Continuous chirality measures in transition metal chemistry

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Received 2nd November 2004
First published as an Advance Article on the web 11th February 2005
DOI: 10.1039/b301406c

The definition of the continuous chirality measure (CCM) is provided and its applications are summarized in this tutorial review, with special emphasis on the field of transition metal complexes. The CCM approach, developed in recent years, provides a quantitative parameter that evaluates the degree of chirality of a given molecule. Many quantitative structural correlations with chirality have been identified for most of the important families of metal complexes. Our recent research has shown that one can associate the chirality measures with, e.g., enantioselectivity in asymmetric catalysis. We also explore a fragment approach to chirality in which we investigate which part of a molecule is responsible for the chirality-associated properties of a given family of compounds.

1. Continuous chirality measures: the concept

Chirality is such a central concept in chemistry and biochemistry, linked to problems which range from the origin of life to modern drugs, that one wonders why its descriptive language is so dull: A molecule is either chiral or not. The awkwardness of this limited language is immediately evident by considering the following series of substituted 2-butanes (see 1): 2-fluorobutane and 2-iodobutane are of course chiral, but so is 2-deuteriobutane, which is only marginally different from the parent achiral butane. The intuition of the reader probably dictates correctly that since the 2-deuterio derivative is actually not that different from the achiral n-butane, its “degree of chirality” is quite small. Likewise the reader may feel that iodobutane is perhaps “more chiral” than fluorobutane, because the iodine atom is much larger than the fluorine atom, and therefore disturbs more the achirality of butane. Increasing even more the 2-substituent, one can perhaps say that 2-phenylbutane is “highly chiral”, but if the very large coronene is used as a substituent, then the chirality of 2-coronenobutane is not so pronounced, because the butyl substituent on the very large polycyclic molecule is just a small disturbance to its achirality.