Molecular Structure of Diphenylchlorophosphine in the Gas Phase

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Abstract — The molecular structure of diphenylchlorophosphine was determined by gas-phase electron diffraction in combination with quantum-chemical calculations. The molecule has the C_1 symmetry with the following torsion angles around the P–C bonds: 140.2(3.1)° ($C^2P^1C^8C^9$) and –95.8(3.1)° ($C^8P^1C^2C^3$). The $ClPC^2$ and $ClPC^8$ bond angles are 101.9(4)° and 99.7°, respectively; the CPC bond angle is 103.1(1.3)°. The results of structural analysis agree with theoretical calculations of the geometry by the B3LYP/6-31G* and HF/6-31G* methods. The molecular geometries of some amines (fluoro- and chlorodiphenylamines) were calculated for comparison.

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