



The Theory of Intermolecular Forces

Anthony Stone

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The theory of intermolecular forces has advanced very greatly in recent years. It has become possible to carry out accurate calculations of intermolecular forces for molecules of useful size, and to apply the results to important practical applications such as understanding protein structure and function, and predicting the structures of molecular crystals. The Theory of Intermolecular Forces sets out the mathematical techniques that are needed to describe and calculate intermolecular interactions and to handle the more elaborate mathematical models. It describes the methods that are used to calculate them, including recent developments in the use of density functional theory and symmetry-adapted perturbation theory. The use of higher-rank multipole moments to describe electrostatic interactions is explained in both Cartesian and spherical tensor formalism, and methods that avoid the multipole expansion are also discussed. Modern ab initio perturbation theory methods for the calculation of intermolecular interactions are discussed in detail, and methods for calculating properties of molecular clusters and condensed matter for comparison with experiment are surveyed.

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