Polysulfonylamine, CLXX [1]. Wasserstoffbrücken in kristallinen Onium-dimesylamiden: Drei Strukturen mit NH_2-substituierten 1,3,5-Triazinium-Kationen (einschließlich Melaminium)

Polysulfonylamines, CLXX [1]. Hydrogen Bonding in Crystalline Onium Dimesylamides: Three Structures Involving NH_2-Substituted 1,3,5-Triazinium Cations (Including Melaminium)

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In order to study hydrogen bonding networks and packing arrangements, preparations and low-temperature X-ray structures are reported for three ionic solids of general formula $BH^+(MeSO_2)_2N^-$, where BH^+ is 2,6-diamino-4-phenyl-1,3,5-triazin-1-ium (compound **1**, tetragonal, space group $P42_1c$, $Z = 8$), 2,4,6-triamino-1,3,5-triazinium or melaminium (**2**, monoclinic, $P2_1/c$, $Z = 4$), and 2,4-diamino-6-methyl-1,3,5-triazin-1-ium (**3**, triclinic, $P1$, $Z = 2$). The asymmetric units consist of cation-anion pairs that display in **1** a [DDD:AAA] three-point hydrogen bond pattern formed by two lateral N-H···O bonds and a central N^+-H···N interaction, in **2** a related pattern, in which the substantial lateral offset of the ions causes the two-centre H bonds to split up into three-centre bonds, and in **3** a [DD:AA] two-point pattern formed by an N-H···N and an N^+-H···O interaction. All NH donors that are not involved in the ion pairs use sulfonyl oxygen atoms and/or non-protonated nitrogen ring-atoms as acceptors to form, in **1** and **3**, discrete cation-anion strands, and in **2** similar strands associated into a three-dimensional network *via* one independent N-H···O bond. The packing topologies of the strands may be viewed as supramolecular analogues to molecular arrangements occurring in crystalline polyaromatic hydrocarbons, *viz*. the sandwich-herringbone pattern in **1** (sustained by $\pi\cdots\pi$ stacking of the triazine rings within the sandwiches and a phenyl-phenyl C-H···π interaction between orthogonal sandwiches), the flattened or γ-type herringbone pattern in **2** (sustained by the unique N-H···O interaction of orthogonal strands), and the pseudo-graphitic β-pattern in **3**. In each packing, weak C-H···A hydrogen bonds (A = O, N) originate from the activated methyl groups of the anions and act as structure-supporting links between the cation-anion strands.

Key words: Di(methanesulfonyl)amide, Nitrogen Heterocycles, Hydrogen Bonding, Cation-Anion Strands, Supramolecular Chemistry