NUMERICAL SIMULATION OF DENSE CESIUM VAPOR EMISSION AND ABSORPTION SPECTRA

Robert Beuc, Mladen Movre, Goran Gatalica, Berislav Horvatić

Institute of Physics, Bijenička cesta 46, HR-10 000 Zagreb, Croatia

Recent *ab initio* calculation of Cs_2 electronic potential curves and electronic transition dipole moments (A. Allouche and M. Aubert-Frécon 2012) [1] provided us with a starting point for a very accurate Cs_2 spectra numerical simulation. We investigated the red and near-infrared (600-1200 nm) absorption and emission spectrum of dense, weakly ionized cesium plasma at high temperatures (600-1500 K). Our study showed that this "semiquantum" numerical spectrum simulation can be a very efficient tool for the diagnostics of hot and dense dimer vapors. It also enabled us to perform modelling of dense alkali vapor light sources.

Tha reduced absorption coefficient for the transition between two electronic molecular states in the semiquantum approximation reads

$$k(\nu,T) = a(\mu,T,\nu)\frac{2\mu k_B T}{\hbar^2}\sum_{V',V'} \exp\left(-\frac{\bar{E}_{V'',\Lambda''}}{k_B T}\right)\left|\left\langle \Phi_{V'',0,\Lambda''}\left|RD(R)\right|\Phi_{V',0,\Lambda'}\right\rangle\right|^2 g\left(\nu-\nu_{V',V'}\right)$$

where

$$a(\mu,T,\nu) = \omega_J \frac{8\pi^3\nu}{3hc}\left(\frac{2\pi}{\mu k_B T}\right)^{3/2}\frac{\left(2-\delta_{0,\Lambda'+\Lambda''}\right)}{\left(2-\delta_{0,\Lambda'}\right)}\frac{2S+1}{(2S_a+1)(2S_b+1)}$$

We analyzed the spectrum in the region 600 - 1200 nm where 11 singlet and 19 triplet cesium molecular transitions contribute to the absorption spectrum, and the total reduced absorption coefficient $\boldsymbol{k_T(\nu, T)}$ is the sum over all the electronic transitions:

$$k_T(\nu,T) = \sum_{i=1}^{30} k_i(\nu,T)$$

$$= a(\mu,T,\nu)\frac{2\mu k_B T}{\hbar^2}\sum_{j=1} \exp\left(-\frac{\bar{E}_j}{k_B T}\right)\left|\left\langle \Phi_{V'',0,\Lambda''}\left|RD(R)\right|\Phi_{V',0,\Lambda'}\right\rangle_j\right|^2 g\left(\nu-\nu_{Tr_j}\right)$$

In the calculation we took into account about 10^7 rovibrational transitions, and the computer time was 6 - 60 s, depending on the temperature of the cesium plasma.

The thermal emission from a uniform emitting layer, of thickness L and with the molecular concentration N, is related to the absorption coefficient $\boldsymbol{k(\nu,T)}$ by Kirchhoff's law [2] :

$$I(\nu,T) = \frac{8\pi h\nu^3}{c^4}\frac{1-e^{-k(\nu,T)N^2L}}{e^{\frac{h\nu}{k_B T}}-1}$$

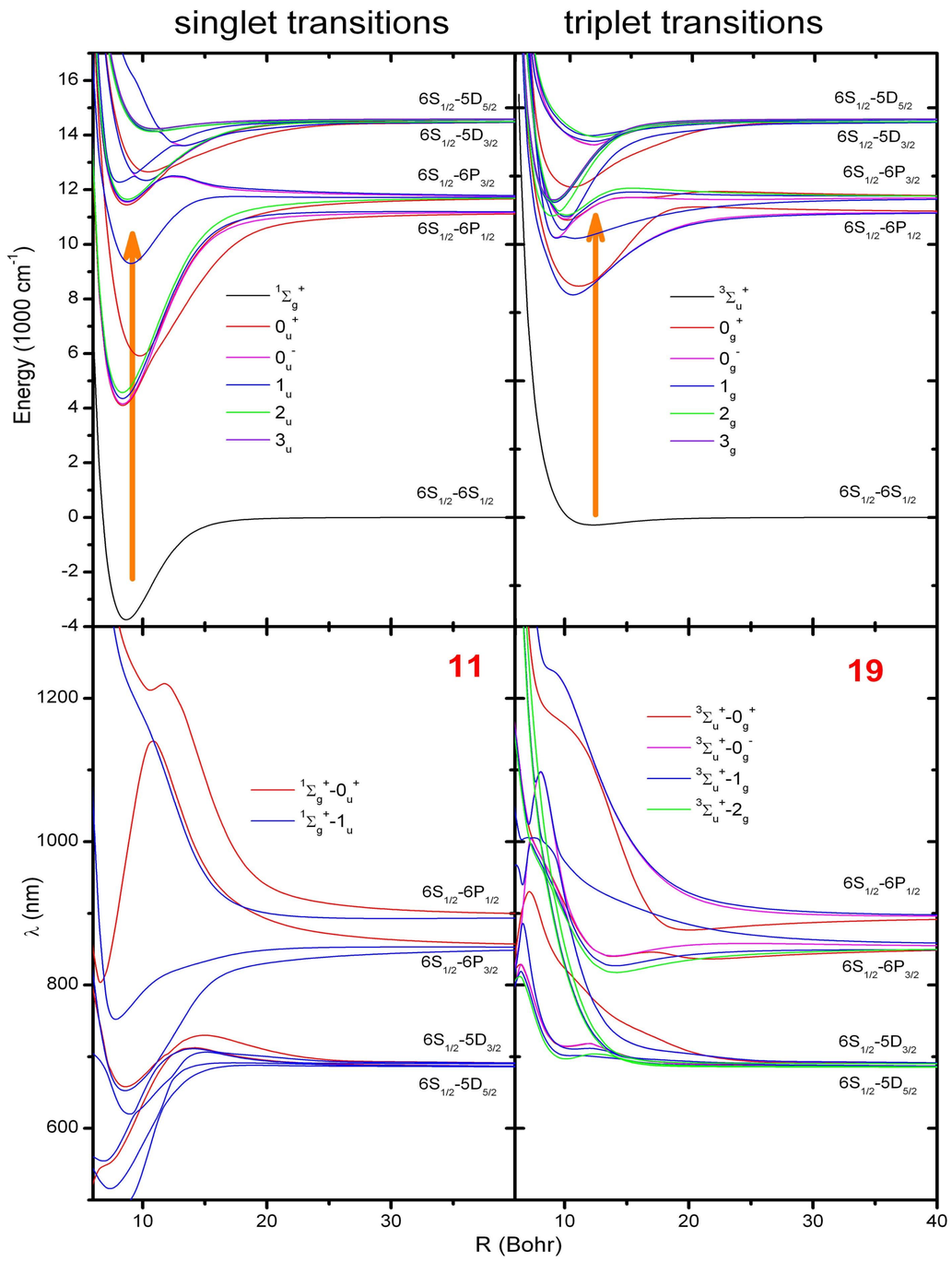
$$= \begin{pmatrix} k(\nu,T)N^2L \ll 1 \\ \frac{h\nu}{k_B T} \gg 1 \end{pmatrix} \Rightarrow \frac{8\pi h\nu^3}{c^4}N^2 L e^{-\frac{h\nu}{k_B T}}k(\nu,T)$$

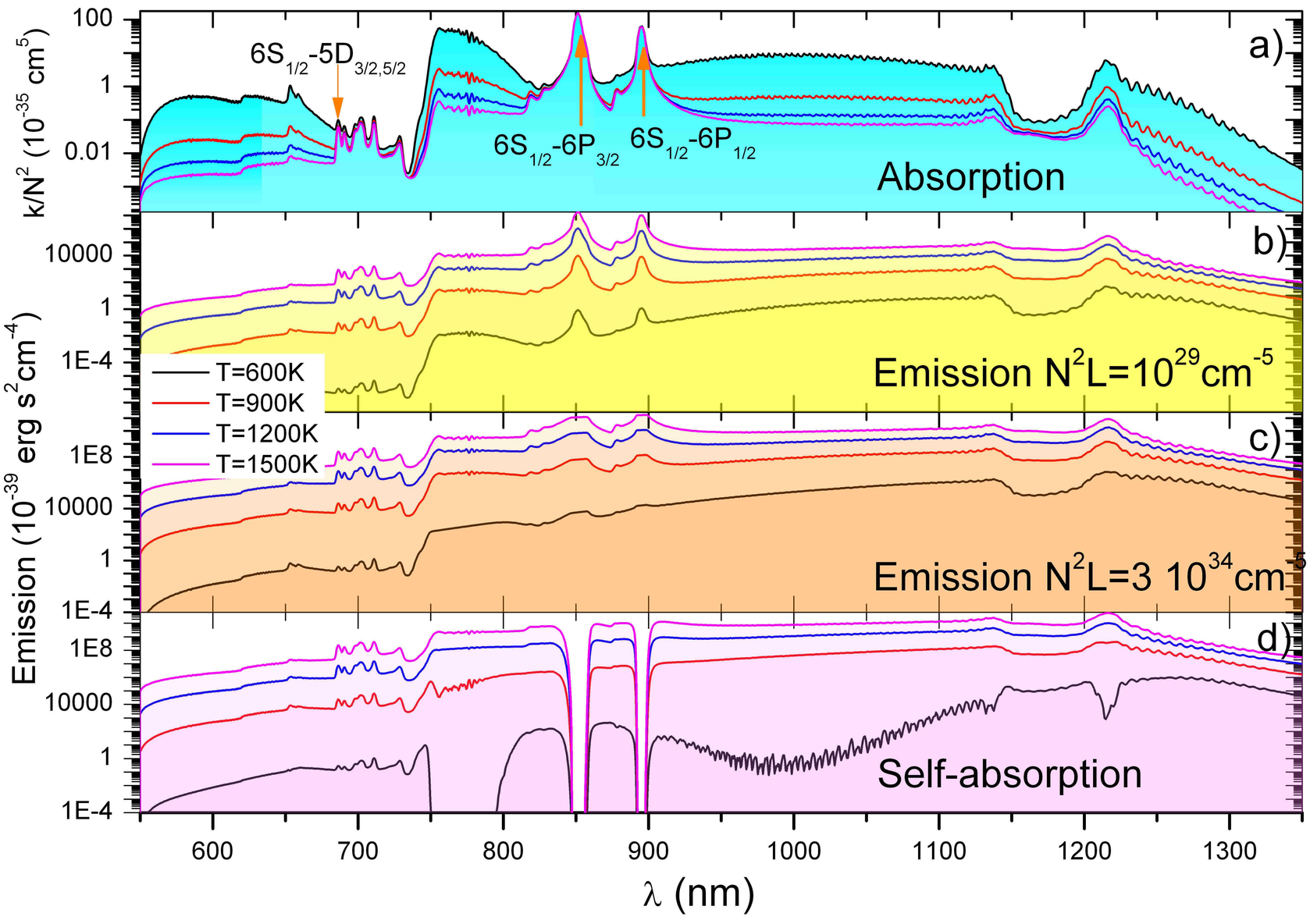
When modelling the total intensity $\boldsymbol{I_T(\nu)}$ of the emission spectrum, one can assume that all excited electronic states are differently thermalized at different temperatures $\boldsymbol{T_i}$, but in this work we have taken that all excited states have the same temperature $\boldsymbol{T}$.

$$I_T(\nu) = \sum_{i=1} I_i(\nu,T_i)$$

The intensity of radiation transmitted through uniform absorbing layer of thickness L and with the molecular concentration N is given by the Lambert-Beer law

$$I_t(\nu,T) = I(\nu,T)e^{-k(\nu,T)N^2L}$$





a) The reduced absorption coefficient for the four different temperatures

b) The intensity of the thermal emission of an optically thin medium ($\boldsymbol{kN^2L \ll 1}$) $\mathbf{N^2L} = 10^{29}$ cm^{-5}

c) The intensity of the thermal emission of an optically thick medium ($\boldsymbol{kN^2L \gg 1}$) $N^2L = 3 \cdot 10^{34}$ cm^{-5}

d) The intensity of thermal emission (case c) transmitted through an optically thick absorbing layer $N^2L = 6 \cdot 10^{35}$ cm^{-5}

[1] A. R. Allouche and M. Aubert-Frécon, J. Chem. Phys. **136**, 114302 (2012)

[2] J. Huennekens, T.G. Walker, and S.C. McClain, J. Chem. Phys. **83**, 4949 (1985)