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Spectroscopy of Cl_2 ($B\,^3\Pi_{0^+_u}$) molecules at high temperatures

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Radiative characteristics of molecular chlorine have been studied using the shock-tube technique. The absolute emission spectroscopy method has been used based on the intensity measurements of the spontaneous NIR radiation of the thermally excited Cl_2 molecules under conditions of local thermodynamic equilibrium. The matrix element of dipole moment and Einstein coefficients for the $B\,^3\Pi_u(0^+_u) \rightarrow X^1\Sigma_g(0^+_g)$ electronic transitions in Cl_2 have been determined. Radiative lifetime of the lowest v-level of the electronic B-state is found to be $\tau_R\,(v'=0) = 50\pm10$ μs. The data obtained correlate well with the series of values $\tau_R\,(v'=0)$ for analogous B-states of other halogens in order of increasing of the mass of molecules.

Приводятся результаты экспериментального исследования радиационных характеристик молекулярного хлора с применением техники ударной трубы. Используется метод абсолютной эмиссионной спектроскопии, который базируется на измерении интенсивности спонтанного ИК излучения термически возбужденных молекул Cl_2 в условиях локального термодинамического равновесия. Определены матричный элемент дипольного момента и коэффициенты Эйнштейна электронного перехода Cl_2 $B\,^3\Pi_u(0^+_u) \rightarrow X^1\Sigma_g(0^+_g)$. Найдено радиационное время жизни нижайшего колебательного уровня электронного B-состояния Cl_2 $\tau_R\,(v'=0) = 50\pm10$ μs. Полученные данные хорошо коррелируют с рядом значений $\tau_R\,(v'=0)$ аналогичных B-состояний галогенов в порядке увеличения массы молекул.

Spectroscopy as a means to study the structure and properties of the excited electron molecular states (ES) is of great scientific interest since it contributes to understanding of elementary physical and chemical processes (excitation, relaxation, energy exchange, reactions) which take place in high temperature media. Molecular chlorine is one of the most interesting objects for spectroscopic studies both from fundamental and applied standpoints. In particular, Cl_2 plays an important role in various technological processes employed for semiconductor materials fabrication in the microelectronic industry (CVD, PVD, etc).

In spite of common knowledge of spectroscopic constants for diatomic molecules [1–3], available data on the transition probability, oscillator strength and radiative lifetimes (Einstein coefficients) for the $B\,^3\Pi_{0^+_u} \rightarrow X^1\Sigma^+_g$ system of Cl_2 are contradictory. This is a point of discussions in the literature over years [4–7].

This work is devoted to spectrophotometric study of actual radiative characteristics of Cl_2 molecules at high temperatures using of the shock tube technique. Using a precise method of absolute emission spectroscopy based on the intensity measurements of the spontaneous NIR radiation of thermally excited molecules under local thermodynamic equilibrium (LTE) conditions, the dipole moment of the $Cl_2(B–X)$ electronic transitions (ET) and radiative lifetimes for the optically active B-state of Cl_2 have been determined.

The experiments were carried out using a classic high temperature shock tube [8] equipped by a set of optical spectral analyzers of "interference filter + photomulti-