Symmetry Operation Measures

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Abstract: We introduce a new mathematical tool for quantifying the symmetry contents of molecular structures: the Symmetry Operation Measures. In this approach, we measure the minimal distance between a given structure and the structure which is obtained after applying a selected symmetry operation on it. If the given operation is a true symmetry operation for the structure, this distance is zero; otherwise it gives an indication of how different the transformed structure is from the original one. Specifically, we provide analytical solutions for measures of all the improper rotations, S_n^p, including mirror symmetry and inversion, as well as for all pure rotations, C_n^p. These measures provide information complementary to the Continuous Symmetry Measures (CSM) that evaluate the distance between a given structure and the nearest structure which belongs to a selected symmetry point-group.

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Introduction

Distance measures are widely used in many fields of modern science,[1] including medical image analysis,[2] computerized image quality evaluation,[3] and linguistics.[4] In the chemical sciences, similarity measures and quantum molecular similarity measures were intensively developed by Mezey et al.[5] in the context of electron density analyses (see also Ref. 6) and shape analyses, and by Carbó-Dorca, Gironés et al.,[7] for instance, in the context of quantum QSAR studies. The use of similarity measures for DNA sequence analysis,[8] is another important example. Our own contribution has been in the areas of symmetry[9,10] chirality[11,12] and shape[13,14] measures. Measuring symmetry and chirality on a continuous scale is a concept that has found already many applications in practically all domains of chemistry.[15–17] The essence of the Continuous Symmetry Measures (CSM)[9,10] approach consists of finding the minimal distance between a given structure and the nearest, searched structure, that belongs to the desired symmetry point group. Yet a more elementary measure has been lacking, that focuses on single operations rather than on the whole group, and is capable of answering the following question:

What is the minimal distance between a given structure and the structure that is obtained after applying the operation?

This distance function is a symmetry measure in the sense that it is zero if the chosen operation is indeed a symmetry operation (i.e., if it leaves the structure in a configuration that is indistinguishable from the original one), but is nonzero otherwise, with its value increasing as the difference between the transformed and the original structure increases. In this report we provide analytical solutions for this problem for all proper and improper rotation operations performed on a discrete set of vertices. Finally, it should be noted that although we focus in this work on symmetry operations, the approach is general, and can be applied to any other operation executed on a molecule.

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