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# High-resolution $\nu_1$ spectrum of propyne: Application of a microcomputer-controlled infrared-acoustic color center laser spectrometer

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Development of a microcomputer-controlled infrared-acoustic color center laser spectrometer capable of scanning in  $100 \text{ cm}^{-1}$  sections over the wavelength range  $2.2\text{--}3.3 \mu\text{m}$  with a resolution of  $0.01 \text{ cm}^{-1}$  ( $300 \text{ MHz}$ ) is reported. Application of the spectrometer to investigation of the  $\nu_1$  spectrum of propyne is demonstrated.

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There has been considerable interest in exploiting infrared-acoustic techniques for high-resolution spectroscopic analysis using tunable laser sources.<sup>1-4</sup> Emphasis has been placed on the development of small volume nonresonant acoustic detectors using  $\text{CO}_2$ ,<sup>3</sup> Spin-Flip Raman<sup>1,2</sup> and Color Center Lasers.<sup>4</sup> Color Center Lasers appear to combine the characteristics of medium laser intensity, broad tunability, and narrow linewidth, which make them particularly appealing for development of a high resolution infrared-acoustic tunable laser spectrometer.

Recently, Kasper *et al.*<sup>5,6</sup> have described a sophisticated minicomputer software/hardware system suitable for controlling commercially available Burleigh Instruments Inc. FCL-20 lasers. This has permitted conversion of the laser into an ultrahigh resolution spectrometer. In the current work, we report development of a less extensive general purpose microcomputer-controlled infrared-acoustic tunable laser spectrometer utilizing an FCL-20. This particular system can be scanned single mode over frequency ranges of  $100 \text{ cm}^{-1}$  at a time using mode-hop scanning. The spectrometer provides a resolution of  $0.01 \text{ cm}^{-1}$  and, with a  $3 \text{ GHz}$  marker cavity, the capability of calibrating the wavenumber scale to better than  $0.01 \text{ cm}^{-1}$  using low pressure reference spectra. High-resolution  $\nu_1$  spectra of propyne are recorded to demonstrate the spectrometer's performance.

Figure 1 illustrates the system, which is similar to that used previously,<sup>4</sup> including the Micromation-Z64 microcomputer with flexible disc unit, a CRT terminal (ACT V), and a EPSON MX-80111F/T printer. The additional hardware involves a four channel digital-to-analog converter (CDC DA-100), eight channel analog-to-digital converter (CDC AD-100), and a stepping motor driver (SAA-1027). Single mode character of the laser is monitored with a high-resolution ( $150 \text{ MHz FSR}$ ) spectrum analyzer (Burleigh CFT500). The software consists of FORTRAN language modules which control the single mode scanning of the laser and store into the disc the digitized spectrum and marker cavity transmission.

The laser frequency is tuned by synchronously scanning the grating and internal etalon. A stepping motor scans the grating via a sine bar drive and the internal etalon length is adjusted by a PZT translator stage. The cavity length is kept fixed so that the frequency tunes with  $300 \text{ MHz}$  ( $0.01 \text{ cm}^{-1}$ ) steps as the laser jumps from one cavity mode to another sequentially. The control program synchronizes the tuning of the grating and internal etalon by utilizing prerecorded data on the tuning characteristics of the sine bar drive and the PZT-translator stage. However, with the microcomputer, the use of extensive look-up tables<sup>5</sup> is not feasible. In practice, the scanning has performed in the following manner:

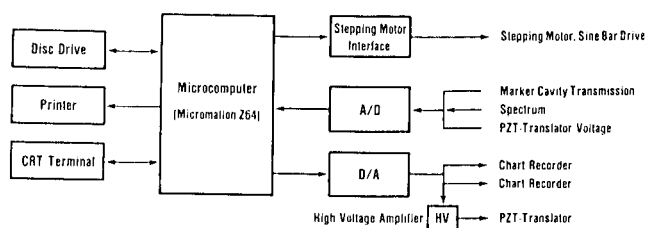
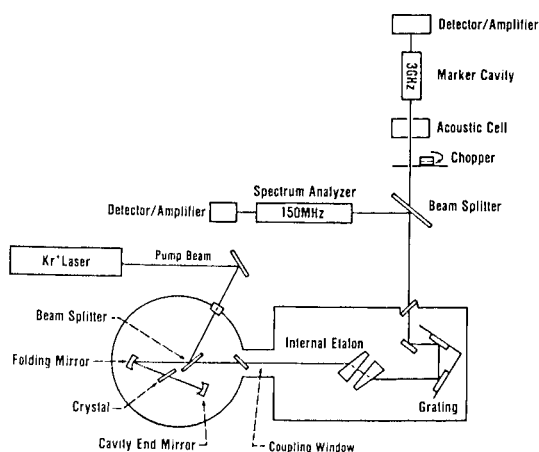


FIG. 1. Experimental arrangement and schematic of computer interface for spectrometer.

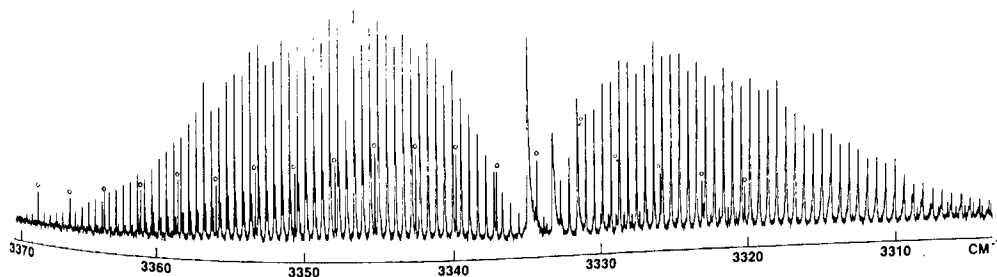


FIG. 2. Infrared-acoustic  $\nu_1$  spectrum of propyne at 303 K. Circled transitions belong to  $\nu_3$  band of HCN. The spectrum also includes weak lines belonging to  $\nu_1 + \nu_{10} - \nu_{10}$  and  $\nu_1 + 2\nu_{10} - 2\nu_{10}$  bands of propyne with Q-branches at 3333.4 and 3331.6  $\text{cm}^{-1}$ , respectively.

(1) PZT-translator stage proves to be nearly linear within the voltage range employed (100–600 V) whereas the sine bar drive exhibited large periodic and semirandom (nonperiodic but reproducible) deviations from the linearity. To ensure the proper synchronization, the sine bar drive was first calibrated against the internal etalon by using the method previously described.<sup>5</sup>

(2) In scanning the spectrum, the voltage on the PZT translator is stepped up at a constant rate. Each time the internal étalon has scanned over 1.2 GHz (4 longitudinal cavity modes), the grating was turned as required according to the sine bar drive calibration data to again center the two tuning elements in frequency.

(3) Because of the limited capacity of expansion, the PZT-translator stage has to be reset each time the internal etalon has scanned over about one of its free spectral ranges (27.3 GHz). The reset points were chosen to be immediately following the frequency marker from the marker cavity and the internal étalon length is set back slightly more than  $\lambda/2$ . Therefore, when scanning is resumed after the reset, the same frequency marker is recorded again. The spectrum initially consists of 1  $\text{cm}^{-1}$  long segments each overlapping about 0.1  $\text{cm}^{-1}$  with the immediate adjacent segments. When storing the data, the control program matches the frequency markers recorded before and after the reset points so that the final digitized spectrum appears to be continuously scanned.

TABLE I. Molecular constants of  $\nu_1$  band in  $\text{CH}_3\text{C}\equiv\text{C-H}$ .<sup>a</sup>

	Ref. 9	Ref. 8	Present work
$\nu_0$		3335.062 ± 0.002	3335.0597 ± 0.0007
$B''$	0.285059	0.28494 ± 0.00005	0.28511 ± 0.00005
$B'$		0.28426 ± 0.00005	0.28443 ± 0.00005
$D_j''$	9.87 × 10 <sup>-8</sup>	(1.7 ± 0.3) × 10 <sup>-7</sup>	(1.6 ± 0.3) × 10 <sup>-7</sup>
$D_j'$		(1.7 ± 0.3) × 10 <sup>-7</sup>	(1.6 ± 0.3) × 10 <sup>-7</sup>

<sup>a</sup> Constants are in  $\text{cm}^{-1}$ . The quoted error limits represent one standard deviation.

We have recorded the propyne  $\nu_1$  spectrum between 3370 and 3305  $\text{cm}^{-1}$  using the mode-hopping scan described above (Fig. 2). To obtain this spectrum, the small volume nonresonant acoustic cell<sup>4</sup> was filled at 2 Torr pressure with propyne. For calibration purposes, 100 m Torr of HCN was added. The HCN wavenumbers were taken from Ref. 7. The marker cavity (Burleigh CF25, 3.030 GHz FSR) provided frequency markers with 0.1  $\text{cm}^{-1}$  separation.

Measured transition frequencies were assigned and fitted to the expression

$$\nu_m^{P,R} = \nu_0 + (B' + B'')m + (B' - B'' - D_j' + D_j'')m^2 - 2(D_j' + D_j'')m^3 - (D_j' - D_j'')m^4.$$

The results of the fit are given in Table I and agree with previous infrared<sup>8</sup> and corresponding ground-state rotational constants determined from microwave spectroscopy.<sup>9</sup> The standard deviation of the measured wavenumbers was 0.004  $\text{cm}^{-1}$ .

#### ACKNOWLEDGMENTS

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