

Crystal Structure and Comparative Study via Hirshfeld Surface Analyses of Charge Transfer Compounds Based on Anthranilic Acid

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INTRODUCTION

Studies of organic-inorganic hybrid materials, including aminoacids and various inorganic acids^{1,2}, have received a great deal of attention in recent years. The need to use these materials is permanently increasing³. Hence, this symbiosis can lead to new rich structure, chemical and physical properties and has secured a good place in various fields of application such as biomolecular science^{4,5}, electronic⁶, nonlinear optics^{7,8}. In order to enrich the varieties in such kinds of hybrid materials and to investigate the influence of hydrogen bonds on the structural features, they have synthesized a new compound; this kind of hydrogen bonding is observed in similar previously studied hybrid compounds¹⁰.

EXPERIMENTAL AND THEORETICAL STUDY

This present work undertakes the crystal structure and comparative study via Hirshfeld surface (HS) analyses of charge transfer of two organic-inorganic hybrid material based on anthranilic acid, which has been obtained by the single crystal X-ray diffraction method. Hirshfeld surface analysis is a powerful tool used to quantify the intermolecular interactions of molecular crystals. The HS⁹ and fingerprint plots¹⁰ presented here are carried out using Crystal Explorer 17.1¹¹.

RESULTS AND DISCUSSION

The structure of the title compound o-carboxyanilinium dihydrogenphosphate, (C₇H₈NO₂⁺, H₂PO₄⁻) (I)¹² crystallizes in the centrosymmetric space group P-1, describes the in-depth structural analysis thereof shows that a single proton transfer occurs. The analyses of the hydrogen bonds of the two compounds (C₇H₈NO₂⁺, H₂PO₄⁻) (I) and (C₇H₈NO₂⁺, H₂AsO₄⁻) (II)² show that the anions and cations are held together via strong and short O—H...O hydrogen bonds, in addition to N—H...O interactions. Complementary Hirshfeld surface analysis was carried out to investigate and quantify the contributions of the different intermolecular interactions of the two compounds. The normalized contact distance (d_{norm}) (Fig. 1), based on d_e (d_e : distance from a point on the surface to the nearest nucleus outside the surface) and d_i (d_i : distance from a point on the surface to the nearest nucleus inside the surface), was calculated via the following expression:

$$d_{norm} = \frac{d_i - r_i^{vdw}}{r_i^{vdw}} + \frac{d_e - r_e^{vdw}}{r_e^{vdw}} \quad (1)$$

Where r^{vdw} is the van der Waals radius of the atom that lies inside the surface of Hirshfeld, while r_e^{vdw}



is the van der Waals radius of the atom that lies outside of the surface of Hirshfeld.

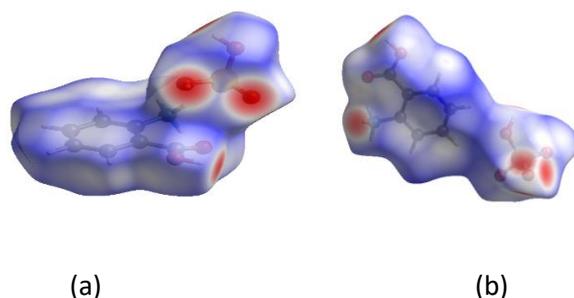


Fig.1. Hirshfeld surface analysis d_{norm} of o-carboxyanilinium dihydrogenphosphate (a) and o-carboxyanilinium dihydrogenarsenate (b).

CONCLUSION

The Single crystal XRD analysis established the supramolecular nature of the two crystals structures. The comparative study via 3D Hirshfeld surface and 2D fingerprint plots of the two compounds (I) and (II) reveal that the structure is dominated by O...H/H...O (52.9,50.3) %, the H...H contacts as the second dominant interactions with (28.2, 25.3) % and C—H... π (11.6,10.5) % contacts successively. Hydrogen bond interactions are the primary contributors to the intermolecular stabilization in the crystal.

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