Molecular Detection for Unconcentrated Gas with \textit{ppm} Sensitivity Using 220-to-320 GHz Dual-Frequency-Comb Spectrometer in CMOS

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Abstract—Millimeter-wave/terahertz rotational spectroscopy of polar gaseous molecules provides a powerful tool for complicated gas mixture analysis. In this paper, a 220-to-320GHz dual-frequency-comb spectrometer in 65-nm bulk CMOS is presented, along with a systematic analysis on fundamental issues of rotational spectrometer, including the impacts of various noise mechanisms, gas cell, molecular properties, detection sensitivity, etc. Our comb spectrometer, based on a high-parallelism architecture, probes gas sample with 20 comb lines simultaneously. It does not only improve the scanning speed by 20×, but also reduces the overall energy consumption to 90 mJ/point with 1 Hz bandwidth (or 0.5 s integration time). With its channelized 100-GHz scanning range and sub-kHz specificity, wide range of molecules can be detected. In the measurements, state-of-the-art total radiated power of 5.2 mW and single sideband noise figure (NF) of 14.6−19.5 dB are achieved, which further boost the scanning speed and sensitivity. Lastly, spectroscopic measurements for carbonyl sulfide (OCS) and acetonitrile (CH₃CN) are presented, with a path length of 70 cm and 1 Hz bandwidth, the measured minimum detectable absorption coefficient reaches $\alpha_{\text{gas, min}}=7.2 \times 10^{-7} \text{ cm}^{-1}$. For OCS, that enables a minimum detectable concentration of 11 ppm. The predicted sensitivity for some other molecules reaches ppm level (e.g. 3 ppm for hydrogen cyanide (HCN)), or 10 ppt level if gas pre-concentration with a typical gain of $10^3$ is used.

Index Terms—terahertz, molecular spectroscopy, CMOS, frequency comb, transceiver.

I. INTRODUCTION

ULTRA sensitive gas sensing is of great importance in environmental monitoring, industrial process control, hazardous agent detection, etc. [1]. It is also gaining increasing interests in clinical disease diagnosis. One important application is the molecular analysis of human exhaled breath [2], [3], which contains abundant volatile organic compounds (VOCs). Many of these VOCs, with concentrations ranging from ppm to ppb levels, have unique physiological basis [4], [5]. For example, hydrogen sulfide, acetone and toluene have strong correlation with halitosis, diabetes and lung cancer, respectively.

Current technologies for gas sensing includes: (1) gas chromatography/mass spectroscopy (GC/MS), which achieves ppb level sensitivity with pre-concentration techniques. However, it is ineffective for the identification of different compounds with similar mass spectra [5]; (2) selected-ion flow-tube mass spectroscopy (SIFT-MS) and proton transfer reaction-mass spectrometry (PTR-MS), which detect ionized molecules produced by gas-phase collisions. They have ppt level sensitivity but the specificity is also limited; (3) mid-Infrared spectroscopy [6] detects the vibrational spectrum of gas molecules, which is sensitive due to the strong absorption intensity in infrared range. However, the limited tunability and linewidth of the light source make it less effective for complicated mixture analysis; (4) MEMS resonator based chemical sensors [7], [8], [9], which measure the variation of resonate frequency after absorption of gas molecules, have promising mass resolution but still suffer from selectivity issue; (5) electrochemical sensors, which is low cost but can only detect specific chemical species.

Rotation of polar gaseous molecules have quantized energy states in millimeter-wave and THz range. When molecules are excited by electromagnetic waves with photon energy matching that of the rotational state transitions, absorption spectral lines can be measured [10], [11]. The absorption intensity, as a result of degenerated quantum state number (increase with frequency) and probability for unoccupied quantum states (decrease with frequency), peaks at low-THz frequencies for most gaseous molecules. THz rotational spectroscopy is a powerful tool for gas sensing over the aforementioned technologies for the following reasons:

1) Simultaneous identification/analysis for a wide range of molecules is enabled through broadband scanning. Molecular spectral lines all follow a quasi-periodic pattern in frequency domain, and the “period” is determined by the dipole moment, weight, etc. of molecules. In fact, a spectroscopic bandwidth of 100 GHz allows the coverage of most of the chemical species under interest, including very light molecules such as hydrogen cyanide (HCN), which has a repetitive spectral line every 88.61 GHz [12].

2) The width of spectral lines in the Doppler-limited regime (at low pressure) is around 1 MHz. The corresponding spectral-line quality factor of $Q \approx 10^6$ leads to ultra-high detection specificity. Spectral overlap from different molecules is highly unlikely. The sub-kHz frequency resolution (at least 3 orders lower than the spectral line width) is also supported by nowadays THz electronics.

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Both of the narrow spectral lines and high quality THz signal sources make THz spectrometers capable of analyzing complex gas mixtures in details.

3) Previously, sensitive THz spectrometers using discrete compound III-V semiconductor components are reported. Working in conjunction with a widely adopted, industrial standard gas pre-concentration gain of $10^7$, ppt-level sensitivity is achieved [13], which is comparable with state-of-the-art gas sensors.

Recently, rapid development of silicon-based THz integrated circuits brings about new opportunities for low-cost, energy-efficient rotational spectrometers at chip scale. As shown in Fig. 1(a), the spectrometer architecture widely adopted in prior arts performs molecular probing using a single tunable tone [14], [15], [16], [17]. Although relatively compact and convenient to implement, it has several disadvantages: (1) the full-band scanning is time consuming. To scan a 100-GHz bandwidth with 10-kHz resolution and 1-ms integration time per point, it consumes $\sim 3$ hours in total. (2) It suffers from power efficiency and sensitivity degradation due to the need for lossy tunable components and low Q-factor resonators to deliver broadband coverage. (3) As discussed in Section II-D, the maximum radiation power density for probing is set by the molecular saturation effect. As a result, an upper speed limit exists for this architecture due to the maximum achievable signal-to-noise ratio (SNR) per frequency step. Besides single-tone spectrometers, a 260 GHz pulse-based radiator with 24.7 GHz bandwidth for spectroscopy has been implemented [18]. However, due to the low duty cycle of pulse modulation, 80% of the RF energy is lost, which leads to low SNR. Without phase locking, it also lacks kHz-level tunability. Pulsed echo spectrometer [19] reduces the required RF power. But it needs to mechanically adjust resonant frequency of the cavity, which slows down the scanning speed. The reported frequency accuracy of its signal source is 0.1 ppm or 10 kHz. In [20], THz comb is generated through nonlinear optics using periodic laser pulses. This approach provides abundant comb lines from 100 GHz to 2 THz with frequency interval of 250 MHz. However, it comes with lower average radiated power and insufficient frequency resolution ($\sim 25$ MHz).

In this paper, a 220-to-320 GHz, dual-frequency-comb spectrometer in 65-nm bulk CMOS process is presented. As shown in Fig. 1(b), the spectrometer probes the gas molecule sample using two counter-propagating comb signals rather than a single tunable tone. Each radiated comb signal has 10 continuous-wave, evenly-spaced frequency tones. Generation and heterodyne detection of the two comb signals are conducted simultaneously. The two comb spectra can also be shifted, so that a 100-GHz bandwidth is seamlessly covered. Through the parallel spectral scanning with the 20 comb lines, the scanning speed is enhanced by a factor of $20 \times$. Since each comb line sweeps within only a small fractional bandwidth, peak efficiency is maintained, breaking the aforementioned bandwidth-efficiency trade-off in single-tone spectrometers. The measured silicon chip achieves state-of-the-art 5.2-mW radiated power and 14.6$\sim$19.5 dB single sideband noise figure (SSB NF). To our best knowledge, these represent the highest power and sensitivity performance in THz silicon electronics.

The operation principles of the THz frontend circuits were originally presented in [21] and later described in details in [22]. In addition to including these contents (Section III) for completeness, this paper mainly focuses on the systematic analysis and design considerations of the work (in Section II), as well as extensive discussions and experiments for molecular sensing (in Section IV), which are not presented in [21] and [22]. In particular, the overall system performance is validated by measurements using OCS and acetonitrile gas samples, which give a minimum detectable absorption coefficient of $\alpha_{\text{gas, min}}=7.2 \times 10^{-7}$ cm$^{-1}$ with 1 Hz bandwidth. For OCS, our spectrometer reaches a minimum detectable concentration of 11 ppm and 0.1 ppb (if using standard gas pre-concentration with a gain of $10^3$). Its sensitivity for some molecules with larger absorption (such as hydrogen cyanide (HCN)) should further reach a few ppm (without pre-concentration) and tens of ppt (with pre-concentration). Finally, conclusions, a comparison with other gas sensors in silicon, as well as perspectives for future work are given in Section V.

II. PERFORMANCE ANALYSIS OF SPECTROSCOPIC SYSTEM

Sensitive spectrometer design requires a comprehensive consideration for the on-chip electronics, molecular properties, gas cell, and their interactions. Systematic analysis and optimizations of these factors will be presented in this section. As is shown later in Section III, the generation and detection of each comb frequency tone are performed by a THz transceiver. 

Fig. 1. (a) Conventional single-tone spectroscopy. (b) Dual-frequency-comb spectroscopy architecture. (c) Wavelength modulation spectroscopy (WMS).
unit in each comb chip (Fig. 4). For each pair of comb tones, the circuit operation are the same as a typical single-tone heterodyne spectrometer shown in Fig. 1(a). In mmW/terahertz range, cascaded heterodyne receiver and square-law detector are preferable over direct square-law power detection due to its higher sensitivity. Normally, standing wave is formed inside the gas cell, which is due to multi-reflection between the inlet and outlet THz-signal windows. It introduces significant periodic RF power variation in frequency domain. The length of gas chamber is about \( \lambda/2 \) of the RF power variation frequency (70 cm gas cell for a variation frequency of 214 MHz). Thus, even if no spectral lines exist, the system has a baseline fluctuation. Wavelength modulation spectroscopy (WMS) [23] with a modulation frequency of \( f_m \) and a deviation frequency of \( \Delta f \) (illustrated in Fig. 1(c)) is adopted, which measures the derivatives of the overall transmission response. Since the derivatives (especially the 2\( n \)th-order derivative) of the baseline are much smaller than that of the spectral lines, this approach effectively reduces the impact from the baseline fluctuation. In addition, for maximum baseband response, \( \Delta f \) is chosen to be half of the full width at half maximum (0.5 \times FWHM) of the spectral line (for output at \( f_m \)) or FWHM (for output at 2\( f_m \)), respectively. Note that analyses throughout this section are based on single-channel circuits (Fig. 1(a)) and the above detection principles, but are also applicable to our comb spectrometer.

### A. Impact of Receiver Noise on Sensitivity

In Fig. 1(a), the received signal power changes according to the gas absorption intensity, which can be expressed as:

\[
\Delta P = P_0 e^{-\alpha_0 L} (1 - e^{-\alpha_{gas}L}) \approx P_0 e^{-\alpha_0 L} \alpha_{gas} L, \tag{1}
\]

where \( P_0 \) is the transmitted signal power, \( \alpha_{gas} \) is the peak absorption coefficient at the center of spectral line, \( \alpha_0 \) and \( L \) are the path loss coefficient and length of the gas cell. Here, we assume \( \alpha_{gas} L \ll 1 \) given the normally low molecule concentration, and no extra loss exists besides path loss and gas absorption.

Next, the overall receiver noise is dominated by the input-referred noise temperature \( T_n = T_0 (F - 1) \) of the mixer, where \( F \) is the mixer noise factor, and \( T_0 \) is the ambient temperature. Therefore, the RMS noise voltage referred at the receiver input side is \( v_{n,RMS} = \sqrt{kT_n f_{ENBW} Z_0} \), where \( k \) is Boltzmann’s constant, \( Z_0 \) is receiver input impedance and \( f_{ENBW} \) is the effective noise bandwidth. To investigate its impact on detection sensitivity, we note that the total voltage at the square-law detector input is:

\[
V_{in}(t) = [V_0 \sin(\omega_0 t) + v_n(t)] \cdot G_{mixture}, \tag{2}
\]

where \( V_0 \) is the amplitude of the receiver input voltage (and equals to \( \sqrt{2Z_0 P_0 e^{-\alpha_0 L}} \) if no gas exists) and \( G_{mixture} \) is the mixer conversion gain. Meanwhile, the square-law detector is modeled as a polynomial function:

\[
V_{out}(t) = C_1 V_{in}(t) + C_2 V_{in}(t)^2 + C_3 V_{in}(t)^3 + \ldots \tag{3}
\]

As a result, the final baseband output of the square-law detector is:

\[
V_{out} = C_2 G_{mixture}^2 V_0^2 / 2 + 2V_0 \sin(\omega_0 t) v_n(t) |_{BB} + \ldots. \tag{4}
\]

The low-pass-filtered detector output signal is then:

\[
V_{s, out} = C_2 G_{mixture}^2 V_0^2 / 2. \tag{5}
\]

Within an output bandwidth of \( \Delta \nu \) at baseband, the second term in (4) represents a down-conversion of both the upper and lower RF sideband noise \( v_n \) around \( \omega_0 \) (i.e., \( f_{ENBW} = 2\Delta \nu \)). Therefore, in (3) the total integrated noise (RMS) at the detector output is:

\[
V_{n, out} = C_2 G_{mixture}^2 V_0 \sqrt{2kT_0 \Delta \nu Z_0}. \tag{6}
\]

Equation (6) is also called Townes noise [10], which is dependent on the input signal power level. If assuming no gas absorption, the baseband SNR (in voltage) of the receiver, with a bandwidth of \( \Delta \nu \), is then:

\[
SNR_{BB}|_{\nu = v} = \frac{V_{s, out}}{V_{n, out}} = \frac{V_0^2}{2V_0^2 (2kT_0 \Delta \nu Z_0)} = \frac{1}{2 \sqrt{P_0 e^{-\alpha_0 L}/kT_0 \Delta \nu}}, \tag{7}
\]

A few conclusions are made out of the above derivations:

1. The ratio between the input RF signal power and the input-referred receiver noise with the same bandwidth of \( \Delta \nu \) is:

\[
SNR_{RF}|_{\nu = v} = \sqrt{I_{DC}/(2q_e \Delta \nu)}. \tag{8}
\]

By comparing (7) with (8), we see that an SNR degradation of \( 2 \times \) or 6 dB occurs. This, verified by our circuit simulation, is important for sensitivity estimation based on electronic RF performance and is later used in our experiments (Section IV).

2. Here, the shot noise of the detector is not included, but will ultimately limit the SNR even if the transmitter and receiver mixer are noise-free. Shot noise results from the charge injection over semiconductor barrier in the detector diode. Its current spectral density is \( i_n^2 = 2q_e I_{DC} \Delta \nu \), where \( q_e \) is the charge of electron, and \( I_{DC} \) is the rectified DC output current. The associated ultimate SNR is therefore:

\[
SNR_{BB, ShotNoise} = \sqrt{I_{DC}/(2q_e \Delta \nu)}. \tag{9}
\]

Note that the current responsivity of a diode is \( \sim 10 \) A/W, meaning that 0.1 mW of input power already leads to an \( SNR_{BB, ShotNoise} \) of \( 5.6 \times 10^7 \), or 160 dB with baseband bandwidth of \( \Delta \nu = 1 \) Hz. This is a few orders of magnitude larger than the \( SNR \) typically achieved by a THz frontend (see Section IV). Therefore, our THz spectrometer is not shot-noise limited.

3. In case of detection with modulation frequency \( f_m \) and frequency deviation \( \Delta f = 0.5 \times FWHM \), the system searches maximum baseband SNR at \( f_m \) when the RF center frequency is \( f_0 = f_s \pm 0.5 \times FWHM \), if a linear approximation rather than Lorentz or Gaussian profile is
assumed, as shown in Fig. 1(c). The maximum baseband SNR is expressed as:

\[ SNR_{BB|v/v} = \frac{\Delta V_{s,\text{out}}}{V_{n,\text{out}}} = \frac{1}{2} \sqrt{\frac{P_0 e^{-\alpha_g L}}{kT_0 \Delta \nu}} (1 - e^{-\alpha_g L \frac{\pi f_m}{\nu}}). \tag{10} \]

If \( \alpha_g L \ll 1 \), (10) is simplified as:

\[ SNR_{BB|v/v} \approx \frac{1}{2} \sqrt{\frac{P_0 e^{-\alpha_g L}}{kT_0 \Delta \nu}} \alpha_g L. \tag{11} \]

It indicates that when \( \alpha_g L \ll 1 \) the molecule concentration (linearly proportional to \( \alpha_g \)) is linearity proportional to the input/output SNR in voltage rather than in power. That means, for example, even if the receiver noise figure is reduced by 20 dB, the sensitivity of the spectrometer (in terms of ppm) is only improved by 10\( \times \). This is later verified by our experiments in Fig. 12. In addition, it should also be noticed that due to the non-ideal profile of spectral lines, the expression of actual SNR differs slightly from (11). For instance, 2 dB SNR degradation is expected for a Lorentzian profile (pressure induced broadening), and 0.6 dB SNR degradation is expected for Gaussian profile (Doppler limited broadening). However, this error can be compensated by choosing a slightly larger \( \Delta f \). Lastly, (11) can also be applied to the detection output at 2\( \Delta m \) with \( \Delta f = \text{FWHM} \), where \( \approx 3 \) dB lower SNR compared with WMS at \( f_m \) is obtained at the center frequency of spectral line (\( f_s \), in Fig. 1(c)).

B. Impact of Transmitter Noise on Sensitivity

The amplitude and phase noise of the transmitter may also affect the sensitivity. To investigate this issue, we assume that the receiver is noiseless, and the IF signal, being a frequency-shifted version of the transmitted signal, is:

\[ V_{in}(t) = [V_0 + a_n(t)] \cos[\omega_0 t + \phi_n(t)] \cdot G_{\text{mixer}}, \tag{12} \]

where \( V_0 \), \( a_n(t) \), \( \omega_0 \) and \( \phi_n(t) \) are the signal amplitude, amplitude noise, carrier frequency and phase noise, respectively. The phase noise \( \phi_n(t) = \phi_p \sin(2\pi f_m t) \) is assumed to have a sinusoidal form [24], where \( \phi_p \) is the peak phase fluctuation, and 2\( \pi f_m \) is the offset frequency from \( \omega_0 \).

First, if an input signal contains only phase noise (\( a_n(t) = 0 \)), and the phase noise is assumed small, (12) is then written as:

\[ V_{in}(t) = V_0 \cos[\omega_0 t + \phi_p \sin(2\pi f_m t)] \cdot G_{\text{mixer}} \approx V_0 G_{\text{mixer}} \left\{ \cos(\omega_0 t) - \frac{\phi_p^2}{2} [\cos(\omega_0 - 2\pi f_m t)] \right\} \tag{13} \]

The 2\( ^{nd} \) and 3\( ^{rd} \) items of (13) refer to the two phase noise sidebands (upper sideband (USB) and lower sideband (LSB) as shown in Fig. 2(a)). If no spectral lines exist at the probing frequency, the amplitudes of two sidebands are equal. After the square-law detection, the two sideband signals will cancel each other. As a result, the detector output voltage after low-pass filtering of (3) is:

\[ V_{\text{out}} \approx \frac{1}{2} C_2 G_{\text{mixer}}^2 V_0^2 + C_1 V_{in}|_{\text{LPF}} + \ldots \tag{14} \]

where the 1\( ^{st} \) term is the desired output. The 2\( ^{nd} \) term is the direct low-pass-filtered component of \( V_{in} \), which includes the phase noise of \( V_{in} \) at offset larger than \( \omega_0 - 2\pi \Delta \nu \). Typically, at 1-MHz offset frequency, the phase noise of THz signal is \(-80 \text{ dBc/Hz} \) for oscillator-based sources and \(-100 \text{ dBc/Hz} \) for multiplier-based sources. Therefore, the IF frequency should be sufficiently high, so that the close-in phase noise does not directly fall into baseband.

If the THz signal touches the spectral line, as shown in Fig. 2(a), PM-to-AM noise is generated. Because the slope of absorption coefficient on the edge of spectral line profile introduces amplitude imbalance on the two phase noise sidebands of (13). After square-law detection, the phase noise of THz signal is then down-converted into amplitude noise in the baseband due to imperfect sideband cancellation. If a linear approximation is assumed for the spectral line profile, and \( \alpha_g L \ll 1 \), the baseband signal at \( f_m \) is expressed as:

\[ \Delta V_{s,\text{out}} \approx C_2 G_{\text{mixer}}^2 \frac{V_0^2}{2} \text{FWHM} \cdot \beta \cdot L. \tag{15} \]

where \( \beta = \alpha_g / \text{FWHM} \) is the slope of line profile. Since \( \Delta V_{s,\text{out}} \) is located at \( f_m \) of baseband, only the phase noise close to frequency offset \( f_m \) matters, as shown in Fig. 2(b). Based on (3) and (13), the PM-to-AM noise at \( f_m \) of baseband is then expressed as:

\[ V_{n,\text{P2A}} \approx C_2 G_{\text{mixer}}^2 \frac{V_0^2}{4} \phi_p \cdot f_m \cdot \beta \cdot L. \tag{16} \]

The SNR in voltage due to PM-to-AM noise can then be calculated using the following equation:

\[ SNR_{P2A|v/v} \approx \frac{\text{FWHM}}{f_m \int_{f_m + \Delta \nu / 2}^{f_m - \Delta \nu / 2} \frac{P_{\text{SSB}}(\nu) d\nu}, \tag{17} \]

where \( P_{\text{SSB}}(\nu) \) is the single sideband phase noise of THz signal at frequency offset \( \nu \), and \( \Delta \nu \) is integration bandwidth. Thus, for one spectral line with \( \text{FWHM} \) of 1 MHz, \( f_m \) of 50 kHz and \( \Delta \nu \) of 1 Hz, the phase noise at 50 kHz frequency...
offset needs to be at least -54 dBc/Hz for SNR of $10^4$. But since $V_{n,P2A}$ decreases linearly with molecule concentration (i.e. smaller $\beta$), PM-to-AM noise only matters under high SNR. It is not a limiting factor for sensitivity, which is defined when SNR=$1$.

Next, if the input contains only amplitude noise (i.e. $\phi_n(t) = 0$), it is similar to the input referred noise of receiver as shown in (4):

$$V_{out} \approx C_2 G_{mixer}^2 \left( \frac{V_0^2}{2} + V_0 a_n(t) + \frac{a_n(t)^2}{2} \right) + \ldots$$ \hspace{1cm} (18)

We note that Townes noise in the 2$^{nd}$ term is again the dominant noise contributor, which results from the close-in amplitude noise of the transmitter signal. Fortunately, many mmWave/terahertz CMOS sources (including ours) are based on heavily-driven nonlinear devices. The voltage swing of these devices is normally saturated or clipped by the power supply rail, which in turn suppresses the amplitude fluctuation caused by device noise. In addition, the power supply noise can potentially modulate the gain of transceiver and introduce amplitude noise to the baseband, and should therefore be maximally suppressed in the design of the entire system. Currently the noise of the receiver still dominates the overall SNR. In the future, however, when THz amplifier (with no device noise. In addition, the power supply noise can potentially modulate the gain of transceiver and introduce amplitude noise to the baseband, and should therefore be maximally suppressed in the design of the entire system. Currently the noise of the receiver still dominates the overall SNR. In the future, however, when THz amplifier (with no squeezing of amplitude noise) becomes available, this issue should be revisited.

C. Spectral Broadening and Effect of Gas Cell Size

Both the inter-molecular collision (i.e. pressure) and the Doppler effect of Brownian motion cause spectral broadening. To achieve absolute specificity, gas pressure should be sufficiently low, so that the linewidth is only limited by Doppler effect, in order to avoid spectral-line overlap. It is noteworthy that optimum pressure increases with frequency [10], and in mmWave/terahertz range, such pressure threshold is $\sim 10$ Pa. In addition, when encapsulated inside a gas cell, molecules also have collisions with the sidewalls of gas cell, leading to additional broadening. Fortunately, this is not a predominant concern for THz spectrometer. Note that a spectral-line absorption $\gamma(f)$ due to collision follows a Lorentzian profile [25]:

$$\gamma(f) \propto \frac{1}{(f - f_0)^2 + (1/\pi \tau)^2};$$ \hspace{1cm} (19)

where $f_0$ is resonance frequency and $\tau$ is the mean free time between molecular collisions. The full width of half maximum (FWHM) of the spectral line is therefore $\sim \frac{1}{\pi \tau}$. At the Doppler-limited pressure level ($\sim 10$ Pa), the value of $\tau$ is $\sim 0.3$ $\mu$s (hence a FWHM of $\sim 1$ MHz), and the mean free path of molecules, determined by molecular diameter $d$ and gas pressure $P$ is:

$$\lambda_0 = \frac{kT_0}{\sqrt{2 \pi d^2 P}}.$$ \hspace{1cm} (20)

As an example, the mean free path for OCS ($d = 8$ Å) is 140 $\mu$m. Even if a WR-3.4 waveguide (aperture size of $860 \times 430$ $\mu$m$^2$) is adopted as gas cell, which enables propagation of a 220-320-GHz TE$_{01}$ wave, its dimension is still a few times larger than the above mean free path, and does not cause significant spectral broadening. In fact, the gas cell in our setup is even $\sim 100 \times$ wider. Hence, the detection specificity is not degraded.

D. Molecular Saturation and Maximum Allowable Signal Power

High incident signal power may deplete the population of unexcited molecules, preventing additional photon absorption if the signal power is further increased. Such saturation effect, occurring at the tip of the spectral line first, not only leads to spectral broadening, but also nonlinear dependency between power absorption and gas concentration. The maximum probing signal power flux $I$ can be estimated by [10]:

$$I = \frac{3e_0 c h (\Delta f)^2}{D^2},$$ \hspace{1cm} (21)

where $e_0$ is the permittivity of vacuum ($8.85 \times 10^{-12}$ F/m), $c$ is the speed of light ($3 \times 10^8$ m/s), $h$ is Planck’s constant ($6.6 \times 10^{-34}$ J·s), $D$ is molecular dipole moment, and $\Delta f$ is the absorption linewidth. The dipole moment of most polar molecules is on the order of $10^{-18}$ esu (in CGS system) or $3.3 \times 10^{-30}$ C·m. Hence, the saturation power flux of a low-THz spectrometer is $\sim 0.3$ mW/mm$^2$. Normally, the gas cell cross-sectional area is large enough that power saturation is avoided; however, if a single-mode WR-3.4 waveguide is used for sensor miniaturization, the maximum allowable signal power reduces to $\sim 0.1$ mW, which is achievable in CMOS circuits (including our chip). This poses a fundamental limit for the SNR (shown in (11)) that a single-tone spectrometer can provide. In Section III-C, we will show how this problem is addressed by our comb spectrometer.

E. Optimum Path Length of Gas Cell and Maximum Achievable Sensitivity

The minimum detectable gas absorption coefficient $\alpha_{gas, min}$ is derived when the spectrometer baseband SNR (shown in (11)) is unity:

$$\alpha_{gas, min} = \frac{4}{I} \sqrt{\frac{kT_n \Delta \nu}{P_0 e^{-\alpha_0 L}}},$$ \hspace{1cm} (22)

A longer gas cell path length $L$ enables stronger absorption but also higher waveguide power loss. In (22), an optimum length $L_{opt}$ exists to achieve the minimal value of $\alpha_{gas, min}$. By having $\frac{d \alpha_{gas, min}(L)}{dL} = 0$, we derive:

$$L_{opt} = \frac{2}{\alpha_0}$$ \hspace{1cm} (23)

and the ultimate $\alpha_{gas, min, achievable}$ by the electronics is:

$$\alpha_{gas, M1N} = 2e\alpha_0 \sqrt{\frac{kT_n \Delta \nu}{P_0}}.$$. \hspace{1cm} (24)

Therefore, the minimum detectable gas concentration is expressed as:

$$\gamma_{min} = \frac{\alpha_{gas, M1N}}{\alpha_{gas, pure}} = \frac{2e\alpha_0}{\alpha_{gas, pure}} \sqrt{\frac{kT_n \Delta \nu}{P_0}},$$ \hspace{1cm} (25)
where \( \alpha_{\text{gas,pure}} \) is the absorption coefficient of pure gas sample.

Currently, most THz spectrometers are based on the propagation of a collimated Gaussian beam inside a bulky gas cell. In the future, if single-mode metal rectangular waveguide is adopted as gas chamber, the optimum gas cell length \( L_{\text{opt}} \) and the associated minimum detectable absorption intensity \( \alpha_{\text{gas,MIN}} \), as a function of path loss \( \alpha_0 \), are plotted in Fig. 3. Here, a signal power of 0.1 mW is assumed, which is the threshold power for molecular saturation (Section II-D). A single sideband noise figure (NF) of 17 dB is assumed. Both metrics are achieved by our CMOS comb spectrometer (see Section IV). For a typical waveguide loss of 0.25 dB/cm (i.e. \( \alpha_0=0.058 \text{ cm}^{-1} \)), the minimum detectable absorption intensity \( \alpha_{\text{gas,MIN}} \) is \( 1.6 \times 10^{-8} \text{ cm}^{-1} \) with 1 Hz bandwidth at 296 K. The optimum gas cell length is \( \sim 35 \text{ cm} \). Table I shows the sensitivity or minimum detectable gas concentration based on the calculated minimum detectable absorption coefficient. A sensitivity at ppm level is predicted. A standard pre-concentration gain of \( 10^3 \) (like the one used in [13]) will further increase the spectrometer sensitivity to ppt level. According to Fig. 3, if low-loss hollow dielectric waveguide is used, the sensitivity can be further improved by \( 2 \sim 3 \times \). Although the gas cell waveguide has an optimum length of 0.1~1 m, they can be folded to shrink the size of the spectroscopy system (in conjunction with the usage of micro vacuum pumps).

### III. COMB-BASED SPECTROSCOPY: DESIGN AND CHIP-SCALE PROTOTYPE

In this section, we present the design of a new spectrometer, which leverages the large integration capability of CMOS technology, in order to improve spectral-scanning speed and sensitivity using parallelism.

#### A. Dual-Frequency-Comb, Bi-Directional Spectrometer

The dual-frequency-comb spectrometer consists of two identical frequency-comb chips. Each chip works under transmitting (TX) and receiving (RX) modes simultaneously. Shown in Fig. 1(b), 10 equally-spaced comb lines with 10 GHz frequency interval are transmitted from Chip A through the gas sample and coupled into Chip B via on-chip antennas. Meanwhile, inside Chip A, the above 10 comb lines are also used as local-oscillator (LO) signals for the heterodyne mixing of another 10 comb lines radiated from Chip B. A 950-MHz frequency offset is also created between the output radiation spectra of Chip A and Chip B as intermediate frequency (\( f_{\text{IF}}=950 \text{ MHz} \)).

Fig. 4 shows the block diagram of the comb chip [21]. The chip is driven by an external Q-band signals (\( f_{\text{ref}} \)) at \( \sim 46 \text{ GHz} \), which is then frequency multiplied by \( 3 \times \). The frequency tripled signal at \( 3f_{\text{ref}} \) is injected into up- and down-conversion chains. The two chains produce evenly-spaced signal tones through cascaded single-sideband (SSB) mixers. Each SSB mixer shifts the frequency of single tone by 5 GHz; such frequency spacing is determined by a static digital frequency divider (\( \div 2 \)), which is built inside each mixer and has a 10 GHz clock input \( f_D \). In simulation, the rejection of
In Fig. 4, this is readily accomplished by tuning the Q-band bandwidth, the comb spectrum only needs to shift by 10 GHz. In summary, a comb spectrum spanning from 220 to 320 GHz and with frequency spacing of 10 GHz is realized.

It is also noteworthy that, to fully cover the 100-GHz bandwidth, the comb spectrum only needs to shift by 10 GHz. In Fig. 4, this is readily accomplished by tuning the Q-band driving signal \( f_{ref} \) from 45 to 46.67 GHz. On top of this, \( f_{ref} \) is wavelength modulated with a modulation frequency of \( f_m \) and frequency deviation of \( \Delta f/6 \), which is needed for molecular-sensing (illustrated in Fig. 1(c)).

B. Design of the Active Molecular Probe

The active molecular probe (AMP) inside each comb stage is the enabling circuit for simultaneous frequency-doubling and radiation of a transmitted comb line, as well as the down-mixing of another received comb line. The 3D structure of AMP is shown in Fig. 5(a), which consists of only one pair of MOSFETs.

For the frequency doubling of the TX mode, the MOSFETs are driven by a differential fundamental \( (f_0) \) signal through microstrip transmission line TL1 (Fig. 5(b)). Meanwhile, a signal feedback through Slot2 is deployed between the transistor drains and AMP inputs, so that the power gain of the transistor pair at \( f_0 \) is boosted to a theoretical limit of \( \sim 4U \) [26], where \( U \) is the unilateral gain. As one example, when \( f_0 \) equals 137.5 GHz, the gain is improved from 7 dB to 12 dB, which enhances the doubler efficiency from 18% to 43% [21]. The high efficiency is also due to the quarter-wavelength Slot1, which translates the virtual ground at the AMP top to high impedance termination at transistor drains. This generates large drain voltage swing, hence stronger nonlinearity.

At \( f_0 \), Slot2 supports the feedback flow of the input differential signal, because its cutoff frequency for the associated quasi-TE mode wave (Fig. 5(b)) is zero. In comparison, at \( 2f_0 \), the generated common-mode signal is blocked by Slot2, because the cutoff frequency for the associated TM-mode wave is \( \sim 6 \text{THz} \). Such mode-filtering mechanism effectively isolates the harmonic signal from the lossy transistor gates (Fig. 5(c)). Meanwhile, 2\( f_0 \) Slot1 is half-wavelength, and works as an on-chip folded-slot antenna, because all the standing waves inside the folded branches are in-phase. Such compact, close-to-device radiator structure achieves 45% radiation efficiency in simulation.

Under the RX mode, the incident wave at \( 2f_0 + f_{IF} \) is coupled by the same reciprocal antenna Slot1. The MOSFETs now behave as a resistive-mode sub-harmonic mixer with the large-power input at \( f_0 \) as LO signal. The IF signal is extracted from the top of AMP through an integrated RF choke (Fig. 5(a)) and an external bias tee. With signal filtering at the output, the down-converted irrelevant comb lines are not presented at baseband. For the entire comb spectrometer, 10 IF channels can be connected to separate external IF amplifiers and detectors for parallel data processing.

C. Advantages of Dual-Frequency-Comb Spectrometer

Compared to prior optical combs based on mode-locked laser pulse [27], [28], the CW-type electronic comb offers excellent tuning capability, phase coherency, and high frequency resolution. It also enables scalability to higher bandwidth through extended cascading of AMP channels. In the dual-frequency-comb architecture, since 10 probing comb pairs work simultaneously, it leads to a much faster scanning speed through parallel operation by at least a factor of 20x. In addition to that, significant spectroscopic performance is gained, due to the following reasons.

Firstly, our chip architecture breaks the bandwidth-efficiency tradeoff of conventional RF-to-THz designs, as mentioned in Section I. By partitioning the overall spectrum, the
required tuning range for each channel is reduced below 4.5%, which allows for high-Q topology (e.g. the dual-transmission-line feedback in AMPs) and keeps peak performance across a broad frequency range. Shown in Fig. 6(a) is a statistic of silicon-based sources above 200 GHz, which exhibits clear inversely proportional dependency between the radiated power and bandwidth. In contrast, our work demonstrates broad bandwidth without degrading the radiated power and noise performance.

Secondly, as is discussed in Section II-D, the maximum radiated power, is limited by the saturation effect of molecules, especially for small-size gas cells. Subsequently, it determines the ultimate sensitivity for a given total scanning time. In our comb, the total radiated power exceeds such limitation while keeping each single tone still below the saturation threshold. Given an fixed total scanning time and total bandwidth, since the integration time per frequency point is 20× longer (i.e. smaller ∆ν in (11)) due to the parallelism, the comb architecture achieves better sensitivity.

Thirdly, the energy efficiency is significantly improved. Due to the aforementioned bandwidth-efficiency tradeoff, the total energy consumption of conventional single-tone spectrometers has a square or cubic dependency over operational bandwidth (Fig. 6(b)). In comparison, without extending scanning time, the energy consumption of dual-frequency-comb spectrometer increases linearly with higher bandwidth (i.e. more cascading comb stages). The simultaneous transmit-receive scheme enabled by our AMP design further reduces the energy consumption by ∼2×. For an fractional bandwidth of ∼40% (this work), the estimated overall energy saving is 10 to 100× compared with conventional spectrometer scheme.

IV. EXPERIMENTAL RESULTS

The comb spectrometer chip is fabricated using TSMC 65-nm bulk CMOS process (f_{max}=250 GHz). The chip size is 3×2 mm² and the die photo is shown in Fig. 7(a). The chip is mounted on an FR-4 PCB with wire bonding. A 1-inch diameter high-resistivity silicon lens is attached to the backside of the chip (shown in Fig. 7(b)), in order to enhance the radiation coupling to free space. The lens has a hemispheric shape, so the beam out of the chip is not further collimated.

![Photograph of: (a) CMOS THz comb transceiver based on 65-nm bulk CMOS process (2×3 mm²) and (b) the packaged chip on PCB with 1-inch diameter silicon lens attached at the backside.](image)

![Measurement results of (a) the spectrum of 10 comb lines from 225-to-315GHz with 10-GHz spacing, (b) the spectrum of 275-GHz comb line with 10-kHz span, (c) the phase noise of the 275-GHz comb line, 10-GHz reference signal and 17.2-GHz LO signal for EHM (16th harmonic) used for comb-line phase noise measurement, (d) effective isotropic radiated power (EIRP), and (e) single sideband noise figure (SSB NF).](image)
results from the limited diameter of silicon lens compared with the dimension of CMOS chip. Each on-chip antenna thus has a non-negligible offset to the geometric center of the lens, and generates radiation beam deviated towards slightly different direction. In the RX mode, the SSB noise figure (NF) of each AMP is measured by using an OML network analyzer frequency extender as the broadband radiation source. Shown in Fig. 8(e), the NF including the loss of the on-chip antennas, ranges from 14.6 to 19.5 dB within the operational bandwidth.

The sample is injected from a gas cylinder with its pressure of the single-mode waveguide mentioned in Section II-E. Fig. 9(a). The demonstration system adopts free space radiation beam. Two CMOS comb chips are used as transceivers, precisely controlled by a turbo molecular pump and a vacuum gauge. Two CMOS comb chips are used as transceivers, which are driven by two phase-synchronized signal sources (with a frequency difference to generate $f_{IF}=950$ MHz). The output/input beams of the chips are collimated using a pair of Teflon lenses, and are coupled to the gas chamber through quartz vacuum windows. Wavelength modulation spectroscopy (WMS) with a modulation frequency $f_m$ of 50 kHz and a frequency deviation $\Delta f$ of 360 kHz is performed. A lock-in amplifier (Stanford Research SR865A) generates the $f_m$ modulation signal and measures the amplifier output envelope of the baseband rectifier, which contains the spectral information. Due to the limited hardware, the molecular spectrum is scanned channel by channel.

Firstly, based on the measured chip performance in Section IV-A, the link budget is calculated to estimate sensitivity. For a typical channel at 275 GHz ($\lambda=1.1$ mm), if no lens nor gas cell is placed, the link SNR can be estimated by:

$$SNR_{\text{linkbudget}} = \frac{P_0 D^2 \lambda^2}{(4\pi L)^2 kT_n} = 92 \text{ dB (} \Delta \nu = 1 \text{ Hz)}$$

where an emitted power $P_0$ of 0.5 mW, an SSB NF of 17 dB, a total path length $L$ of 1 m and a typical directivity $D$ of 10 dB are used. When the loss from vacuum windows, gas cell and internal reflection is included, the SNR will be even lower. Fortunately, with the well-aligned Teflon lenses, which increase the link budget by $\sim$20 dB, the actual SNR reaches 98 dB (1-Hz bandwidth) in our measurement. This indicates that our spectrometer has a minimum detectable absorption of $\alpha_{\text{gas,min}} = 7.2 \times 10^{-7} \text{ cm}^{-1}$ according to (22). The maximum detectable absorption of the current system is $6.6 \times 10^{-2} \text{ cm}^{-1}$, which corresponds to 99% absorption over a 70 cm path. Therefore, the dynamic range of the current system is 50 dB.

**B. Demonstration of THz Spectroscopy**

A spectroscopy experimental setup is built as shown in Fig. 9(a). The demonstration system adopts free space radiation and a 70 cm gas cell with 2 inches diameter instead of the single-mode waveguide mentioned in Section II-E. The sample is injected from a gas cylinder with its pressure precisely controlled by a turbo molecular pump and a vacuum gauge. Two CMOS comb chips are used as transceivers, which are driven by two phase-synchronized signal sources (with a frequency difference to generate $f_{IF}=950$ MHz). The output/input beams of the chips are collimated using a pair of Teflon lenses, and are coupled to the gas chamber through quartz vacuum windows. Wavelength modulation spectroscopy (WMS) with a modulation frequency $f_m$ of 50 kHz and a

$$\text{Measured}$$

**Fig. 10.** Measured spectrum of OCS using WMS at $f_m$: (a) full band spectrum versus the recorded integrated intensity (LGINT) from JPL molecular catalog and (b) details of OCS spectral lines at 231.061 GHz and 316.146 GHz, respectively.
The entire spectrum is recorded by WMS at 100-GHz bandwidth with 10-kHz step size and 1-kHz integration bandwidth. Details of two OCS spectral lines at 231.061 GHz and 316.146 GHz are shown in Fig. 11(b), as is illustrated in Fig. 1(c).

Next, spectroscopy for carbonyl sulfide (OCS) is investigated. Fig. 10(a) presents the measured spectrum of OCS from 220- to 320 GHz under 10-Pa pressure, which matches the JPL molecular catalog [12], and exhibits a period of 12.15 GHz. The FWHM of the spectral line is 83 mV and the measured baseband RMS noise voltage $V_{\text{noise}}$ is 2.8 $\mu$V/Hz; as a result, the output SNR$_{v/v}$ is $2.9 \times 10^4$ (or 89.2 dB) with 1 Hz bandwidth. We note that this matches the theoretical calculation of $3.0 \times 10^4$ very well, which further validates our analysis in Section II-A.

At the pressure of 10 Pa, the spectrum of another molecule, acetonitrile (CH$_3$CN), between 220 to 320 GHz with a period of 18.4 GHz is also measured and shown in Fig. 11(a). Details of two spectral sections within 220.2- to 220.8 GHz and 312.1- to 312.7 GHz are given in Fig. 11(b), which again agree with the JPL molecular catalog [12]. The peak absorption coefficient for the 294.251-GHz spectral line (at 10 Pa) is 0.017 cm$^{-1}$. An output baseband SNR$_{v/v}$ of $7.4 \times 10^3$ is measured for 1 Hz bandwidth. This is lower than the theoretical SNR derived from (11), mainly because the pressure-broadening effect for acetonitrile is more significant at 10 Pa, and the frequency deviation that we used ($\Delta f = 360$ kHz) does not optimally match the larger molecular linewidth ($\sim 2$ MHz).

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The volume ratio of the two gas samples is of the gas mixture is 10 Pascal. The sensitivity is determined by the baseline ripple, WMS at 2 \( f \) \( s \) from the spectrum of an OCS and CH\(_3\)CN gas mixture. The pressure of the OCS gas mixture is 10 Pascal. The volume ratio of the two gas samples is 10 Pascal. The sensitivity is determined by the baseline ripple, WMS at 2 \( f \) \( s \) from the spectrum of an OCS and CH\(_3\)CN gas mixture. The pressure of the OCS gas mixture is 10 Pascal. The volume ratio of the two gas samples is 10 Pascal. The sensitivity is determined by the baseline ripple, WMS at 2 \( f \) \( s \) from the spectrum of an OCS and CH\(_3\)CN gas mixture. The pressure of the OCS gas mixture is 10 Pascal. The volume ratio of the two gas samples is 10 Pascal. The sensitivity is determined by the baseline ripple, WMS at 2 \( f \) \( s \) from the spectrum of an OCS and CH\(_3\)CN gas mixture. The pressure of the OCS gas mixture is 10 Pascal. The volume ratio of the two gas samples is 10 Pascal. The sensitivity is determined by the baseline ripple, WMS at 2 \( f \) \( s \) from the spectrum of an OCS and CH\(_3\)CN gas mixture. 

Lastly, there is one possible error that the TX spurs shown in Fig. 8(a) probe the spectral lines, which are then subsequently down-converted into IF band by mixing with corresponding LO spurs in the RX. However, in simulation, the LO-power-dependent mixer conversion loss is 84 dB, and the resultant inter-modulation components in IF band are \( \sim 100 \) dB lower than the actual IF signals. Thus, it is not a limiting factor of the sensitivity. For validation, Fig. 13(a) presents the measured spectrum of an OCS and CH\(_3\)CN gas mixture. The pressure of the gas mixture is 10 Pascal. The volume ratio of the two gas samples is \( V_{\text{OCS}} : V_{\text{CH}_3\text{CN}} \approx 1 : 60 \). To further reduce the baseline ripple, WMS at 2 \( f \) \( m \) is performed. The measured spectra (shown in Fig. 13(b) and Fig. 13(c)) are examined; no false spurs are observed besides the superposed OCS and CH\(_3\)CN spectra.

VI. Conclusions

A CMOS dual-frequency-comb spectrometer is presented in this paper. A comparison between this work and previous publications is given in Table II. Through a parallel spectral scanning using 20 comb lines, this spectrometer achieves more than 20\( \times \) speed enhancement and breaks the bandwidth-efficiency tradeoff in conventional circuit design. A total radiated power of 5.2 mW and a 14.6-to-19.5 dB SSB NF are obtained in measurements, which are not only the best among all silicon-based THz electronics, but also even comparable with the performance of compound semiconductor devices (e.g. GaAs Schottky-barrier diode). The measured minimum detectable absorption coefficient of this work is 7.2 \( \times \) 10\(^{-7} \) cm\(^{-1} \), which is higher than the prior work in silicon, but still two orders lower than that reported in [13]. This is mainly because of the lower on-chip antenna gain (10 dBi versus 25 dBi in [13] for TX and RX). Such problem can be solved in the future by implementing multiple coherent radiators for each comb channel (hence higher antenna gain).

In addition, fundamentals of frequency scanning spectrometer are discussed and validated. The measured SNR matches the theoretical prediction. The Townes noise due to square-law detection is the major limiting factor for sensitivity so far, which leads to a linear dependency of SNR versus gas concentration. It is an interesting issue to be addressed before we encounter shot noise. Based on the current silicon semiconductor technology, the sensitivity of a fully-optimized spectrometer should reach below 1-ppm level (or below 10-ppt with pre-concentration).

This technology is expected to be applied in future biomedical areas. The concentration of volatile organic compounds (VOCs) in human exhaled breath ranges from ppm to ppb level [1], [4], and the fluctuation of specified VOCs, normally at ppm level, can be utilized as bio-markers for disease diagnosis. As shown in this work, sufficient sensitivity is provided by silicon-based rotational spectrometers. This enables fast, non-invasive monitoring/analysis of human health conditions.

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References


<table>
<thead>
<tr>
<th>Ref.</th>
<th>Spectrometer Architecture</th>
<th>Technology</th>
<th>Frequency (GHz)</th>
<th>TX Radiated Power (mW)</th>
<th>RX SSB Noise Figure (dB)</th>
<th>Path Length (m)</th>
<th>Minimum Detectable Absorption (cm$^{-1}$) with 1-Hz bandwidth</th>
</tr>
</thead>
<tbody>
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<td>[11]</td>
<td>Single-Tone</td>
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<td>~1$^1$</td>
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<tr>
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<td><strong>This Work</strong></td>
<td><strong>Dual-Frequency-Comb</strong></td>
<td><strong>65nm CMOS</strong></td>
<td><strong>220~320</strong></td>
<td><strong>5.2$^5$</strong></td>
<td><strong>14.6~19.5</strong></td>
<td><strong>0.7</strong></td>
<td><strong>7.2×10$^{-7}$</strong></td>
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</table>

$^1$ The reported radiated power and noise figure are estimated from performance of typical VDI instrument.

$^2$ $\alpha_{\text{gas.min}}$=0.017 cm$^{-1}$/100 Pa/0.008 Pa=2.7×10$^{-5}$ cm$^{-1}$ is calculated based on CH$_3$CN with pressure of 6×10$^{-5}$ Torr (0.008 Pa).

$^3$ The reported SNR is 300 with 0.01 s integration time.

$^4$ $\alpha_{\text{gas.min}}$=0.0013 cm$^{-1}$/1000=4.3×10$^{-10}$ cm$^{-1}$ is calculated based on 248.28 GHz spectral line of CH$_3$OH with pressure of 13 Pa. Its absorption coefficient is 0.0013 cm$^{-1}$ based on [40]. The measured SNR is 30 based on Fig.18 of [14]. The integration time hasn’t been specified.

$^5$ The reported power is EIRP, which includes the antenna gain of the chip.

$^6$ Effective path length is larger than physical length due to multi-reflection inside high Q semiconfocal cavity.

*Total radiated power of THz comb. The average radiated power is 0.5 mW for each comb line.*

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