Vibrational circular dichroism spectra for large systems and systems with heavy elements

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Vibrational circular dichroism (VCD) intensities are proportional to the rotational strengths which are defined as the imaginary part of the scalar product between the electric and magnetic dipole transition moments for vibrational transitions. We have implemented the calculation of VCD spectra as proposed by Cheeseman [1] in TURBOMOLE by extending the modules mpshift (for the magnetic part) and aoforce (for the vibrational/electric part). Calculation of the VCD spectrum of the icosahedral C_{420} cluster takes 170 hours on a single CPU if symmetry is exploited, the CPU effort being dominated by the vibrational part.

For systems with heavy elements we followed van Wüllen's suggestion [2] to ensure gauge invariance when using effective core potentials (ECPs) in calculations of magnetic properties and employed this also for VCD spectra. We confirmed the gauge invariance for both the chemical shielding tensors and the VCD spectra for e.g. $Co(ppy)_3$, ppy=2-Phenylpyridine, and the heavier homologue $Ir(ppy)_3$.

[1] Cheeseman, J. R., Frisch, M. J., Devlin, F. J., Stephens, P. J., *Chem. Phys. Lett.* **1996**, *252*, 211.
[2] van Wüllen, C., *J. Chem. Phys.* **2012**, *136*, 114110.