LOW ENERGY COMPLEX-FORMING DYNAMICS ON ATOM-DIATOM REACTIONS

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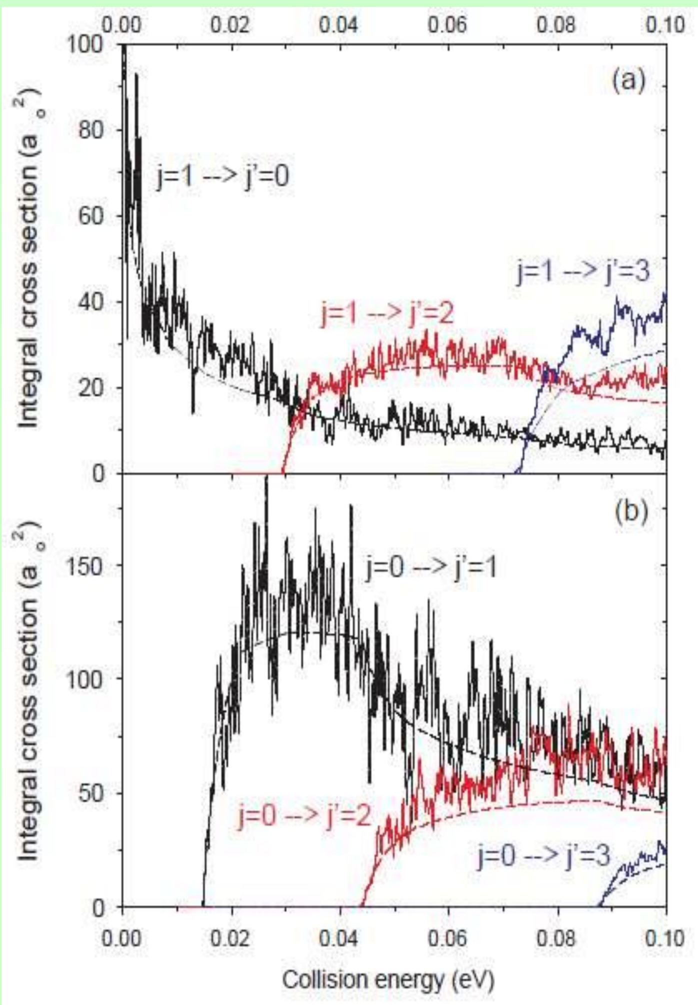
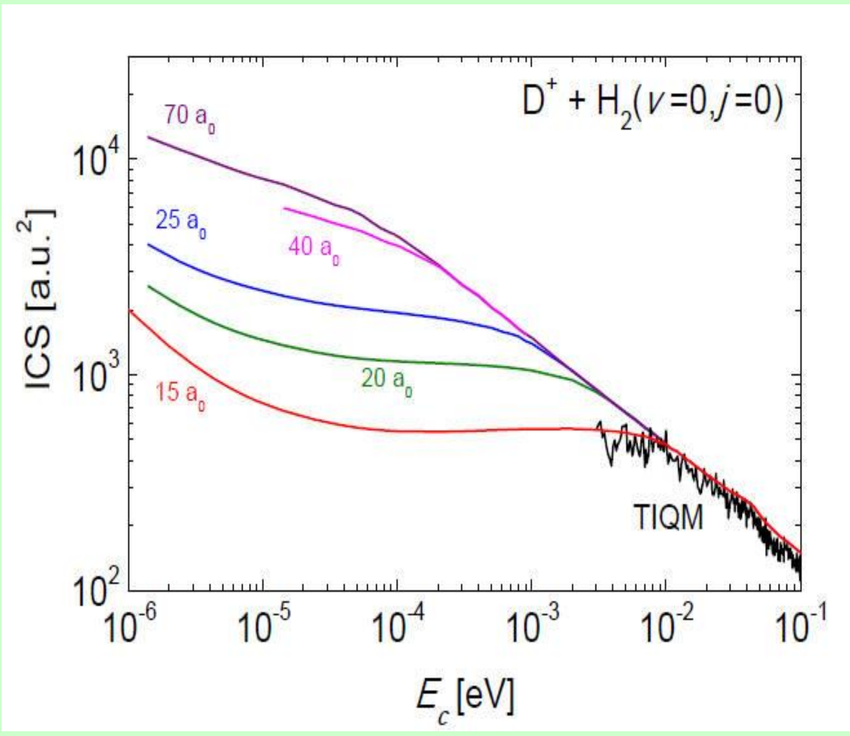
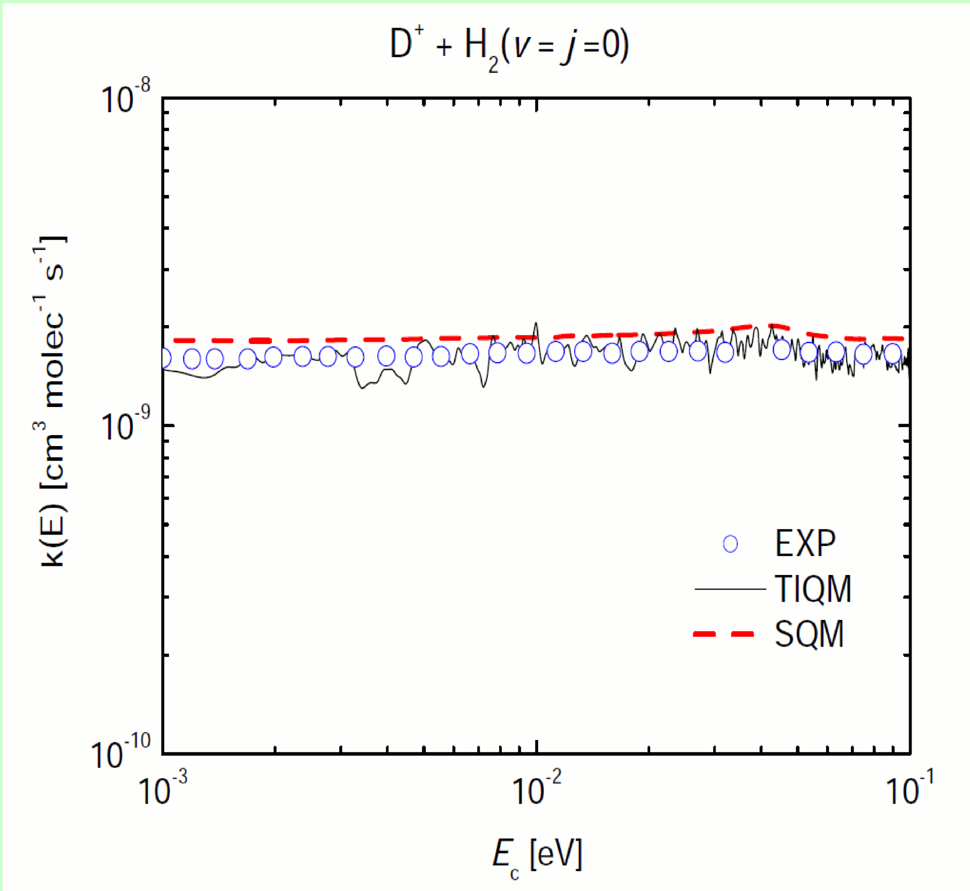
The dynamics of atom-diatom reactions can vary with the collision energy, and direct and insertion pathways can compete [1]. Recent work has treated low energy collisions by means of statistical methods thus revealing the possible complex-forming character of the process at such energy regimes [2,3]. We have been studying the H^{+}+H_2 process [4,5] and isotopic variants, such as D^{+} +H_2 [6,7], by means of a statistical quantum model (SQM) [8,9] in comparison with exact quantum mechanical (EQM) methods and experimental results. Interestingly the main dynamical features are conveniently reproduced. A similar investigation for LiYb+Li →Li_2+Yb [10] revealed the energy range at which the process corresponds mainly to a S-wave dynamics and the apparent limits of a statistical description.

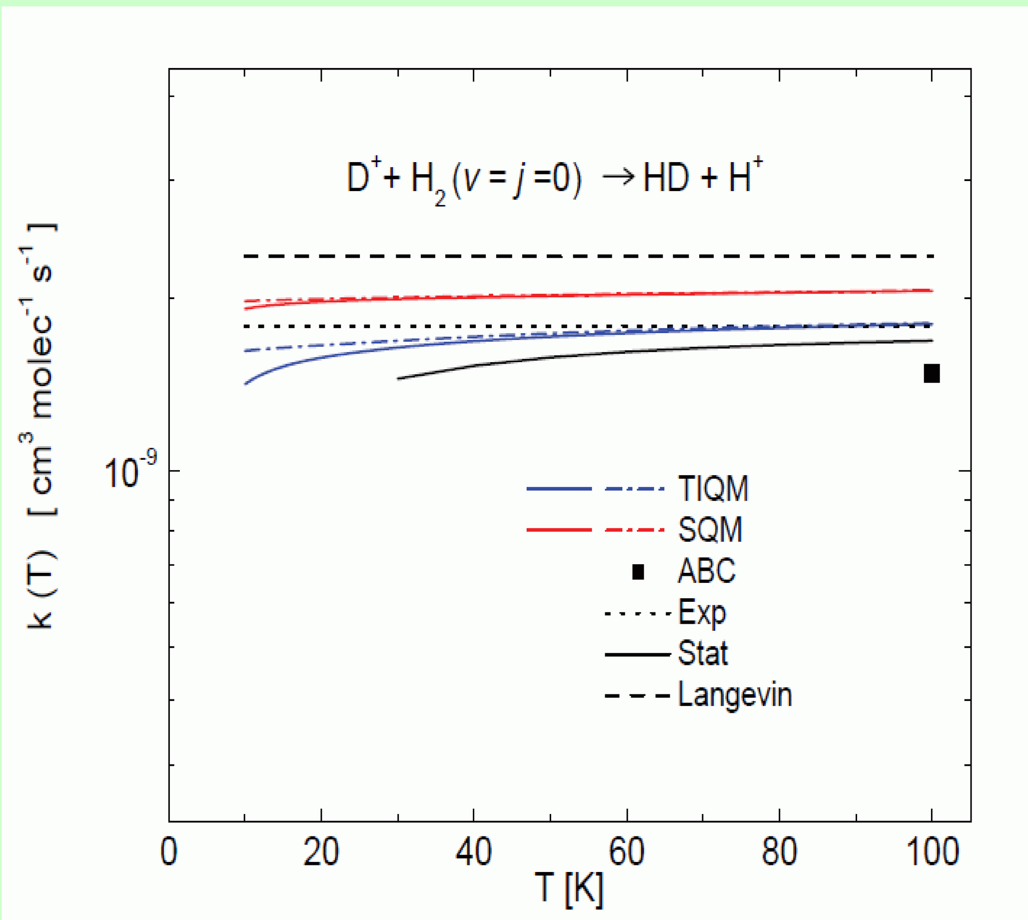


Ortho-para transitions in H^{+} + H_2 can be described by means of statistical techniques at low energies [4]. EQM cross sections are fairly well described below 0.1 eV by SQM and the corresponding rate constants [4] have been used in astrophysical models [11,12].

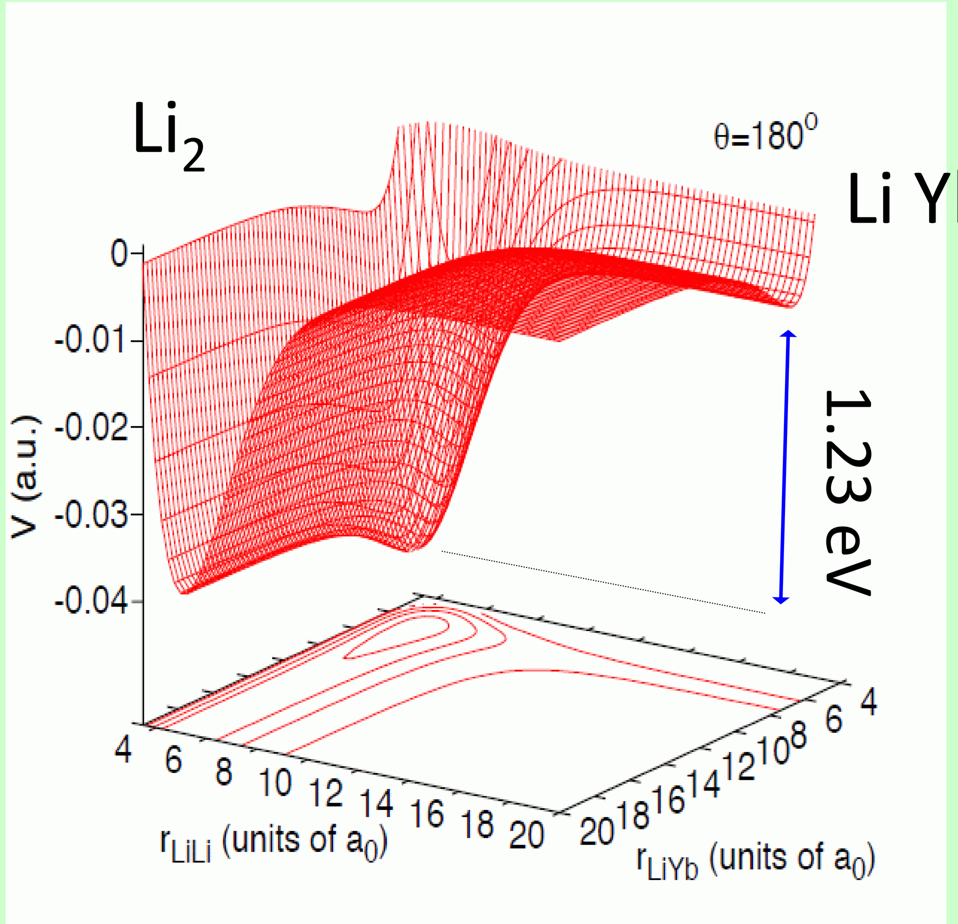




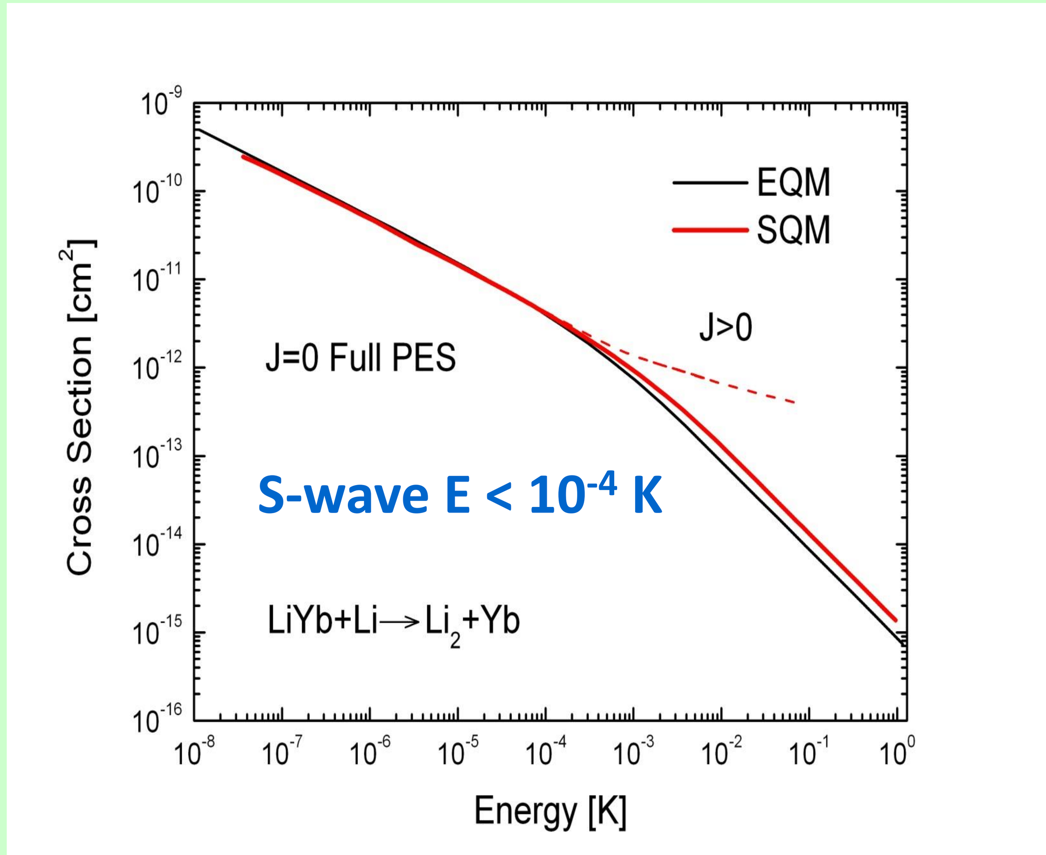
Cross sections have to be calculated with an appropiate description of the corresponding asymptotic region. Limits of the validity of the SQM cross sections depending on Rmax are shown at the left. Rate coefficients in comparison with EQM and experiment (right) shows good agreement.



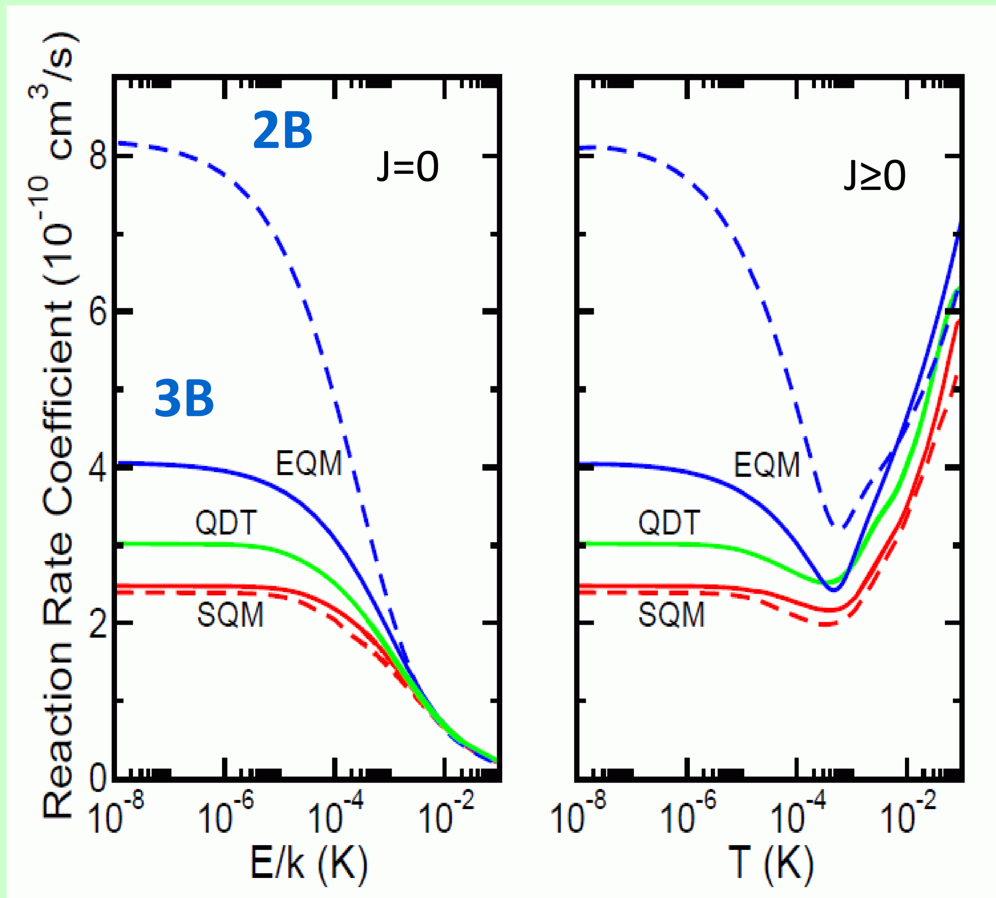
Behaviour of the rate constants at low temperature also depends on the calculation of the cross sections at the low energy regime. On the left, comparison of different approaches.



$^{6}Li^{174}Yb$+^{6}Li →$^{6}Li_2$+^{174}Yb mediated by a deep potential well at the linear geometry



Essentially S-wave process below 10^{-4} K. SQM cross sections in good agreement with EQM results



Rate coefficients for $^{6}Li^{174}Yb$(v=j=0)+^{6}Li

References

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