Chiroptical spectroscopy of flexible molecules at low and room temperature

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Chiroptical spectroscopy, *i.e.* the even response of a chiral molecule to a circular polarized light (CPL), is a unique tool for determining absolute configurations. It is also very sensitive to conformational isomerism and molecular interactions.

I will first illustrate the sensitivity of chiroptical spectroscopy to molecular conformation on the example of photoelectron circular dichroism (PECD) of 1-indanol under supersonic jet conditions. PECD is as a forward-backward asymmetry in the photoelectron angular distribution with respect to the light propagation, for chiral molecules photo-ionised by CPL. 1-indanol is a flexible bicyclic molecule for which two conformers resulting from the ring inversion can be advantageously isolated in the gas phase under controlled supersonic expansion conditions. Changing the nature of the carrier gas allows trapping both conformers, when helium is used, or only one, in argon. The PECD is dramatically different in the two carrier gases, leading to the conclusion that it differs in both magnitude and sign for the two conformers.[1]

The second part of my talk will focus on vibrational circular dichroism (VCD) spectroscopy, *i.e.* the very small difference in absorption between left and right CPL by a chiral molecule in the IR. I will discuss how VCD of chiral diols in the solid state gives information that are complementary to those obtained on their clusters in the gas phase at low temperature, under supersonic jet conditions.[2]

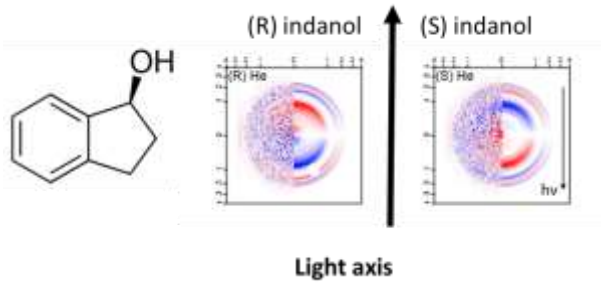

Figure 1: The 1-indanol molecule and raw (half left) and Abel-inverted (half right) difference images (Left CPL – Right CPL) of the photoelectron distribution in helium.

[1] Dupont, J.; Lepere, V.; Zehnacker, A.; Hartweg, S.; Garcia, G. A.; Nahon, L., Photoelectron Circular Dichroism as a Signature of Subtle Conformational Changes: The Case of Ring Inversion in 1-Indanol. *The Journal of Physical Chemistry Letters* **2022**, *13* , 2313.
[2] Jähnigen, S.; Zehnacker, A.; Vuilleumier, R., Computation of Solid-State Vibrational Circular Dichroism in the Periodic Gauge. *The Journal of Physical Chemistry Letters* **2021**, 12, 7213.