# AB INITIO STUDY OF MAGNETOCHIRAL BIREFRINGENCE. CAN THE DISCREPANCIES BETWEEN THEORY AND EXPERIMENT BE RESOLVED?

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The study is an extension of previous work by Coriani *et al.* [J. Chem. Phys. **117**, 6417 (2002)] on magnetic field induced axial birefringence in chiral systems. It concerns six closed-shell chiral molecules (methyloxirane, fluoro- and methylcyclopropanone, carvone, limonene and proline). In previous work, carried out at Hartree-Fock level employing analytical response theory, the computed birefringence was found to be up to three orders of magnitude weaker than measured in experiment. Also note that disagreement still exists between experimentalists on the magnitude of the effect.

Here we extend work of Coriani and co-workers to account for correlation, environmental, conformational and tautomeric effects in an attempt to find the causes for the abovementioned disagreements. We employ density functional theory with a B3LYP functional to take care of correlation effects. The B3LYP approach is validated by the results of coupled-cluster CCSD calculations for the smaller system (methyloxirane) and it is found to perform well. Since experiments (carried out to date on the three heavier molecular systems out of the six listed above) takes place in pure liquids or in water solution, we analyse the effects of environment by exploiting the polarizable continuum model (PCM) with, in some cases for the aqueous solutions, explicit inclusion of extra solvent molecules. Conformational effects in the condensed phase are also studied. Tautomerism was taken into account, in the case of proline, by including some zwiterionic structures in our model.

Although the refinement of the model yields significant improvement over previous results, the discrepancy between computational model and experimental data remains.