

Konkurrierende Liganden: Theophyllin als nicht- und stark koordinierender Ligand in Quecksilber(II)-Komplexen

Competing Ligands: Theophylline as Non- and Strongly Coordinating Ligand in Mercury(II) Complexes

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[{Hg(CF₃)₂}(ThpH)(H₂O)](H₂O) (**1**), [{Hg₄(Thp)₄}(ClO₄)₄(H₂O)₈](H₂O)₄ (**2**), [{Hg(ThpH)₂}(NO₃)](NO₃) (**3**) and {Hg(Thp)Cl}(H₂O) (**4**) (ThpH = theophylline, C₇H₈N₄O₂) have been synthesized by slow evaporation of aqueous solutions of the mercuric salts Hg(CF₃)₂, Hg(ClO₄)₂, Hg(NO₃)₂, or HgCl₂ and theophylline. Their crystal structures were determined on the basis of single crystal X-ray data. The coordination polymers **1** and **2** crystallize with triclinic symmetry, *P* $\bar{1}$ (no. 2), with *a* = 468.8(2), *b* = 1256.4(5), *c* = 1445.5(6) pm, α = 67.15(3), β = 89.21(3), γ = 89.40(3)° and *a* = 833.6(1), *b* = 1862.7(2), *c* = 2182.9(2) pm, α = 111.61(1), β = 90.98(1), γ = 95.51(1)°, respectively. **3** and **4** crystallize with monoclinic symmetry, *Pc* (no. 7), *a* = 1194.1(1), *b* = 1258.8(2), *c* = 735.5(2) pm, β = 96.96(2)° and *P*2₁/*n* (no. 14), *a* = 1069.0(2), *b* = 911.6(1), *c* = 1089.9(2) pm and β = 96.87(2)°. In **1** the theophylline molecules are non-coordinating to mercury and leave the Hg(CF₃)₂ molecule unchanged. Only weak electrostatic attractions to one keto-oxygen atom of theophylline and one water molecule hold this co-crystallisate together. In **2**, the theophyllinate anion, Thp[−], strongly coordinates with both N(7) and N(9) to Hg^{II} forming a large ring with eight Hg atoms that incorporates the water molecules. One sort of nitrate ions in **3** is weakly attached to Hg^{II} with the theophylline molecules still bound strongly through N(9). The chloride ligand and the theophyllinate ion seem to have the same strengths as ligands in **4** as they are both attached to Hg^{II} with the shortest distances possible.

Key words: Mercury, Bis(trifluormethyl)mercury, Mercuric Nitrate, Mercuric Chloride, Theophylline