Schwingungsspektren und Normalkoordinatenanalyse der Tetrahalogeno-*closo*-1,2-diphosphahexaborane $P_2B_4X_4$, X = Cl, Br

Vibrational Spectra and Normal Coordinate Analysis of the Tetrahalogeno-*closo*-1,2-diphosphahexaboranes $P_2B_4X_4$, X = Cl, Br

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Tetrahalogeno-*closo*-1,2-diphosphahexaboranes, Vibrational Spectra, Normal Coordinate Analyses, Force Constants

High resolution vibrational spectra of the tetrahalogeno-*closo*-1,2-diphosphahexaboranes $P_2B_4X_4$, X = Cl, Br have been measured at low temperatures (20 - 60 K). The boron-halogen stretching vibrations are observed below 370 cm^{-1} while the P-P valence vibrations are found at 414 (Cl) and 372 cm^{-1} (Br). Due to the presence of the boron isotopes ^{10}B and ^{11}B the P-P stretching vibrations and the cage modes in the region of 550 to 1200 cm^{-1} are split. Based on the crystallographic data of $P_2B_4Cl_4$ normal coordinate analyses have been performed. Using a set of 16 force constants (e.g. f_d(PP) = 1.35 (X = Cl) and 1.20 (Br), f_d(BB) = 1.30 / 1.65 (Cl) and 1.45 / 1.60 (Br), f_d(BX) = 4.40 (Cl) and 3.53 (Br) mdyn / Å) a good agreement of observed and calculated frequencies has been achieved.