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HIGH TEMPERATURE OPTICAL SPECTRA OF DIATOMIC MOLECULES: QUANTUM-MECHANICAL, SEMIQUANTUM AND SEMICLASICAL APPROACH

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We developed a full quantum-mechanical procedure for calculating the absorption spectra of diatomic molecules, based on the Fourier grid Hamiltonian method for determining energies and the corresponding wave functions. A molecule in a box concept enables that all transitions between the bound, free, and quasibound states can be treated as bound-bound transitions. Using the classical FranckCondon principle and the stationaryphase approximation, we developed a semiquantum simulation method of the spectrum. The approximation is in very good agreement with fully quantummechanical calculations, while its consumption of computer time is lower by four orders of magnitude. Coupled channel quantummechanical and semiquantum approaches correctly describe the optical spectra in the case of non-adiabatic mixing. Both methods were tested on the absorption spectra of potassium and rubidium molecules in the red and nearinfrared region. In the case of local thermodynamic equilibrium the spontaneous emission coefficient and the linear absorption coefficient are related by Kirchhoffs law, which enables the semiquantum approximation of the diatomic molecules emission spectra as well. Using the latest ab initio calculations of electronic potentials and dipole moments of cesium molecules, we made a numerical simulation of the red and nearinfrared (600 - 1300 nm) absorption and emission spectrum of a dense cesium vapor for temperatures within the range 600 - 1500 K. The generalized Airy approximation of the canonical oscillating integrals was applied to the semiclassical calculation of thermally averaged spectral profiles of optical transitions of diatomic molecules, where the characteristic difference potential curve has a few critical points. Our study suggests that the semiquantum and semiclassical numerical simulation of the absorption/emission spectra can be an efficient tool for the diagnostics of hot vapors and are suitable for the determination of the number density and temperature of the vapors of diatomic molecules.