

Polysulfonylamine, CXXVII [1]

Wasserstoffbrücken in kristallinen Onium-dimesylamiden: Ein robustes Achtring-Synthon als Bestandteil dreidimensionaler Wasserstoffbrückenmuster

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Hydrogen Bonding in Crystalline Onium Dimesylamides: A Robust Eight-Membered Ring Synthon as a Component in Three-Dimensional Hydrogen Bonding Patterns

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In order to study crystal packings and hydrogen bonding frameworks, low-temperature X-ray structures were determined for three onium salts of general formula $\text{BH}^+(\text{MeSO}_2)_2\text{N}^-$, where BH^+ is acetamidinium (**1**, monoclinic, space group $P2_1/c$, $Z = 4$), guanidinium (**2**, monoclinic, $P2_1/c$, $Z = 4$), or 4,6-diamino-2-thioxo-2,3-dihydropyrimidinium (**3**, monoclinic $P2_1/n$, $Z = 4$). In every case the ions create three-dimensional $\text{N}-\text{H}\cdots\text{N}/\text{O}$ networks, in which all N–H donors of the cations and four (in **1**) or five (**2**, **3**) acceptors of the anion are involved; non-conventional secondary bonds, *e.g.* $\text{C}-\text{H}\cdots\text{O}/\text{N}$, do not play an important role in the packings. For the isotopic structures **1** and **2**, congruencies and dissimilarities of the hydrogen bonding patterns are discussed in detail. Despite the structural and chemical differences between the cations and the way in which they are attached to the anion, each of the three structures displays a robust eight-membered ring synthon [$\text{N}_2 = \text{R}_2^2(8)$, antidromic] constructed *via* two-centre hydrogen bonds from a *syn, syn*-sequence $\text{H}-\text{N}-\text{C}(\text{sp}^2)-\text{N}-\text{H}$ of the respective cation and a V-shaped $\text{O}-\text{S}(\text{sp}^3)-\text{N}$ fragment of the anion. Although the networks in **2** and **3** contain several $\text{N}-\text{H}(\cdots\text{O})_2$ three-centre interactions, the two-point connectivity of the synthon is distinctly preserved. The results indicate that the $(\text{MeSO}_2)_2\text{N}^-$ ion may be utilized in crystal engineering as a dependable building block.