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13. ABSTRACT (Maximum 200 words)

During the period covered by the U.S. Air Force grant a Broida type oven was constructed allowing the spectroscopic investigation of the A O^+ and X O^+ electronic states of the BiF molecule. Potential energy curves for the A and X states were constructed up to v = 25 and v = 36 respectively, much farther than previously known. Except a drastic change in the nature of the BiF (X O^+) band strength, the dissociation energy is estimated 40 000 cm^{-1} almost twice the calculated current value. We are currently constructing a new BiF source in order to better determine the electronic structure of low-lying states of BiF.

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This technical report has been reviewed and is approved for publication.

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Final Scientific Report - GRANT AFOSR - 88 - 0347

During the period covered by the U.S. Air Force grant, a Broida type oven was constructed in order to investigate the spectroscopy of the low-lying states of the BiF molecule. Moderate resolution spectra of the chemiluminescence from the Bi + F_2 reaction were recorded by using the Fourier transform instrument by Jean Vergès at the Aimé Cotton Laboratory in Paris. These spectra allowed an extended vibrational analysis of the BiF AO^+ and XO^+ electronic states (1). From these data, potential energy curves for the A and X states were constructed up to v = 25 and v = 36, respectively, much farther than previously known. LeRoy-Bernstein long range analysis applied to the vibrational constants obtained for the BiF ground state yielded an estimate for the dissociation energy of 40 000 cm^{-1}, almost twice the current value of 21 200 cm^{-1} (2). Since the highest observed level of the ground state, v = 36, lies only 6 400 cm^{-1} below this energy, a drastic change in the nature of the BiF bond as it is stretched would be necessary to conform with the current value of the BiF bond strength. Only experimental observation of higher vibrational levels of the BiF X state will resolve this question.

We attempted to improve the BiF emission intensity from our Broida oven in order to extend the knowledge of the BiF ground state closer to the dissociation energy. Unfortunately, the temperature range obtainable with our current apparatus is limited to less than 600°C in the reaction zone where the major product of the Bi + F_2 reaction is BiF_3 and hence any increase in F_2 density results in a decrease of the BiF A-X emission intensity. However, at temperatures above 700°C, the BiF_3 + 2 Bi - 3 BiF reaction begins to dominate (3). We are currently constructing a new Broida oven that will operate in the 900-950°C range to exploit this reaction, so much higher BiF densities can be achieved. With this new source we will observe A-X emission to much higher X state levels. This apparatus will also operate at pressures up to several torr where several new band systems appear (4).

We have also built a BiF emission source based on microwave excitation. This apparatus consists of two separate ovens with independant temperature control in order to produce both Bi and BiF_3 vapor. These are entrained in a F_2/He mixture and flowed through a microwave discharge cavity. The BiF A-X and B-X emission is intense while the fluorescence of the so-called C_1-X_3 and C_2-X_2 systems is relatively weak, as shown in Fig. 1. Assignments of the electronic states responsible for the C_1-X_3 and C_2-X_2 bands have been suggested in Ref. 5. We attempted to observe high resolution Fourier Transform spectra of these systems to better characterize these poorly known states of BiF. However, the presence of strong Bi resonance lines prevented observation of these weak bands under high resolution.

The X_1 state, predicted by ab-initio calculations (2) to lie some 7 600 cm^{-1} above the ground state, has recently been observed by Devore et al. under low resolution conditions (4). We will attempt to obtain high resolution emission spectra using our high temperature Broida oven source and as confirm the assignments of ref. 4. The X_1 state may also be populated by energy transfer from the near-resonant process : BiF (XO^+) + O_2 ($^1\Delta_g$) → BiF (X_1) + O_2 ($^3\Sigma_g^-$). We will also try to record BiF X_1 - XO^+ emission spectra in the 7600 cm^{-1} region in order to characterize the X_1 state. We will also obtain IR emission spectra from the system reported in ref. 6. In addition, a King furnace is being installed to obtain BiF from the thermolysis of BiF3 at temperature of 1 200-1 300° C so that high resolution Fourier transform absorption spectra can be recorded. These new investigations will yield information of the electronic structure of low-lying states of BiF as well as provide a more precise determination of the BiF bond strength.

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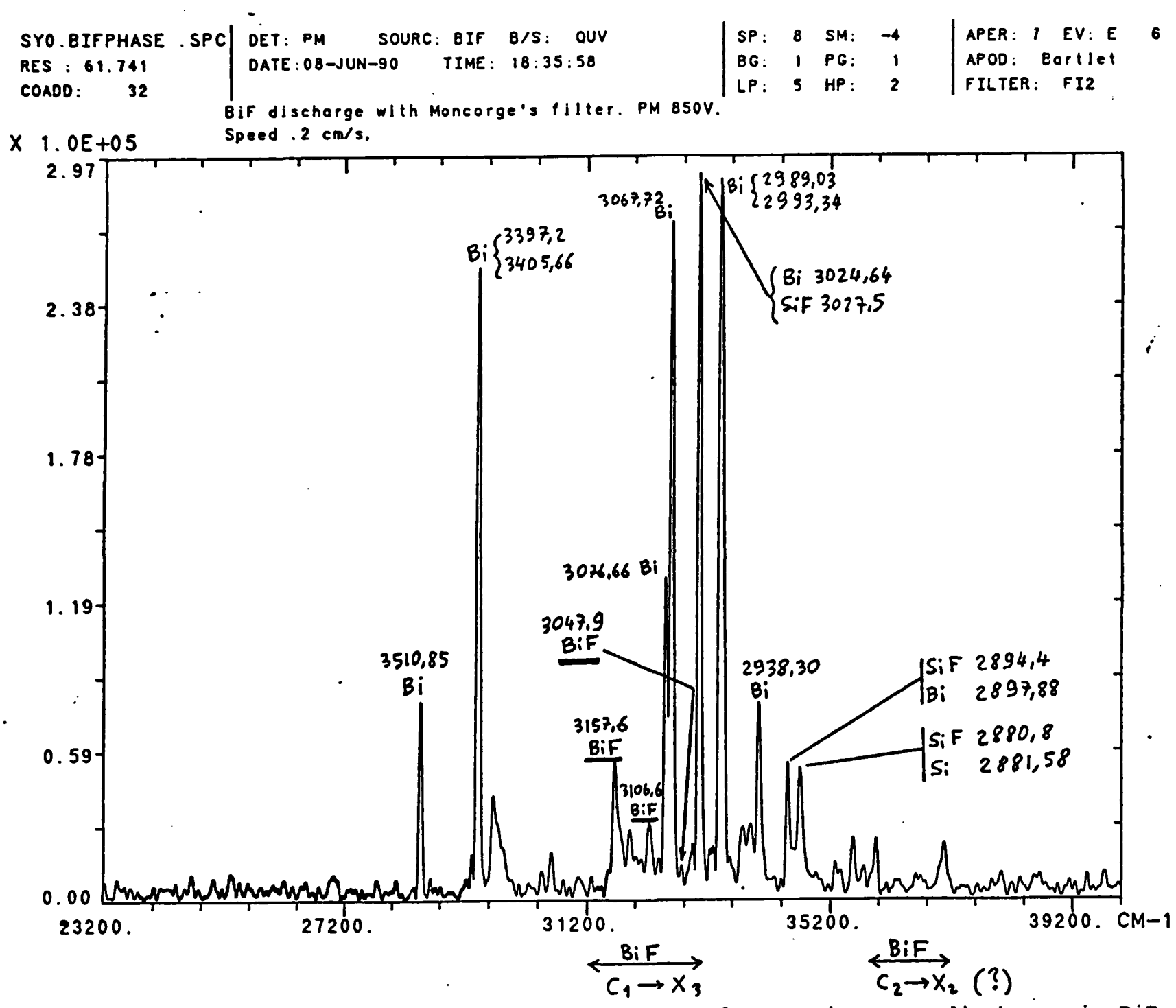

Fig 1 : Fourier Transform low resolution spectrum from a microwave discharge in BiF