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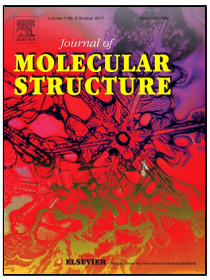

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Complexation of different transition metals with 4-(4-carboxyphenyl)-1,2,4-triazole: Synthesis, Crystal structure and Hirshfeld surfaces

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Abstract: Four new complexes based on the 4-(4-carboxyphenyl)-1,2,4-triazole (Hcpt) ligand, {[Co(cpt)$_2$(H$_2$O)$_4$]·H$_2$O}(**1**), {[Cr(cpt)$_2$(H$_2$O)$_4$]·10H$_2$O}(**2**), {[Fe(cpt)$_2$(H$_2$O)$_4$]·10H$_2$O}(**3**), {[Zn(cpt)$_2$(H$_2$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[Co(cpt)$_2$(H$_2$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[Cr(cpt)$_2$(H$_2$O)$_4$] or [Fe(cpt)$_2$(H$_2$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℃, while the loss of coordinated water molecules in **4** is in the temperature range of 190 -260℃. Hirshfeld surface shows that the N–H···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