Quantification of Symmetry

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A new mathematical criterion is suggested for symmetry ranking, i.e. determination of an "absolute symmetry scale" for discrete, finite groups. The criterion is based on both, the periods (orders) of each group element and the order of the group itself. This is different from the current criteria which consider only the orders of the groups themselves. The symmetry ranking, based on the new criterion, is applied to the symmetry point groups.

Introduction

The symmetry quantification is often used implicitly in physics and chemistry as can be seen from the statements that systems have "higher" or "lower" symmetry. The notions of "higher" and "lower" symmetries are crucial in the descriptions of many practical phenomena, e.g. Jahn-Teller effect. The interest in symmetry quantification has recently been revived in two different fields of science: (i) The study of biological systems [1] has shown that living organisms prefer more symmetric patterns to less symmetric ones. (ii) Kanis et al. [2] have introduced a "continuous symmetry measure" (CSM) in chemistry, which enables one to evaluate the amount of particular symmetry existing in an arbitrary geometrical configuration. Furthermore, these authors have shown that CSM and symmetry quantification has practical use in demonstrating that a direct relationship exists between an observable property (hyperpolarizability) and centrosymmetricity content. In the CSM method, the symmetry content of a particular geometric configuration is expressed by a real, positive number $S(G)$. This number (symmetry measure) quantifies symmetry with respect to a particular reference structure, e.g. how much D_{6h} symmetry is contained in the lower C_i symmetry. The CSM method is very useful, but is limited by the necessary presence of a reference structure and the calculation of spatial coordinates. The work of Kanis et al. [2] suggests that symmetry is a continuous, intensive, structural property. The logical sequel of this argument is that it should then be possible to compare different symmetries directly, e.g. one might ask whether a regular cube or an octahedron is more symmetric?

The CSM method does not provide a direct answer to such questions since it is tied to the number of vertices and (implicitly) spatial coordinates of a particular structure. In order to address this question on a more general level one must turn to group theoretical considerations because, as Armstrong [3] has pointed out, "numbers measure size, groups measure symmetry".

The purpose of this work is to discuss the quantification of symmetry in a more general sense and it's relevance (or the lack of it) to observable properties. We shall devise an "absolute symmetry scale", without any reference to spatial coordinates, by introducing a new mathematical criterion.

Discussion

Some criteria for symmetry quantification of objects which can be described by finite, discrete symmetry groups had been suggested previously by Rosen [4]. He postulated that the higher the order of the symmetry group which describes an object, the higher it's symmetry. If the symmetry groups are isomorphic, then the objects could be considered "equally symmetrical". There are, however, many non-isomorphic symmetry groups of the same order, and the question of their symmetry ranking remains unresolved. If symmetry quantification is to be done through consideration of symmetry groups, then one must consider, besides group order, the order of individual elements of the group.

We are proposing, for this purpose, a new parameter, the symmetry quantifier ($\boldsymbol{s}_\mathbf{q}$)

$$\boldsymbol{s}_\mathbf{q} = \Sigma_j \, n_j \, p_j \,, \tag{1}$$

where n_j is the number of elements of period p_j in class j.

The ranking of symmetry groups can then be reduced to the calculation of $\boldsymbol{s}_\mathbf{q}$; the group with a larger $\boldsymbol{s}_\mathbf{q}$ has a higher symmetry rank.

The definition of s_q is based on the notion that *both* the number and order of symmetry elements should be

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Table 1. The ranking of important symmetry point groups based on s_q values. s_q values are given in parenthesis, next to the group symbol. The symbols printed in bold designate sets of isomorphic groups [5].

$I_h(603) > D_{10d}(271) > S_{20}(231) > \mathbf{D_{9d}}(219) > I(211)$
$> D_{10h}(207) > D_{8d}(203) > \mathbf{C_{9h}}(183) > S_{16}(171)$
$> O_h(159) > C_{10h}(147) > \mathbf{D_{7d}}(137) > \mathbf{C_{7h}}(129)$
$> D_{8h}(119) > D_{6d}(101) > C_{8h}(87) = T_h(87) > \mathbf{D_{10}}(83)$
$> \mathbf{D_9}(79) > S_{12}(77) > D_{6h}(73) > O(67) > \mathbf{C_{10}}(63)$
$> C_9(61) > \mathbf{D_8}(59) > \mathbf{D_7}(57) > C_{6h}(49) > \mathbf{C_8}(43)$
$= C_7(43) > D_{4h}(39) > \mathbf{D_6}(33) > T(31)$
$= D_5(31) > C_{4h}(23) > \mathbf{C_6}(21) = C_5(21) > \mathbf{D_4}(19)$
$> D_{2h}(15) > \mathbf{D_3}(13) > \mathbf{C_4}(11) > \mathbf{D_2}(7)$
$= C_3(7) > \mathbf{C_2}(3)$

considered when deciding overall symmetry ranking for a particular group. The order of the individual symmetry operator (element) gives the number of symmetrically equivalent positions of an object that can be reached after applying symmetry transformation associated with this element. Again, this is in keeping with the accepted notion that e.g. the C_6 axis is "twice more symmetrical" than C_3. The derivation of periods for elements of symmetry point groups had been reported in [5].

With the aid of character tables [6] and by using s_q one may arrange all important molecular symmetry groups according to their symmetry rank (Table 1) and create and "absolute symmetry scale".

It is worth noting two important points concerning the present listing. Isomorphic groups have the same number of elements of any particular order and consequently the same s_q value and symmetry rank. The ranking of symmetries proposed in this work is new and sometimes differs from the conventional one suggested by Rosen [4], e.g. D_2 and C_3 are equally symmetrical in our classification, but $D_2 > C_3$ in Rosen's. The reason is that the latter classification is based solely on group orders.

The method used for calculating s_q will be demonstrated on the O_h point group. The O_h group consists of 10 elements:

$$O_h = E + 8C_3 + 6C_2 + 6C_4 + 3C_2' + i + 6S_4 + 8S_6 + 3\sigma_h + 6\sigma_d .$$

The periods (p) for all symmetry elements were derived in [5] and can be used directly:

$$p(E) = 1,\ p(C_3) = 3,\ p(C_2) = 2,\ p(C_4) = 4,$$
$$p(C_2') = 2,\ p(i) = 2,\ p(S_4) = 4,\ p(S_6) = 6,$$
$$p(\sigma_h) = 2,\ p(\sigma_d) = 2,$$

from which it then follows that

$$s_q(O_h) = 1\times1 + 8\times3 + 6\times2 + 6\times4 + 3\times2 + 1\times2 + 6\times4 + 8\times6 + 3\times2 + 6\times2 = 159 .$$

How do these symmetry ranking criteria relate to observable properties? Isomorphic molecules are considered to be equally symmetrical, and yet their properties differ widely. A few examples will suffice: molecules of C_2 symmetry are chiral while those of the isomorphic symmetries C_s and C_i are not; molecules of C_{nv} symmetry are polar while the isomorphic D_n ones are not. The source of these differences lies in the fact that the quantum mechanical operator which describes a certain physical property Π must commute with every symmetry operator (element) Σ_i in the MSG if it's expectation value is to be non-zero. In mathematical language: if $[\Pi, \Sigma_i] = 0$ for every i, then $\langle \Pi \rangle \neq 0$. This condition is not fulfilled for some isomorphic groups and, hence the molecular properties differ. The isomorphism is an abstract concept which considers only intra-group relationships between elements and not the types of symmetry elements themselves. The nature at the molecular level does not recognize isomorphism or homomorphism, but it would be interesting to see if the more complex biological system do.

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