

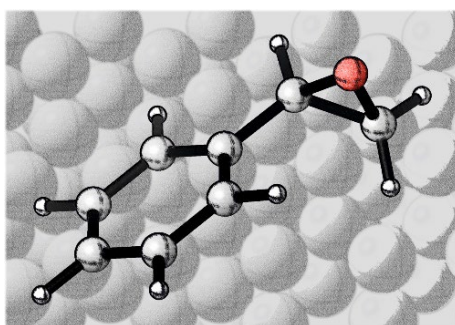
# VCD spectroscopy under cryogenic conditions: Of matrix effects and photochemistry of chiral molecules

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Vibrational Circular Dichroism (VCD) spectroscopy measures the small difference in the absorption of left- and right circular polarized infrared light by a chiral sample. It allows for the unambiguous assignment of absolute configurations by comparison of experimental and computationally predicted spectra.<sup>1</sup> It is also highly sensitive to even very subtle differences in structures, such as conformational changes induced by solute-solvent interactions,<sup>2</sup> and we utilize this conformational sensitivity to probe intermolecular interactions of interest in catalysis<sup>3</sup> and supramolecular chemistry.<sup>4-6</sup>

In this talk I will focus on our activities to combine VCD spectroscopy with the matrix-isolation technique as sample preparation method for the isolation of small molecules and reactive intermediates. Highlighting some recent results, we show that trapping chiral molecules in solid rare gas matrices can help us understand problems faced in the interpretation of solution phase spectra. These challenges in the analysis are, for instance, flat potential energy surfaces<sup>7</sup> or rapidly rearranging photoisomerization products.<sup>8</sup> Matrix effects were found to occasionally make the interpretation of MI-VCD spectra quite challenging,<sup>9</sup> and we also implemented a setup to record MI-VCD spectra in para-hydrogen matrices. Comparison with experimental VCD spectra recorded in liquified rare gases helped us to reveal further matrix-effects in MI-VCD spectra and to benchmark computational approaches for the prediction of anharmonic VCD intensities.<sup>10-11</sup>



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