

Structure of Dinitrato Sodium with Imidazolium Cation
(C₃H₅N₂)[Na(NO₃)₂]

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Abstract

Imidazole, an aromatic heterocyclic, classified as an alkaloid, is present as an antifungal agent in commercial pharmaceutical products [1-2]. A novel 3D crystal structure of the title compound $\{(C_3H_5N_2)[Na(NO_3)_2]\}_n$ (C₃H₅N₂=Imidazolium cation) has been synthesized via hydrothermal procedure. Its molecular structure was determined by single X-ray diffraction analysis. The compound crystallizes with space group P21/c and the cell parameters are $a = 3.5875$ (3) Å, $b = 24.8548$ (17) Å, $c = 8.819$ (6) Å, $\beta = 95.546$ (4) °, $V = 1782.7$ (5) Å³, and $Z = 4$ ($R_1 = 0.034$). The NaI ion is coordinated by eight O atoms from three bidentate nitrate anions and two O atoms from two monodentate nitrate anions, displaying a bicapped trigonal-prismatic geometry. The imidazolium cation is essentially planar. In the crystal, the NaI ions are connected by bridging nitrate ligands, forming layers parallel to (010). The imidazolium cations are sandwiched between these layers. Weak C—H...O hydrogen bonds link the layers into a three-dimensional network. In addition, π – π interactions between the imidazolium rings [centroid–centroid distance = 3.588 (3) Å] are observed.

Key words: Hydrothermal synthesis, crystal structure, sodium nitrate, imidazole.