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VIBRATIONAL AND ROTATIONAL CONSTANTS FOR THE $A^2\ \Sigma^+$ STATE OF THE $^{15}N^{16}O$ MOLECULE*

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The 8 bands of the γ system of the $^{15}N^{16}O$ molecule have been photographed and measured. The vibrational and rotational constants for the $A^2\Sigma^+$ state were obtained and the spin-splitting constant was estimated.

In the course of investigations of the NO molecule a number of the γ system bands $A^2\Sigma^+ - X^2\Pi$ were obtained. Eight of them: 0—3, 0—4, 1—4, 1—5, 1—6, 2—6, 2—7 and 3—4 lying in the region 2600 Å − 2800 Å were measured and analysed. The spectrum was photographed in ninth and tenth orders of the two metre plane-grating PGS-2 spectrograph (VEB Carl Zeiss, Jena), at reciprocal linear dispersion of about 0.4 Å/mm. The light source was an ordinary discharge tube with a quartz window. The tube was filled with a N_2+O_2 mixture (where the nitrogen contained about 95% of the $^{15}N_2$). The thorium lines from a hollow cathode lamp were used as the standard spectrum [1]. A partial analysis of the experimental data was made and the more accurate vibrational and unknown rotational constants for the $A^2\Sigma^+$ state of the $^{15}N^{16}O$ molecule were obtained.

The vibrational constants were found according to the method of Jenkins and McKellar [see, p. 188 [2]], which permits one to eliminate one of two electronic states. Then, by resolving the 77 equations, we obtained the following differences of the vibrational quanta:

$$G(1)-G(0)=2300.6007(67)\ \mathrm{cm}^{-1},\qquad G(3)-G(2)=2237.235(25)\ \mathrm{cm}^{-1},$$
$$G(2)-G(1)=2269.1547(65)\ \mathrm{cm}^{-1},\qquad G(3)-G(0)=6807.046(18)\ \mathrm{cm}^{-1},\qquad (1)$$

and the differences of the rotational constants:

$$B_0-B_1=0.017825(19)\ \mathrm{cm}^{-1},\qquad B_2-B_3=0.017894(32)\ \mathrm{cm}^{-1},$$
$$B_1-B_2=0.017957(19)\ \mathrm{cm}^{-1},\qquad B_0-B_3=0.053676(42)\ \mathrm{cm}^{-1}.\qquad (2)$$

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* Dedicated to Prof. I. Kovács on his 70th birthday

The numbers in parentheses are the standard deviations. The vibrational constants were calculated from obtained values (1). Table I presents them together with their standard deviations. The data in the second column [3] are the values obtained from band heads and they are less accurate. Data in the third column were calculated from isotopic relations which were applied to the best data for the $^{14}N^{16}O$ molecule [4].

The rotational constants were obtained using the combination differences $\Delta_2F(J)$ and the calculated differences of the rotational constants (2). The 290 equations were obtained in this way. The following values were calculated by means of the least squares method:

$$\begin{gathered} B_0=1.91636(11)\,\mathrm{cm}^{-1}, \quad 10^6\cdot D_0=5.132(72)\,\mathrm{cm}^{-1}, \\ 10^6\cdot\Delta D=(D_v-D_{v+1})\cdot 10^6=0.323(72)\,\mathrm{cm}^{-1}, \\ 10^3\cdot\gamma=10^3\cdot\gamma_v=-1.14(38)\,\mathrm{cm}^{-1}. \end{gathered} \tag{3}$$

The rotational constants which are shown in Table II are calculated in the following way:

α_e as a weighted value from data (2) (assuming $\gamma_e=0$);
β_e was assumed to be equal to ΔD;
B_e was obtained from B_0 (data (3)) and α_e, as well as D_e from D_0 and β_e.

Table I

Vibrational constants for $A^2\Sigma^+$ state of the $^{15}N^{16}O$ molecule [cm^{-1}]

Constant	Present results	After [3]	Results from isotopic relations for $^{14}N^{16}O$ After [4]
0	1	2	3
ω_e	2331.61(15)	2331.0(1.1)	2331.85
ω_ex_e	15.380(95)	15.77(39)	15.819
ω_ey_e	−0.076(16)	0*	−0.044

* assumed value

Table II

Rotational constants for $A^2\Sigma^+$ state of the $^{15}N^{16}O$ molecule [cm^{-1}]

Constant	Present results	Results from isotopic relations for $^{14}N^{16}O$	
		After [5]	After [4]
0	1	2	3
B_e	1.91636(11)	1.9269	1.92408
α_e	0.017892(29)	0.0181	0.01736
$10^6\cdot D_e$	5.293(74)	5.8	5
$10^6\cdot\beta_e$	0.323(72)	0.3	0*

* assumed value

Since the constants B_e, α_e, D_e, β_e for the $A^2\Sigma^+$ states of the $^{15}N^{16}O$ molecule are not known they are compared with other ones obtained from isotopic relations. These relations are applied to the best known data for the $^{14}N^{16}O$ molecule [4], [5]. Our spin-splitting constant $10^3 \cdot \gamma = -1.14(38)\,\mathrm{cm}^{-1}$ (assumed to be equal for all vibrational states) is in rough agreement with the results obtained [6—8] for the $^{14}N^{16}O$ molecule.

For the $A^2\Sigma^+$ state of the $^{15}N^{16}O$ molecule the only data available are those of Freedman and Nicholls [8] whose values are as follows:

$$B_1 = 1.895851(95)\,\mathrm{cm}^{-1}, \quad 10^6 \cdot D_1 = 5.488(2800)\,\mathrm{cm}^{-1}$$

$$10^2 \cdot \gamma = -1.303(355)\,\mathrm{cm}^{-1}.$$

The respective values calculated from our data in Table II are:

$$B_1 = 1.89847(11)\,\mathrm{cm}^{-1}, \quad 10^6 \cdot D_1 = 4.808(102)\,\mathrm{cm}^{-1}$$

$$10^3 \cdot \gamma \cong 10^3 \cdot \gamma = -1.14(38)\,\mathrm{cm}^{-1}.$$

It is not clear to us why the agreement is not quite satisfactory.

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References

1. A. Giacchetti, J. Opt. Soc., *60*, 474, 1970.
2. G. Herzberg, Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules, D. Van Nostrand, New York, 1950.
3. H. Cisak, J. Danielak and M. Rytel, Acta Phys. Polon. *A37*, 67, 1970.
4. R. Engleman, Jr., and P. E. Rouse, J. Mol. Spectr. *37*, 240, 1971.
5. I. Deézsi, Acta Phys. Hung., *9*, 125, 1958.
6. T. Bergman and R. N. Zare, J. Chem. Phys., *61*, 4500, 1974.
7. R. Wallenstein and H. Zacharias, Opt. Com., *25*, 363, 1978.
8. R. Freedman and R. W. Nicholls, J. Mol. Spectr. *83*, 223, 1980.