Polysulfonylamine, CLXXX [1]. Bis(triphenylphosphoranyliden)ammonium-di(methansulfonyl)amid: Eine Kristallstruktur mit CH/π-Wechselwirkungen zwischen Methyl- und Phenylgruppen

Polysulfonylamines, CLXXX [1]. Bis(triphenylphosphoranylidene)ammonium Di(methanesulfonyl)amide: A Crystal Structure Featuring Methyl-Phenyl CH/π Interactions

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The structure of $[Ph_3PNPPh_3][(MeSO_2)_2N]$ (monoclinic, $P2_1/c$, $Z' = 1$; single-crystal X-ray diffraction at -140 °C) displays chains of relatively small anions, surrounded by four parallel columns of bulky cations, giving a rectangular array. In contrast to a previously reported series of onium dimesylamides with smaller cations, interanion hydrogen bonding C_{Me}–H$\cdots$O, originating from the inductively activated methyl groups, is not observed in the present structure. In consequence, the packing arrangement is determined by multiple phenyl embraces between cations, weak cation-anion hydrogen bonds C_{Ph}–H$\cdots$O/N and, most notably, by methyl-phenyl CH/π interactions between anions and cations. One methyl group forms two C–H$\cdots\pi$ contacts to different phenyl rings (hydrogen-to-centroid distances: 272 and 285 pm), the other lies in a tripodal mode above an aromatic ring plane (hydrogen-to-centroid distances: *ca.* 330 pm).

Key words: Activated Methyl Groups, Methyl-Phenyl CH/π Interactions, Weak Hydrogen Bonding, Multiple Phenyl Embraces, Sulfonamides