

Selection of optimal frequencies near $\lambda = 4.5 \mu\text{m}$ for detecting nitrous oxide (N_2O) absorption in the atmosphere

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The absorption spectra of N_2O , H_2O vapor, CO , and CO_2 isotopes were analyzed in the spectral range $\lambda = 4\text{--}5 \mu\text{m}$, where a strong absorption band ν_3 of N_2O centered at $\sim 2225 \text{ cm}^{-1}$ is located. To measure the absorption of N_2O in a real atmosphere in the presence of absorption of interfering atmospheric gases (H_2O vapor, CO , $^{12}\text{CO}_2$, $^{13}\text{CO}_2$), a number of N_2O absorption lines near $\lambda = 4.5 \mu\text{m}$ (vibrational-rotational band ν_3) and the corresponding radiation frequencies were selected, where the relative influence of the absorption of interfering atmospheric gases is minimal and amounts to no more than 2.2 %. For practical use, three optimal frequencies of rotational absorption lines in the ν_3 N_2O band near $4.5 \mu\text{m}$ are recommended, where the maximum sensitivity of N_2O detection is achieved with a minimum relative influence of the absorption of interfering atmospheric gases: 2234.01 cm^{-1} (line $R(12)$ N_2O); 2234.75 cm^{-1} (line $R(13)$ N_2O); 2240.43 cm^{-1} (line $R(21)$ N_2O). In this case, the minimum relative influence of the absorption of interfering atmospheric gases (1.8 %) is observed on the $R(21)$ absorption line of the ν_3 N_2O band.

Keywords: laser gas analysis of the atmosphere, photoacoustic gas analyzer of N_2O , detection of N_2O absorption, absorption band ν_3 of N_2O .

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Introduction

The problem of detecting harmful gas compounds in the surrounding atmosphere is rather relevant. The analysis of data from observations of the Global Atmosphere Watch network shows that the averaged concentrations of the main greenhouse gases (CO_2 , CH_4 , N_2O) on the surface of Earth in 2024 reached unprecedented high values [1]: CO_2 — $(423.9 \pm 0.2) \text{ ppmV}$, CH_4 — $(1942 \pm 2) \text{ ppbV}$, N_2O — $(338.0 \pm 0.1) \text{ ppbV}$.

Detection of nitrous oxide (N_2O) in the atmosphere, in various technological processes, in medicine etc. is of great interest. Nitrous oxide is released into the atmosphere from the soil, and also when mineral fertilizers are produced. Nitrous oxide differs by high greenhouse activity, which is 298 times higher than in CO_2 [2]. When processing natural gas, even a minor impurity of N_2O ($\sim 0.1 \text{ ppm}$) may complicate the technological processes in polymerization of ethylene and propylene [3]. High concentration of N_2O in an exhalation of a human being may be a sign of serious chronic diseases [4,5].

Currently the most sensitive and selective methods of gas analysis are gas chromatography (GC) and mass-spectrometry (MS), and also combinations of such methods, which gained wide practical use [6]. However, GC–MS methods may to a full extent be implemented only in

laboratory conditions, moreover, they are practically unable to operate in a real time mode.

Contrary to the GC–MS methods, the methods of laser spectroscopy make it possible to study the gas composition of atmosphere by measurement of absorption of gas impurities in a real time mode in the field conditions at a sampling site [7,8]. Laser gas analyzers built on laser photoacoustic spectroscopy (LPAS) [8–10], have high sensitivity, simplicity, reliability, are used in practice.

The aim of this paper is to determine the optimal frequencies of emission for detection of nitrous oxide absorption in the atmosphere near $\lambda = 4.5 \mu\text{m}$, where N_2O molecule has a strong vibration-rotation (VR) absorption band ν_3 , with the use of the LPAS method in the conditions of the presence of background absorption of disturbing atmospheric gases (water vapor, CO , CO_2) on the basis of the data from the spectral base HITRAN [11].

Brief review on detection of N_2O absorption

Find below a brief review of some papers dedicated to the detection of absorption of N_2O impurity with different spectroscopic methods in the middle IR-range for the last ~ 30 years.

Paper [12] describes a solid-state laser spectrometer of the middle IR-range (DFG, $\lambda = 3.98\text{--}4.62\mu\text{m}$), using which, N_2O absorption was detected at frequency of $\nu = 2236\text{ cm}^{-1}$ ($4.47\mu\text{m}$); sensitivity of $(1\sigma) \sim 2$ ppbV N_2O was achieved. Paper [13] presents a spectrometer ($\lambda = 2.88\text{--}3.02\mu\text{m}$) with pumping from a diode laser and Nd:YAG-laser. At frequency of $\nu = 3447.67\text{ cm}^{-1}$ ($\lambda = 2.90\mu\text{m}$) for the $P(33)$ N_2O absorption line, the detection sensitivity was 2.5 ppmV. In paper [14] absorption of N_2O was detected with a QEPAS-sensor using emission of a quantum cascade laser (QCL, $\nu = 2198.3\text{--}2195.5\text{ cm}^{-1}$). Absorption of N_2O was measured on line $P(30)$ (2195.633 cm^{-1}), parameter $(1\sigma) = 4$ ppbV was measured at integration time of $\tau = 3$ s, and also parameter $NNEA = 1.5 \cdot 10^{-8}\text{ cm}^{-1} \cdot \text{W} \cdot \text{Hz}^{-1/2}$.

In paper [15] the absorption of N_2O was detected by the CAES method in the spectral range of $\lambda = 4.52\text{--}4.53\mu\text{m}$ using a optical parametric oscillator (OPO) pumped from a pulse Nd:YAG-laser. In opinion of the authors, the spectral range of $4.52\text{--}4.53\mu\text{m}$ is the best to detect N_2O . Operation at these wavelengths helps to avoid noise from other gases of atmosphere, such as CO_2 and vapors of H_2O . Taking into account 2%-uncertainty of measurements and effective value of N_2O absorption cross section of around $6 \cdot 10^{-19}\text{ cm}^2$, the limit of detection of 10 ppbV of N_2O . In paper [16] the measurement of N_2O absorption was implemented using emission of QCL ($\lambda = 4.6\mu\text{m}$) and a multi-pass cell, at $\nu = 2178.2\text{ cm}^{-1}$ ($4.591\mu\text{m}$) the sensitivity of detection of 2.5 ppmV N_2O was achieved. In paper [17] a QEPAS-sensor is described for the measurement of the concentration of impurity N_2O using QCL emission of ($\lambda = 4.6\mu\text{m}$). For the $P(41)$ N_2O absorption line on $\nu = 2169.6\text{ cm}^{-1}$ ($4.609\mu\text{m}$) and $p = 100$ Torr the minimum limit of detection was 23 ppbV N_2O , and the parameter $NNEA = 2.91 \cdot 10^{-9}\text{ cm}^{-1} \cdot \text{W} \cdot \text{Hz}^{-1/2}$.

In paper [18] the detection of NO and N_2O absorption was carried out using CEAS method. Two optical resonators were used (one for each gas), built from spherical mirrors with high reflection coefficient. Sensitivity improvement was achieved by application of absorption spectroscopy with amplification in the resonator. To measure N_2O absorption, a narrowband QCL ($\lambda = 4.53\mu\text{m}$) was used. Various mixtures of Ar+NO and Ar+ N_2O were measured in the range from 100 ppbV to 10 ppmV. Relative uncertainty of the results did not exceed 13%.

In paper [19] an experimental setup is described, which is made of a multi-pass cell, a QCL ($\lambda = 7.73\mu\text{m}$) and a detector with thermoelectric cooling. At $\nu = 1297.05\text{ cm}^{-1}$ ($\lambda = 7.71\mu\text{m}$) the minimum level of detection was 1.7 ppbV N_2O at $p = 80$ Torr and time of integration $\tau = 2$ s. In paper [20] a multifunctional laser system is presented based on an IR parametric oscillator of light ($\lambda = 1.41\text{--}8.48\mu\text{m}$) for remote probing of various gases in the atmosphere (including NO_2 , N_2O) using a lidar of differential absorption. To record absorption of N_2O , wavelengths 1.588 and $1.615\mu\text{m}$ were used. At diffuse reflection of probing laser pulses from an object and the

distance of 500 m, the sensitivity of ~ 3.4 ppm N_2O was achieved experimentally.

In paper [21] a QEPAS-system is presented for detection of low concentrations of gas impurities. The source of emission was a pulse matrix from 32 QCLs, emitting in the spectral range of $\nu = 1190\text{--}1340\text{ cm}^{-1}$ ($\lambda = 7.46\text{--}8.40\mu\text{m}$). At time of integration $\tau = 10$ s the sensitivity of detection below 60 ppbV N_2O was achieved, which makes it possible to monitor nitrous oxide at the global atmospheric level.

In paper [22] a QEPAS-sensor is described for detection of absorption of N_2O . QCL emission was used at frequency of $\nu = 1297.05\text{ cm}^{-1}$ ($\lambda = 7.71\mu\text{m}$). The sensitivity of 5 ppbV N_2O was obtained at time of integration of $\tau = 100$ ms. In paper [23] a QEPAS-sensor is presented with a source of QCL. Measurements were carried out in the range of $\nu = 2100\text{--}2250\text{ cm}^{-1}$ ($\lambda = 4.44\text{--}4.76\mu\text{m}$). At $\nu = 2212.35\text{ cm}^{-1}$ ($4.52\mu\text{m}$) the detection limit was $(1\sigma) = 7$ ppbV N_2O , the parameter $NNEA = 5.4 \cdot 10^{-9}\text{ cm}^{-1} \cdot \text{W} \cdot \text{Hz}^{-1/2}$. In paper [24] a QEPAS-sensor is described on the basis of ICL ($\lambda = 4.57\mu\text{m}$) for measurement of N_2O absorption. At frequency of $\nu = 2191.4\text{ cm}^{-1}$ ($4.56\mu\text{m}$) the minimum detection limit was 230 ppbV N_2O at $p = 250$ Torr and integration time of $\tau = 0.1$ s, parameter $NNEA = 6.17 \cdot 10^{-8}\text{ cm}^{-1} \cdot \text{W} \cdot \text{Hz}^{-1/2}$. In paper [25] a QEPAS-sensor was presented using QCL ($\lambda = 7.84\mu\text{m}$) for detection of N_2O impurity. At frequency of emission $\nu = 1275.49\text{ cm}^{-1}$ at integration time of $\tau = 0.1$ s minimum detection limit was 9 ppbV N_2O .

In paper [26] the N_2O absorption bands were studied in the middle IR-range (bands of 3.9 and $4.5\mu\text{m}$), suitable for remote probing by method of differential absorption onboard of an airplane from the altitude of 5 km. Simulation demonstrated that the preferable option was the position of the spectral dip between the two strong absorption lines N_2O in the $4.5\mu\text{m}$ band, and also in a weaker absorption band $3.9\mu\text{m}$. Both options meet the requirements to the measurement of N_2O concentration for quantitative assessment of emissions in agricultural areas or point sources (measurement accuracy 0.5%, spatial resolution 500 m). As you can see from the presented brief review of the papers dedicated to detection of N_2O impurity absorption by spectroscopic methods, different authors used sources of emission of the middle IR-range, the wavelengths of which get into different N_2O absorption bands near 2.9 , 3.9 , 4.5 and $7.71\mu\text{m}$, and also in the near IR-range ($\sim 1.6\mu\text{m}$).

Analysis of absorption spectra

Fig. 1 presents the N_2O absorption spectrum in the middle IR-range ($\lambda = 2.5\text{--}20\mu\text{m}$), in which you can see several vibration-rotation N_2O absorption bands of various intensity. The strongest VR-band of absorption of ν_3 N_2O is located near $\nu = 2225\text{ cm}^{-1}$ ($4.49\mu\text{m}$) [11,27].

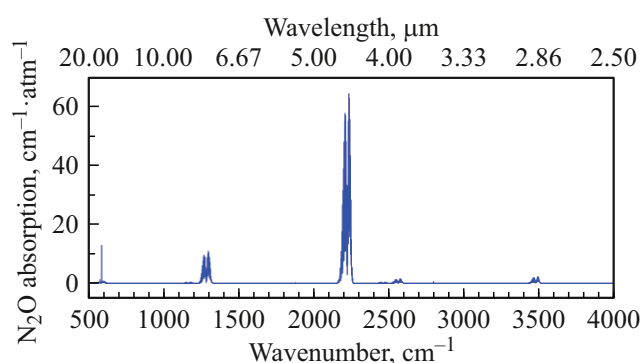


Figure 1. Spectrum of N_2O molecule absorption in the middle IR-range ($\lambda = 2.5\text{--}20 \mu\text{m}$) [11].

This is the absorption band that makes nitrous oxide one of the most dangerous greenhouse gases in the atmosphere [1,2]. Besides, Fig. 1 shows weaker short-wave bands of N_2O absorption, whose centers are located at frequencies of 588.9 cm^{-1} ($16.98 \mu\text{m}$), $\sim 1285 \text{ cm}^{-1}$ ($7.78 \mu\text{m}$), $\sim 2557 \text{ cm}^{-1}$ ($3.91 \mu\text{m}$), $\sim 3475 \text{ cm}^{-1}$ ($2.88 \mu\text{m}$). In the near IR-range ($\lambda = 0.7\text{--}2.5 \mu\text{m}$) weak overtones of the main VR bands of N_2O absorption in the middle IR-range are also located.

Vibration rotation ν_3 N_2O absorption band consists of two *P*- and *R*-branches (Fig. 2), which have the structure corresponding to various rotation numbers *J*. The most intense *R*-branch of N_2O absorption is located to the right on the scale of the frequencies, where the strongest is the rotation absorption band *R*(16) with the center at $\nu = 2236.93 \text{ cm}^{-1}$ ($4.47 \mu\text{m}$) [11,27]. Fig. 2 presents the absorption spectra of some atmospheric gases (N_2O , vapors of H_2O , CO , $^{12}\text{CO}_2$, $^{13}\text{CO}_2$), which have VR absorption bands in the spectral range of $\nu = 2000\text{--}2500 \text{ cm}^{-1}$ ($\lambda = 4\text{--}5 \mu\text{m}$) [11]. Note that in process of measurement of N_2O impurity absorption in the real atmosphere, absorption of impurities of the specified disturbing atmospheric gases. Using data from the spectral base HITRAN [11] let us conduct certain assessments of effect from absorption of disturbing gases when absorption of N_2O is measured in the atmosphere in the spectral range of $\nu = 2180\text{--}2260 \text{ cm}^{-1}$ ($\lambda = 4.43\text{--}4.59 \mu\text{m}$), where the strong VR absorption band is located ν_3 for N_2O molecule [11,27].

Concentration of H_2O vapors in the ambient air undergoes considerable variations depending on the weather. Thus, at pressure of 1 atm and temperature of 23°C at relative humidity of $RH = 100\%$ (dew point) the absolute humidity of air reaches the value of 20.6 g/m^3 [28], which is $\sim 25635 \text{ ppm H}_2\text{O}$ [28]. The atmosphere model by IAO (Institute of Atmospheric Optics, Tomsk, Russia) for mid-latitudes suggests averaged air humidity in the ground-level air atmosphere in summer at the level of $15600 \text{ ppm H}_2\text{O}$, in winter — $5880 \text{ ppm H}_2\text{O}$ [29]. The American model of atmosphere for mid-latitudes suggests other averaged values of air humidity: in summer — $18600 \text{ ppm H}_2\text{O}$,

in winter — $4320 \text{ ppm H}_2\text{O}$ [11]. For our simulation of absorption spectra of atmospheric gases near $\lambda = 4.5 \mu\text{m}$, let us take the averaged concentration of water vapors in the air equal to $15600 \text{ ppm H}_2\text{O}$ in accordance with the IAO model [29], which at temperature of 23°C corresponds to relative air humidity $RH \approx 55\%$ [28].

The background concentration of carbon monoxide (CO) impurity in the atmosphere according to experimental study [30] varies in the range of $75\text{--}175 \text{ ppb}$, therefore, for our simulation we select the average level of $\sim 120 \text{ ppb CO}$. Currently the average background concentration of carbon dioxide (CO_2) in the atmosphere reaches $\sim 420 \text{ ppm}$ [1]. According to the adopted standard Belemnitella Americana (PDB) [31,32] the ratio of isotope content $^{13}\text{C}/^{12}\text{C} = \delta^{13}\text{C} = 1.12372\%$ is accepted as a reference of zero value, therefore, for our simulation we select the concentration of $^{13}\text{CO}_2$ isotope impurity in the atmosphere equal to $\sim 4.7 \text{ ppm}$.

Let us analyze the relative impact (share) of each of the listed gas impurities at the measurement of N_2O absorption in the real atmosphere. For this purpose let us introduce the new relative parameters $A_i(\nu)$, which represent the ratio of absorption of $\alpha_i(\nu)$ disturbing gases in the atmosphere (H_2O

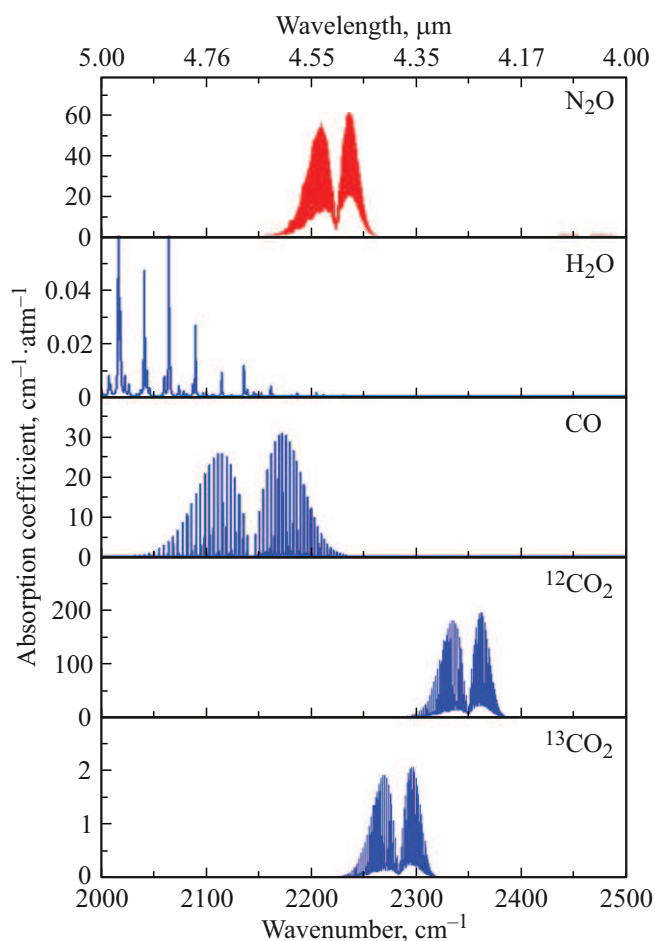


Figure 2. Absorption spectra of N_2O , H_2O , CO , $^{12}\text{CO}_2$, $^{13}\text{CO}_2$ in the interval of $\nu = 2000\text{--}2500 \text{ cm}^{-1}$ ($\lambda = 4\text{--}5 \mu\text{m}$) [11].

vapors, CO, $^{12}\text{CO}_2$, $^{13}\text{CO}_2$) to absorption (optical thickness) of the background concentration of the target substance (N_2O) in the atmosphere in the specified spectral range of frequencies ν (i.e. practically the ratio of optical thicknesses at the conventional length of optical path $l = 1$ cm):

$$A_{[\text{H}_2\text{O}/\text{N}_2\text{O}]}(\nu) = \alpha_{\text{H}_2\text{O}}(\nu)/\alpha_{\text{N}_2\text{O}}(\nu),$$

$$A_{[\text{CO}/\text{N}_2\text{O}]}(\nu) = \alpha_{\text{CO}}(\nu)/\alpha_{\text{N}_2\text{O}}(\nu),$$

$$A_{[^{12}\text{CO}_2/\text{N}_2\text{O}]}(\nu) = \alpha_{^{12}\text{CO}_2}(\nu)/\alpha_{\text{N}_2\text{O}}(\nu),$$

$$A_{[^{13}\text{CO}_2/\text{N}_2\text{O}]}(\nu) = \alpha_{^{13}\text{CO}_2}(\nu)/\alpha_{\text{N}_2\text{O}}(\nu),$$

$$A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu) = \alpha_{\text{ATM}}(\nu)/\alpha_{\text{N}_2\text{O}}(\nu),$$

where $\alpha_i(\nu) = k_i(\nu) \cdot p_i'$ — absorption [cm^{-1}] of selected gas impurities in the atmosphere, $k_i(\nu)$ and p_i' — coefficients of absorption [$\text{cm}^{-1} \cdot \text{atm}^{-1}$] and partial pressures [atm, ppm] of the selected gas impurities in the atmosphere, $\alpha_{\text{ATM}}(\nu) = \alpha_{\text{H}_2\text{O}}(\nu) + \alpha_{\text{CO}}(\nu) + \alpha_{^{12}\text{CO}_2}(\nu) + \alpha_{^{13}\text{CO}_2}(\nu)$ — total absorption [cm^{-1}] of disturbing gases in the atmosphere, $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu)$ — ratio [rel. units] of the total absorption of disturbing gases in the atmosphere to the absorption of the background concentration of N_2O in the atmosphere.

Using the data from the spectral base HITRAN [11] the calculations were conducted for the parameters $A_i(\nu)$ for the selected list of gases at the following background concentrations of these impurities in the atmosphere selected previously: 330 ppb N_2O [1], 15600 ppm H_2O [29], 120 ppb CO [30], 420 ppm $^{12}\text{CO}_2$ [1], 4.7 ppm $^{13}\text{CO}_2$ [31,32]. To simulate the absorption spectra, in HITRAN [11] they used the following conditions: spectral range of simulation 2000–2500 cm^{-1} , simulation pitch of spectra 0.01 cm^{-1} , temperature 296 K, pressure 1 atm, Lorentzian apparatus function, apparatus resolution 0.1 cm^{-1} . Names and frequencies of N_2O absorption lines in VR-band ν_3 were taken from paper [27].

Fig. 3 presents the absorption spectrum of N_2O molecule (P -branch of VR-band ν_3) [11] and estimated parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu)$ in the spectral range of $\nu = 2175$ –2224 cm^{-1} . As you can see from Fig. 3, b , minimum total relative influence of disturbing gases absorption in the atmosphere (vapors of H_2O , CO, $^{12}\text{CO}_2$, $^{13}\text{CO}_2$) (i.e. ratio of optical thicknesses) in P -branch of VR-band ν_3 N_2O is observed only in two lines of absorption $P(24)$ and $P(8)$ N_2O (annotated and marked with vertical dashed lines of red color), where parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu_j) \approx 2.6$ –3%. In another two lines $P(30)$ and $P(28)$ of the same band, parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu_j) \approx 3$ –3.2%. In other absorption lines in P -branch of the VR-band ν_3 N_2O the relative effect of the total absorption of disturbing gases in the atmosphere is even higher and is not of practical interest for gas analysis of the atmosphere. Note that in the strongest absorption line in P -branch of VR-band ν_3 N_2O (line $P(16)$, annotated and marked in Fig. 3 with vertical dashed line of blue color), parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(P16) \approx 11\%$, which makes this absorption line hardly practically suitable for measurement

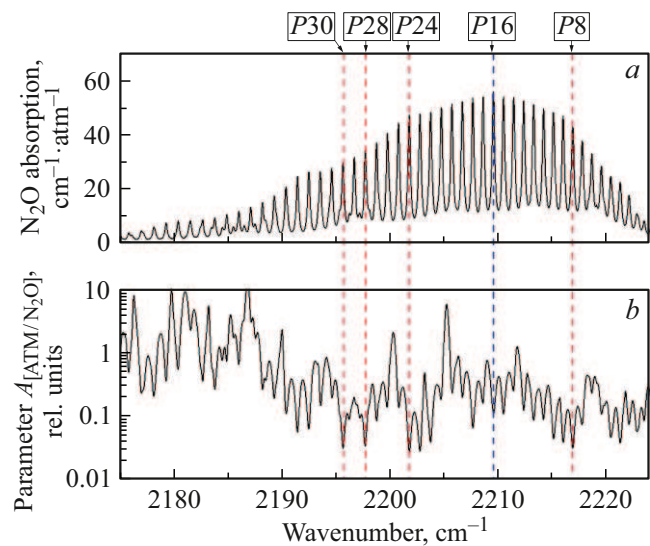


Figure 3. (a) Coefficient of N_2O absorption in VR-band ν_3 (P – branch) [11]; (b) ratio of total absorption of disturbing gases in the atmosphere (H_2O vapors — 15600 ppm, CO — 120 ppb, $^{12}\text{CO}_2$ — 420 ppm, $^{13}\text{CO}_2$ — 4.7 ppm) to absorption of background concentration of N_2O (330 ppb) at pressure of 1 atm and temperature of 23°C.

of N_2O absorption in the atmosphere in the presence of disturbing atmospheric gases.

Fig. 4 presents the N_2O absorption spectrum in the spectral range of $\nu = 2225$ –2255 cm^{-1} and results of estimation of the relative influence of total absorption of disturbing gases in the atmosphere in R -branch of the VR-band of ν_3 N_2O absorption. As you can see from Fig. 4, b , the minimum relative influence of disturbing gases in the atmosphere (ratio of optical thicknesses) in the specified spectral range on absorption of N_2O (330 ppb) is observed at line $R(21)$, where parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(R21) = 1.8\%$, and also at lines $R(6)$, $R(12)$, $R(13)$ N_2O , where parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu_j) \approx 2.15$ –2.3% (annotated and marked in Fig. 4 with vertical dashed lines of red color). Taking into account the fact that coefficient of N_2O absorption in R -branch of VR-band ν_3 is somewhat higher than in P -branch (Fig. 3,4), the optimal frequency of emission for measurement of N_2O absorption in the atmosphere at minimum influence of disturbing gases must be selected from a rather short list of marked rotation absorption lines of short-wave band ν_3 N_2O : $R(6)$, $R(12)$, $R(13)$, $R(21)$. Note that in the entire VR-band ν_3 N_2O in the strongest rotation line of absorption $R(16)$ (annotated and marked in Fig. 4 with a vertical dashed line of blue color) parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(R16) \approx 3.7\%$, i.e. is quite close to minimum values (~ 1.8 –2.3%) in other adjacent rotation lines of N_2O absorption.

The table presents frequencies of emission from [11,27], and also results of calculation of parameters $A_i(\nu_j)$ and $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu_j)$ in the individual rotation lines identified in process of analysis in P - and R -branches of VR-band of ν_3

Parameters of separate lines of N_2O absorption in band ν_3

Line of absorption N_2O [27]	Frequency, cm^{-1} [27]	Frequency, cm^{-1} [11]	Absorption N_2O [11], $\text{cm}^{-1}\cdot\text{atm}^{-1}$	Parameter $A_{[\text{H}_2\text{O}/\text{N}_2\text{O}]}(\nu_j)$, rel. units	Parameter $A_{[\text{CO}/\text{N}_2\text{O}]}(\nu_j)$, rel. units	Parameter $A_{[^{12}\text{CO}_2/\text{N}_2\text{O}]}(\nu_j)$, rel. units	Parameter $A_{[^{13}\text{CO}_2/\text{N}_2\text{O}]}(\nu_j)$, rel. units	Parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu_j)$, rel. units
$P(30)$	2195.6322	2195.62	29.14	0.02704	0.00253	0.000426	$7.3993 \cdot 10^{-6}$	0.03
$P(28)$	2197.6983	2197.69	33.79	0.03009	0.00204	0.000388	$1.0476 \cdot 10^{-5}$	0.03252
$P(24)$	2201.7485	2201.74	46.87	0.02474	0.000751	0.000297	$1.2947 \cdot 10^{-5}$	0.0258
$P(16)$	2209.5225	2209.51	55.50	0.07092	0.03696	0.00134	$5.3588 \cdot 10^{-5}$	0.10927
$P(8)$	216.8593	2216.84	42.70	0.02732	0.000268	0.00195	0.000393	0.02993
$R(6)$	2229.4284	2229.42	39.08	0.02131	$5.7161 \cdot 10^{-5}$	0.000555	0.00108	0.02299
$R(12)$	2234.0208	2234.01	59.10	0.01755	$4.5628 \cdot 10^{-5}$	0.00128	0.0027	0.02158
$R(13)$	2234.7616	2234.75	59.40	0.01793	$1.5134 \cdot 10^{-5}$	0.000745	0.00331	0.022
$R(16)$	2236.9427	2236.93	61.37	0.02629	$2.0843 \cdot 10^{-5}$	0.0026	0.00788	0.03679
$R(21)$	2240.4392	2240.43	54.82	0.01429	$6.3501 \cdot 10^{-6}$	0.000707	0.00299	0.018

N_2O absorption, where the minimum influence of disturbing atmospheric gases is observed. As you can see from the presented results of calculation, among the selected rotation lines of N_2O absorption, the highest relative influence is provided by absorption of H_2O vapor (everywhere more than 1.7%, apart from the line $R(21)$ N_2O). In other lines of N_2O absorption (table) the influence of other disturbing atmospheric gases is less noticeable (apart from line $P(16)$ N_2O , where the abnormally high influence of absorption of CO is observed— 3.7%). The most suitable rotation lines for measurement of absorption of N_2O in the atmosphere under the conditions of the disturbing atmospheric gases (H_2O vapor, CO , $^{12}\text{CO}_2$, $^{13}\text{CO}_2$) are rotation lines of N_2O absorption in R -branch of VR -band ν_3 , listed in the lower part of the table: $R(6)$, $R(12)$, $R(13)$, $R(21)$.

Let us introduce a new parameter:

$$B_{[\text{N}_2\text{O}/\text{ATM}]} = k_{\text{N}_2\text{O}}(\nu)/A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu),$$

equal to the ratio of N_2O absorption coefficient [11] to the value of parameter $A_{[\text{ATM}/\text{N}_2\text{O}]}(\nu)$ that we calculated (table). The essence of the new parameter $B_{[\text{N}_2\text{O}/\text{ATM}]}$ consists in the following. Selection of the optimal working frequency of laser emission often depends on the value of absorption coefficient of the target gas impurity. Usually the frequency of laser emission is selected so that it is within the maximum of absorption of the target gas impurity. However, the above analysis of the relative influence of disturbing gases in the atmosphere at the measurement of N_2O absorption (ratio of optical thicknesses) demonstrated that such selection is not always right (see the example with the $P(16)$ N_2O absorption line, Fig. 3, table). Therefore, it is suggested to select the optimal frequency of laser emission so that it is within the maximum values of target gas impurity absorption coefficient at minimum relative influence of total absorption of disturbing gases in the atmosphere. This criterion to a certain extent is compliant with a new parameter $B_{[\text{N}_2\text{O}/\text{ATM}]}$ in the field of its maximum values.

Fig. 5 presents the N_2O absorption spectrum [11] and estimated parameter $B_{[\text{N}_2\text{O}/\text{ATM}]}$ in the spectral range of

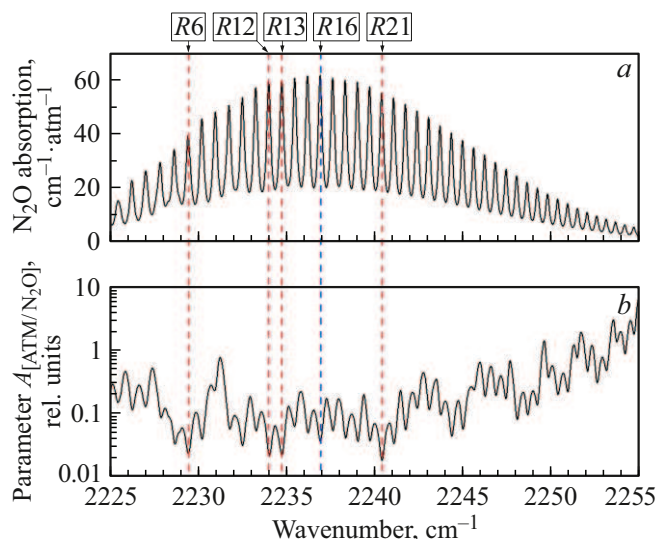


Figure 4. (a) Coefficient of N_2O absorption in ν_3 band (R -branch) [11]; (b) ratio of total absorption of disturbing gases in the atmosphere (H_2O vapor, CO , CO_2) to absorption of background concentration of N_2O (330 ppb) at pressure of 1 atm and temperature of 23°C .

$\nu = 2185\text{--}2255\text{ cm}^{-1}$ (entire VR -band of ν_3 N_2O absorption). As you can see from Fig. 5, b , in the VR -band of ν_3 N_2O absorption the maximum value of parameter $B_{[\text{N}_2\text{O}/\text{ATM}]}$ ≈ 3050 rel. units is obtained on the rotation line of $R(21)$, and slightly lower values ($\sim 2700\text{--}2740$ rel. units) are observed in another two rotation lines $R(12)$ and $R(13)$, which confirms our previous conclusions regarding the selection of the optimal frequency of laser emission. Note that consideration of parameter $B_{[\text{N}_2\text{O}/\text{ATM}]}$ has shortened even more the list of possible N_2O absorption lines (down to three lines in R -branch of VR -band ν_3) to organize the measurement of N_2O absorption in real atmosphere under the conditions of influence from disturbing atmospheric gases (H_2O vapor, CO , $^{12}\text{CO}_2$, $^{13}\text{CO}_2$).

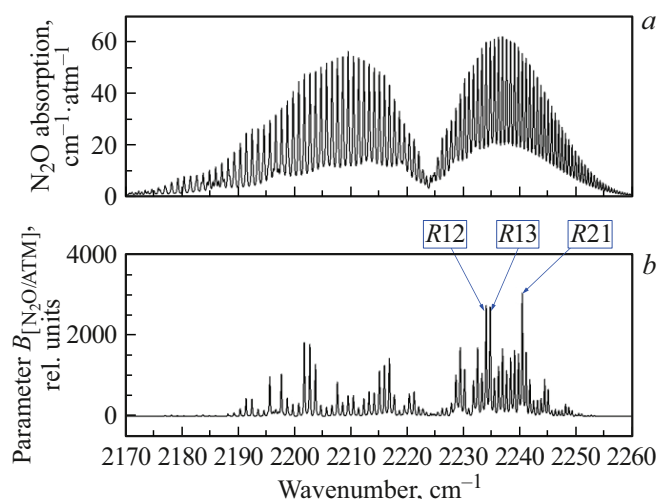


Figure 5. (a) Spectrum of N₂O absorption in VR-band ν₃ [11]; (b) graphic illustration of the value of parameter $B_{[N_2O/ATM]} = k_{N_2O}/A_{[ATM/N_2O]}$ in VR-band of absorption ν₃ of N₂O molecule.

Discussion of results

As a result of the completed analysis of N₂O, H₂O vapor, CO, CO₂ isotopes absorption spectra in the frequency range of 2170–2260 cm⁻¹ a list of N₂O absorption lines was determined in VR-band ν₃ and their corresponding frequencies of emission, where the relative influence of absorption of disturbing atmospheric gases on absorption of N₂O (ratio of optical thicknesses) does not exceed 1.8–2.3% (parameter $A_{[ATM/N_2O]}(\nu)$) (Fig. 3, 4, table). The list of selected lines of nitrous oxide absorption with relative influence of absorption of disturbing atmospheric gases of not more than 2.6% contains only five lines of VR-band ν₃ N₂O: P(24), R(6), R(12), R(13), R(21). At the same time the minimum value of parameter $A_{[ATM/N_2O]}(R21) = 1.8\%$ is observed at rotation line of R(21) N₂O absorption ($\nu = 2240.43$ cm⁻¹).

Review of parameter $B_{[N_2O/ATM]}(\nu)$ provides an additional criterion for selection of the optimal frequencies of emission, where the target gas impurity absorption coefficient is maximum at minimum relative influence of disturbing atmospheric gases (Fig. 5). According to this criterion (maximum value of parameter $B_{[N_2O/ATM]}(\nu)$), the most suitable lines for detection of nitrous oxide absorption in real atmosphere are rotation lines of absorption R(12), R(13), R(21) of VR-band ν₃ N₂O.

The most variable factor determining the absorption of disturbing atmospheric gases is absolute air humidity. For our simulation, we selected the average content of moisture in the air (15600 ppm H₂O) in the ground-level air atmosphere for the summer of mid-latitudes using IAO model [29], which corresponds to relative air humidity $RH \approx 55\%$ at temperature of 23°C [28]. Note that in summer when temperature and absolute air humidity increase, the relative influence of absorption of H₂O vapor

on the change of the background absorption of N₂O in atmosphere may increase 2.3-fold maximum. For winter of mid-latitudes at lower temperatures IAO model [29] suggests average content of moisture in air 5880 ppm H₂O (which corresponds to $RH \approx 97\%$ at temperature of 0°C [28]), i. e. 2.6 times less than in the summer. Therefore, to measure the composition of the atmosphere in winter conditions, the relative influence of absorption of H₂O vapor near $\lambda = 4.5 \mu\text{m}$ noticeably drops, but the relative influence of other disturbing gases (CO, CO₂) remains at not more than 1%.

Therefore, according to the results of the conducted analysis of absorption spectra from HITRAN [11], to measure absorption of nitrous oxide in real atmosphere with the use of laser photoacoustic gas analyzer N₂O (analog of the instrument from our papers [33,34]), three optimal frequencies of emission were selected in the VR-band of ν₃ N₂O absorption with the minimum (~ 1.8 – 2.2%) relative influence of absorption of disturbing atmospheric gases (H₂O vapor, CO, CO₂ isotopes):

- 1) $\nu(R(12) \text{ N}_2\text{O}) = 2234.01 \text{ cm}^{-1}$,
- 2) $\nu(R(13) \text{ N}_2\text{O}) = 2234.75 \text{ cm}^{-1}$,
- 3) $\nu(R(21) \text{ N}_2\text{O}) = 2240.43 \text{ cm}^{-1}$.

Note that the results of our simulation conflict with the statement of the authors of paper [15] that the spectral range $\lambda = 4.52$ – $4.53 \mu\text{m}$ is the best to detect N₂O, and operation at these wavelengths makes it possible to avoid noise from other gases of atmosphere (CO₂ and H₂O vapor). The specified spectral range 4.52 – $4.53 \mu\text{m}$ ($\nu = 2207$ – 2212 cm^{-1}) includes several lines of absorption of VR-band ν₃ N₂O: from P(13) to P(18) [11,27]. The specified rotation lines of absorption in P-branch of VR-band ν₃ N₂O according to our calculations the relative influence of disturbing atmospheric gases (H₂O vapor, CO, CO₂ isotopes) is from 6 to 12% (Fig. 3, b). However, a more favorable situation for measurement of nitrous oxide absorption is observed in R-branch of VR-band ν₃ N₂O (Fig. 4, b), where the relative influence of absorption of disturbing atmospheric gases is around 2%.

Note that paper [26] also simulated a similar procedure for selection of the optimal frequencies of emission for implementation of remote probing of N₂O impurity in atmosphere at the minimum influence of absorption of disturbing atmospheric gases using an airborne lidar of differential absorption onboard of an airplane from the altitude of 5 km, using the reflection of probing pulses from the surface of the Earth. The variant with account of temperature dependence that the authors [26] chose as the preferable one was the position of the spectral dip between the two strong absorption lines R(28) and R(29) N₂O in band $4.5 \mu\text{m}$, and also in a weaker absorption band $3.9 \mu\text{m}$.

Conclusion

The absorption spectra of N₂O, H₂O vapor, CO, CO₂ isotopes were analyzed in the spectral range of

$\nu = 2000\text{--}2500 \text{ cm}^{-1}$ ($\lambda = 4\text{--}5 \mu\text{m}$), where the strongest VR-band of absorption of ν_3 N_2O is located in the middle IR-range with the center at $\sim 2225 \text{ cm}^{-1}$ ($4.5 \mu\text{m}$) [11,27]. To measure the absorption of the target substance N_2O impurity in real atmosphere (at background concentration of N_2O — 330 ppb [1]) in presence of the absorption of disturbing atmospheric gases (H_2O vapor — 15600 ppm [29], CO — 120 ppb [30], $^{12}\text{CO}_2$ — 420 ppm [1], $^{13}\text{CO}_2$ — 4.7 ppm [31,32]), several rotation lines of N_2O absorption in VR-band ν_3 were selected, as well as the corresponding frequencies of emission near $\lambda = 4.5 \mu\text{m}$, where the relative influence of total absorption of disturbing atmospheric gases is minimum and is $\sim 2\%$. For use within a laser photoacoustic gas analyzer of N_2O , three optimal frequencies of rotation lines are recommended in VR-band of absorption ν_3 N_2O , where the maximum sensitivity of detection is implemented at the minimum relative influence of absorption of disturbing atmospheric gases: $\nu_{R12} = 2234.01 \text{ cm}^{-1}$ — line $R(12)$ N_2O , $\nu_{R13} = 2234.75 \text{ cm}^{-1}$ — line $R(13)$ N_2O , $\nu_{R21} = 2240.43 \text{ cm}^{-1}$ — line $R(21)$ N_2O . At the same time in rotation line $R(21)$ of VR-band of ν_3 N_2O absorption the minimum (1.8%) relative influence of total absorption of disturbing atmospheric gases is observed.

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Conflict of interest

The authors declare no conflict of interest.

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