The decisive role of hydrogen-bonds in chiral discrimination - unraveled by quantum chemical means

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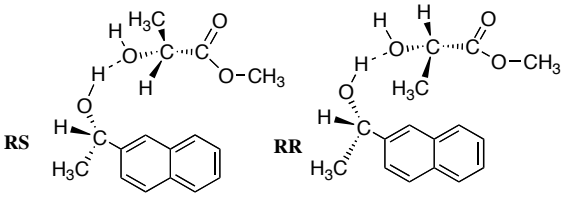
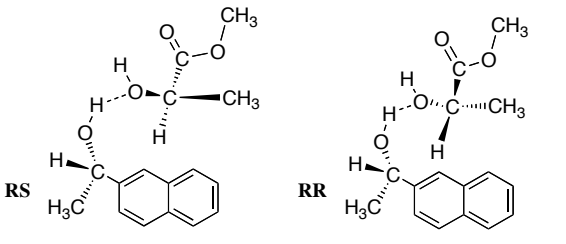
The investigation and understanding of chiral discrimination of pairs of homo- and heterochiral molecules is a challenge for both experimentalists and computational chemists. Limited success has been accomplished by analyzing molecular properties such as the chirodiastaltic energy, geometry, NMR magnetic shieldings or NMR spin-spin coupling constants. Vibrational spectroscopy is a sensitive tool for detecting H-bonding and therefore it should also distinguish H-bonding in pairs of homo- and heterochiral molecules.

The information contained in the vibrational spectra is difficult to decode, which complicates the discrimination of H-bonding in homo- and heterochiral molecules. However, the normal vibrational modes of a molecule provide all information needed to determine its local vibrational modes. The local vibrational modes, as first described by Konkoli and Cremer, lead to an accurate description of bonding, which can be exploited when distinguishing H-bonding in pairs of homo- and heterochiral molecules or to assess the role of H-bonding in chiral recognition.[1-3] Based on experimental, DFT, and CCSD(T) data, we will present an explanation for the formation of homo- and heterochiral molecules.

S or R methyl-lactate, conf. 1



S or R methyl-lactate, conf. 2



[1] Zou, W., Kalescky, R., Kraka, E., Cremer, D. Relating Normal Vibrational Modes to Local Vibrational Modes with the help of an Adiabatic Connection Scheme. *J. Chem. Phys.* 137:084114-1-084114-11, 2012.

[2] Freindorf M, Kraka E, Cremer D. A Comprehensive Analysis of Hydrogen Bond Interactions Based on Local Vibrational Modes. *Int. J. Quant. Chem.*, 112: 3174-3187, 2012.

[3] Kraka E, Freindorf M, Cremer D. Chiral Discrimination by Vibrational Spectroscopy utilizing Local Modes. *Chirality*, 25:185-196, 2013.