

Inner Dihedral

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15/10/2019

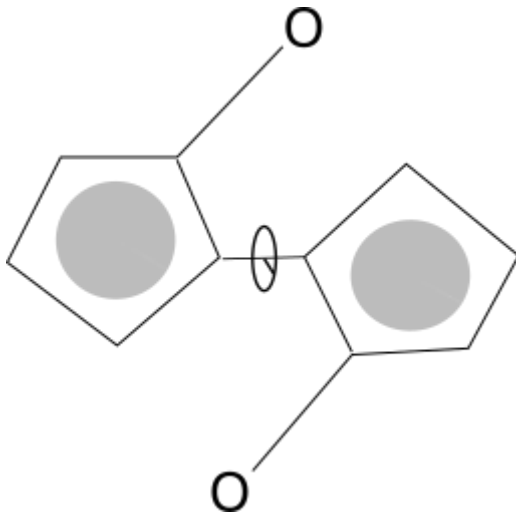


Figure 1: Schematic showing the 'inner dihedral'. In this configuration, the dihedral angle has a value of $\psi = 0$

Functions and Formulas

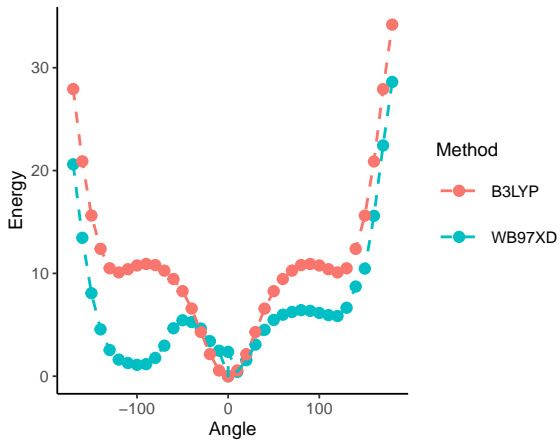
For organic molecules, dihedral parameters are often fitted with a dihedral with the form of a Ryckaert-Belleman function,

$$V_{rb}(\phi_{ijkl}) = \sum_{n=0}^5 C_n \cos(\psi)^n$$

where $\psi = \phi - 180^\circ$. We will initially use this functional form for our fitting as it is supported in Gromacs 5.1.4.

QCC results

Results when continuous scan performed



MD results

