

**On One Hand But Not the Other:  
*Ab Initio* Calculations of Optical Rotation Dispersion  
and Circular Dichroism Spectra**

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Although the phenomenon of optical activity in chiral molecules was first observed almost two hundred years ago, only in the last decade have quantum chemical models achieved sufficient maturity to allow the rigorous first-principles calculation of these properties. This talk will address the current state of the art in first-principles methods for predicting optical rotation and circular dichroism in chiral species. In particular, we will consider the ability of highly correlated *ab initio* methods such as coupled cluster theory to provide accurate optical activity data at non-absorbing wavelengths for both rigid and flexible molecules, including [4]triangulane, 2-chloropropionitrile, epichlorohydrin, methyloxirane, and methylthiirane, with comparisons to both gas-phase and solution-phase experimental results.

“*Ab Initio* Calculation of Molecular Chiroptical Properties,” T.D. Crawford, *Theor. Chem. Acc.* **115**, 227-245 (2006).

“*Ab Initio* Calculation of Optical Rotation in (*P*)-(+)-[4]Triangulane,” T.D. Crawford, L.S. Owens, M.C. Tam, P.R. Schreiner, and H. Koch, *J. Am. Chem. Soc.* **127**, 1368-1369 (2005).

“Coupled Cluster Calculations of Optical Rotatory Dispersion in (*S*)-Methyloxirane,” M.C. Tam, N.J. Russ, and T.D. Crawford, *J. Chem. Phys.* **121**, 3550-3557 (2004).