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A NEW BAND SYSTEM OF BiF MOLECULE IN THE REGION λ6200-λ7000 Å

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ABSTRACT

A reinvestigation of the electronic spectrum of BiF, has revealed the presence of a new system of bands, degraded to longer wavelengths, in the region λ6200-λ7000 Å. The band heads could be represented by the following vibrational quantum formula.

$$v = 16114.4 + 399.3(V'+1/2) - 3.4(V'+1/2)^2$$
$$- 535.3(V''+1/2) + 2.7(V''+1/2)^2$$

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INTRODUCTION

The spectrum of the BiF molecule is wellknown to consist of a number of band systems disignated as $A-X_1$, $B-X_1$, C_1-X_2, C_2-X_2 and C_3-X_1. As the $A-X_1$, $B-X_1$ and C_3-X_1 systems were observed in absorption, it is known that X_1 is the ground state of the BiF molecule. From a rotational analysis of the $A-X_1$ system, Rao and Rao[1] have attributed the ground state X_1 to the $^3\Sigma^- 0^+$ state of the ground state electron configuration

$$(z\sigma)^2 (y\sigma)^2 (x\sigma)^2 (w\pi)^4 (v\pi)^3 \quad \ldots \quad 0^+(^3\Sigma^-).$$

The levels X_2 and X_3 were tentatively attributed by them to the $^1\Delta$ and $^1\Sigma^+$ states of the same ground state configuration. Later, from a rotational analysis of the C_2-X_2 (λ2850-λ2650) Å and C_1-X_2 (λ3050-λ3250) Å systems, the states X_2 and X_3 were attributed to the $^1\Delta$ and $^1\Sigma^+$ states respectively by Mohanty et al[2] and Chaudhary et al[3,4].

The present paper deals with the analysis of a new system of bands of the BiF molecule observed in the region λ6200-λ7000 Å, disignated as A_2-X_2.

EXPERIMENTALL

The spectrum of BiF has been excited in a R.F.(40 MHz) discharge from a 500 watt oscillator, using specpure BiF_3, in a conventional quartz discharge tube. In addition to all the previously known systems, the spectrum when photographed on a Hilger three-prism glass littrov spectrograph, revealed the existence of new bands degraded to longer wavelengths in the Photographic infrared region λ6200-λ7000 Å., as shown in Fig. 1.

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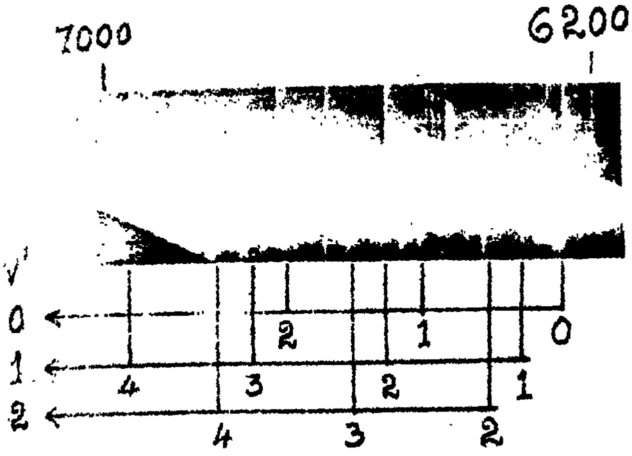

Fig. 1. A new A_2-X_2 system of BiF molecule

ANALYSIS

Unsuccessful attempts have been made to fit the observed single headed bands, as an extension of the wellknown visible A-X_1 system. However, the bands could be analysed into a separate brief system. The analysis has become simple with the identification of the three prominent V''-progressions $V'=0,1,2$. The wavenumber, intensity and classification data of the bands of the new system are given in Table I. The heads are represented by the following quantum formula to within an accuracy of about ± 1 Cm^{-1}.

$$v = 16114.4 + 399.3(V'+1/2) - 3.4(V'+1/2)^2 - 535.3(V''+1/2) + 2.7(V''+1/2)^2$$

It is seen from the above data that the lower state constants

TABLE -I

Band Head data of the A_2-X_2 system of the BiF molecule

Wavenumber (Cm^{-1})	Assignment	Intensity	ν_{obs} - [illegible]
16046.1	0,0	10	[illegible]
15907.3	1,1	4	-1.2
15769.4	2,2	2	-0.1
15516.2	0,1	9	0.7
15383.9	1,2	3	0.1
15250.6	2,3	3	0.4
14990.0	0,2	6	-1.3
14864.7	1,3	9	0.2
14736.7	2,4	4	0.4
14351.0	1,4	9	0.4

are in fairly good agreement with those of the $X_2(^1\Sigma^+)$state, (ω_e" = 535.0 Cm^{-1}). Because of the observed single headed nature of the bands, the upper state (disignated as A_2) can reasonably be attributed to a $^1\Sigma^+$ state, arising from the first excited electron configuration

$(z\sigma)^2\ (y\sigma)^2\ (x\sigma)^2\ (w\pi)^3\ (v\pi)^3\quad \ldots\ ^3\Sigma^-,\ ^3\Sigma^+,\ ^3\Delta,\ ^1\Sigma^+,\ ^1\Sigma^-,\ ^1\Delta.$

However, this conclusion has to be confirmed from a rotational analysis of the system under high resolution. By analogy with the energy levels of isoelectronic molecule SbF, this system may be disignated as A_2-X_2 system of BiF molecule.

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