GENERALIZED EQUATIONS FOR THE INERTIAL TENSOR OF A WEAKLY BOUND COMPLEX

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A variety of methods have been employed for deriving intermolecular structural parameters from observed rotational constants of weakly bound complexes. Among these are methods that use formulas expressing the moments of inertia of the complex in terms of intermolecular coordinates and the known moments of inertia of the free monomers. While such formulas are available for a number of specific geometries, general forms have not been given. In this talk, equations are presented for the inertial tensor components of a weakly bound complex in terms of intermolecular coordinates and moments of inertia of the individual moieties. The result is a generalization of similar equations existing in the literature and allows for the use of up to three angles to specify the orientation of an asymmetric rotor within a complex. The angles used are well suited to treating the large amplitude motion characteristic of weakly bound systems and the resulting expressions should be useful in the analysis of the rotational constants of weakly bound systems with complicated geometries.