Molecular structure and association of diphenylguanidine in solution.

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Streszczenie

An experimental and theoretical study of the structure and aggregation of diphenylguanidine (DPhG) in non-polar and low-polarity solvents (CCl_4, C_6H_6, C_2HCl_3 and $CHCl_3$) was performed. Dipole moments, IR spectra and average molecular weight measurements as a function of concentration demonstrate that DPhG is strongly associated in the solvents studied. The dimerization constant in CCl_4 is 192 ± 7 dm^3mol^{-1}. Experimental results and a theoretical discussion on the basis of MNDO-PM3 and -AM1 methods show that in low-polarity solvents DPhG exists in the form of an asymmetric tautomer, the same as was found in the solid-state structure.

Adres publiczny

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