Die starke und schwache Wasserstoffbrücken in den Kristallstrukturen von 8-Hydroxychinolinium- und 8-Aminochinolinium-dimesylamid

Polysulfonilamines, CLI [1].

Strong and Weak Hydrogen Bonding in the Crystal Structures of 8-Hydroxyquinolinium and 8-Aminoquinolinium Dimesylamide

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Hydrogen Bonding, Ion Catemers, Arene Stacking

In order to study hydrogen bonding networks and packing arrangements in ionic organic crystals, low-temperature X-ray structures were determined for two chemically related onium salts BH+(MeSO2)2N−, where BH+ is 8-hydroxyquinolinium (1; monoclinic, space group P21/c, Z′ = 1) or 8-aminoquinolinium (2; monoclinic, P21/n, Z′ = 1). The packings are governed by strong hydrogen bonds, π-π stacking interactions and weak hydrogen bonding. In both compounds, hydrogen bonds using the NH/OH donors of the cations and O/N acceptors of the anion result in simple chain polymeric structures, which extend parallel to the y axis and are propagated by translation (1) or 21 transformation (2). Moreover, an intramolecular N–H···O hydrogen bond is present in the 8-hydroxyquinolinium cation. As a common feature, the anion substructures are pervaded by hexagonal channels parallel to y, each one accommodating either two separate stacks of translation related cations (1) or a unique (merged) stack of inversion related cations (2). The crystal cohesion is reinforced by numerous weak hydrogen bonds of the types C=H···O=S and CH2=H···O=S, the latter creating in each structure a topologically different double-chain ribbon of anions. All C–H···O contacts taken into consideration have normalized parameters d(H···O) ≤ 268 pm and θ(C–H···O) ≥ 126°.