SPascal SPECSGROUP saes high vacuum KYMA

Contribution ID: **37** Type: **Poster**

Conformer-Selective and Induced Photoelectron Circular Dichroism

Photoelectron Circular Dichroism (PECD), the forward/backward asymmetry in the angular distribution of the electrons resulting from the ionization of a chiral molecule by a circularly polarized light [1], is a very sensitive probe of molecular structure [2, 3, 4]. While it was historically studied using synchrotron facilities, recent developments show PECD using laser setups, both in the femto- and nanosecond time scale [5]. Using a ns-laser and a resonance-enhanced multiphoton ionization energy scheme, it is possible to selectively ionize different conformers of the same molecule in the gas phase, which enhances the analytical potential of PECD. One major drawback of this phenomenon is the need of an accessible excited electronic state, *i.e.* the presence of a chromophore within the molecule.

To tackle the issue, we thought of using a method already evidenced for circular dichroism in absorption [6, 7]. More specifically, it is the use of molecular complexes, separated in two moieties. One part is chiral, but does not have a chromophore, and the other is a non-chiral moiety with a chromophore. We recorded induced PECD [8] of methyloxirane (MOx) via a molecular complex with phenol (PhOH) using VUV synchrotron radiation. In the gas phase, using helium as a carrier gas, we were able to form PhOH-MOx complexes whose structure and orbitals were previously calculated, showing a non-chiral HOMO located solely on the PhOH moiety. However, what we saw is a non-zero chiroptical response originating from the ionization of the complex, due to the electron scattering off the chiral molecular potential. Using this method, it is possible to enlarge the scope of PECD as an analytical tool, allowing to gain extensive molecular information of chiral molecule, as well as conformer-specific chiroptical response for virtually any system.

We then successfully applied this technique using a ns-laser 2 photon energy scheme, providing conformer-selective PECD results. We first applied it to a single molecular system 1-indanol [9], before confirming our synchrotron-based results on conformer selected Phe:MOx molecular complexes.

1. I. Powis, J. Chem. Phys. (2000), 112, 1
2. J. Dupont, V. Lepère, A. Zehnacker, S. Hartweg, G. A. Garcia, L. Nahon, J. Phys. Chem. Lett. (2022), 13, 2313-2320
3. R. Hadidi, D. K. Božanić, H. Ganjitabar, G. A. Garcia, I. Powis, L. Nahon, Commun. Chem. (2021) 4, 72
4. S. Turchini, J. Phys.: Condens. Matter (2017) 29, 503001
5. H. Lee, S. T. Ranecky, S. Vasudevan, N. Ladda, T. Rosen, S. Das, J. Ghosh, H. Braun, D. M. Reich, A. Senftleben, T. Baumert, Phys. Chem. Chem. Phys. (2022) 24, 27483
6. S. Allenmark, Chirality (2003) 15, 409
7. P. Rizzo, M. Beltrani, G. Guerra, Chirality (2010) 22, E67
8. E. Rouquet, M. Roy-Chowdhury, G. A. Garcia, L. Nahon, J. Dupont, V. Lepère, K. Le Barbu-Debus, A. Zehnacker, Nat. Commun (2023) 14, 6290
9. E. Rouquet, J. Dupont, V. Lepère, G. A. Garcia, L. Nahon, A. Zehnacker, Angew. Chem. Int. Ed. (2024) 63, e202401423

Primary author: Mr ROUQUET, Etienne (Synchrotron SOLEIL)

Co-authors: Dr ZEHNACKER, Anne (Institut des Sciences Moléculaire d'Orsay); Dr GARCIA, Gustavo (Synchrotron SOLEIL); Dr DUPONT, Jennifer (Institut des Sciences Moléculaire d'Orsay); Dr NAHON, Laurent (Synchrotron SOLEIL); Dr LEPÈRE, Valéria (Institut des Sciences Moléculaire d'Orsay)

Presenter: Mr ROUQUET, Etienne (Synchrotron SOLEIL)

Session Classification: Poster Session