

Research article-Synthesis, crystal structure determination and Hirshfeld surface analysis of three new salt forms of creatinine with hydro-bromic acid, 3-amino-benzoic acid and 3,5-di-nitro-benzoic acid

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Synthesis, crystal structure determination and Hirshfeld surface analysis of three new salt forms of creatinine with hydrobromic acid, 3-aminobenzoic acid and 3,5-dinitrobenzoic acid

Nirmalram Jeyaraman Selvaraj¹, Udhayasuriyan Sathya¹, Sundaramoorthy Gomathi², Samson Jegan Jennifer³, Logesh Mathivathanan⁴, Ibrahim Abdul Razak³

Affiliations + expand
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Abstract

Creatinine, a biologically important compound, is used to analyze kidney function and kidney diseases in the human body. The salt form of creatinine is used in the formation of drug materials like anti-HIV, antifungal, antiprotozoal, antiviral and antitumour compounds. Here we report the solid-state structures of three new crystalline salts, namely, creatininium (2-amino-1-methyl-4-oxo-4,5-dihydro-1H-imidazol-3-ium) bromide, $C_4H_8N_3O^+Br^-$ (I), creatininium 3-aminobenzoate, $C_4H_8N_3O^+C_7H_6NO_2^-$ (II), and creatininium 3,5-dinitrobenzoate, $C_4H_8N_3O^+C_7H_4N_2O_6^-$ (III). These salts have been

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Abstract

Creatinine, a biologically important compound, is used to analyze kidney function and kidney diseases in the human body. The salt form of creatinine is used in the formation of drug materials like anti-HIV, antifungal, antiprotozoal, antiviral and antitumour compounds. Here we report the solid-state structures of three new crystalline salts, namely, creatininium (2-amino-1-methyl-4-oxo-4,5-dihydro-1H-imidazol-3-ium) bromide, $C_4H_8N_3O^+Br^-$ (I), creatininium 3-aminobenzoate, $C_4H_8N_3O^+C_7H_6NO_2^-$ (II), and creatininium 3,5-dinitrobenzoate, $C_4H_8N_3O^+C_7H_4N_2O_6^-$ (III). These salts have been synthesized and characterized by single-crystal X-ray diffraction and Hirshfeld surface analysis. The structural chemistry of salts (I)-(III) and their crystal packing are discussed in detail. The primary interaction between the creatinine cation and the acid anion in the three salts is N-H...Br/O hydrogen bonds. In salt (I), the creatinine cation and bromide anion are connected through a pair of N-H...Br hydrogen bonds forming $R_4^2(8)$ and $R_4^2(12)$ ring motifs. In salts (II) and (III), the creatinine cation interacts with the corresponding anion via a pair of N-H...O hydrogen bonds. The crystal structure is further stabilized by C-H...O and O-H...O hydrogen bonds with the ring motifs $R_2^2(8)$, $R_2^1(7)$ and $R_2^1(6)$. Furthermore, the crystal structures are stabilized by π - π , C-H... π , C-O... π and N-O... π stacking interactions. The contributions made by each hydrogen bond in maintaining the crystal structure stability has been quantified by Hirshfeld surface analysis.

Keywords: Hirshfeld surface analysis; benzoate; bromide; comparative analysis; creatinine; crystal structure; intermolecular interactions; salt; two-dimensional fingerprint plot.

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