Low-Energy Inelastic Magnesium-Hydrogen Collisions

D.S. Rodionov[1], A.K. Belyaev[1]

E-mail: *virtonoobne@bk.ru*

Available quantum calculations of cross sections for inelastic processes in Mg + H and $Mg^+ + H^-$ collisions, that is, the processes of astrophysical interest, are analyzed. It is shown that cross sections with large values are calculated with high accuracy. The calculations include all transitions between the nine lowest adiabatic $MgH(^2\Sigma^+)$ molecular states, with the uppermost of those diabatically extended to the ionic molecular state in the asymptotic region. Calculations also include transitions between five lowest adiabatic $MgH(^2\Pi)$ molecular states. The inelastic cross sections with large values are stable with respect to a number of channels treated. The non-adiabatic nuclear dynamical calculations have been performed by means of the reprojection method in the framework of the Born–Oppenheimer approach, which provides reliable physical results.

1 Aims

The measurement of abundances of chemical elements in stellar atmospheres, as interpreted from stellar spectra, is of fundamental importance in modern astrophysics. Inelastic processes in collisions of different atoms with hydrogen atoms are important for the non-local thermodynamic equilibrium modeling of stellar spectra which is the main tool for obtaining relative and absolute chemical abundances [1, 2].

Magnesium is of particular astrophysical interest since it is an α-element produced by supernovae of type II. The spectral lines of such α-element provide diagnostic tools to study distribution with time of chemical abundances in stellar populations [2, 3, 4]. Neutral Mg lines give many spectral features in different wavelength ranges and are easily observed in spectra of late-type stars, even in the most extreme metal-poor stars, e.g. the oldest stars in the Galaxy. Thus, the need for investigation of inelastic collisions of hydrogen atoms with magnesium atoms is well justified.

2 Methods and results

Non-adiabatic nuclear dynamical calculations have been performed by means of the reprojection method [5] in the framework of the standard Born–Oppenheimer approach, which provides reliable physical results. The method takes into account

[1] Herzen State Pedagogical University, St. Petersburg, Russia

V. Grinin et al. (eds) Radiation mechanisms of astrophysical objects. Yerevan: Edit Print, 2017, pp. 265–266.

non-vanishing asymptotic non-adiabatic matrix elements, provides the correct incoming and outgoing asymptotic total wave functions, and removes non-adiabatic transitions between atomic-state channels in the asymptotic region. The present analysis of the reprojection procedure within the reprojection method shows a reliable convergence with respect to a number of channels treated.

We have performed full quantum calculations [6, 7] of cross sections and rate coefficients for all excitation and de-excitation processes for all transitions between the eight lowest atomic states of Mg in inelastic collisions with H, as well as for mutual neutralization processes in $Mg^+ + H^-$ collisions and their inverse processes, the ion-pair formation ones, involving these Mg atomic states.

The first group of partial processes consists of the processes with large values of the cross sections, typically larger than $10\,Å^2$ for endothermic processes. The processes with the largest cross sections are $Mg(3s4s\,^1S) + H \to Mg^+ + H^-$, $Mg(3s4s\,^1S) + H \to Mg(3s3d\,^1D) + H$, $Mg(3s4p\,^3P) + H \to Mg(3s3d\,^3D) + H$. The present calculations show that these cross sections are rather stable with respect to variation of a number of channels treated.

The second group consists of inelastic processes with moderate values of cross sections, typically with the values between $0.1\,Å^2$ and a few $Å^2$. This is the largest group. The processes of these two groups are important for astrophysical applications [2].

The third group consists of the processes with low cross sections. The inelastic processes for transitions between, from and to low-lying states (including the ground one) are typically in this group due to large energy splittings, which result in small non-adiabatic transition probabilities.

Acknowledgments. The work was partly supported by Ministry for Education and Science (Russian Federation).

References

1. *P.S. Barklem*, J. Phys. Conf. Ser., **397**, 012049, 2012.
2. *Y. Osorio, P.S. Barklem, K. Lind et. al.*, Astron. Astrophys., **579**, A53, 2015.
3. *R. Cayrel, E. Depagne, M. Spite et. al.*, Astron. Astrophys., **416**, 1117, 2004.
4. *K. Fuhrmann*, Mon. Not. Roy. Astron. Soc., **384**, 173, 2008.
5. *A.K. Belyaev*, Phys. Rev. A, **82**, 060701(R), 2010.
6. *A.K. Belyaev, P.S. Barklem, A. Spielfiedel et. al.*, Phys. Rev. A, **85**, 032704, 2012.
7. *M. Guitou, A. Spielfiedel, D.S. Rodionov et. al.*, Chem. Phys., **462**, 94, 2015.