Conformation of *ortho*-fluorosubstituted biphenyls in CCl_4 solution: molecular dynamics simulation.

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The molecular dynamics simulation of 2,2′-difluorobiphenyl, 2,6-difluorobiphenyl and 2,6,2′,6′-tetrafluorobiphenyl was performed in the CCl_4 solution, in order to reproduce the solvent influence on the conformation of these molecules. Parameters necessary for the description of the intrinsic rotational potential were obtained from *ab initio* calculations. The solvent influence was assumed to be van der Waals solute-solvent interaction, described by the GROMOS96 force field. The solvent tended to decrease a dihedral angle and a volume of the solute molecule. The correlation between the solvent effect energy and the molecular volume was observed, including earlier results obtained for biphenyl.

Słowa kluczowe

Biphenyl, Rotational potential, MD simulation, Solvent influence

Adres publiczny

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