

# An intrinsic measure for the reliability of calculated VCD band signatures

Gábor Magyarfalvi, Sándor Góbi, György Tarczay

<sup>1</sup>Laboratory of Molecular Spectroscopy, Eötvös Loránd University, Budapest, Hungary

gmagyarf@elte.hu

We present a novel measure that improves the reliability of the assignment procedure for vibrational circular dichroism (VCD) spectra. Interpretation and assignment of VCD spectra is only possible through the comparison of experimental and computed results, but agreement is rarely perfect.

The new criterion extends the useful robustness concept introduced by Nicu and Baerends [1] and enables spectroscopists to single out bands with unreliable VCD intensities. These bands, selected purely on a simple theoretical measure can be disregarded during analysis and determination of absolute configuration. [2]

We extensively use the new criterion, denoted as robustness in our studies on the conformational equilibria of flexible molecules, such as carboxylic acids and their dimers, amino acid derivatives and small peptide models.

[1] V. P. Nicu, E. J. Baerends, *Phys. Chem. Chem. Phys.*, 2009, **11**, 6107–6118

[2] Góbi, S.; Magyarfalvi, G. *Phys. Chem. Chem. Phys.*, 2011, **13**, 16130–16133