

Extension of the range of resonator scanning spectrometer into submillimeter band and some perspectives of its further developments

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Abstract

Extension of the working frequency of modern resonator spectrometers into submillimeter wave range is described. Experimental record of atmospheric absorption spectrum covering 45–370 GHz range is demonstrated for the first time, and measured water vapor $J'_{ka'}, kc' - J_{ka, kc} = 5_{1,5} - 4_{2,2}$ at 325 GHz line parameters are presented. For the first time pressure lineshift for the 325-GHz water vapor line is measured. Further extension of working range is discussed. New estimations of physical limits of time needed for measurements of absorption in the whole Backward Wave Oscillator (BWO) range are given for phase continuous synthesizer regime. Basic schemes of fast broadband continuous phase synthesized sources are discussed. Verification of the previous measurements of water vapor $3_{1,3} - 2_{2,0}$ at 183 GHz line parameters is presented. Comparisons with ringdown resonator spectrometers are given.

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1. Introduction

Development of modern millimeter-wave resonator spectrometer [1] led to some new results obtained by its use [1–4]. Highest for resonator spectrometers sensitivity $\sim 4 \times 10^{-9} \text{ cm}^{-1}$ was reached and continuous atmosphere absorption spectra at 44–98 GHz and 113–200 GHz were obtained for the first time [1]. Precise line shape investigation showed that at atmospheric pressure water vapor $3_{1,3} - 2_{2,0}$ at 183 GHz line shape follows Van Vleck–Weisskopf profile up to 20 half-widths from the line center within experimental accuracy [1]. Introduction of sample substitution method for the exclusion of the apparatus function permitted to observe the 183-GHz atmospheric water vapor line down to far wings in the range 130–205 GHz

and to measure with unprecedented accuracy the air broadening parameter of that line [2]. In [2] for the first time the atmospheric gases line shift parameter for the 183-GHz water vapor line was observed and measured in laboratory. The directly measured integrated intensity for the 183-GHz water vapor line coincides with a value given in GEISA and HITRAN databases [2] within 0.4%. Turning to another most important atmospheric molecule of oxygen, the line mixing coefficient was measured experimentally for the first time for weak 1^- oxygen fine structure line at 118 GHz [3]. Refined value of pressure broadening was also obtained [3]. Record of the absorption profile of the oxygen 60-GHz band at atmospheric pressure in the range 45–96 GHz was obtained for laboratory air and pure oxygen with noise level of about $\pm 0.05 \text{ dB/km}$. From this record, the revised first-order line mixing coefficients were deduced and for the first time the quantitative assessment of second-order mixing effects was obtained [4]. Observation of broadband continuous spectra of absolute atmospheric absorption with

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high sensitivity including the intervals between the discrete absorption lines gave the possibility to investigate absorption in atmospheric continuum. A refined set of Millimeter-wave Propagation Model (MPM) parameters was derived from the new data [4]. Obtained parameters of atmospheric lines are used in, e.g., MASTER database [5] and other atmospheric databases.

Having in mind proved usefulness and high parameters of new resonator spectrometer, it is of interest to investigate further possibilities of extension of its frequency range and improvement of its parameters. Improved parameters of modern resonator spectrometer [1] were obtained mainly by introduction of the fast locked-in sources of radiation scanning the frequency band with continuous phase. So prospects of improvements of such sources and extension of the frequency band scanned with continuous phase are of interest. It is of interest also to make comparisons with some other resonator spectrometers. In the present paper the extension of the working frequency of modern resonator spectrometers into submillimeter wave range is described. Possibility of atmospheric absorption spectrum study in continuous range of 45–370 GHz is demonstrated for the first time. Experimentally measured 325-GHz water vapor line collisional parameters are presented. Pressure line shift for the 325-GHz water vapor line is measured for the first time. Further extension of the spectrometer frequency working range is discussed. New estimations of physical limits of time needed for measurements of absorption in the whole BWO range are given for continuous phase digital frequency scanning. Basic schemes of fast broadband continuous-phase synthesized sources are discussed. Verification of the previous measurements of the 183-GHz line parameters is presented. Comparisons with ringdown resonator spectrometers are given.

2. Verification of earlier measured 183 GHz water vapor line parameters

Verification of the 183-GHz line parameters measured earlier in [2] at atmospheric pressure was done by measurements in [6] by spectrometer with Radio-Acoustic Detection of absorption (RAD) at sample pressures differing by hundreds of times (Torr range).

Table 1 contains experimental values of the broadening and shifting parameters of the $3_{1,3}-2_{2,0}$ water vapor line at 183 GHz by the pressures of main atmospheric gases, N_2

and O_2 , obtained by resonator spectrometer [2] and RAD spectrometer [6]. Theoretical values of these parameters [7] are also presented in Table 1.

Comparison of the experimental values obtained by two spectrometers shows their agreement within the statistical errors quoted. Experimental values agree well also with theoretical ones. Some difference exists only between experimental and theoretical values of the shift parameter by N_2 pressure. Agreement within statistical errors of values of the pressure broadening and shifting parameters measured by two different types of spectrometers at pressures differing by hundreds of times makes values obtained very reliable.

This result leads to the important conclusion, that modern resonator spectrometer permitted to reach at atmospheric pressure the accuracies of measurements of broadening and shifting parameters nearing the ones obtainable earlier in the best traditional microwave spectrometers at common (low) pressures of the gas sample.

3. Extension of the frequency range of modern resonator spectrometer into submillimeter wave band

Extension of the frequency range of modern resonator spectrometer into submillimeter wave band is very desirable having in mind permanent extension of the range of frequencies used for atmosphere physics, astrophysics and remote sensing studies even well beyond the Terahertz. All these studies need supporting laboratory measurements.

In the present work, the range of modern resonator spectrometer, constituting earlier [1–4] 45–205 GHz, was extended up to 370 GHz, i.e., into submillimeter region. Two BWO's were added to the previously used: OB-24 (180–260 GHz) and OB-30 (260–380 GHz). We did not have in our disposal unidirectional elements for that range of frequencies, which were used in our previous work for better stability of the phase lock-in system. But experiments showed that stable regime of the phase lock-in system in strongly frequency (phase) dependent tract including high-quality resonator can be achieved by extension of the lock-in system bandwidth up to 5–7 MHz. Such an extension was found easier to achieve at frequencies of phase/frequency detector operation near 350 MHz, not 35 MHz, as in previous studies. Reference signal for phase/frequency detector (PFD) was obtained then by

Table 1
Experimental values of the broadening and shifting parameters of the $3_{1,3}-2_{2,0}$ water vapor line at 183 GHz by the pressures of main atmospheric gases, N_2 and O_2 , measured by resonator spectrometer [2] and RAD spectrometer [6]

	Tretyakov et al. meas. [2]	Golubiatnikov meas. [6]	Gamache calc. [7], 296 K
Width/ N_2	4.24(4) 299 K	4.230(7) 302 K	4.41
Shift/ N_2	−0.091(24) 299 K	−0.092(10) 302 K	−0.140
Width/ O_2	2.57(5) 298.6 K	2.580(5) 301 K	2.46
Shift/ O_2	−0.084(30) 298.6 K	−0.097(5) 301 K	−0.099

For comparison theoretical values of these parameters [7] are also presented.

multiplication of the frequency of the same digital direct synthesizer (DDS) as in previous works [1–4].

Fig. 1 presents laboratory atmosphere absorption spectrum experimentally obtained by new version of spectrometer at atmospheric pressure in the continuous frequency range 45–370 GHz. Resonator modes (experimental points) are following each 0.38 GHz and are not shown separately. The record consists from 6 sub-ranges corresponding to 6 different radiation sources used. Recording and processing of the spectrum were carried out by the same way as in our previous studies [2]. The record corresponds to temperature 296 K, pressure 730 Torr and absolute humidity 5.3 g/m³. The highest frequency sub-band spectrum record (250–370 GHz) was made using a mixture of pure nitrogen with water vapor as a sample. Small variations of absorption related to variations of ambient parameters (temperature, pressure, and humidity) during each sub-band spectrum recording as well as their minor differences between different days of the experiment (each sub-band record requires at the present time near one working day including time for the radiation source change) were taken into account by use of MPM as described in details in [4].

The highest sub-band spectrum record includes water vapor $5_{1,5}-4_{2,2}$ line at 325 GHz. Broadening and shifting parameters of this line by the pressure of nitrogen were measured in the present work. In the processing of the $5_{1,5}-4_{2,2}$ water vapor line record at 325 GHz the effect of neighboring weaker not resolved $10_{2,9}-9_{3,6}$ water vapor line at 321 GHz on the observed absorption profile was taken into account. Absorption profile of the $10_{2,9}-9_{3,6}$ line for our experimental conditions was calculated using MPM program ([4] and references therein) and subtracted from experimental data. This approach in which parameters of the 321-GHz line were not varied was justified because the 321-GHz water vapor line is about 40 times weaker than line at 325 GHz. For calculation of the shifting parameter, the non-shifted (at low pressures) value of 325-GHz line frequency measured in [9] was used.

Obtained in the present work parameters of 325 GHz water vapor line are presented in Table 2. Pressure shift parameter for the line $5_{1,5}-4_{2,2}$ at 325 GHz was measured for the first time. Experimental values of broadening parameter obtained in previous study [8] and theoretical values [7] for broadening and shifting parameters are also presented in Table 2 for comparison. We plan to make in separate work full comparative measurements of the parameters of the line $5_{1,5}-4_{2,2}$ at 325 GHz also by two spectrometers (resonator and RAD) as was done for $3_{1,3}-2_{2,0}$ line at 183 GHz in [2,6].

Now on the basis of the results obtained it becomes possible to estimate some perspectives of further extension of the frequency range of the modern resonator spectrometer. In the present study, no need of unidirectional elements was demonstrated. Earlier BWO phase lock-in in the whole continuous range of the existing BWO's (up to about 1.2 THz) was demonstrated by us (see, e.g., [10] and review paper [11]). Fast BWO frequency control with continuous phase using direct digital synthesizer (DDS) at the frequency of phase detector is described by us earlier [1,11], and it is independent on the BWO frequency range because control is applied at intermediate frequency of the BWO lock-in system. One desirable change with extension of the range of the modern resonator spectrometer into sub-millimeter range would be the change of the spectrometer receiver from videodetector (as in [1–4]) to the more

Table 2

Experimental values of the broadening and shifting parameters of the $5_{1,5}-4_{2,2}$ water vapor line at 325 GHz by the pressure of nitrogen N₂, measured in this work

	This work, meas., 298 K	Colmont et al. [8], meas., 300 K	Gamache [7], calc., 296 K
Width/N ₂	4.05(5)	4.011(30)	4.156
Shift/N ₂	−0.020(16)	—	−0.101

For comparison, experimental value of the broadening parameter measured in [5] and theoretical value of broadening and shifting parameters by pressure of N₂ [7] are also presented.

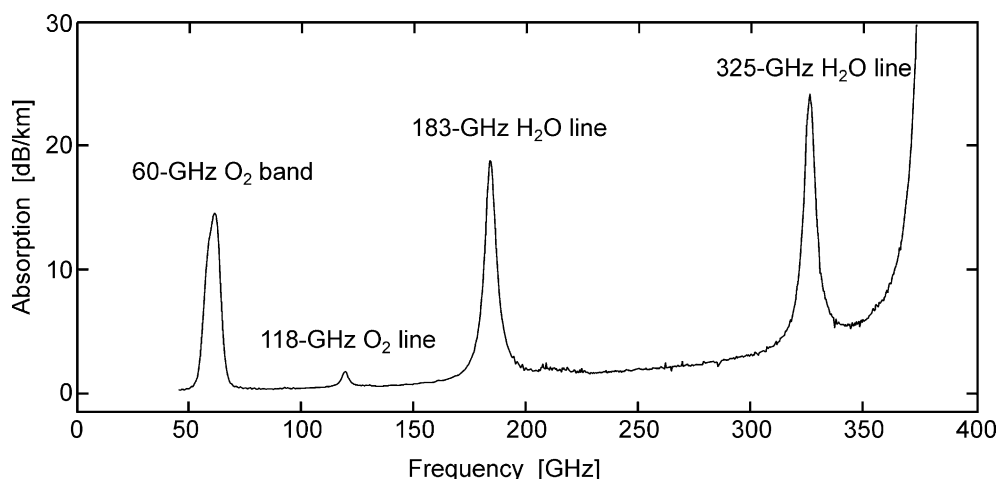


Fig. 1. Laboratory atmosphere absorption spectrum experimental record in 45–370 GHz range. See text for details.

sensitive receivers such as hot electron InSb bolometer or superheterodyne receiver. Use of superheterodyne receiver could be desirable as faster receiver. Multiplier-mixer working in the whole BWO range is described by us in [10,11]. We have experience in operation of Fabry–Perot resonators by microwave technique at least up to 600 GHz [12]. So at the present moment we do not see any principal difficulty in extension of the working range of modern resonator spectrometers further into submillimeter band maybe up to the highest BWO frequency of about 1.2 THz.

4. Re-evaluation of physical time limitations of modern resonator spectrometer experiment

The most important improvement defining the best parameters of the modern resonator spectrometer was the introduction in it of the fast continuous phase digital scanning of the source frequency by the special synthesizer [1]. However, presented in the paper [1] estimation of one of important characteristics of new spectrometer—the minimal time needed for spectroscopical experiment—was done too cautiously, in fact, without taking into consideration possibilities of shortening of the experiment time with continuous phase source frequency switching. Among other reasons, the cautiousness appeared due to absence at that time of the quantitative calculations of the resonator excitation in conditions of fast digital scanning of the source frequency with continuous phase frequency switching. Later these calculations were made by us in [13] together with development of the algorithm of the resonator parameters recovery in conditions of fast digital frequency scanning.

Let us consider regimes of synthesizer frequency scanning in resonator spectrometer. First regime is when condition of continuous phase of signal is not fulfilled with frequency switching. This case is typical for most part of microwave frequency synthesizers using so-called indirect synthesis of the output frequency. To measure resonator response in the regime with phase jumps when frequency of radiation exciting the resonator is switched, one has to wait after each switching till previously excited oscillations are decayed and newly excited oscillations with new phase arise. Both these processes demand times of the order of several resonator time constant $\tau = 1/\pi\Delta f$, where Δf is the resonator response FWHM. Then measurements of, e.g., a hundred points to characterize resonant curve of one mode of the resonator will demand time of the order of several hundreds of the resonator time constant. It is well known, that the time necessary for resonance curve profile recording in conditions of continuous (analog) scanning of frequency can be by the order of magnitude equal to the resonator time constant τ . So digital scanning of resonance curve with phase jumps at every step is at least time consuming by physical reasons.

We used in [1–4] synthesized frequency radiation source in millimeter wave band permitting to accomplish fast digital phase continuous scanning of the source frequency within 200 MHz around the frequency defined by micro-

wave synthesizer of the range of 8–18 GHz. The produced response can be practically the same as one obtained by continuous scanning of the free-running radiation source, but with the frequency precisely known and controlled at each instant. Correspondingly estimated times necessary for experiment on measurement of the resonance curve width by the scanning of synthesized continuous phase signal are strongly shortened as compared with estimations in [1]. As it is shown in [13] the time, earlier estimated by us as necessary for taking of one (from one hundred) point on the resonance curve, now can be taken as time enough for taking the whole profile of the resonance curve, and, moreover, can be significantly shortened in comparison with 10τ taken in [1]. Correspondingly estimated time required for obtainment of the absorption spectrum in the whole waveguide band can be shortened in comparison with the time estimated in [1] by several hundred times. If in [1] this estimation corresponded to the time of the order of one second, now estimated time can constitute only a few tens of milliseconds. Thus, record of 100 frequency points of one resonator eigen mode resonance curve at 1 μ s per point and about 100 modes to scan within entire BWO frequency range requires altogether 10 ms for the experiment time not including the switching time between modes that will be discussed later. Results of [13] show that necessary accuracy of recovery of the resonance width (i.e., sensitivity of the spectrometer) can be provided by fast enough passing of the resonance curve and averaging of the treatment results of repeated fast scans.

5. Principal scheme of continuous phase synthesizers for the broad BWO band

For full use of possibilities of the modern resonator spectrometer it would be very desirable to construct the system of fast precise continuous phase frequency control in as broad as possible frequency range, constituting in the limit the whole range of BWO. Experiments described in [10,11] show possibility of obtaining of beat signal between the BWO oscillation and harmonic of reference microwave synthesizer big enough for phase lock-in of the BWO frequency in the whole continuous BWO bandwidth (about 100 GHz). For this the specially constructed broadband multiplier-mixer was used. Now corresponding extension is needed for the system of fast BWO frequency control with continuous phase of oscillations.

We suggested the basic principle of such system in [11]. Let us consider it now in more details taking into consideration progress in digital, microwave and radiofrequency technique achieved since publication of [11]. Block-diagram of the proposed BWO based synthesizer in millimeter and submillimeter wave bands able to fast frequency scanning with continuous phase of oscillations almost in the whole waveguide band is presented in Fig. 2. The BWO frequency in this system is defined as

$$f_{\text{bwo}} = nf_{\text{mw}} \pm mf_{\text{rf}},$$

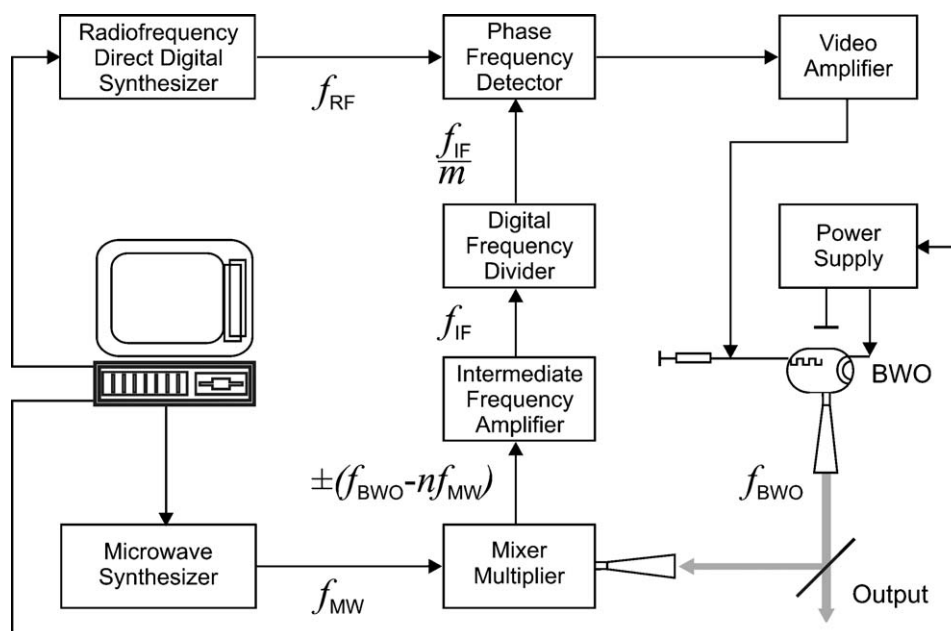


Fig. 2. Block-diagram of the fast continuous phase broadband BWO-based synthesizer in millimeter and submillimeter wave bands. Frequencies of signals are shown besides corresponding arrows. BWO frequency $f_{\text{BWO}} = nf_{\text{MW}} \pm f_{\text{rf}}$, where f_{MW} is microwave synthesizer frequency, n is harmonic number for microwave synthesizer, m is division number for digital frequency divider, f_{rf} is frequency of continuous phase radiofrequency direct digital synthesizer.

where f_{MW} is microwave synthesizer frequency, n is a harmonic number for microwave synthesizer, m is a division factor of intermediate frequency by digital frequency divider, f_{rf} is frequency of continuous phase radiofrequency direct digital synthesizer (DDS).

At any fixed frequency of microwave synthesizer BWO frequency can be scanned phase continuously by scanning of the DDS frequency. Limits of such scanning can be extended by the use of a digital frequency divider (DFD) of the intermediate frequency signal and corresponding increase of intermediate frequency and its bandwidth, and also by increase of DDS and phase frequency detector (PFD) frequency. Increase of the role of second term mf_{rf} in the equation above can in fact almost exchange roles of microwave and radiofrequency (DDS) synthesizers, when most part of scanning would be done by DDS, and change of the first term nf_{MW} (microwave synthesizer frequency or n) would be done only a few times in the whole waveguide band.

Let us consider in short quantitative characteristics of elements and possible characteristics of the whole system. Useful review of existing status and perspectives of digital signal processing including DFD, DDS, etc. is presented in [14] and references therein. Description of separate elements necessary for construction of aforementioned system with high parameters one can find, e.g., in [14–16]. Situation in this field is changing rapidly, and references mentioned reflect rather lower estimations of necessary parameters. Nevertheless, at the moment already exist DDS able to synthesize frequencies from DC to higher than 400 MHz (1 GHz clock frequency) with 0.2 Hz resolution, and switching times down to a few nanoseconds, low noise broadband intermediate frequency amplifiers up to at

least 40 GHz and DFD (both static and dynamic) up to 70–80 GHz. These parameters permit to realize even by moderate estimations bandwidth of fast continuous phase tuning of the order of 10–20 GHz with switching times of a few nanoseconds, and cover the whole bandwidth of BWO (~ 100 GHz) with only a few first term switching steps.

In the recent time, several companies began to produce also the fast microwave synthesizers, able to cover (within some limits) frequency ranges with continuous phase (see, e.g., [17,18]), which can be used as the reference. Variants of their use will depend on concrete type of synthesizer. In any case, use of such synthesizers permit to decrease time of first term switching steps between parts of the spectrum covered by continuous phase frequency control.

The most practical at the moment seems to be realization of the frequency scanning regime, in which frequency of the synthesized source jumps from one resonator mode to the next (making necessary scanning of each resonance curve), and slow following of the average frequency of BWO is produced by the control of the BWO high voltage supply. In that case it is possible to scan the whole BWO bandwidth with existing lock-in output amplifiers having dynamic range about ± 10 V (at about 100 MHz/V BWO frequency/voltage slope), the working point of which will be kept near the middle of the amplifier characteristic.

6. Comparison with some other resonator spectrometer schemes

Millimeter wave (170–260 GHz) resonator spectrometer for continuum absorption measurements using non-stabilized (free-running) BWO as radiation source and ring-down receiving of the signal from the excited resonator

modes had been described in the recent paper [19]. In the spectrometer [19] the high voltage scanning of the frequency of non-stabilized BWO radiation leads to consecutive excitation of the consecutive modes of the Fabry–Perot resonator. Each excited mode radiates the ringdown signal which is received by InSb helium bolometer. Decay of the signal characterizes the mode quality factor Q . Among other factors Q depends on radiation absorption by the sample introduced into the resonator. Large size of the resonator (10 m length) leads to values of $Q \sim 5 \times 10^6$. These parameters correspond to $\Delta F = 15$ MHz interval between two consecutive longitudinal modes and at the average frequency $f \sim 200$ GHz width of the resonance $\Delta f = f/Q \cong 40$ kHz.

It is of interest to analyze this type of spectrometers in comparison with the type developed by us. It is reasonable to make comparison of principal physical parameters of spectrometers assuming equal conditions (parameters of resonator, receiver and integration time).

First of all it is worth to note that ultimate sensitivity of “time” and “frequency” approach must be the same in equal conditions because in both devices considered at each moment only one spectral interval is excited (see, e.g. [20]).

However, resonator spectrometer with non-stabilized BWO scanning frequency band by the scanning of BWO high voltage, described in [19], has important unremovable deficiency. Namely, in the free-running BWO spectrometer one has to scan the whole frequency range including empty intervals between modes of interest. In [19], the “free spectral range,” i.e., interval between two neighboring modes constitutes $\Delta F/\Delta f = 375$ times of the width of the resonance. In these conditions, the useful time is evidently much less than the total time of scanning. The scanning speed must not exceed the one defined by the demand that for efficient excitation of the oscillations in the resonator the time of excitation must be at least of the order of the cavity time constant ($\tau = 3.3 \times 10^{-6}$ s [19]). This gives speed of frequency scanning as $\Delta f/\tau \approx 12$ GHz/s and total scanning time for 90 GHz range ~ 7.4 s. Our rough estimation of the total scanning time coincides by the order of magnitude with the value “about 3 s” given by authors of [19]. This coincidence confirms that in [19] scanning of the whole frequency range was performed with the speed of frequency scanning limited by necessity of enough excitation of resonator modes when passing them. Counting as useful time the sum of time of excitation and ringdown time (several τ s), one must conclude that ratio of useful to useless time (“duty cycle”) constitutes in described in [19] spectrometer about one percent. This deficiency is unremovable because switching of the frequency of the free-running BWO precisely to the next mode is impossible due to the irregularities in such scale of the BWO characteristics.

In contrast, spectrometer with the phase lock-in BWO can simply miss “empty” intervals of frequencies by switching precisely to the known frequency of the next mode. Frequency of the next mode of the Fabry–Perot resonator can be easily computed using known formula from positions of

previous modes, central frequencies of which were defined automatically during the scan. Then phase lock-in BWO frequency can be precisely addressed to this mode frequency. Time of observing of the resonance curve of the one mode in phase-locked with continuous phase scanning spectrometer can be done also of the order of τ [13], and aforementioned two order loss in duty cycle intrinsic to the free-running BWO spectrometer is absent in phase-locked with continuous phase BWO spectrometer. This gives two orders of magnitude gain either in useful signal integration time during the same time of experiment or in the total time needed for scanning the whole bandwidth with the same parameters as compared with free-running BWO spectrometer.

It is worth to note that the gain aforementioned is connected not with frequency domain spectrometer principle, but with fast continuous phase precise broadband source frequency control, and the same gain as compared with free-running BWO can be obtained in time domain spectrometer similar to [19] but having the fast precise broadband source frequency control, permitting not to scan “empty” parts of the spectrum.

Another important gain connected with precise frequency control in phase-locked BWO spectrometers is evident—the spectrometer permits to measure not only continuum absorption, but also parameters of the molecular spectral lines in the range studied. Examples of accuracy were shown above [1–4]. In contrast with [1–4] authors of [19] do not mention measured parameters of the observed by them water vapor line at 183 GHz (Figs. 12 and 16 of [19]). Spectrometer with phase-locked with continuous phase BWO, as is described in Section 1 and Ref. [1–4], permitted to measure not only pressure line broadening parameters, but also such more subtle effects as pressure line shift and pressure line coupling parameters.

7. Conclusion

In summary, in the present paper the extension of the working frequency of modern resonator spectrometer into submillimeter wave range is described. The spectrometer for the first time gave possibility of studies of atmospheric absorption spectrum in the continuous 45–370 GHz range. Collisional parameters of the 325-GHz water vapor line was measured in pure nitrogen at atmospheric pressure and compared with previous data. Pressure shift for the 325-GHz water vapor line was measured for the first time. Perspectives of further extension of the spectrometer working frequency range are discussed. New estimations of physical limits of time needed for measurements of absorption in the whole BWO range are given for fast digitally controlled BWO-based frequency synthesized radiation sources with continuous phase frequency switching, showing possibility by two orders of magnitude improvement of existing instruments abilities. Basic scheme of fast broadband continuous phase synthesized sources is discussed. Verification of the previous measurements of 183 GHz line

parameters is presented which gave results coinciding with experimental errors for different types of spectrometers and differing by hundreds of times in sample pressures. Comparisons with resonator spectrometers using free-running radiation source are given.

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