

Title: Unraveling chiral-self recognition using Symmetry-Adapted Perturbation Theory (SAPT) and its derivatives, Functional-group SAPT (F-SAPT) and F-SAPT difference analysis

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Chirality and chiral molecules have attracted a lot of attention from chemists and biochemists from the beginning of chemistry because of their importance and functions in chemistry and biochemistry. Chiral discrimination, the ability of chiral molecules to differentiate weak intermolecular interactions from their mirror image, is explored for dimers of propylene oxide and oxiranemethanol (glycidol). In the matter of chiral discrimination, chirodiastaltic energy, which is defined as the energy difference between homochiral (RR) and heterochiral (RS) diastereomers is explored to elucidate the origin of chiral discrimination in the two adjacent interacting chiral molecules. The case studies for the present work are propylene oxide (PO) dimers and glycidol dimer complexes.

The origins of chirodiastaltic energy are elucidated by employing several symmetry-adapted perturbation theory (SAPT) analyses including conventional SAPT, functional-group SAPT (F-SAPT), and F-SAPT difference analysis in order to distinguish direct and indirect substitution effects of $H \rightarrow CH_3$ and $H \rightarrow CH_2OH$ in propylene oxide and glycidol, respectively. It is found that the largest diastereomeric energy differences correlate to the fluctuations of the electrostatic and dispersion contributions of SAPT. To complement our finding, the harmonic frequency shifts relative to noninteracting propylene oxide and glycidol molecules were computed for all the conformations of propylene oxide dimers and glycidol dimer structures to get insight into the effect of chiral interactions. It is shown that the largest frequency shifts are related to hydrogen bonding effects of the O-H stretch mode in glycidol dimers and chiral discrimination effects in propylene oxide complexes.