CN violet system spectrum used as a molecular pyrometer and the influence noise to signal ratio on the temperature values

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Abstract. The CN violet system (\(B^2\Sigma^+ \rightarrow X^2\Sigma^+)\) molecular emission spectrum is frequently observed in plasma sources containing hydrocarbons and nitrogen mixture. We have simulated the spectrum of (0,0) and (1,1) bands of this system for different rotational and vibrational temperatures. The influence of the noise to signal ratio has been studied, if the noise to signal ratio is about 10% we found an error of 6% at temperature 3000K and 10% at 6000K.

1. Introduction
The violet system of CN molecule is a good tool for diagnosing plasmas containing this molecule, the molecular constants and the lines structure are well-known, and it is present in most of the plasma sources containing hydrocarbon and nitrogen in mixture for a temperature between 2000K and 6000K.

Czernykowski (1987) has simulated CN violet system to measure temperature in Electrobûleurs plasma [1]. Bontemps-Faure in 1997 uses this system for temperature measurements in arc plasma [2]. In 2004, Lino Da Silva used the violet system of CN to study the radiative properties of the plasma surrounding a vehicle through a planetary atmosphere at hypersonic speed [3].

In the previous publications, we have proposed a numerical method based on the simulation of molecular spectrum for studying the distribution temperature in modified arc Macker [4] and [5], and in transferred arc [6]. To determine \(N_2^+ / N_2\) ratio and the temperature distribution in Glidarc [7], we have made the simulation of both systems first negative and second positive one simultaneously.

In this paper, we have used this method based on the simulation of the (0,0) and (1,1) bands of CN molecular violet system. The method proposed permit to evaluate, by comparing point to point a real spectrum with the simulated one, temperature and apparatus function, approximated by the gauss function (the half-width at \(1/e\) height). Moreover, it is shown, by noised spectra simulation, the influence of noise to signal ratio at the calculated temperature values.

2. Simulation of the (\(B^2\Sigma^+ \rightarrow X^2\Sigma^+)\) spectrum of CN

2.1. The violet system of CN molecule
A complete description of the spectral terms of the diatomic molecules may be found, e.g. in [9] and [10], or in our previous publications [5] and [7].

The violet system of molecule diatomic CN corresponds to radiative transitions between the \(B^2\Sigma^+\) and \(X^2\Sigma^+\) electronic state (\(A = 0\)) at 3.32 eV and 0 eV respectively. We are interested in the (3858Å,
3888Å) spectral range covering the (0,0) and (1,1) bands. The coupling is type (b) Hund case [9]. The absolute rotational emission line intensity of the molecule is given by

\[ I_{ul} = C \sigma \Delta S_{J',J} \exp \left( -\frac{\hbar c F(J')}{kT} \right) \]  

(1)

where \( C \) is a normalization constant, \( \sigma \) is the wave number, \( S_{J',J} \) is the Hönl-London factors, \( h \) and \( c \) are the conventional physical constants, \( F(J') \) is the spectral terms and \( T \) is the temperature (marks ' concern the lower spectral term and the marks " are for the upper one). Formulae for \( S_{J',J} \)-factors for the (b) Hund case are taken from Kovacs [9] and the spectral terms are those of Budo [10].

2.2. Numerical simulation

Line intensities are calculated when a state of thermodynamic equilibrium is fully reached and the corresponding temperature of the gas, considered from a macroscopic and thermodynamic point of view, are the same. In reality, within laboratory plasmas, we usually have to deal with a local thermal equilibrium state instead of thermodynamic equilibrium state.

It is possible, when the population of discrete energy levels follow Boltzmann's Law, to attribute a corresponding temperature for each corresponding energy distribution; electronic, \( T_e \), vibrational \( T_v \) and rotational \( T_r \). In a non-equilibrium plasma \( T_r, T_v \) and \( T_e \) may differ from the kinetic temperature \( T_g \) of heavy species. Taking into account the strong coupling between translational and rotational energy states, the temperature derived from experiments is, in a general case, close to the gas kinetic temperature [11] and [12]. Thus, \( T_g \) can be deduced from \( T_r \), measured by using the rotational structure of molecular spectra.

All the spectral constants are taken from Herzberg [8]. Computed spectrum of individual lines for a given temperature is then convoluted with our apparatus function approximated by the gauss function whose \( \Delta X \) (the half-width at 1/e height):

\[ I_0 = \int_{v_0 - \Delta X}^{v_0 + \Delta X} I_v \exp \left( -\frac{(v - v_0)^2}{\Delta X^2} \right) dv \]  

(2)

where \( \tau = 2.5 \Delta X \) and \( v_0 \) is the wave number of the line.

An integrated cell (pixel) of simulated spectrum is chosen according to the cell of experimental spectrum under consideration. We can, following the situation, group several cells in one.

Practically, for each given set of values (\( \Delta X, T_r \)), the line intensities of this band are normalized to its maximum. Examples of simulated spectra, normalized to 100, are shown in figures 1, 2 and 3 for different sets of \( (T_v, T_r, \Delta X) \) values.

A quick analysis of these simulated spectra shows that and vibrational temperature has a great influence on the height of the band head (1.1) figure 1.

The apparatus function has essentially influenced the resolution of the rotational line structure. Particularly, if \( \Delta X \) is too high, only the shape of the band can be used to determine the rotational temperature. The rotational temperature has a significant influence on the rotational line structure.

3. Numerical method for rotational temperature evaluation

To evaluate the \( T_r \) from a given real spectrum, we have chosen to compare this spectrum point-by-point with spectra simulated at different values of \( \Delta X, T_r \). In our experiments the following procedure was applied. (i) The measured spectrum was corrected for the continuous background, which was assumed to be linear in the studied spectral range. (ii) The experimental spectral intensity was normalized to the maximum value, which was set to 100. (iii) The experimental data were compared with that of the simulated spectrum. The minimization procedure was used to minimize \( E(T_r, \Delta X) \) as a function of \( T_r, and \Delta X \) defined as:
\[ E(T_r, DX) = \frac{1}{N} \left[ \sum_{i=1}^{N} (I_i^r - I_i^s)^2 \right]^{1/2} \]  \hspace{1cm} (3)

\( I_i^r \) and \( I_i^s \) are respectively the intensities of the real and simulated i-th pixel of the spectrum containing \( N \) points. If the choice of the spectrum reference origin (background) is a bad one, the result will be affected. To avoid this error, we fix several origins, and our computer program searches the best origin to find the \( E(T) \) at minimum.

**Figure 1.** Effect of the vibration temperature \( T_v \) (\( T_r = 2000K \) DX = 0.075Å).

**Figure 2.** Effect of rotational temperature \( T_r \) (\( T_v = 5000K \) DX = 0.075Å).

**Figure 3.** Effect of the apparatus function DX (\( T_r = T_v = 4000K \)).
4. Application to simulated noisy spectra
In order to test the sensitivity of the temperature estimator, we applied this method when a noisy spectrum was used instead of the experimental one. The synthetic spectra were calculated for known apparatus functions, temperatures, and noise was introduced using a random number generator. Examples of simulated spectra noised, normalized to 100, are shown in figure 4 for different sets of N/S ratio. We can see that the rotational spectra are very deformed for the high N/S values.

![Simulated Spectrum](image)

Figure 4. Effect of noise to signal ratio (N/S) \((T_v = T_r = 4000K\) and \(Dx = 0.075\text{Å}\)).

5. Results and discussion
Calculations were performed for noise-to-signal ratios N/S equal to 1%, 5%, 10% and 20% and for temperatures of 3000 and 6000 K. The results obtained are given in table 1.

The results are satisfactory since the relative error in the temperatures is of the same order of magnitude as the noise-to-signal ratio, even if the last one was relatively high. Given that when the concentration of emitting molecule is relatively weak, the spectrum of molecular emission seems immersed in the continuous background noise. In other words, the ratio noise / signal depends strongly on the molecular concentration, we can therefore, using this method to determine at what temperature the emission is maximum and hence its concentration.

| Noise/signal % | 3000k | 6000k |
|---------------|-------|-------|
| 1%            | 1.5%  | 3%    |
| 5%            | 4%    | 7%    |
| 10%           | 6%    | 10%   |
| 20%           | 11.5% | 18.5% |

Table 1. Evolution of the relative error on the temperature with noise/signal ratios.

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