Atomic Data for Inelastic Processes in Collisions of Beryllium and Hydrogen

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The recently proposed model approach is applied to low-energy inelastic beryllium-hydrogen collisions for the purpose of obtaining quantum data for inelastic processes in beryllium-hydrogen collisions. The cross sections and the rate coefficients for the excitation, de-excitation, mutual neutralization and ion-pair formation processes are calculated.

1 Introduction

Atomic and molecular data on the inelastic processes in low-energy collisions of beryllium with hydrogen are important for astrophysical modeling of stellar atmospheres. Accurate quantum calculations are time-consuming and require accurate quantum-chemical input data. For this reason, it is important to develop and apply reliable model approaches, e.g. the approach described in [1, 2]. The approach is developed within the framework of the Born–Oppenheimer formalism and based on the asymptotic method [1] for construction of potential energy curves and on the multichannel formula [2] for calculations of non-adiabatic transition probabilities. It has been shown [2] that the data obtained by the model approach and by full quantum calculations are in good agreement for processes with large cross sections, i.e. the processes of the main interest for astrophysical applications.

2 Brief theory

A transition probability for a single passing of a non-adiabatic region created by molecular states k and $k+1$ is calculated within the Landau–Zener model [3]

$$p_k = \exp\left(-\frac{\xi_k^{LZ}}{v}\right), \quad \xi_k^{LZ} = \frac{\pi}{2\hbar}\sqrt{\frac{Z_k^3}{Z_k''}}\Bigg|_{R=R_c}, \tag{1}$$

with Z_k being a local minimum of an adiabatic splitting (see [3] for details). The total probability for a transition from an initial state i to a final state f is obtained by the multichannel formula [2]

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$$P_{if}^{tot} = 2p_f(1-p_f)(1-p_i)\prod_{k=f+1}^{i-1} p_k \left\{1 + \sum_{m=1}^{2(f-1)} \prod_{k=1}^{m} \left(-p_{f-\left[\frac{k+1}{2}\right]}\right)\right\} \times \left\{1 - \frac{\prod_{k=i}^{F} p_k^2 \left(1 + \sum_{m=1}^{2(i-1)} \prod_{k=1}^{m} \left\{-p_{i-\left[\frac{k+1}{2}\right]}\right\}\right)}{\sum_{m=1}^{2F} \prod_{k=1}^{m} \left(-p_{F+1-\left[\frac{k+1}{2}\right]}\right)}\right\}, \quad (2)$$

where F is a total number of open channels. The cross sections and rate coefficients are calculated as usual.

3 Results

Cross sections and rate coefficients of inelastic low-energy beryllium-hydrogen collisions for 12 covalent states and one ionic are calculated. The labels are shown in Fig. 1, where the channel $j = 13$ corresponds to the ionic one, $Be^+(2s\ ^2S)+H^-$. Rate coefficients are presented in Fig. 1 in form of heatmap. It is seen that the largest rate coefficients correspond to non-adiabatic transitions between the ionic state, the $Be(2s3p\ ^{1,3}P)$, $Be(2s3d\ ^3D)$ and $Be(2s3s\ ^1S)$ states.

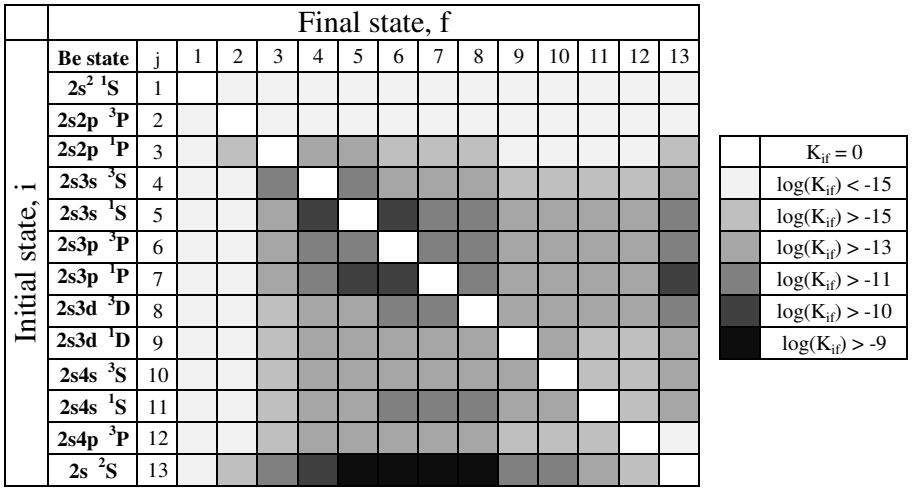

Figure 1: Calculated rate coefficients for Be+H, Be^++H^- collisions for $T = 6000$ K.

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References

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