2.431(3)	Pr(2)–O(6)#6	2.326(3)	K(1)–O(15)	2.561(4)
Pr(1)–O(12)#10	2.395(3)	Pr(2)–O(7)	2.663(3)	K(1)–O(16)	2.414(4)
Pr(1)–O(14)#2	2.692(3)	Pr(2)–O(8)	2.579(3)	K(1)–O(17)	2.395(4)
Pr(1)–O(15)	2.580(3)	Pr(2)–O(13)	2.498(3)		

Symmetry codes:

- 1** #1 –x + 1/2, –y –1/2, –z + 1; #3 –x + 1, –y –1, –z + 1; #4 x, y –1, z;
2 #1 –x + 1/2, –y + 3/2, –z + 1; #2 –x, –y + 1, –z + 1; #4 x, y –1, z;
3 #1 –x + 1/2, –y + 3/2, –z + 2; #2 –x, –y + 2, –z + 2; #3 x, y + 1, z;
4 #1 –x + 1/2, –y –1/2, –z + 1; #2 –x, –y, –z + 1; #3 –x + 1/2, –y + 1/2, –z + 1;
5 #1 –x + 1/2, –y + 3/2, –z + 1; #2 –x, –y + 1, –z + 1; #3 –x + 1/2, –y + 1/2, –z + 1;
6 #1 –x + 3/2, –y + 1/2, –z; #2 –x + 1, –y + 1, –z; #3 –x + 3/2, –y + 3/2, –z;
7 #2 –x + 1, –y + 1, –z; #5 x, y + 1, z; #9 x –1, y, z;
8 #2 –x + 1, –y + 1, –z + 2; #5 x, y –1, z; #8 x + 1, y, z;
9 #1 –x + 2, –y + 2, –z + 2; #2 –x + 1, –y + 1, –z + 2; #3 x + 1, y, z; #4 –x, –y + 1, –z + 1; #5 –x + 1, –y + 1, –z + 1; #6 x, y, z + 1; #7 –x + 1, –y + 2, –z + 1; #8 –x + 2, –y + 1, –z + 2;
10 #2 –x, –y + 2, –z + 1; #3 x, y + 1, z; #5 –x + 1, –y + 1, –z + 1; #6 –x, –y + 1, –z + 1; #7 –x + 1, –y + 1, –z; #8 –x, –y + 2, –z; #10 x + 1, y, z.

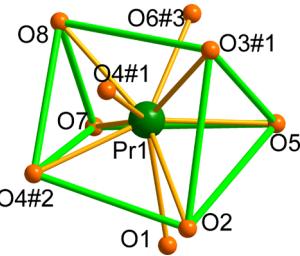


Fig. S1 The distorted tricapped trigonal prism coordination polyhedron of Pr(III) ion in **2**.

Symmetry code: #1, $0.5 - x, 1.5 - y, 1 - z$; #2, $x, -1 + y, z$; #3, $-x, 1 - y, 1 - z$.

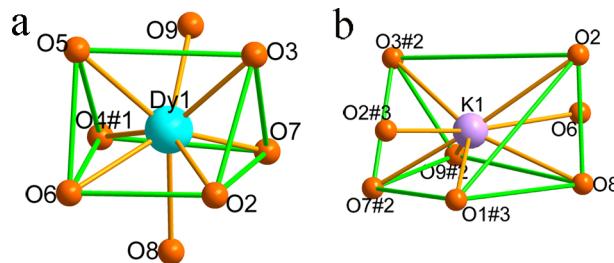


Fig. S2 The distorted bicapped trigonal prism coordination polyhedra of Dy(III) ion (a) and K^+ (b)

in **8**. Symmetry code: #1, $1 + x, y, z$; #2, $x, -1 + y, z$.

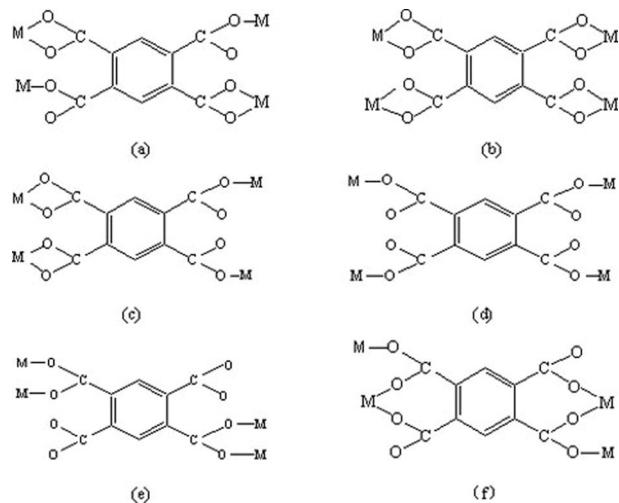


Fig. S3 μ_4 coordination modes of pma ligand in transition metal and lanthanide complexes (a-e being in reported complexes and f in compounds **7** and **8**).

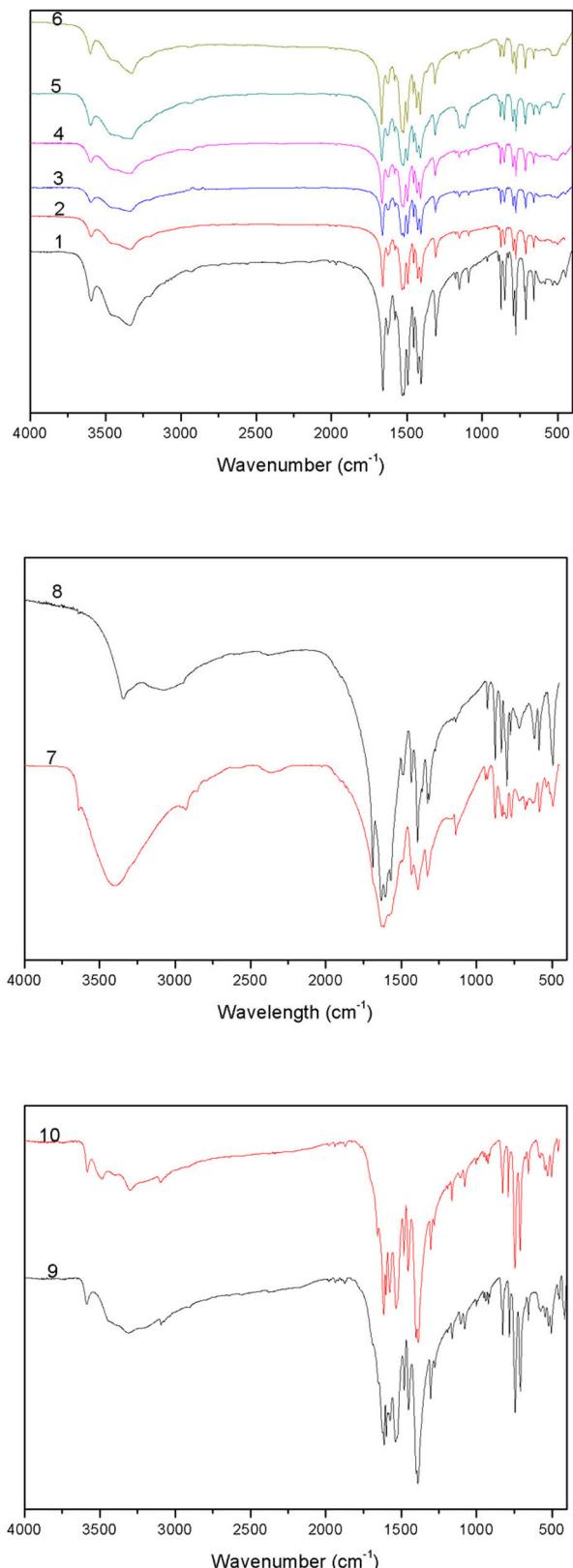


Fig. S4 The IR spectra of complexes **1-10**.