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DESYMMETRIZATION AND DEGREE OF CHIRALITY

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Abstract

Chiral objects, viewed as distorted derivatives of achiral ones, may be represented by points in a configuration space that is spanned by a set of symmetry coordinates derived for the symmetry group of the achiral object of highest symmetry. We propose a measure (d) that quantifies the displacement of the representative point for a chiral object away from the *nearest* point representing an achiral object in such a multi-dimensional configuration space. If the symmetry coordinates are chosen so as to yield a similarity invariant measure, then the values d_i obtained for a series of i chiral objects can serve as a basis for comparing the degrees of chirality of these objects. The chirality of triangles in E^2 is studied by this method, and it is shown that the most chiral triangle in terms of this measure corresponds to one that is infinitely flat, and that may be approached but is never attained. This result is compared to others obtained previously for the same system by the use of different measures of chirality.

1. Introduction

According to Kelvin's original definition, an object is termed *chiral* if, and only if, it is not superposable on its mirror image (enantiomorph) [1]. Clearly, while enantiomorphs cannot be *superposed* on one another so as to make all their parts coincide, they may nonetheless be *superimposed*, i.e. placed upon one another. There have been a number of suggestions, based on this notion, that the chirality of an object may be quantified by evaluating the extent to which its two enantiomorphs may be superimposed or overlapped. For instance, in a straightforward extrapolation of Kitaigorodskii's idea [2], it has been proposed that the fraction of non-overlapping volumes, under the condition of maximal overlap of the enantiomorphs, may be regarded as a measure of chirality: if the objects are achiral, then there will be no non-overlapping volumes, and the fraction will thus have a value of zero [3]. The notion of maximal overlap of enantiomorphs also underlies a scheme by Kuzmin and Stelmakh, who have attempted to obtain a measure of chirality by superimposing two enantiomorphous sets of point masses representing enantiomeric molecules in a

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reduced system of coordinates [4]. We term measures – such as the fraction mentioned above – whose underlying rationale is the maximal overlap of enantiomorphs *overlap measures of chirality*.

An alternative approach that is based on symmetry considerations alone may be developed from the recognition that chiral objects are distinguished from achiral ones by the absence in their point groups of improper rotations, or symmetry operations of the second kind (σ, i, or S_n) [5]. A desymmetrization of an achiral object into a chiral one may be brought about by shifting points in the former that are invariant under improper rotations into positions where they would no longer remain invariant (thereby destroying symmetry elements of the second kind in the achiral object). A precedent for this type of approach exists, in a qualitative sense, in a definition of an achiral object as (pro)^p-chiral if it can be systematically desymmetrized by at most p steps into a chiral object [6(a)]. In this paper, we show how such a desymmetrization may be quantified, and how this quantification may serve as a basis for expressing a degree of chirality.

2. Method

The problem of quantifying the distortion of a chemical molecule from a more symmetrical reference structure has been addressed by Murray-Rust, Bürgi and Dunitz [7,8], who set out to attach a quantitative meaning to statements of the type "the molecule has *approximate* T_d symmetry". In terms of their method, a given nuclear configuration is represented by a point in a multi-dimensional space spanned by a set of symmetry coordinates ($\mathbf{S}_i$) for the (more symmetric) reference structure. The spatial coordinates of the representative point are given by displacements along the $\mathbf{S}_i$'s, which are linear combinations of the internal coordinates that transform according to the irreducible representations of the molecular symmetry (point) group ($\mathbf{G}$) of the reference structure, with the origin of the space representing that structure. The magnitudes of these displacements then serve as the basis for quantifying the deformation of the observed configuration away from the reference structure.

In general, any point that lies on an $\mathbf{S}_i$ transforming as the irreducible representation $\Gamma_j(\mathbf{G})$ is transformed into itself by those operations of $\mathbf{G}$ whose character in $\Gamma_j(\mathbf{G})$ equals that of the identity operation. The point group composed of these operations is called the kernel $\mathbf{K}(\mathbf{G}, \Gamma_j)$ of the representation. In general, more than one class of elements is represented in Γ_j by the same matrix. By contrast, the set of distinct matrices forms another group $\mathbf{H}(\mathbf{G}, \Gamma_j)$, the homomorphic image of $\mathbf{G}$, with $\mathbf{K}$ serving as the kernel of the homomorphism. Points lying on planes or in spaces transforming as degenerate representations may also be transformed into themselves by operations (R) not belonging to the kernel. These operations, together with those of the kernel, constitute a group called the co-kernel $\mathbf{CoK}(\mathbf{G}, \Gamma_j, R)$. Kernel symmetries are easily determined from character tables, while co-kernel symmetries have been derived by McDowell [9], and have later been listed together with the symmetries of $\mathbf{H}$ by Murray-Rust, Bürgi and Dunitz [8].

Such a multi-dimensional nuclear configuration space for the molecular point group **G** is thus composed of a number of subspaces – one for each irreducible representation Γ_j – whose symmetries are those of the groups $\mathbf{H}(\mathbf{G}, \Gamma_j)$. Each subspace is spanned by symmetry coordinates which necessarily have the kernel symmetry of that representation, and for degenerate representations the subspaces will also contain coordinates whose symmetry conforms to that of the co-kernel. Since every point in the space uniquely defines a given nuclear configuration, i.e. a given set of bond angles and distances, it follows that points lying along these coordinates represent nuclear configurations whose symmetries conform to those of the respective kernels and co-kernels. Some of these symmetries will be *achiral*, in the sense that their groups contain improper rotations that are prerequisites for achirality [5]. A point (C) representing a given *chiral* nuclear configuration (M) may therefore be thought of as lying in a general position in the configuration space, a certain distance $\boldsymbol{d}$ from the nearest point on an achiral coordinate. This point, which we denote p^1-C, represents a (pro)^1-chiral configuration whose single-step desymmetrization leads to the chiral configuration M. In the context of the configuration space, this desymmetrization corresponds to the displacement of a representative point from p^1-C to C, and the distance $\boldsymbol{d}$ can thus be taken as a measure of this desymmetrization.

We have previously [10] defined a *measure of chirality* $\chi(M)$ as a continuous, real-valued, and similarity invariant function of the molecular model M, in the interval $[-1, 1]$, such that $\chi(M) = 0$ if M is achiral, and $\chi(M) = -\chi(M')$, where M' is the enantiomorph of M. The *degree of chirality* was defined as $|\chi(M)|$. If the symmetry coordinates have been constructed so as to give a similarity invariant representation of M (i.e. a representation that is dependent only on the *shape*, and not the *size* of M), then the measure $\boldsymbol{d}$ will also be similarity invariant. Now, if it can be shown that the configuration space thus constructed is bounded as a consequence of geometrical restrictions on the values adopted by the internal coordinates, then the range of $\boldsymbol{d}$ may be normalized to the interval $[0, 1]$. The measure $\boldsymbol{d}$ then has all the attributes of a measure for the degree of chirality and, since it is not premised on the generation of the enantiomorphous object (M'), $\boldsymbol{d}$ constitutes what we call a *non-overlap measure* for the degree of chirality.

A configuration space constructed by the use of a set of symmetry coordinates that are not similarity invariant differs in an important way from a multi-dimensional space that is spanned by similarity invariant symmetry coordinates. In the former, each point represents a unique nuclear configuration, characterized by a unique set of internal coordinates. In the latter, by contrast, each point represents a family of configurations all of the same shape, but of different sizes. In this sense, the latter type of space would be more correctly referred to as a "conformation space", where the term "conformation" is used here as a general description of the shape of a molecule [11]; in the context of our approach, the term is therefore not limited to its common meaning as a characteristic of torsional isomers.

We shall illustrate the above approach by analyzing the conformation space of triangles confined to the Euclidean plane (E^2), and we shall derive the "most chiral"

triangle in terms of this method. The system of triangles was chosen for the reason that two recently completed analytic studies of the chirality of triangles – employing both overlap and non-overlap measures – offer an interesting comparison [10, 12, 13].

3. Conformation space of triangles in E^2

The shape of a triangle (or, in the context of this paper, its conformation), is fully defined by a minimum of two variables (two angles), although a third (a side) would be necessary to fix its size (or configuration). In order to construct a suitable set of symmetry coordinates, a reference geometry of sufficiently high symmetry needs to be chosen, so that all possible deformations of the "molecule" may be mapped in the parameter space. Scalene, isosceles, and equilateral triangles in E^2 belong to the two-dimensional point groups C_1, D_1, and D_3, respectively [10]. As the achiral reference group, we chose $\mathbf{G} = D_3$, a two-dimensional group that is isomorphic with C_{3v}, in that the three σ_v elements in E^3 correspond to lines of reflection in E^2. Our choice of internal coordinates α, β, and γ – the angles subtended at the respective vertices A, B, C – as a basis set ensures that the symmetry coordinates will be similarity invariant, since the angles determine the shape of the triangle only, and not its size. They transform as $A_1 + E$; three symmetry coordinates derived by standard methods [14, 15] may be chosen as:

$$\mathbf{S}_1(A_1) = (1/\sqrt{3})(\Delta\alpha + \Delta\beta + \Delta\gamma),$$

$$\mathbf{S}_{2a}(E) = (1/\sqrt{6})(2\Delta\alpha - \Delta\beta - \Delta\gamma),$$

$$\mathbf{S}_{2b}(E) = (1/\sqrt{2})(\Delta\beta - \Delta\gamma),$$

where Δ refers to the deviation from the angles in the reference structure (the D_3 equilateral triangle). Note, however, that the values of the reference angles are important only for the totally symmetric representation, since they cancel out in the others; for these, one can consequently use the internal angles (α, β, γ) in evaluating displacements along the $\mathbf{S}_i$'s.

For the one-dimensional representation, $\mathbf{K} = \mathbf{G}$ and $\mathbf{H} = 1$, since any point along the totally symmetric coordinate must be transformed into itself [8]. Following Murray-Rust, Bürgi and Dunitz [8], we will indicate the symmetry group ($\mathbf{H}$) of the space spanned by the degenerate representation by the Hermann–Mauguin symbol $3m$ (where m, in this case, refers to a line of reflection). We do so in order to avoid confusion between the group $\mathbf{H}$ and the groups $\mathbf{G}$, $\mathbf{K}$, or $\mathbf{CoK}$; for the latter, the Schoenfliess symbols will be used. Accordingly, the degenerate representation has $\mathbf{K} = C_1$ and $\mathbf{CoK} = D_1$, the latter corresponding to the C_s co-kernel symmetry of C_{3v} in E^3.

Clearly, there must be a redundancy amongst the symmetry coordinates, since one of the internal coordinates is dependent on the other two. Indeed, it can be seen

that the positive and negative deviations of the angles in the A_1 representation will cancel each other out, since their sum must always remain zero. The similarity invariant space of triangles is therefore adequately represented in terms of just the E coordinates. A projection of this space onto the plane defined by S_{2a} and S_{2b} is shown in fig. 1.

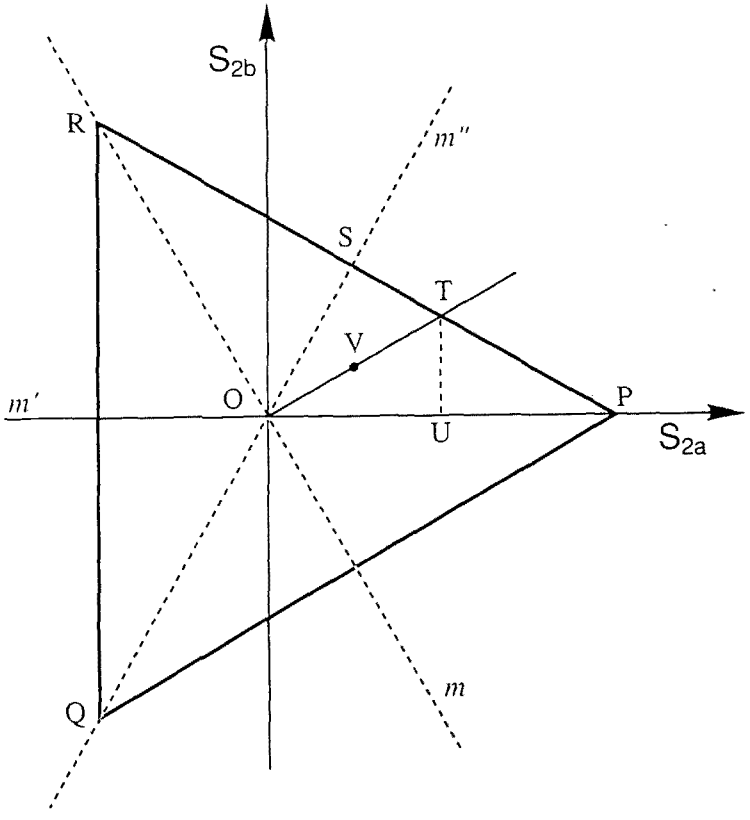

Fig. 1. Diagram of the conformation space for triangles. The dimensions of S_{2a} and S_{2b} are any angular measures. The space has symmetry $3m$, with point O as the point of threefold rotation, and lines m, m', m'' representing the lines of reflection. Section OSP corresponds to one of the six asymmetric units. The significance of points S, T, U, and V is discussed in the text.

4. Discussion

The triangular conformation space QPR depicted in fig. 1 may be used to describe any deformation of the equilateral triangle. The boundaries are the lines RQ, QP, and PR, which result naturally from the limitations placed on the values that the internal angles of a triangle may adopt. Point Q, for example, represents a triangle with $\alpha = \beta = 0°$ and $\gamma = 180°$, point P has $\alpha = 180°$ and $\beta = \gamma = 0°$, with QP hence

representing all configurations for which $\beta = 0°$ and $\alpha + \gamma = 180°$. Such triangles, in which at least one angle is 0° and all three vertices are thus collinear, will be called "degenerate". Similarly, lines RQ and PR correspond to degenerate triangles with $\alpha = 0°$ and $\gamma = 0°$, respectively. On the other hand, line QS – excluding points Q and S – maps all (non-degenerate) isosceles triangles for which $\alpha = \beta$ between the extremes of the degenerate triangles S ($\alpha = \beta = 90°$, $\gamma = 0°$) and Q. The six asymmetric units that compose the conformation space reflect the six possible permutations of α, β, and γ, and they are, of course, a function of the $3m$ symmetry of the point group $\mathbf{H}(D_3, E)$.

The lines of reflection m, m', and m'' [corresponding to the coordinates $S_{2b} = -\sqrt{3}\, S_{2a}$, $S_{2b} = 0$, and $S_{2b} = \sqrt{3}\, S_{2a}$, respectively] constitute special positions of the conformation space. These lines map achiral geometries that maintain D_1 co-kernel symmetries, such that conformations along m have $\alpha = \gamma$, those along m' have $\beta = \gamma$, and those on m'' have $\alpha = \beta$. We refer to these coordinates as *achiral coordinates*.

A representative point C will therefore lie in a general position in the conformation space when it represents a given *chiral* triangle, while in the case of an *achiral* triangle the point will lie in a special position on one of the achiral coordinates – or at the special point O if it is equilateral. Any systematic desymmetrization of an equilateral triangle to yield a given non-equilateral one would correspond to a displacement of the representative point at O until it becomes coincident with C. This displacement, in turn, may be broken down into the resultant of two consecutive displacements, the first proceeding along any achiral coordinate and the second (which may be zero) in a perpendicular direction away from it. In terms of the definition [6(a)] of prochirality mentioned above, the D_3 equilateral triangle may hence be seen to be $(\text{pro})^2$-chiral, the origin corresponding to a point that we therefore denote as p^2-C. Note that any point C in the conformation space will have this as its $(\text{pro})^2$-chiral point. (In accord with the method of [6(a)], two is the maximum number of steps in which an achiral object in E^2 may be desymmetrized into a chiral one.) All triangles represented by points on the achiral coordinates, except for the point p^2-C, are $(\text{pro})^1$-chiral.

The displacement of C along an achiral coordinate therefore measures the desymmetrization of the $(\text{pro})^2$-chiral geometry, while the perpendicular displacement away from it measures the desymmetrization of the $(\text{pro})^1$-chiral geometry, i.e. the deformation of the chiral triangle away from its closest achiral precursor. Since each asymmetric unit is bordered by two achiral coordinates, there will in general be two distances (d_1 and d_2) that could be considered. However, we are interested only in knowing the displacement from the *nearest* achiral point, and hence define our measure of the degree of chirality $\boldsymbol{d}$ as the shorter of the two, i.e.

$$\boldsymbol{d} = \min\{d_1, d_2\}.$$

The shortest perpendicular distance of a general point C to either of the achiral coordinates bordering an asymmetric unit may readily be calculated; in the asymmetric unit OSP (for which $\alpha \geq \beta \geq \gamma$), for example, the distances to the coordinates m' and m'' are $d_1 = (1/\sqrt{2})(\Delta\beta - \Delta\gamma)$ and $d_2 = (1/\sqrt{2})(\Delta\alpha - \Delta\beta)$. Note that the reference angle once again cancels out, so that the internal coordinates themselves may be substituted for the deviations, and the distance is thus simply a function of the differences between the angles.

The most chiral triangle will be the one whose representative point is at a maximum distance from the achiral coordinates, and it may be evaluated as follows. Consider, for example, the asymmetric unit OSP (see fig. 1): line OT (which corresponds to all triangles with $\beta = 60°$) is the bisector of angle $\angle SOP$, and thus represents all geometries that are equidistant from the two achiral coordinates bordering this unit. The perpendicular projections from point T onto the achiral coordinates are the maximum perpendicular distances that can be realized within this asymmetric unit, and hence represent the maximum displacement from achirality, i.e. the maximum degree of chirality. The triangle corresponding to point T would thus appear to be the most chiral. Figure 2(a) depicts graphically the deformation of the equilateral triangle that

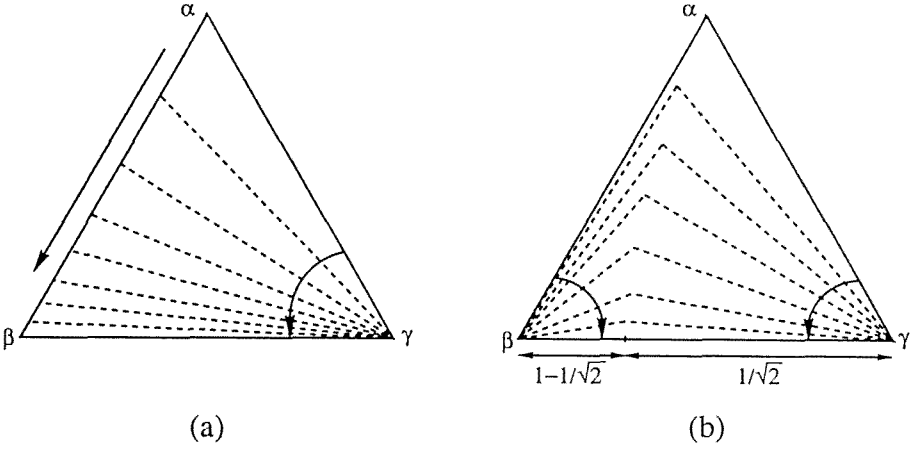

Fig. 2. (a) Deformation of the equilateral triangle towards maximum chirality as mapped by line OT in fig. 1, and (b) the corresponding deformation as mapped by the chirality function employed in [10,12]. Note that in (b) both β and γ tend to zero, as the ratio of sides $a:b:c$ tends toward $1:1/\sqrt{2}:(1 - 1/\sqrt{2})$.

is mapped by line OT, and it shows that the limit of this deformation, point T, corresponds to a degenerate triangle in which the vertices A and B (at angles α and β, respectively) and the corresponding sides a and b have become coincident, but with $\alpha = 120°$, $\beta = 60°$, and $\gamma = 0°$.

This result gives rise to contradictory interpretations: on the one hand, in the limit at point T the internal angles indicate that the triangle has a chiral conformation ($\alpha \neq \beta \neq \gamma$; $\alpha \neq \gamma$), whereas on the other hand, one might assume that when two of

the vertices are coincident, i.e. when two sides are coincident and therefore equal, an achiral, though degenerate, triangle obtains. This contradiction arises out of the contrasting perspectives that are employed in making the respective deductions. The former corresponds to an interpretation that keeps rigidly within the (mathematical) confines of the symmetry coordinate measure, while the second goes beyond this – as the use of the word "assume" shows – in that it is informed by other geometrical principles, namely, that a triangle with two equal sides must be isosceles, and therefore achiral. A second complication arises from the fact that whereas it is possible to construct a degenerate triangle from the coordinates of point T, the reverse mapping is not feasible: when two vertices are coincident, it is impossible to define uniquely the three angles α, β, and γ, and to map such degenerate triangles onto the conformation space.

The only way in which these difficulties can be avoided is by excluding the boundaries of the conformation space from consideration as triangles, i.e. by defining triangles in terms of three non-collinear points. *Under this condition, the most chiral triangle emerges as one that is infinitely flat and approachable only as a limit, with one angle of 60°, another that is arbitrarily close to zero, and a third that is arbitrarily close to 120°.* As a further consequence of the above restriction, the configuration space of triangles, while bounded, is rendered open.

The unique nature of the boundaries of the conformation space may give rise to an apparently counterintuitive interpretation, since the results suggest that as the equilateral triangle is deformed into progressively more chiral triangles, an achiral geometry – a one-dimensional line segment – is approached more and more closely. However, the loss of chirality in the limit is a natural consequence of the reduction in dimensionality that occurs at point T, since chirality is an extrinsic property and depends on the dimension in which a body is embedded: when the dimension of the space is higher than that of the body, the body must be achiral [10].

The two p^1-C points (U, S; see fig. 1) on m' and m'' whose displacements in the direction of T both yield, *in the limit*, the most chiral triangle, respectively represent an isosceles triangle with $\alpha = 120°$ and $\beta = \gamma = 30°$, and the degenerate isosceles triangle mentioned above. In both cases, the p^1-$C \rightarrow T$ displacement is accompanied by a total absolute angular change of 60°, with $d_1 = d_2 = \boldsymbol{d} = (1/\sqrt{2})(60°) \approx 42.4°$. This value defines the least upper bound (i.e. supremum) for $\boldsymbol{d}$ in the conformation space for triangles. The most chiral *right* triangle in the asymmetric unit OSP lies at point V on the line OT, with $\alpha = 90°$, $\beta = 60°$, $\gamma = 30°$, and the representative points for its (pro)^1-chiral conformations ($\alpha = 90°$, $\beta = 45°$, $\gamma = 45°$) and ($\alpha = 75°$, $\beta = 75°$, $\gamma = 30°$) on m' and m'', respectively, are both equidistant from V, with $\boldsymbol{d} = (1/\sqrt{2})(30°) \approx 21.2°$.

5. Comparison with previous results

In the first of our prior studies of the chirality of triangles [10,12], we employed an overlap measure of chirality that was determined by maximizing the intersecting

area [T^*] resulting from the superimposition in E^2 of a given triangle and its enantiomorph, and then taking the function

$$\chi(T) = 1 - \{[T^*]/[T]\},$$

where [T] is the area of the triangle, as the degree of chirality. Clearly, this function is zero for achiral geometries ($T^* = T$), while it tends towards unity for chiral triangles, and it is also similarity invariant. Our second study [13] utilized a chirality product function which takes the form

$$P(e) = (a - b)(b - c)(c - a),$$

where a, b, c are the sides (e) of the triangle. This function may be transformed into the similarity invariant measure of chirality [13]

$$\chi(e) = (1 - b/a)(1 - c/b)(1 - a/c).$$

The exploration of the conformation space of triangles that we are presenting here is in some respects comparable to the previous investigation [13] of (what we there called) the shape space of triangles by means of the measure $\chi(e)$. Our use of the term "conformation space" in place of "shape space" is a deliberate attempt to couch the discussion and the illustration of the technique presented in this paper in its proper historical context, and in a language that is intended to unambiguously illustrate its chemical relevance. After all, Murray-Rust, Bürgi and Dunitz originally proposed the use of symmetry coordinates explicitly for the description of "*nuclear arrangements of molecules* [our emphasis] that can be regarded as being distorted versions of more symmetrical reference structures" [8].

Both of the spaces mentioned above contain six segments, but only in the conformation space discussed in this paper do they constitute true asymmetric units, in the sense that the complete space may be constructed by the operations of the group $3m$ on any one of the units. The six segments of the shape space comprise three pairs that arise from the labeling convention [13] adopted for the triangular vertices (or the sides, or the angles) in the following manner. Consider, for example, applying the labels (a, b, and c) to the sides of a given scalene triangle, with $a < b < c$. When the labels a and b are transposed, the sense of cyclic directionality of the labels has to reverse. Therefore, in order to preserve the same sense for both inequalities $a < b < c$ and $b < a < c$, as required by the convention, enantiomorphs of the triangle will have to be considered. The two segments of the shape space in which the representative points for the enantiomorphs will be found hence represent enantiomorphous triangles labeled in the same sense, and according to the two permutations above. The same argument applies to the other two pairs of permutations, with a and b as the longest sides, respectively. Thus, as a consequence of the labeling convention, the shape space of the preceding study [13] maps heterochiral triangles, while the conformation space of the present study maps homochiral triangles. A conformation

space could be constructed to represent heterochiral triangles by adopting a similar labeling convention, but the distinction between enantiomorphs would then be reflected only in different positions of their representative points, not by differences in the measure $\boldsymbol{d}$: as a measure for the degree of chirality, $\boldsymbol{d}$ is an unsigned quantity and therefore does not carry any information about handedness. With $\chi(e)$, on the one hand, enantiomorphous triangles have differently signed values of the measure, and the subdivision of the shape space into heterochiral segments is therefore much more meaningful than it would be in the present study.

The three measures differ in what they reveal to be the most chiral right triangle, and in the degree of chirality of this triangle as a fraction of the supremum on the value of the chirality measure. The overlap measure yields a triangle with $\alpha = 90°$, $\beta = \arcsin 2^{-1/3} \approx 52.5°$, and $\gamma = \arccos 2^{-1/3} \approx 37.5°$, while the geometric chirality product yields one with $\alpha = 90°$, $\beta \approx 71.2°$, and $\gamma \approx 18.8°$. Expressed as a fraction of the supremum on the value of the chirality measure, the degrees of chirality of the former two right triangles are ≈ 0.67 and ≈ 0.07, respectively, while for the most chiral right triangle found in the present study ($\alpha = 90°$, $\beta = 60°$, $\gamma = 30°$), the fraction has a value of 0.5.

Both previously employed measures yield the most chiral triangle as an infinitely flat one, as does the measure developed in the present study. However, the limit that is approached is not the same in all three cases: the measures $\boldsymbol{d}$ and $\chi(e)$ both yield the limiting triangle depicted in fig. 2(a), whose ratio of sides $a:b:c = 1:1:0$, while the overlap function $\chi(T)$ yields the limiting triangle shown in fig. 2(b), for which the ratio is $1:1/\sqrt{2}:(1-1/\sqrt{2})$. In the first study [10, 12], the degenerate triangle with altitude zero had to be excluded since its area is zero, leading to an indeterminate expression for $\chi(T)$. With the chirality product function, only the degenerate triangle corresponding to the limit of the deformation depicted in fig. 2(a) had to be excluded, since only in this case does one of the sides become zero, leading to a similarly indeterminate expression for $\chi(e)$. For all other degenerate triangles, no such problems were encountered since three line segments can be identified for any triangle whose vertices are non-coincident. Indeed, we made the point that in the limit of a completely flat triangle, $\chi(e)$ becomes a measure of one-dimensional chirality [13]. Despite the differences between them, *all three chirality measures have independently revealed the most chiral triangle to be one that is infinitely flat and that can be approached only as a limit.* Whether a similar result might obtain for systems in higher dimensions, e.g. a tetrahedron in E^3, is a question that yet remains to be answered, and that we intend to address in a subsequent publication.

Irrespective of the answer to the question posed above, we wish to emphasize a point that may have been lost through our choice of an extremely abstract "molecule" on which to demonstrate the applicability of this method. The approach that we have outlined in the present paper is generally applicable to any geometric object, and may as readily be applied to quantifying the degree of chirality of distorted tetrahedral molecular models in E^3 as it was here to a selection of hypothetical triangles restricted to E^2. Furthermore, the present method does not require the generation of the

enantiomorphous image; all that is necessary is the choice of a reference geometry and a set of basis parameters that will make the derived symmetry coordinate representation similarity invariant.

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