

**Molecular Universe ESR Position
Team 21**

- **Location of Appointment :** Warsaw, Poland
- **Team Leader (contact person):** Robert Moszynski
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- **Various URL :** <http://www.chem.uw.edu.pl/>
- **Duration of Appointment (in months) :** 36
- **Starting Date :** 01-05-2005
- **Requirements with respect to candidate :** M.Sc. in physics/chemistry
- **Title of Research project :** Theoretical studies of collisional processes between light colliders and molecules of astrophysical interest
- **General Introduction** There is a need for accurate rate constants for rovibrational (de)excitation between molecules of astrophysical interest such as water, formaldehyde, and long polycarbonic chains, and light colliders mostly abundant in the interstellar space such as helium atoms and hydrogen molecules. The full set of rate constants at low temperatures for a given collisional process is rarely available from the experiments, even though its knowledge is essential for the construction of astrophysical models describing various environments such as the interstellar clouds.
- **Abstract of Research Project** The research will involve state-of-the-art ab initio calculations of the potential energy surfaces for collisional complexes of astrophysical interest and the collisional dynamics of rovibrational (de)excitation at low temperatures. Symmetry-adapted perturbation theory of intermolecular forces will be used to compute accurate intermolecular potentials for the collisional complexes. The quantum dynamics of the collisional processes will be treated nearly exactly including the intramolecular vibrations of the colliding molecules. For some collisional systems more elaborate approaches will be developed, and specific computer codes will be written. This includes in particular collisions involving rovibrational excitations for complexes with intramolecular vibrational motions carrying internal angular momenta, and collisional processes for complexes described by several (coupled) potential energy surfaces. In the latter case the question of couplings between surfaces and possible long-range diabatization models will be addressed.
- **Applications** Letter of application together with the cv and the list of the university courses taken and their grades should be addressed to the team leader by May 1, 2005. Two recommendation letters from researchers familiar with the applicant's undergraduate studies should be sent to the same address. Strong background in quantum chemistry and molecular physics is required. Qualified female candidates are encouraged to apply.