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Structure of Sodium 3-Benzylcarbamoyl-1-methyl-2,2-dioxo-1*H*-2λ^6,1-benzothiazine-4-olate

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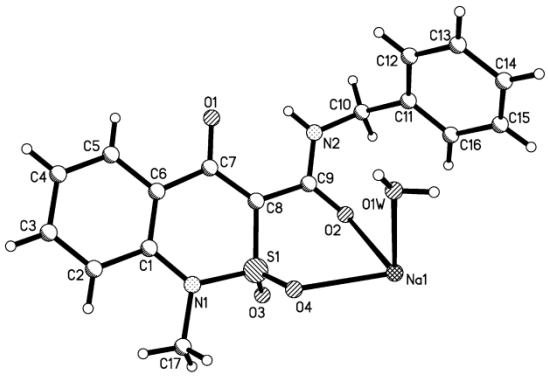
Numerous studies of the spatial structure of derivatives of 1-R-4-hydroxy-2,2-dioxo-1*H*-2λ^6,1-benzothiazine-3-carboxylic acids – esters, hetaryl-, alkylamides and anilides carried out with the help of X-ray crystallographic analysis have shown that, as a rule, the thiazine nucleus that forms their base is in a *"half-chair"* conformation or in an intermediate conformation between a *"twist-bath"* and a *"sofa"* [1-3].

However, in the case of sodium 3-benzylcarbamoyl-1-methyl-2,2-dioxo-1*H*-2λ^6,1-benzothiazine-4-olate obtained by crystallization from water a completely different result is observed. The dihydrothiazine ring of this compound unexpectedly appeared to be flat with the accuracy of 0.02 Å. The cyclic nitrogen atom has a planar configuration, the sum of bond angles centralized on it is 360°. The carbamide group of the substituent at C(8) atom is coplanar with the endocyclic C(7)-C(8) double bond (the torsion angle is C(7)-C(8)-C(9)-N(2) 5.5(6)°). Apparently, it is stabilized by formation of the intramolecular hydrogen bond N(2)-H…O(1) (H…O 1.95 Å N-H…O 136°) and leads to lengthening the C(7)-C(8) 1.405(6) Å bond. The benzyl fragment is in *ap*-conformation in relation to the C(8)-C(9) bond (the torsion angle is C(8)-C(9)-N(2)-C(10) -177.9(3)°), and the aromatic cycle is orthogonal to the plane of the carbamide fragment and turned towards the N(2)-C(10) bond (the torsion angles are C(9)-N(2)-C(10)-C(11) -80.2(6)°; N(2)-C(10)-C(11)-C(16) 104.4(5)°). The steric repulsion between atoms of the methyl substituent and the bicyclic fragment causes lengthening the C(17)-N(1) bond up to 1.502(9) Å compared to its mean value 1.469 Å.

The coordination polyhedron of a sodium cation is a distorted octahedron. A pair of sodium cations is linked with two bridging anions by the chelated type coordinating by atoms O(2), O(3) and O(4). In the terminal each sodium atom is coordinated by O(1) atom of the third anion binding pairs of atoms of sodium and by a water molecule. As a result, the infinite polymer chain is formed in the crystal.



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[2] Ukrainets, I.V.; Petrusova, L.A.; Dzyubenko, S.P.; Liu, Y. // Chem. Heterocycl. Comp. – 2014. – Vol. 50, No. 4. – P. 564.

[3] Ukrainets, I.V.; Petrusova, L.A.; Sim, G.; Bereznyakova, N.L. // Chem. Heterocycl. Comp. – 2015. – Vol. 51, No. 1. – P. 97.