Self-association of N,N'-dialkylthiourea derivatives in non-polar solvents.

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Streszczenie

The paper consists of the joint studies of average molecular weight, dipole moments and the IR spectra of symmetric dialkyl, from dimethyl to dihexyl, thioureas, performed in function of concentration in low polar solvents, with the aim to determine those substances' relative ability of self-aggregation and the form of the subsequent aggregates. The studies were accompanied by the DFT calculations at B3PW91/6-31+G(d,p) level. It was demonstrated that association in CCl_4 and benzene is much stronger than in chloroform and 1,2-dichloroethane, which results from the competition of interaction of acidic CH groups of solvent molecules with sulfur atom of thioureas. By way of comparing the association constant with the related values for urea derivatives it was shown that the aggregation ability of thioureas is clearly lower than of ureas. This results from the fact that the basicity of sulfur atom is lower than of the oxygen one. Interesting difference between urea and thiourea derivatives is the dependence of dipole moments on concentration, when in urea derivatives dipole moment systematically grow with concentration, showing predominance of near-linear aggregation, in thioureas with shorter chains dipole moments decrease with concentration. Increase the size of chains leads to some preference of linear aggregation – dipole moments increase in non-active solvents. It can be explained by change the conformation in direction of trans–trans forms. Such conclusion was supported by results of DFT calculations.

Słowa kluczowe

Model of self-association, Dipole moments, Average molecular weight, FT-IR spectra, DFT calculation, N

Adres publiczny

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