

THE Q BRANCH OF 21¹0-01¹0 BAND OF N₂O

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The vibration-rotation spectra of N₂O are among the most thoroughly investigated IR spectra in the literature. Recently, the observation made by C. Amiot et al. gave molecular constants with great precision^[1]. There is, however, no information yet on the Q branch of the 21¹0-01¹0 band.

Our measurements were made by using a Laser Analytics model LS-3 tunable diode laser source IR spectrometer. The principle and operation of the apparatus have been described elsewhere^[2]. The gas cell was a multipass White cell with a path length set at 12m, and the N₂O pressure was 1.5 torr. The resulting spectra is shown in Fig. 1. The whole spectra obtained are composed of 4 regions. Between 2577.1 and 2578.8 cm⁻¹, 37 lines of the Q branch were observed, most of which were well separated, while a few lines were mutually overlapping. The half-width of any single line, about 0.006 cm⁻¹, was somewhat broader than the Doppler width.

The calculated and observed line positions are given in Table 1. For the calculation of line positions, the following formulae were used:

$$\begin{aligned} \nu_{c-d} &= \Delta\nu_0 + (B'_c - B'_d)J(J+1) - (D'_c - D'_d)[J(J+1)]^2 \\ &\quad + (H'_c - H'_d)[J(J+1)]^3, \\ \nu_{d-c} &= \Delta\nu_0 + (B'_d - B'_c)J(J+1) - (D'_d - D'_c)[J(J+1)]^2 \\ &\quad + (H'_d - H'_c)[J(J+1)]^3. \end{aligned}$$

The constants *B*, *D*, *H*'s used here are those of Amiot et al. and are given in Table 2.

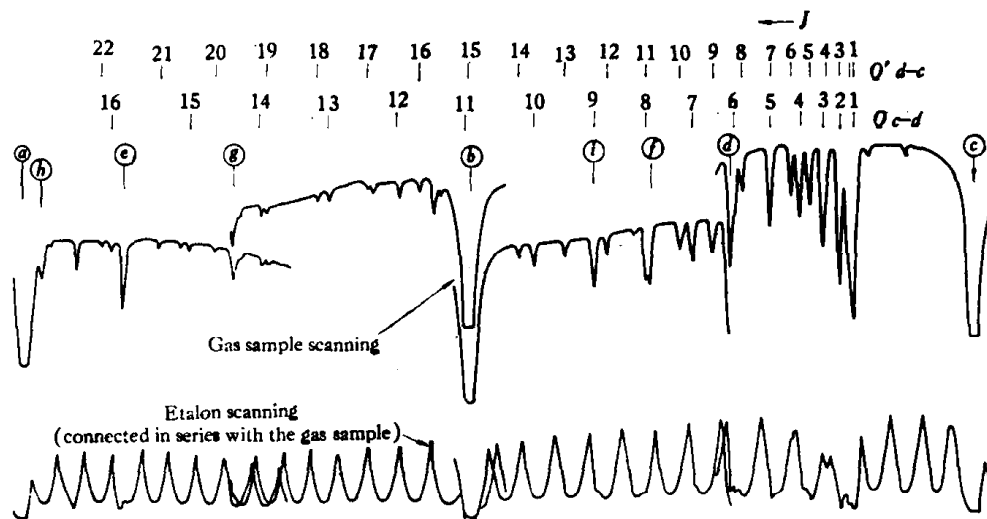


Fig. 1

Table 1

Calculated Value			Observed Value	(C—O)×10 ⁻³ (cm ⁻¹)
$Q(J)$ (c—d band)	$Q'(J)$ (d—c band)	Mean		
$Q(1)$ 2577.0774	$Q'(1)$ 2577.0811	0.0793	0.0803	—1
	$Q(2)$ 0.0721	0.0721	0.0726	—0.5
$Q(2)$ 0.0609	$Q'(3)$ 0.0585	0.0597	0.0605	—0.8
$Q(3)$ 0.0361	$Q'(4)$ 0.0405	0.0383	0.0370	1.3
	$Q'(5)$ 0.0179	0.0179	0.0170	0.9
$Q(4)$ 0.0032		0.0032	0.0021	1.1
	$Q'(6)$ 2576.9908	0.9908	0.9895	1.3
$Q(5)$ 2576.9619	$Q'(7)$ 0.9592	0.9606	0.9607	—1
	$Q'(8)$ 0.9231	0.9231	0.9225	0.6
$Q(6)$ 0.9124		0.9124	0.9107	1.7
	$Q'(9)$ 0.8825	0.8825	0.8854	—2.9
$Q(7)$ 0.8547		0.8547	0.8568	—2.1
	$Q'(10)$ 0.8374	0.8374	0.8391	—1.7
$Q(8)$ 0.7887	$Q'(11)$ 0.7878	0.7883	0.7901	—1.8
	$Q'(12)$ 0.7338	0.7338	0.7347	—0.9
$Q(9)$ 0.7145		(0.7158)	0.7165	—0.7
	$Q'(13)$ 0.6752	0.6752	0.6750	0.2
$Q(10)$ 0.6321		0.6321	0.6298	2.3
	$Q'(14)$ 0.6122	0.6122	0.6090	3.2
$Q(11)$ 0.5414	$Q'(15)$ 0.5447	—	—	—
	$Q'(16)$ 0.4728	0.4728	0.4775	4.7
$Q(12)$ 0.4425		0.4425	0.4455	—0.3
	$Q'(17)$ 0.3964	0.3964	0.3986	—2.2
$Q(13)$ 0.3354		0.3354	0.3357	—0.3
	$Q'(18)$ 0.3155	0.3155	0.3166	—1.1
	$Q'(19)$ 0.2303	0.2303	0.2306	—0.3
$Q(14)$ 0.2200		0.2200	0.2203	—0.3
	$Q'(20)$ 0.1406	0.1406	0.1428	—2.2
$Q(15)$ 0.0964		0.0964	0.0987	—2.3
	$Q'(21)$ 0.0465	0.0465	0.0461	0.4
$Q(16)$ 2575.9646		0.9646	0.9650	—0.4
	$Q'(22)$ 2575.9480	0.9480	0.9482	—0.2

Table 2

Some Spectral Constants of N₂O

Vibration State	B	D	H
21 ¹ °O	0.4158451	1680.4×10 ⁻¹⁰	3.4×10 ⁻¹³
21 ¹ dO	0.4169188	1585.9×10 ⁻¹⁰	6.4×10 ⁻¹³
01 ¹ °O	0.4191775	1785.2×10 ⁻¹⁰	—
01 ¹ dO	0.4199695	1792.2×10 ⁻¹⁰	—

 $\Delta\nu_0$ for transition 21¹°—01¹° = 2577.08563.

Several foreign lines that do not belong to the Q branch are also shown in Fig. 1. They are:

- ② $R(15)$, ⑥ $R(16)$ and ③ $R(17)$ of band $20^{\circ}0-00^{\circ}0$,
- ④ $P(13)$ and ⑤ $P(14)$ of the band $22^{\circ}0-02^{\circ}0$,
- ⑦ $R(34)$ and ⑧ $R(33)$ of the band $30^{\circ}0-10^{\circ}0$,
- ⑨ $P(5)$ and ① $P(4)$ of the band $22^{\circ}0-02^{\circ}0$

Except for the line ① overlapping with $Q(9)$ and the strong line ⑥ covering entirely $Q(11)$ and $Q'(15)$, all the remaining lines are well separated. Lines ④, ⑦, ⑧ and ⑤ are taken as the frequency standards in the four scan regions respectively. Following Amiot, the frequencies corresponding to the above 4 lines are:

- ④ $-2576.9055 \text{ cm}^{-1}$;
- ⑦ $-2576.7951 \text{ cm}^{-1}$;
- ⑧ $-2576.1742 \text{ cm}^{-1}$;
- ⑤ $-2575.9856 \text{ cm}^{-1}$.

In Table 1, the greatest deviation between the calculated and measured line positions is shown to be about $4 \times 10^{-3} \text{ cm}^{-1}$. A single line may be shifted by 0.004 cm^{-1} when measured in different regions. The source of error is due both to the nonlinearity of the laser scan and to the noncoincidence between the sample and etalon scans. On the other hand, we can see that any two adjacent lines always have approximately the same deviation, whether they are in the same band or not. This fact confirms the accuracy of Amiot's work.

REFERENCES

- [1] Amiot, C. & Guelachvili, G., *J. Mol. Spectr.*, **59**(1976), 171—190.
- [2] Nill, K. W., *Laser Focus*, **13** (1977), 2: 32