

## Post-doctoral position in Raman Optical Activity

Would you like to contribute to a major research project?

Join the Institute of Molecular Sciences ([ISM](#)) – of the University of Bordeaux!

ISM brings together a community of organic and physical-chemical researchers interested in molecular structures, and working on their design, synthesis, characterization, reactivity and analysis in various environments. The Institute's expertise is based on a number of key skills: theorists in quantum chemistry, molecular and reaction dynamics, synthetic organic chemists, physical-chemical experimentalists (spectroscopy, photochemistry, molecular recognition and analysis), working in 10 research groups and 3 technical platforms. The position is within the Molecular Spectroscopy Group ([GSM](#)) and an Infra-Red and Vibrational Spectroscopy platform (SIV).

### Context:

As part of the research project CAORSS - Understanding by Raman Optical Activity of Solvent Structuring, funded by the ANR, we are recruiting a **Post-Doctoral position in Raman Optical Activity**.

The project is based on Raman Optical Activity (ROA) spectroscopy studies of chiral molecules or molecular structures. In addition to the direct determination of absolute configuration, this technique will be used to highlight electronic resonance effects, weak interactions with solvents, molecular complexation and chiral induction. Recently, a new chiral spectroscopy has been identified: eCP/Raman[1].

In this context, this project focuses on the study of linear tri-metallic complexes[2] exhibiting intense resonant Raman Optical Activity signals, as well as chiral induction on the solvent. The study of chiral induction, solvent effects and complexation of small molecules by cryptophane cage molecules[3] will also be addressed. Experimental measurements will be accompanied by theoretical developments and numerical simulations to interpret the fundamental origin of the observations.

The activity of this position is mainly dedicated to experimental optical activity studies in the Molecular Spectroscopy Group (GSM) with N. Daugey, T. Buffeteau and Y. Danten.

1. Li, G.; Alshalalfeh, M.; Kapitán, J.; Bouř, P.; Xu, Y. Electronic Circular Dichroism-Circularly Polarized Raman (eCP-Raman): A New Form of Chiral Raman Spectroscopy. *Chemistry A European J* **2022**, 28 (20). <https://doi.org/10.1002/chem.202104302>.
2. Cortijo M, Valentín-Pérez Á, Rosa P, Daugey N, Buffeteau T, Hillard EA. Resolution, structures, and vibrational circular dichroism of helicoidal trinickel and tricobalt paddlewheel complexes. *Chirality*. 2020;32(6):753-764. doi:[10.1002/chir.23211](https://doi.org/10.1002/chir.23211)
3. Daugey N, Brotin T, Vanthuyne N, Cavagnat D, Buffeteau T. Raman Optical Activity of Enantiopure Cryptophanes. *J Phys Chem B*. 2014;118(19):5211-5217. doi:[10.1021/jp502652p](https://doi.org/10.1021/jp502652p)

#### Main activities:

As such you will be responsible for preparing and carrying out spectral measurements on chiral samples. Studies in solution will be carried out using Raman Optical Activity Spectroscopy, supplemented by optical spectroscopy (UV absorption, ECD, IR, VCD). Experimental data will be processed with Origin and/or Python. Results will be interpreted by comparison with theoretical chemistry calculations in DFT, using software or programs in development.

#### # Optical Activity Spectroscopy

- Prepare chiral or chiral-structured samples.
- Perform Raman Optical Activity and optical spectroscopy measurements.
- Process data, write reports and disseminate results.
- Contribute to evolution of measurement protocols, data processing and instrumentation

#### # Spectroscopy calculations

- Quantum chemistry calculations of optical activity spectroscopy
- Compare theory and experiment
- Interpret results

#### # Bibliography and scientific dissemination

- Write reports and articles
- Communicate results
- Supervise undergraduate and graduate internships

#### Your skills:

Holder of a PhD in Physical Chemistry, Chemistry or Physics, you justify a first experience in the domain.

- You are autonomous, rigorous and have the spirit of initiative
- Proficiency in chemical analysis, optical experimentation and spectroscopy
- You are familiar with programming languages (e.g. Python, Origin, Octave) and are comfortable with computer and mathematical tools for the exploitation of results
- You enjoy and know how to work as a team
- Fluency in English in an international work environment and basic French wished

Do you recognize yourself? Apply!

#### More information:

By joining the ISM, on the CAORSS project, you will work on a multidisciplinary research project. This fundamental research project brings together nine scientists from the ISM, the ICMCB of Bordeaux, the ENS Chimie of Lyon, the LCT of Namur (Belgium).

**NB: the position is based in a laboratory in the Restrictive Zone, which requires an investigation prior to hiring, which can take up to 8 weeks.**

Based in Talence – access by tramway line B (stop « Arts et Métiers ») buses, bike.  
The laboratory is near the city-centre of Bordeaux and about 60 Km of the Atlantic coast.

13-month fixed-term contract

Salary gross: 2700€ per month according the salary grid

Job Benefits:

50 days of vacation from the first year of collaboration

Refill of 75% of the subscription to the public transport

Participation in the private healthcare up to 15€ / month

Leisure, sport and culture for all staff

Disabled-friendly establishment

Possibility of staff parking

Sustainable mobility package for commuting – work

Recruitment process: Applications are reviewed as they arrive.

Candidates selected for an interview will be contacted by the Recruitment Officer for a first pre-qualification phone conversation. An interview with the supervisor will then be organised by videoconference.

**Interested applicants should send a CV, brief statement of qualifications and basis for interest in the position, copies of up to 3 relevant publications, and the email addresses of 2 appropriate references.**

Link to job offer: <https://www.u-bordeaux.fr/universite/travailler-a-l-universite/offres-emploi/post-doctoral-position-raman-optical-activity>

**Please note that to be admissible**, you must apply to the job offer or send e-mail with your documents at: [job-ref-nxnzf8uqz6@emploi.beetween.com](mailto:job-ref-nxnzf8uqz6@emploi.beetween.com)