

Structure of aggregates of dialkyl urea derivatives in solutions.

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2010

Czasopismo

Journal of Physical Chemistry
B

Numer woluminu

114

Strony

15905-15912

DOI

10.1021/jp107096q

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Combined IR spectroscopy, dipole moment, and average molecular weight measurements and DFT calculations on the self-aggregation of *N,N'*- and *N,N*-dialkylureas in solvents of different polarities were performed. It was found that, to acquire a better understanding of the mechanisms of associations, the simultaneous use of all of these methods is required. It was found that symmetric dialkyl derivatives of urea associate much more strongly, giving in CCl_4 even a 12-fold mass of monomers, in contrast to asymmetric ones, where the average molecular weight reaches only a 2-fold mass of monomers. The very strong influence of solvents was discovered. The aggregation is much weaker in more polar chloroform and 1,2-dichloroethane leading to only a 2-fold increase in the average molecular weight. A strong influence of the symmetry of dialkylurea molecules was also found. Dipole moments of symmetric *N,N'*-dialkylurea increase with concentration, suggesting a rather linear arrangement of vectors in an aggregate. For asymmetric *N,N*-derivatives dipole moments decrease with concentration. DFT calculations were used to predict the form of aggregation.

Adres publiczny

<https://doi.org/10.1021/jp107096q>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>