

High-Resolution Fourier-Transform IR Spectroscopic Determination of Impurities in Silicon Tetrafluoride and Silane Prepared from It

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Received February 15, 2006

Abstract—The impurity compositions of silicon tetrafluoride and silane prepared from it have been determined by high-resolution Fourier-transform IR spectroscopy. In the spectra of SiF₄ samples differing in purity, we have identified rovibrational bands arising from Si₂F₆O, SiF₃OH, HF, SiF₃H, SiF₂H₂, SiH₃F, CH₄, CO₂, and CO impurities. Their detection limits lie in the range 9×10^{-5} (CO₂) to 3×10^{-3} mol % (Si₂F₆O). In the spectra of SiH₄ samples of different purity, we have detected CH₄, CO₂, SiF₃H, SiF₂H₂, and SiF₄ impurities. Their detection limits lie in the range 8×10^{-5} (CO₂) to 1×10^{-3} mol % (SiF₄).

DOI: 10.1134/S0020168506080231

INTRODUCTION

Silicon tetrafluoride, SiF₄, is a large-scale by-product in the manufacture of phosphoric fertilizers and some ore dressing processes [1]. On the other hand, silicon tetrafluoride has recently received considerable attention as one of the cheapest and most attractive precursors to silicon, which is being used increasingly in industrial applications. Unfortunately, the procedures proposed to date are inferior in efficiency and cost to the existing industrial processes for silicon manufacturing [2]. At the same time, in the approach recently developed by Devyatykh et al. [3] for producing isotopically enriched ²⁸Si, ²⁹Si, and ³⁰Si—thermal decomposition of an appropriate isotopically enriched silane—silicon tetrafluoride is essentially the only silicon-containing volatile precursor with consideration for the known advantages of using volatile fluorides in centrifugal isotopic enrichment processes. The key steps of this approach are the synthesis and purification of silicon tetrafluoride, isotopic enrichment, conversion to isotopically enriched silane, purification and decomposition of the silane, and preparation of polycrystalline silicon—from several grams for the rare isotopes ²⁹Si and ³⁰Si to hundreds of grams and, in the future, several kilograms for ²⁸Si.

In devising processes for the synthesis and purification of isotopically enriched SiF₄ and SiH₄, an important issue is the ability to monitor a number of impurities in these substances, primarily those containing hydrogen, oxygen, and carbon.

High-resolution (up to 0.01 cm⁻¹) Fourier-transform IR (FTIR) spectroscopy is used rather rarely to determine impurities in the gas phase, primarily because only a limited number of laboratories have appropriate vacuum instruments at their disposal. In contrast to diode laser spectroscopy, this method provides information about the chemistry and state (clustering, complexing, adsorption) of impurities in a broad spectral range, typically from 400 to 5000 cm⁻¹. Its sensitivity depends primarily on the integral absorption coefficient of the analytical line or band and the intensity of the absorption spectrum of the host substance and impurities in the spectral range in question. The sensitivity of high-resolution IR spectroscopy is typically 10⁻⁵ to 10⁻³ mol % and may reach in some cases 10⁻⁷ to 10⁻⁶ mol % [4, 5].

A literature search revealed no reports on the use of high-resolution FTIR spectroscopy for determining the impurity composition of silicon tetrafluoride or silane. At the same time, IR spectroscopic techniques employing nonvacuum diffraction instruments (with a resolu-

tion of several cm^{-1}) were used in a number of studies [6–9] for semiquantitative analysis of SiF_4 . In the case of hexafluorodisiloxane, $\text{Si}_2\text{F}_6\text{O}$, whose analytical band at 839 cm^{-1} has a full width at half maximum of about 10 cm^{-1} , this approach is justified if the content of this impurity is no lower than 10^{-2} to 10^{-1} mol \% [6]. At the same time, in the case of light impurities, such as H_2O , HF , CO_2 , and CO , whose bands have a rather complex rovibrational structure, the data reported by Sviderskii et al. [8] and Nikonov et al. [9] appear questionable, especially those for water.

In this paper, we examine the possibility of using high-resolution (up to 0.01 cm^{-1}) FTIR spectroscopy for determining the impurity composition of isotopically unmodified silicon tetrafluoride and silane prepared from it.

EXPERIMENTAL

We analyzed the IR spectra of SiF_4 and SiH_4 samples differing in purity. Note that, to assign impurity bands with more confidence, we also measured the IR spectra of concentrates of high- and low-boiling impurities taken from a fractional column. In addition, we used silane samples prepared by a fluoride-free process.

The IR absorption spectra of silicon tetrafluoride and silane were measured in the range 400 to 4500 cm^{-1} on a Bruker IFS-120 HR high-resolution vacuum (residual pressure, $\leq 3.9\text{ Pa}$) FTIR spectrometer, with the gas cells constantly kept in the cell compartments. In most measurements, we used a multipass gas cell with a 975-cm pathlength (for studies of silane) and a gas cell with a 20-cm pathlength (for silicon tetrafluoride) made of stainless steel 12Kh18N10T, with indium-gasketed CaF_2 and ZnSe windows. Through the leak-in system, passing through a vacuum flange, the cells were connected to turbo and roughing pumps, which ensured a residual pressure in the cells no higher than 130 Pa . The gas pressure in the cells was varied from 1.3×10^3 to $78 \times 10^3\text{ Pa}$ and was monitored by an MKS Baratron 722A pressure sensor with an accuracy of 0.5% . Spectra were measured with a resolution of 0.01 to 0.1 cm^{-1} using liquid-nitrogen-cooled MCT and InSb detectors. The signal was acquired over 250 – 900 scans. Before measurements, we recorded the absorption of evacuated empty cells. The results were subsequently used as a background spectrum, I_0 . Determination of H_2O and CO_2 required more careful, longer time preparation of the experimental setup. In view of this, the instrument and cells were pumped for several days.

In assigning absorption bands and lines of impurities in the gas phase, we used earlier data for SiF_4 and SiH_4 [10, 11], HITRAN Database resources [12] (HF , H_2O , CO , CO_2 , and CH_4 molecules), and earlier data

for hexafluorodisiloxane, trifluorohydroxysilane, and fluorosilanes [13–21].

In quantitative determination of impurities, we used the standard Bouguer–Lambert–Beer equation:

$$p = \frac{RTc_0}{AlN_A}B. \quad (1)$$

Here, p is the partial pressure of the impurity (mm Hg), B is the integrated intensity of the spectral line or band (cm^{-1}), $R = 6.236 \times 10^4\text{ mm Hg cm}^3/(\text{mol K})$ is the gas constant, T is the absolute temperature (K), $c_0 = 2.9979 \times 10^{10}\text{ cm/s}$ is the velocity of light in vacuum, A is the integral absorption coefficient (IAC) of the line or band ($\text{cm}^2/(\text{s molecule})$), l is the optical pathlength (cm), and $N_A = 6.022 \times 10^{23}\text{ mol}^{-1}$ is the Avogadro number.

Knowing the partial pressure of an impurity and the total pressure in the cell, one can calculate the percentage of the impurity:

$$C = p/p_{\text{total}} \times 100\%. \quad (2)$$

Here, C is the molar percent of the impurity, p is its partial pressure, and p_{total} is the total pressure in the cell.

HF , H_2O , CO , CO_2 , and CH_4 impurities, for which reliable values of analytical lines are available, were determined to within 5% accuracy. For $\text{Si}_2\text{F}_6\text{O}$, SiF_3OH [14], and fluorosilanes [21], we used the IAC values determined earlier for the entire rovibrational band by first-principles quantum-chemical calculations. This significantly increased the pooled error of determination, which was at least 50% according to our estimates. The detection limits for the above impurities were estimated using the 3σ criterion.

Silicon tetrafluoride was prepared by decomposing sodium hexafluorosilicate and was purified by low-temperature fractional distillation [22]. Silane was synthesized by reacting silicon tetrafluoride with calcium hydride and was then purified by low-temperature fractional distillation [22].

RESULTS AND DISCUSSION

Figures 1 and 2 show wide-scan IR absorption spectra of silicon tetrafluoride and silane. As seen, the spectra of both compounds contain very strong intrinsic absorption bands in the ranges 950 – 1350 and 1750 – 2100 cm^{-1} for SiF_4 and 1700 – 2400 and 700 – 1200 cm^{-1} for SiH_4 . These bands are due to fundamental modes, composite modes, and overtones. The absorption lines of individual impurities lie on the wings of the strongest bands or heavily overlap with them and are, therefore, rather difficult to identify even at the maximum resolution in this study (0.01 cm^{-1}). Consider in greater detail

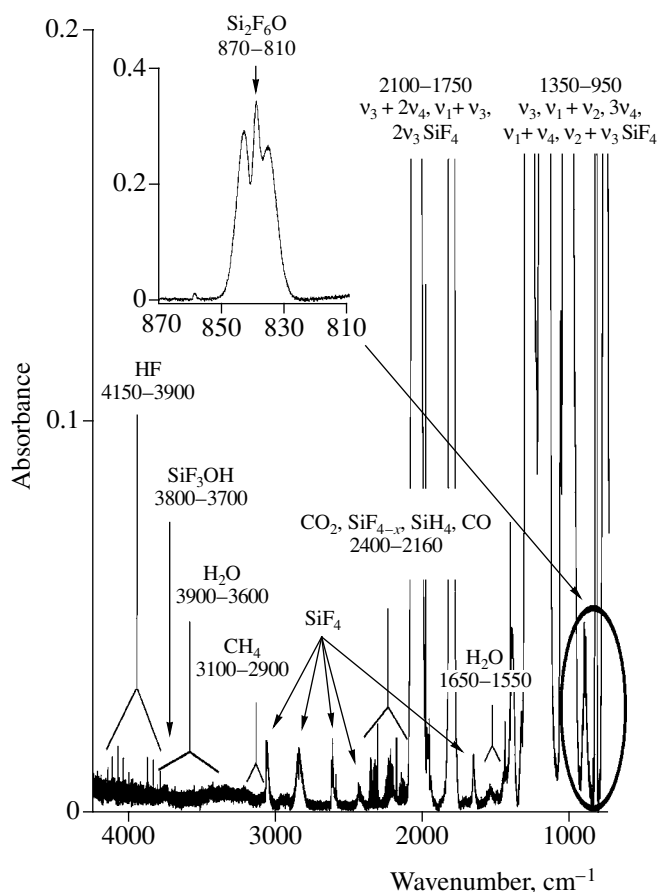


Fig. 1. Absorption spectrum of SiF_4 in the range 750–4250 cm^{-1} ($p(\text{SiF}_4) = 7.8 \times 10^4$ Pa, $l = 20$ cm, 0.05-cm^{-1} resolution) showing fundamental and composite absorption bands; the arrows mark impurity absorptions. Inset: absorption band of $\text{Si}_2\text{F}_6\text{O}$.

the spectral ranges containing impurity-related absorption lines.

3950–4150 cm^{-1} . This spectral range includes the *R* branch of the absorption band of the ν_1 fundamental transition of molecular hydrogen fluoride—one of the major impurities in SiF_4 and SiH_4 . According to Krasnov et al. [23], the absorption band of HF is centered at 3960 cm^{-1} . As seen in Fig. 3, the spectrum of SiF_4 before purification shows well-resolved lines at 4109.94, 4075.29, 4038.96, and 4000.99 cm^{-1} , which correspond to an HF content of $(5.0 \pm 0.5) \times 10^{-4}$ mol %.

3600–3900 cm^{-1} . This spectral range is of interest primarily because it contains absorption lines belonging to the stretching modes ν_1 and ν_3 of molecular water. The content of molecular water in silicon tetrafluoride, a substance highly reactive with moisture, is the subject of much controversy. At the same time, according to preliminary studies of gas-phase SiF_4 hydrolysis [14], supplemented later by experiments

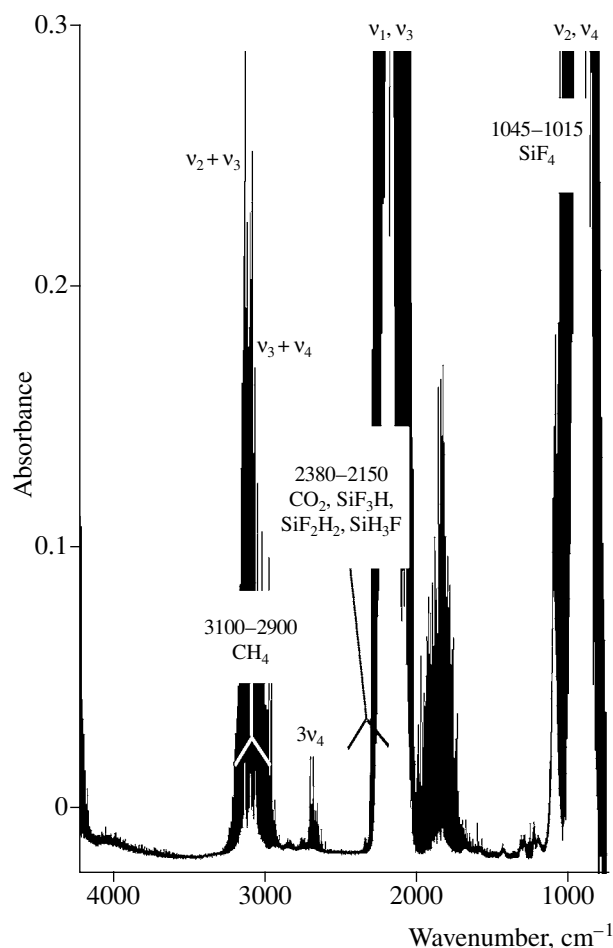
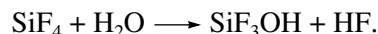


Fig. 2. Absorption spectrum of SiH_4 in the range 750–4250 cm^{-1} ($p(\text{SiH}_4) = 6.5 \times 10^3$ Pa, $l = 20$ cm, 0.1-cm^{-1} resolution) showing fundamental and composite absorption bands; the arrows mark impurity absorptions.

with heavy water (the results will be presented in a subsequent communication), a mixture of silicon tetrafluoride and water may be stable for a rather long time. It can be concluded therefore that the portion of the spectrum of water shown in Fig. 4, recorded after the cell and instrument had been treated as described in the EXPERIMENTAL section, is indeed due to the molecular water in silicon tetrafluoride, $(6 \pm 1) \times 10^{-3}$ mol % in this sample. In none of the SiH_4 samples studied did we find H_2O levels above the detection limit in our measurements, 1×10^{-3} mol %.

According to low-resolution IR spectroscopic studies of impurities in silicon tetrafluoride [24], the spectral range under consideration may contain a band peaked at 3762 cm^{-1} . As shown in detailed experimental and theoretical studies [14], this band is due to stretches of the OH group of trifluorohydroxysilane, SiF_3OH , forming according to the simplified scheme



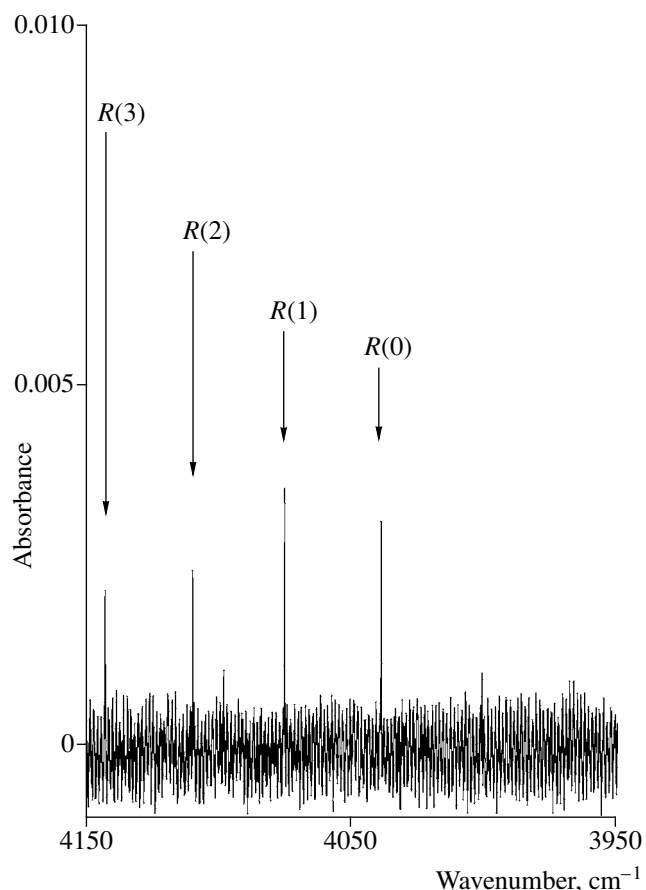


Fig. 3. Portion of the *R* branch of the rovibrational absorption band ν_{HF} in the spectrum of SiF_4 before purification ($p(\text{SiF}_4) = 2.6 \times 10^3$ Pa, $l = 975$ cm, 0.01-cm^{-1} resolution) and positions of analytical rotational lines (4000.99 , 4038.96 , 4075.29 , and 4109.94 cm^{-1}).

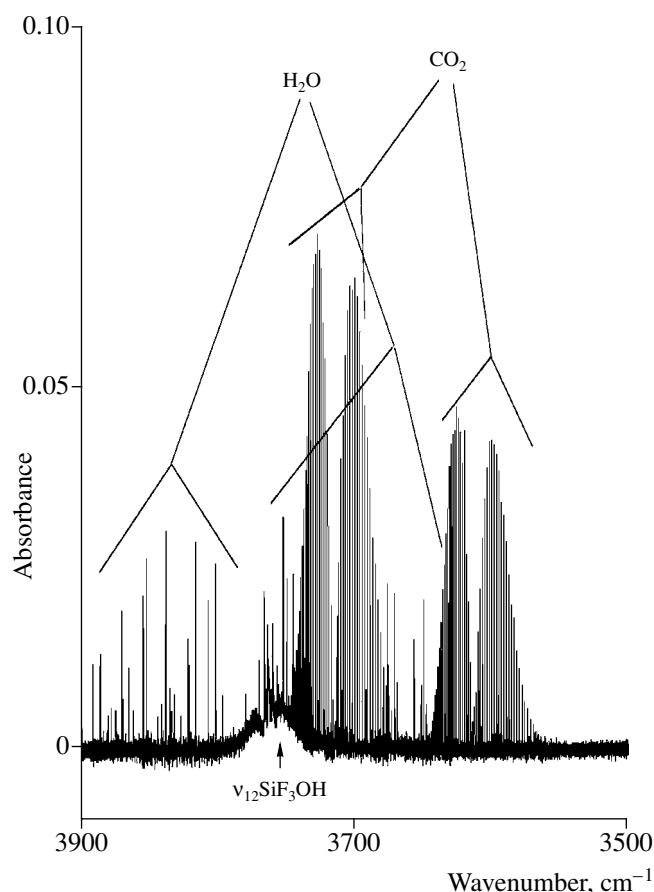


Fig. 4. Rovibrational absorption bands of H_2O (ν_1 and ν_3), CO_2 (Fermi-resonance bands), and SiF_3OH (ν_{12} at 3762 cm^{-1}) impurities in SiF_4 before purification; $p(\text{SiF}_4) = 5.8 \times 10^3$ Pa, $l = 975$ cm, 0.01-cm^{-1} resolution.

The formation of this intermediate in silicon tetrafluoride hydrolysis is typical of unpurified SiF_4 . The SiH_4 samples showed no impurity-related absorption in the spectral range in question.

2800–3200 cm^{-1} . This spectral range includes rovibrational components of stretching modes of light hydrocarbons, $\text{C}_1\text{--C}_4$. The strongest lines belong to the stretching mode ν_3 of methane [12]. Several of our silicon tetrafluoride samples contained CH_4 , at a level no higher than 1×10^{-3} mol %, even in impurity concentrates.

Rovibrational lines of methane impurity in silane are difficult to reveal because the stretching band ν_3 of methane overlaps with the $\nu_2 + \nu_3$ and $\nu_3 + \nu_4$ absorption bands of SiH_4 . In view of this, to identify the absorption bands of methane impurity in silane we used the spectrum, taken under the same conditions, of silane prepared by a fluoride-free process.

Figure 5 shows a portion of the spectrum of silane prepared by a fluoride-free process and containing CH_4

at a level no higher than a few times 10^{-6} mol % (according to gas chromatography data) (curve 1), a portion of the spectrum of silane prepared from SiF_4 with no subsequent purification (curve 2), and the difference spectrum of curves 1 and 2 (curve 3). The resultant spectrum is in perfect agreement with the reference spectrum for this portion of the ν_3 band of silane [12]. According to our data, the methane content of the sample is $(8 \pm 4) \times 10^{-3}$ mol %, in good agreement with the gas chromatography results.

2100–2400 cm^{-1} . This spectral range is rather informative for assessing the impurity compositions of silicon tetrafluoride and silane because it includes the following absorption bands of typical impurities:

2349.5 cm^{-1} , the ν_3 band of carbon dioxide, CO_2 [12];

2316.7 cm^{-1} , the ν_1 band of trifluorosilane, SiF_3H [15, 16];

2251.6 cm^{-1} , the ν_1 band of difluorosilane, SiF_2H_2 [17];

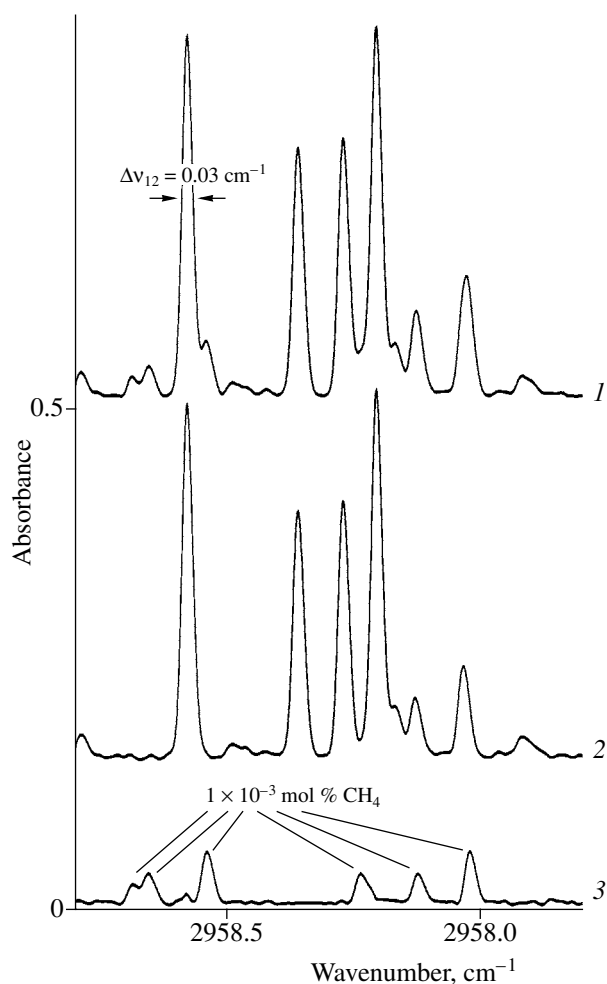


Fig. 5. Rotational components of the rovibrational absorption band ν_3 of SiF_4 impurity in SiH_4 ($p(\text{SiH}_4) = 1.3 \times 10^3$ Pa, $l = 975$ cm, 0.01-cm^{-1} resolution): (1) SiH_4 sample prepared from SiF_4 with no subsequent purification, (2) SiH_4 sample prepared by a fluoride-free process and containing CH_4 at a level no higher than a few times 10^{-6} mol %, (3) difference spectrum of curves 1 and 2.

2216.8 cm^{-1} , the ν_1 band of fluorosilane, SiFH_3 [18–20];

2143 cm^{-1} , the band of carbon monoxide, CO [12].

In addition to these impurities in silicon tetrafluoride, this spectral range includes the ν_1 band of SiH_4 , centered at 2188 cm^{-1} . This, in turn, impedes determination of impurities in silane. Figure 6 shows a portion of the spectrum of an SiF_4 sample containing all of the above impurities.

In the case of silane, of all the above impurities only CO_2 is sufficiently easy to identify, owing to the absorption in the range $2350\text{--}2400\text{ cm}^{-1}$, where the absorption in silane is very weak. The analytical range $2150\text{--}2350\text{ cm}^{-1}$ of fluorosilanes overlaps almost entirely with the strong absorption lines of silane. As a

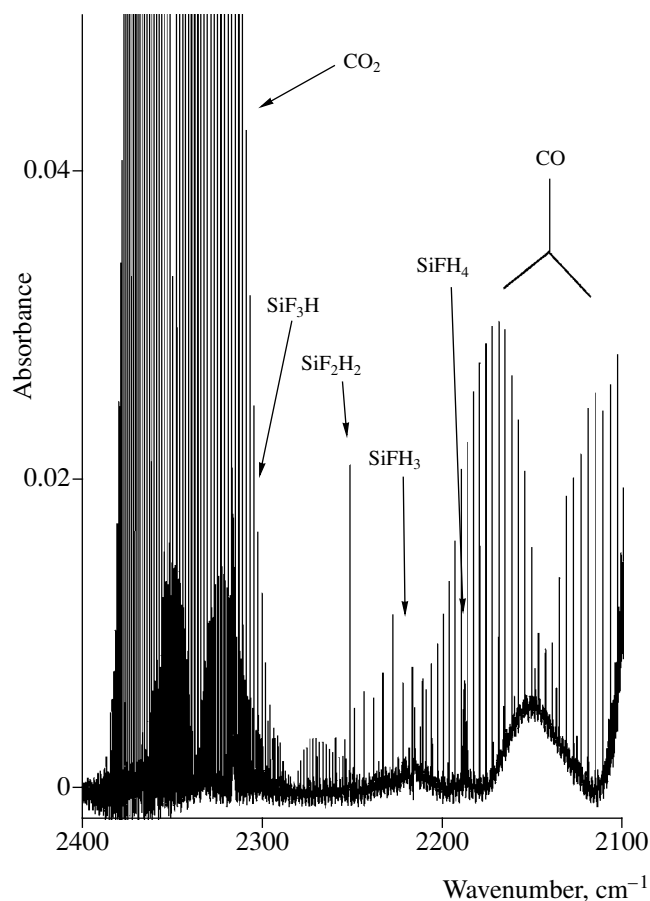


Fig. 6. Rovibrational bands of CO_2 (ν_3), SiF_3H (ν_1), SiF_2H_2 (ν_1), SiFH_3 (ν_1), SiH_4 (ν_1), and CO (ν_1) impurities in a concentrate taken from the top part of a fractional column; $p(\text{SiF}_4) = 4.7 \times 10^3$ Pa, $l = 975$ cm, 0.01-cm^{-1} resolution.

result, only the absorption in trifluorosilane, SiF_3H , may be identified with certainty. Using the above-mentioned procedure—subtraction of the spectrum of silane prepared by a fluoride-free process from that of “fluoride” silane—we obtained the ν_1 band of trifluorosilane with a well-defined $R\text{--}Q\text{--}P$ profile (Fig. 7). The SiF_3H content of silane samples prepared from silicon tetrafluoride varied from $(8 \pm 6) \times 10^{-2}$ to $(1 \pm 0.7) \times 10^{-2}$ mol %.

1500–1700 cm^{-1} . This spectral range includes absorption lines of the ν_2 bending mode of water molecules, whose behavior in SiF_4 and SiH_4 was mentioned above. At the same time, it lies within the transmission window of silicon tetrafluoride, so that the absorption lines in this range can be used as analytical. Note, however, that the MCT detector used in this spectral range ensured a notably smaller signal-to-noise ratio in comparison with the range $3600\text{--}3900\text{ cm}^{-1}$ (InSb detector) at the same signal intensity.

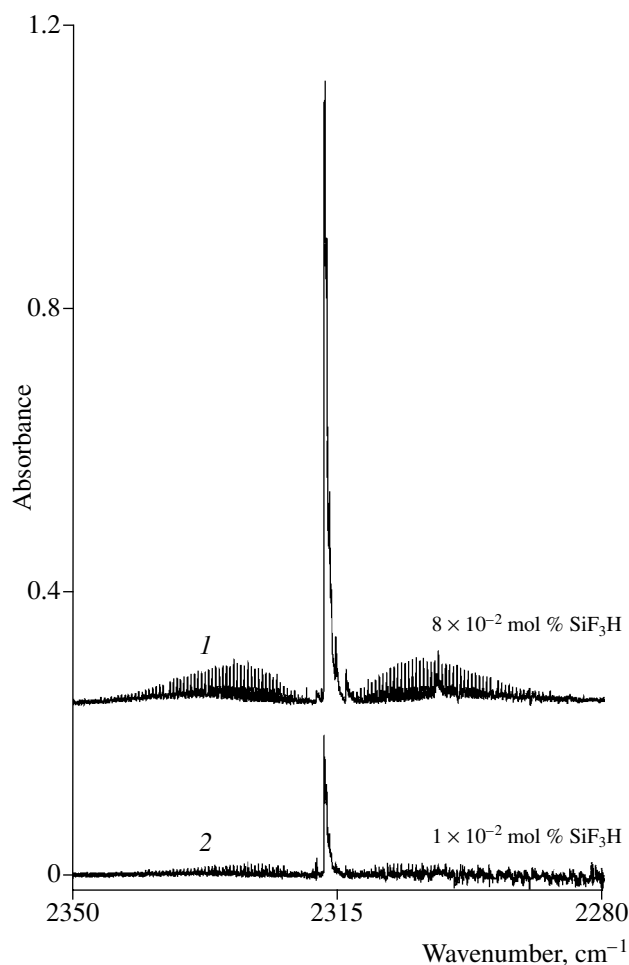


Fig. 7. Rovibrational band ν_1 of SiF_3H in SiH_4 samples (1) before and (2) after purification; $p(\text{SiH}_4) = 1.3 \times 10^3$ Pa, $l = 975$ cm, 0.01-cm^{-1} resolution.

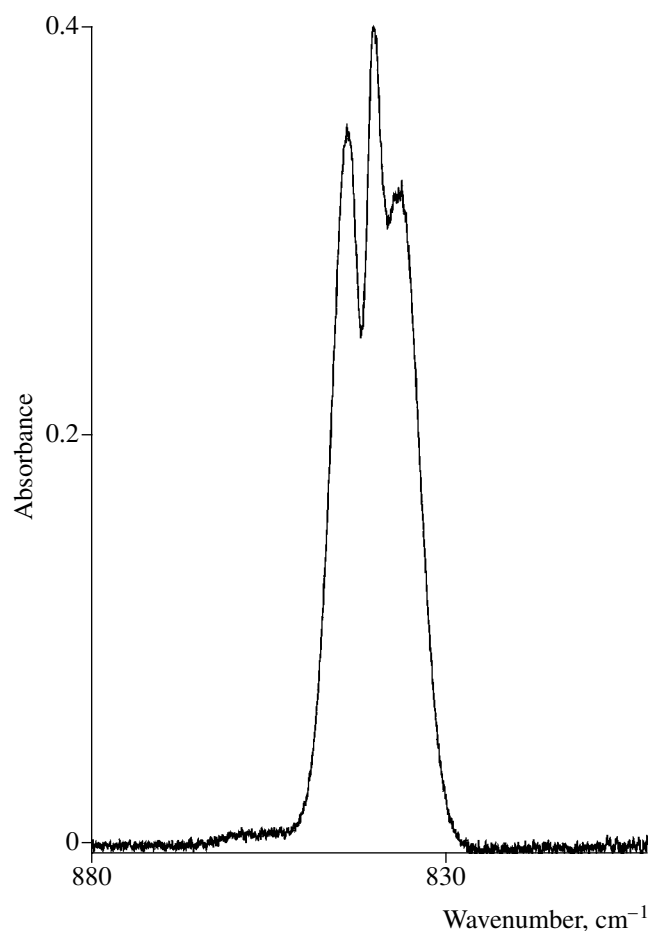


Fig. 8. Absorption band of $\text{Si}_2\text{F}_6\text{O}$ in SiF_4 in the range $850\text{--}900\text{ cm}^{-1}$; $p(\text{SiF}_4) = 6.5 \times 10^3$ Pa, $l = 10$ cm, 0.05-cm^{-1} resolution.

1015–1045 cm^{-1} . This range can be used for determination of silicon tetrafluoride impurities in silane owing to the very strong band at 1031.4 cm^{-1} . The IAC of this band has been recently refined by Burtsev et al. [25]. The detection limit of SiF_4 might be lower by at least one order of magnitude, but this is prevented by the overlap of the analytical band at 1031.4 cm^{-1} with the bending bands ν_2 and ν_4 of silane.

800–880 cm^{-1} . The strongest band in this spectral range is the ν_{14} band (centered at 839 cm^{-1}) of hexafluorodisiloxane, $\text{Si}_2\text{F}_6\text{O}$, a product of partial silicon tetrafluoride hydrolysis [6, 13] (Fig. 8). This substance is among the most important oxygen-containing impurities in silicon tetrafluoride and was found in all of the silicon tetrafluoride samples studied here. In the spectra of the silane prepared from silicon tetrafluoride, this impurity was not detected.

The table summarizes the analytical results for the impurities in silicon tetrafluoride and silane samples

differing in purity. Note that high-resolution FTIR spectroscopy is currently the only tool for simultaneous determination of H_2O , $\text{Si}_2\text{F}_6\text{O}$, and SiF_3OH in SiF_4 and SiH_4 at impurity concentrations low enough for practical applications. This technique offers a rather low detection limit of CO_2 and enables determination of a number of fluorine-containing impurities, which is crucial for the successful implementation of the technology in question. Unfortunately, in the case of fluorosilanes the error of determination is rather large, first, because of the strong intrinsic absorption in SiF_4 and SiH_4 in the spectral ranges in question and, second, because of the use of IACs found by quantum-chemical calculations [14, 21], which are known to be still inferior in accuracy to experimental techniques. On the other hand, according to our results the total content of fluorine in the form of fluorine-containing molecules (excluding difluorosilane) in the silane sample is 0.12 mol %, which is in reasonable agreement with chromatography data (0.17 mol %) [23]. Moreover, IR

Impurity compositions of SiF₄ and SiH₄ samples before and after purification

Impurity	Molar percent				DL, mol %
	SiF ₄		SiH ₄		
	before purification	after purification	before purification	after purification	
Si ₂ F ₆ O	2 ± 1	0.2 ± 0.1	<DL	<DL	1 × 10 ⁻³
SiF ₃ OH	(2 ± 1) × 10 ⁻²	<DL	<DL	<DL	1 × 10 ⁻³
HF	(5.0 ± 0.5) × 10 ⁻⁴	<DL	<DL	<DL	5 × 10 ⁻⁴
H ₂ O	(6 ± 1) × 10 ⁻³	<DL	<DL	<DL	1 × 10 ⁻³
SiH ₄	<DL	<DL			1 × 10 ⁻³
SiF ₃ H	(4 ± 2) × 10 ⁻³	<DL	(8 ± 6) × 10 ⁻²	(1.0 ± 0.7) × 10 ⁻²	1 × 10 ⁻³
SiF ₂ H ₂	(2 ± 1) × 10 ⁻³	<DL	NA	NA	1 × 10 ⁻³
SiH ₃ F	≤DL	<DL	(7 ± 5) × 10 ⁻²	(3 ± 2) × 10 ⁻³	1 × 10 ⁻³
SiF ₄			(6 ± 4) × 10 ⁻³	<DL	5 × 10 ⁻⁴
CH ₄	≤DL	<DL	(8 ± 4) × 10 ⁻³	<DL	1 × 10 ⁻³
CO ₂	(5.0 ± 0.5) × 10 ⁻²	(3 ± 0.3) × 10 ⁻³	(4 ± 0.5) × 10 ⁻⁴	<DL	8 × 10 ⁻⁵
CO	(4.0 ± 0.4) × 10 ⁻³	≤DL	NA	NA	1 × 10 ⁻³

Note: DL = detection limit, NA = not analyzed.

spectroscopy offers the possibility of identifying the chemical nature of impurities.

CONCLUSIONS

High-resolution FTIR spectroscopy can be used to analyze the impurity composition of silicon tetrafluoride and silane prepared from it. Using this technique, we detected a variety of impurities in SiF₄ samples of different purity: SiF₃H, SiF₂H₂, SiH₃F, CH₄, CO₂, CO, and the products of partial SiF₄ hydrolysis under the action of moisture (HF, SiF₃OH, Si₂F₆O, and molecular water). H₂O and SiF₃OH impurities in silicon tetrafluoride were detected with certainty for the first time. The detection limits of these impurities lie in the range 9 × 10⁻⁵ (CO₂) to 3 × 10⁻³ mol % (Si₂F₆O). In SiH₄ samples of different purity, we detected CH₄, CO₂, SiF₃H, SiF₂H₂, and SiF₄ impurities. Their detection limits lie in the range 8 × 10⁻⁵ (CO₂) to 1 × 10⁻³ mol % (SiF₄).

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