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

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The crystal structure determination of \([[(\eta^4\text{-cod})\text{Pt(N}_3\text{)}_2]]\) from powder diffraction data is reported [1]. The detailed X-ray powder diffraction study of \([[(\eta^4\text{-cod})\text{PtX}_2]] (X = \text{Cl, N}_3)\) and \([[(\eta^4\text{-cod})\text{PtMeX}] (X = \text{Cl, I, N}_3)\) is presented as well as the single crystal structures of \([[(\eta^1\text{-cod})\text{PtMeX}] (X = \text{I, N}_3)\). Additionally, all complexes of the type \([[(\eta^4\text{-cod})\text{PtX}_2]]\) and \([[(\eta^4\text{-cod})\text{PtMeX}] \text{ (COD = cis,cis-1,5-cyclooctadiene, X = Cl, I and N}_3)\) were compared via \(^1\text{H}, ^{13}\text{C}\{^1\text{H}\}\) 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.