Oral presentation

Continuous Symmetry and Chirality Measures – Powerful Descriptors for Structural Analysis

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Symmetry and chirality stand in the heart of numerous natural phenomena. In chemistry, it is frequently perceived as a driving force that controls the shape of molecular structures, defines selection rules for the interaction of light and matter, and determine the mechanisms of change. While perfect symmetry is conceptually appealing, numerous experimental and computational studies show that actual structures are only approximately symmetric due to e.g., conformational flexibility, dynamics, crystallization conditions, chemical processes, and the physical environment. In many of these cases, describing the molecules at hand from the perspective of their deviation from the original symmetric or achiral geometry provides deeper understanding of the molecular systems, can highlight anomalous cases, and shed light on mechanisms of symmetry breaking. Such a description is based on the treatment of symmetry and chirality as continuous quantitative parameters of the molecular structure, rather than binary properties. This approach was originally developed by Avnir and co-workers in the early 90's of the 20th century [1-2], in the form of the continuous symmetry measure (CSM) and the continuous chirality measure (CCM). These intuitively defined three-dimensional geometrical descriptors quantify the level of distortion with respect to the nearest symmetric (or achiral) structure. Major algorithmic improvements introduced in recent years [3-5] significantly increased the accuracy and speed of calculation and paved the way to analyze a huge variety of structures as well as sets of related molecules that appear in crystallographic unit cells. The CSM and CCM have the ability to detect even minute structural changes of the studied molecules across chemistry, including organic, inorganic, and biochemical systems. Its applications to study small molecules, unit cells of crystals and protein homomers will be presented.

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