Sultam and Sultim Structures, Part 2 [1].
Functionalized Novel Cyclic Sulfin- and Sulfonamides: A Comparison of Hydrogen Bonding Formation in Sulfoxides and Sulfones

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The stable hydroperoxides rac-cis-2a,d and 4a,c were synthesized by oxidation of the salts 1. The 3-hydroxy sultims rac-cis-3a,b and sultams 5a,e were obtained by reduction of the corresponding hydroperoxides 2 and 4. Crystal structure analyses were performed for compounds 3b, 4a, 5a, 5e and revealed a variety of intermolecular contacts leading to cyclodimers, tetramers and polymers. In carboxylic esters 4a and 5a, cyclodimers with a 20- or 22-membered ring are formed via ‘head-to-tail’ CO///H-O hydrogen bonds and \( \pi/\pi \)-interactions, without participation of the \( \text{SO}_2 \) group. The 1,1-dioxide 4c, which has no carbonyl substituent, forms a tetrameric unit by combining two symmetry independent molecules through strong OO-H///O-S-O and short nonclassical O-S-O///H-C hydrogen bonds. The sultam 1,1-dioxide 5e, bearing a highly substituted 2-phenyl ring, exhibits in the solid state strong intermolecular O-S-O///H-O hydrogen bonds and forms the first polymer chain in this cyclic sulfonamide series. In sultims 2a, 3a and 3b, but not in 2d, strong intermolecular S-O///H-O hydrogen bonds are observed and polymer chains originate from the c-glide plane (space group \( P2_1/c \)) in 2a and from two symmetry independent molecules in 3a. In the 1-oxide 2d a ‘head-to-head’ dimer was found with two strong SO///H-OO hydrogen bonds in a 14- or 16-membered ring. Short nonclassical C-H///O-C interactions connect the dimers to form polymeric chains.