

STRUCTURE DETERMINATION OF $[(h^4\text{-cod})\text{Pt}(\text{N}_3)_2]$ FROM X-RAY POWDER DIFFRACTION DATA

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The crystal structure determination of $[(h^4\text{-cod})\text{Pt}(\text{N}_3)_2]$ from powder diffraction data is reported [1]. The detailed X-ray powder diffraction study of $[(h^4\text{-cod})\text{PtX}_2]$ ($X = \text{Cl}, \text{N}_3$) and $[(h^4\text{-cod})\text{PtMeX}]$ ($X = \text{Cl}, \text{I}, \text{N}_3$) is presented as well as the single crystal structures of $[(h^4\text{-cod})\text{PtMeX}]$ ($X = \text{I}, \text{N}_3$). Additionally, all complexes of the type $[(h^4\text{-cod})\text{PtX}_2]$ and $[(h^4\text{-cod})\text{PtMeX}]$ (COD = *cis,cis*-1,5-cyclooctadiene, $X = \text{Cl}, \text{I}$ and N_3) were compared via ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{195}\text{Pt}\{^1\text{H}\}$ NMR spectroscopy. From chemical shifts and bond lengths, the influences of the chemical environments at the platinum centers on the strength of the Pt-methyl bonds is revealed and will be discussed.

Powder diffraction methods are increasingly becoming a sophisticated tool in small molecule structural investigations. Structure determination from single crystal data is nowadays a more or less routine procedure in chemical laboratories for compounds up to about 30 atoms per molecule. In the case of powder diffraction this is still a task. The condition precedent for such a study is the application of new methods for structure determination.

For the ab-initio structure determination as well as the Rietveld refinements of the other compounds the software package TOPAS [2] has been used. The software solves structures in real space by simulated annealing technique using complex rigid bodies in combination with lattice energy minimization techniques including user-defined force fields.

[1] Frank Stowasser, European J. of Inorganic Chemistry (2001), in prep.

[2] A.A. Coelho, J. Appl. Cryst. 33 (2000), pp. 899-908.