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THE ROLE OF IMPERFECT SYMMETRY IN NATURE, ART, MATHEMATICS, AND CHEMISTRY: APPROXIMATE SYMMETRY AND SYMMETRY DEFICIENCY MEASURES

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Mezey, P. G. (1990) A Global Approach to Molecular Symmetry: Theorems on Symmetry Relations between Ground and Excited State Configurations, *Journal of American Chemical Society*, 112, 3791-3802.
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Abstract: *Approximate symmetry is a concept that is fundamental for most fields of natural sciences, and it is also an important feature of art. Perfect symmetry is an abstraction of mathematics, seldom, if ever actually realized. Nevertheless, with reference to the ideal, perfect symmetry, it is possible to evaluate, analyse, and appreciate both the scientific relevance and the artistic value of approximate symmetries. Here we shall focus on two such approaches, one based on the concept of symmetry deficiency that also leads to precise measures for the degree of missing symmetry, and on the concept of symmorphy, a generalization of symmetry that also*

allows for approximate symmetry, yet preserves some of the elegant mathematical tools, such as group theory, which have been found so powerful in utilizing symmetry in chemistry, atomic physics, and even in biology. With these concepts in mind, it is also possible to study and appreciate approximate symmetry in artistic productions.

1 INTRODUCTION

Approximate symmetry is often perceived as a somewhat vague concept that is not easily suitable for precise analysis. This perception is reinforced by the contrasting elegance of perfect symmetry, and the powerful mathematical tools available for its study. Specifically, group theory is a highly evolved chapter of mathematics that is ideally suited for the type and level of complexity presented by symmetry in the ordinary three-dimensional space. However, approximate symmetry also can be treated by precise mathematical tools, and among these tools topology provides the most versatile and practical approaches. Here we shall be concerned primarily with two approaches: with a family of *symmetry deficiency measures*, and with the notion of *symmorphy*, leading to *symmorphy groups*. Symmetry deficiency measures and the symmorphy group approach have been studied and applied to a variety of fields [see references Mezey (1982-2004)], mostly in chemistry, but the generality of the approach provides suggestions for precise studies of approximate symmetry in other fields of natural sciences as well as art.

2 SYMMETRY DEFICIENCY MEASURES AND SYMMORPHY

One conceptually simple way of quantifying approximate symmetry is by comparisons to actually symmetric, ideal objects. Of course, this requires a choice of an object with the required, exact symmetry. For example, a clover with irregularly placed four leaves, having no other than trivial symmetry, has no four-fold symmetry axis, yet it might be regarded as having an approximate four-fold rotational symmetry. How close is the actual, approximate symmetry to an ideal four-fold rotational symmetry? For simplicity, let us assume that we are dealing with a clover pressed unto a planar cardboard, that is, we are dealing with a planar object, with approximate four-fold rotational symmetry. In fact, all we shall consider is the planar outline S of the clover on the cardboard. We assume that the symmetry operation referring to four-fold rotational symmetry is denoted by R, and we shall denote the area of this outline by A(S). One may ask the question: what is the smallest area outline E(S,R) that contains the actual outline S, and also has a perfect fourfold rotational symmetry? There must exist such an outline, but it need not be unique: it is possible that two our more such minimum area outlines exist, each containing the actual outline S of the clover. Yet, for any such outline E(S,R) the area enclosed must have the same value, that is, the area measure is unique. For a given clover outline S we may denote this area by A(E(S,R)). Similarly, one may consider the maximum area four-fold symmetry outlines I(S,R) inscribed within the outline S, which need not be unique, yet their area measure must have a unique value A(I(S,R)). The relative differences between these areas, DE(S,R) = [A(E(S,R)) – A(S)] / A(S) and DI(S,R) = [A(I(S,R)) – A(S)] / A(S) can serve as measures of symmetry deficiency (measures of missing symmetry) of the original outline S, with respect to the four-fold rotational symmetry R. It is clear that the same procedure is applicable to any planar object S and to any symmetry operator R, furthermore, by replacing area A with volume V, the approach is applicable to approximate symmetries in three dimensions. The three-dimensional version of these symmetry deficiency measures have been applied to molecular electron densities, and the same procedure is equally applicable to any object of art, whether a planar drawing or three-dimensional sculpture. Whereas in symmetry, as the very word indicates it, some of the metric properties, such as two or more distances, are the same; by contrast, in symmorphy [Mezey (1989, 1990a, 1993)], some of the morphological properties are the same. If the family of symmetry operators is extended to a much larger family of operators which do not necessarily preserve the metric properties, such as distances, but preserve the overall morphology of the objects, then a new algebraic structure, a symmorphy group is obtained, formed by all symmorphy operators acting on the given object. The symmorphy group approach is an extension of the point symmetry group approach where the set of symmetry operators is extended to include all symmorphy operators. For any given object S the symmorphy group G(S) is the set of all homeomorphisms (continuous, one-to-one, and onto transformations) of the space which leave the shape of the object S unchanged, where the group operation is the application of one such homeomorphism after another. Evidently, all symmetry operations of the object (if there are any beyond trivial symmetry) are elements of the symmorphy group, but these groups usually have far more elements than the corresponding symmetry groups.

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