Photodissociation of oxygen molecules upon the absorption in Shumann-Runge bands in various environments: modeling study

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Photodissociation of molecular oxygen plays an important role in the photochemistry of the atmosphere and can be used for the initiation of combustion in different combustible mixtures due to production of highly reactive atomic oxygen upon absorption of resonance laser radiation [1, 2]. For the analysis and modeling of photochemical processes both in the atmosphere and in the combustible mixtures it is needed to calculate the photodissociation rate with rather high accuracy upon the exposure of the mixture to solar radiation or to resonance laser radiation at given wavelength. As is known, O_2 molecules strongly absorb the ultraviolet radiation in the Shumann-Runge and Hertzberg systems.

In order to estimate the photodissociation rate it is necessary to reproduce the ultraviolet spectrum of O_2 molecules in different mixtures and at various values of temperature and pressure. This paper does address the calculations of the spectrum of Shumann-Runge bands in air and in H_2-O_2(air) mixture as well as the estimation of the photodissociation rate upon exposure of the mixture to ArF laser radiation at 193.3 nm wavelength. The variation of the composition of H_2-O_2(air) mixture with temperature $T_0 = 700 - 800$ K and pressure $P_0 = 0.5 - 1$ atm during the laser pulse duration ($\tau_p = 40$ ns) is also calculated. It should be emphasized that applied methodology for the calculation of O_2 spectrum in the Shumann-Runge bands allows us to reproduce with high accuracy the data on spectrum of Shumann-Runge system in the atmosphere reported elsewhere [3]. As an example Figure depicts the spectrum of O_2 molecule in the range of wavelength numbers $\nu = 51500 - 52000 \mathrm{cm}^{-1}$ for the stoichiometric H_2-air mixture at $T_0 = 800$ K and $P_0 = 1$ atm. On the basis of this methodology the values of photodissociation rate were calculated in the different sections of ArF laser beam propagating through the cell filled by the stoichiometric H_2-air mixture. The composition of the mixture in these sections was predicted by using the numerical simulation taking into account the detailed chemistry in the H_2-air system.

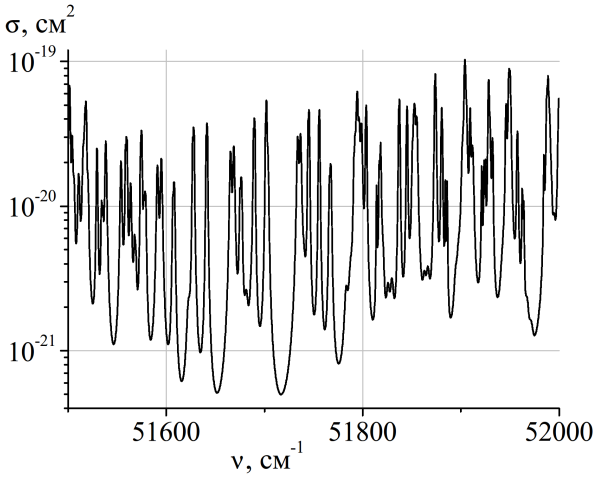

Figure 1: *Absorption cross section of O_2 molecule in the range of wavelength $\nu = 51500 - 52000 cm^{-1}$ for the stoichiometric H_2-air mixture at $T_0 = 800$ K and $P_0 = 1$ atm.*

We acknowledge the support by the EU FP7 IRSES Project – NOCTURNAL ATMOSPHERE

References

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