match no.1 p. 121 1975

GRAPH THEORY AS A BASIS FOR THE SYMMETRY GROUPS OF NON-RIGID MOLECULES

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Abstract:

A new method for derivation of symmetry groups of nonrigid molecules, based on the concept of isometry of nuclear configurations, is presented. With any nuclear configuration, defined by a certain number of interval coordinates, we associate a graph, whose vertices and edges are valued by nuclear charge and mass and by internuclear distances, respectively. The group of mappings of this graph onto itself defines the internal isometric group, which, together with the covering group, generates the full isometric group. Representations of this groups on the distance-set, the coordinate vectors of the nuclei and the dynamical variables of the rotation-internal-motion Hamiltonian are illustrated by a few examples.

The isometric group is the generalization of the covering group of rigid molecules to nonrigid molecules and may in a strictly analogous manner be used in the construction of symmetry groups of the rotation-internal-motion Hamiltonian and the Born-Oppenheimer problem of nonrigid molecules. Application to the stereochemistry of nonrigid molecules leads to a necessary and sufficient symmetry criterion of optical activity of this wide class of molecules, in analogy to the well known Kelvin criterion for rigid molecules.