

Polysulfonylamine, CLXVII [1].

Wasserstoffbrücken in kristallinen Onium-dimesylamiden:

Ein robustes Dreipunktmuster als Bestandteil eines 2D-, eines zweifach verwobenen 2D- und eines 3D-Wasserstoffbrücken-Netzwerks

Polysulfonylamines, CLXVII [1]. Hydrogen Bonding in Crystalline Onium Dimesylamides:
A Robust Three-Point Pattern Integrated into a 2D, a Twofold Interwoven 2D, or a
3D Hydrogen-Bond Network

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As an exercise in crystal engineering, preparations and low-temperature X-ray structures are reported for three ionic solids of general formula $\text{BH}^+(\text{MeSO}_2)_2\text{N}^-$, where BH^+ is 2,4,6-triaminopyrimidinium (compound **1**, triclinic, space group $P\bar{1}$, $Z = 2$), 2,6-diaminopyridinium (**2**, monoclinic, $C2/c$, $Z = 8$), or 2,4-diaminopyrimidin-6(1*H*)-on-3-ium (**3**, monoclinic, $P2_1/c$, $Z = 4$). As a common feature, the onium cations in question exhibit a trifunctional hydrogen-bond donor sequence H-N-C-N(H)-C-N-H that is complementary to a W-shaped O-S-N-S-O fragment of the anion. Consequently, each structure displays a [DDD:AAA] three-point hydrogen-bond pattern formed by two lateral N-H \cdots O bonds and a central N-H \cdots N interaction. This grouping is integrated as a robust supramolecular synthon into two-dimensional (**1**, **2**) or three-dimensional (**3**) hydrogen-bond networks, in which all good donors and all good acceptors are involved (excepting one S=O group in **2**). In structure **1**, the approximately planar cation-anion layers are perfect mosaics composed of 6-membered pyrimidine heterocycles and seven crystallographically independent types of 8-, 10-, 12- or 24-membered rings based upon hydrogen bonding. In contrast, the corresponding layers in structure **2** are marred by large 40-membered voids; in order to achieve dense packing, the imperfect layers adopt a strongly corrugated shape and interpenetrate to form twofold interwoven and nearly planar double-layers. Each structure features close C-H \cdots O contacts consistent with weak hydrogen bonding; in the layer structures **1** and **2**, some of these interactions serve as links between adjacent or interwoven layers.

Key words: Di(methanesulfonyl)amide, Nitrogen Heterocycles, Supramolecular Synthon,
Three-Point Hydrogen-Bond Pattern, Twofold Interwoven 2D Network