Quantum-Chemical Method for Determination of Effective Structure-Energy Parameters of Multiparticle Interaction in Solutions of Polar Substances

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Abstract—A new method is developed for the determination of equilibrium value of effective structure-energy parameter of multiparticle interaction (Onsager radius of a molecule) in solutions of polar compounds. The method is based on the results of quantum-chemical calculations of the dependence of an electric dipole moment of the studied molecule in the ground state on the dielectric properties of the individual solvents that are applied. Additinal data were obtained that confirmed an opinion that by its physical sense the Onsager radius of a molecule was a value close to van der Waals radius of the same molecule which can be found using known methods of quantum chemistry and structural chemistry for isolated molecules (gas phase). It was shown by an example of solutions of 4-dimethylaminochalcone and several phthalimide and *N*-methylphthalimide derivatives that the results of determination of Onsager and van der Waals radii of all the studied molecules using three independent methods are in good quantitative agreement confirming their validity.

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