CURRICULUM VITAE ANNE ZEHNACKER-RENTIEN

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Position

Directeur de recherche CNRS
Head of « Centre Laser de l'Université Paris Sud (CLUPS)
Head of the team "Interactions moléculaires: structure et dynamique" of the ISMO Institute.

Present activities

Member of the advisory Editorial Board of Phys Chem. Chem. Phys since 2008
Member of the driving committee of the excellence cluster PALM "Physique, Atomes, Lumière, Matière" (Physcis, Atoms, Light, Matter"),
Member of the board of the Physical Chemistry division of the French Chemical Society.
Member of the "Physical Chemistry" evaluation section of the CNRS (section 13) 2012-2016).
Chair of the Gordon Research Conference "Molecular and Ionic Cluster" 2014

Field of research

My work focuses on laser spectroscopy and photophysics of organic molecules in the gas phase and on elementary photo-induced processes (electron and proton transfer). I am especially interested in the molecular description of the forces responsible for molecular recognition in isolated systems, in particular for chiral recognition. I also study the influence of stereochemical factors on the spectroscopy and the dynamics of the electronic excited state, involving for example photofragmentation, electron and proton transfer. To this end, my group combines laser spectroscopy, supersonic expansions or ion traps with theoretical chemistry calculations and vibrational circular dichroism in solution.

Scientific Production

1 plenary introductive lecture and 35 invited lectures in International Conferences.
86 publications (h-index 25).

Publications from 2011 to 2015

1. Intrinsic folding proclivities in cyclic β-peptide building blocks: configuration and heteroatom effects analyzed by conformer-selective spectroscopy and quantum chemistry
M. Alauddin, Eric Gloaguen, V. Brenner, B. Tardivel, M. Mons, A. Zehnacker-Rentien, V. Declerck, D. J. Aitken
Chemistry - A European Journal. Accepted for publication (2015)

2. Exotic Protonated Species Produced by UV-Induced Photofragmentation of a Protonated Dimer: Metastable Protonated Cinchonidine
I Alata, D Scuderi, V Lepere, V Steinmetz, F Gobert, L Thiao-Layel, K. Le Barbu-Debus, A. Zehnacker
The Journal of Physical Chemistry A 10.1021/acs.jpca.5b06506 (2015)

3. Diastereo-specific conformational properties of neutral, protonated and radical cation forms of (1 R, 2 S)-cis-and (1 R, 2 R)-trans-amino-indanol by gas phase spectroscopy
A Bouchet, J Klyne, G Piani, O Dopfer, A Zehnacker
Physical Chemistry Chemical Physics DOI: C5CP00576K (2015)

4. Spectroscopic Study of Jet-Cooled Deuterated Porphycenes: Unusual Isotopic Effects on Proton Tunneling
ET Mengesha, A Zehnacker-Rentien, J Sepioł, M Kijak, J Waluk
The Journal of Physical Chemistry B (2015) 119, 2193–2203

5. Direct Spectroscopic Evidence of Hyperconjugation Unveils the Conformational Landscape of Hydrazides
E Gloaguen, V Brenner, M Alauddin, B Tardivel, M Mons, Anne Zehnacker-Rentien, Valérie Declerck, David J Aitken
Angewandte Chemie (2014) 126 (50), 13976-13979

6. IR–UV spectroscopy of jet-cooled 1-indanol: Restriction of the conformational space by hydration
A Bouchet, J Altnöder, M Broquier, A Zehnacker
Journal of Molecular Structure (2014) 1076, 344-351

7. Chirality effects in gas-phase spectroscopy and photophysics of molecular and ionic complexes: contribution of low and room temperature studies
A Zehnacker
International Reviews in Physical Chemistry (2014) 33 (2), 151-207

8. Unraveling non-covalent interactions within flexible biomolecules: from electron density topology to gas phase spectroscopy
R Chaudret, B De Courcy, J Contreras-Garcia, E Gloaguen, A Zehnacker-Rentien, M Mons, J-P Piquemal
Physical Chemistry Chemical Physics (2014) 16 (21), 9876-9891

9. Structural Characterization of the UV-Induced Fragmentation Products in an Ion Trap by Infrared Multiple Photon Dissociation Spectroscopy
D Scuderi, V Lepere, G Piani, A Bouchet, A Zehnacker-Rentien
The Journal of Physical Chemistry Letters (2013) 5 (1), 56-61

10. How do Pseudoenantiomers Structurally Differ in the Gas Phase? An IR/UV Spectroscopy Study of Jet-Cooled Hydroquinine and Hydroquinidine
A Sen, V Lepere, L Barbu-Debus, A Zehnacker
ChemPhysChem (2013) 14 (15), 3559-3568

11. Mass spectrometry study and infrared spectroscopy of the complex between camphor and the two enantiomers of protonated alanine: the role of higher-energy conformers in the enantioselectivity of the dissociation rate constants.
A Sen, K Le Barbu-Debus, D Scuderi, A Zehnacker-Rentien
Chirality (2013) 25 (8), 436-443

12. Structural Rearrangement in the Formation of Jet-Cooled Complexes of Chiral (S)-1, 2, 3, 4-Tetrahydro-3-isoquinolinemethanol with Methyl Lactate: Chirality Effect in Conformer Selection
A Mahjoub, K Le Barbu-Debus, A Zehnacker
The Journal of Physical Chemistry A (2013) 117 (14), 2952-2960

13. Chirality-dependent balance between hydrogen bonding and London dispersion in isolated (±)-1-indanol clusters
J Altnöder, A Bouchet, JJ Lee, KE Otto, MA Suhm, A Zehnacker-Rentien
Physical Chemistry Chemical Physics (2013) 15 (25), 10167-10180

14. Conformational analysis of quinine and its pseudo enantiomer quinidine: a combined jet-cooled spectroscopy and vibrational circular dichroism study
A Sen, A Bouchet, V Lepère, K Le Barbu-Debus, D Scuderi, F Piuzzi, A Zehnacker-Rentien
The Journal of Physical Chemistry (2012) A 116 (32), 8334-8344

15. Excited-state intramolecular proton transfer reaction modulated by low-frequency vibrations: An effect of an electron-donating substituent on the dually fluorescent bis-benzoxazole
J Sepioł, A Grabowska, P Borowicz, M Kijak, M Broquier, C Jouvet, C Dedonder-Lardeux, A Zehnacker-Rentien
The Journal of Chemical Physics (2011) 135 (3), 034307

16. Role of Conformational Isomerism in Solvent-Mediated Charge Transfer in Chiral (S) 1, 2, 3, 4-Tetrahydro-3-isoquinoline Methanol (THIQM): Condensed-Phase to Jet-Cooled Spectroscopic Studies
A Chakraborty, N Guchhait, K Le Barbu-Debus, A Mahjoub, V Lepère, Anne Zehnacker-Rentien
The Journal of Physical Chemistry (2011) A 115 (34), 9354-9364

17. Jet-cooled hydrates of Chiral (S) 1, 2, 3, 4-tetrahydro-3-isoquinoline methanol (THIQM): structure and mechanism of formation
K Le Barbu-Debus, A Sen, M Broquier, A Zehnacker
Physical Chemistry Chemical Physics (2011) 13 (31), 13985-13991

18. The role of weak hydrogen bonds in chiral recognition
D Scuderi, K Le Barbu-Debus, A Zehnacker
Physical Chemistry Chemical Physics (2011) 13 (40), 17916-17929

Invited talks from 2011 to 2015:

1. **XVII Congreso Argentino de Fisicoquímica y Química Inorgánica** Cordoba Argentine Chiral recognition in molecular and ionic complexes: the role of minor interactions. May 2011
2. **Wresmol** Cordoba Argentine. Hydrogen-bonded complexes of a chiral chromophore. Mai 2011
3. **Anharmonicity in medium-sized molecules and clusters** Marne la Vallée. Chiral recognition in molecular complexes in the gas phase: low-frequency modes. April 2012.
4. **Gordon Conference on Atomic and Molecular Interactions**. Stonehill (Etats Unis). Stereochemical effects in the photophysics of quinine derivatives. July 2012
5. **22nd International Conference on High Resolution Molecular Spectroscopy** Prague (République thèque) Chiral Recognition in Molecular Complexes in the gas phase. September 2012.
6. **"Journées André Collet de la chiralité" (JACC 2012)**Stereochemical effect in the structure and photophysics of quinine derivatives. Dinard October 2012.
7. **Core-to-Core International Symposium on Ionization Induced Switching** Stereochemical effect in the structure and photophysics of quinine derivatives. Marseille March 2013.
8. **Korean-French Joint Symposium "Recent Progresses in Laser Spectroscopy and Reaction Dynamics"** Stereochemistry effects in alkaloid derivatives" Ajou (Corée) September 2013
9. **Core to core German Japanese Symposium**. Berlin "Chirality effects: low and room temperature studies". December 2014
10. **COST Molecules in action** (Marne la Vallée) "Photostability of gas-phase alkaloids"
11. **2015 CRL Forum** "Photostability of gas-phase alkaloids" Tokyotech Ookaya (Japon) October 2015
12. **PACIFICHEM** "Photostability of gas-phase alkaloids" Honolulu December 2015

Seminars :

1. **Université de Genève Département de chimie.** Chiral recognition in molecular and ionic complexes: the role of secondary interactions. March 2011
2. **Institut de Chimie Physique de l'Académie des Sciences de Varsovie.** Chiral recognition in molecular and ionic complexes: the role of minor interactions. February 2012
3. **Université de Kaiserlautern** Chiral recognition in molecular and ionic complexes. December 2012.
4. **Laboratoire de Physique des Lasers Université Paris 13 Villetaneuse** Le rôle des interactions faibles dans la reconnaissance chirale. December 2013
5. **Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin** Stereochemical effects in cinhona alkaloids. December 2013
6. **Journées LiDYL/ISMO (CEN Saclay)** Applications de la spectroscopie vibrationnelle à la compréhension des effets de chiralité 28 March 2014

7. **Desy Hamburg**. Chiral recognition in spectroscopy and photophysics of weakly bound complexes in the gas phase**.** 26 June 2015
8. **Laboratoire Francis Perrin (CEN Saclay)** 21 November 2014 Effets de stéréochimie dans la structure et la dynamique de biomolécules
9. **Laboratoire Francis Perrin /Saclay** Réunion de lancement de l'ANR ESBODYR. 28 November 2014 Désactivation des états excités des alcaloïdes dérivés de la quinine neutres ou protonés
10. **Université technique de Berlin** 18 December 2014 Séminaire de type « tutorial » Applications of the Non-Covalent Interaction Method to stereochemical effects.
11. **Institut de Chimie Physique de l'Académie des Sciences de Varsovie**. « stereochemical effects in spectroscopy and photophysics of quinine derivatives " 28 January 2015

Awards

CNRS bronze medal (1992)
Award of the Physical Chemistry division - French Chemical Society (2003)