

# Cubic Icosahedra? A Problem in Assigning Symmetry

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In recent years, there has been movement toward interdisciplinary work in the sciences. However, as with moving between nations, there can be language barriers for scientists from one discipline who try to begin work in another. In this communication, I draw attention to a difference in symmetry language between the standard usage in chemistry (and in physics) and a very different one that has come to be adopted in virology, and that is now beginning to enter chemistry; students need to be made aware of this. I also attempt to explore how this strange confusion may have come about.

From courses on the basic ideas of symmetry, chemistry students know that the point groups<sup>1</sup> of the tetrahedron ( $T_d$ ) and octahedron ( $O_h$ ) are often classified together as “cubic”, meaning having four three-fold axes. Given the excitement in recent years over “Buckyballs”, they will probably also have some acquaintance with the icosahedral group  $I_h$ , and will know that this has a much higher symmetry than other polyhedral groups, and is classified separately. Later, if the students move over to work in the biological sciences, they are likely to encounter work on viruses at some time. They may then be startled to find that in many virology textbooks<sup>2</sup> those viruses that have approximately icosahedral symmetry are described as “cubic”. One teaching Web site even claims that “icosahedral symmetry is identical to cubic symmetry” (1).

I examine first what symmetry considerations may lie behind this confusion and then give a brief history of the alternative, but mistaken, usage. This is traced to a very significant paper in virology, whose authority has been great enough to allow the error to spread widely. Several points along the way may be of wider interest.

## The Relation of Icosahedral and Cubic Symmetries

Most introductions to symmetry ideas treat these classes completely separately, though the somewhat gnomonic statement that the symmetries of the tetrahedron, octahedron, and icosahedron “are all closely related to that of a cube” appears in early editions of *Inorganic Chemistry*, by Shriver, Atkins, and Langford (2). There is a relationship between cubic and icosahedral symmetry, but it is not one that is immediately obvious.<sup>3</sup> Formal group theory can of course be used to analyze this problem (3), but a pictorial approach may be more useful. Figure 1 shows an icosahedron inscribed within a cube<sup>4</sup>; in this combination, the symmetries of both bodies are reduced. Versions of this diagram can be found in Shriver, Atkins, and Langford (2), accompanying the comment mentioned above, and in Caspar and Klug (4). Six of the icosahedron edges lie within cube faces; four are visible in Figure 1 and have been emphasized with heavy lines. Four of the original ten 3-fold axes of the icosahedron are preserved in the combination. These four  $C_3$  axes coincide with the cube body

diagonals and with the  $C_3$  axes of the cube; one of these is picked out as a dash-dot line. Because of the existence of this set of four  $C_3$  axes, an icosahedron can form the repeat unit of a cubic crystal structure (4).

All six of the icosahedron edges in the cube faces are shown in Figure 2, where the other edges have been removed for clarity. The symmetry elements that are common to both the cube and the icosahedron interchange all components of both bodies, but their effects are most easily seen using these six edges.<sup>5</sup> These common elements are the four  $C_3$  axes, the three  $C_2$  axes through cube faces coincident with the dotted lines in Figure 2, the inversion center, four  $S_6$  axes collinear with the  $C_3$  axes, and three planes of symmetry defined by opposite pairs of these six edges.<sup>6</sup> These elements are those of the group  $T_h$ , which is thus a subgroup of both  $O_h$  and  $I_h$ . The correlation of all the elements of the three groups is shown in Table 1. Although  $T_h$  is not often encountered in chemistry courses, a number of important examples are known.<sup>7</sup>

There is a similar relationship between the rotation groups  $I$ ,  $O$ , and  $T$  (5); the appropriate table can be generated from Table 1 by removing the column showing the inversion center, and all the other columns to the right of this one.<sup>8</sup> Although for chemists the centrosymmetric  $I_h$ ,  $O_h$ , and  $T_h$  are the useful groups, the rotation groups are the significant ones for a discussion of virus structures.

## The Symmetry Language of Virology

In 1956, shortly after their famous DNA work, Crick and Watson published a letter to *Nature* that revolutionized structural work in virology (6). There had been earlier suggestions that viruses might be built up from multiples of smaller units, and for spherical viruses, Crowfoot-Hodgkin (7) had pointed out that where these crystallize with cubic lattices, the smaller units must occur in multiples of 12. This number arises from the effect of the four three-fold axes of the cubic lattice, or in the language of point groups, this is the order of the simplest cubic group, that of the tetrahedral rotation group  $T$ . Before the Crick and Watson letter appeared, such multiple units would have been expected to have either octahedral or tetrahedral symmetry, that is, one of the five types,  $O_h$ ,  $O$ ,  $T_d$ ,  $T_h$ , and  $T$ , that chemists call cubic.

The paradigm shift introduced by Crick and Watson was the idea that a lattice with cubic symmetry can also be generated by packing units that have icosahedral symmetry. Reasons for this have been explained above: the icosahedral groups  $I$  or  $I_h$  include the cubic groups  $T$  or  $T_h$  as subgroups. Molecules of living matter are homochiral, and a symmetry plane or inversion center would convert a left-handed unit into a (nonexistent) right-handed example, so the *only possible* symmetry elements here are rotation axes. Consequently, the icosahedra concerned have  $I$  symmetry,

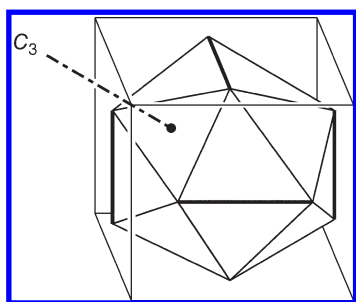


Figure 1. A regular icosahedron inscribed in a cube. The dash-dot line shows one of the four 3-fold axes that coincide with the four cube body diagonals. These axes are common to both units; the heavy lines are icosahedron edges that lie within cube faces (see Figure 2).

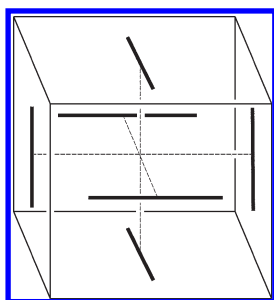


Figure 2. A regular icosahedron inscribed in a cube (as in Figure 1), but only those edges of the icosahedron that lie within cube faces are shown. The dotted lines show the positions of the three  $C_2$  axes that are common to both units (see also Table 1).

not the more familiar  $I_h$  symmetry.  $I$  includes five-fold axes, so the multiples of smaller units that make up the virus structure<sup>9</sup> are now of 60, the order of  $I$ , the icosahedral rotation group.

Unfortunately, perhaps to shorten their text, Crick and Watson did not present an argument of the type given above<sup>10</sup> in their letter. Instead they stated that icosahedral symmetry can be classed as cubic and defined a cubic class of symmetry as one that "must contain at least four three-fold axes and three two-fold axes, arranged as for a tetrahedron." In this citation, the words "at least" are critical. If accepted, they allow the inclusion of icosahedral symmetry within the classification "cubic", and they seem to be original to the authors. No reference is given for this definition, and it contrasts with one that had been given earlier, in the standard work by Landau and Lifschitz (8). This classifies *only* the five octahedral and tetrahedral symmetries as cubic; icosahedral symmetry is handled separately. Landau had worked with most of the major figures in theoretical physics of the period, so his opinion should be representative of the standard usage at this time. There can be no doubt that Crick and Watson intended to classify icosahedral as cubic; this occurs several times in the letter, and in their discussion of the Platonic solids as potential models for virus structures, all five of these are classed as having "cubic" symmetry.

If classifications of symmetry were concerned only with crystal structures, there might be some logic to this reclassification of icosahedral symmetries. However, spectroscopists and chemists need to deal with more or less isolated units, and there are good reasons to reject this amalgamation of different symmetry types. Mathematically, the group  $I$  belongs to the important class of simple groups (6, 9); the cubic groups do not.

Table 1. A Correlation of Elements in the Groups  $I_h$ ,  $T_h$ , and  $O_h$

Group	Element									
$I_h$	$6C_5$	$10C_3$	—	—	$15C_2$	$i$	$6S_6$	$10S_8$	$15\sigma$	—
$T_h$	—	$4C_3$	—	—	$3C_2$	$i$	—	$4S_6$	$3\sigma_d$	—
$O_h$	—	$4C_3$	$6C_2^a$	$3C_4$	$3C_2$	$i$	—	$3S_4$	$4S_6$	$3\sigma_h$ $6\sigma_d$

<sup>a</sup>These  $6C_2$  lie along  $\{110\}$  directions of the cube, and as can be seen in Figure 1, they have no counterpart in the other two groups. The other  $3C_2$  are indicated in Figure 2.

Icosahedral symmetry has *five* sets of four 3-fold axes that can be chosen, in Crick and Watson's words, to be "arranged as for a tetrahedron" (i.e., the circumscribing cube in Figure 1 is only one of five that can be drawn<sup>11</sup>); cubic symmetries have only one such set.

A more obviously chemical objection is that the *maximum* degeneracy in any of the cubic groups is *three*, whereas in icosahedral symmetry it is *five*; correspondingly, any cubic field splits the 5-fold degenerate set of d orbitals into doubly and triply degenerate sets, but an icosahedral field, such as that at the center of a  $C_{60}$  molecule, does not split this set. Finally, the use by Crick and Watson of the words "at least" requires that spherical atoms and ions, with an infinite number of axes, be classified as cubic. Of course in a lattice such as NaCl, the ions are in a cubic field, so their symmetry is reduced to cubic, but as free ions, they have a much higher symmetry than cubic.

Nevertheless, the term "cubic virus", meaning an approximately spherical or icosahedral virus, has become widespread in textbooks and works of reference in virology. This is almost certainly the result of following the lead of the Crick and Watson letter, and most of these works cite this. The letter had a transforming influence on the field, and it would be unreasonable to blame virologists for accepting a statement, which is almost an aside, and adopting a convention that appeared to have considerable authority behind it. However, this mistaken convention is likely to present difficulties for chemists who venture into the area, and it is also appearing in chemistry.

### Problems for Chemistry and Suggestions for Teaching

There are two examples where widely used chemistry textbooks, which have gone through several editions, have conflated icosahedral and cubic symmetries. In one textbook (10), a decision tree for assigning point groups showed all three polyhedral groups as cubic, but this has been corrected in a more recent edition (11). In the other textbook (12), the next edition will be corrected (13). A warning about the confusion is given in a Web site about symmetry operations and character tables (14).

There is a different example that may have more serious consequences for chemistry. Viruses are clear examples of self-assembly and of encapsulation, and both of these topics are of considerable interest in contemporary chemistry, so it is not surprising that chemists should be looking to virology for ideas. However, this leaves open the possibility of transmitting this incorrect symmetry language from virology into the chemical research literature, and this is beginning to happen. In major reference volumes, statements can be found such as "The Platonic solids comprise a family of five convex uniform polyhedra which possess cubic symmetry" (15), and "Three types of cubic symmetry exist; namely tetrahedral, octahedral and

icosahedral" (16). Both of these statements are clearly following the lead of the Crick and Watson letter.

Chemists should be made aware of this potential stumbling block, particularly because it can now be found in some chemistry textbooks. Some discussions of point symmetries suggest that there is no molecular example of  $I$  symmetry, but if the concept "molecule" includes viruses, this is clearly incorrect, and it might be appropriate to mention viruses here when discussing point groups. The constraint imposed on the symmetry of virus structures by the handedness of the units of living matter is a useful connection between chirality and symmetry, which are often taught in very different courses. Finally, despite the objection above, the Crick–Watson letter is a particularly beautiful instance of the application of symmetry to solve an important problem, and working through this could be a useful and interesting exercise for advanced students.

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### Notes

- Standard Schoenflies symmetry labels of point groups are used here, but in the virology literature, if symbols are used, the Hermann–Mauguin system is employed. The same is true for the chemistry textbooks that use the mistaken virology convention, so that instead of the symbols  $T$ ,  $O$ , and  $I$  for pure rotation groups, the symbols 23, 432, and 532 appear.
- A list of such textbooks has been provided for the reviewers, but it is not my intention to criticize individual authors, nor is it being suggested that the virology community is in any way to blame for the mistake, because they have been relying on an article that carries great authority (see below).
- Even among professional mathematicians, the correlation of cubic and icosahedral symmetries can cause problems. In the classic text by Hilbert and Cohn-Vossen (17), it is claimed that "the octahedral group is a subgroup of the icosahedral group". It will become clear in the following discussion that this is not true; see particularly Table 1. The English translation of this text appeared shortly before the letter being discussed here, and the two mistakes have similarities. A very similar statement to that in ref 17 occurs in a much more recent text on geometry (18).
- This diagram has been attributed to Euclid (4), but in fact was first drawn by the great artist of the early Renaissance, Piero della Francesca, who was also a mathematician of substantial ability (19–22). Piero's drawing is available (23).
- For example, the  $C_3$  axis shown in Figure 1 is now seen to interchange all six of these edges; the three adjacent to the front top left corner are rotated into each other, as are the other three.
- These opposite pairs of edges also define three perpendicular rectangles, which have the proportions of the "golden ratio" (24), and the operations of the symmetry elements may equally be considered as interchanging these "golden rectangles". The golden ratio also appears in the character tables for icosahedral symmetry (25).

- As expected from Figure 1, examples of  $T_h$  can be found as modifications of both  $I_h$  and  $O_h$  symmetries.  $Cs_3C_{60}$  has a structure (26) that can be described using Figure 1, where the unit cell has  $C_{60}$  units at the cube corners and at the body-center, and the Cs ions are at the corners of the icosahedron, so that both the  $C_{60}$  units and the icosahedron have  $T_h$  rather than  $I_h$  symmetry. Cubic distortions from  $I_h$  to  $T_h$  symmetry have been predicted for the hypothetical molecules  $B_{80}$ ,  $Si_{60}$ , and  $Ge_{60}$  (27, 28), and  $T_h$  symmetry can be found experimentally in appropriately substituted fullerenes (29). In "octahedral" symmetry,  $T_h$  occurs in hexa-coordinated complexes  $ML_6$ , where L has a local  $C_{2v}$  symmetry, and the principal ligand planes include the heavy lines of Figure 2. Examples include complexes of nitrite, both monodentate (30, 31) and bidentate (32); nitrate (33); and water (34, 35).
- An alternative approach, which leads to the same conclusion, can be developed by using the concept of the orbit of a group. This concept is described by Quinn, Fowler, and Redmond (25, Chapter 2); the illustrations of the regular orbit of  $T_h$  on p 51 of this work can be correlated with appropriate ones for orbits of  $I_h$  and  $T_h$  symmetry.
- More accurately, this is the number of particles that make up the structure of the virus coat: the RNA of the virus is enclosed within this icosahedral protein shell.
- Caspar and Klug (4) presented an argument of this type later, but their article did not address the error described here.
- The set of five cubes, which together have icosahedral symmetry, is illustrated in a rotatable image in (36).

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