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Experimental and theoretical conformational analysis of methylene- and cyanophosphines and their oxides

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Abstract

The structure of a great number of methylenephosphine oxides 1-11 and cyanophosphines and their oxides 12-18 was studied by semiempirical PM3 and ab initio RHF/6-31G** calculations. Obtained results are in good agreement with experimental data (dipole moments, Kerr effect, IR spectroscopy). In 12-18 the contribution of interactions of CN group or Ph ring with lone pair of electrons (LPE) of the P atom, d-orbitals of the P atom, or P=O group is absent.

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Keywords

Conformational analysis, Cyanophosphines and their oxides, Methylenephosphine oxides, Quantum chemical calculations