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NOTE

Symmetry Group of Molecules

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In this paper, a novel discussion on symmetry group of molecules in a finite universe is presented.

Key Words: Symmetry, Molecule, Group theory.

A rigid molecule is defined as being such that the barriers between its versions are insuperable and there are no observable tunneling splittings. For non-rigid molecules, there are one or more contortional large amplitude vibrations such as inversion or internal rotation that give rise to tunneling splittings. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intra-molecular dynamics which can be studied more easily resorting to group theory.

Following Smeyers[1], the non-rigid molecule group will be strictly defined as the complete set of the molecular conversion operations, which commute with a given nuclear Hamiltonian operator, limited to large amplitude motions. In addition, these molecular conversation operations have been expressed in terms of physical operations, such as rotations, internal rotations, inversions, similarly as in the Altmann's theory, rather than in terms of permutations and permutations-inversions[2,3].

The molecular symmetry group is first defined by Longuet-Higgins[4]. Although there have been earlier works that suggested the need for such a framework. Bunker and Papoušek[5] extended the definition of the molecular symmetry group to linear molecules using an extended molecular symmetry.

Computing the non-rigid molecule groups using wreath product formalism was first introduced by Balasubramanian[6]. He then found some methods for computing the character table of wreath product groups[7-10] and applied his method to solve some problem related to the enumeration of molecules.

In some research papers, Ashrafi *et al.*[11-20], applied the computer algebra system GAP[21] to find symmetry and non-rigid group of some molecules. In this paper, we continue his approach to present some new aspects of symmetry of molecules. The notation we use is standard and the reader may consult references[22,23].

In this section we first describe some notation which will be kept throughout. Suppose X is a set. The set of all permutations on X, denoted by S_X, is a group which is called the symmetric group on X. In the case that, X = {1, 2,…, n}, we denote S_X by S_n or Sym(n). Also, for a group G and a subset A of G, <A> is the subgroup of G generated by A.

In the early 1920s Alexander Friedmann showed that using one assumption, the equations of general relativity can be solved to show that a finite universe must have a larger density of matter and energy inside it than an infinite universe would have. In fact, there is a certain critical density, 10^{-29} g/cm^3, which is equivalent to about 5 hydrogen atoms per cubic meter, that determines the overall structure of the universe. If the density of the universe is lower than this value, the universe must be infinite, whereas a greater density would indicate a finite universe. These two cases are referred to as an open and closed universe, respectively.

Thus finiteness of the universe is one of the most important questions in some branches of physics. Here we assume that the universe is finite and consider the point group symmetry of molecules. We first introduce some notations.

Suppose we have N atoms in the universe, say $U = \{x_1, x_2, \ldots, x_N\}$ and $M = \{y_1, y_2, \ldots, y_r\}$ is a subset of R^3. A function $f: M \longrightarrow M$ is called an isometry, if it is one-to-one, onto and for all i,j, $1 \leq i,j \leq r$ we have $|x_i - x_j| = |f(x_i) - f(x_j)|$. The set of all isometries of M is denoted by Iso(M). It is easy to see that Iso(M) is a group under composition of functions. Since the set of all positive numbers is infinite, the probability of having 4 atoms a, b, c and d such that |a-b| = |c-d| is zero. This shows that for every molecule M, Iso(M) is trivial. On the other hand, some of the symmetry elements of a molecule are isometries of Iso(M) and so in a finite universe the point group symmetry of a molecule may be different from its point group in an infinite universe.

Conclusion

The small group library of GAP contains the structure and character table of all groups with order ≤ 2000 except from 1024, groups of order 5^5, 7^4 and groups of orders p^2q and pqr, where p, q and r are primes. Thus GAP is very useful for research and education in chemistry. Our discussion in Section 2.3 shows that it is reasonable to accept the universe is infinite. We have several examples which show that the symmetry group of a molecule is depended critically to our accuracy in computing the Cartesian coordinates of atoms in the molecule under consideration.

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