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Continuous symmetry measures. VI. The relations between polyhedral point-group/subgroup symmetries

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We extend our analysis of the symmetry content of the classical polyhedra [1] to the analysis of the degree of polyhedral subgroup symmetries. The quantitative levels of the hierarchical polyhedral symmetries series of O_h, D_{4h} and D_{2h} of hexacoordinated structures, as well as the relations between them, serve as an example. A distinction is made between two types of measures: quantitative evaluation of the degree of symmetry, and quantitative evaluation of the degree of content of a reference shape.

KEY WORDS: symmetry, hexacoordination, polyhedra, symmetry subgroups, continuous symmetry, octahedron, bipyramid, shape measure

1. Background

In the past several years we have developed a general methodology for measuring, on a quantitative scale, the degree of symmetry (and chirality) content in a given (distorted) structure [1,2]. A number of novel-type correlations between symmetry or chirality and molecular properties have been consequently revealed [3–15]. The Continuous Symmetry Measure (CSM), which seeks the minimal distance to the desired perfect symmetry, has been backed both by a general algorithm [16] and by several specific algorithms and computational tools [2] tailored for specific needs. Of relevance here is the symmetry measurement tool developed for the family of the classical polyhedral symmetries [1]. Specifically, it allows the determination of the degree of the highest polyhedral symmetry, and more generally it allows the quantitative evaluation of the content of any given shape, symmetric or not, in any structure. Here we develop further the analysis of polyhedral symmetries by addressing two issues. First, whereas in [1] we described the evaluation of the highest possible symmetry, here we develop

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the methodology for evaluating subgroups symmetries content. And second, we clarify the distinction between measuring the symmetry content in cases where the specifics of the reference symmetric structure are unknown, and cases where such a structure is predetermined or preselected. Since the family of molecular polyhedra which are characterized by symmetry subgroups is by far larger then the family of polyhedral molecules characterized by the highest possible symmetry, the following is a necessary addition to the arsenal of programs devised to determine the symmetry and chirality contents on a continuous level. In particular, the measurement of the degree of subgroup symmetries provides an interesting mean of analyzing the hierarchical relations between them on a quantitative level. We recall that a common practice in structural analysis is to plot the relation between specific geometric parameters, say, changes in bond lengths as a function of angle changes [17] and references therein. The quantitative symmetry approach provides a new type of global-parameter analysis: how do values of relevant symmetries of a structure relate to each other. A detailed study of the relation between the degree of symmetries which are not a subgroups series – the degree of tetrahedricity (T_d) and of D_{4h} square planarity in tetracoordinated complexes – was published recently [6].

To demonstrate the methodology and the relations between a hierarchical set of polyhedral symmetries, we have selected to concentrate on the series of O_h, D_{4h} and D_{2h} symmetry content of hexacoordinated structures. In addition to the central role of this coordination, this selection continues the O_h-hexacoordination analysis in [1] and the recent detailed analyses [8,9] of the quantitative degree of chirality of a large library of hexacoordinated compounds the structures of which lie on the Bailar D_3-twist route.

2. The polyhedral-symmetry measurement methodology: Subgroups and reference shapes

2.1. The distance to symmetry

According to the CSM methodology [1,2,16] (for other approaches, see [18–20], given a (distorted) structure composed of N vertices (either the ligands only, or the ligands and the central atom) the coordinates of which are Q_k ($k = 1, 2, \ldots, N$), one searches for the vertex coordinates of the nearest perfectly G-symmetric object (G being a specific symmetry group), $\widehat{P}_k$. Once at hand, the symmetry measure is defined as

$$S(\mathrm{G}) = \min \frac{\sum_{k=1}^{N} |Q_k - P_k|^2}{\sum_{k=1}^{N} |Q_k - Q_0|^2} \cdot 100, \tag{1}$$

where P_k is the set of coordinates of the searched reference shape before minimization, Q_0 is the coordinate vector of the center of mass of the investigated structure,

$$Q_0 = \frac{1}{N} \sum_{k=1}^{N} Q_k, \tag{2}$$

and were the denominator is a mean square size normalization factor. It was proven elsewhere [1,16] that the bounds are $100 \geqslant S \geqslant 0$: if a structure has the desired G-symmetry, $S(\mathrm{G}) = 0$ and the symmetry measure increases as it departs from G-symmetry, reaching maximal value (not necessarily 100). All $S(\mathrm{G})$ values, regardless of G or of the structure are on the same scale and therefore comparable. One can compare the degree of, say, perfect octahedricity ($\mathrm{O_h}$-ness), $D_{4\mathrm{h}}$-ness, $\mathrm{D_{2h}}$-ness and $\mathrm{D_{3h}}$-ness of various distorted hexacoordinated complexes; one can compare the $\mathrm{D_{2h}}$-ness of complexes with different coordination numbers; or one can compare different symmetry contents of different complexes.

The main computational problem is to find the nearest structure that has the desired symmetry, namely, how to minimize equation (1) to get the set of $\widehat{P}_k$. Several methods, both general and problem-specific, have been constructed towards this goal [1,2,16]. We continue here the development of the method described in [1], which uses for the minimization procedure of equation (1) an input structure which has the desired symmetry but which is not of minimal distance to the distorted one. This *prototype symmetric structure*, the coordinates of which are P_{0k}, undergoes minimizations which transform it to the desired set of vertices, which is the closest to the distorted Q_k. For instance, if one wishes to determine the degree of $\mathrm{D_{4h}}$-ness (or tetragonality [21,22]) of a distorted hexacoordinated compound, then the prototype symmetric structure is a square-based octahedron with some arbitrary z-elongation. Such an arbitrary $\mathrm{D_{4h}}$-square bipyramid (located at P_{0k}, scaled to an r.m.s. size of 1 and placed at the origin) is used as a starting input for the minimization procedures. These minimizations constitute of the orientation, the scale and the z-elongation, i.e., the height-to-base ratio,[1] h/b. It has been shown [1] that in terms of the prototype symmetric structure, P_{0k}, minimization of equation (1) leads to

$$S(\mathrm{G}) = \left[1 - \frac{\left(\sum_{k=1}^{N} P_{0k}^{\mathrm{t}} R^{\mathrm{t}} Q_k\right)^2}{N \sum_{k=1}^{N} |Q_k|^2}\right] \cdot 100. \tag{3}$$

Here, R is a rotation (3×3) matrix (and the upper index, t, shows the transposition of the matrix or vector).

2.2. *The distance to a predetermined shape*

Specific structural-parameter minimizations such as the z-elongation/contraction are not needed for the five regular Platonic polyhedra, the shapes of which are uniquely defined. Another useful case where specific structural minimizations are not needed is when the shape of the prototype structure is decided upon *a priori* [23]. Consider again determining $S(\mathrm{D_{4h}})$ of a hexacoordinated structure. An available option is to make an *a priori* decision on what is the suitable or desired specific reference shape of the

[1] Translation needs not be minimized if the center of masses of Q_k and P_{0k} coincide. Minimization over all possible vertex-labeling is needed, but can be avoided if the correspondence between the two sets (Q_k and P_{0k}) is given (which in most instances can be the case). Other minimizations may be needed, as dictated by specific cases.

square bipyramid. We term this shape the *ideal reference shape* (i-rs), which in our case is an ideal square bipyramid (i-sbp). One can decide for instance that ideality is reflected by the z-elongation with a height to base ratio (h/b) of 1. In this case one determines not $S(\mathrm{D_{4h}})$ but S(i-sbp), using the shape of the i-sbp as a prototype structure. Of course, the symmetry of that nearest ideal structure is $\mathrm{D_{4h}}$ as well, but $S(\mathrm{D_{4h}}) \leqslant S$(i-sbp) because a general $\mathrm{D_{4h}}$ bipyramid can have any h/b ratio and, therefore, is usually closer than the ideal one. Generally, since more than one definition of ideality is possible, the resulting S(i-rs) (but not S(G)) will depend on the selected definition;[2] and S(i-rs) will be $\leqslant S$(G), if the i-rs is a specific member of a family of the G-symmetric structures.

To summarize, the CSM methodology offers therefore two different options: either to determine purely the *symmetry content* by searching for the nearest specific structure which carries the desired symmetry; or, it can function as a *shape-content measure* where the distance to a specific, preselected prototype structure is searched. In fact, the preselected structure needs not be symmetric at all, and from that point of view, equation (3) is a general shape-content measure. Both optional applications of the CSM methodology are of use and will be demonstrated below.

3. $\mathrm{O_h}$, $\mathrm{D_{4h}}$ and $\mathrm{D_{2h}}$ symmetry measures in hexacoordination and relations between them

3.1. The measurement of $\mathrm{D_{4h}}$

In [1] we answered the question, what is the degree of perfect $\mathrm{O_h}$-ness of a distorted hexacoordinated structure, defining perfectness after Plato as having all edges of equal length. Specifically, we analyzed there the tetragonal distortion – $\mathrm{O_h}$ to $\mathrm{D_{4h}}$ – because of its central role in removing $\mathrm{O_h}$ degeneracies [24] and asked how much $\mathrm{O_h}$-ness is there in $\mathrm{D_{4h}}$ structures. Here we proceed down the hierarchy of symmetry, and ask a different question, namely, what is the degree of the symmetry of a distorted hexacoordinated structure with respect to a subgroup of $\mathrm{O_h}$? While we shall concentrate on the evaluation of the degree of $\mathrm{D_{4h}}$-ness (or tetragonality) and $\mathrm{D_{2h}}$-ness, the following treatment is general in its principles and can be easily adapted for other $\mathrm{O_h}$ symmetry subgroups down to $\mathrm{C_1}$, for octacoordinated subgroups of $\mathrm{O_h}$ (the cube), and in fact, for the measure of any polyhedral symmetry subgroup.

While for measuring the degree of octahedricity one has in hand, as explained above, the specific relevant prototype shape (figure 1 with a square base ($\alpha = 90^\circ$) and with height to base edge length ratio (h/b) of $2^{-1/2}$), for the determination of the $\mathrm{D_{4h}}$-ness degree one needs to minimize over all h/b values of the square based bipyramid. As an example for a low symmetry hexacoordinated structure for which we wish to

[2] Taking another example from the $\mathrm{C_{60}}$-fullerene and its distorted anions, one can either determine $S(\mathrm{I_h})$ for which the hexagon/pentagon edge ratio should be minimized; or one may wish to take the structure of $\mathrm{C_{60}}$-fullerene as the ideal $\mathrm{I_h}$ prototype and then the edge ratio is an input. The latter is what was done in [1], where the distinction between $S(\mathrm{I_h})$ and $S(\mathrm{C_{60}}$-fullerene) was not clear.

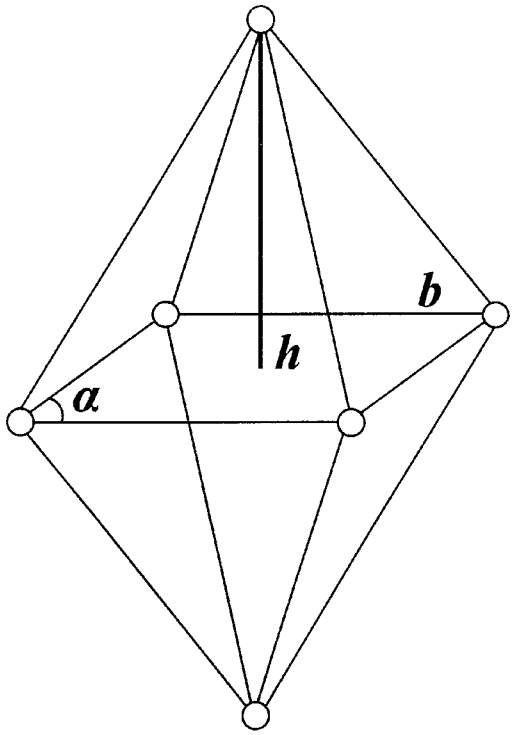

Figure 1. The parameters of the bipyramid used in this report. The base angle, α, the base edge size, b, and the height, h.

determine $S(\mathrm{D_{4h}})$, let us consider the family of $\mathrm{D_{2h}}$-hexacoordinated bipyramids, characterized by a rhombus base of various base α angles, maintaining the $h/b = 2^{-1/2}$ ratio (figure 1). The evaluation of $S(\mathrm{D_{4h}})$ of a $\mathrm{D_{2h}}$-bipyramid belonging to this family, say, a specific one with $\alpha = 60^\circ$, is carried out as follows:

1. The coordinates of the center of mass of the starting $\mathrm{D_{2h}}$-octahedron (figure 1, $\alpha = 60^\circ$) are calculated and the polyhedron is placed at the origin of Cartesian coordinates (i.e., at $Q_0 = 0$, equation (2)). The orientation and size are arbitrary (or selected for convenience of computation; in this example, for instance, the rhomboid base was in the x–y plane and the height coincides with the z-direction).

2. The prototype shape, a $\mathrm{D_{4h}}$-square bipyramid with an arbitrary h/b ratio is placed at the origin of the coordinates as well (the same $Q_0 = 0$) with either an arbitrary orientation or a conveniently selected one (e.g., height coincides with the z-direction), and its r.m.s. size is scaled to 1. The vertex labeling of $\{P_{0k},\ k = 1, 2, \ldots, N\}$ in this specific example was predetermined. As explained above, this defines the starting prototype shape, the distance of which to the coordinates of the $\mathrm{D_{2h}}$-bipyramid is to be minimized.

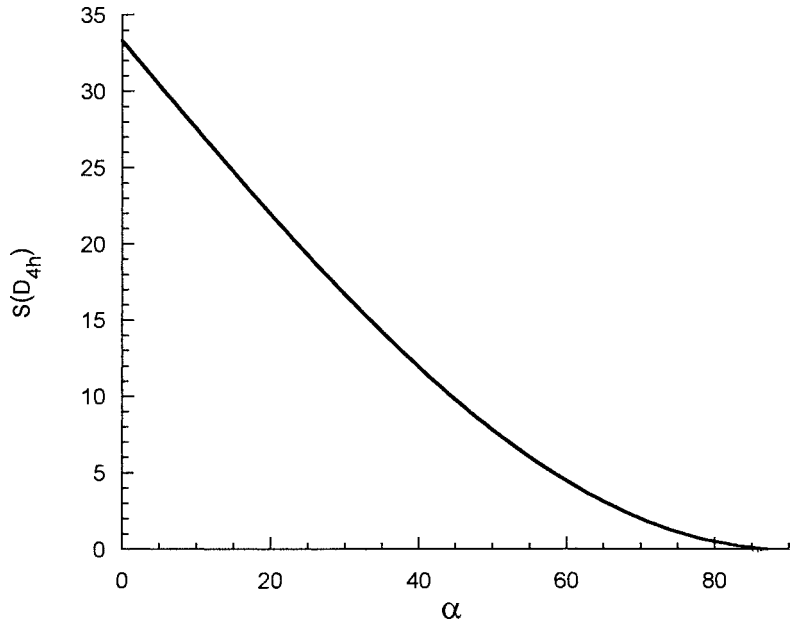

Figure 2. The degree of D_{4h} symmetry in a D_{2h}-bipyramid as a function of the base angle α (figure 1).

3. The transformation of the set P_{0k} in order to yield the desired set of $\widehat{P}_k$, namely, the set which is closest to Q_k, is determined by the various minimizations described above and in [1], and by minimizing over the h/b ratio, which is carried out by changing gradually the prototype h/b input.

4. The symmetry-content value, $S(D_{4h}$-square bipyramid), is then calculated from equation (3), and the coordinates of the nearest symmetric structure are obtained. The nearest D_{4h}-square bipyramid is characterized by an h/b ratio of 0.732 and the $S(D_{4h})$ value of that specific D_{2h} bipyramid is 4.47. Finally we note that whereas the analyzed structures do not contain, for simplicity, a polyhedron center atom, such an atom may be added and the analysis procedure is the same – see [6–9] for examples.

Let us now proceed to a full analysis of this case. Figure 2 shows the full picture, namely, $S(D_{4h})$ as a function of α of the D_{2h}-bipyramid. For $\alpha = 90°$, $S(D_{4h})$ is zero, as it should be, reflecting the fact that D_{2h} is a subgroup of D_{4h}; and therefore, as α decreases, the shape gets farther from being a D_{4h} structure, i.e., its $S(D_{4h})$ value increases. For each of the α values of the D_{2h}-bipyramid, the nearest D_{4h} square bipyramid is different, and its shape is characterized by a specific h/b value. Figure 3 shows these shapes in terms of h/b as a function of $S(D_{4h})$, and, by comparison with figure 2, it is seen that as α decreases, the nearest D_{4h}-octahedron becomes more elongated.

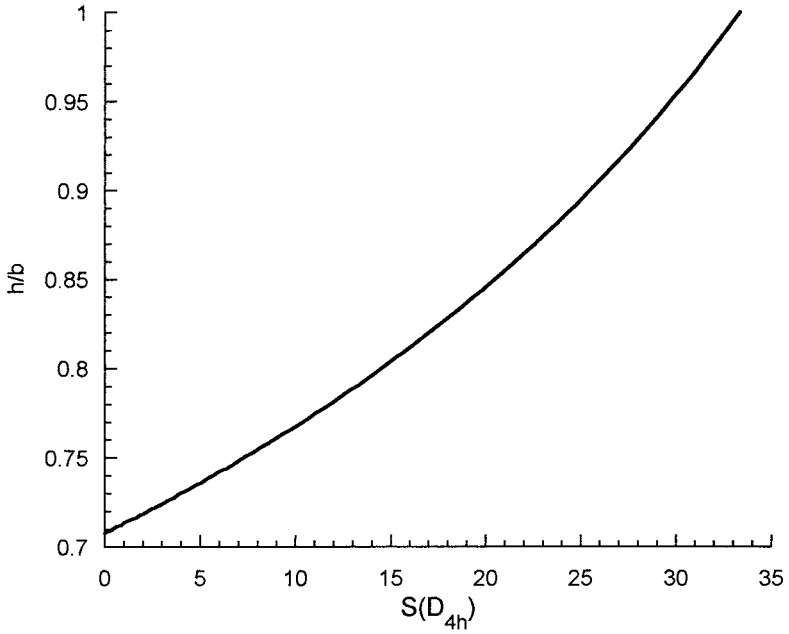

Figure 3. The height-to-base ratios (h/b) of the D_{4h}-bipyramids, which are nearest to the D_{2h}-bipyramids of figure 2, as a function of their degree of D_{4h}-symmetry.

3.2. *Quantitative relations between* O_h, D_{4h} *and* D_{2h} *symmetries*

Interesting insight on the relations between the continuous symmetry values of D_{2h}, D_{4h} and O_h is obtained by following the minimization of h/b, which led to figure 2. The search for the h/b ratio in a perfect D_{4h}-square bipyramid which leads to the minimal $S(D_{4h})$ value for several $D_{2h}(h/b = 2^{-1/2})$ rhombic bipyramids is shown in figure 4. Let us analyze, for instance, the $\alpha = 60^\circ$ curve which searches for the nearest D_{4h} to the D_{2h}, $\alpha = 60^\circ$ pyramid. From left to right, one sweeps over the h/b ratio and determines the (yet non-minimal) S measure, i.e., the distance to a *certain* D_{4h}-bipyramid characterized by a specific h/b value. The line passes through a minimum at $h/b = 0.732$, which characterizes the searched nearest D_{4h}-structure, providing the minimal $S(D_{4h})$ value of 4.47. Seen in figure 4 is the full picture behind figure 3 as well. As α decreases, the minimal $S(D_{4h})$ value is shifted to higher h/b values; i.e., as α decreases, the hexacoordinated structure is farther from a D_{4h}-bipyramid.

Figure 4 demonstrates the second capability of the CSM methodology. On each of the curves one has in each point the distance between *specific* shapes, i.e., it provided the content degree of one shape in the another shape. For instance, point (I) on the $\alpha = 60^\circ$ line is the distance of a $D_{2h}(\alpha = 60^\circ, h/b = 2^{-1/2})$-structure to a D_{4h}-structure characterized by $h/b = 0.44$; and since, in general, the distance from structure A to B must be also the distance from B to A, point (I) also determines the degree of the $D_{2h}(\alpha = 60^\circ, h/b = 2^{-1/2})$ shape in a $D_{4h}(h/b = 0.44)$-bipyramid. As explained in section 2, the CSM methodology also allows one to determine the degree of the con-

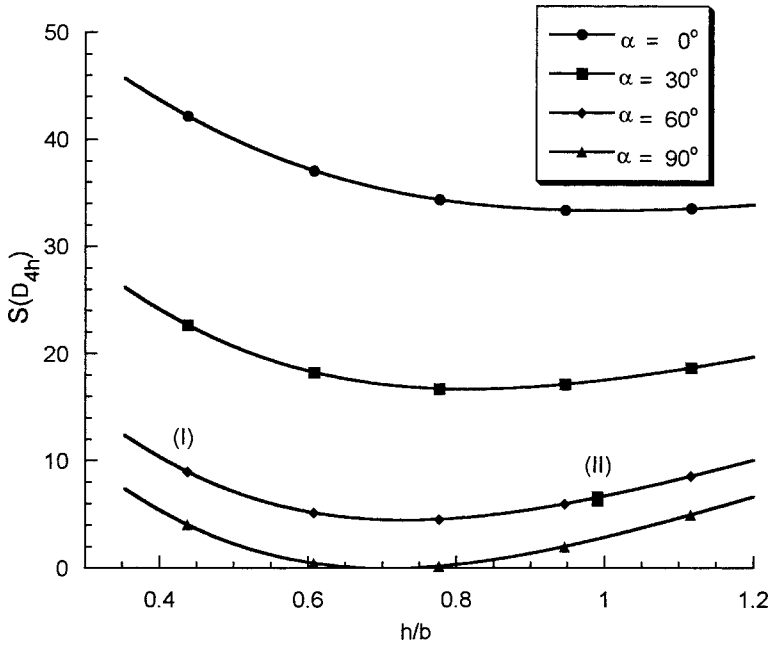

Figure 4. The two faces of the Continuous Symmetry measures approach. On one hand, shown is the search for the h/b ratio in a perfect D_{4h}-square bipyramid which leads to the minimal $S(D_{4h})$ values for several $D_{2h}(h/b = 2^{-1/2})$ rhombic bipyramids; this is a search for *symmetry content*. On the other hand, this figure also shows how to find the degree of content of *specific shapes*: point (I) on the $\alpha = 60°$ line is the distance of a $D_{2h}(\alpha = 60°, h/b = 2^{-1/2})$-structure to a specific D_{4h}-structure characterized by $h/b = 0.44$. And, suppose that a $D_{4h}(h/b = 1)$-bipyramid is defined as the ideal square bipyramid; then the distance of the $D_{2h}(\alpha = 60°, h/b = 2^{-1/2})$-structure to it is point (II). The $\alpha = 90°$ line provides information on the octahedricity level, $S(O_h)$.

tent of an ideal reference shape. Returning to the example given there suppose that we have selected a $D_{4h}(h/b = 1)$-bipyramid representing ideality, then the distance of the $D_{2h}(\alpha = 60°, h/b = 2^{-1/2})$-structure to that reference shape, namely its S(i-sbp) value, is point (II) on the $\alpha = 60°$ line (figure 4); and as explained above, it must be that S(i-sbp) $\geqslant S(D_{4h})$ as is indeed the case (figure 4).

Next let us comment on the relation between D_{2h}, D_{4h} and O_h, which becomes evident from the $\alpha = 90°$ line of figure 4. This line – like the lower-α lines – searches for the nearest D_{4h}-octahedron to a $D_{2h}(h/b = 2^{-1/2})$-bipyramid; but $\alpha = 90°$ introduces yet another meaning here because this specific D_{2h}-bipyramid is in fact a perfect O_h-octahedron. This is seen, for instance, in figure 3 where the line reaches the minimal value of $S(D_{4h})$ $(= S(O_h)) = 0$ at $h/b = 2^{-1/2}$. It follows that the $\alpha = 90°$ line also indicates the distance of tetragonally distorted octahedra (D_{4h}-bipyramids) from perfect O_h-ness. In fact, figure 4 provides information on $S(O_h)$ not only for the $\alpha = 90°$ line, but for all other α values. In general, $S(O_h)$ of the $D_{2h}(h/b = 2^{-1/2})$-bipyramids are the $S(D_{4h})$ values of the lines in figure 4 at $h/b = 2^{-1/2}$. The full picture of $S(O_h)$ as a function of α is given in figure 5(a). Comparing it to figure 2 ($S(D_{4h})$ as

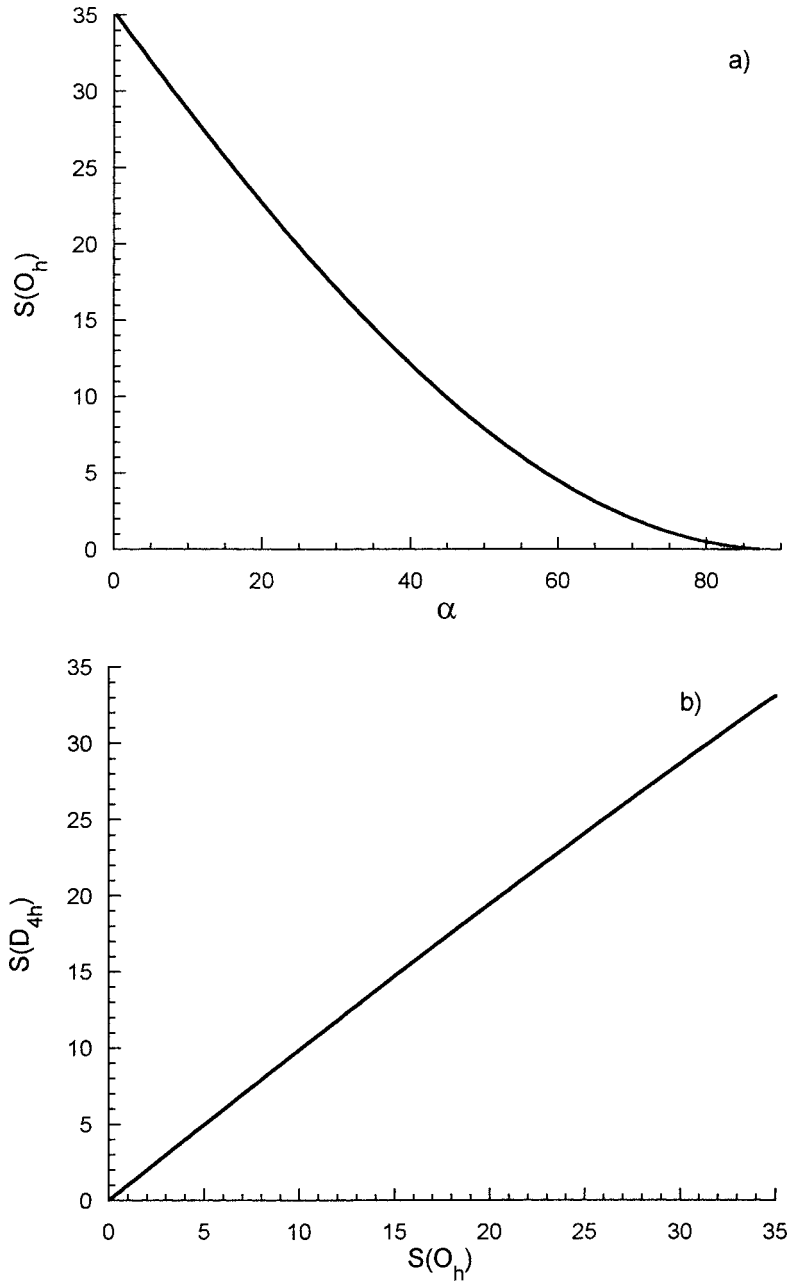

Figure 5. (a) $S(O_h)$ as a function of α of the D_{2h}-bipyramids and (b) comparison of the $S(O_h)$ and $S(D_{4h})$ values.

a function of α) it is seen that, as expected, the $S(O_h)$ values are always larger than the $S(D_{4h})$ values reflecting the fact that any (distorted) hexacoordinated structure is farther from the higher O_h symmetry than from D_{4h} symmetry; and yet the two val-

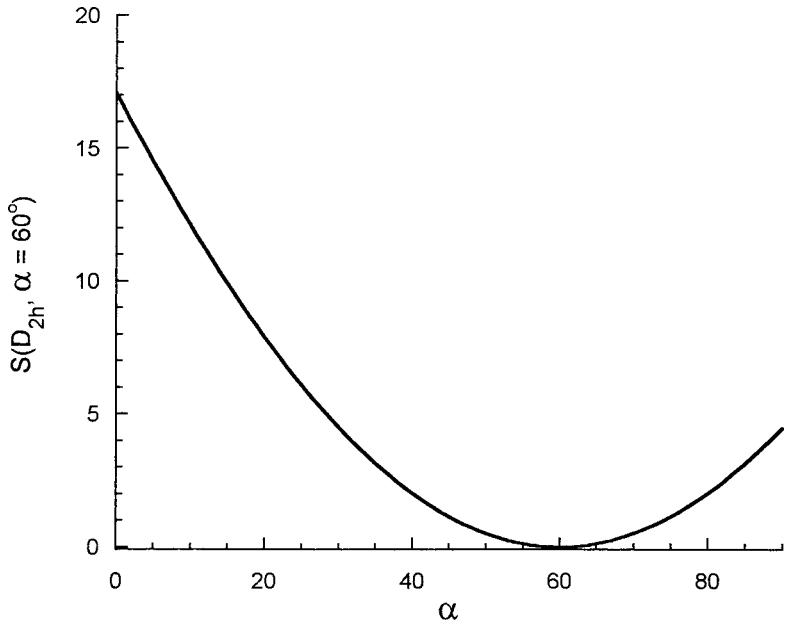

Figure 6. The distance between shapes within the same family. Defining a specific $D_{2h}(\alpha = 60°)$-bipyramid as a target shape, its content within all other D_{2h}-bipyramids is shown, as a function of α of these pyramids.

ues are quite close (figure 5(b)), and it is only at the lower α values – the more distorted D_{2h}-octahedra – that significant differences between the two measures – $S(O_h)$ and $S(D_{4h})$ – emerge. This can be understood by recalling that in the high α angle range, the $S(G)$ value in both cases is close to zero, making the difference between them small.

Another interesting feature of our methodology is its ability to analyze distances within members of a family of structures. Continuing with the same example, we now select the specific $D_{2h}(\alpha = 60°)$-bipyramid, define it as our target shape, and determine the shape content of an $S(D_{2h}(\alpha = 60°)$-bipyramid) in all of the other D_{2h}-bipyramids. The result, shown in figure 6, is a curve which passes through a minimum of zero at $\alpha = 60°$ (the distance of the target structure to itself), and therefore, in the interval of $30° \leqslant \alpha \leqslant 90°$ there are pairs of different D_{2h}-structures, equally distant within each pair, from the target $D_{2h}(\alpha = 60°)$ shape. We have termed structures of equal $S(G)$ value as *isosymmetric*;[3] likewise, structures of equal distance to a specific reference shape are termed *iso-shaped* structures. Figure 6 can be further generalized in 3D presentation to all intra-group distances within the D_{2h}-family (not shown).

[3] For this as well as other concepts that have emerged from treating symmetry as a continuous structural property, see [5,25].

4. Conclusion

We have demonstrated that the Continuous Symmetry Measures (CSM) methodology, which has been used so far mainly for the analysis of the content of specific symmetries, is also useful in revealing the relation between the quantitative degree of a point group and its subgroups. In fact, if one wishes to obtain a full profile of the symmetry characteristics of distorted polyhedral structures, then required are both the hierarchical-symmetry analyses of the type summarized here, and the analysis of characteristic point groups which are not of subgroup relations. The latter is the topic of a forthcoming report on the quantitative relation between O_h and prismatic D_{3h} of hexacoordinated compounds [26].

An important feature highlighted in this report is the CSM methodology to evaluate the degree of any one shape in any other one shape, symmetric or not. The consequences and applications of this generalization go beyond the specific problem solved here, as it allows one to define ideality without being limited to structures characterized by a symmetry point group, as the specific chemical problems may require.

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