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### Remote Temperature Determination from Maximum Intensity line in Molecular Emission Fundamental Band

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## REMOTE TEMPERATURE DETERMINATION FROM MAXIMUM <sup>①</sup> INTENSITY LINE IN MOLECULAR EMISSION FUNDAMENTAL BAND <sup>②</sup>

**Key Words:** Temperature Measurement; Molecular Emission Spectra; Fourier  
Transform Infrared Spectroscopy; Remote Sensing

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### Abstract

A remote sensing method for estimating the temperature of hot gas is described. The method is based on the relation between the rotational quantum number  $J'$  corresponding spectral line of maximum intensity in the fine structure of rotation-vibration emission band of diatomic molecules and the temperature  $T$ . The advantages of the method are very easy, rapid and accurate. In this paper the condition using the method is discussed.

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## INTRODUCTION

In remote Fourier transform infrared emission spectroscopy, if the temperature of hot gas could be estimated by remote sensing molecular emission spectra the concentration of each gaseous species may be quantitatively measured. Over a decade ago a number of the methods of estimating hot gas temperature using its infrared absorption spectra, such as band—fitting methods<sup>(1)</sup>, graphical methods<sup>(2)</sup>, two—line methods<sup>(3,4)</sup> etc. , have been completed in the laboratories. Herget et al. <sup>(4,5)</sup> have developed a graphical method to measure the temperature of industrial stack plumes with remote sensing infrared molecular emission spectra. More recently Junde Wang et al. <sup>(6)</sup> have improved Herget's method to utilize remote Fourier transform spectrometer for measuring rotation—vibration emission spectra of diatomic molecules to estimate rough combustion temperature of smokeless high luminosity infrared pyrotechnics and the solid propellant. However these methods are complicated for measuring and calculating process.

Because the relative molecule population of exited rotational energy states is strongly temperature dependent, there is a quantitative relation between the rotational quantum number  $J'$  and the gaseous temperature  $T$ . To simplify the measuring and calculating process we have applied the rotational quantum number  $J'$  corresponding spectral line of maximum intensity in the fine structure of rotation—vibration emission band of the molecules using remote sensing Fourier transform infrared spectrometer. The calculated temperature is in remarkable good agreement with the temperature measured by other methods. The advantages of the present method are very easy, rapid and accurate.

## Theory

According to the theory of molecular spectra<sup>(7)</sup>, if thermal equilibrium exists among the molecules being considered, molecular emission spectral line intensity  $I_{\nu,\nu'}$  is proportional to the number  $N_{\nu,\nu'}$  of molecules in any given initial state( $\nu', J'$ )

$$I_{\nu,\nu'} \propto N_{\nu,\nu'} \quad (1)$$

For any given initial state ( $\nu', J'$ ) the relative number  $N_{\nu', J'}$  of molecules with energy  $E_{\nu', J'}$  can be shown to be proportional to the Boltzmann factor

$$N_{\nu', J'} \propto g_{\nu', J'} \exp\left(-\frac{E_{\nu', J'}}{kT}\right) \quad (2)$$

where  $k$  is the Boltzmann constant and  $g_{\nu', J'}$  is the degeneracy of the state ( $\nu', J'$ ). Because the vibrational states are nondegenerate and rotational degeneracy is  $2J' + 1$ , the rotation-vibration state degeneracy is  $g_{\nu', J'} = 2J' + 1$ .

The relative number  $N_{\nu', J'}$  of molecules with energy  $E_{\nu', J'}$  has the following relationship

$$N_{\nu', J'} \propto (2J' + 1) \exp[-J'(J' + 1)B_e h/kT] \quad (3)$$

where  $h$  is Planck's constant.

From Eqns(1) and (3), we obtain

$$I_{\nu', J'} \propto (2J' + 1) \exp[-J'(J' + 1)B_e h/kT] \quad (4)$$

In Eqn(4) the Boltzmann factor  $\exp[-J'(J' + 1)B_e h/kT]$  decreases and degeneracy  $g_{\nu', J'} = 2J' + 1$  increases with increasing  $J'$ , so there is a maximum of intensity occurring in each branch at about the same  $J'$  value. The  $J'$  of the maximum intensity line strongly depends on hot gas temperature  $T$  and increases with increasing temperature  $T$ , i.e., its running number  $m$  increases with increasing temperature  $T$ .  $m$  is an integral running number which takes the values  $1, 2, \dots$  for the R branch (that is,  $m = J' + 1$ ) and the values  $-1, -2, \dots$  for the P branch (that is,  $m = -J'$ ).

$$T = \frac{B_e}{A} (2J' + 1)^2 \quad (5)$$

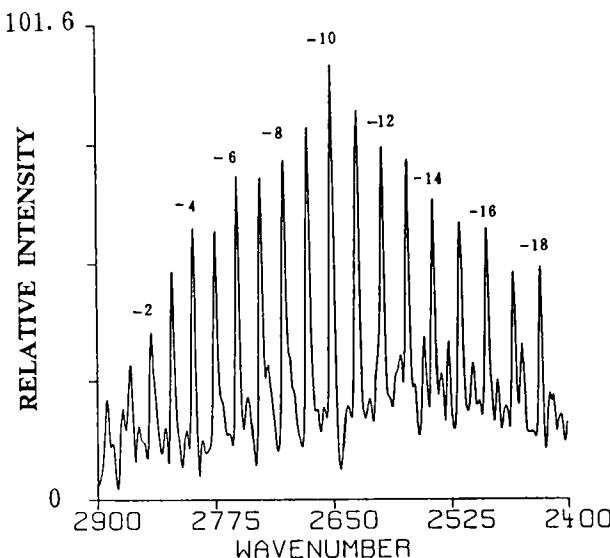


Fig. 1. Fine structure of the P-branch of the principal emission band (fundamental) of HCl at  $2885.9\text{cm}^{-1}$ .

The numbers above the individual lines are the  $m$  values.

Where  $A = 2k/h = 0.416 \times 10^{11}\text{K}^{-1} \cdot \text{sec}^{-1}$ ,  $J'$  corresponds to the maximum intensity line.

Form the R or P branch of the vibration-rotation emission spectrum of the molecules hot gas temperature  $T$  is satisfactorily given by Eqn (5).

## RESULTS

We have applied the remote measured temperature method to discuss plume temperatures of three types.

1. The infrared spectrum of the solid propellant containing a large quantities of ammonium perchlorate ( $\text{NH}_4\text{ClO}_4$ ) and magnesium powders is recorded on a NICOLET 170 Remote Source FT-IR Spectrometer (Resolution is  $4\text{cm}^{-1}$  in spectra). Fig. 1 is fine structure of P-branch of the principal emission band of chlorine hydride molecules (HCl) in solid propellant flare at  $2885.9\text{cm}^{-1}$ .

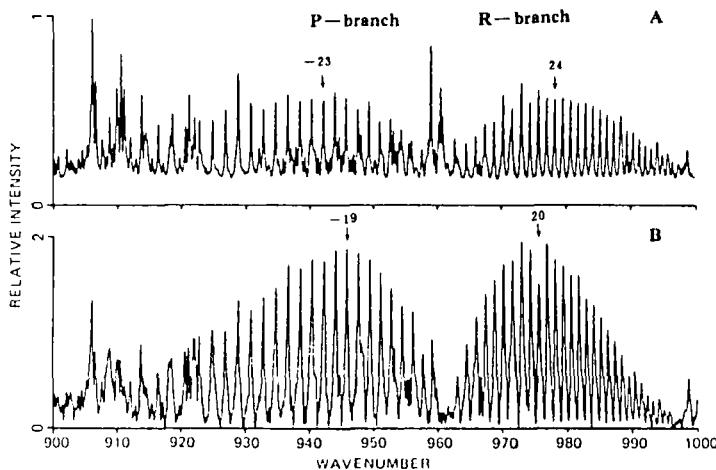


Fig. 2. A. Emission spectrum of carbon dioxide from a carbon monoxide boiler.  
 B. Emission spectrum of carbon dioxide from a coal-burning power plant (from Herget and Brasher<sup>[4]</sup>).

The running number  $m$  of the maximum spectral line intensity is  $-10$ , i.e.,  $J' = -m = 10$ . For HCl the rotational constant  $B_e$  is  $3.16 \times 10^{11} \text{ sec}^{-1}$ . From Eqn(5) we can obtain the flare temperature of the solid propellant

$$T = 3349.9 \text{ K}$$

In addition, the measured temperatures by both remote FT-IR from emission rotation-vibration band of molecules<sup>[6]</sup> and modified sodium line reversal method<sup>[8]</sup> equal 3371.5 and 3365.5 K, respectively. It is seen that there is a good agreement for the results obtained by three measured temperature methods.

2. Fig. 2 shows  $\text{CO}_2$  emission spectra from the plumes of the carbon monoxide boiler and coal-burning power plant. From Fig. 2A we can find that the running numbers for R- and P-branches of  $\text{CO}_2$  emission spectrum from the plume of the carbon monoxide boiler are 24 and  $-23$ , re-

Table 1. Compare results obtained by this method with other methods

Methods Temperature, K Hot gas	Present method	Other methods of molecular spectra	Modified sodium line rever— sal method
Solid Propel— lant flare	3349. 9	3371. 0 <sup>(6)</sup>	3365. 1 <sup>(6,8)</sup>
Plume of the carbon monox— ide boiler	637. 2	633 <sup>(6)</sup>	—
Plume of a coal—burning power plant	434. 6	444 <sup>(6)</sup>	—

spectively. The rotational constant  $B_e$  of  $\text{CO}_2$  is  $0.12 \times 10^{11} \text{ sec}^{-1}$ . From Eqn (5) we can obtain the plume temperature

$$T = 637.2 \text{ K} \quad \text{for R—and P—branches}$$

The plume temperature measured by remote infrared emission graphical method<sup>(4)</sup> is

$$T = 620 \text{ K} \quad \text{for R—branch}$$

$$T = 645 \text{ K} \quad \text{for P—branch}$$

The average value of R—and P—branches is  $\bar{T} = 633 \text{ K}$ .

There is a good agreement for results obtained from the present method and graphical method<sup>(4)</sup>.

3. Fig. 2B shows that the running numbers for R—and P—branches of  $\text{CO}_2$  emission spectrum from the plume of a coal—bruning power plant are 20 and—19, respectively. The plume temperature is obtained from Eqn (5)

$$T = 434.6 \text{ K} \quad \text{for R—and P—branches.}$$

The plume temperature obtained by remote infrared emission graphical method<sup>[4]</sup> is

$$\begin{array}{ll} T = 430K & \text{for R-branch} \\ T = 458K & \text{for P-branch} \end{array}$$

Their average value is  $\bar{T} = 444K$ .

It is agreement in the results obtained from two methods.

## CONCLUSIONS

1. We summarize above results obtained by several methods in Table 1.

From Table 1 it is seen that the remote temperatures estimated by the present method are in agreement with several methods.

2. The present method is much more easy, rapid and accurate than several other methods for the measuring and calculating process.

3. When we utilize the method for estimating temperature of hot gas it is noteworthy

(1) In the fine structure of the rotation—vibration emission band of molecules the change of spectral line intensity with the running number  $m$  of spectral line must be remarkable, i. e. , in the beginning spectral line intensity increases with increasing running number  $m$  , then after the spectral line intensity reaches a maximum value the spectral line intensity decreases with increasing  $m$ .

(2) In the fine structure of the rotation—vibration emission band the number of the spectral lines must be greater. Thus the higher spectral interferometer system is necessary . Generally , resolution  $4 - 0. 125\text{cm}^{-1}$  in spectra is enough.

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