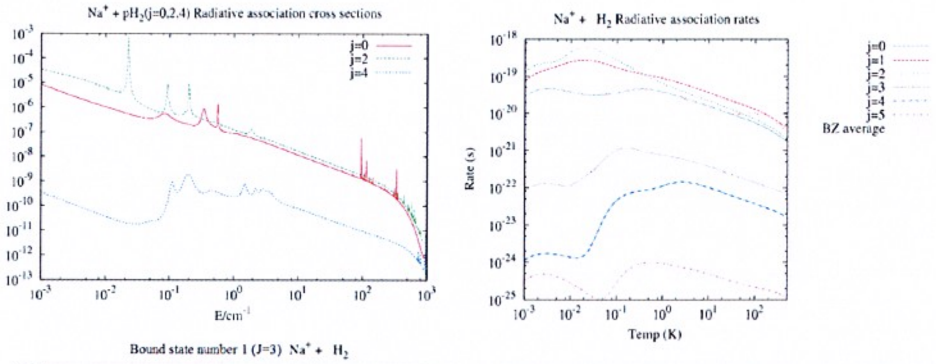
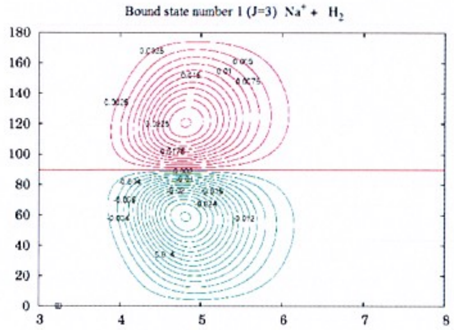
STSM report of Daria Burdakova

I conducted my STSM at Institut des Sciences Molculaires in Bordeaux under the supervision of professor Thierry Stoecklin during the period of 15th September to 27th October. The purpose for this mission was that I would learn how to use a program that performs radiative association (RA) calculations, for triatomic systems, that was written by Thierry Stoecklin[1].

Radiative association is an important process in interstellar chemistry, explaining the formation of polyatomic species. In RA two fragments combine while lowering the energy of the formed complex by emitting a photon. Due to the low density of the interstellar clouds, formation of molecules through RA becomes more probable than the reaction where a third molecule carries away the excess energy.

The calculations were performed on the $Na^+ + H_2$. To obtain rate coefficients and cross sections, the first step is to calculate the bound states (wave functions and energies). The bound states are calculated using discrete variable representation (DVR). The largest values of J that could give bound states and the total number of bound states were 24 respectively 428 for para H_2 and 21 respectively 387 for ortho H_2. The second step is to recalculate the bound states on a radial grid that is adapted to dynamic calculations. These results are used to calculate cross sections and rate constants. We used the rigid rotor 2d potential and the dipole moments calculated by Buchachenko et al[2] for the$Na^+ + H_2$ collision as a function of the R and theta Jacobi coordinates. The two first figures below shows cross sections for J=0,2,4 and rates for J=0,1,2,3,4,5 plus a curve showing the Boltzmann average of the rates. The last figure is a visualization of the first bound state with J=3 with R on the x-axis and theta on the y-axis.





[1] *Phys. Chem. Chem. Phys.*, 2013, **15**, 13818

[2] *J. Chem. Phys.*, 2008, **129**, 184306

Daria Burdakova

Supervisor in Bordeaux: Thierry Stoecklin, research director