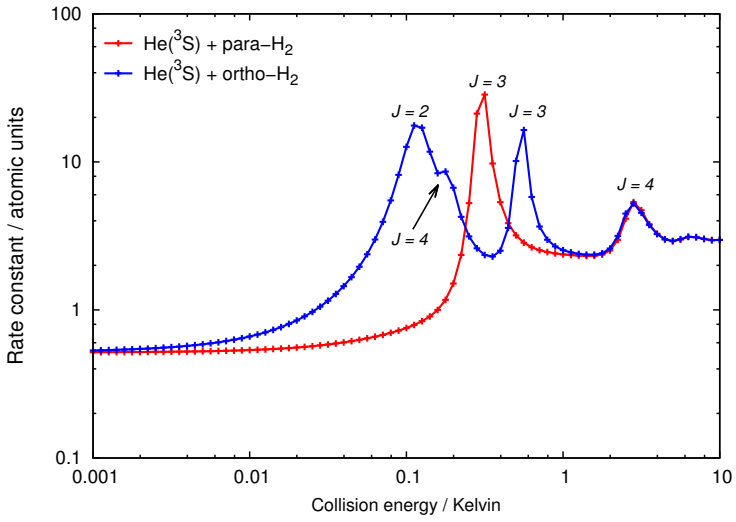
# Theoretical modeling of Penning ionization reaction between molecular hydrogen and metastable helium

(Final report from the STSM of Wojciech Skomorowski in the laboratory of Prof. Ad van der Avoird at the Institute for Molecules and Materials, Radboud University in Nijmegen)

The goal of the STSM was to calculate rate constants for Penning ionization process in the collisions between molecular hydrogen and metastable helium atom in the $^3S$ state. Our plan was to apply a method for coupled-channels quantum reactive scattering, which was developed a few years ago in the Nijmegen Theoretical Chemistry group [Janssen *et al.*, Phys. Rev. Lett. 110, 063201 (2013)]. This approach is a single-arrangement reactive scattering method in which only the reactant configuration is explicitly taken into account, and was originally designed to describe reactive collisions of two NH radicals in magnetic fields.

The first task was to modify the original code and to adapt it to the properties and symmetry of our collisional system. To this end, we (*i*) introduced correct treatment of rotational state of $H_2$ (only even $j$'s allowed in case of collision with para-$H_2$ or only odd $j$'s in case of ortho-$H_2$), (*ii*) removed unnecessary transformation of the scattering matrix from the coupled to the decoupled representation, (*iii*) fixed all numerical prefactors to get correct cross sections for field-free calculations in the coupled basis set, where the total angular momentum $J$ of the collisional complex is rigorously conserved. In the next step we performed comparative tests of the modified code against other available scattering codes with standard short-range boundary conditions, allowing only for elastic or inelastic processes (but not for reactive collisions). When these tests gave satisfactory results, as a final step, we could start running calculations with reactive short-range boundary conditions to get reactive cross sections. In our case we worked only with the real part of the interaction potential between $H_2$ and He($^3S$), which is purely repulsive at short range, and, in consequence, would not allow any flux to enter reactive channels – all these channels are closed in such a case. To overcome this problem, we introduced a model in which the interaction potential becomes constant and attractive at any intermolecular separation smaller than some $R_0$ distance. In this way we allowed part of the incoming flux to transmit irreversibly into short range and populate reactive channels. In this model reactive collisions can occur due to quantum tunneling through the potential barrier. We checked that the height of this barrier is not essential for general shape and structure of the reactive cross sections. The $R_0$ inner point was chosen in such a way, that it guarantees the full convergence of the elastic cross sections.

The attached figure presents the calculated rate constants for collisions of para-$H_2$ and ortho-$H_2$ with He($^3S$) as a function of collisional energy $E$, where the original *ab initio* potential was employed. An inspection of this figure shows that the reaction rates are largely determined by shape resonances, which may occur at different energies for para-$H_2$ and ortho-$H_2$. This is because the anisotropic part of the interaction makes the effective potentials for collisions with para-$H_2$ and ortho-$H_2$ different.




Results of our calculation will be directly used to interpret the ongoing experiments on Penning ionization carried out in the group of Dr. Ed Narevicius at Weizmann Institute of Science. In the near future we would like to extend this approach and apply it to the collisions between $H_2$ and He in the $^3P$ state. This is a much more challenging task because here the interactions take place on three adiabatic surfaces simultaneously.