Schwingungsspektren und Normalkoordinatenanalyse von Hexathiocyanatoplatinat(IV), Kristallstruktur von $[Py_2CH_2][Pt(SCN)_6]$

Vibrational Spectra and Normal Coordinate Analysis of Hexathiocyanatoplatinate(IV), Crystal Structure of $[Py_2CH_2][Pt(SCN)_6]$

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Hexathiocyanatoplatinate(IV), IR Spectra, Raman Spectra, Normal Coordinate Analysis, Crystal Structure

By treatment of $[PtCl_6]^{2-}$ with an excess of SCN^- in aqueous solution $[Pt(SCN)_6]^{2-}$ is formed. The X-ray structure determination on a single crystal of $[Py_2CH_2][Pt(SCN)_6]$ (orthorhombic, space group $Pna2_1$, a = 15.5084(9), b = 11.8444(11), c = 13.2830(9)Å, Z = 4) shows, that the thiocyanate groups are exclusively S-coordinated with average Pt-S distances of 2.378Å and Pt-S-C angles in the range from 103.1° to 108.1°. Based on the molecular parameters of the X-ray determination the low temperature (10 K) IR and Raman spectra have been assigned by normal coordinate analysis. The valence force constant is f_d(PtS) = 1.62 mdyn/Å.

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