Spectroscopic Investigation of the System $TeCl_4/[NEt_4]PF_6$ in Solution and the Crystal Structure of $[NEt_4]_2[Te_2Cl_{10}]$

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Z. Naturforsch. **59b,** 1209 – 1213 (2004); received July 21, 2004

Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

Solutions containing $TeCl_4$ and $[NEt_4][PF_6]$ in CH_2Cl_2 were investigated by means of UV/vis and NMR spectroscopy in order to study the complex chemistry of $TeCl_4$ with the $[PF_6]^-$ anion. The results show formation of $[TeCl_5]^-$ and strong interactions of $[PF_6]^-$ with a tellurium containing species, presumably $[TeCl_3]^+$. The life time of the Te^{IV}-PF_6 complex is long enough to give different signals in the ^{19}F NMR spectrum of a solution containing excess $[PF_6]^-$. Even a fivefold excess of Cl^- ions over $[PF_6]^-$ does hardly lead to a dissociation of $[TeCl_3 \cdots PF_6]$. Crystals of $[NEt_4]_2[Te_2Cl_{10}]$ were obtained from a 4:1 solution of $[NEt_4]PF_6$ and $TeCl_4$ in CH_2Cl_2. The compound crystallizes in the triclinic space group P1, $a = 0.82626(7)$, $b = 1.04260(8)$, $c = 1.9915(3)$ nm, $\alpha = 84.641(9)$, $\beta = 84.891(9)$, $\gamma = 75.208(6)^\circ$ ($T = 295$ K). Slight variations in the molecular environment can have a substantial influence on the interatomic distances within the Te_2Cl_2 bridge of the $[Te_2Cl_{10}]^{2-}$ ion. This conclusion is confirmed by *ab initio* calculations.

Key words: Tellurium, ^{19}F NMR Spectroscopy, UV/vis Spectroscopy, Single Crystal X-Ray Diffraction, *ab initio* Calculations