

Molecular dynamics study of biphenyl and 3,5,3',5'-tetrafluorobiphenyl in CCl₄ solution.Autorzy

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Streszczenie

The molecular dynamics simulation of biphenyl and 3,3',5,5'-tetrafluorobiphenyl was performed in CCl₄ solution, in order to reproduce the solvent influence on the shape of these molecules. The rotation around a single bond between the phenyl rings was analyzed. Parameters necessary for the description of the *intra* potential were obtained from ab initio calculations. The solvent influence was assumed to be van der Waals solute- solvent interaction, described by the gromos 96 force field. Forces acting inside the solute molecule dominated its conformation. The solvent tended to minimize the dihedral angle and the volume of a solute molecule. *meta* substitution did not influence conformational properties of biphenyl.

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