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1,3,5-TRIS(PENTAFLUOROPHENYL)-2,4,6-TRICHLOROBORAZINE

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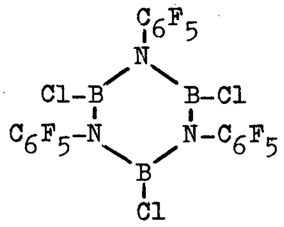
While B-perfluoroarylborazinederivatives (1, 2) and N-polyfluoroalkylborazines (2, 3) are known, N-perfluoroarylborazines have not been described yet. Since especially the hydrolytic properties are more influenced by the substituents at the nitrogen atoms than at the boron atoms of the borazine ring (4), we have prepared 1,3,5-tris(pentafluorophenyl)-2,4,6-trichloroborazine.

1,3,5-tris(β-trifluoroethyl)-2,4,6-trichloroborazine (2) and 1,3,5-triphenyl-2,4,6-trichloroborazine (5, 6, 7, 8, 9) can be obtained by thermal dehydrohalogenation of the respective aminoboranes, but 1,3,5-tris(pentafluorophenyl)-2,4,6-trichloroborazine is not produced by an analogous reaction. Addition of tertiary bases leads to the formation of small amounts of the desired compound, which, however, cannot be isolated in a pure state from the reaction mixture.

It has been found that the compound triethylamine-boron(III)chloride in the presence of an excess of triethylamine by addition of pentafluoroaniline is readily converted into 1,3,5-tris(pentafluorophenyl)-2,4,6-trichloroborazine.

$$3\ Et_3N + 3\ BCl_3 \longrightarrow 3\ Et_3N.BCl_3$$

$$3\ Et_3N.BCl_3 + 3\ Et_3N + 3\ C_6F_5NH_2 \longrightarrow$$



$$+ 6\ Et_3NHCl$$

The preparation must be carried out under complete exclusion of moisture, since the compound is extremely sensitive towards moisture [(B)O-H str. at 3650 cm^{-1}]. The B-N ring-stretching frequency is found at 1369 cm^{-1}, only slightly lower than in 1,3,5-triphenyl-2,4,6-trichloroborazine (5).

1,3,5-tris(pentafluorophenyl)-2,4,6-trichloroborazine appears to be useful as a starting material for other substituted borazines to be published elsewhere.

Preparation: 29,2 g BCl_3 are condensed under stirring in a solution of 50,5 g triethylamine in 150 ml toluene. 45,8 g pentafluoroaniline dissolved in 100 ml toluene are dropwise added. The reaction mixture is heated under reflux and stirring for 25 hours. After cooling the resulting suspension is filtered and the crystalline materials extracted with 150 ml dry benzene for 6 hours. After removal of the benzene the crystals are sublimed at 10^{-3} torr and 185°. Yield: 42 %. Mp. (in vacuo) 254°. Mol.wt.calcd. 682. Found 700 (cryosc. in benzene).

Anal. Calcd. for $C_{18}B_3Cl_3F_{15}N_3$: C 31,70; N 6,16; Cl 15,60
Found : C 31,18; N 5,98; Cl 14,32

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