

26th June 2014 - 10:00
Building 99, Seminar Room I & II (EG)

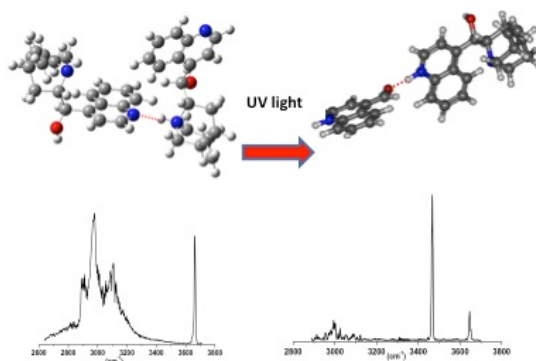
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Chiral recognition in spectroscopy and photophysics of weakly-bound complexes in the gas phase

Chirality and more generally stereochemistry effects play a key-role in molecular recognition. Spectroscopic study of weakly bound neutral or ionic complexes isolated in the gas phase brings information on these effects at the molecular level.¹

Neutral systems studied by combining IR and UV spectroscopy in supersonic jet conditions with *ab initio* calculations will be presented first.²⁻³ It will be shown that chiral recognition is governed by a subtle balance between different interactions, and often rest on interactions much weaker than those ensuring the cohesion of the complex. UV or IR photofragmentation of alkaloids isolated in an ion trap will then be presented. CID and UV fragmentation experiments of cinchona alkaloid protonated dimers lead to different fragmentation pathways, which are highly sensitive to chirality. MS3 experiments coupling both UV and IR excitations allow characterizing the photofragments and determining the specific photofragmentation mechanism.⁴



1. Zehnacker, A. Chirality Effects in Gas-Phase Spectroscopy and Photophysics of Molecular and Ionic Complexes :Contribution of Low and Room Temperature Studies. *International Reviews in Physical Chemistry* 2014, DOI: 10.1080/0144235X.2014.911548.
2. Scuderi, D.; Le Barbu-Debus, K.; Zehnacker, A. The Role of Weak Hydrogen Bonds in Chiral Recognition. *Physical Chemistry Chemical Physics* 2011, 13, 17916-17929.
3. Altnoeder, J.; Bouchet, A.; Lee, J. J.; Otto, K. E.; Suhm, M. A.; Zehnacker-Rentien, A. Chirality-Dependent Balance between Hydrogen Bonding and London Dispersion in Isolated (+)-1-Indanol Clusters. *Physical Chemistry Chemical Physics* 2013, 15, 10167-10180.
4. Scuderi, D.; Lepere, V.; Piani, G.; Bouchet, A.; Zehnacker-Rentien, A. Structural Characterization of the UV-Induced Fragmentation Products in an Ion Trap by Infrared Multiple Photon Dissociation Spectroscopy. *Journal of Physical Chemistry Letters* 2014, 5, 56.

Host: Melanie Schnell - CFEL Molecular Physics seminar