Aggregation of *N, N*'-diallylurea and *N, N*'-diallylthiourea in solutions.

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Streszczenie

Joint studies by IR spectroscopy, dipole moments, average molecular weight measurements and DFT calculations on the self-aggregation of *N*,*N*′-diallylureas and *N*,*N*′-diallylthioureas in solvents of different polarities were performed.

Simultaneous uses of all these methods are required for better understanding the mechanism of aggregation and the effects of different polarity of solvents. In this study also the measurements of IR spectra in polarized light were additionally performed, which gives information on arrangement of aggregates in liquid crystal matrix—built of 4-CN biphenyl derivative. It was demonstrated that in such conditions two forms of dimers the linear and cyclic ones are in equilibrium with different arrangements according the axis of CN group.

Słowa kluczowe

Self-association constants, Dipole moments, Polarized IR-LD spectra, N,N′-diallylurea, N,N′-diallylthiourea

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