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NOTE

Synthesis and Crystal Structure of New Pb(II) Complex with *p-tert*-Butyl Benzoic Acid

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A new Pb(II) complex of formula $[Pb(PTBA)_2H_2O]$ (PTBA = *p-tert*-butyl benzoic acid) has been synthesized and the crystal structure was characterized by single crystal X-ray diffraction. The complex crystallizes in the system and belongs to space group: triclinic, P-1 with a = 6.6964(7)Å, b = 12.5782(12)Å, c = 13.9056(14)Å, α = 91.8640(10)°, β = 101.141(2)°, γ = 97.5670(10)°, V = 1137.1(2)Å^3, Z = 2, Dc = 1.693 Mg/cm^3, Mr = 579.63, μ(moKo) = 7.445 mm^{-1}, F(000) = 564. R = 0.0282 and wR = 0.0575 for 3943 observed reflections with I >σ(I). The crystal structure analysis indicates that the Pb(II) ion is five-coordinated by two PTBA ligand molecules and one water molecule.

Keywords: Pb(II) complex, *p-tert*-Butyl benzoic acid, Synthesis, Crystal structure.

Recently, the crystal engineering of using ligands and metal ions through self-assembly to form coordination compounds has much attention because of their ascinating structural diversity and potential applications as functional materials[1-8]. In this paper, the self-assembly synthesis and crystal structure of a complex $[Pb(PTBA)_2H_2O]$ (PTBA = *p-tert*-butyl benzoic acid) are reported.

All reagents were of AR grade and used without further purification. IR spectra were record on a Nicolet 380 spectrophotometer. Elemental analyses for C, H and N were performed on a Elementar Vario EL-III analyzer. The crystal structure was determined by Bruker Smart-1000 CCD area-detector diffractometer.

Synthesis: 20 mL 0.20 M aqueous solution of *p-tert*-butyl benzoic acid sodium salt, 20 mL 0.20 M aqueous solution of $Pb(NO_3)_2$ and 15 mL 0.30 M alcohol solution (C_2H_5OH:H_2O = 1:1) of $Cu(phen)_2{\cdot}Cl_2$ were mixed together under stirring condition for 1 h. After being filtered, the solution was kept at room condition for 10 d and then the lump shaped colourless crystals were collected. Yield 48 %. IR spectrum (KBr, ν_{max}, cm^{-1}): 3442, 3049, 1620, 1514, 1382, 848, 723. Elemental analysis (%): Calcd. for $C_{22}H_{28}N_2O_5Pb$: C,45.59; H,4.87; found: C, 45.54; H, 4.94.

A single crystal (0.23 mm × 0.20 mm × 0.12 mm) was selected for crystallographic data collection at 298(2) K and structure determinated with graphite monochromatic MoK_α radiation (λ = 0.71073 Å). A total of 5985 reflections were collected in the range of 2.28° ≤ θ ≤ 25.02°, of which 3943 reflections were unique with R_{int} = 0.0212 and R = 0.0282 and wR = 0.0575, where $w = 1/[s^2(F_0^2) + (0.0561P)^2 + 0.0000P]$, $P = (F_0^2 + 2F_0^2)/3$. The maximum and minimum peaks on the final difference Fourier map are corresponding to 0.738 and -1.032 e/Å^3 (CCDC No. 994482), respectively.

The atomic coordinates and thermal parameters are listed in Table-1 and the selected bond lengths and bond angles in Table-2, respectively. Fig. 1 shows diagram of the molecular

TABLE-1
NON-HYDROGEN ATOMIC COORDINATES (× 10^4) AND THERMAL PARAMETERS (× 10^{3}Å^2)

Atom	X	Y	Z	U(eq)
Pb(1)	7259(1)	-247(1)	4161(1)	39(1)
O(1)	9135(5)	1572(3)	4903(3)	48(1)
O(2)	5863(5)	1147(3)	4969(3)	43(1)
O(3)	4115(5)	-91(3)	2811(3)	50(1)
O(4)	7116(6)	812(4)	2712(3)	64(1)
O(5)	11179(5)	390(3)	3777(3)	50(1)

TABLE-2
SELECTED BOND LENGTHS (Å) AND BOND ANGLES (°)

Bond	Length	Angle	(°)	Angle	(°)
Pb(1)-O(2)	2.433(3)	O(2)-Pb(1)-O(4)	89.32(14)	O(2)-Pb(1)-O(2)#1	69.76(13)
Pb(1)-O(4)	2.445(4)	O(2)-Pb(1)-O(1)	52.59(11)	O(4)-Pb(1)-O(2)#1	129.90(12)
Pb(1)-O(1)	2.542(4)	O(4)-Pb(1)-O(1)	78.22(14)	O(1)-Pb(1)-O(2)#1	116.16(11)
Pb(1)-O(3)	2.569(4)	O(2)-Pb(1)-O(3)	81.42(12)	O(3)-Pb(1)-O(2)#1	79.35(12)
Pb(1)-O(5)	2.799(3)	O(4)-Pb(1)-O(3)	52.11(13)	O(2)-Pb(1)-O(5)	114.47(12)

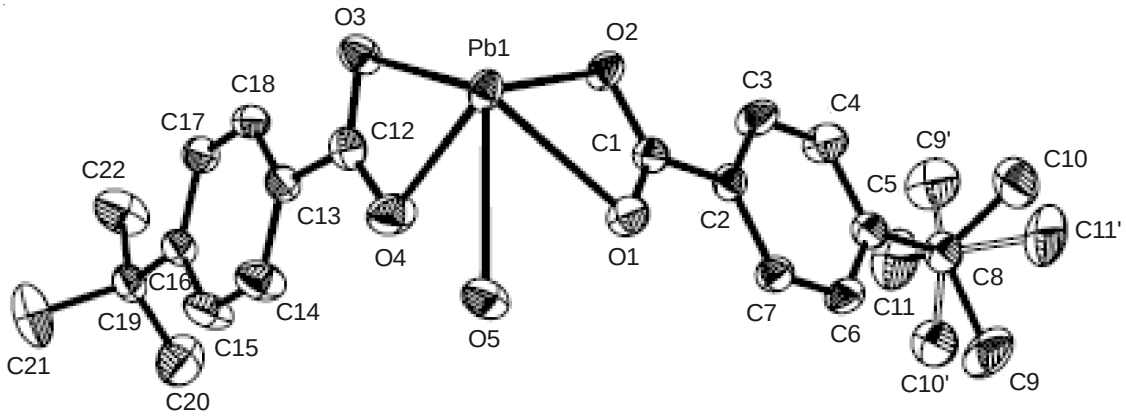

Fig. 1. Molecular structure of the complex $[Pb(PTBA)_2H_2O]$

structure of the complex $[Pb(PTBA)_2H_2O]$. Fig. 2 shows a perspective view of the crystal packing in the unit cell. As shown in the Fig. 1, the center metal ions has five coordinated by five O atoms from two PTBA molecules and one water molecule.

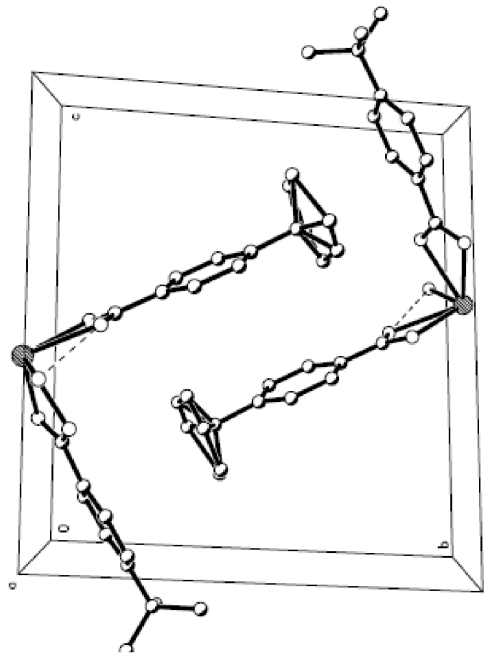

Fig. 2. Molecular packing arrangement in the unit cell

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