Polysulfonylamine, CXL [1].

N-Cycloalkylidimesylamine \( C_nH_{2n-1}N(SO_2CH_3)_2 \):

Synthesen \((n = 3–6)\), Festkörper-Molekülstrukturen \((n = 4–6)\) und Rolle schwacher Wasserstoffbrücken C–H···O in den Kristallstrukturen

Wiebke Schaper, Ilona Lange, Dagmar Henschel, Oliver Moers,
Armand Blaschette und Peter G. Jones

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

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


N-Cycloalkyl Di(methanesulfonyl)amines, Carbon-Nitrogen Bond Lengthening, Weak Hydrogen Bonds

The new disulfonylamines \( R–N(SO_2Me)_2 \), where \( R = \) cyclopropyl (1), cyclobutyl (2), cyclopentyl (3) or cyclohexyl (4), were prepared according to an established one-step procedure (condensation of RNH\(_2\) with two equivalents of MeSO\(_2\)Cl, NaH as basic auxiliary).

Whereas the structure determination for 1 was marred by severe disorder, compounds 2–4 have been characterized by low-temperature X-ray diffraction (2: monoclinic, space group \( P2_1, Z' = 2 \), pseudo-\( P2_1/c \) packing; 3: triclinic, \( P\bar{1}, Z' = 1 \); 4: orthorhombic, \( Pbca, Z' = 1 \)). The four independent molecules display puckered carbocycles, whereby the electronegative (MeSO\(_2\))\(_2\)N substituent occupies an equatorial position, leading to short intramolecular C–H···O contacts (2: angles of ring pucker \( \varphi = 30–33^\circ \); 3: envelope conformation, \( \varphi \approx 40^\circ \); 4: chair conformation, \( \varphi_1 \approx \varphi_2 \approx 51^\circ \)). In accordance with known congener structures, the C(sp\(^3\))–N(S)\(_2\) moieties feature trigonal-planar N configurations and unusually long C–N bonds (ranges for 2–4: C–N 148.8–150.8 pm, S–N 166.6–168.9 pm, S–N–S 118.3–119.3\(^\circ\)).

The three crystal packings are governed by a plethora of weak intermolecular hydrogen bonds C(sp\(^3\))–H···O, and a thorough survey of these interactions reveals that the inductively activated methyl groups are distinctly more efficient hydrogen bond donors than the methine and methylene ring groups. In each structure, the principal hydrogen bonds create layer substructures parallel to a unit cell face, which are cross-linked by the remaining C–H···O contacts to form three-dimensional networks.