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Conformational analysis of mono-and bis(dimethoxyphosphoryl)benzenes

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Abstract

Conformational analysis of mono-and bis(dimethoxyphosphoryl)benzenes with substituents in the benzene ring was performed by the method of dipole moments, IR spectroscopy, and quantum-chemical calculations (DFT B3LYP/6-31G*). Comparison of all calculated and experimental data shows that the compounds studied exist as equilibrium mixtures of conformers with preferred gg orientation of the phosphoryl and methoxy groups. © Pleiades Publishing, Inc., 2006.

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