A Microwave Fourier Transform Spectrometer in the Range from 18 to 26.4 GHz with Increased Sensitivity Using Circular Waveguides.
Measurements of Isotopomeres of Carbonylsulfide and of Methane

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We present a microwave Fourier transform spectrometer in the region of 18 to 26.4 GHz with an increase in sensitivity roughly by a factor of ten in comparison to a former set up. Measurements of rotational transitions of isotopomers of carbonylsulfide, OCS, in natural abundance and of rovibrational transitions of methane, CH_4, illustrate the improvement.

Introduction

In 1985 we published the design and performance of a microwave (MW) Fourier transform (FT) spectrometer operating in the frequency region from 18 to 26.4 GHz (K-band) [1]. Meanwhile we extended the MWFT-technique to the V-band (26.4 to 40 GHz) [2]. The sensitivity of the V-band spectrometer could be improved considerably by use of a circular instead of a rectangular waveguide as a sample cell [3]. We expected a similar enhancement of the sensitivity of our K-band spectrometer with application of this special MW-technique.

Experimental Details

A detailed block diagram of the spectrometer is given in Figure 1. A circular waveguide with diameter of 23.8 mm and length of 36 m is used as the sample cell.

A backward wave oscillator (1) generating MW-radiation in the frequency range from 8 to 16 GHz is phase stabilized via the directional coupler (6), attenuator (7), mixer (8) and synchronizer (4). The reference frequency which is multiplied in (8) is provided by the radio frequency (RF) synthesizer (3), which also provides the common 10 MHz reference for the synchronizers (4) and (51), and the multipliers (66) and (67). Passing the directional coupler (9) and the attenuators (10) and (12), the microwaves reach via the coaxial transition (13), directional coupler (14) and isolator (15) the active frequency doubler (16). An X-band waveguide is used for the transmission line (11), which has an attenuation of approximately 8 dB over the length of 36 m. With the directional coupler (14) the input power for the frequency doubler (16) may be adjusted with an optional power meter. The isolator (15) reduces reflections. The frequency of (1) is chosen half of the frequency of the transition to be investigated. The advantage is, that frequencies in the range from 9 to 13.2 GHz can be transmitted with lower attenuation, and radio interference with the detection system is reduced. The input power for the travelling wave tube amplifier (TWTA) (24), which amplifies the pulses to a 1 to 10 Watt level, can be monitored with the power meter (18). With the PIN-switches (20) to (22) MW-pulses of 30 to 2000 ns length can be formed. The isolator (19) reduces reflections produced by the PIN-switches. A 0°/180° phase modulation of the MW-pulses (PAPS [4, 5]) is achieved by a biphase modulator (23). The PIN-switches (25) and (27) prevent the TWTA-noise from reaching the detection system during the sampling period. They further reduce the cw-microwave radiation leaked through (19) to (25). The circular H_{01} (TE_{01}) mode is formed by the Marie transition (29). All other modes, which might be created, are attenuated by a mode filter (31) between sample cell (30) and a second Marie transition (32), which converts the circular mode back to the rectangular H_{10} (TE_{10}) mode. The isolators (28) and (33) reduce reflections in the cell (30). They should be with low VSWR to reduce the delay time between the end

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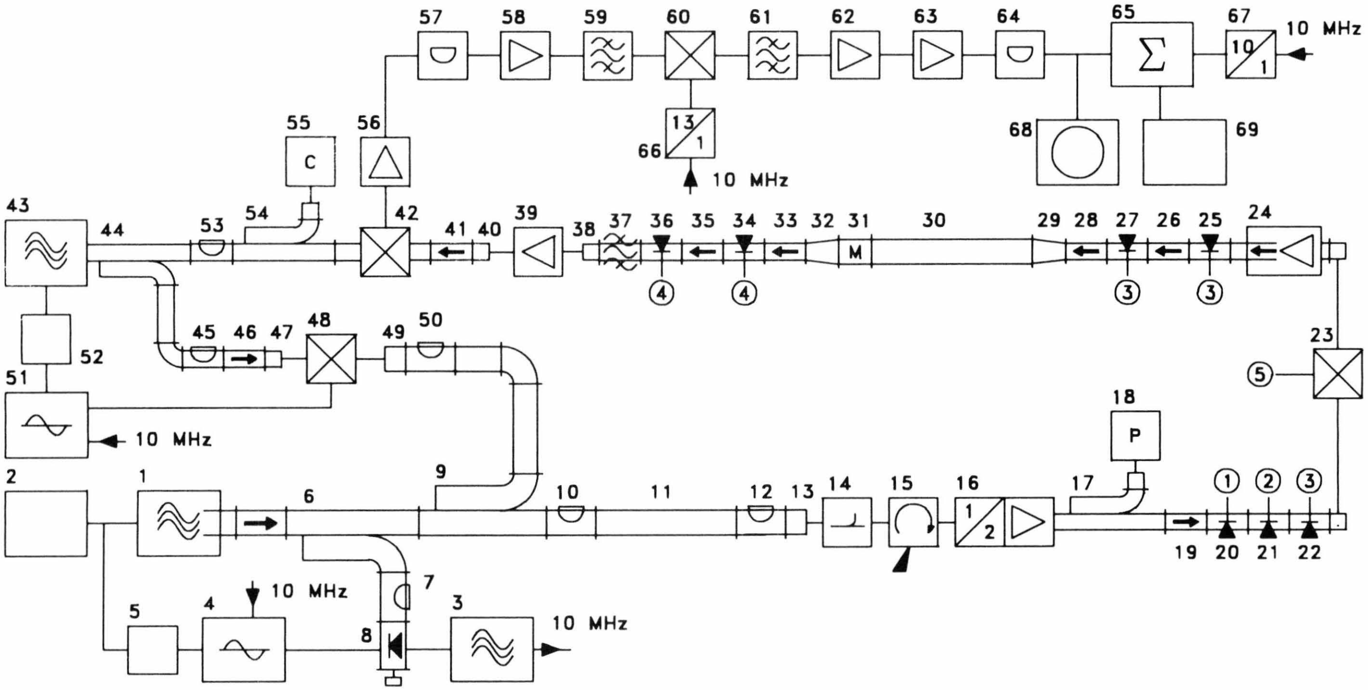

Fig. 1. Set up of a microwave Fourier transform spectrometer in the frequency band 18–26.4 GHz (K-band) with a sample cell of circular cross section.

BW	3 dB bandwidth	NF	noise figure	IL	insertion loss
IF	intermediate frequency	X	X-band, 8–12.4 GHz	K	K-band, 18–26.4 GHz
IS	isolation	co	coaxial	wg	waveguide

1 carcinotron (backward wave oscillator, BWO) 8–16 GHz, 50–100 mW, CSF, CO 521 A, with isolator.
2 power supply, FXR, Z 817 A.
3 synthesizer, 5 kHz–2720 MHz, Rhode and Schwarz, SMPD.
4 synchronizer, IF 30 MHz, Schomandl, FDS 30.
5 matching device.
6 wg directional coupler, X, 10 dB.
7 wg variable attenuator, X.
8 wg mixer with diode 1N23, X.
9 wg directional coupler, X, 10 dB.
10 see 7.
11 wg, 36 m, approximately 8 dB attenuation, X.
12 see 7.
13 wg–co transition, X.
14 co directional coupler, SMA.
21 see 20. 22 see 20.
23 biphase modulator (double balanced mixer), RHG, DMK2-18, SMA.
24 traveling wave tube amplifier, 18–26.4 GHz, 10 W or 1 W, Hughes 8010 H or 1077 H with output isolator, K.
25 wg PIN switch, Alpha Industries, 979K03, K.
26 see 19. 27 see 20.
28 wg isolator, VSWR 1:1.15 max, IS 30 dB, K.
29 Marie transition, 18–26.5 GHz, IL 0.15 dB, VSWR 1:1.2 max, Gamma Corporation, 108797, K.
30 circular wg sample cell, diameter 23.825 mm, length 36 m with 3 vacuum connections, volume 16 l, IL 8–6 dB for 18–19.3 GHz, 6–4 dB for 19.3–22.3 GHz, 4–2 dB for 22.3–26.4 GHz, Evered, C 89.
40 see 38. 41 see 28.
42 wg mixer with bias, Honeywell, K5100N, K.
43 MW-sweeper, 18–26 GHz, HP, 8690 B and 8696 A, K.
44 see 17. 45 wg variable attenuator, K.
46 see 19. 47 see 38.
48 co balanced mixer, RHG, DMS1-26.
49 see 38. 50 see 45.
51 synchronizer, IF 160 MHz, constructed by R. Schwarz.
52 see 5. 53 see 45. 54 see 17.
55 MW-counter with power meter, 10 Hz–26.4 GHz, Systron Donner, 6030, SMA.
56 IF-amplifier 160 MHz, BW 50 MHz, gain 35 dB, NF 2.5 dB, RHG, ICFH160LN, SMA.
57 co attenuator, 3 dB, SMA.

15 co isolator, IS 17 dB, SMA.
16 active frequency doubler, 9–13.2 to 18–26.4 GHz, output 15 dBm, Avantek, 260X2-31, K-SMA.
17 wg directional coupler, 10 dB, K.
18 power meter with sensor, Hewlett Packard (HP), 435 B and 8485 A.
19 wg isolator, K.
20 wg PIN switch, IS > 50 dB, IL < 1 dB, AEG PS42, K.
31 mode filter, 18–26.5 GHz, IL 0.2 dB, VSWR 1:1.2 max, TE_{11} mode rejection 8 dB, Gamma Corporation, 108798.
32 see 29. 33 see 28. 34 see 20. 35 see 28.
36 see 20.
37 wg bandpass filter, 18–26.4 GHz, Epsilon Lambda, 1305 B.
38 wg–co transition, HP, K281C, K-SMA.
39 MW-amplifier, gain 38 dB, NF 8 dB max, Avantek, AMT-26038, SMA.
58 IF-amplifier, 160 MHz, BW 50 MHz, gain 25 dB, NF 3.5 dB, RHG, ICFT16050, SMA.
59 BP-filter, 160 MHz, BW 20 MHz.
60 IF-mixer, MiniCircuits, ZAD-1.
61 BP-filter, 30 MHz, BW 10 MHz.
62 amplifier, Avantek, GPD 461–463.
63 see 62, optional. 64 co variable attenuator.
65 signal averager and control unit [4].
66 multiplier 10 to 130 MHz.
67 multiplier 10 to 100 MHz.
68 oscilloscope.. 69 personal computer.

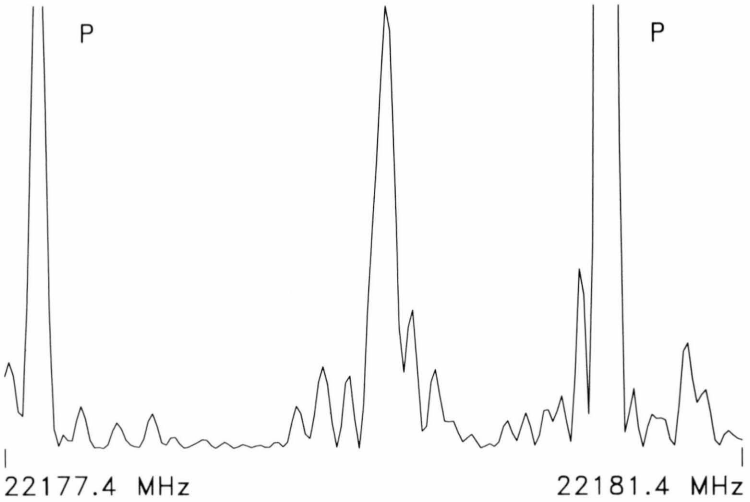

Fig. 2. A 4 MHz section out of a 50 MHz scan of the rotational power spectrum of the $J=2-1$ transition in the vibrational ground state of carbonylsulfide, $^{18}O^{13}C^{34}S$, in natural abundance. Absorption coefficient $4 \cdot 10^{-11}$ cm^{-1} [6]. Temperature 20 °C, pressure 3 mTorr (0.4 Pa), polarizing frequency 22 179.4 MHz, transition frequency 22 179.453 MHz. 128 000 K averaging cycles (29 minutes). P: coherent perturbations caused by averager switching frequencies.

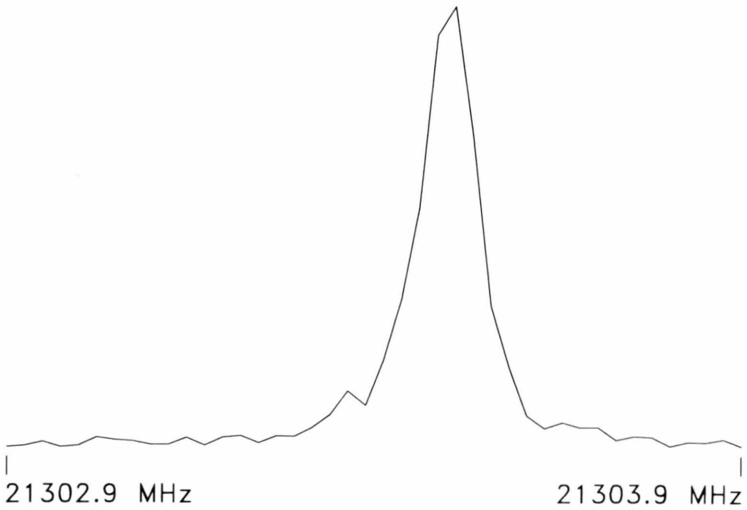

Fig. 3. A 1 MHz section out of a 50 MHz scan of the $J=15$, A1, 1–A2, 1, transition of methane, CH_4. Sample interval 10 ns, 1024 data points supplemented with 3072 zeros prior to Fourier transformation, temperature 20 °C, pressure 0.5 mTorr (0.07 Pa), polarizing frequency 21 303.3 MHz, line frequency 21 303.467 MHz, 16 000 *k* averaging cycles (220 sec). HWHH 45 kHz.

of the MW-pulse and the start of the sampling period. The detection system is protected from the strong MW-pulse by the PIN-switches (34) and (36). The PIN-switches (20, 21, 22, 25, 27, 34, 36) are marked by ①, ②, ③ and ④ for identification. The timing diagram for the spectrometer is given in Fig. 2 of [1]. The molecular signal passes a bandpass filter (37) to reduce harmonics generated by the PIN-switches (34) and (36). The signal is amplified (39) and fed into the MW-mixer (42). The local oscillator (43) is phase stabilized to the second harmonic of (1) by the MW-mixer (48) and the synchronizer (51) with 160 MHz intermediate frequency. So the resulting local frequency is $\nu_{\mathrm{loc}} = \nu_{\mathrm{Si}} + 160$ MHz or $\nu_{\mathrm{loc}} = \nu_{\mathrm{Si}} - 160$ MHz. The frequency and power of the local oscillator can be monitored with a MW-counter (55). The isolator (41) reduces reflections of the local frequency into (42) leaking through it. The downconverted molecular signal is amplified (56, 58), downconverted a second time to intermediate frequencies around 30 MHz (60), amplified (62, 63) and fed into the signal averager (65) [4] following the usual procedure [5].

Table 1. Measured $J = 2-1$ transitions of carbonylsulfide (OCS) of various isotopomeres in natural abundance in different vibrational states $v_1 v_2^l v_3$. Absorption coefficients in cm^{-1} [6], frequencies in MHz.

$^{18}O^{13}C^{34}S$	$0\,0^0\,0$	$4.06 \cdot 10^{-11}$	22 179.455
$^{16}O^{13}C^{34}S$	$0\,2^0\,0$	$1.56 \cdot 10^{-10}$	23 715.379
$^{16}O^{12}C^{32}S$	$0\,1^1\,1$	$1.01 \cdot 10^{-10}$	24 212.120
$^{16}O^{12}C^{32}S$	$0\,1^1\,1$	$1.01 \cdot 10^{-10}$	24 237.971
$^{16}O^{12}C^{32}S$	$0\,5^1\,0$	$8.89 \cdot 10^{-11}$	24 450.562
$^{16}O^{12}C^{32}S$	$0\,5^1\,0$	$8.89 \cdot 10^{-11}$	24 523.223

Table 2. Measured rovibrational transitions of methane in the vibrational ground state. Frequencies in MHz. Designation see [7].

13	(F2, 3)–(F1, 1)	19 360.513
14	(E2) –(E1)	19 288.639
14	(F1, 2)–(F2, 1)	18 506.477
15	(A1, 1)–(A2, 1)	21 303.466
15	(F1, 2)–(F2, 1)	22 588.190
15	(F2, 3)–(F1, 1)	24 297.655
16	(E3) –(E2)	18 562.529
17	(A2, 1)–(A1, 1)	21 837.842
17	(E2) –(E1)	26 486.120
17	(F2, 3)–(F1, 2)	24 883.308
17	(E2) –(E1)	26 486.112
18	(E3) –(E2)	18 529.011
18	(F2, 4)–(F1, 2)	20 414.863

Q4	(F1)	3, 4	18 750.359
Q5	(F2)	4, 3	18 106.617
Q6	(F2)	1, 1	18 708.502
Q6	(F1)	3, 3	19 412.690
Q8	(F1)	5, 5	20 183.975
Q9	(F2)	5, 4	21 859.842
Q11	(F2)	6, 7	19 598.342
Q12	(F1)	6, 6	23 137.040

Table 3. Measured transitions of methane in the excited vibrational state $v_4 = 1$. Frequencies in MHz. Designation see [9, 10].

Performance

The sensitivity of the spectrometer was tested with various isotopomers of carbonylsulfide in natural abundance. In Fig. 2 we give an example of the $^{18}O^{13}C^{34}S$ $J = 2-1$ transition in the vibrational state $v_1 v_2^l v_3 = 00^00$ with an absorption coefficient of $\alpha = 4 \cdot 10^{-11}$ cm^{-1} according to [6]. 128 000 k averaging cycles with a measuring time of 29 minutes were used. The signal to noise (S/N) ratio in the power spectrum is estimated as 16. The search for weaker lines was hindered by the coherent perturbing signals (P) coming from multiples of one sixteenths of the averager clock frequency 100/16 = 6.25 MHz and subharmonics thereof. For the band from 26 to 40 GHz we reached a S/N ratio of 22 in the power spectrum, as can be seen from Fig. 3 of [3], where the power spectra of lines with $\alpha = 1.3 \cdot 10^{-10}$ cm^{-1} and $\alpha = 1.9 \cdot 10^{-10}$ cm^{-1} are presented. So the sensitivity is of comparable magnitude.

The resolution is illustrated in Figure 3. There we give a rovibrational transition of methane, CH_4. According to [7] it is the $J = 15$, A1, 1 – A2, 2 transition. The measured line width is 45 kHz HWHH. The Doppler width may be calculated according to [8] as 33 kHz HWHH. As wall broadening is not included we may state that we reach experimentally nearly the Doppler width.

In Table 1 we give a list of transitions of isotopomers of OCS, which have not yet been measured or measured with presently available precision. The assignment was taken from Table 3 of [6].

In Table 2 we give a list of rovibrational transitions of methane, which were not yet measured. The assignment was taken from the calculation of the spectrum in [7, 9, 10]. These measurements also illustrate the sensitivity of the new instrument.

Acknowledgements

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