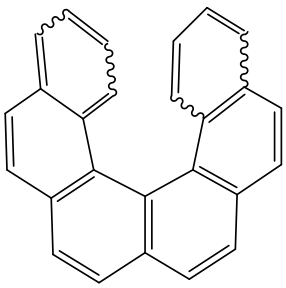
Matrix effects in MI-VCD spectra: The effect of temperature and concentration

Grassin, C.,[1] Merten, C.,[2]
[1] corentin.grassin@rub.de, Ruhr Universität Bochum, Germany
[2] Ruhr Universität Bochum, Germany

In Matrix Isolation (MI)[1] the compound of interest is trapped in an inert gas at cryogenic temperature to avoid dimerization and/or thermal relaxation. In combination with Infrared (IR) spectroscopy, MI gives a broad choice of studies from isomerism to photochemistry or aggregate clustering. Vibrational Circular Dichroism (VCD) spectroscopy is the chiral version of IR spectroscopy and measures the difference between left and right circular polarized IR light absorbed by a chiral molecule. Typically employed to solution phase measurements, the sensitivity of VCD has been shown to be of added benefit for the investigation of intermolecular interactions[2]. Both IR and VCD spectra need to be compared with computations to determine if the expected structure is the one experimentally obtained. VCD coupled to MI (MI-VCD)[3] offers a better resolution than VCD solution thanks to the narrow line width. In turn, it is also much more prone to matrix cage effects[4], which can hardly be predicted computationally.

Our group already encountered MI-VCD specific matrix effects and was able to explain it by distortion around the lowest energy conformer[5]. These effects cannot be predicted and can only be treated individually. To further investigate such matrix site effects and to give some experimental guidelines on how to avoid them, we studied two compounds having different sizes. Despite the bulkiness of hexahelicene **1**, 5 K difference during the deposition is enough for the VCD spectra to be different in Argon. Besides an influence of the temperature, we also found the concentration of styrene oxide **2** to influence the spectral quality. Under different experimental conditions, it shows such matrix effects in Argon, but not in Nitrogen matrix. In both cases, the IR spectra are not affected. In this contribution, we report the MI-IR and MI-VCD spectra of **1** and **2** and discuss the effects of the deposition conditions.



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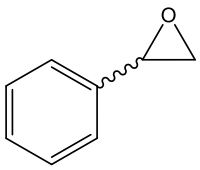

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