

Exploring Molecular Structure with Symmetry, Chirality and Shape Measures

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Symmetry and chirality stand in the heart of numerous natural phenomena and are directly linked to the electronic structure and reactivity of molecules. Visualization of symmetry at the molecular level can be an eye-opener experience that promotes the development of visual-spatial abilities and high order thinking skills. Nevertheless, perfect symmetry is not as frequent as may be expected, and the situation of approximate symmetry is by far more abundant. Continuous symmetry measures, are molecular descriptors that quantify the distance of a given structure from the nearest symmetric structure with the same connectivity map. Through the years these measures were extended to measure chirality and shape, and were applied in numerous structural studies. The recently developed CoSyM website (<https://csm.ouproj.org.il>) provides free online calculators of these descriptors for molecules and protein homomers. This development paved the way to introduce this rather intuitive concept into the undergraduate chemistry curriculum. Here a brief introduction to the topic is presented with specific examples that deepen our understanding of molecular structure.

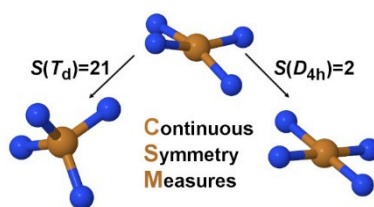


Figure 1