Sultam and Sultim Structures, Part 3 [1]. Strong and Weak Hydrogen Bonds in 3-Oxosultams, 3-Oxosultims and 3-Alkoxysultams

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Dedicated to Professor Dr. Klaus Schulze on the occasion of his 70th birthday

In order to study hydrogen bonding networks in cyclic sulfin- and sulfonamides, X-ray structures were determined for 3-oxosultams **3a, c – e**, 3-alkoxysultams **5b, f** and 3-oxosultim **2f**, all of which show predominantly weak intermolecular hydrogen bonds. The 3-oxosultam **3a** forms tetrameric units by combining two symmetry-independent molecules through weak aromatic C-H···O-S-O hydrogen bonds without participation of the carbonyl groups. The 3-oxosultam **3c**, with two chloro substituents in the N-aryl ring show a polymer arrangement of the molecules through intermolecular association of the SO_2 and CO groups also with the aromatic H-atoms of the aryl rings. Sultam **3d** shows the first polymer chain in the 3-oxosultam series by the strong O-H···O=C hydrogen bonds without participation of the SO_2 group. Two new 'head-to-head' dimers with a 10-membered ring are found for 3-alkoxysultams **5b**, **5f** through weak C-H···O-S-O hydrogen bonds. In the 3-oxosultim **2f** weak intermolecular hydrogen bonds are observed to form a two-dimensional network with the two methylene groups, the carbonyl function and the chloro atom but, surprisingly, without the strong S-oxide acceptor group.

Key words: Sultims, Sultams, Intermolecular Hydrogen Bonds