

# Polysulfonylamine, CL [1]. Wasserstoffbrücken in kristallinen Onium-dimesylamiden: Ein robustes Achtring-Synthon in den Strukturen von Methyluronium- und 1,1-Dimethyluronium-dimesylamid.

Polysulfonylamines, CL [1]. Hydrogen Bonding in Crystalline Onium Dimesylamides: A Robust Eight-Membered Ring Synthon in the Structures of Methyluronium and 1,1-Dimethyluronium Dimesylamide

Dagmar Henschel, Thomas Hamann, Oliver Moers, Armand Blaschette und Peter G. Jones

Institut für Anorganische und Analytische Chemie der Technischen Universität, Postfach 3329, D-38023 Braunschweig

Sonderdruckerfordernungen an Prof. Dr. A. Blaschette oder Prof. Dr. P. G. Jones. Fax: +49(0) 5313915387. E-mail: p.jones@tu-bs.de

Z. Naturforsch. **57b**, 113–121 (2002); eingegangen am 31. Oktober 2001

Di(methanesulfonyl)amide, Uronium, Hydrogen Bonding

Methyluronium dimesylamide (**1**) and 1,1-dimethyluronium dimesylamide (**2**) have been prepared by proton transfer reactions of the strong nitrogen acid  $\text{HN}(\text{SO}_2\text{Me})_2$  with the corresponding ureas and characterized by low-temperature X-ray diffraction (**1**: orthorhombic, space group  $P2_12_12_1$ ,  $Z' = 1$ ; **2**: orthorhombic,  $Pna2_1$ ,  $Z' = 2$ ). Compound **2** appears to be the first crystallographically established 1,1-dimethyluronium salt. As a common feature, the three independent formula units consist of ion pairs held together by an eight-membered ring synthon [ $\text{N}_2 = \text{R}_2^2(8)$ , antidromic] constructed from a *syn,syn*-sequence  $\text{H}-\text{O}-\text{C}(\text{sp}^2)-\text{N}-\text{H}$  of the cation and a V-shaped  $\text{O}-\text{S}(\text{sp}^3)-\text{N}$  fragment of the anion *via* homonuclear two-centre hydrogen bonds. The surplus  $\text{N}-\text{H}$  donors form hydrogen bonds to  $\text{O}=\text{S}$  acceptors in adjacent formula units, leading to a three-dimensional network (**1**) or a pseudo- $2_1$  symmetric helical catemer of alternatingly inequivalent formula units (**2**). In both structures, the activated methyl groups give rise to numerous short interionic  $\text{C}-\text{H}\cdots\text{O}$  contacts, the more prominent of which are analyzed in terms of weak hydrogen bonding [cut-off criteria:  $d(\text{H}\cdots\text{O}) \leq 270$  pm,  $\theta(\text{C}-\text{H}\cdots\text{O}) \geq 130^\circ$ ].