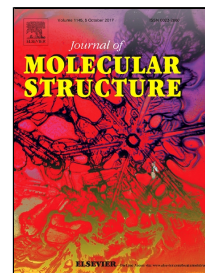


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Complexation of different transition metals with 4-(4-carboxyphenyl)-1,2,4-triazole: Synthesis, Crystal structure and Hirshfeld surfaces

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Abstract: Four new complexes based on the 4-(4-carboxyphenyl)-1,2,4-triazole (Hcpt) ligand, $\{[\text{Co}(\text{cpt})_2(\text{H}_2\text{O})_4] \cdot \text{H}_2\text{O}\}$ (**1**), $\{[\text{Cr}(\text{cpt})_2(\text{H}_2\text{O})_4] \cdot 10\text{H}_2\text{O}\}$ (**2**), $\{[\text{Fe}(\text{cpt})_2(\text{H}_2\text{O})_4] \cdot 10\text{H}_2\text{O}\}$ (**3**), $\{[\text{Zn}(\text{cpt})_2(\text{H}_2\text{O})_2]\}$ (**4**) have been synthesized and characterized by elemental analysis, single crystal X-ray diffraction and TGA. For complexes **1**, **2**, and **3**, they almost have the same coordination mode that only one nitrogen atom of triazole are involved in the coordination, while in the complex **4**, only the group COO^- participates in the coordination. In the crystal structure of **1**, each structural unit $[\text{Co}(\text{cpt})_2(\text{H}_2\text{O})_4]$ is linked to another by hydrogen bonding formed by the lattice water molecules, thus forming a one-dimensional chain structure; In the crystal structure of **2** or **3**, each structural unit $[\text{Cr}(\text{cpt})_2(\text{H}_2\text{O})_4]$ or $[\text{Fe}(\text{cpt})_2(\text{H}_2\text{O})_4]$ forms a two-dimensional layered structure by intermolecular hydrogen bonds from the coordinated water molecule and the group COO^- . The results of thermogravimetric analysis show that the loss of lattice water and coordinated water molecules in **1**, **2** and **3** is below 120°C , while the loss of coordinated water molecules in **4** is in the temperature range of $190 - 260^\circ\text{C}$. Hirshfeld surface shows that the $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonding interaction plays a significant role towards the conformation of the basic structure of these complexes.

Keywords: 4-(4-carboxyphenyl)-1,2,4-triazole; Metal complex; Crystal structure; Hirshfeld surface

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