

## Spectrum of the $^{15}\text{N}^{17}\text{O}$ isotopologue in the region of $1.86\ \mu\text{m}$ . Determination of the „Dunham-type“ constants

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The absorption spectrum of the  $^{15}\text{N}^{17}\text{O}$  molecule in the range  $5200\text{--}5500\ \text{cm}^{-1}$  was recorded for the first time using a Bruker IFS-125M Fourier spectrometer with a spectral resolution of  $0.0056\ \text{cm}^{-1}$ . Analysis of the spectrum made it possible to detect the vibration-rotation lines of the 3-0 band of the main transitions in the  $X^2\Pi$  electronic state of the  $^{15}\text{N}^{17}\text{O}$  molecule. For the main transitions  $^2\Pi_{1/2} - ^2\Pi_{1/2}$  and  $^2\Pi_{3/2} - ^2\Pi_{3/2}$ , 149 positions of rotational lines were registered in the three branches with the maximum value of the rotational quantum number  $J = 29.5$ . It was for the first time possible to determine the parameters of  $\Lambda$ -splitting in this band. The positions and relative intensities of both the components of the  $\Lambda$ -doublets and the centers of 31 unresolved doublets were determined. The frequencies of the registered transitions and the transition frequencies in the 1-0 vibrational band, weighted in accordance with experimental uncertainties, were jointly processed using two models. As a result of the processing, spectroscopic parameters were determined for vibrational states  $v = 0, 1, 3$ , as well as „Dunham-type“ constants for the  $^{15}\text{N}^{17}\text{O}$  isotopologue. Using the found „Dunham-type“ constants, model calculations of transition frequencies in vibrational bands 1-0, 2-0, 3-0 up to  $J = 35.5$  were performed. A comparison of the calculated transition frequencies with those given in the Exomol project was made.

**Keywords:**  $^{15}\text{N}^{17}\text{O}$  isotopologue, experimental spectrum, vibration band 3-0, spectroscopic constants, „Dunham-type“ constants.

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A molecule of nitrogen monoxide  $^{14}\text{N}^{16}\text{O}$  is a diatomic stable radical, the spectrum of which is the subject of multiple studies in infrared and microwave areas. The interest in this molecule is caused by its chemical activity, which manifests itself in atmospheric chemistry, burning processes, as well as physiological and pathological processes occurring in live organisms. Nitrogen monoxide is present in the atmosphere of Earth and other planets.

The main electronic state of NO molecule is a doublet  $^2\Pi$ , made of two components  $^2\Pi_{1/2}$  and  $^2\Pi_{3/2}$ , having a total electronic angular momentum relative to the internuclear axis, designated as  $\Omega$ ,  $\Omega = |\Lambda + \Sigma|$  and equal to  $1/2$  and  $3/2$  accordingly. Doublet split into two components occurs due to spin-orbit interaction. Each component of the doublet, in its turn, remains doubly degenerate by sign  $\Lambda$  (projection of orbital angular momentum onto the internuclear axis of the molecule), the so called  $\Lambda$ -doubling. The vibrational-rotational spectrum of the molecule in this case consists as though of two: the spectrum for the state  $^2\Pi_{1/2}$  and the spectrum for the state  $^2\Pi_{3/2}$ . Besides, apart from transitions  $^2\Pi_{1/2} \rightarrow ^2\Pi_{1/2}$ ,  $^2\Pi_{3/2} \rightarrow ^2\Pi_{3/2}$  within the states called the main bands, there are transitions observed between the components  $^2\Pi_{1/2} \leftrightarrow ^2\Pi_{3/2}$ , which are called the satellite bands.

This paper is the continuation of the studies of nitrogen monoxide and its isotopologues spectra [1–4]. The review of the literature on experimental studies of infrared spectra

of nitrogen monoxide isotopologues may be found in the papers [1,2,5–8]. The studies of the isotopologue spectra are rather scarce, and for the isotopologue  $^{15}\text{N}^{17}\text{O}$  there is only one paper known in the  $5.4\ \mu\text{m}$  range [5]. In this paper the spectrum of the fundamental band (1-0) of this isotopologue was recorded in the Fourier-spectrometer with resolution  $2.7 \cdot 10^{-3}\ \text{cm}^{-1}$  at pressure 1.35 Torr. The authors were able to resolve  $\Lambda$ -doublets and define the spectroscopic constants for vibrational states  $v = 0, 1$ . In the known base of spectroscopic information, HITRAN, there is data for the NO molecule only for three isotopologues  $^{14}\text{N}^{16}\text{O}$ ,  $^{15}\text{N}^{16}\text{O}$  and  $^{14}\text{N}^{18}\text{O}$  with the natural abundance of 0.993974, 0.003654 and 0.001093, accordingly. The data calculated using the parameters of spectral lines for the isotopologue  $^{15}\text{N}^{17}\text{O}$  may be found only in the ExoMol project [6], where the authors specify the list of the lines „NOname“, representing the extensive variational calculations for six isotopologues of this molecule. To calculate the energy levels, the project uses the combination of two methods: the method of effective Hamiltonians and the variation method.

The objective of this paper is to determine the parameters of Dunham type for the isotopologue  $^{15}\text{N}^{17}\text{O}$  using the new experimental data in  $1.86\ \mu\text{m}$  range and their use for the simulation of the spectrum of this molecule.

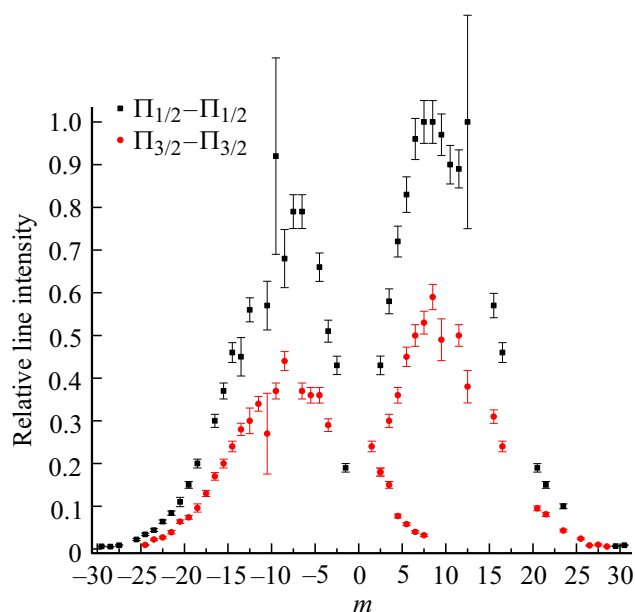
## Experiment

To study the spectrum of nitrogen monoxide, a mixture from IZOTOP company was chosen, which is represented by two isotopologues: 80%  $^{15}\text{N}^{18}\text{O}$  and 20%  $^{14}\text{N}^{16}\text{O}$ . As a result of isotope exchange all six isotopologues of nitrogen monoxide are produced in such mix. The absorption spectrum of nitrogen oxide was recorded in the range of  $4000\text{--}7000\text{ cm}^{-1}$  with the help of Fourier spectrometer Bruker IFS-125M with the spectral resolution  $0.0056\text{ cm}^{-1}$ . To achieve the full optical path of  $2400\text{ cm}$ , a multi-way cuvette with length of  $60\text{ cm}$  was used. The spectrometer was equipped with a halogen lamp as a source of light, germanium photodetector and beam splitter from  $\text{CaF}_2$ . The sample pressure was measured by sensor AIR-20/M2-N with accuracy of  $0.03\text{ mbar}$ . The averaged interference pattern was considered by the Merz phase correction method with phase resolution of  $1\text{ cm}^{-1}$ . The triangular apodization was used. Thermal stabilization of the room made it possible to perform long-term recording. Signal-to-noise ratio in the recorded spectra was about 650 for strong lines. The absorption spectrum of nitrogen oxide was recorded at temperature of  $297 \pm 1\text{ K}$  and gas pressure of  $16\text{ mbar}$ . The spectrum was calibrated along the lines of water vapor present in the mixture as an admixture. The calibration accuracy was  $0.0014\text{ cm}^{-1}$ .

## Methods and results

### Determination of the spectral lines parameters

The recorded spectrum was analyzed in the in the range  $5200\text{--}5500\text{ cm}^{-1}$ , where the vibrational-rotational lines of the band  $3\text{-}0$  were first found for the main transitions between the electron states  $^2\Pi_{1/2}$  and  $^2\Pi_{3/2}$  of the molecule  $^{15}\text{N}^{17}\text{O}$ . The lines of these bands were identified on the basis of the calculated data presented in the ExoMol project [6]. To determine the parameters of the line, MultiFit software [9] was used with the Voigt model for the line contour. For the molecule  $^{15}\text{N}^{17}\text{O}$  the total 149 positions of rotational lines were recorded in the three branches of the main subbands  $^2\Pi_{1/2}\text{--}^2\Pi_{1/2}$  and  $^2\Pi_{3/2}\text{--}^2\Pi_{3/2}$ . The maximum value of the rotational quantum number  $J$  was 29.5. All  $\Lambda$ -doublets in the recorded spectrum were not spectrally resolved. For the majority of them in the case when the split was more than  $4.5 \cdot 10^{-3}\text{ cm}^{-1}$ , it was possible to obtain the positions and relative intensities of each component of the doublet, while, the self-broadening parameter was fixed by the value from HITRAN [8] for the main isotopologue, and intensities of the components „e“ and „f“ were deemed equal. The number of the remaining unresolved  $\Lambda$ -doublets was 31, and for them the positions of the center and the total intensity of the doublet were found. We neglected the shift of the line position by pressure, taking into account the smallness of the full mix pressure. Therefore, the analysis defined the positions (transition frequencies  $\nu_{\text{obs}}$ ) 149 of spectral lines



**Figure 1.** Dependence of the experimental relative intensities of lines on rotational quantum number  $m$ . The parameter  $m$  adopts values  $-J$ ,  $J$  and  $J + 1$  for  $P$ -,  $Q$ - and  $R$ -branches accordingly.

and their relative intensities for the molecule  $^{15}\text{N}^{17}\text{O}$  (A1, Appendix). In the table the transition frequencies are given in units  $\text{cm}^{-1}$ , since the spectroscopy widely uses the wave number of energy level  $\tilde{E} = E/hc$  ( $\text{cm}^{-1}$ ). The same table presents our estimates of the error for the positions of the lines  $\Delta\nu_{\text{obs}}$  and relative intensities  $\Delta I_{\text{obs}}$ . Absolute intensities were not defined, since the value of the partial pressure of the considered isotopologue is not known. The distribution of the relative intensities of the lines in branches in the observed spectrum is illustrated by Fig. 1.

### Determination of the spectroscopic parameters of the vibrational state $v = 3$ and parameters of „Dunham type“

In the laboratory of theoretical spectroscopy of the Institute of Atmospheric Optics of the Siberian Branch of the Russian Academy of Sciences the software was developed, making it possible on the basis of the model of effective Hamiltonians for various electronic states of stable diatomic radicals [1] to process the experimental energy levels, and the transition frequencies in the individual vibrational bands or a system of bands. As a result of such processing, the spectroscopic parameters of vibrational states, or the molecular constants of „Dunham type“ for individual electronic states of the considered molecule, are defined. The molecular constants of „Dunham type“ found in this way make it possible to simulate the spectrum of radicals in the ranges that are experimentally unknown as of today. The software was based on the effective Brown Hamiltonian [10], which describes the spin-orbit and spin-rotational interactions.

**Table 1.** Spectroscopic parameters for the vibrational states  $v = 0, 1, 3$  in the molecule  $^{15}\text{N}^{17}\text{O}$  ( $\text{cm}^{-1}$ )

Parameter	State $v = 0$	State $v = 1$	State $v = 3$	State $v = 2$ Calculation <sup>c</sup>
$T$	58.3952739 <i>0</i>	1875.177691(16) <i>1816.766455(88)</i>	5429.81843(17)	3665.6519
$A$	123.13744 <sup>a</sup> <i>123.13744</i>	122.901029(24) <i>122.90102(14)</i>	122.39989(29)	122.6549
$A_d \cdot 10^4$	1.624(10) <sup>b</sup> <i>1.496(26)</i>	1.550(9) <i>1.453(26)</i>	1.369(13)	1.460
$B$	1.58950546(78) <i>1.5895337(24)</i>	1.57357029(78) <i>1.5735982(52)</i>	1.5416150(12)	1.55761
$D \cdot 10^6$	4.7984(27) <i>4.785(18)</i>	4.8139(22) <i>4.804(14)</i>	4.8432(25)	4.8299
$p \cdot 10^3$	10.59(2) <i>10.52(11)</i>	10.58(2) <i>10.51(12)</i>	10.564(26)	10.570
$q \cdot 10^6$	83.465 <sup>a</sup> <i>83.465</i>	81.09(30) <i>1.1(16)</i>	79.84(98)	80.92
$q_d \cdot 10^8$				-1.595

Note. The italic font is used to identify the spectroscopic constants from the paper [5].

<sup>a</sup> Effective constants  $A$  and  $q$  for the ground state were fixed by the values taken from [5].

<sup>b</sup> The parameter  $\gamma$  was fixed by zero, since  $A_d$  and  $\gamma$  are dependent.

<sup>c</sup> The calculation of the authors is made from the found molecular constants of „Dunham type“.

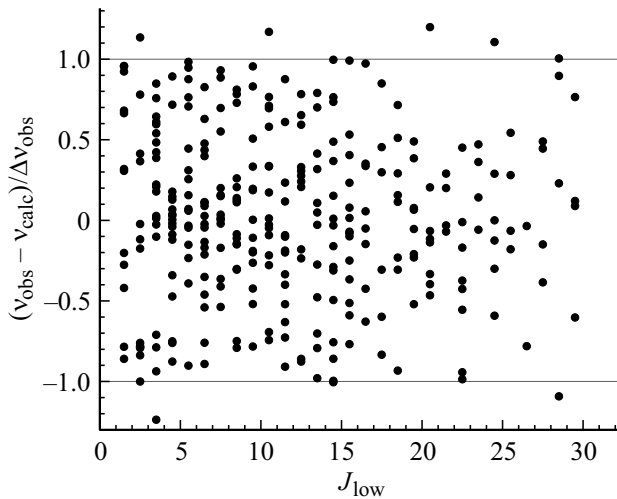
The experimental values of the transition frequencies in the vibrational band 1-0 [5] and the new experimental data on the transition frequencies in the band 3-0 were used to model the values of the energy levels of the isotopologue  $^{15}\text{N}^{17}\text{O}$ . To process the data, the file was made comprising 306 transition frequencies. It included 126 values of the transition frequencies from the vibrational band 1-0 [5], 118 values of the transition frequencies for the resolved  $\Lambda$ -doublets and doubled values of the frequencies of unresolved doublets from the band 3-0. All data included in the file that are weighted in accordance with the experimental errors were processed by the software code using the non-linear least square method. The experimental error of the transition frequencies in the band 1-0 varied within  $(0.1-1) \cdot 10^{-3} \text{ cm}^{-1}$ . The experimental error that we assessed for the frequencies of resolved  $\Lambda$ -doublets in the band 3-0 varied within  $(0.15-2) \cdot 10^{-3} \text{ cm}^{-1}$ , and for the frequencies of unresolved doublets was equal to  $4 \cdot 10^{-3} \text{ cm}^{-1}$ . The wave numbers of the vibrational-rotational energy levels for the electron state  $^2\Pi$  were found by diagonalization of the effective Hamiltonian matrix for the lower and upper vibrational states. First, the developed file of the transition frequencies was used to find the spectroscopic parameters of the vibrational states  $v = 0, 1, 3$ . Such processing with the standard deviation of 0.57 made it possible to determine 18 spectroscopic parameters for the specified three states. The found values of the parameters and their comparison with the ones known in the literature are given in Table 1.

As one can see from Table 1, the obtained spectroscopic parameters for  $v = 0, 1$  are well matched with the ones

given in [5]. For the vibrational parameter  $T$  there is a difference related to selection of the lower energy level value, from which the count is taken. Absence of data on the frequencies of satellite transitions prevented us, as well as the authors of the paper [5], from determining the parameter of the spin-orbit interaction  $A$  for this isotopologue. Therefore, this parameter was fixed by the value taken from the paper [5], where it was recalculated on the basis of the isotopic ratios from the value for the main isotopologue. The same was done for the parameter of the spin-rotational interaction  $q$ . Its value was fixed and recalculated from the value for the main isotopologue [5]. The found spectroscopic parameters recover the known experimental data within the limits of the specified experimental accuracy, but prevent from making prediction calculations in the intervals that are not available for the experiment. Such simulation would require molecular constants of „Dunham type“ when the spectroscopic parameters of the effective Hamiltonian are represented in the form of a series by the vibrational quantum number ( $v + 1/2$ ):

$$P_v = \sum_{i=0} Y_i (v + 1/2)^i,$$

where the coefficients of „Dunham type“  $Y_i$  are determined for each parameter  $P_v$ , and  $i$  determines the degree of polynomial. Therefore, the composed file of experimental frequencies was processed in accordance with the model using molecular constants of „Dunham type“. As a result of this processing with the standard deviation of 0.55, 16 molecular constants of „Dunham type“ were defined for the isotopologue  $^{15}\text{N}^{17}\text{O}$ . The found constants and their



**Figure 2.** Dependence of the relative deviations  $(\nu_{\text{obs}} - \nu_{\text{calc}}) / \Delta \nu_{\text{obs}}$  for the transition frequencies from the rotational quantum number of the lower vibrational state  $J_{\text{low}}$ .

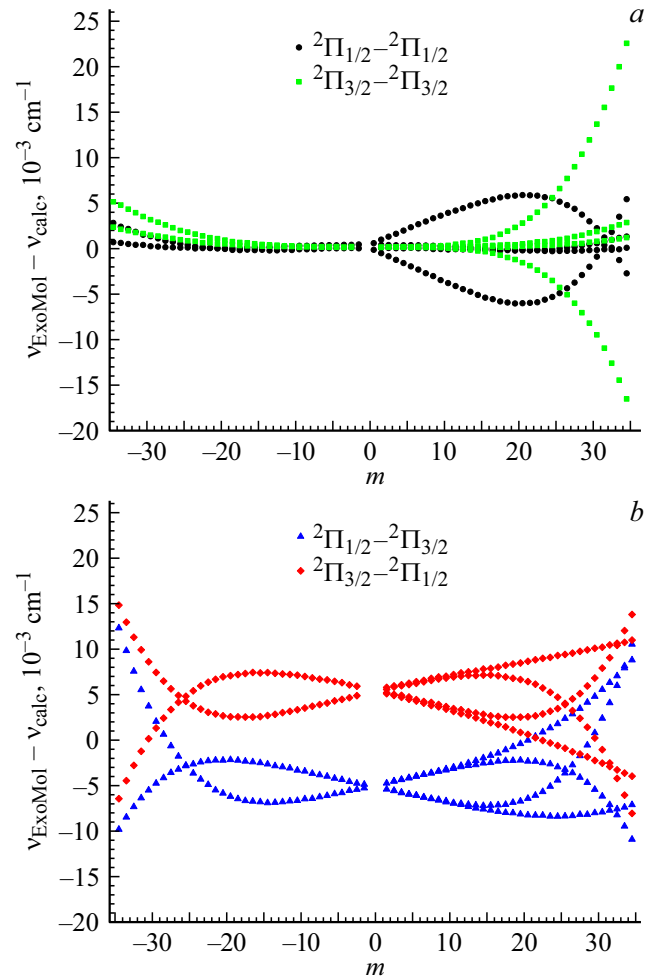
**Table 2.** Molecular constants of „Dunham type“ ( $\text{cm}^{-1}$ ) for  $^{15}\text{N}^{17}\text{O}$   $0 \leq v \leq 3$

Parameter	1	$(v + 1/2)$	$(v + 1/2)^2$
$G_V$	-859.8615538	1843.090487(55)	-13.154034(26)
$A_V$	123.25191 <sup>a</sup>	-0.22692(11) -0.22748(59) -0.22654(61)*	$-4.749(49) \cdot 10^{-3}$ $-4.749(49) \cdot 10^{-3}$ $-4.79(23) \cdot 10^{-3}$
$A_{VD} \cdot 10^5$	16.48(11)	-0.627(44)	-0.050(16)
$B_V$	1.59746256(75) 1.5974790(101) 1.5974795(84)*	-0.01590712(27) -0.0158992(117) -0.158991(135)*	$-1.403(13) \cdot 10^{-5}$ $-1.83 \cdot 10^{-5}$ $-1.83(44) \cdot 10^{-5}$
$D_V \cdot 10^6$	4.7917(25) 4.7755(90) 4.7954(88)*	$1.527(47) \cdot 10^{-2}$ $1.90(78) \cdot 10^{-2}$ $1.39(75) \cdot 10^{-2}$	
$p_V \cdot 10^2$	1.0597(21)	-0.00105(17)	
$q_V \cdot 10^5$	8.384 <sup>a</sup>	-0.117(28)	
$q_{VD} \cdot 10^8$	-1.59(42)		

*Note.* The italic font highlights the values of constants found in the paper [5], the asterisk (\*) marks the values of the same paper calculated using the isotopic ratios. The equilibrium constant  $A_e$  of spin-orbit interaction was fixed by the value for the main isotopologue [5]. The equilibrium value of the constant of  $q_e$  was fixed and recalculated using isotopic ratios from the value for the main isotopologue [2].

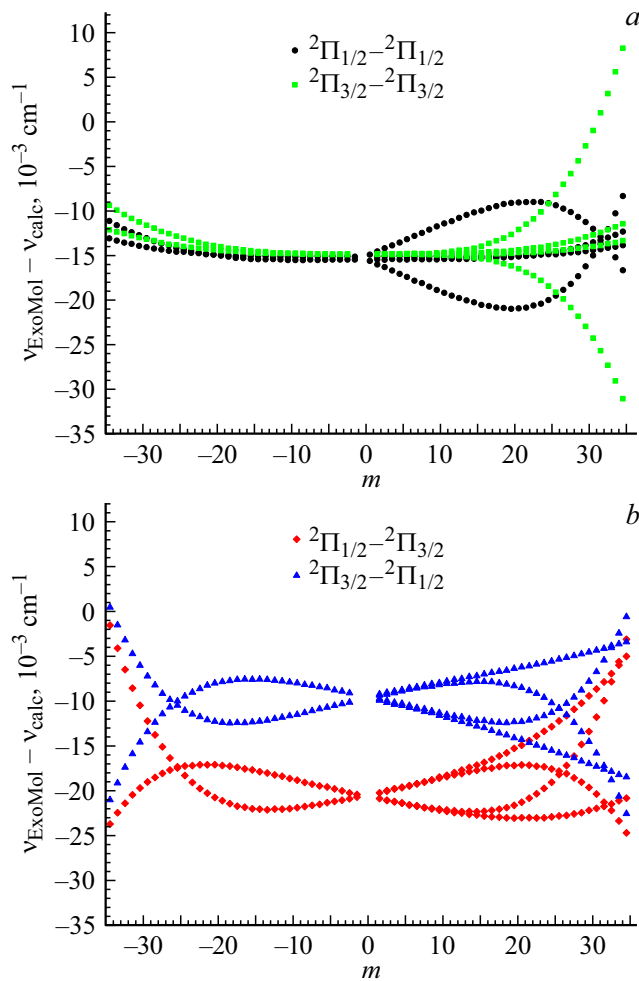
<sup>a</sup> See notes to Table 1.

comparison with the ones published in [5] are given in Table 2. It should be noted that the values of constants of „Dunham type“ from Table 2 are well matched between each other. The value of the equilibrium constant of spin-orbit interaction  $A_e$  is fixed by the value for the main isotopologue [5]. The equilibrium value of the constant of  $\Lambda$ -doubling  $q_e$  was also fixed and recalculated using isotopic ratios from the value for the main isotopologue [2].



**Figure 3.** Deviations of the values calculated in this paper for the transition frequencies in the vibrational band 3-0 from the ones given in [6]; the parameter  $m$  takes the values  $-J, J$  and  $J + 1$  for  $P$ -,  $Q$ - and  $R$ -branches, accordingly:  $a$  — for the main bands  ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{1/2}$ ,  ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{3/2}$ ;  $b$  — for the satellite bands  ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{3/2}$ ,  ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{1/2}$ .

The quality of processing is demonstrated by Fig. 2, which presents the dependence of the relative deviations for the transition frequencies  $(\nu_{\text{obs}} - \nu_{\text{calc}}) / \Delta \nu_{\text{obs}}$  from the rotational quantum number  $J$  of the lower vibrational state  $J_{\text{low}}$ . From Fig. 2 one can see that the relative deviation of the calculated transition frequencies exceeds one only for six lines from the vibrational band 3-0, and this means that the found constants of „Dunham type“ recover the experimental data within the experimental accuracy. The found molecular constant of „Dunham type“ made it possible to perform model interpolation calculations of energy levels in the vibrational state  $v = 2$  and to accordingly calculate the transition frequencies in the vibrational band 2-0 for the electronic states  ${}^2\Pi_{1/2}$  and  ${}^2\Pi_{3/2}$  with account of  $\Lambda$ -doubling for the isotopologue  $^{15}\text{N}^{17}\text{O}$ . Using the found constants of „Dunham type“ we also calculated the spectroscopic parameters for the vibrational state  $v = 2$ . These data are given in Table 1. Fig. 3 and 4 show the comparison of



**Figure 4.** Deviations of the values calculated in this paper for the transition frequencies in the vibrational band 2-0 from the ones given in [6]; the parameter  $m$  takes the values  $-J, J$  and  $J + 1$  for  $P$ -,  $Q$ - and  $R$ -branches, accordingly: *a* — for the main bands  ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{1/2}$ ,  ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{3/2}$ ; *b* — for the satellite bands  ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{3/2}$ ,  ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{1/2}$ .

the calculated values of the transition frequencies obtained in this paper with the values from the ExoMol project [6] for the vibrational band 3-0 and for the band 2-0 predicted with the help of the found constants of „Dunham type“. The comparative calculation was given to  $J = 35.5$ , which by five values exceeds the value of the rotational quantum number of the last observed energetic level. The differences between the two calculations for the main transitions (Fig. 3, *a*) in the band 3-0, exceeding experimental errors, are observed only for the transition frequencies in  $Q$ -branch and become substantial for the transitions with  $J \geq 28.5$ . For the satellite transitions in the same band (Fig. 3, *b*), apart from deviations in  $Q$ -branch, there is a systematic shift of the line positions by the value  $\sim 0.005\ \text{cm}^{-1}$ . This shift is explained by the difference in the values of constants of spin-orbit interaction  $A_e$ , used in this paper and the ExoMol project [6]. Deviations in  $Q$ -branch for the main and satellite transitions are related to the accuracy of

determination of the spin-rotational interaction constants  $p_V$  and  $q_V$ . For more accurate determination of these constants, the experimental data on the frequencies of resolved  $\Lambda$ -doublets in  $Q$ -branch, where  $\Lambda$ -doubling manifests itself most evidently, are not sufficient. In the ExoMol project [6] for calculation of  $\Lambda$ -doubling in the transition frequencies of various isotopologues, isotope-independent constants of „Dunham type“ are used, which are determined on the basis of the known experimental data by  $\Lambda$ -split for the main isotopologue. For the molecule  ${}^{14}\text{N}^{16}\text{O}$  spin-rotational split was observed only in  $Q$ -branch of the vibrational band 3-0 ( $J_{\text{max}} = 2.5$ ) [11], and also in branches  $P$  and  $R$  of the band 3-1 of the main transitions to  $J_{\text{max}} = 16.5$  [12]. Such experimental information is obviously insufficient for the precise determination of the parameters of spin-rotational interaction in the vibrational band 3-0. Fig. 4 shows the comparison of our predictive calculations of the transition frequencies in the band 2-0, made using the found constants of „Dunham type“, with the calculations from the ExoMol project [6]. The calculations in this vibrational band are characterized by the same differences as for the band 3-0, i.e. the differences arising from using various values of the constant of spin-rotational interaction, and the differences related to the insufficient accuracy of spin-orbit interaction parameter determination. It should be noted that for the predicted band 2-0 (Fig. 4, *a, b*) there is also systematic shift of  $0.015\ \text{cm}^{-1}$ , which is determined by the accuracy of parameter  $G_V$  for this band.

## Conclusion

This paper for the first time registered the spectrum of molecule  ${}^{15}\text{N}^{17}\text{O}$  in range of  $5200\text{--}5500\ \text{cm}^{-1}$ , and its analysis was performed. The analysis found 149 vibrational-rotational lines presenting  $\Lambda$ -doublets in the band 3-0 of the main transitions between electronic states  ${}^2\Pi_{1/2}$  and  ${}^2\Pi_{3/2}$  with the maximum value of the rotational quantum number  $J = 29.5$ . For the first time the parameters of  $\Lambda$ -split were determined in this band. The positions and relative intensities were determined for the individual components of  $\Lambda$ -doublets and for the centers of 31 unresolved doublets. All values are presented in Table A1 (Appendix). The joint weighted processing of the transition frequencies was performed in the vibrational band 1-0 [5] and frequencies of registered transitions using two models. As a result, the spectroscopic parameters were determined for the vibrational states  $v = 0, 1, 3$ , and also the constants „of Dunham type“ for the isotopologue  ${}^{15}\text{N}^{17}\text{O}$ . The found constants of „Dunham type“ were used for model calculations of the transition frequencies in the vibrational bands 1-0, 2-0, 3-0 to  $J = 35.5$ . The calculated transition frequencies were compared to the ones given in the ExoMol project [6].

## Appendix

Table A1. Parameters of molecule band 3-0 lines  $^{15}\text{N}^{17}\text{O}$ 

Identification			$\nu_{\text{obs}}, \text{cm}^{-1}$			$\nu_{\text{obs}} - \nu_{\text{calc}}, 10^{-3} \text{cm}^{-1}$		Relative $I_{\text{obs}}$	
$\Omega$	Branch	$J_{\text{low}}$	$e$	$f$	$\Delta\nu_{\text{obs}} \cdot 10^3$	$e$	$f$	$e/f^a$	$\Delta I_{\text{obs}}, \%$
1/2	P	1.5	5366.9992	5366.9896	4.0	2.70	3.81	1.9E-01	5.3
1/2	P	2.5	5363.7185	5363.7101	1.5	-1.15	1.20	4.3E-01	5.0
1/2	P	3.5	5360.3497	5360.3390	1.5	0.34	0.33	5.1E-01	5.0
1/2	P	4.5	5356.8859	5356.8748	1.5	0.31	-0.23	6.6E-01	5.0
1/2	P	6.5	5349.6779	5349.6671	1.5	0.21	-0.24	7.9E-01	5.0
1/2	P	7.5	5345.9338	5345.9233	1.5	0.22	-0.04	7.9E-01	5.0
1/2	P	8.5	5342.0963	5342.0863	2.0*	0.42	0.50	6.8E-01	10.0
1/2	P	9.5	5338.1657	5338.1544	2.0*	1.04	-0.39	9.2E-01	25.0
1/2	P	10.5	5334.1411	5334.1326	2.0*	1.23	2.31	5.7E-01	10.0
1/2	P	12.5	5325.8101	5325.8009	1.5	0.41	0.33	5.6E-01	5.0
1/2	P	13.5	5321.5042	5321.4955	2.0*	-0.12	0.14	4.5E-01	10.0
1/2	P	14.5	5317.1054	5317.0962	1.5	0.15	-0.45	4.6E-01	5.0
1/2	P	15.5	5312.6125	5312.6039	1.5	0.03	-0.38	3.7E-01	5.1
1/2	P	16.5	5308.0261	5308.0181	1.5	-0.12	-0.21	3.0E-01	5.1
1/2	P	18.5	5298.5730	5298.5653	1.5	0.17	-0.28	2.0E-01	5.2
1/2	P	19.5	5293.7056	5293.6986	1.5	-0.06	-0.26	1.5E-01	5.3
1/2	P	20.5	5288.7449	5288.7391	2.0*	-0.08	0.40	1.1E-01	5.6
1/2	P	21.5	5283.6908	5283.6848	1.5	-0.02	-0.13	8.4E-02	5.9
1/2	P	22.5	5278.5429	5278.5376	1.5	-0.25	0.00	6.4E-02	6.3
1/2	P	23.5	5273.3019	5273.2974	1.5	-0.06	0.51	4.4E-02	7.2
1/2	P	24.5	5267.9672	5267.9631	1.5	-0.17	0.41	3.4E-02	7.9
1/2	P	25.5	5262.5393	5262.5359	1.5	-0.11	0.82	2.2E-02	11.2
1/2	P	27.5	5251.4019		4.0	-1.52	1.98	8.4E-03	19.4
1/2	P	28.5	5245.6965		4.0	0.88	3.98	5.3E-03	14.8
1/2	P	29.5	5239.8949		4.0	0.35	3.05	5.9E-03	14.5
1/2	R	1.5	5379.1580	5379.1689	1.5	-0.55	-0.27	4.3E-01	5.1
1/2	R	2.5	5381.9678	5381.9785	1.5	-0.26	0.03	5.8E-01	5.0
1/2	R	3.5	5384.6839	5384.6945	1.5	0.01	0.25	7.2E-01	5.0
1/2	R	4.5	5387.3055	5387.3151	1.5	-0.54	-1.06	8.3E-01	5.0
1/2	R	5.5	5389.8343	5389.8449	1.5	-0.07	0.53	9.6E-01	5.0
1/2	R	6.5	5392.2686	5392.2788	1.5	-0.32	0.05	1.0E+00	5.0
1/2	R	7.5	5394.6091	5394.6191	1.5	-0.32	0.00	1.0E+00	5.0
1/2	R	8.5	5396.8553	5396.8651	1.5	-0.46	-0.19	9.7E-01	5.0
1/2	R	9.5	5399.0082	5399.0173	1.5	0.25	0.03	9.0E-01	5.0
1/2	R	10.5	5401.0656	5401.0749	1.5	-0.06	0.02	8.9E-01	5.0
1/2	R	11.5	5403.0278	5403.0381	1.5	-1.10	0.18	1.0E+00	5.0
1/2	R	14.5	5408.3495	5408.3581	1.5	-0.04	0.04	5.7E-01	5.0
1/2	R	15.5	5409.9327	5409.9411	1.5	-0.08	-0.13	4.6E-01	5.0
1/2	R	19.5	5415.3093	5415.3168	1.5	0.11	-0.32	1.9E-01	5.2
1/2	R	20.5	5416.4129	5416.4207	1.5	-0.23	-0.24	1.5E-01	5.3
1/2	R	22.5	5418.3304	5418.3382	1.5	-0.59	-0.61	1.0E-01	5.7
1/2	R	28.5	5421.7545	5421.7544	4.0	3.63	-4.36	6.6E-03	14.1
1/2	R	29.5	5421.9758	5421.9864	4.0	-2.40	0.24	8.6E-03	13.1
3/2	P	3.5	5359.3888		4.0	-0.02	0.08	2.9E-01	5.1
3/2	P	4.5	5355.8260		4.0	0.00	0.30	3.6E-01	5.1
3/2	P	5.5	5352.1663		4.0	0.21	0.61	3.6E-01	5.1
3/2	P	6.5	5348.4092		4.0	-0.10	0.50	3.7E-01	5.1
3/2	P	8.5	5340.6057		4.0	-0.37	0.53	4.4E-01	5.1
3/2	P	9.5	5336.5598		4.0	-0.39	0.71	3.7E-01	5.1
3/2	P	10.5	5332.4183		4.0*	-0.07	1.33	2.7E-01	35.1
3/2	P	11.5	5328.1801		4.0	-0.80	0.90	3.4E-01	5.1
3/2	P	12.5	5323.8472		4.0*	-0.72	1.28	3.0E-01	10.1
3/2	P	13.5	5319.4186		4.0	-1.06	1.34	2.8E-01	5.1
3/2	P	14.5	5314.8952		4.0	-1.19	1.51	2.4E-01	5.2

Table P1. Continuation

Identification			$\nu_{\text{obs}}, \text{cm}^{-1}$			$\nu_{\text{obs}} - \nu_{\text{calc}}, 10^{-3} \text{cm}^{-1}$		Relative $I_{\text{obs}}$	
$\Omega$	Branch	$J_{\text{low}}$	<i>e</i>	<i>f</i>	$\Delta\nu_{\text{obs}} \cdot 10^3$	<i>e</i>	<i>f</i>	<i>e/f</i> <sup>a</sup>	$\Delta I_{\text{obs}}, \%$
3/2	<i>P</i>	15.5	5310.2769		4.0	-1.46	1.64	2.0E-01	5.2
3/2	<i>P</i>	16.5	5305.5678	5305.5627	2.2	2.13	0.48	1.7E-01	5.3
3/2	<i>P</i>	17.5	5300.7592	5300.7542	1.5	0.73	-0.49	1.3E-01	5.4
3/2	<i>P</i>	18.5	5295.8573	5295.8533	1.5*	0.15	0.37	9.6E-02	10.7
3/2	<i>P</i>	19.5	5290.8624	5290.8571	1.5	0.71	0.07	7.4E-02	6.1
3/2	<i>P</i>	20.5	5285.7741	5285.7665	1.5	1.78	-0.68	6.4E-02	6.3
3/2	<i>P</i>	21.5	5280.5895	5280.5841	1.5*	0.29	0.39	3.9E-02	10.5
3/2	<i>P</i>	22.5	5275.3111	5275.3026	1.5*	-1.40	-3.90	2.7E-02	10.7
3/2	<i>P</i>	23.5	5269.9431	5269.9362	1.5	0.69	0.20	2.2E-02	9.5
3/2	<i>P</i>	24.5	5264.4775	5264.4749	2.5	-1.47	2.77	9.2E-03	12.9
3/2	<i>Q</i>	1.5	5370.9071		4.0	0.02	0.12	2.4E-01	5.1
3/2	<i>Q</i>	2.5	5370.6621		4.0	0.25	0.45	1.8E-01	5.3
3/2	<i>Q</i>	3.5	5370.3193		4.0	0.50	1.00	1.5E-01	5.3
3/2	<i>Q</i>	4.5	5369.8774		4.0	-0.43	0.57	7.7E-02	6.0
3/2	<i>Q</i>	5.5	5369.3382		4.0	-0.64	0.96	5.8E-02	6.5
3/2	<i>Q</i>	6.5	5368.7012		4.0	-0.83	1.67	4.0E-02	7.4
3/2	<i>Q</i>	7.5	5367.9675	5367.9639	1.5	-0.04	0.18	3.2E-02	8.1
3/2	<i>R</i>	1.5	5378.7149		4.0	0.35	0.25	1.8E-01	5.2
3/2	<i>R</i>	2.5	5381.5918		4.0	0.20	0.10	3.0E-01	5.1
3/2	<i>R</i>	3.5	5384.3700		4.0	0.15	-0.05	3.6E-01	5.1
3/2	<i>R</i>	4.5	5387.0494		4.0	0.13	-0.17	4.5E-01	5.0
3/2	<i>R</i>	5.5	5389.6298		4.0	0.27	-0.13	5.0E-01	5.0
3/2	<i>R</i>	6.5	5392.1109		4.0	0.41	-0.19	5.3E-01	5.0
3/2	<i>R</i>	7.5	5394.4930		4.0	0.85	0.15	5.9E-01	5.0
3/2	<i>R</i>	8.5	5396.7748		4.0*	0.36	-0.34	4.9E-01	10.0
3/2	<i>R</i>	10.5	5401.0404		4.0	0.75	-0.35	5.0E-01	5.0
3/2	<i>R</i>	11.5	5403.0223		4.0*	-0.43	-1.63	3.8E-01	10.1
3/2	<i>R</i>	14.5	5408.3704	5408.3742	1.5	-1.45	0.71	3.1E-01	5.1
3/2	<i>R</i>	15.5	5409.9539	5409.9568	1.5	-0.94	0.29	2.4E-01	5.2
3/2	<i>R</i>	19.5	5415.2841	5415.2847	1.5	0.58	-0.77	9.5E-02	5.7
3/2	<i>R</i>	20.5	5416.3642	5416.3661	1.5	-0.52	-0.57	8.1E-02	5.9
3/2	<i>R</i>	22.5	5418.2261	5418.2266	1.5	0.74	-0.83	4.3E-02	7.2
3/2	<i>R</i>	24.5	5419.6831	5419.6855	1.5	-0.51	-0.04	2.4E-02	9.1
3/2	<i>R</i>	25.5	5420.2619	5420.2631	1.5	0.36	-0.33	8.2E-03	13.3
3/2	<i>R</i>	26.5	5420.7370	5420.7403	2.0*	-1.60	-0.15	1.0E-02	15.5
3/2	<i>R</i>	27.5	5421.1145	5421.1171	1.5	-0.19	0.68	5.6E-03	14.6

Note. \* Overlapping lines.

<sup>a</sup> For the split doublets there is intensity of one component (intensity of components „*e*“ and „*f*“ are equal), and for the non-split doublets the half-intensity of the doublet was provided.

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## Conflict of interest

The authors declare that they have no conflict of interest.

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