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Research Article

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Study on novel structure of Pr complex, $C_{14}H_{19}PrN_2O_{14}$

Hai-Xing Liu[1,*], Zhang-Xue Yu[1], Yu-Feng Li[1], Lin-Tong Wang[1], Kai-Qi Ye[2] and Hui Cao[3]

[1]*College of Chemistry and Chemical Engineering, Weifang University, Weifang, P.R. China*
[2]*College of Chemistry, State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, P.R. China*
[3]*College of Biological Engineering, Weifang University, Weifang, P.R. China*

ABSTRACT

A novel Pr complex $C_{14}H_{11}PrN_2O_{10}\bullet4(H_2O)$ has been synthesized from a hydrothermal reaction and the crystal structure has been determined by means of single-crystal X-ray diffraction. Monoclinic, P2(1). a=14.078(3) Å, b = 11.250(2) Å, c =12.957(3) Å, $\alpha = 90^\circ$, $\beta = 102.00(3)^\circ$, $\gamma = 90^\circ$. V=2007.3(7) Å^3. Z=4. R_1 =0.0371, wR_2 =0.0897, T=293(2) K. The Pr atom is nine-coordinated by two N atoms from two 2,6-pyridine dicarboxylic acid moleculars and seven O atoms. The molecular structure stabilized by the O-H…O hydrogen-bonding interactions.

Keywords: Pr complex; structure analysis; hydrogen bonding

INTRODUCTION

Receptors are usually designed to recognise desired guest molecules based on hydrogen bonding interactions between the functional groups of hosts and guests [1-3]. Dicarboxylic acids and their complex have attracted the attention owing to their wide role in many biological processes. In solid state, the arrangements of differently designed receptors and guests containing carboxylic acid moiety are important in supramolecular chemistry and crystal engineering [4-9]. Coordination bonding, hydrogen bonding, π–π stacking interactions and electrostatic interactions are all responsible for the architectures of supramolecules in many cases [10-12]. Pyridine-2,6-dicarboxylic acid is known to constitute a stable chelate with metal ions and oxometal cations and can still display widely varying coordination demeanour functioning as a bidentate, tridentate, meridian or bridging ligand [13, 14]. It is a versatile N–O-chelating agent with limited steric hindrance and can further provide the ability to form polymeric complexes by bridging interaction under suitable conditions [15-19]. Lanthanide complexes have received attention due to a wide field of applications [20-22]. Some lanthanide complexes are biological probes for medical diagnosis and drug development [23, 24]. In this paper, the Pr complex is reported.

EXPERIMENTAL SECTION

All commercially obtained reagent-grade chemicals were used without further purication. A mixture of $Pr(NO_3)_36H_2O$ (0.01 mmol, 0.004g), 2,6-bipyridine dicarboxylic acid (0.1mmol, 0.02g), boric acid (0.2mmol, 0.012g) and salicylic acid (0.1mmol, 0.014g) were added into 10 mL water with 10%(v/v) ethanol and heated for 10h at 403K. 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.

The crystal data was collected on a Bruker smart CCD Area Detector.
A colorless block single crystal with dimensions of 0.43 x 0.40 x 0.39 mm was selected for measurement. Diffraction data of the single crystal were collected by ψ-ω scan mode using a graphite-monochromatic Mo *K*α

rediation (λ=0.71073 Å) at 293(2) K on a Bruker Smart Apex CCD diffractometer.

RESULTS AND DISCUSSION

The title complex crystal structure is shown in Fig.1. It is built up Pr cation, two 2,6-pyridine dicarboxylic acid anion and water molecular. The crystal data and structure refinement is shown in Table 1. The Pr atom is nine-coordinated by two N atoms from two 2,6-pyridine dicarboxylic acid moleculars and seven O atoms. The distances d(Pr-O) are in the range of 2.451-2.559 Å. The bond lengths d(Pr-N) are 2.619 and 2.621 Å. The angles of O3-Pr1-O6, N1-Pr1-N2, O9-Pr1-N2 are 82.76, 111.88, 133.62°, respectively. The torsion angles of O8-Pr1-N1-C1, N2-Pr1-N1-C5, O6-Pr1-O3-C6 are 23.6, 117.8, 68.1, respectively. Selected bond lengths and bond angles are shown in Table 2.

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

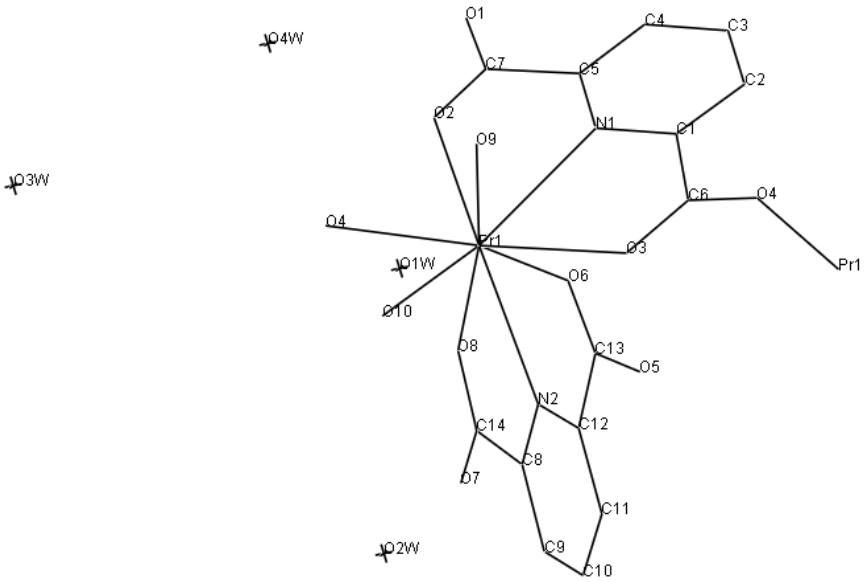

Fig.1 The molecular structure of $C_{14}H_{19}N_2O_{14}Pr$

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

Empirical formula	$C_{14}H_{19}N_2O_{14}Pr$
Formula weight	580.22
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 14.078(3) Å alpha = 90°. b = 11.250(2) Å beta = 102.00(3)°. c = 12.957(3) Å gamma = 90°.
Volume	2007.3(7) $Å^3$
Z, Calculated density	4, 1.920 Mg/m^3
Absorption coefficient	2.504 mm^{-1}
F(000)	1152
Crystal size	0.43 x 0.40 x 0.39 mm
Theta range for data collection	3.01 to 25.04°.
Limiting indices	-16<=h<=16, -13<=k<=13, -13<=l<=15
Reflections collected / unique	15256 / 3551 [R(int) = 0.0670]
Completeness to theta = 25.04	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4417 and 0.4123
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3551 / 0 / 280
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0892
R indices (all data)	R1 = 0.0377, wR2 = 0.0897
Largest diff. peak and hole	2.617 and -1.439 e. $Å^{-3}$

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

Pr(1)-O(9)	2.451(3)
Pr(1)-O(8)	2.480(2)
Pr(1)-O(10)	2.485(3)
Pr(1)-O(2)	2.514(2)
Pr(1)-O(3)	2.545(3)
Pr(1)-O(6)	2.559(2)
Pr(1)-N(1)	2.619(3)
Pr(1)-N(2)	2.621(3)
N(1)-C(1)	1.337(4)
N(1)-C(5)	1.338(4)
N(2)-C(8)	1.333(5)
N(2)-C(12)	1.335(5)
O(1)-C(7)	1.245(4)
O(2)-C(7)	1.264(4)
O(3)-C(6)	1.263(4)
O(4)-C(6)	1.250(4)
O(5)-C(13)	1.288(5)
O(5)-H(5)	0.8200
O(6)-C(13)	1.224(5)
O(7)-C(14)	1.240(4)
O(8)-C(14)	1.264(4)
C(1)-C(2)	1.396(5)
C(1)-C(6)	1.507(4)
C(2)-C(3)	1.375(5)
C(3)-C(4)	1.385(5)
C(4)-C(5)	1.390(5)
C(5)-C(7)	1.512(5)
C(8)-C(9)	1.388(6)
C(8)-C(14)	1.517(5)
C(9)-C(10)	1.377(7)
C(10)-C(11)	1.371(7)
C(11)-C(12)	1.388(6)
C(12)-C(13)	1.502(5)
O(9)-Pr(1)-O(8)	80.58(9)
O(9)-Pr(1)-O(4)#1	72.33(9)
O(8)-Pr(1)-O(4)#1	75.57(9)
O(9)-Pr(1)-O(10)	141.73(9)
O(8)-Pr(1)-O(10)	98.02(10)
O(4)#1-Pr(1)-O(10)	70.36(8)
O(9)-Pr(1)-O(2)	85.98(9)
O(8)-Pr(1)-O(2)	153.03(8)
O(4)#1-Pr(1)-O(2)	78.11(8)
O(10)-Pr(1)-O(2)	78.39(10)
O(9)-Pr(1)-O(3)	72.55(9)
O(8)-Pr(1)-O(3)	75.72(8)
O(4)#1-Pr(1)-O(3)	137.47(8)
O(10)-Pr(1)-O(3)	144.61(9)
O(2)-Pr(1)-O(3)	122.20(8)
O(9)-Pr(1)-O(6)	140.53(9)
O(8)-Pr(1)-O(6)	122.95(9)
O(4)#1-Pr(1)-O(6)	139.60(9)
O(10)-Pr(1)-O(6)	71.51(9)
O(2)-Pr(1)-O(6)	81.68(8)
O(3)-Pr(1)-O(6)	82.76(8)
O(9)-Pr(1)-N(1)	75.48(9)
O(8)-Pr(1)-N(1)	135.20(8)
O(4)#1-Pr(1)-N(1)	129.43(8)
O(10)-Pr(1)-N(1)	123.98(10)
O(2)-Pr(1)-N(1)	61.57(8)
O(3)-Pr(1)-N(1)	61.25(8)
O(6)-Pr(1)-N(1)	65.65(8)
O(9)-Pr(1)-N(2)	133.62(9)
O(8)-Pr(1)-N(2)	61.95(8)
O(4)#1-Pr(1)-N(2)	118.62(9)
O(10)-Pr(1)-N(2)	73.97(10)
O(2)-Pr(1)-N(2)	139.05(9)
O(3)-Pr(1)-N(2)	72.46(10)
O(6)-Pr(1)-N(2)	61.27(8)
N(1)-Pr(1)-N(2)	111.88(9)
C(1)-N(1)-C(5)	119.1(3)
C(1)-N(1)-Pr(1)	120.8(2)
C(5)-N(1)-Pr(1)	118.5(2)
C(8)-N(2)-C(12)	118.5(3)

C(8)-N(2)-Pr(1)	120.0(2)
C(12)-N(2)-Pr(1)	121.4(2)
C(7)-O(2)-Pr(1)	124.6(2)
C(6)-O(3)-Pr(1)	126.0(2)
C(6)-O(4)-Pr(1)#2	143.7(2)
C(13)-O(5)-H(5)	109.5
C(13)-O(6)-Pr(1)	124.0(2)
C(14)-O(8)-Pr(1)	127.0(2)
N(1)-C(1)-C(2)	122.3(3)
N(1)-C(1)-C(6)	114.8(3)
C(2)-C(1)-C(6)	122.9(3)
C(3)-C(2)-C(1)	118.2(3)
C(2)-C(3)-C(4)	119.8(3)
C(3)-C(4)-C(5)	118.6(3)
N(1)-C(5)-C(4)	121.9(3)
N(1)-C(5)-C(7)	114.9(3)
C(4)-C(5)-C(7)	123.2(3)
O(4)-C(6)-O(3)	126.5(3)
O(4)-C(6)-C(1)	117.6(3)
O(3)-C(6)-C(1)	115.9(3)
O(1)-C(7)-O(2)	126.0(3)
O(1)-C(7)-C(5)	118.0(3)
O(2)-C(7)-C(5)	115.9(3)
N(2)-C(8)-C(9)	122.4(4)
N(2)-C(8)-C(14)	114.5(3)
C(9)-C(8)-C(14)	123.1(4)
C(10)-C(9)-C(8)	118.3(4)
C(11)-C(10)-C(9)	120.1(5)
C(10)-C(11)-C(12)	118.0(4)
N(2)-C(12)-C(11)	122.8(4)
N(2)-C(12)-C(13)	112.9(3)
C(11)-C(12)-C(13)	124.4(4)
O(6)-C(13)-O(5)	124.6(4)
O(6)-C(13)-C(12)	120.1(3)
O(5)-C(13)-C(12)	115.3(3)
O(7)-C(14)-O(8)	125.9(3)
O(7)-C(14)-C(8)	117.9(3)
O(8)-C(14)-C(8)	116.1(3)

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