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NOTE

Hydrothermal Synthesis and Crystal Structure of Cobalt(II) Complex with Imidazole Ligand

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A new cobalt(II) complex with m.f. $C_{40}H_{50}N_{12}O_4Co$ has been synthesized by the hydrothermal reaction of imidazole with $Co(NO_3)_2$ and sodium *tert*-butylbenzoate. The structure was characterized by IR and X-ray single crystal structure analysis. The crystal is in a monoclinic system, space group P2(1)/n with a =10.4215 (11) Å, b = 15.5263 (15) Å, c = 13.5857(12)Å, α = 90º, β = 106.8790 (10)º, γ = 90º, V = 2103.6 (4) Å^3, Z = 2, Mr = 821.85, D_c = 1.298 Mg/cm^3, μ = 0.463 mm^{-1}, F(000) = 866, T = 298(2) K, R = 0.0393, wR = 0.0955 for 10488 reflections with I>2σ (I). In the molecular structure unit, metal ion octahedral geometry coordinated by six N atoms from six imidazole molecules.

Keywords: Cobalt complex, Hydrothermal synthesis, Crystal structure.

Recently, the complexes polymers of imidazole and its derivatives with transition metal ions have much attention because of their potential applications in magnetism, catalysis, photochromic property and bioactivities, *etc.*[1-7]. In this paper, the hydrothermal synthesis and crystal structure of a complex $[Co(ImH)_6]\cdot(PTBBA)$ (ImH = imidazole, PTBBA = *tert*-butylbenzoic acid) are reported.

All reagents were of AR grade and used without further purification. IR spectra were recorded on a Nicolet 380 FT-IR spectrophotometer. The crystal structure was determined by Siemens SMART CCD area-detector diffractometer.

Synthesis: Aqueous solution of imidazole (20 mL, 5 mmol), $Co(NO_3)_2$ (5 mmol) and sodium *tert*-butylbenzoate (5 mmol) was carried out in a autoclave and heated to 150 ºC for three days. After cooling to room temperature, the red cylindrical crystals were collected by filtration. Yield 44 %. IR spectrum (KBr, ν_{max}, cm^{-1}): 3105-2620, 1590, 1560, 1520, 1380, 1071, 937, 833, 748, 667.

Structure determination: A single crystal (0.30 mm × 0.2 mm × 0.18 mm) was selected for crystallographic data collection at 298 (2) K and structure determinated with graphite monochromatic MoK_α radiation (γ = 0.71073 Å). A total of 10488 reflections were collected in the range of 2.18º ≤ θ ≤ 25.01º, of which 3714 reflections were unique with R_{int} = 0.0366 and R = 0.0393 and wR = 0.0955, 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 0.288 and -0.321 e/Å^3, 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 structure of the complex $[Co(ImH)_6]\cdot(PTBBA)$. 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 octahedral geometry coordinated by six N atoms from six imidazole molecules. The independent component, $[Co(ImH)_6]^{2+}$ cation and PTBBA anion are connected by N-H···O hydrogen bonds.

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

Atom	X	Y	Z	U(eq)
Co(1)	5000	5000	5000	39(1)
N(1)	5011(2)	6043(1)	3910(1)	44(1)
N(2)	4677(2)	6795(1)	2486(2)	53(1)
N(3)	3060(2)	5419(1)	5102(1)	44(1)
N(4)	1501(2)	6352(1)	5123(2)	64(1)
N(5)	5932(2)	5828(1)	6292(1)	44(1)
O(1)	5354(2)	7069(1)	9405(1)	60(1)
O(2)	4252(2)	7373(1)	10525(1)	60(1)

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

Bond	Length	Angle	(°)	Angle	(°)
Co(1)-N(5)	2.1644(18)	N(5)-Co(1)-N(3)	88.71(7)	N(5)#1-Co(1)-N(3)	91.29(7)
Co(1)-N(3)	2.1658(18)	N(5)-Co(1)-N(1)	91.12(7)	N(5)-Co(1)-N(1)#1	88.88(7)
Co(1)-N(1)	2.1970(18)	N(3)-Co(1)-N(1)	90.53(7)	N(3)-Co(1)-N(3)#1	180.0
N(1)-C(1)	1.318(3)	N(1)-C(1)-N(2)	112.1(2)	N(3)#1-Co(1)-N(1)	89.47(7)
N(2)-C(1)	1.333(3)	N(4)-C(4)-N(3)	112.0(2)	N(1)#1-Co(1)-N(1)	180.0
N(3)-C(4)	1.321(3)	O(2)-C(10)-O(1)	123.3(2)	N(1)-C(1)-N(2)	112.1(2)

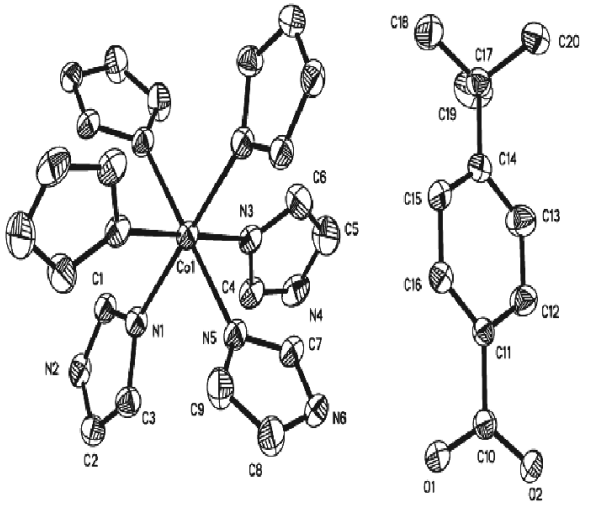

Fig. 1. Molecular structure of the complex $[Co(ImH)_6]\cdot(PTBBA)$

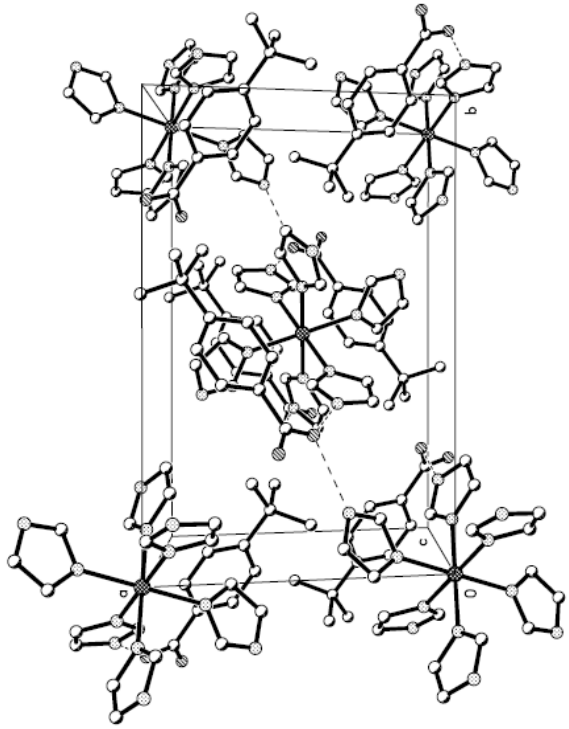

Fig. 2. Molecular packing arrangement in the unit cell

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