

Synthesis, X-ray crystallography, and Hirshfeld surface analysis of a New Carbacylamidophosphate

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Carbacylamidophosphates (CAPH) with moiety $-\text{C}(\text{O})\text{NHP}(\text{O})-$ are important inorganic ligands in the synthesis of metal complexes such as transition metals, lanthanides, and Sn(IV) with biological and pharmacological activities [1,2]. Besides, the biological activity behavior of CAPH, its seemed efficient ligands in coordination chemistry either as O,O'-bidentate chelates in neutral and deprotonated form or in a monodentate fashion via oxygen of the phosphoryl group [3,4]. $\text{Cl}_2\text{HCC}(\text{O})\text{NHP}(\text{O})[\text{NHC}_6\text{H}_{11}]_2$ was synthesized and characterized by IR spectroscopy and elemental analysis. The structure of CAPH was determined by single-crystal X-ray crystallography technique. The compound crystallizes in triclinic system, space group $P1$, unit cell $a = 4.8182(3)\text{\AA}$, $b = 11.6693(6)\text{\AA}$, $c = 16.3611(9)\text{\AA}$, $\alpha = 84.171(4)^\circ$, $\beta = 86.836(4)^\circ$, $\gamma = 85.947(4)^\circ$, $Z=2$. In the crystalline lattice of CAPH, there are $\text{O}p\cdots\text{NH}_{\text{amine}}$ and $\text{O}c\cdots\text{NH}_{\text{amide}}$ hydrogen bonds between adjacent molecules led to one dimensional polymer along the c-axis. There are also weak intramolecular hydrogen bonds CAPH adopts a 3D supramolecular structure. The main non-covalent intermolecular interactions were also studied by Hirshfeld surface analysis and fingerprint plots.

Keywords: Carbacylamidophosphate, X-ray crystallography, Hirshfeld surface analysis

References

- [1] S. Nikpour, N. Dorosti, F. Afshar, M. Kubicki, *Appl Organomet Chem.* **2020**;e5724.
- [2] N. Dorosti, F. Afshar, F. Ghaziani, Kh. Gholivand, S. Zarabi, *Inorganica Chimica Acta*, **2019**, 489, 140-149.
- [3] Kh. Gholivand, M. Rajabi, N. Dorosti, F. Molaei, *Appl Organomet Chem*, **2015**, 29, 739-745.
- [4] F. Ghaziani, F. Afshar, Y. Maghsoud, Kh. Gholivand, *Journal of Molecular Structure*, **2019**, 1181, 61-70.