

Co-crystal structure of a dinuclear (Zn-Y) and a trinuclear (Zn-Y-Zn) complexes derived from a Schiff base ligand

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The very dynamic field of research for the design and synthesis of heteropolynuclear complexes of d and f-block elements has made it possible to generate original structures with interesting properties in various fields such as magnetism, optics, catalysis and luminescence.

The present investigation describes the synthesis and structural study of two complexes. The complex 1 is a Heterotrinnuclear complexes synthesis which was used to generate three dimensional complexes formulated as $[\{Ni(L)\}(K)\{Ni(L)\}](SCN)$. The compound crystallizes in the Monoclinic system Space group P21/c with the following unit cell dimensions $a = 11.5891(13) \text{ \AA}$, $b = 17.307(2) \text{ \AA}$, $c = 19.781(2) \text{ \AA}$ and $\beta = 92.368(10)^\circ$, $R1 = 0.1172$. In the compound the ligand H2L is hexadentate. In the unit the coordination environment of the Ni metal can be described as distorted square, the alkaline metal K is octacoordinated.

The complex 2 is a co-crystal which was a three dimensional supramolecular complexes. formulated as $[Y\{Zn(L)(SCN)\}(SCN)_2] \cdot [Y\{Zn(L)(SCN)\}_2(DMF)_2] \cdot (NO_3)$. It crystallizes in the triclinic space group P-1 with unit cell parameters: $a = 14.8987(7) \text{ \AA}$, $b = 15.6725(8) \text{ \AA}$, $c = 19.2339(10) \text{ \AA}$, $\alpha = 94.610(4)^\circ$, $\beta = 103.857(4)^\circ$, $\gamma = 101.473(4)^\circ$, $R1 = 0.063$. Heterodinuclear unit $[Y\{Zn(L)(SCN)\}(SCN)_2]$ is co-crystallized with a heterotrinnuclear unit $[Y\{Zn(L)(SCN)\}_2(DMF)_2] \cdot (NO_3)$. In the dinuclear moiety, the ligand is hexadentate and in the trinuclear unit, it is pentadentate with one of the oxygen methoxy group remaining uncoordinated. The coordination environment Zn metal is square pyramidal. In the dinuclear unit the Y(III) is hexacoordinated while it is octacoordinated in the trinuclear unit. The environment of the Y(III) can be described as a distorted octahedral geometry in the dinuclear and as a distorted square antiprism in the trinuclear units respectively.

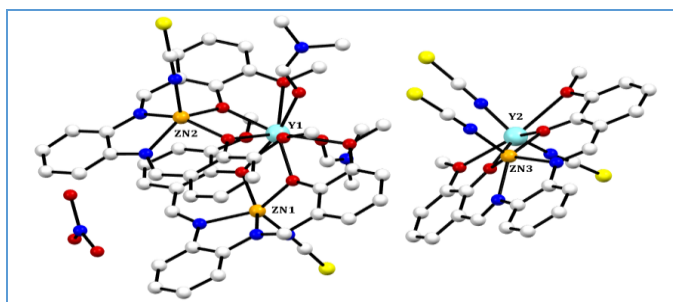


Figure 1. Co-Crystal structure

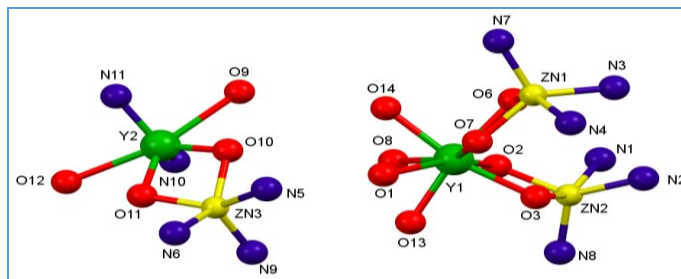


Figure 2. Environment around metals (Y and Zn) with donor atoms

Keywords: complex; antiprism; co-crystal; Schiff base; heteronuclear