

Donor-Akzeptor-Komplexe von Halogenidionen mit

1,4-Diiodtetrafluorbenzol

Donor-Acceptor Complexes of Halide Ions with 1,4-Diiodtetrafluorobenzene

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1,4-Diiodtetrafluorobenzene, Donor-Acceptor Complexes, Crystal Structure

(Ph₄P)X as well as (Me₄N)X (X = Cl, Br, I) react with 1,4-diiodtetrafluorobenzene in CH₂Cl₂ and CH₃CN solutions, respectively, to give the donor-acceptor complexes (Ph₄P)₂[(C₆F₄I₂)Cl₂]·4 CH₂Cl₂ (**1**), (Ph₄P)₂[(C₆F₄I₂)Br₂]·2 CH₂Cl₂ (**2**), (Me₄N)[(C₆F₄I₂)Cl] (**3**), (Me₄N)[(C₆F₄I₂)Br]·CH₃CN (**4**), (Ph₄P)₂[(C₆F₄I₂)₃Br₂]·4 CH₂Cl₂ (**5**), (Ph₄P)₂[(C₆F₄I₂)₃I₂] (**6**) and (Me₄N)₂[(C₆F₄I₂)₃I₂] (**7**). All complexes have been characterized by single X-ray crystallographic structure determinations.

1: Space group P $\bar{1}$, Z = 1, lattice dimensions at 203 K: $a = 1090.2(1)$, $b = 1206.2(1)$, $c = 1242.8(1)$ pm, $\alpha = 91.84(1)^\circ$, $\beta = 106.60(1)^\circ$, $\gamma = 99.84(1)^\circ$.

2: Space group P $\bar{1}$, Z = 1, lattice dimensions at 233 K: $a = 1129.7(2)$, $b = 1183.9(1)$, $c = 1293.4(1)$ pm, $\alpha = 65.52(1)^\circ$, $\beta = 65.74(1)^\circ$, $\gamma = 89.02(1)^\circ$.

3: Space group P2₁/n, Z = 4, lattice dimensions at 243 K: $a = 714.8(1)$, $b = 2405.7(3)$, $c = 930.8(1)$ pm, $\beta = 96.38(1)^\circ$.

4: Space group P2₁/c, Z = 4, lattice dimensions at 203 K: $a = 1400.8(1)$, $b = 1669.9(2)$, $c = 795.9(1)$ pm, $\beta = 102.81(1)^\circ$.

5: Space group Pbc_a, Z = 4, lattice dimensions at 223 K: $a = 2106.0(4)$, $b = 1566.8(3)$, $c = 2445.8(4)$ pm.

6: Space group P $\bar{1}$, Z = 1, lattice dimensions at 203 K: $a = 1150.9(1)$, $b = 1278.9(1)$, $c = 1292.9(2)$ pm, $\alpha = 65.47(1)^\circ$, $\beta = 82.07(1)^\circ$, $\gamma = 83.62(1)^\circ$.

7: Space group Pbc_a, Z = 4, lattice dimensions at 223 K: $a = 1210.5(5)$, $b = 1429.0(6)$, $c = 2470.3(12)$ pm.

In all complexes the acceptor molecule C₆F₄I₂ coordinates with the halide donor ions in linear arrangements C-I···X⁻. In **1** and **2** the halide ions act as terminal donors to form the dianionic species [X···I-C₆F₄-I···X]²⁻ (X = Cl, Br). Complexes **3** and **4** form polymeric anionic zigzag chains with μ -X⁻ bridges and bond angles I···Cl···I of 77.2° and I···Br···I of 74.3°. Complexes **5** - **7** are characterized by three-dimensional anionic networks via μ_3 -X⁻ bridging halide ions and μ -bridging 1,4-diiodtetrafluorobenzene molecules.

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