Study on structure of Pr compound, Pr (C_3 H_6O_9)·2(H_2O)

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Abstract. A Pr compound $Pr(C_3O_9H_6)\cdot 2(H_2O)$ has been synthesized from a hydrothermal reaction and the crystal structure has been determined by means of single-crystal X-ray diffraction. The Pr atom is coordinated by nine O atoms. The Pr compound exhibits extensive O-H…O hydrogen-bonding interactions.

1. Introduction

Metal coordination polymers have attracted much attention due to their varieties of structures and potential applications as new materials for molecular recognition, ion exchange, catalysis, and luminescence [1-5]. Lanthanide coordination polymers have attracted interest due to larger coordination spheres, and unique magnetic and luminescence properties [6, 7]. Carboxylate groups coordinate to lanthanide ions in different method, chelating bidentate, bridging bidentate and bridging tridentate, leading to different structures of lanthanide carboxylate complexes [8, 9]. In this paper, the novel Pr complex is reported.

2. Experimental

All commercially obtained reagent-grade chemicals were used without further purication. A mixture of $Pr(NO_3)_3\cdot 6(H_2O)$ (0.1mmol, 0.044g), 2,6-bipyridine dicarboxylic acid (0.1mmol, 0.02g), H_3BO_3 (0.2mmol, 0.012g) and $(NH_4)_2C_2O_4$ (0.2mmol, 0.028g) were added into 10 mL water with 10%(v/v) ethanol and heated for 9h at 393K. The solution was obtained by filtration after cooling the reaction to room temperature. Colorless single crystals suitable for X-ray measurements were obtained after a few weeks.

3. Results and discussions

The title complex crystal structure is shown in Fig.1. The crystal data and structure refinement is shown in Table 1. The Pr atom is coordinated by nine O atoms from three oxalic acid and three water molecular. One oxalic acid molecular bridges two Gd atoms. The Pr-O distances are in the range of 2.470-2.576 Å. The angles of O-Pr-O are in the range of 62.8-143.9°. Selected bond lengths and bond angles are shown in Table 2.

The molecular structure stabilized by the O-H…O hydrogen bonding interactions.

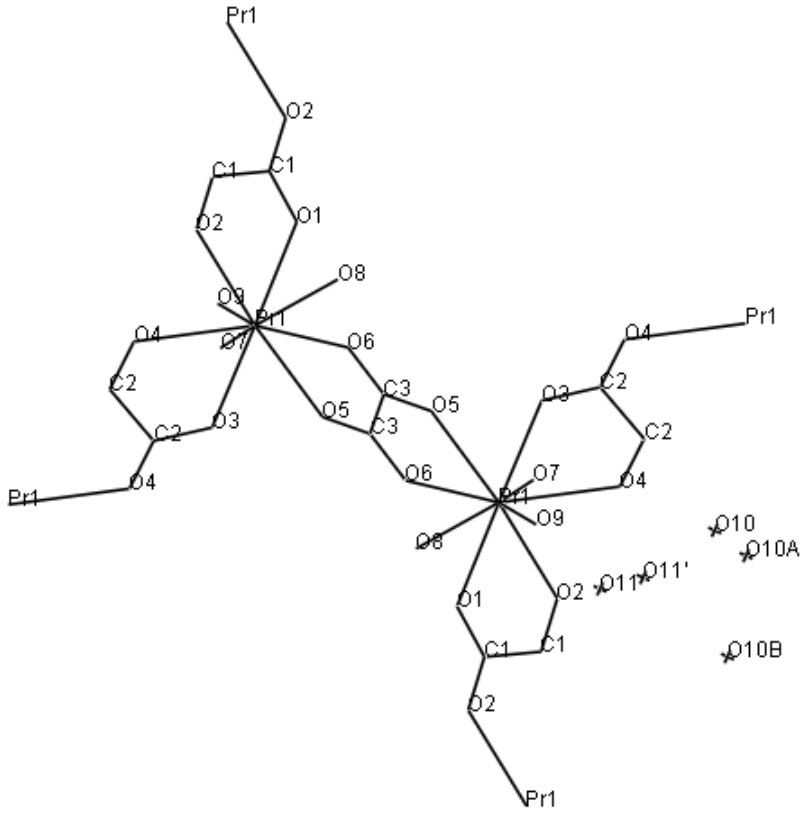

Fig.1 The molecular structure of $Pr(C_3O_9H_6)\cdot 2(H_2O)$

Table 1. Crystal data and structure refinement for the title complex.

Formula		$C_3H_6O_9Pr\ 2(H_2O)$	
Formula Weight		358.99	
Crystal System		Monoclinic	
Space group		P21/c	
a, b, c [Å]	11.2574(15)	9.6493(13)	10.3557(15)
alpha, beta, gamma [°]	90	114.666(3)	90
V [$Å^3$]		1022.3(2)	
Z		4	
D(calc) [g/cm^3]		2.332	
Mu(MoKa) [/mm]		4.811	
F(000)		684	
Crystal Size [mm]		0.09 x 0.12 x 0.13	
Data Collection			
Temperature (K)		296	
Radiation [Å]		MoKa 0.71073	
Theta Min-Max [°]		2.0, 25.0	
Dataset		0: 13 ; -11: 0 ; -12: 11	
Tot., Uniq. Data, R(int)		1752, 1752, 0.000	
Observed data [I > 2.0 sigma(I)]		1278	
Refinement			
Nref, Npar		1752, 142	
R, wR2, S		0.0505, 0.1380, 1.07	
$w = 1/[\s^2(Fo^2)+(0.0819P)^2]$		where $P=(Fo^2+2Fc^2)/3$	
Max. and Av. Shift/Error		0.01, 0.00	
Min. and Max. Resd. Dens. [$e/Å^3$]		-1.23, 1.65	

Table 2. Select bond lengths [Å] and angles [°] for the title complex.

Pr1	-O1	2.524(10)	O4	-C2	1.234(18)
Pr1	-O3	2.528(11)	O5	-C3	1.272(15)
Pr1	-O5	2.518(8)	O6	-C3	1.266(17)
Pr1	-O7	2.502(10)	O7	-H7A	0.8600
Pr1	-O8	2.549(11)	O7	-H7B	0.8500
Pr1	-O9	2.511(10)	O8	-H8A	0.8500
Pr1	-O6_a	2.470(9)	O8	-H8B	0.8500
Pr1	-O4_b	2.576(10)	O9	-H9B	0.8500
Pr1	-O2_c	2.489(9)	O9	-H9A	0.8500
O1	-C1	1.246(16)	C1	-C1_c	1.533(17)
O2	-C1	1.242(17)	C2	-C2_b	1.539(18)
O3	-C2	1.267(17)	C3	-C3_a	1.531(18)

O1 -Pr1 -O3	137.1(3)	O4_b -Pr1 -O8	135.8(3)
O1 -Pr1 -O5	125.0(3)	O2_c -Pr1 -O8	80.8(3)
O1 -Pr1 -O7	126.5(3)	O6_a -Pr1 -O9	75.4(3)
O1 -Pr1 -O8	69.0(3)	O4_b -Pr1 -O9	74.5(3)
O1 -Pr1 -O9	67.9(3)	O2_c -Pr1 -O9	88.7(3)
O1 -Pr1 -O6_a	71.6(3)	O4_b -Pr1 -O6_a	140.9(3)
O1 -Pr1 -O4_b	117.9(3)	O2_c -Pr1 -O6_a	136.2(3)
O1 -Pr1 -O2_c	64.6(3)	O2_c -Pr1 -O4_b	67.0(3)
O3 -Pr1 -O5	70.5(3)	Pr1 -O1 -C1	120.0(8)
O3 -Pr1 -O7	95.3(3)	Pr1_c -O2 -C1	120.4(8)
O3 -Pr1 -O8	143.9(3)	Pr1 -O3 -C2	123.4(9)
O3 -Pr1 -O9	71.9(3)	Pr1_b -O4 -C2	120.6(8)
O3 -Pr1 -O6_a	84.5(3)	Pr1 -O5 -C3	119.6(8)
O3 -Pr1 -O4_b	62.8(3)	Pr1_a -O6 -C3	120.9(8)
O2_c -Pr1-O3	129.2(3)	Pr1 -O7 -H7B	112.00
O5 -Pr1 -O7	74.6(3)	H7A -O7 -H7B	125.00
O5 -Pr1 -O8	73.6(3)	Pr1 -O7 -H7A	114.00
O5 -Pr1 -O9	127.0(3)	H8A -O8 -H8B	109.00
O5 -Pr1 -O6_a	65.2(3)	Pr1 -O8 -H8A	110.00
O4_b -Pr1 -O5	117.1(3)	Pr1 -O8 -H8B	111.00
O2_c-Pr1-O5	144.3(3)	Pr1 -O9 -H9B	111.00
O7 -Pr1 -O8	72.2(4)	Pr1 -O9 -H9A	111.00
O7 -Pr1 -O9	144.7(3)	H9A -O9 -H9B	109.00
O6_a -Pr1 -O7	137.4(3)	O1 -C1 -O2	125.1(12)
O4_b -Pr1-O7	70.5(3)	O2 -C1 -C1_c	118.4(11)
O2_c-Pr1-O7	74.1(3)	O1 -C1 -C1_c	116.5(12)
O8 -Pr1 -O9	136.1(4)	O3 -C2 -C2_b	114.7(13)
O6_a -Pr1-O8	83.2(3)	O4 -C2 -C2_b	118.5(12)

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