

## THE MEASUREMENT OF SYMMETRY: BRIDGING ORDER AND DISORDER

David Avnir<sup>(a)</sup>, Omer Katzenelson<sup>(a)</sup>, Shahar Keinan<sup>(a)</sup>, Mark Pinsky<sup>(a, b)</sup>,  
Yariv Pinto<sup>(a)</sup>, Yair Solomon<sup>(a)</sup> and Hagit Zabrodsky Hel-Or<sup>(c)</sup>

*Address:* The Institute of Chemistry<sup>(a)</sup>, The Lise Meitner Minerva Center for Computational Quantum Chemistry<sup>(a)</sup> and The Institute of Earth Sciences<sup>(b)</sup>, The Hebrew University of Jerusalem, Jerusalem 91904; and Department of Mathematics and Computer Science<sup>(c)</sup>, Bar-Ilan University, Ramat Gan 52900, Israel.  
Email: david@chem.ch.huji.ac.il

The concept of symmetry has attracted virtually all domains of intellectual activity and has strongly influenced the sciences and the arts. It has functioned as a condensed language for the description and classification of the order within shapes and structures; as an identifier of inherent correlations between ordered structure and physical properties of matter; and as a guideline in artistic and practical aesthetic design. Our study of symmetry has been based on the following thesis: *Symmetry provides a rare realization of Nature, beyond the atomic level.*

The motivation of our studies has been rooted in the stark recognition that much more often than not, natural objects, are *not* symmetric. To realize it one should refine the resolution of observation - spatial or temporal - up to the point where it becomes evident. It appears that symmetry serves in many such instances as an approximate, idealized descriptive language of the physical world, beyond the scale of atoms. While it is true that an imprecise language helps in grasping complex situations and in identifying first order trends, the danger of missing the full picture because of the vague description, is always awaiting the user of the current symmetry language.

This motivation has led us to propose that it is natural to evaluate on a quantitative scale, how much of a given symmetry there is in a structure. Thus, we are treating symmetry as a structural property of continuous behaviour, complementary to the classical discrete point of view. A continuous symmetry scale should be able to express quantitatively how far is a given disordered structure from ideal symmetry, at any temporal resolution,

at any spatial resolution, and with respect to any symmetry. Towards this goal, we have designed a general symmetry measurement tool, which is based on a definition which is minimalistic. Our answer to the question “How much of a given symmetry there is in a given structure?” is then:

*Find the minimal distances that the points of a shape have to undergo, in order for it to attain the desired symmetry.*

In order to translate this definition into practice, we have developed the Continuous Symmetry Measure methodology and computational tool. Using this measurement procedure it is possible to evaluate quantitatively how much of any symmetry exists in a non-symmetric configuration; what is the nearest symmetry of any given configuration; and what is the actual shape of the nearest symmetric structure (see Figure).

We have demonstrated the feasibility and versatility of our approach on two levels. The first one is purely geometric. Here we developed solutions for specific problems such as:

- \* evaluation of the degree of bilateral symmetry;
- \* measurement the symmetry content of distorted classical Platonic polyhedra;
- \* assessment of the symmetry content of objects which contain an element of randomness in their construction;
- \* analysis of the concepts of left/right handedness and mirror symmetry; and more.

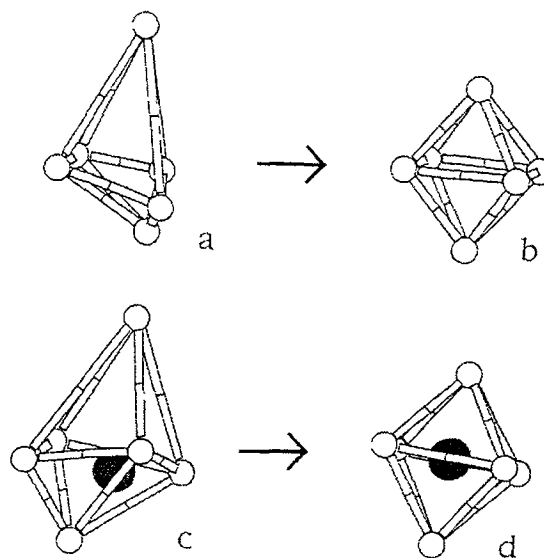
The second level concentrated on applications of the symmetry measure to real problems of the natural sciences. Examples include symmetry analyses of molecules, of crystals, of dynamically changing structures, of small (3-12 molecules) clusters and of large disordered aggregates; of enzymes and their activities, and more. Three major findings emerged:

- I. The symmetry measure describes Nature in a well behaved way: Its trends of change agree with intuition and reflect what is visible to the eye and what has been expected on a qualitative level, before measurement was possible.
- II. Hitherto unknown quantitative correlations between symmetry and physical/chemical/biochemical properties have been revealed.
- III. Far more than before, the importance of a global-shape descriptor for the quantitative observation and analysis of Nature, in distinction from the classically specific geometry descriptors, has been revealed.

In the context of this Symposium, it is important to emphasize that the Continuous Symmetry Measure methodology is applicable, beyond the molecular level analysis, to most other domains of the natural sciences, of the social sciences, and of the arts, where symmetry is an issue, either as a real feature or as an abstract one. Indeed, in separate papers in this Symposium we present the first quantitative assessment in archeology of the degree of symmetry of hand-axes of early man and its correlation to other parameters (Saragusti et al.); the assessment of the orientation of symmetric objects from their images - of relevance to design problems - and the evaluation of facial symmetry (Hel-or et al.); and in yet another on-going project we explore the possible correlation between evolutionary selection, perception of beauty and attractiveness, and the quantitative degree of bilateral symmetry.

Readers are encouraged to contact us on issues of symmetry measurement in all domains of intellectual activities. We shall provide, free of charge, access to our computer programs. Readers with background in the natural sciences are directed for more technical details to references listed in <http://chem.ch.huji.ac.il/~david/index.html>.

*Review:* D. Avnir, O. Katzenelson, S. Keinan, M. Pinsky, Y. Pinto, Y. Salomon and H. Zabrodsky Hel-Or, "The Measurement of Symmetry and Chirality", in "Concepts in Chemistry", D. H. Rouvray, Ed., Research Studies Press, Somerset, 1996, Chapter 9, p.283.



**Figure:** How much tetrahedrality is there in the distorted tetrahedron **a**?; and how much octahedrality in the distorted octahedron **c**? On a scale from zero (perfectly symmetric) to 100, both have a symmetry value of 15. The polyhedra **b** and **d** are the nearest perfectly symmetric objects to **a** and **c**, respectively. Having equal symmetry values, **a** and **c** are equally distant from being fully symmetric - they are *iso-symmetric* objects.