Ab initio method for solving the radiative properties of the S_2 molecule

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Here we adopted *ab initio* method for solving the radiative properties of the S_2 molecule from the molecular structure. In this work, we consider the electronic angular momentum and spin orbit coupling. The potential energy curves and transition dipole moment of the S_2 molecule are obtained from *ab initio* calculations as shown in **Figure 1 (a)**. The Schrödinger equation of nuclear motion is solved to obtain the rovibronic line lists, including rovibronic energy levels and Einstein coefficients and so on, using Duo program[1]. The cross sections are obtained by ExoCross program[2]. The temperature dependence absorption cross sections of the B $^3\Sigma_u^-$–X $^3\Sigma_g^-$ transition are shown in **Figure 1 (b)**, including 298, 3000, 5000 and 10000 K. As the temperature increases, the absorption cross sections cover an increased area over the band. The impact of the coupling effect on the cross section is shown in **Figure 1 (c)**, including the electronic angular momentum and spin orbit coupling between B $^3\Sigma_u^-$ and B″ $^3\Pi_u$ states. At wavenumbers between 2000 and 8000 cm^{-1}, the cross section increases by about 4 orders of magnitude. Expected significant impact of coupling effect on absorption cross section at high temperatures.

The obtained absorption cross sections, along with the flow-filed parameters such as number density, can be further used to compute the radiative characteristic parameters such as absorption and emission coefficients, which in turn can be used to develop corresponding spectral band models, to simulate the radiative transport properties and to predict the radiative heat flow of high temperature gases.

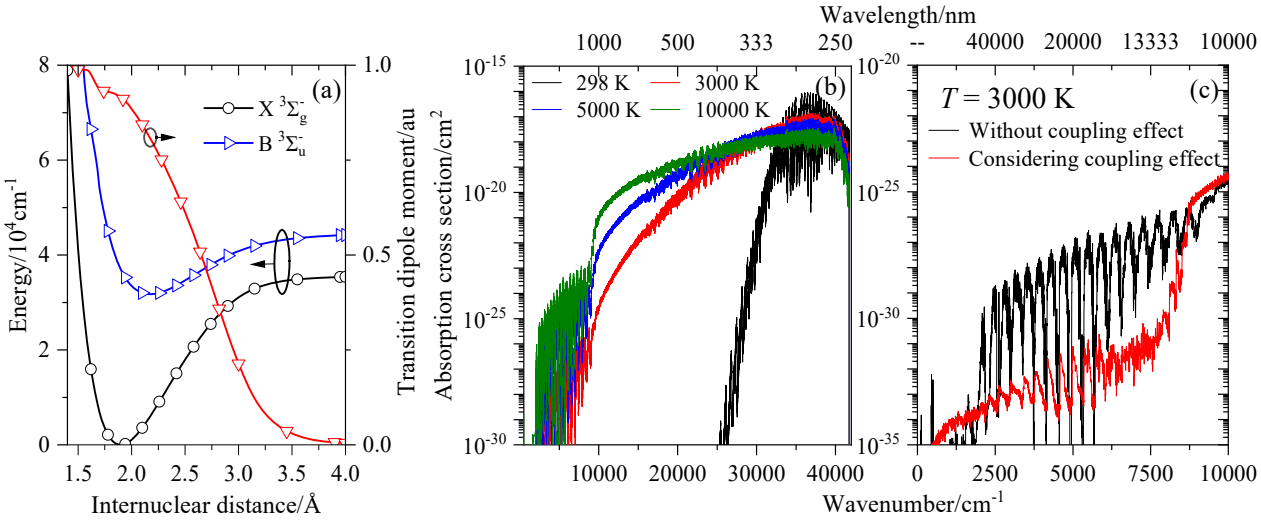

Figure 1. (a) potential energy curves and transition dipole moment, (b) temperature dependence of the S_2 cross sections, from bottom to top: T = 298, 3000, 5000 and 10000 K, (c) the influence of coupling effect on the absorption cross section

[1] Yurchenko S N, Lodi L, Tennyson J, et al. Duo: a general program for calculating spectra of diatomic molecules. Computer Physics Communications, 2016, 202: 262-75.
[2] Yurchenko S N, Al-Refaie A F, Tennyson J. ExoCross: a general program for generating spectra from molecular line lists. Astronomy & Astrophysics, 2018, 614: A131.

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