Molecular Universe Experienced Researcher Position
Team 8

- **Location of Appointment :** Grenoble (FR)
- **Team Leader (contact person):** P. Valiron
- **Address :** Laboratoire d'Astrophysique, Observatoire de Grenoble, BP 53, F-38041 GRENOBLE Cedex 9, FRANCE
- **e-mail :** valiron@obs.ujf-grenoble.fr
- **Telephone :** +33 4 76 51 47 87 or +33 4 76 63 55 16
- **Fax :** +33 4 65 44 88 21
- **Various URL :** http://www-laog.obs.ujf-grenoble.fr/ valiron or http://www-laog.obs.ujf-grenoble.fr/Recherche/AstrophysiqueMoleculaire/presentation.htm
- **Category of Position :** Experienced Researcher
- **Duration of Appointment (in months) :** 12
- **Starting Date :** 2006
- **Requirements with respect to candidate :** PhD in theoretical chemical physics or physical chemistry; Experience with quantum chemistry and collision codes would be useful; Interest in astrochemistry would be an advantage.
- **Title of Research project :** Collisional excitation of interstellar ammonia by hydrogen molecules: a full dimensional study
- **Abstract of Research Project**

A one year postdoctoral position is available to work with the molecular astrophysics Team at the Universite de Grenoble 1, under the direction of Pierre Valiron on the calculation of inelastic processes between ammonia and hydrogen molecules in the gas phase and at astrophysical relevant temperatures (ie T less than 1000K).

General Introduction :
NH_3 is very abundant in the interstellar medium and it has long been considered as an extremely good temperature probe. Its doubly and triply deuterated forms have been recently detected in protostellar environments with a spectacular isotopic enrichment. As the intensities of the observed emission lines depend on a complex competition between radiative and collisional processes, a good knowledge of state-to-state collisional excitation rates is necessary to interpret spectra. Collisions with hydrogen molecules are particularly important since H_2 is the most abundant colliding partner in the dense interstellar medium. The molecular astrophysics Team at the Universite de Grenoble 1 has acquired a great experience in the computation of high-dimensional potential energy surfaces (PES) and the postdoctoral fellow is expected to take a leading role in the treatment of the collision dynamics including all degrees of freedom.

Methods :
We use state-of-the-art ab initio quantum chemistry methods to compute the PES. A first difficulty will be to provide an efficient analytic fit of the PES including explicitly the inversion tunneling coordinate and, possibly, all internal coordinates. The recent experience acquired by the team on the similar H_2O-H_2 system should prove useful. The treatment of the dynamics will also be very challenging, in order to properly account for vibrational motions. The postdoctoral fellow is expected to take a leading role in both these aspects of the project.

Application :
The position is available immediately but a start date up to October 2006 is possible. Informal enquiries should be directed to Pierre Valiron in the first instance, enclosing a detailed CV and if possible the names and contact details of two referees. Qualified female candidates are specifically encouraged to apply. An extra year, for a total duration of 2 years, may be available depending upon funding.

References :
Please visit our website for a complete list of the Team's publications.