Quenching of excited Na due to He collisions

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ABSTRACT

The quenching and elastic scattering of excited Sodium by collisions with Helium have been investigated for energies between 10^{-13} eV and 10 eV. With the *ab initio* adiabatic potentials and nonadiabatic radial and rotational couplings obtained from multireference single- and double-excitation configuration interaction approach, we carried out scattering calculations by the quantum-mechanical molecular-orbital close-coupling method. Cross sections for quenching reactions and elastic collisions are presented. Quenching and elastic collisional rate coefficients as a function of temperature between 1 μK and 10,000 K are also obtained. The results are relevant to modeling non-LTE effects on Na D absorption lines in extrasolar planets and brown dwarfs.

1. Introduction

In cool stellar and planetary atmospheres, the electron abundance is extremely low so that thermalization is only possible through collisions of the dominant neutral species, H_2, He, and H. Typically, neutral cross sections are much smaller than those due to electrons, so that the level populations of the atmospheric constituents may display departures from equilibrium. Unfortunately, these cross sections are generally not available for collision energies typical of stellar/planetary environments. In this work, we investigate collisions of Na with He through the elastic scattering channels, $Na(3s\ ^2S) + He \rightarrow Na(3s\ ^2S) + He$ and $Na(3p\ ^2P^o) + He \rightarrow Na(3p\ ^2P^o) + He$, and the inelastic scattering channel, $Na(3p\ ^2P^o) + He \leftrightarrow Na(3s\ ^2S) + He$.

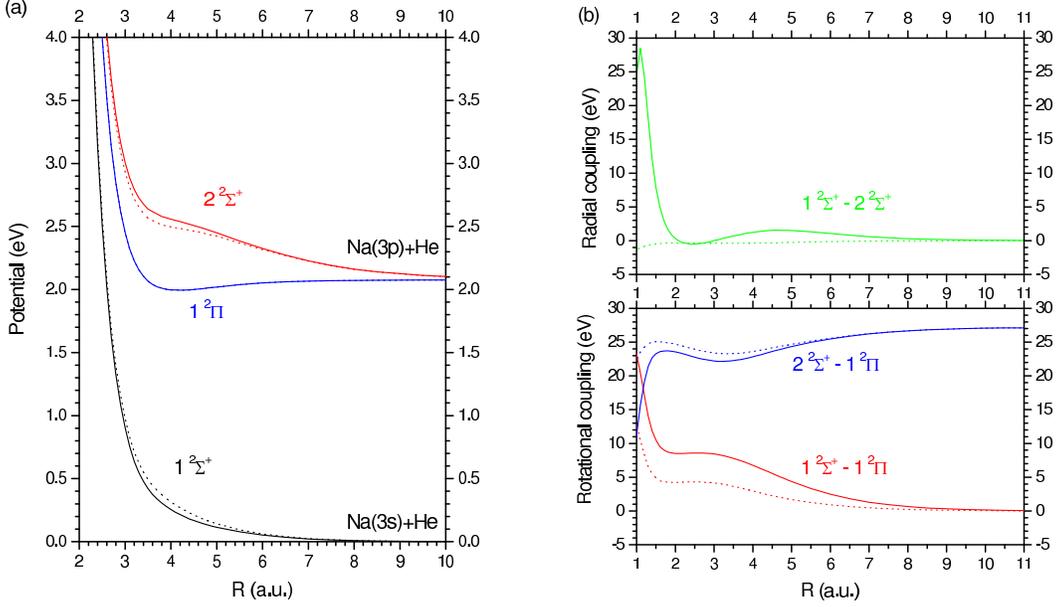# 2. Theoretical Methods and Results

Fig. 1.— Adiabatic (Solid curves) and diabatic (dotted curves) potentials (a) and couplings (b) for Na-He.
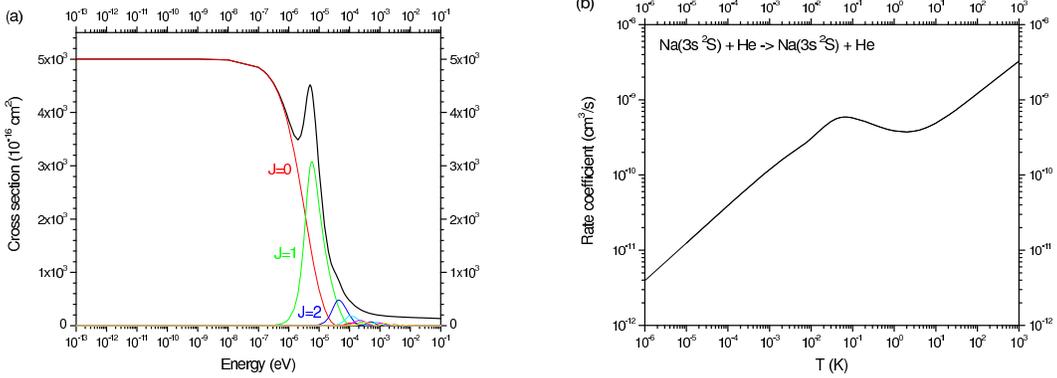

Fig. 2.— Elastic total and partial cross sections (a) and rate coefficients (b) for $1\ ^2\Sigma^+$ state.

The adiabatic potential energy curves and nonadiabatic radial and rotational couplings were obtained using the multireference single- and double-excitation configuration interaction (MRD-CI) method (Krebs & Buenker 1995). The quantum-mechanical MOCC approach (Zygelman 1992) is used in the present scattering calculations. An unitary transformation is applied to convert adiabatic potentials and nonadiabatic couplings into diabatic representation. A coupled set of second-order differential scattering equations can then be solved using the log-derivative method of Johnson (Johnson 1973) to obtain scattering cross sections.

In Fig. 1, we display the comparison of adiabatic and nonadiabatic results to diabatic results. Elastic total cross sections with low partial-wave analysis and rate coefficients are presented in Fig. 2-4. In Fig. 5 and 6, the state-to-state cross sections, total cross sections and rate coefficients for quenching and excitation processes are illustrated.
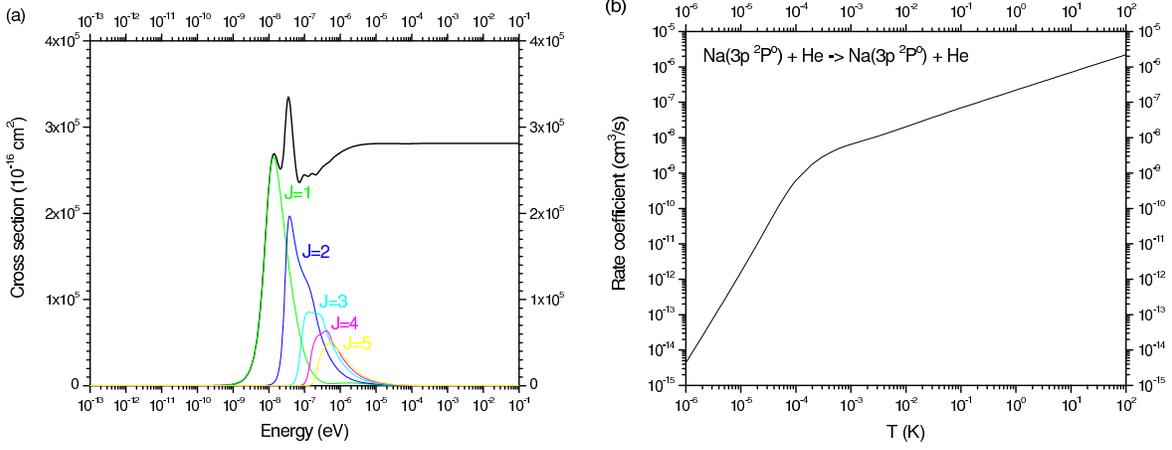

Fig. 3.— Elastic total and partial cross sections (a) and rate coefficients (b) for $1\ ^2\Pi$ state.
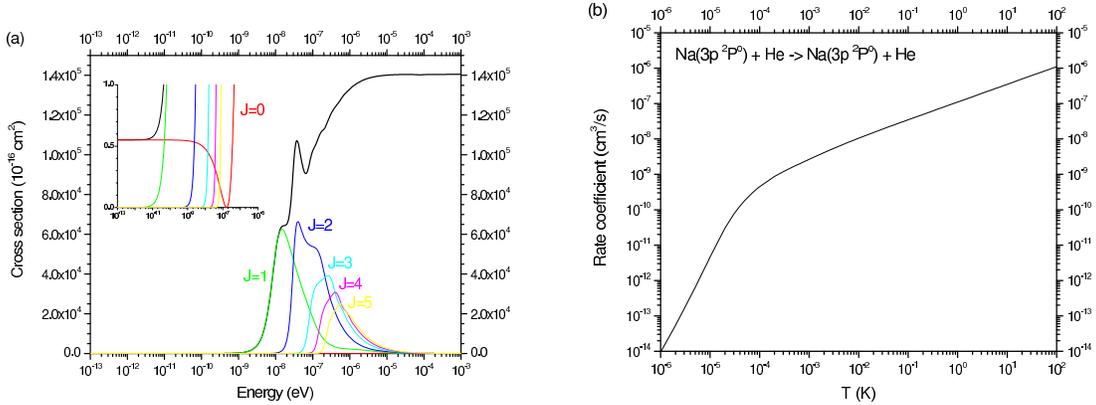

Fig. 4.— Elastic total and partial cross sections (a) and rate coefficients (b) for $2\ ^2\Sigma^+$ state.

3. Summary

We have investigated elastic and inelastic collisions of Na with low-energy He. Elastic cross sections for each of three molecular states are analyzed by their partial cross sections to explain wiggles and peaks of cross sections. Several distinct orbiting resonances occuring on quenching and excitation cross sections are due to quasi-bound states of the quasimolecule. The threshold of Na(3p)+He results in the rapid drop of excitation cross sections.
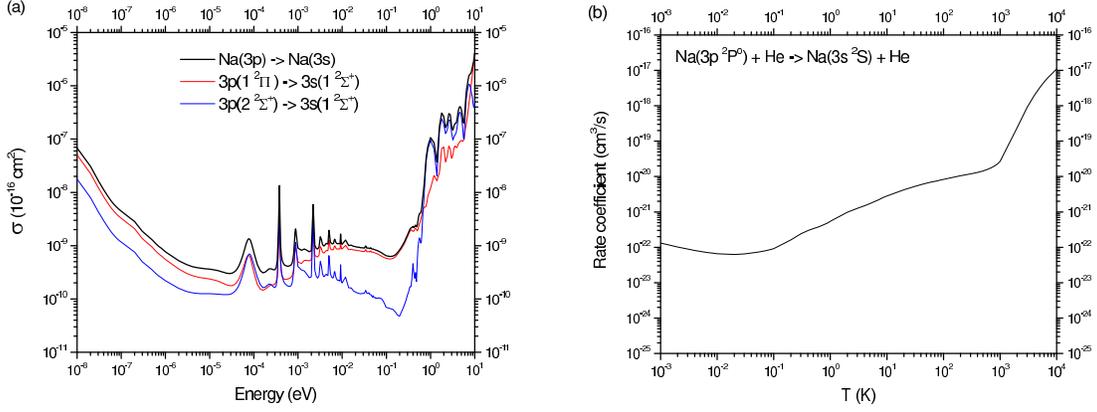
Fig. 5.— Quenching cross sections (a) and rate coefficients (b) for Na($3p\ ^2P^o$) + He → Na($3s\ ^2S$) + He.
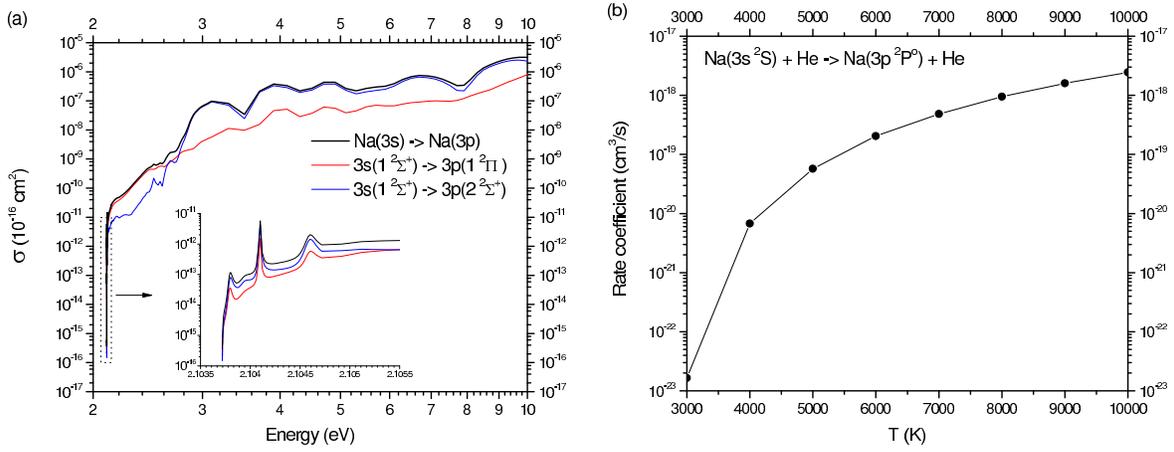
Fig. 6.— Excitation cross sections (a) and rate coefficients (b) for Na($3s\ ^2S$) + He → Na($3p\ ^2P^o$) + He.

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