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Modelling of molecular nano-sized clusters with the methods of quantum chemistry

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Abstract

With the methods of quantum chemistry calculations have been carried out of the effects of solvent on chemical shift of the nuclei of phosphorous ^{31}P. In modeling the structures of molecular clusters of phosphorous-containing molecules in the solution methods of molecular mechanics (MM), combined method of quantum mechanics and molecular mechanics (QM/MM), as well as the method of density functional DFT have been used. Calculations of constants of nuclear magnetic screening have been carried out with the use of calibration-invariant atomic orbitals (GIAO) and the basic set 6-31G(d,p) within the limits of density functional DFT with functional UB3LYP. Calculation results are compared with the experimental NMR data.