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Calculations of 31P Magnetic Shielding Constants of Derivatives of Betaine and Phosphine Molecules Dissolved in Different Solvents by Using Supermolecular Model and Combined Methods of Quantum Chemistry and Molecular Mechanics

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Abstract

Spatial structures of molecular clusters modeling a solvate shell around phosphorus-containing methyl- and butyl-derivatives of phosphine and betaine molecules dissolved in different solvents (acetone, toluene, formamide) have been calculated by using different variants of density functional theory (unrestricted Becke three-parameter Lee-Yang-Parr [UB3LYP], Perdew-Burk--Ernzerhof [PBE], optimized exchange functional [OPTX] developed by Handy and Cohen in conjunction with Lee-Yang-Parr [LYP] correlational functional [OLYP]) with 6-31G(d,p) and 6-31G++(d,p) basis sets. The 31P magnetic shielding constants for the structures are calculated with the usage of gauge-including atomic orbitals in UB3LYP/6-31G(d,p) and 6-31G++(d,p) methods. The modeling of molecular clusters is done by using the supermolecular model, the molecular mechanics method and the combination of quantum chemistry and molecular mechanics methods (QM/MM). The own N-layered integrated molecular orbital method (ONIOM) has been applied for modeling and calculating of isotropic 31P nucleus magnetic shielding of clusters of trimethylphosphine and trimethylbetaine molecules dissolved in acetone using combinations of UB3LYP/6-31G(d,p) (higher level) and unrestricted Hartree-Fock (UHF)/6-31G(d,p) (lower level) methods. Applicability of the ONIOM approach and different ways of modeling to the calculation of 31P nucleus magnetic shielding constants is studied. A comparison of the results obtained by the density functional theory, ONIOM and MM methods is given. © 2011 Springer-Verlag.

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