The Ellipsoid Model of Polyatomic Molecules and its Use

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Molecular structure is the main factor determining the character and intensity of an intermolecular interaction. The energy of interaction of polyatomic molecules forms a complex surface, which is impossible to use for practical tasks. The application of isotropic model potentials is the only possible way for calculations to proceed. However, the simplification of the structure to spherical particles is inadmissible, because it leads to more serious mistakes. In this work it is proposed to model polyatomic molecules by a rotational ellipsoid constructed strictly by laws of mechanics.

The following procedures are performed. The main moments of inertia and the respective rotation radius on the main axes are calculated. These values are used for the construction of an ellipsoid with a rigid surface. The analogs of the main moments of inertia for polarizability are calculated by the same method. The value of the polarizability on the main axes allows the construction of an ellipsoid of polarizabilty around the rigid surface.

Since the main rotation is realized around the axis with the largest moment of inertia, an oblong ellipsoid of revolution was obtained. Geometrical characteristics of the model correspond completely to the molecular conformation, including the rotational isomers. Besides, the thickness of the polarizability layer determines important characteristics for the energy of interaction, e.g. for a rigid molecule, for which the repulsion steepness is important.

The model obtained allows a reasonable approach to the selection of efficient potentials of intermolecular interaction. All characteristics of the model which are used for non-spherical potentials are functions of the molecular structure and thus its interaction is described more completely as compared to spherical potentials. Besides, more high precision is provided by the different approaches to the prediction of properties of so-called convex molecules with the realization of the ellipsoid model.