Investigation of the Chirality of Enantiomers through Information Theory

S. Janssens[a)], A. Borgoo[a)], P. Bultinck[b)], C. Van Alsenoy[c)] and P. Geerlings[a)]
a) Free University of Brussels (VUB), Department of General Chemistry (ALGC), Pleinlaan 2, 1050 Brussels, Belgium
b) Ghent University (UGent), Department of Inorganic and Physical Chemistry, Krijgslaan 281 (S-3), 9000 Ghent, Belgium
c) University of Antwerp (UA), Department of Chemistry, Universiteitslaan 1, 2610 Antwerp, Belgium

In this work [1] we probed the Kullback-Leibler information entropy as a chirality measure, as an extension of previous studies on molecular quantum similarity evaluated for different enantiomers (enantiomers possessing two asymmetric centra in [2], with a single asymmetric carbon atom in [3] and with a chiral axis in [4]). The entropy was calculated using the shape functions of the R and S enantiomers considering one as reference for the other, resulting in an information theory based expression useful for quantifying chirality. It was evaluated for 5 chiral halomethanes possessing one asymmetric carbon atom with H, F, Cl, Br and I as substituents. To demonstrate the general applicability, a study of two halogen-substituted ethanes possessing two asymmetric carbon atoms has been included as well. Avnir's Continuous Chirality Measure (CCM) [5] has been computed and confronted with the information deficiency. By these means we quantified the dissimilarity of enantiomers and illustrated Mezey's Holographic Electron Density Theorem in chiral systems [6]. A comparison is made with the optical rotation and with the Carbó similarity index.

As an alternative chirality index, we recently also calculated the information deficiency in a way which is consistent with experiments as VCD spectroscopy and optical rotation measurements. The entropy calculates the difference in information between the shape function of one enantiomer and a normalized shape function of the racemate. Comparing the latter index with the optical rotation reveals a similar trend.

[1] S. Janssens, A. Borgoo, C. Van Alsenoy, P. Geerlings, *J. Phys. Chem. A*, **112**, 10560 (2008).
[2] S. Janssens, C. Van Alsenoy, P. Geerlings, *J. Phys. Chem. A*, **111**, 3143 (2007).
[3] G. Boon, C. Van Alsenoy, F. De Proft, P. Bultinck, P. Geerlings, *J. Phys. Chem. A*, **110**, 5114 (2006).
[4] S. Janssens, G. Boon, P. Geerlings, *J. Phys. Chem. A*, **110**, 9267 (2006).
[5] H. Zabrodsky, D. Avnir, *J. Am. Chem. Soc.*, **117**, 462 (1995).
[6] P.G. Mezey, *Mol. Phys.*, **96**, 169 (1999).