

Conformation isomerism of 1-indanol probe by PhotoElectron Circular Dichroism

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PhotoElectron Circular Dichroism (PECD) allows measuring the forward/backward asymmetry of the angular distribution of photoelectrons with respect to the axis of light propagation following the ionization of a chiral molecule by circularly polarized light.¹ This technique is very sensitive to the molecule conformations. That is why we applied it to a flexible chiral molecule derived from indane. 1-indanol shows two quasi-isoenergetic conformers connected by a ring inversion motion whose relative population depends on the carrier gas.²

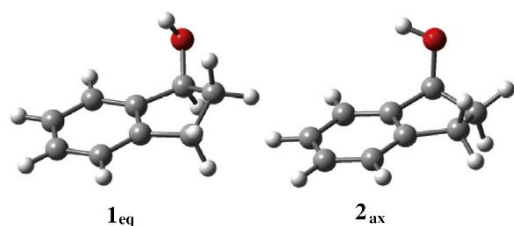


Figure 1. Conformers of 1-indanol present in a supersonic jet in argon (1_{eq}) and in helium (1_{eq} et 2_{ax}).

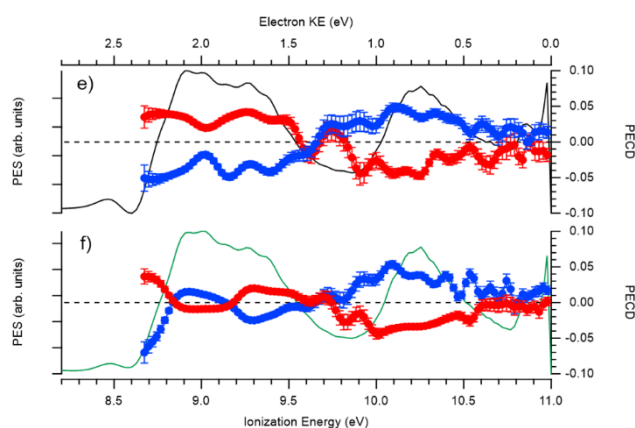


Figure 2. Photoelectron spectra in argon (black) and in helium (green). PECD spectra of R-indanol (blue) and of S-indanol (red) recorded at $h\nu=11\text{eV}$

The photoelectron (PES) and PECD spectra of S-indanol and R-indanol under supersonic conditions were recorded for both gases at several photon energies on the DESIRS beamline at the synchrotron SOLEIL. In helium, two conformers were probed at the same time while in argon only one conformer was probed. First, the PECD spectra show a very nice expected mirroring effect between the two enantiomers in the same gas. On the other hand, clear differences between the two gases due to the contributions of two or one conformers are observed. The experimental results were supplemented by quantum calculations to better understand the nature of the orbitals ionized in these conditions.

[1] S. Daly, M. Tia, G. A. Garcia, L. Nahon, I. Powis, *Angew. Chem. Int. Ed.* 2016, 55, 11054–11058

[2] A. Bouchet, J. Altnöder, M. Broquier, A. Zehnacker, *Journal of Molecular Structure* 1076 (2014) 344–351