

MS30-P38 Synthesis and X-ray structural study of two new polymorphs coordination complexes based on imidazol derivative

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Polymorphism is very common among pharmaceutical substances. As the polymorphs possess different internal organization within the solid, they often show different melting points, solubilities, chemical reactivity or stability. These can appreciably influence pharmaceutical properties such as dissolution rate and bioavailability. It is therefore important to evaluate the polymorphism in early stages of new formulation studies.

We report here the synthesis, crystallographic study and hydrogen bond interactions of two new polymorph coordination complexes based on imidazol derivative and Cobalt.

Polymorph (I) is triclinic with space group P-1 and cell parameters $a=7.0882(8)$ Å, $b=11.9322(12)$ Å, $c=14.1882(15)$ Å, $\alpha=71.417(5)^\circ$, $\beta=86.927(5)^\circ$, $\gamma=83.489(5)^\circ$, $V=1129.9(2)$ Å³, and $Z=2$. Polymorph (II) is monoclinic with space group P 21/n and cell parameters $a=7.5554(2)$ Å, $b=13.0466(5)$ Å, $c=23.3958(9)$ Å, $\beta=94.405(2)^\circ$, $V=2299.36(14)$ Å³, and $Z=4$.

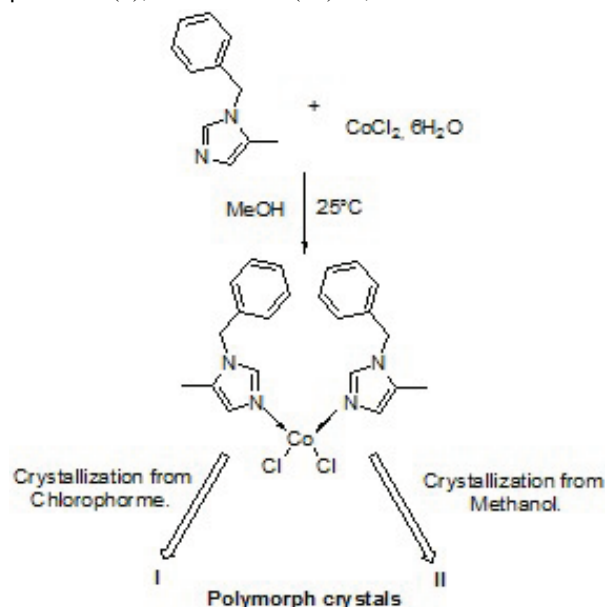


Figure 1. Scheme

Keywords: Polymorphism, single crystal, hydrogen bond, imidazol derivatives

MS30-P39 The role of methanol molecule in supramolecular assembling of $[\text{MoO}_2\text{L}(\text{CH}_3\text{OH})] \cdot \text{CH}_3\text{OH}$ and $[\text{MoO}_2\text{L}(\text{CH}_3\text{OH})]$ Schiff base type complexes

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Investigations of Schiff base molybdenum(VI) complexes have been stimulated by discovery of molybdenum in a number of redox enzymes and their efficiency as catalysts both in heterogeneous and homogenous reactions. Reactions of tridentate O,N,O Schiff base ligands H_2L with $[\text{MoO}_2(\text{acac})_2]$ afforded a series of distorted octahedral *cis*- MoO_2^{2+} complexes of the $[\text{MoO}_2\text{L}(\text{CH}_3\text{OH})] \cdot \text{CH}_3\text{OH}$ (**1-4**) and $[\text{MoO}_2\text{L}(\text{CH}_3\text{OH})_3]$ (**5**) type. Coordinated CH_3OH molecule, positioned *trans* to oxido oxygen atom, could be readily removed from first coordination sphere of molybdenum(VI) cation, yielding a $[\text{MoO}_2(\text{L})]$ intermediate responsible for catalytic activation of substrates during Lewis acid catalyzed transformations.

The supramolecular architecture of complexes is dominated by two types of hydrogen bonds (HB): $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$. The supramolecular motif shaped by $\text{O}-\text{H}\cdots\text{O}$ HB in **2**, **3** and **4** differs in comparison with that formed by the same type of HB in **1** and **5**.

The infinite chains in **2**, **3** and **4** are shaped via the $\text{O}-\text{H}\cdots\text{O}$ HB which include the coordinated CH_3OH oxygen atom, CH_3OH solvent molecule and the oxido oxygen atom of the complex molecule (Fig. 1a). On the contrary, the supramolecular dimers in **1** are formed by two molecules of solvent CH_3OH and two complex molecules via the phenolate oxygen atom and oxygen atom from coordinated CH_3OH (Fig. 1b). Formed dimers are condensed with complex molecules via $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bond which form centrosymmetric puckered 15-membered ring. (Figure 1b). Complex **5** does not contain solvent molecule of crystallization and the main supramolecular synthon formed via $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond is centrosymmetric dimer between the $-\text{OH}$ group of coordinated methanol and the oxygen donor atom of five-membered chelate ring of another complex molecule (Fig. 1c).

The determination of supramolecular role of CH_3OH molecules is essential in the context of complexes solubility and their catalytic activity in the conditions of epoxidation.

