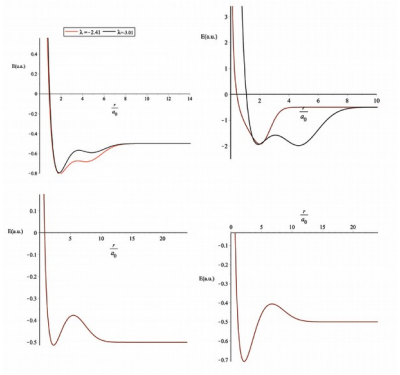
An analytical fit of adiabatic potential energy surface

F. Iacob[1], N. Pop[2]
[1]*Faculty of Physics, West University of Timişoara, Romania*
[2]*Department of Fundamental of Physics for Engineers, Politehnica University of Timisoara, Romania*

Astrochemical models at the molecular level deals with chemical reactions described as collision between two molecules. The conditions in the interstellar medium (ISM) are extreme and mostly the chemistry can be viewed as a collision with interest in the abundances of surface species through the use of rate equations by giving the reaction rate coefficients for chemical reactions.
In order to obtain a better description of the collision between two molecules, a form for the molecular interaction potential should be assumed. Usually, a Lennard Jones potential is employed. The first theory of ion-molecule reactions was proposed by P. Langevin.
Determining theoretically a rate coefficient first one focuses on electronic calculations for calculating potential energy surfaces (PES), in BO approximation, further used to study the motion of the nuclei (collision dynamics).
In this work an analytical expression of potential energy surface is derived and used to describe especially the cases where the present data fully support a model [sor94] that assumes that there are potential barriers or bottle necks.

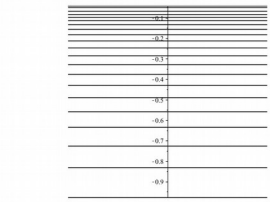


$$V^{s}_{\lambda,\mu}(r) = \sum_{k=0 \vee k=1}^{s} C_k r^{2k-p} \exp(-\mu r^2),$$

$$C_k = \mathrm{sgn}(\lambda)\,\frac{(\lambda+k)}{\mu^{\pm k}\,k!}\,.$$

$$C_k = \mathrm{sgn}(\lambda)\,\frac{(\lambda\mu+k)\mu^{k-1}}{k!}\,.$$

$$E_{n,J} = \frac{\epsilon}{2}(4\nu_{n,J} + 2J + 3)$$



The normalized eigenvalues ($s = 6$, $\lambda = -10$, $\mu = 0.02$)

Figure 1

Figure 2

The figure 1 shows some combinations of parameters for the analytical expression of potential [iac15]. The evaluation of energies in Schrodinger dynamics has been made (figure 2).
It is an open question whether one can classify reactions with nonstandard temperature dependences with a few simple reaction mechanisms based on simple properties of the potential energy surface such as barriers or wells. Low temperature experiments have shown [asv04a] that there can be significant deviations from such simple models. This may be due to subtle details of the potential energy surfaces such as small barriers or bottle necks which are not yet known with the accuracy required for low temperature reactions. In addition it is rather sure although not yet understood quantitatively with exception of simple systems [ger90] that symmetry selection rules play a pivotal role in replacing in a group of identical atoms just one by an isotope or vice versa.

References:

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