Catalog of Spectral Positions

LASER COMPONENTS®

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C_2H_4

C_2H_6

C_3H_2

ClPO

CO

CO_2

$^{12}CO_2$

$^{13}CO_2$

CS

D_2O-CO

Ethylen

HC_3N

HCO

H_2CO

HeH^+

H_2F^+

HNO_2

HNO_3

HO_2

H_2O

LiBr

NCO

NH_3

N_2O

NO

NO_3

NS

Si_2

$SiCl^+$

SiH

SiH_4

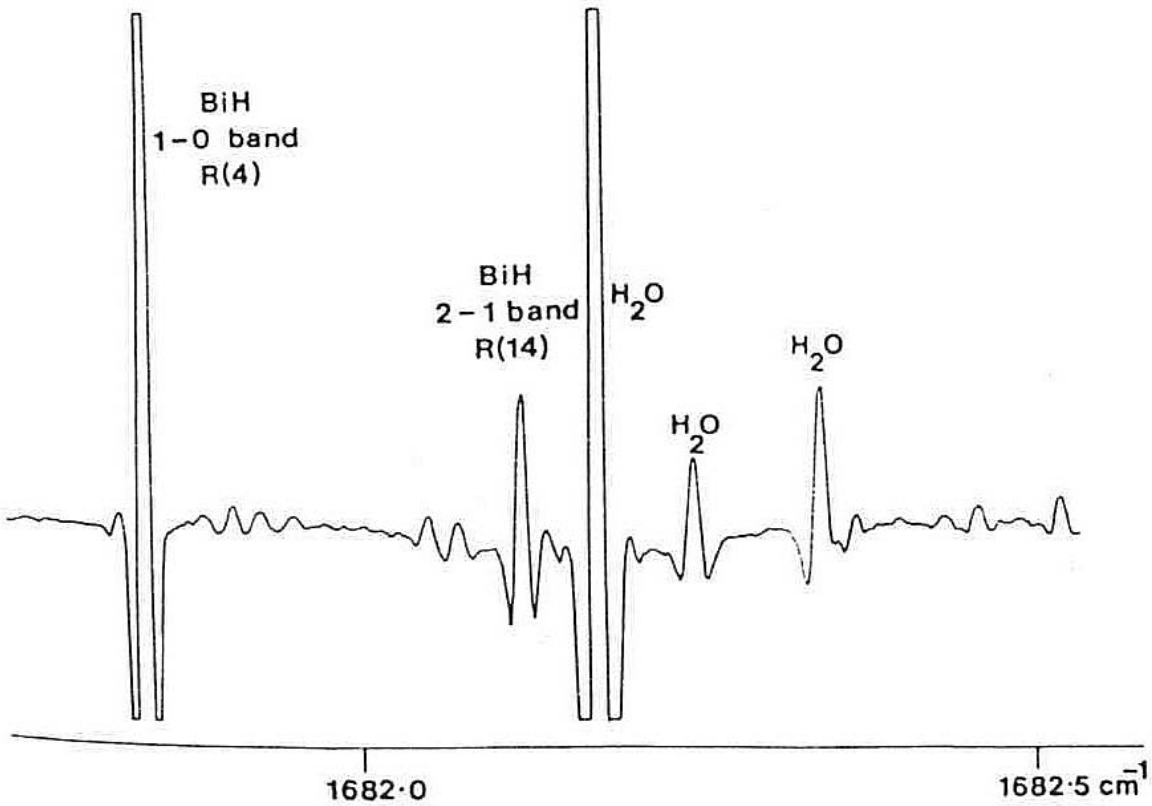
SO_2

SPECTRUM 1681.8

Start wavelength
$\lambda = 1681.8\ cm^{-1}$

End wavelength
$\lambda = 1682.5\ cm^{-1}$

Molecules: H_2O, BiH



A "typical" spectrum from the diode laser study of BiH (91). The BiH was made in a hot cell by the reaction of Bi vapour with 25 Torr of hydrogen at 1000 °C. The molecular lineshape is a second derivative because the technique of frequency modulation with lock-in detection at twice the modulation frequency was used. This modulation scheme gives a flatter baseline than lock-in detection at the modulation frequency.

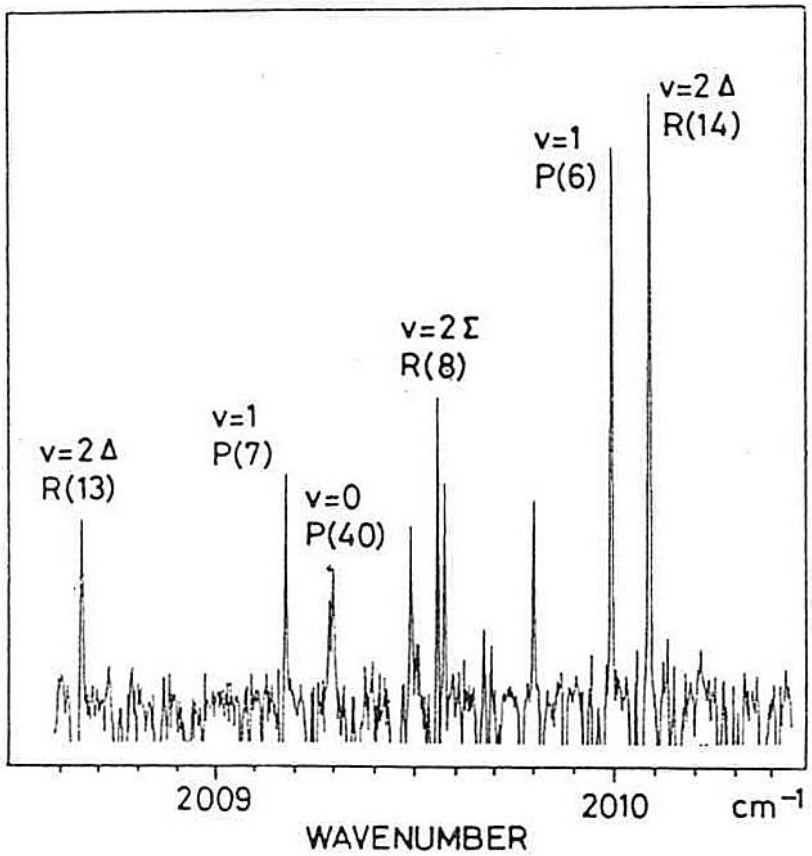
Reference:
Peter F. Bernath, *Annual Review of Physical Chemistry* **41**, 91-122 (1990).

SPECTRUM 2008.5

Start wavelength
$\lambda = 2008.5\ cm^{-1}$

End wavelength
$\lambda = 2010.5\ cm^{-1}$

Molecules: C_3



A part of the observed spectrum of C_3, produced by the 193 nm photolysis of an allene and H_2 mixture with the partial pressures of 0.1 and 0.35 Torr, respectively. The ordinate shows the absorption intensity in an arbitrary scale. Many strong lines of allene going downward were cut for the sake of clarity.

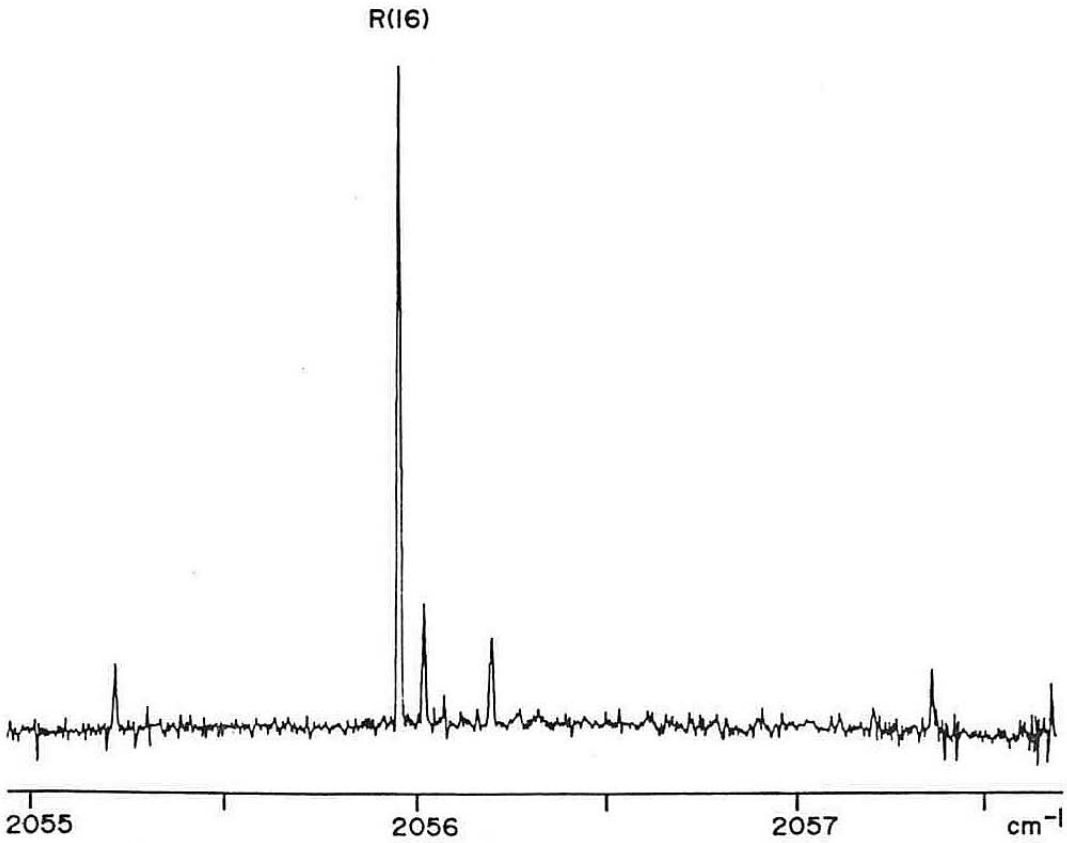
Reference:
K. Kawaguchi et al., *J. Chem. Phys.* **91** (4), (1989).

SPECTRUM 2055

Start wavelength
$\lambda = 2055\ cm^{-1}$

End wavelength
$\lambda = 2057.5\ cm^{-1}$

Molecules: C_3



The *R* (16) transition of the ν_3 band of C_3 recorded with a time-resolved infrared spectrometer. The C_3 molecule was produced by the 193 nm photolysis of an allene and H_2 mixture with the partial pressures of 0.1 and 0.35 Torr, respectively. The spectrum was obtained with a gate of 90 µs duration with 20 µs delay from the excimer laser shot.

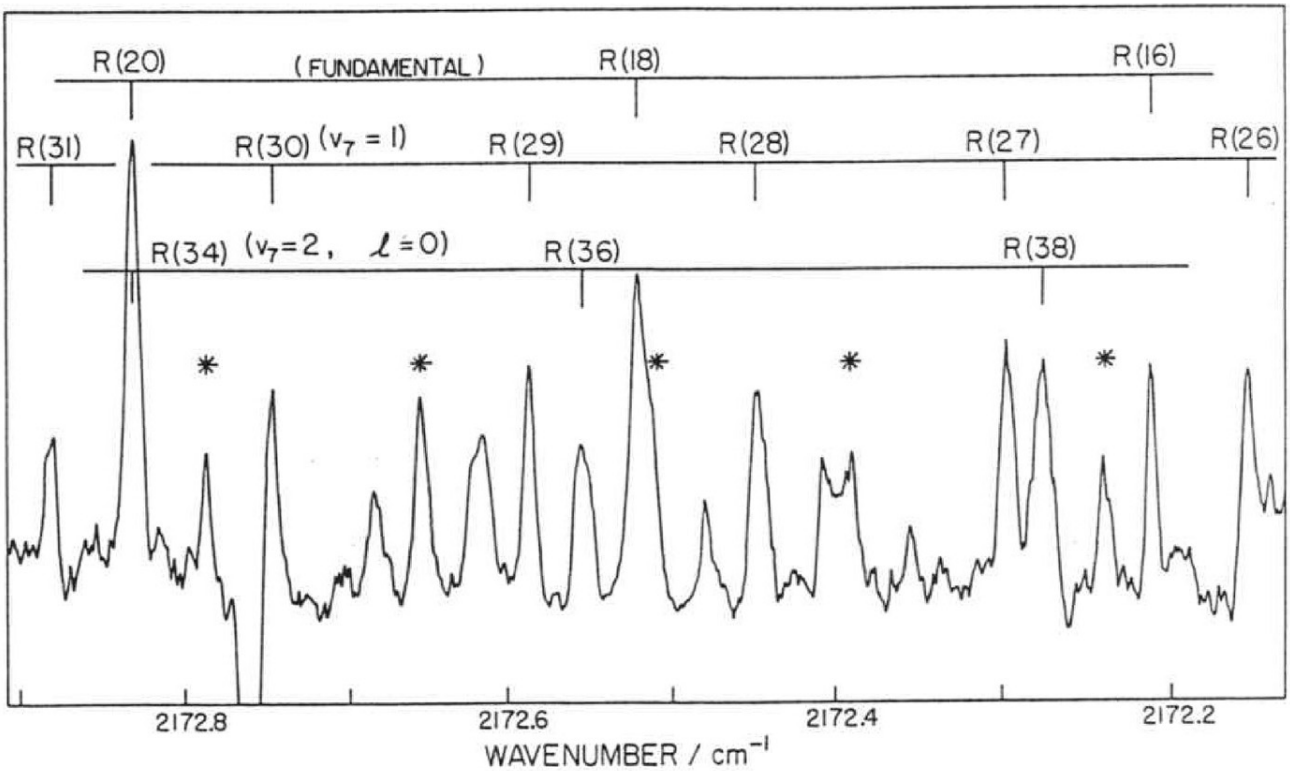
Reference:
K. Matsumura et al., *J.Chem.Phys.* **89** (6), (1988).

SPECTRUM 2172.2

Start wavelength
$\lambda = 2172.2\ cm^{-1}$

End wavelength
$\lambda = 2172.8\ cm^{-1}$

Molecules: C_5



A portion of the spectrum of C_5, as recorded using a tunable diode laser source. The three most prominent bands analyzed in this paper are shown directly, while lines belonging to the $\nu_5 = 1$ hot band, whose assignment is somewhat less certain, are indicated with asterisks. Note that the intensity scale is not uniform due to laser power variations and also that the wave number scale is not necessarily exactly linear. The negative feature at 2172.76 cm^{-1} is due to CO, present as an impurity in the discharge.

Reference:
N. Moazzen-Ahmadi, A. R. W. Mc Kellar, T. Amano, *J. Chem.Phys.*, **91** (4), (1989).

SPECTRUM 1849

Start wavelength
$\lambda = 1849\ cm^{-1}$

End wavelength
$\lambda = 1849.2\ cm^{-1}$

Molecules: CCH

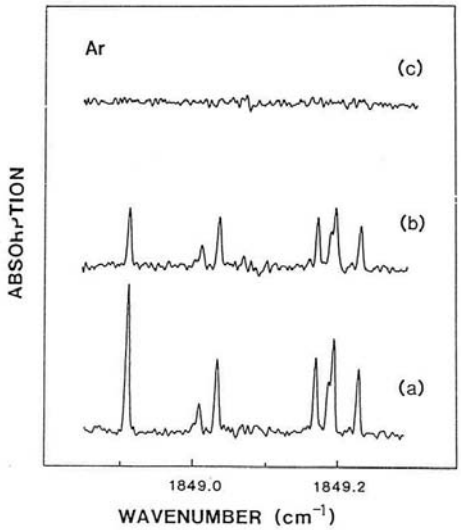


Figure 1

Time resolved infrared spectra of products derived from the 193 nm photolysis of an acetylene and Ar mixture with the partial pressures of 0.8 and 1.2 Torr, respectively. Trace (a) was obtained with a gate of 1 µs duration without delay from the excimer laser shot at $t = 0$, trace (b) with a 1 µs gate with 1 µs delay and trace (c) with a 5 µs gate with 2 µs delay.

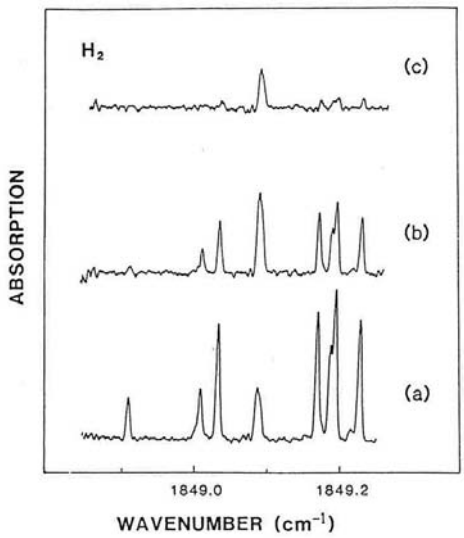


Figure 2

Time resolved infrared spectra obtained with the same conditions as for the spectra of Fig. 1, except that Ar is replaced by H_2 with the partial pressure of 1.2 Torr. A new line appears at 1849.1 cm^{-1}, whereas the line at 1849.9 cm^{-1} reduces intensity very much.

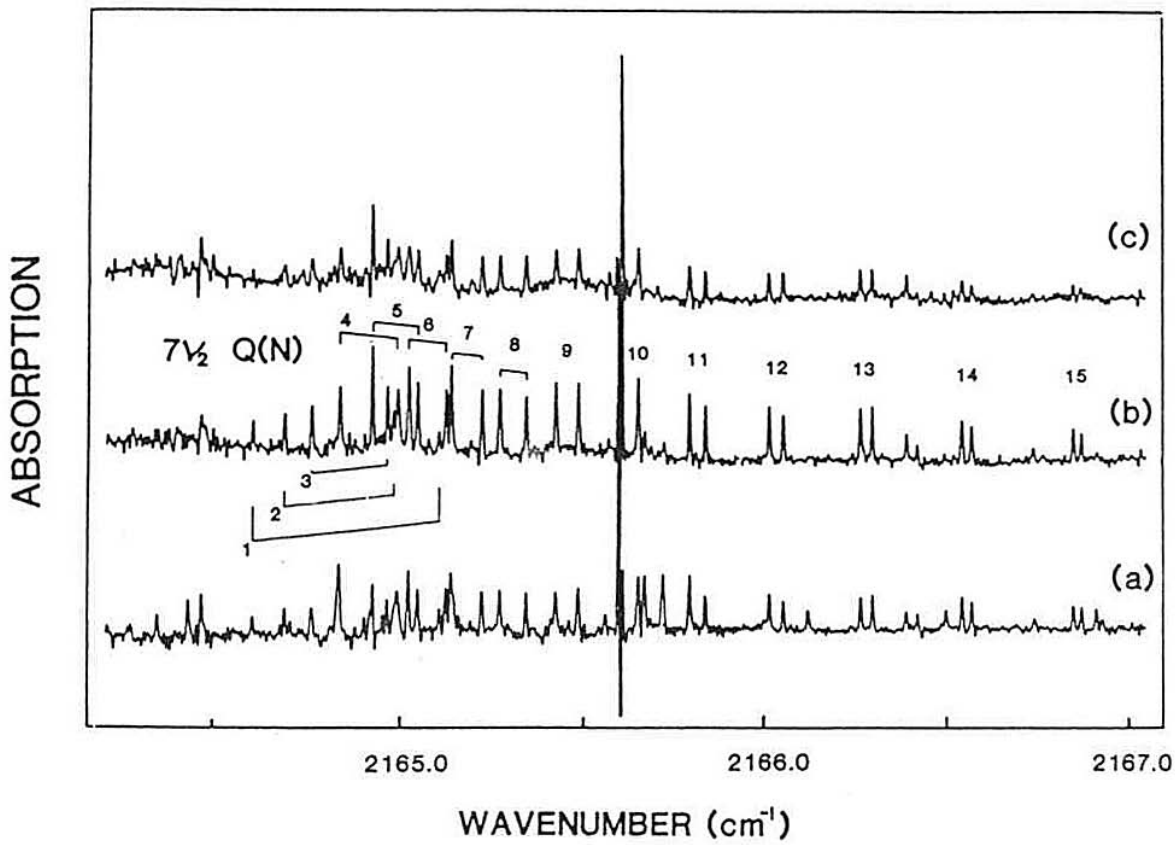
Reference:
H. Kanamori, *J. Chem. Phys.* **87** (1) (1987).

SPECTRUM 2165

Start wavelength
$\lambda = 2165\ cm^{-1}$

End wavelength
$\lambda = 2167\ cm^{-1}$

Molecules: CCH



Time resolved infrared spectra of the $7\nu^1_2$ band, recorded under the same conditions as those applied to the spectra of Fig. 1. A *Q*-branch series is identified; it starts around 2165 cm^{-1} and extends to higher frequency as *J* or *N* increases. The *N* number is indicated. The splittings of high-*N* lines are primarily due to spin-rotation interaction [Hund's case (b)], whereas the spin-orbit interaction predominates in the splittings of a few lowest-*N* transitions [Hund's case (a)]. A strong line at 2165.6 cm^{-1} is the *R* (5) transition of carbon monoxide which is produced by the photolysis of acetone included in the sample of acetylene as an impurity.

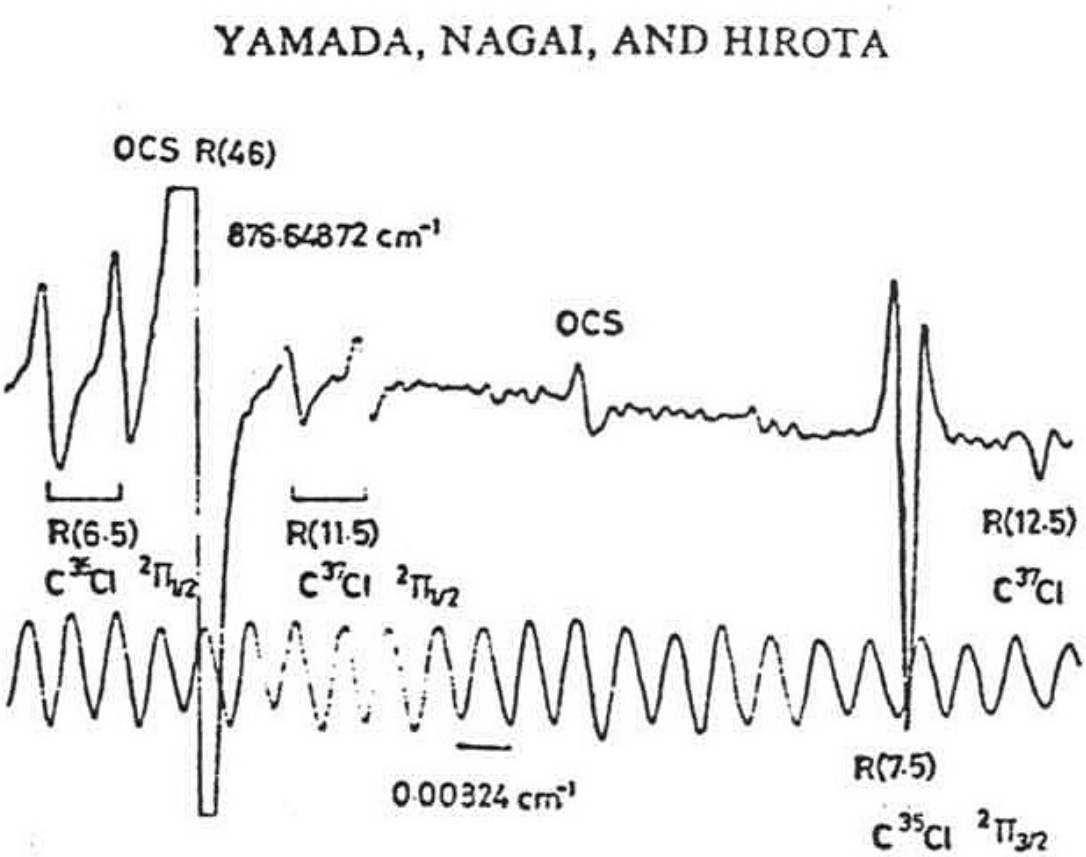
Reference:
H. Kanamori et al., *J. Chem. Phys.*, **89** (7), (1988).

SPECTRUM 876.65

Start wavelength
$\lambda = 876.65\ cm^{-1}$

End wavelength
$\lambda = 876.70\ cm^{-1}$

Molecules: CCL



A part of the CCl spectra. Two $^2\Pi_{22}$ lines, *R* (7.5) of $C^{35}Ci$ and *R* (12.5) of $C^{37}Cl$ appear as second derivatives because of Zeeman modulation, whereas two $^2\Pi_{1/2}$ lines, *R*(6.5) of $C^{35}Cl$ and *R*(11.5) of $C^{37}Cl$, as well as two OCS lines are observed as first derivatives by "source" modulation due to stray magnetic field pick-up. The OCS *R*(46) line is used as a standard. The lower trace shows fringe patterns obtained from the air-spaced etalon.

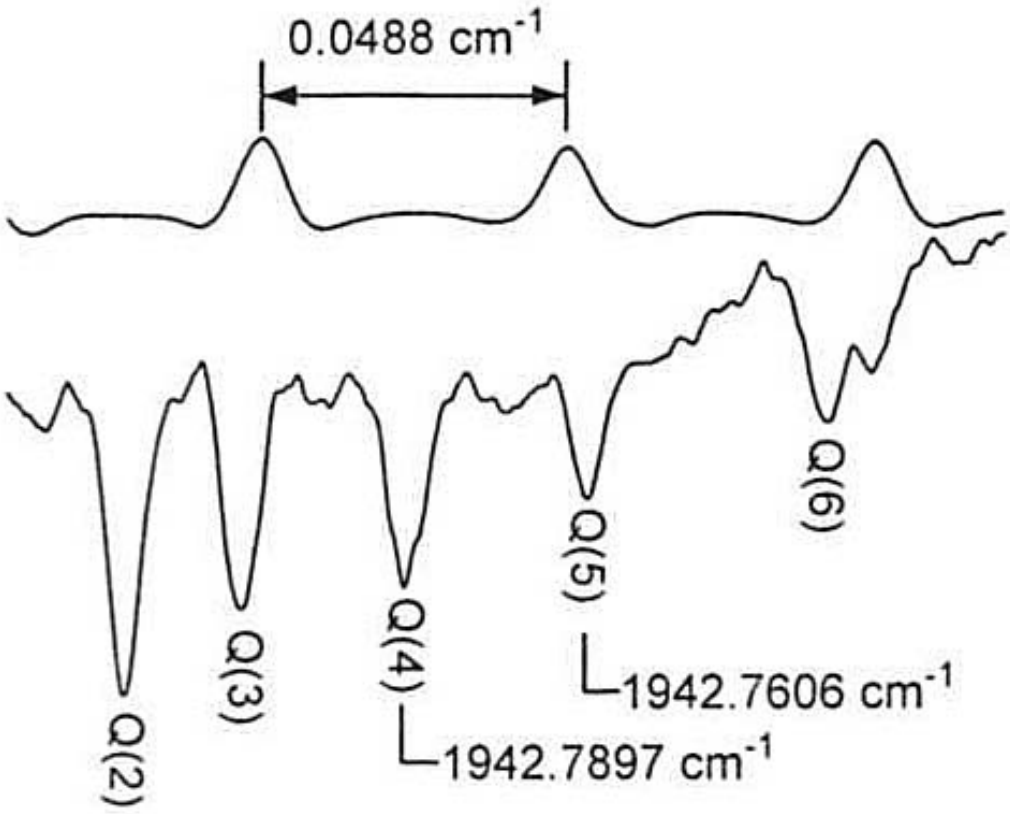
Reference:
C. Yamada, K. Nagi, E. Hirota, *J. Mol. Spectrosc.* **85**, 416-426 (1981).

SPECTRUM 1942.76

Start wavelength
$\lambda = 1942.76\ cm^{-1}$

End wavelength
$\lambda = 1942.78\ cm^{-1}$

Molecules: CCO



The lower trace shows the observed spectrum of CCO near the band center of (100) – (000) of the $\tilde{a}^1\Delta$ electronic state and the upper trace shows the etalon signal used for wave number interpolation. The five lowest *J* lines in the Q branch are identified. The line to the lower frequency side of Q (6) has not been identified.

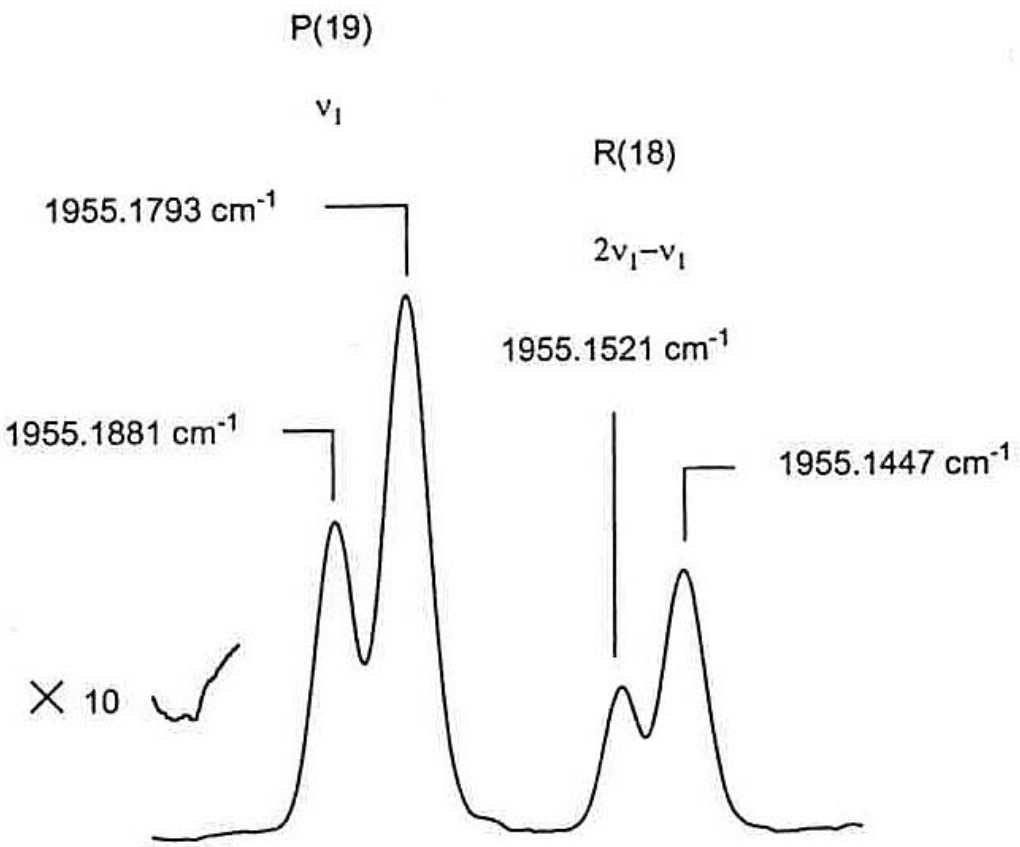
Reference:
N. Moazzen-Ahmadi , R. T. Boeré, *J. Chem.Phys.* **110** (2), (1999).

SPECTRUM 1955.18

Start wavelength
$\lambda = 1955.18\ cm^{-1}$

End wavelength
$\lambda = 1955.14\ cm^{-1}$

Molecules: CCO



The observed spectrum of CCO in the region of the R (18) line of the $2\nu_1 - \nu_1$ difference band. For the identification of the individual components see Table 1. The doublet to the higher frequency side of R (18) is the P (19) of the ν_1 band.

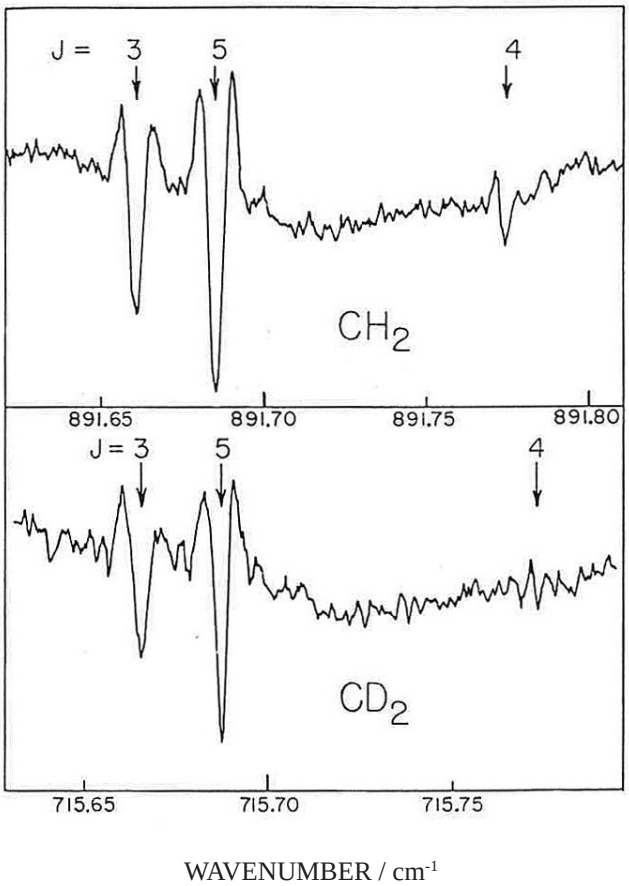
Reference:
N. Moazzen-Ahmadi, R. T. Boeré, *J. Chem.Phys.* **108** (16), (1988).

SPECTRUM 715.65

Start wavelength
$\lambda = 715.65\ cm^{-1}$

End wavelength
$\lambda = 715.75\ cm^{-1}$

Molecules: CH_2, CD_2



The $4_{04} - 4_{13}$ transitions in the ν_2 fundamental bands of CH_2 (top) and CD_2 (bottom) observed using a tunable diode laser and Zeeman modulation. In each case the absorption path was about 8 m and the recorder time constant was 3 s. The F_2 spin component (J = 4) appears to be much weaker then F_1 (J = 5) and F_3 (J = 3) because it is less efficiently Zeeman modulated.

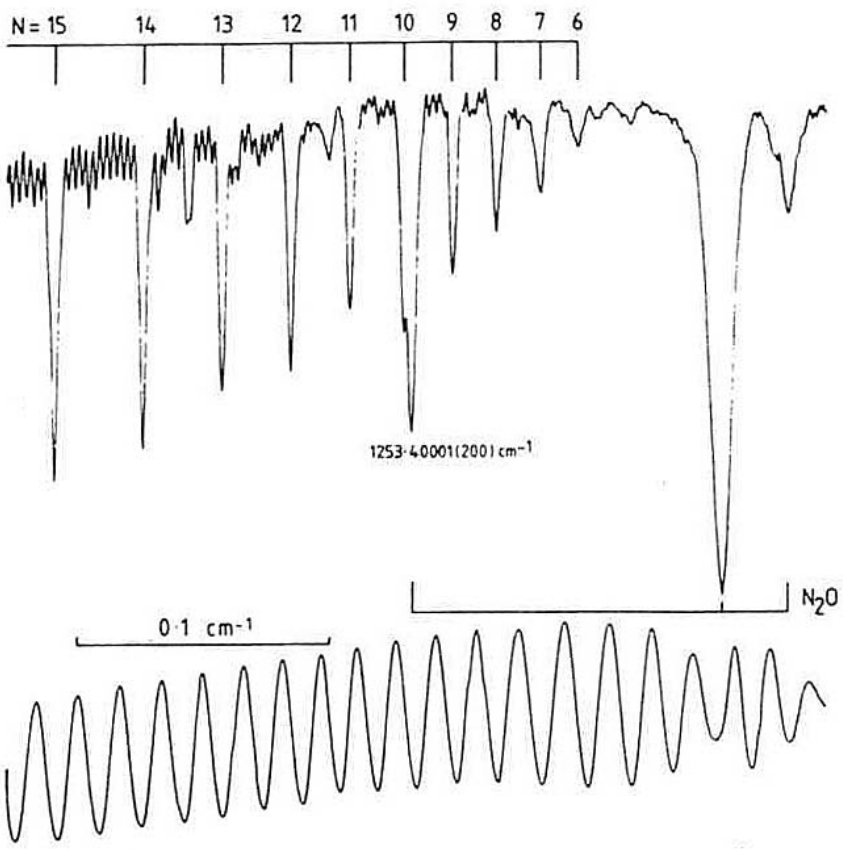
Reference:
A. R. W. Mc Kellar, K. Yamada, E. Hirota, *J. Chem.Phys.* **79** (3), (1983).

SPECTRUM 1252.5

Start wavelength
$\lambda = 1252.5\ cm^{-1}$

End wavelength
$\lambda = 1254.2\ cm^{-1}$

Molecules: CF_2



$^{R}Q_5(N)$ branch of $CF_2(X^1A_1)$ near 1253 cm^{-1}, with superimposed N_2O calibration spectra. The fringe pattern from the 7.6 cm Ge etalon used for relative calibration is shown at the bottom of the diagram.

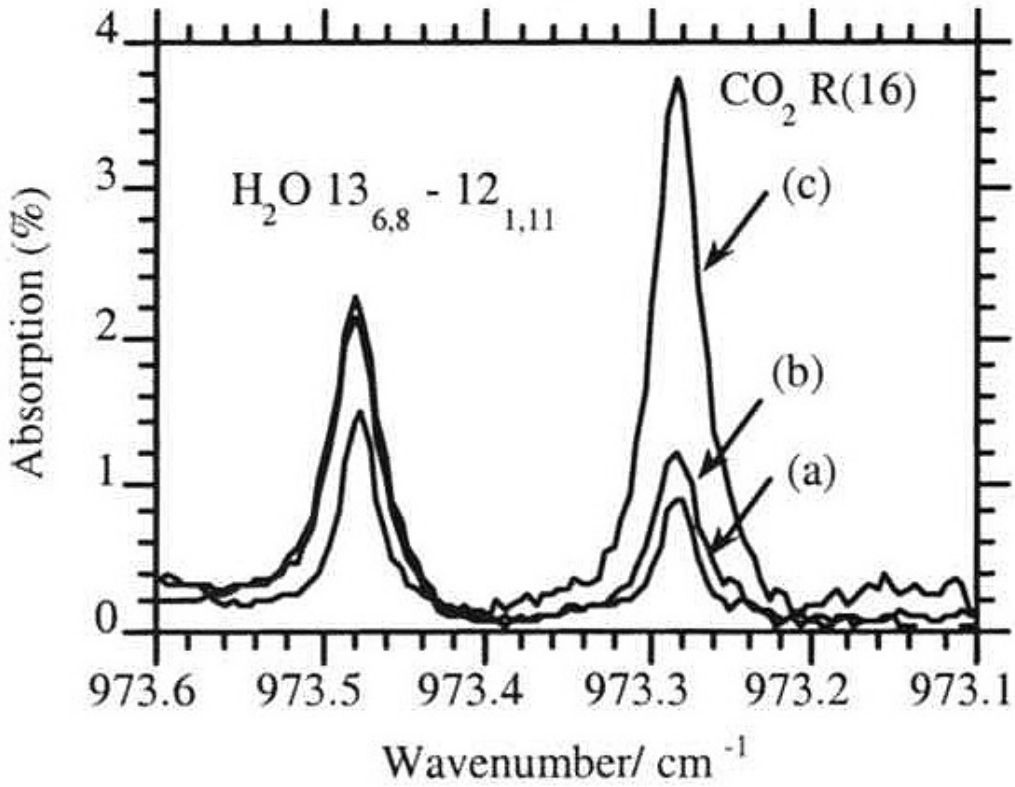
Reference:
P. B. Davies, W. Lewis-Bevan, *J. Chem. Phys.*, ***75*** (12), (1981)

SPECTRUM 973.2

Start wavelength
$\lambda = 973.2\ cm^{-1}$

End wavelength
$\lambda = 973.5\ cm^{-1}$

Molecules: CF_2CH_2



Portion of the atmosphere in the laboratory recorded at reduced pressure using a path length of 101 m. The laser drive current was 5A, the pulse length 232 ns, the repetition rate 5 kHz and the substrate temperature -1.52 °C. An average of 64000 scans was used: (a) cell pressure 50.5 Torr, (b) pressure 104.5 Torr, (c) carbon dioxide contained in human breath that was added to the sample; the pressure was then reduced to 103.2 Torr. The very weak water line has almost the same percentage absorption in traces (b) and (c). However, it is evident that a large increase in the percentage of absorption due to carbon dioxide has occurred in trace (c) in comparison to trace (b).

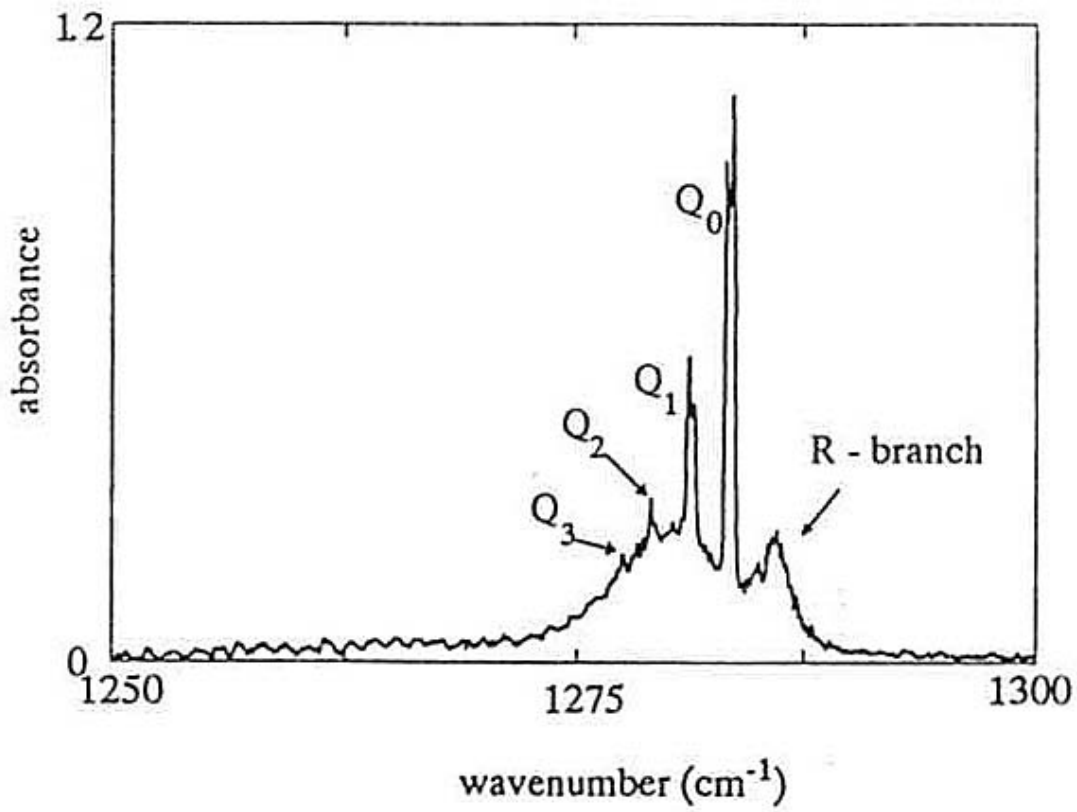
Reference:
M. T. McCulloch, E. L. Normand, N. Langford, G. Duxbury, *J. Opt. Soc. Am. B* **20** (8), (2003).

SPECTRUM 1250

Start wavelength
$\lambda = 1250\ cm^{-1}$

End wavelength
$\lambda = 1300\ cm^{-1}$

Molecules: CF_4



The IR absorption spectrum of CF_4.

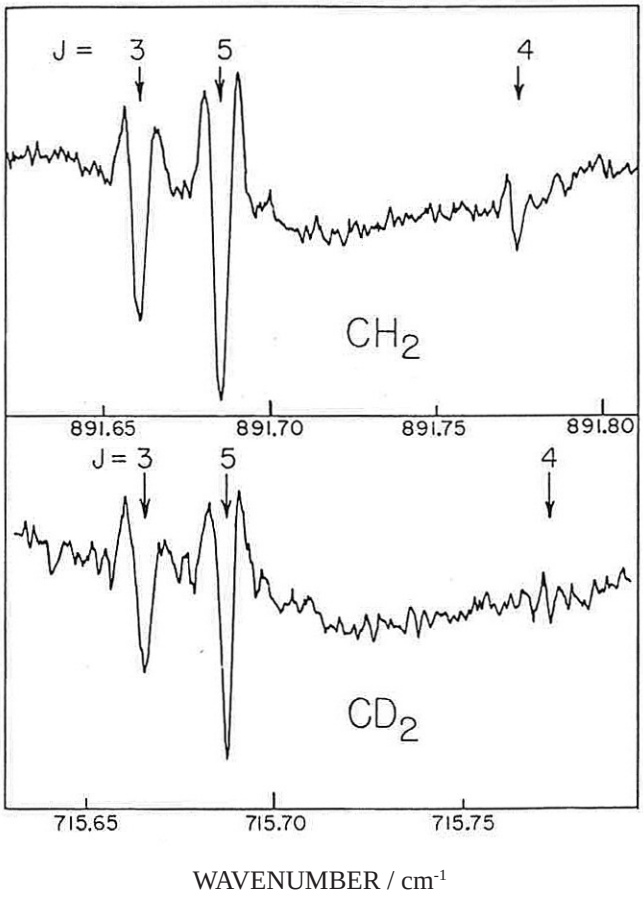
Reference:
G. M. W. Kroesen, F. J. de Hoog, *Applied Physics A, Material Science and Processing* **56** (6), (1993).

SPECTRUM 715.65

Start wavelength
$\lambda = 715.65\ cm^{-1}$

End wavelength
$\lambda = 715.75\ cm^{-1}$

Molecules: CH_2, CD_2



The $4_{04} - 4_{13}$ transitions in the ν_2 fundamental bands of CH_2 (top) and CD_2 (bottom) observed using a tunable diode laser and Zeeman modulation. In each case the absorption path was about 8 m and the recorder time constant was 3 s. The F_2 spin component (J = 4) appears to be much weaker then F_1 (J = 5) and F_3 (J = 3) because it is less efficiently Zeeman modulated.

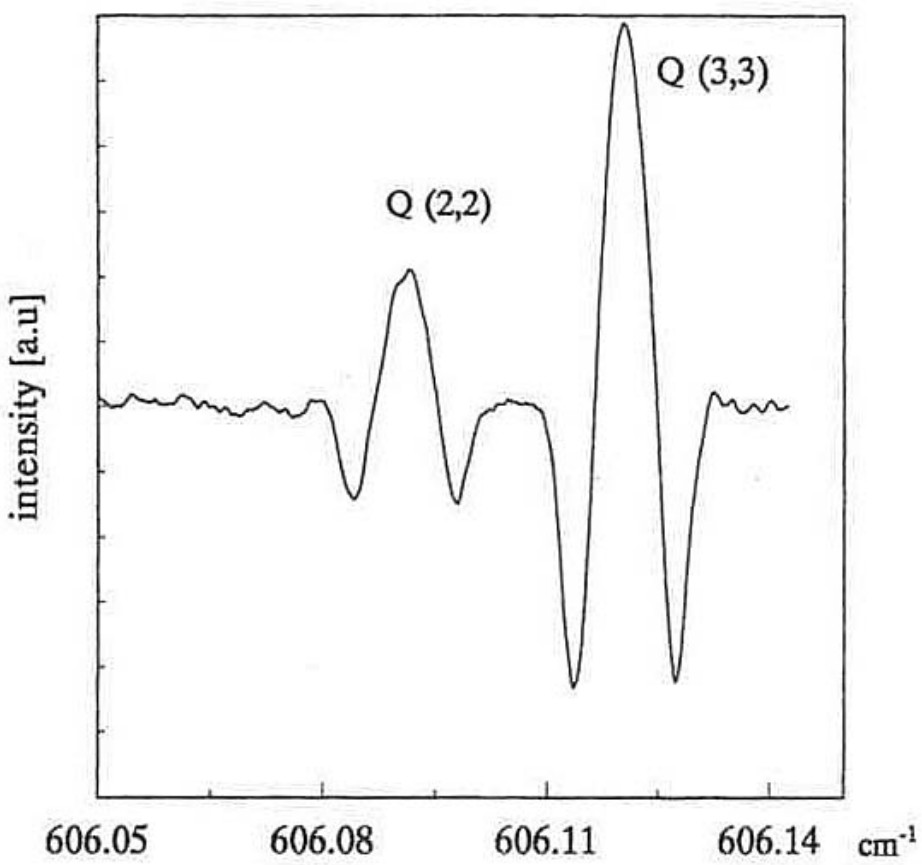
Reference:
A. R. W. Mc Kellar, K. Yamada, E. Hirota, *J. Chem.Phys.* **79** (3), (1983).

SPECTRUM 606.05

Start wavelength
$\lambda = 606.05\ cm^{-1}$

End wavelength
$\lambda = 606.14\ cm^{-1}$

Molecules: CH_3



The Q (2,2) and Q (3,3) absorption lines of the ν_2 fundamental of the methyl radical recorded with 2*f* detection. The radical was produced in a discharge mixture containing 200 m Torr CH_4 and 200 m Torr H_2.

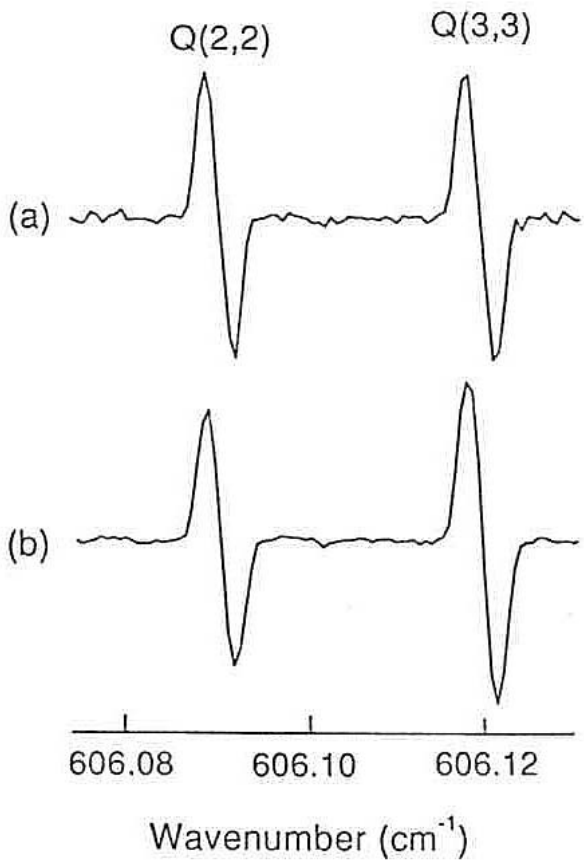
Reference:
W. Y. Fan, J. Röpcke, P. B. Davies, *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films* **14** (5), 2970-2972 (1996).

SPECTRUM 606.08

Start wavelength
$\lambda = 606.08\ cm^{-1}$

End wavelength
$\lambda = 606.12\ cm^{-1}$

Molecules: CH_3



The Q (2, 2) and Q (3, 3) transitions of the ν_2 fundamental band of the methyl radical, generated in the pulsed thermolysis nozzle. The distances between the nozzle and the laser are (a) 10 mm and (b) 5 mm, respectively.

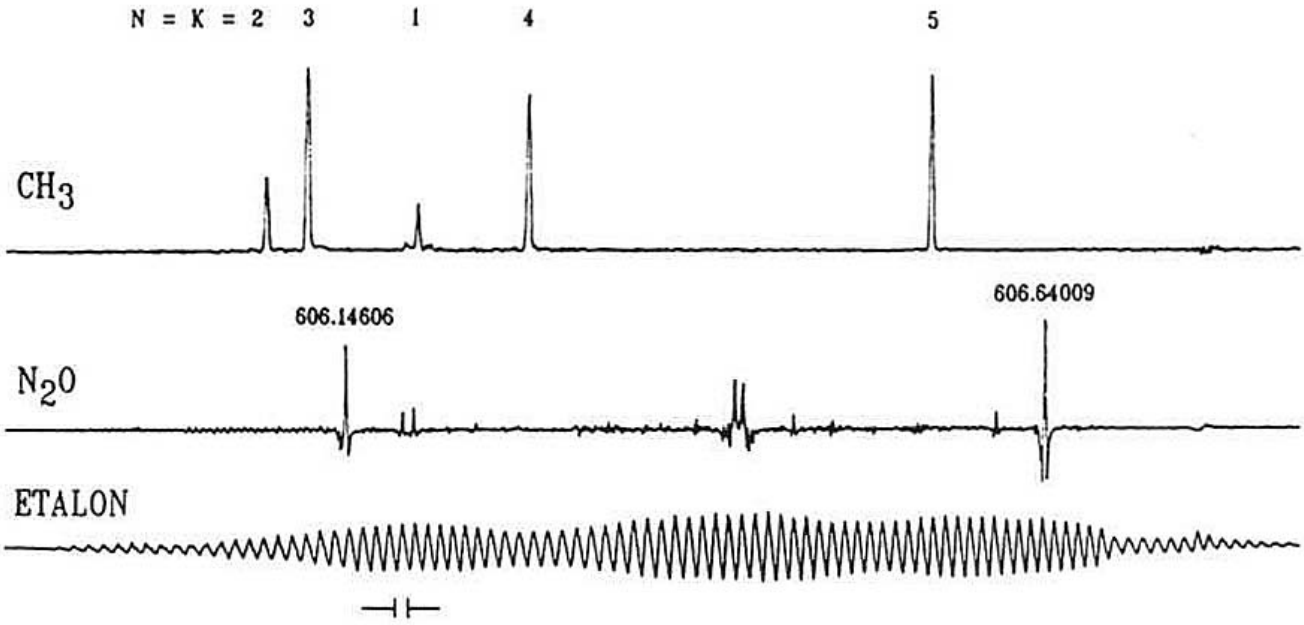
Reference:
P. B. Davies, *Spectrochimica Acta Part A* ***55***, 1987-1997 (1999).

SPECTRUM 606.1

Start wavelength
$\lambda = 606.1\ cm^{-1}$

End wavelength
$\lambda = 606.4\ cm^{-1}$

Molecules: CH_3, N_2O



A portion of the CH_3 spectrum of the ν_2, out-of-plane bending mode, $N = K$ Q branch head. Depicted, left to right, are the $N = K = 2, 3, 1, 4, 5$ transitions. Also shown is the N_2O absorptions used to calibrate the wavenumber of the CH_3 transitions and the etalon interference pattern used to interpolate between the upper two traces.

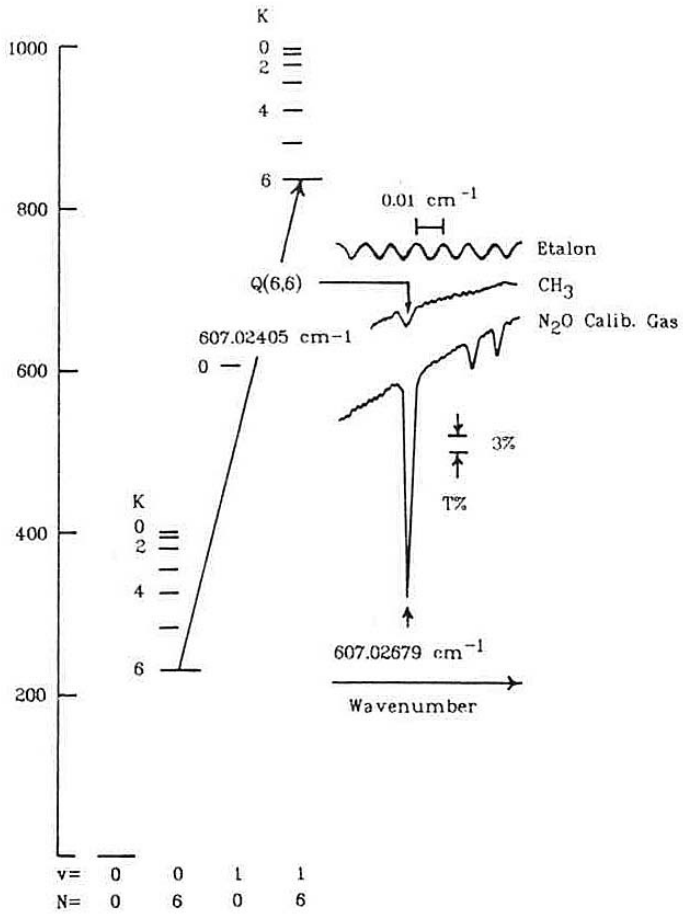
Reference:
D. K. Gaskill, V. Kolubatev, N. Bottka, R. S. Sillmon and J. E. Butler, *J. Crystal Growth* **77**, (1986).

SPECTRUM 607.02

Start wavelength
$\lambda = 607.02\ cm^{-1}$

End wavelength
$\lambda = 607.03\ cm^{-1}$

Molecules: CH_3, N_2O



The Q(6,6) rotational feature of the ν_2 fundamental vibrational mode of the CH_3 radical is presented as the middle trace in the right hand portion of the figure. A portion of the N_2O reference spectrum is shown on the lower trace. The left side of the figure displays the relevant energy levels involved in this transition. The methyl radical was formed by the decomposition of the TMG over the susceptor at 600 °C.

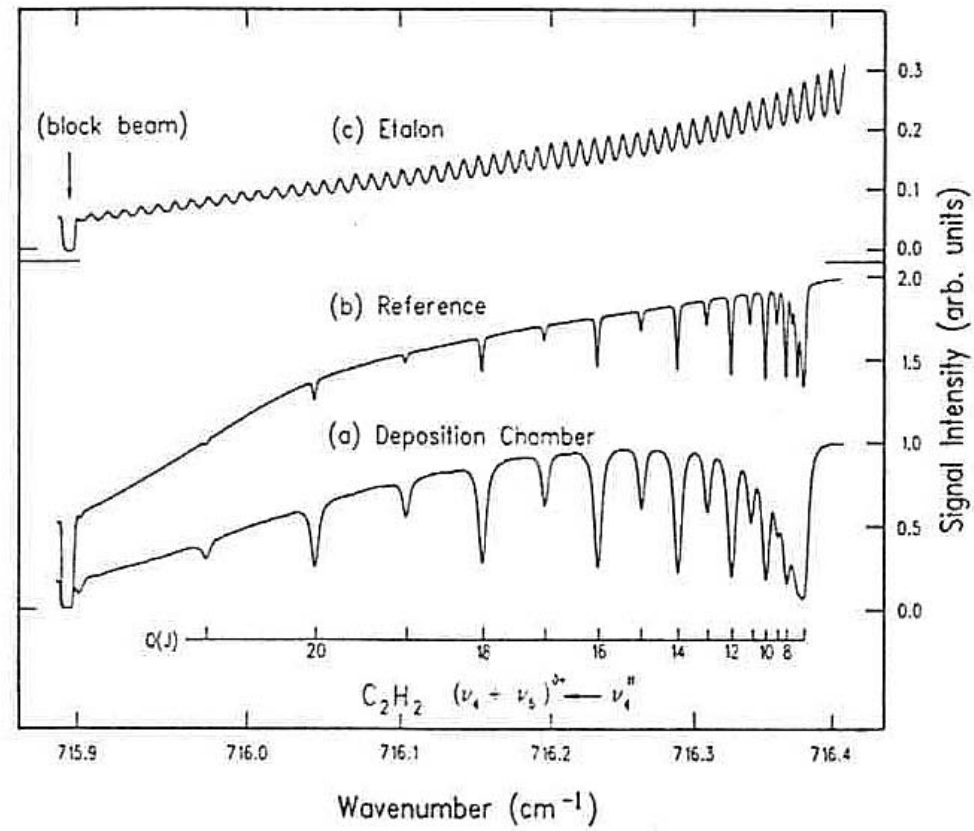
Reference:
J. E. Butler, N. Bottka, R. S. Sillmon, D. K. Gaskill, *Crystal Growth* **77**, 163 (1986).

SPECTRUM 716.4

Start wavelength
$\lambda = 716.4\ cm^{-1}$

End wavelength
$\lambda = 715.9\ cm^{-1}$

Molecules: CH_3, C_2H_2



Results of an infrared diode laser scan of the ($\nu_4 + \nu_5 - \nu_4$) Q-branch band head near 716 cm^{-1}. The traces shown are (a) absorption from the deposition gas-phase environment (20 passes, effective path length ~0.5 m), (b) absorption from a room-temperature cell containing ~0.1 Torr of C_2H_2, and (c) etalon trace (free-spectral range ~0.01 cm^{-1}). The average C_2H_2 temperature in the deposition chamber is estimated from the relative line intensities of the ($J = 8$ - 21) Q-branch lines and found to be in the range 200-300° C. The linewidths in (a) are larger than (b) because of pressure broadening.

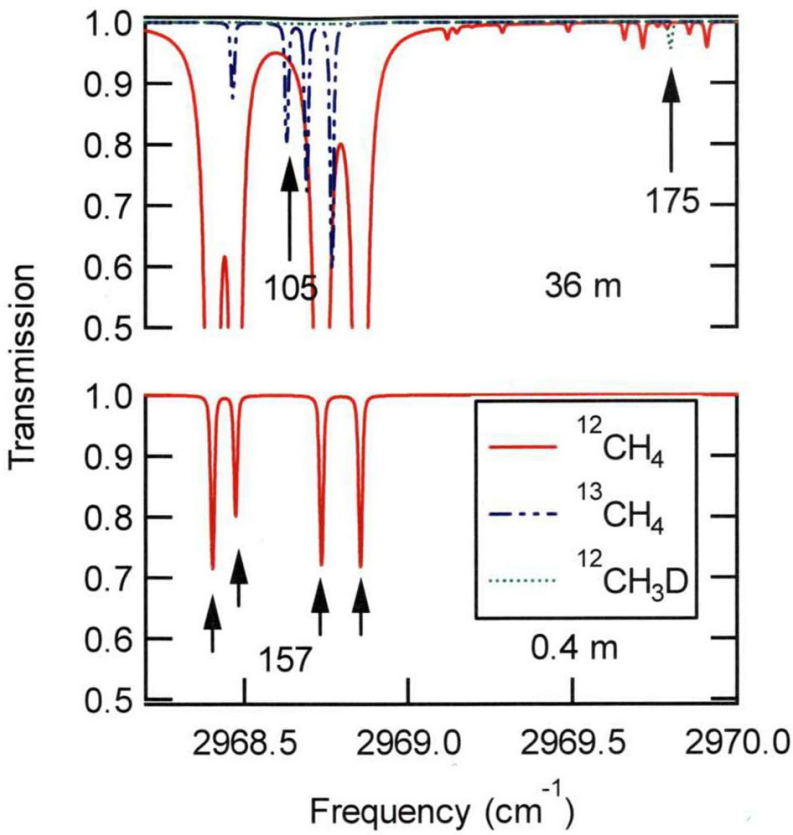
Reference:
F. G. Celii, J. E. Butler, *Annual Review of Phys. Chemistry* **42**, 643-684 (1991).

SPECTRUM 2968.5

Start wavelength
$\lambda = 2968.5\ cm^{-1}$

End wavelength
$\lambda = 2970\ cm^{-1}$

Molecules: $^{13}CH_4$, $^{12}CH_4$, $^{12}CH_3D$



Simulated sample cell transmission for a suitable set of lines for CH_4. The upper panel shows the transmission through a 36 m pathlength and the lower panel shows the transmission through a 40 cm pathlength. The lower state energy levels (in cm^{-1}) are noted below the lines.

Reference:
J. B. McManus, M. S. Zahniser, D. D. Nelson, L. R. Williams, C. E. Kolb, *Spectrochemica Acta* **58**, 2505-2517 (2002).

SPECTRUM 500

Start wavelength
$\lambda = 500\ cm^{-1}$

End wavelength
$\lambda = 4000\ cm^{-1}$

Molecules: CO, CO_2, H_2O, CH_4

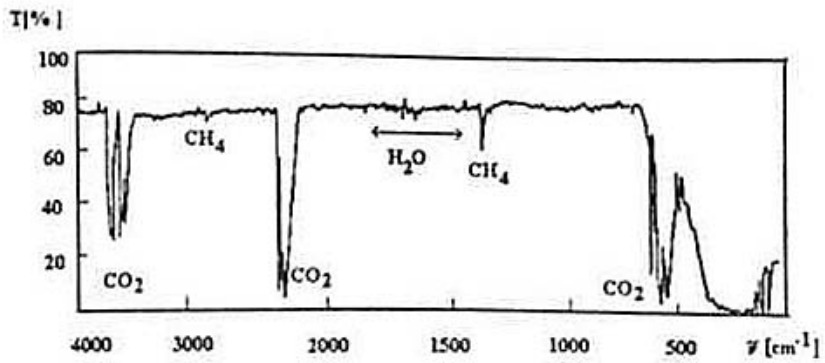
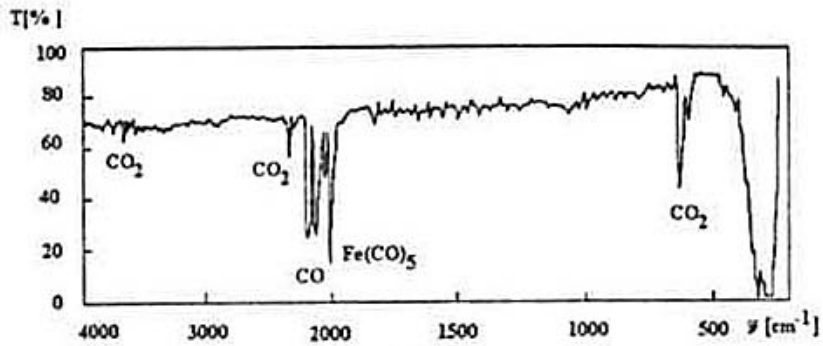


Figure 3. The IR absorption spectrum of CO_2.



(a)

The IR absorption spectrum of CO_2.

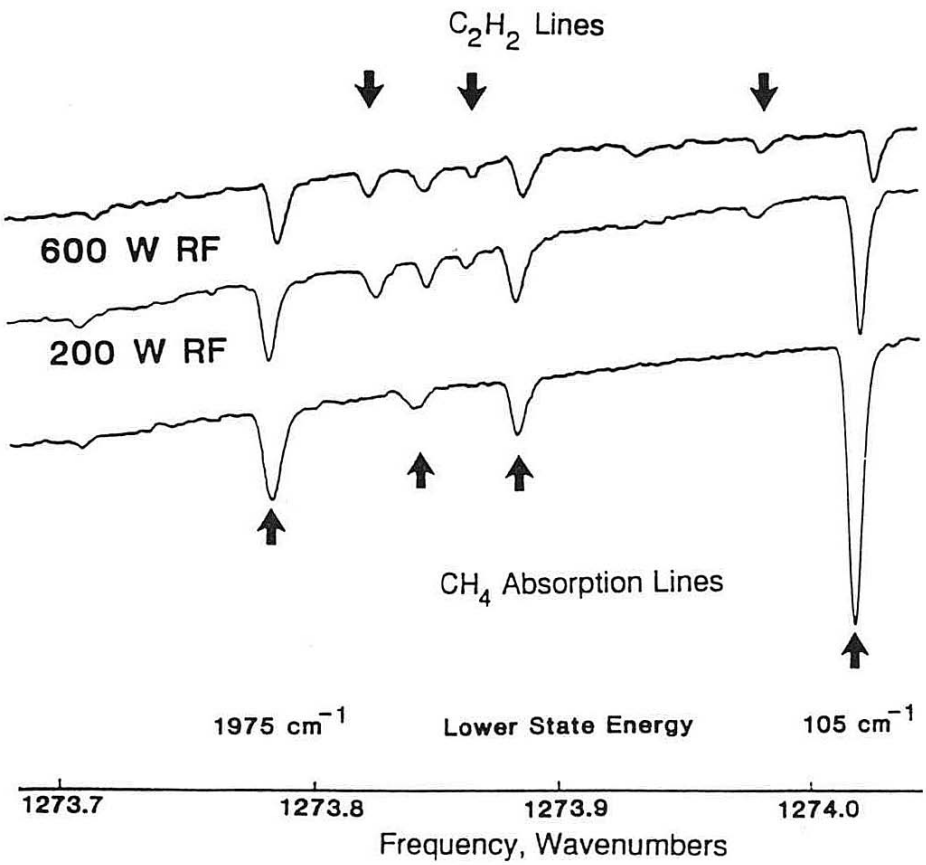
Reference:
M. Morvová, *Czechoslovak Journal of Physics*, **47** (2), (1997).

SPECTRUM 1273.7

Start wavelength
$\lambda = 1273.7\ cm^{-1}$

End wavelength
$\lambda = 1273.8\ cm^{-1}$

Molecules: CH_4, C_2H_2



Infrared spectral region used in CH_4 dissociation fraction and temperature measurement (lower trace, plasma off, upper traces, plasma on).

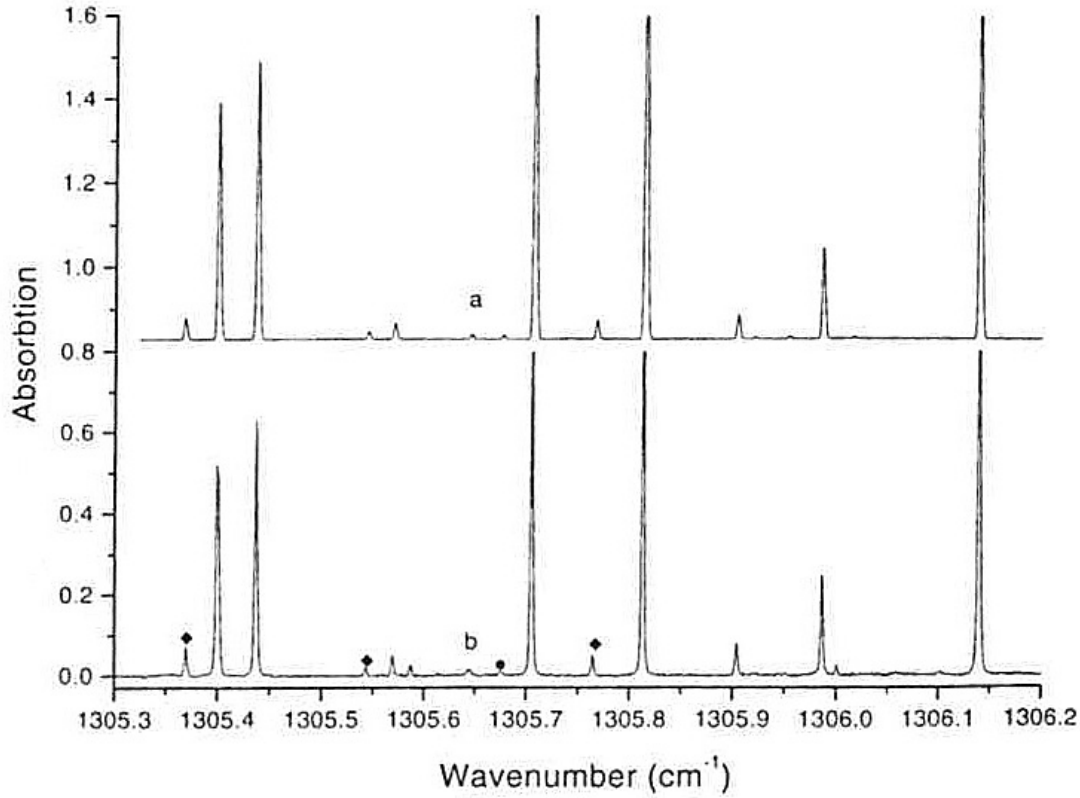
Reference:
J. Wormhoudt, *Final Technical Report* (1990).

SPECTRUM 1305.3

Start wavelength
$\lambda = 1305.3\ cm^{-1}$

End wavelength
$\lambda = 1306.2\ cm^{-1}$

Molecules: CH_4



Sample calculated (a) and experimental (b) spectra in the ν_4 band region of methane. Symbols are ♦ for octad-pentad lines and • for pentad-dyad lines.

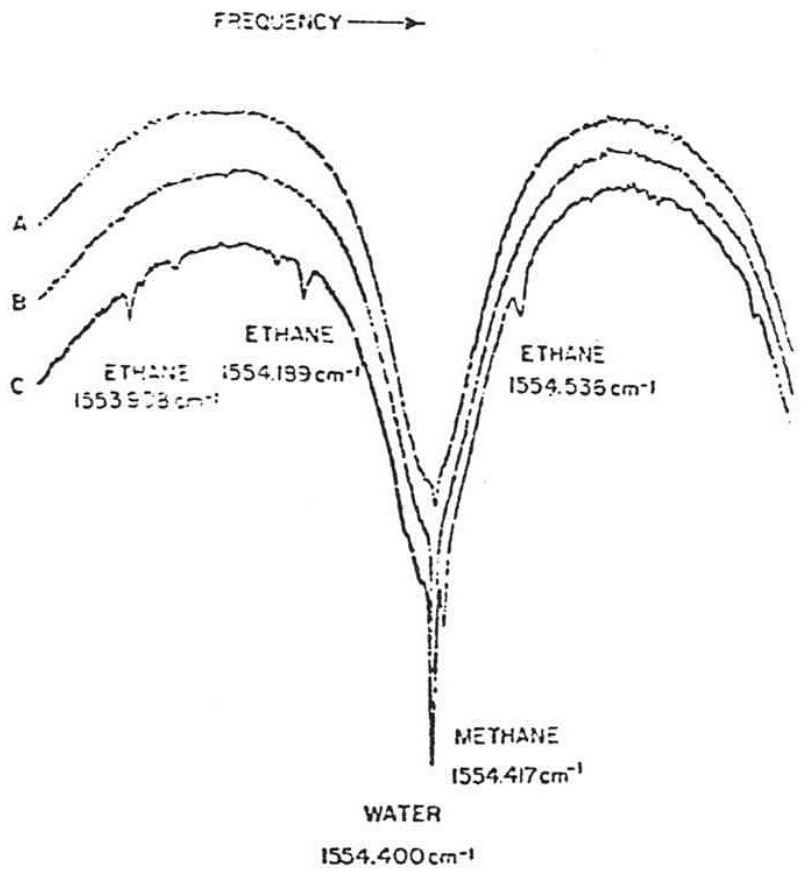
Reference:
D. V. Kalinin, D. K. Bronnikov, Y. u. G. Selivanov, T. Gabard, J. - P. Champion, J. - C. Hilico, *Journal of Quantitative Spectroscopy & Radiotive Transfer* **62**, 13-27 (1999).

SPECTRUM 1553.97

Start wavelength
$\lambda = 1553.97\ cm^{-1}$

End wavelength
$\lambda = 1554.54\ cm^{-1}$

Molecules: H_2O, CH_4, C_2H_4



Transmission spectra in the 1553 cm^{-1} region. The 50 cm^2 samples of either cigarette smoke (C) or room air containing 11.73 mm H_2O (B) were examined at a cell pressure of 12 Torr. Lock-in amplifier gain was 25 mV with a 0.3-sec time constant. Scan rate was 0.0077 cm^{-1} sec^{-1}. The background (A) and etalon calibration spectra (D) are also shown.

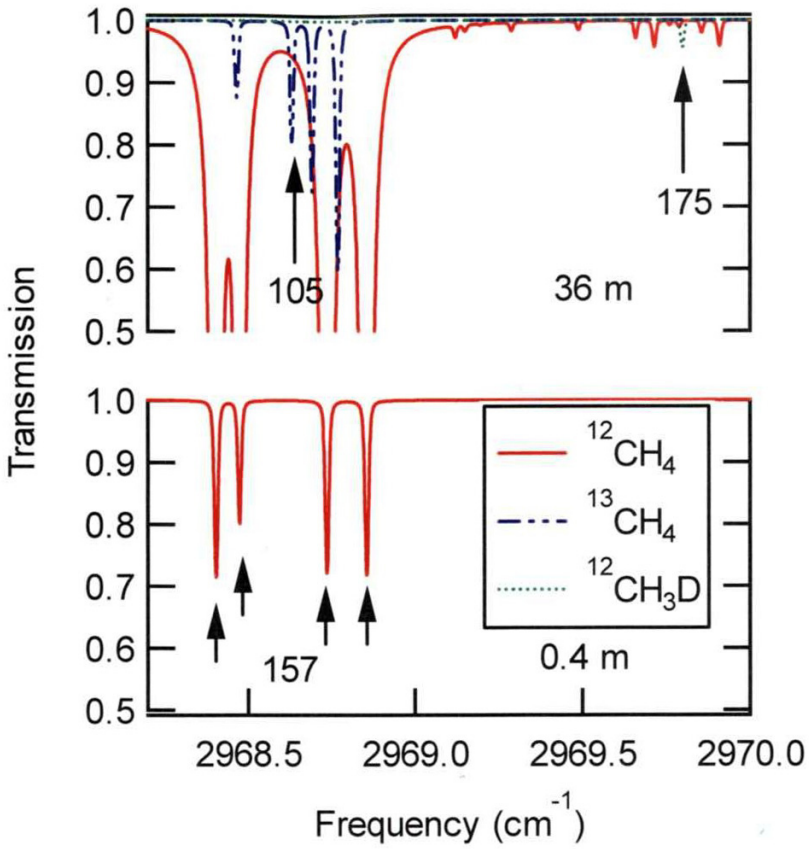
Reference:
G. T. Forrest, *APPLIED OPTICS* **19** (13), (1990).

SPECTRUM 2968.5

Start wavelength
$\lambda = 2968.5\ cm^{-1}$

End wavelength
$\lambda = 2970\ cm^{-1}$

Molecules: $^{13}CH_4$, $^{12}CH_4$, $^{12}CH_3D$



Simulated sample cell transmission for a suitable set of lines for CH_4. The upper panel shows the transmission through a 36 m pathlength and the lower panel shows the transmission through a 40 cm pathlength. The lower state energy levels (in cm^{-1}) are noted below the lines.

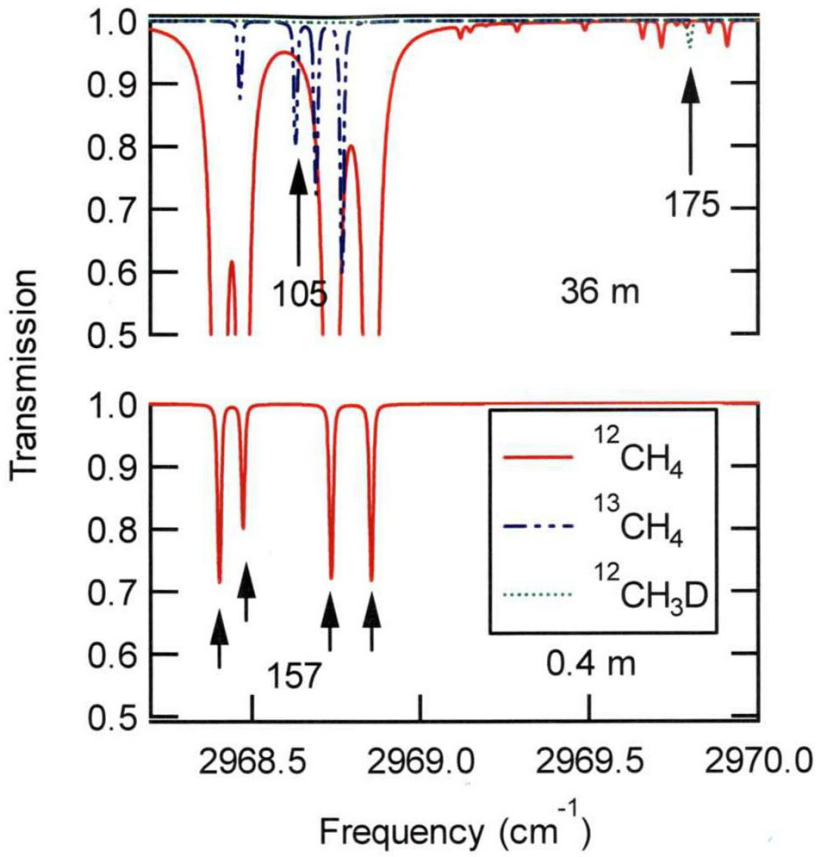
Reference:
J. B. McManus, M. S. Zahniser, D. D. Nelson, L. R. Williams, C. E. Kolb, *Spectrochemica Acta* **58**, 2505-2517 (2002).

SPECTRUM 2968.5

Start wavelength
$\lambda = 2968.5\ cm^{-1}$

End wavelength
$\lambda = 2970\ cm^{-1}$

Molecules: $^{13}CH_4$, $^{12}CH_4$, $^{12}CH_3D$



Simulated sample cell transmission for a suitable set of lines for CH_4. The upper panel shows the transmission through a 36 m pathlength and the lower panel shows the transmission through a 40 cm pathlength. The lower state energy levels (in cm^{-1}) are noted below the lines.

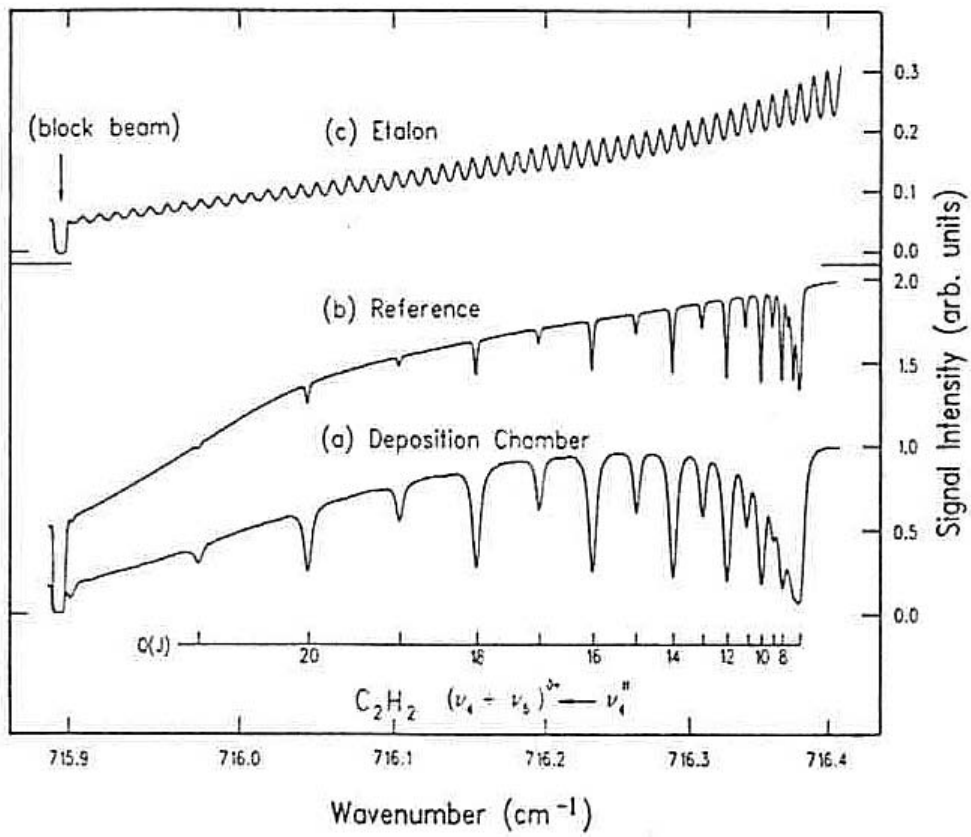
Reference:
J. B. McManus, M. S. Zahniser, D. D. Nelson, L. R. Williams, C. E. Kolb, *Spectrochemica Acta* **58**, 2505-2517 (2002).

SPECTRUM 716.4

Start wavelength
$\lambda = 716.4\ cm^{-1}$

End wavelength
$\lambda = 715.9\ cm^{-1}$

Molecules: CH_3, C_2H_2



Results of an infrared diode laser scan of the $(\nu_4 + \nu_5 - \nu_4)$ Q-branch band head near 716 cm^{-1}. The traces shown are (a) absorption from the deposition gas-phase environment (20 passes, effective path length ~0.5 m), (b) absorption from a room-temperature cell containing ~0.1 Torr of C_2H_2, and (c) etalon trace (free-spectral range ~0.01 cm^{-1}). The average C_2H_2 temperature in the deposition chamber is estimated from the relative line intensities of the ($J = 8$-21) Q-branch lines and found to be in the range 200-300° C. The linewidths in (a) are larger than (b) because of pressure broadening.

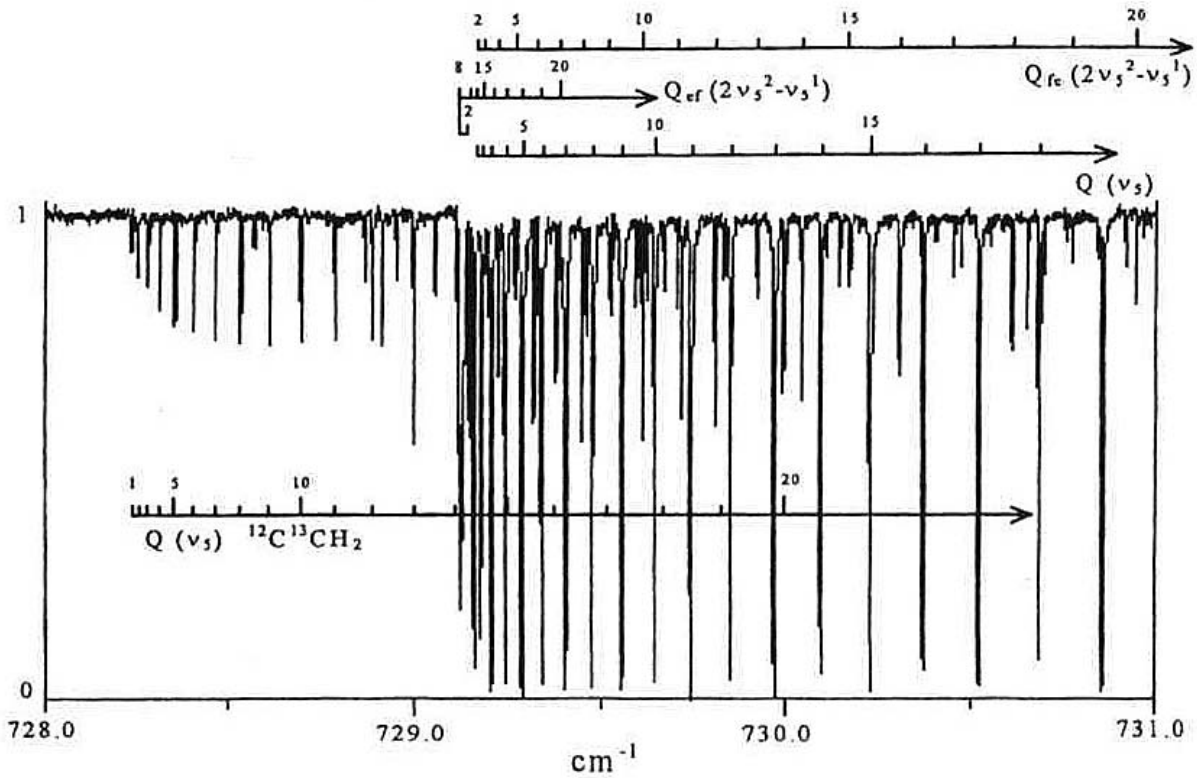
Reference:
F. G. Celii, J. E. Butler, *Annual Review of Phys. Chemistry* **42**, 643-684 (1991).

SPECTRUM 728

Start wavelength
$\lambda = 728\ cm^{-1}$

End wavelength
$\lambda = 731\ cm^{-1}$

Molecules: C_2H_2



Portion of spectrum #2 of Table1, around the Q-branch of the ν_5 band of C_2H_2 at 730 cm^{-1}.

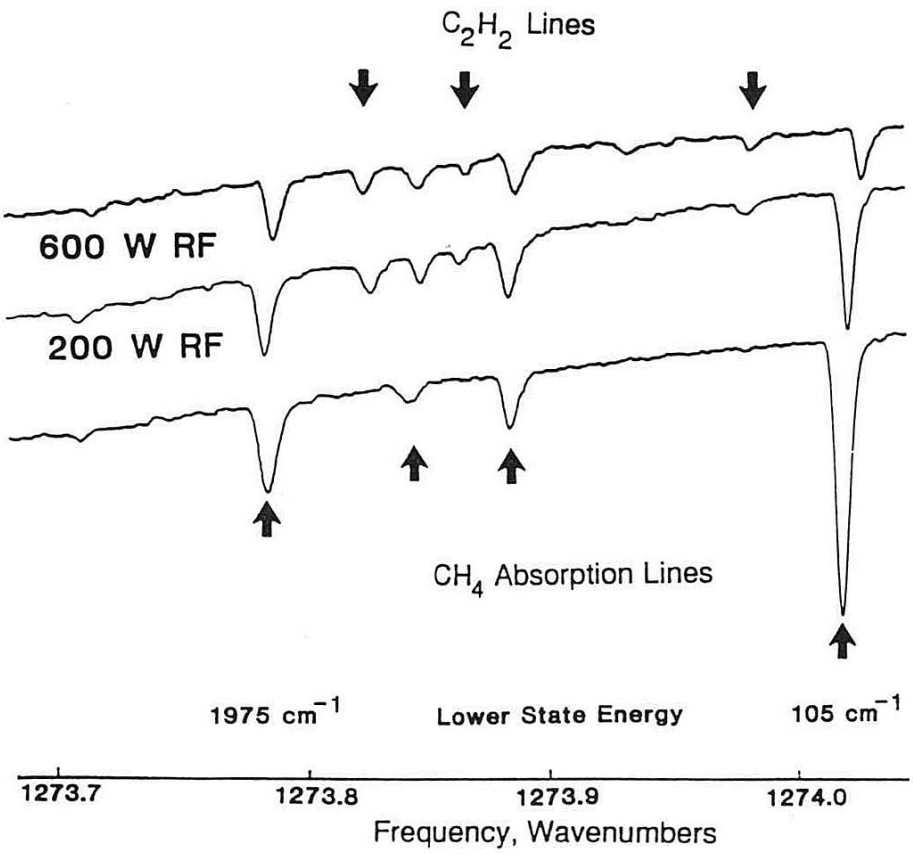
Reference:
D. Jacquemart, C. Claveau, J. Y. Mandin, V. Dana, *Journal of Quantitative Spectroscopy & Radiative Transfer* **69**, 81-101 (2001).

SPECTRUM 1273.7

Start wavelength
$\lambda = 1273.7\ cm^{-1}$

End wavelength
$\lambda = 1273.8\ cm^{-1}$

Molecules: CH_4, C_2H_2



Infrared spectral region used in CH_4 dissociation fraction and temperature measurement (lower trace, plasma off, upper traces, plasma on).

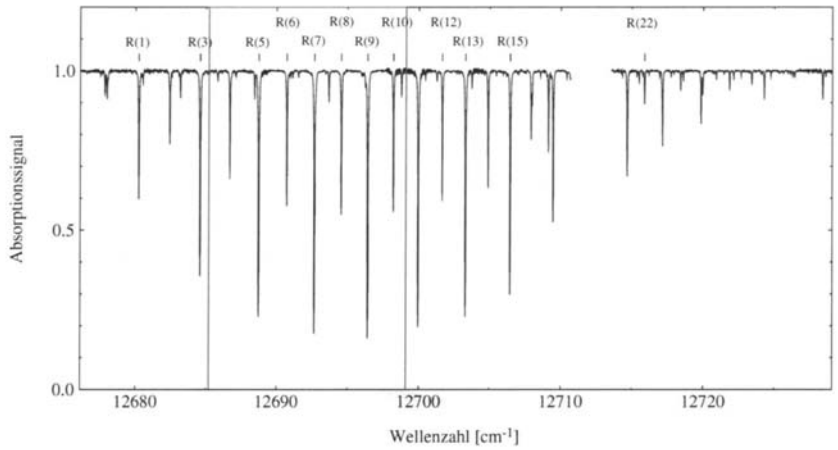
Reference:
J. Wormhoudt, *Final Technical Report* (1990).

SPECTRUM 12680

Start wavelength
$\lambda = 12680\ cm^{-1}$

End wavelength
$\lambda = 12720\ cm^{-1}$

Molecules: C_2H_2



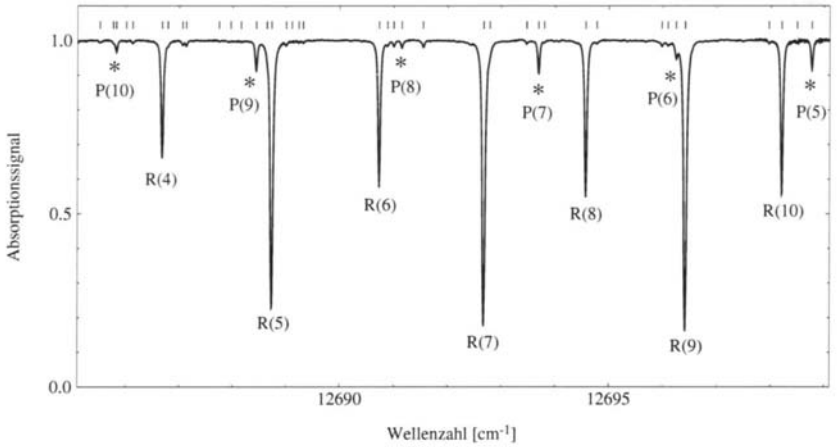


Abb. Oben: Ausschnitt aus dem Spektrum des Acetylens in dem *R*-Zweig der $\nu_1 + 3\nu_3$-Bande. Markiert sind diejenigen Linien, die verbreiterungsspektroskopisch untersucht wurden;
Abb. Unten: vergrößerter Ausschnitt aus der oberen Abbildung.

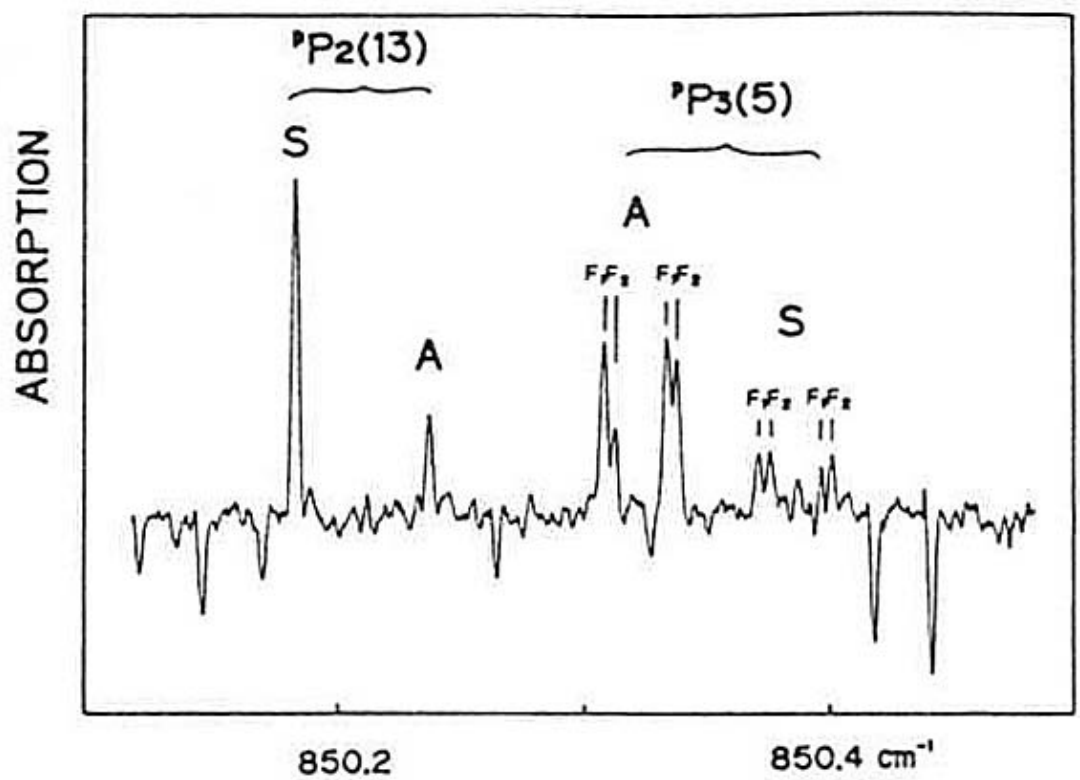
Reference:
Hamid Valipour, *Dissertation „Messung druckinduzierter Effekte an Absorptionslinien von Acetylen", Technische Universität Berlin (2001).*

SPECTRUM 850

Start wavelength
$\lambda = 850\ cm^{-1}$

End wavelength
$\lambda = 850.5\ cm^{-1}$

Molecules: C_2H_3



The $^PP_2(13)$ and $^PP_3(5)$ transitions of the vinyl radical, observed in the same way as trace B of Fig. 1. The latter shows spin-rotation splittings as well as *K*-type doubling, whereas only one *K*-doubling component is seen for the former. The spin-rotation splitting is not resolved for this transition. Lines pointing downward correspond to depletion of the precursor, vinyl bromide.

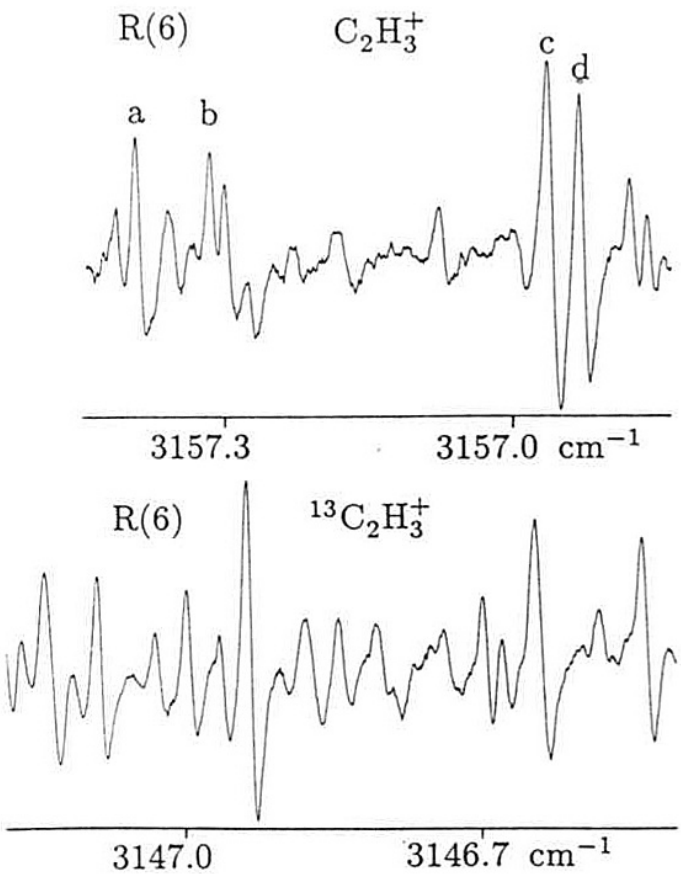
Reference:
H. Kanamori et al., *J. Chem. Phys.* **92** (1), (1990).

SPECTRUM 3157.0

Start wavelength
$\lambda = 3157.0\ cm^{-1}$

End wavelength
$\lambda = 3157.3\ cm^{-1}$

Molecules: $C_2H_3^+$



A comparison of the *R* (6) transitions of $C_2H_3^+$ and $^{13}C_2H_3^+$. The latter transitions split into more components because of the symmetry argument summarized in Table III in reference.

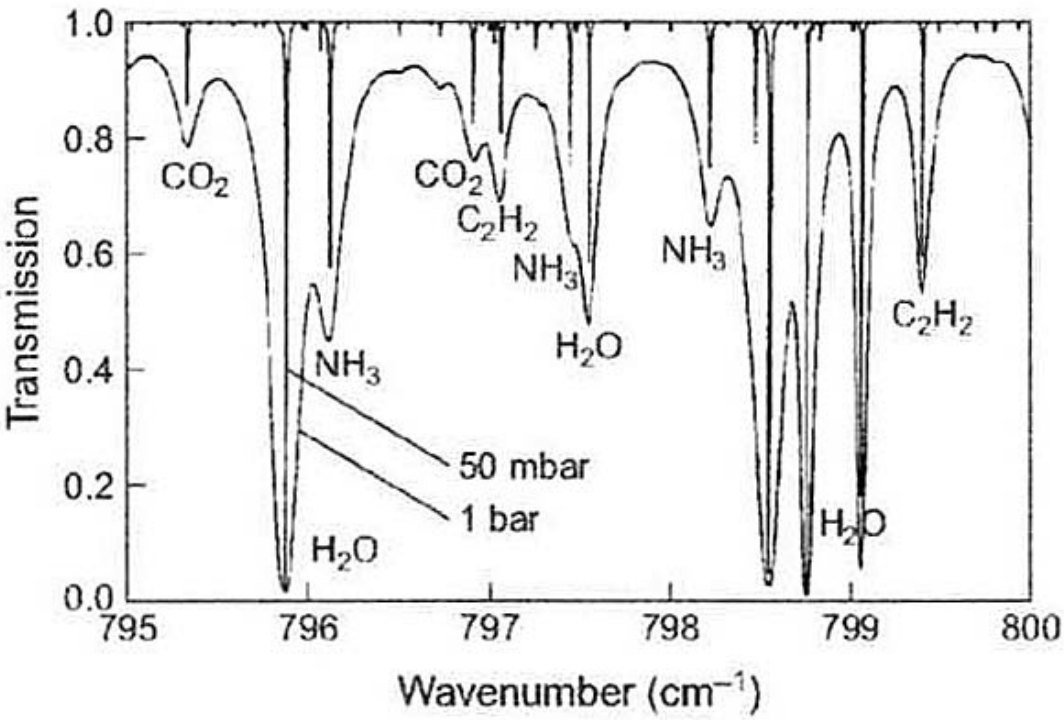
Reference:
M. W. Crofton, M. F. Jagod, B. D. Rehfuss, T. Oka, *J.Chem. Phys.* **91** (9), (1989).

SPECTRUM 795

Start wavelength
$\lambda = 795\ cm^{-1}$

End wavelength
$\lambda = 800\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4, NH_3



Transmission spectrum of a gas mixture typical for emissions of technical combustion containing H_2O, CO_2, NH_3 and C_2H_2 in N_2 at 470 K and 1 m optical path. (Taken from ref. 2). Such a mixture can be found in combustion exhaust to the atmosphere. While at atmospheric pressure the absorption lines merge, at low pressure (50 mbar) lines are only Doppler broadened and well isolated.

Reference 1:
M. Tacke, F. Wienhold, R. Grisar, H. Fischer, F. - J. Lübken, *Encyclopedia of Analytical Chemistry R.A. Meyers (Ed.) © John Wiley & Sons Ltd*, 2033-2065 (2000).

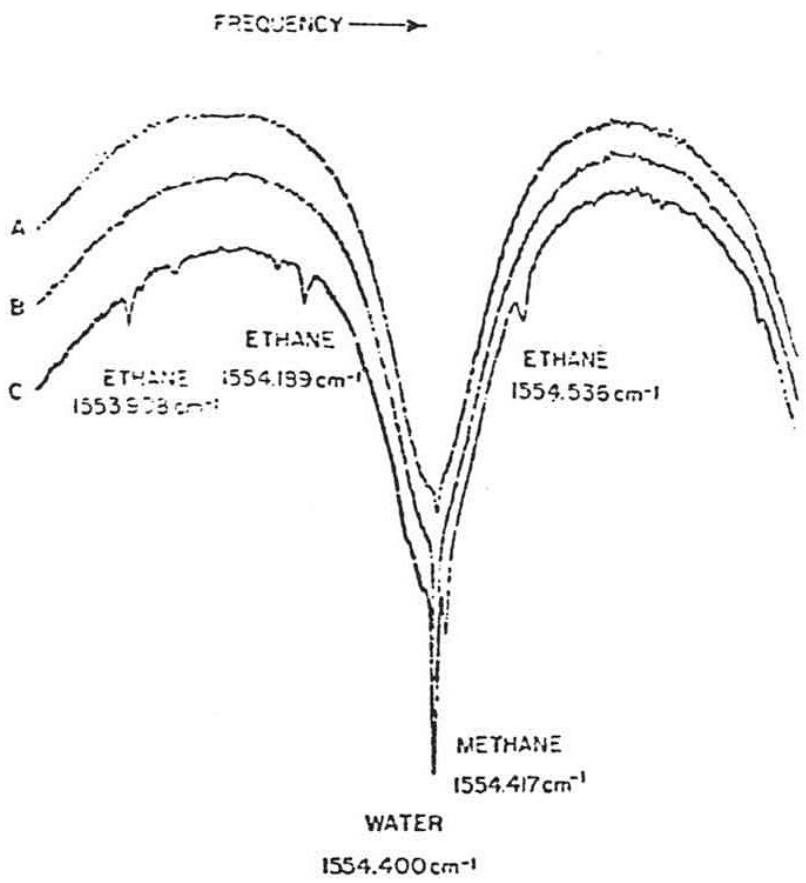
Reference 2:
U. von Zahn et al., *J. Geophys. Res.*, 102, 7443-7456 (1990).

SPECTRUM 1553.97

Start wavelength
$\lambda = 1553.97\ cm^{-1}$

End wavelength
$\lambda = 1554.54\ cm^{-1}$

Molecules: H_2O, CH_4, C_2H_4



Transmission spectra in the 1553 cm^{-1} region. The 50 cm^2 samples of either cigarette smoke (C) or room air containing 11.73 mm H_2O (B) were examined at a cell pressure of 12 Torr. Lock-in amplifier gain was 25 mV with a 0.3-sec time constant. Scan rate was 0.0077 cm^{-1} sec^{-1}. The background (A) and etalon calibration spectra (D) are also shown.

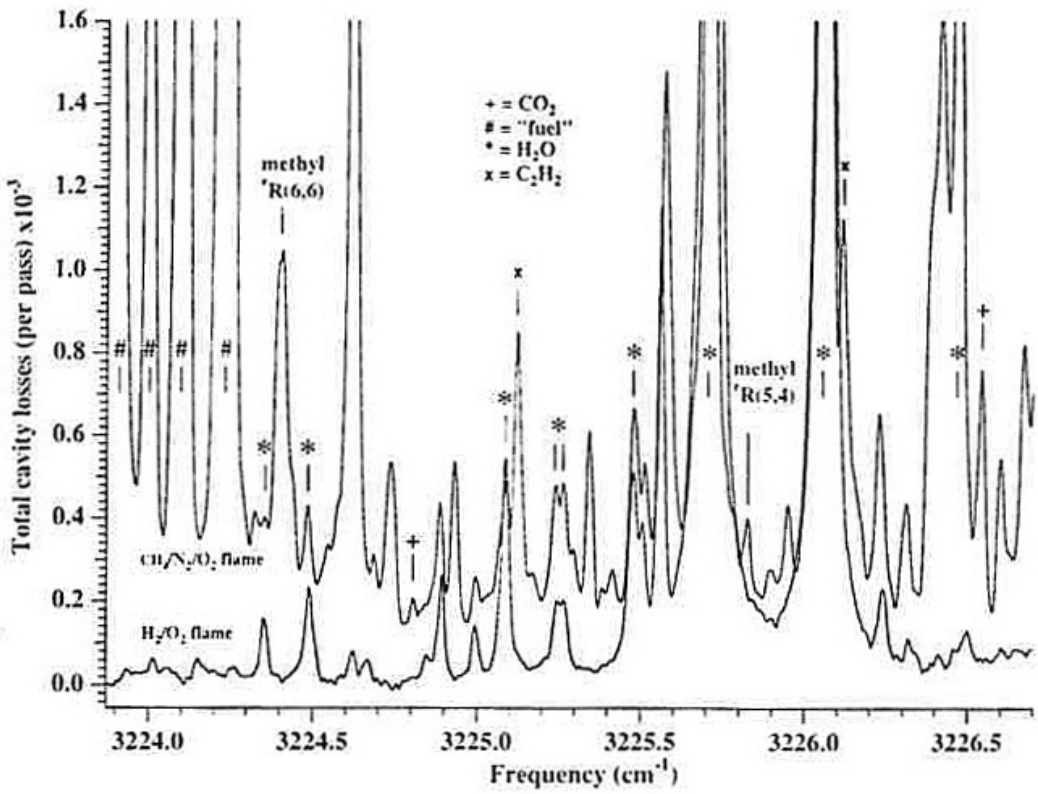
Reference:
G. T. Forrest, *APPLIED OPTICS* **19** (13), (1990).

SPECTRUM 3224.4

Start wavelength
$\lambda = 3324.4\ cm^{-1}$

End wavelength
$\lambda = 3226.5\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4



High resolution IR-CRLAS spectra obtained in the 3 micron region in a 37.5 Torr $CH_4/N_2/O_2$ (upper trace) and $H_2/N_2/O_2$ (lower trace) flame. Comparison of the two scans readily identifies likely H_2O features, which frequently overlap methyl transitions. In these data, the unique ability to obtain data for reactants (# = fuel and x = C_2H_2), Intermediates (CH_3) and products (* = H_2O and + = CO_2) in the infrared spectral region is demonstrated.

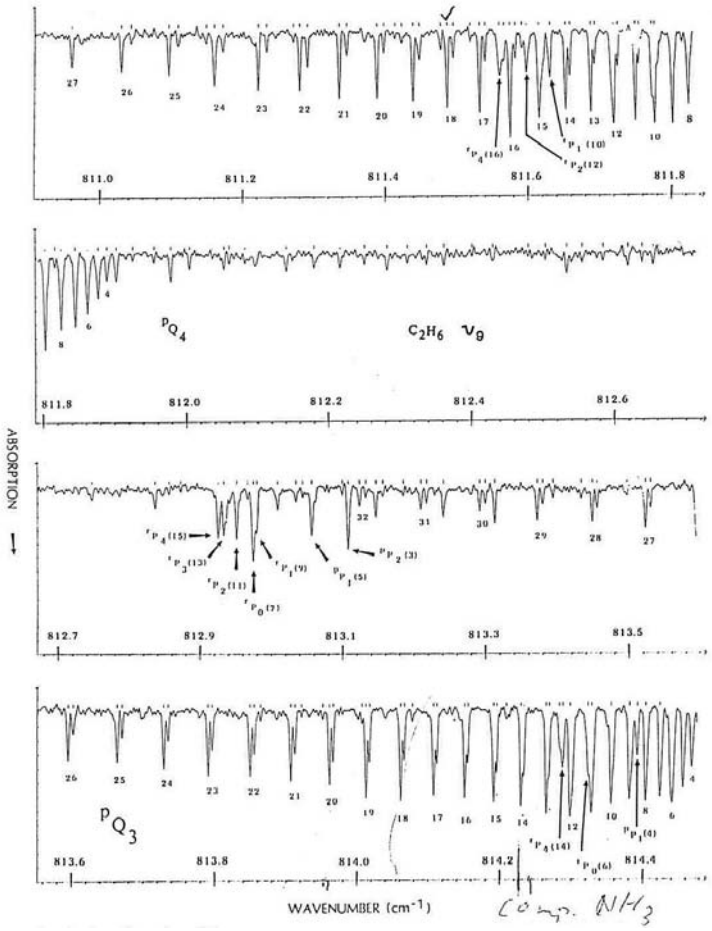
Reference:
J. J. Scherer et al., *J. Chem. Phys.* **107** (16), (1997).

SPECTRUM 811

Start wavelength
$\lambda = 811\ cm^{-1}$

End wavelength
$\lambda = 814\ cm^{-1}$

Molecules: C_2H_6



A small portion of the FTIR spectrum of the ν_9 band of C_2H_6. The *J* numbering of the two *Q* branches in the figure is indicated by integer labels. *P*-branch transitions falling in the region are indicated.

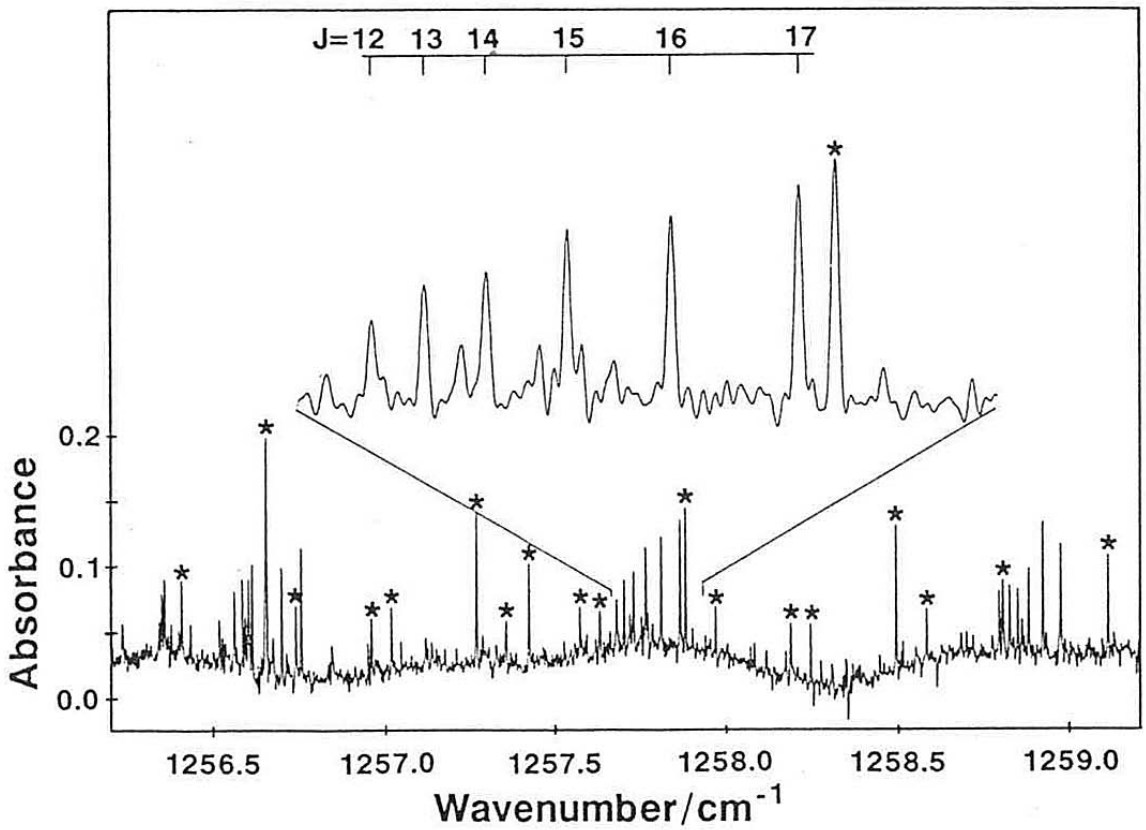
Reference:
L. Henry et al., *Ethane Spectrum*

SPECTRUM 1256.5

Start wavelength
$\lambda = 1256.5\ cm^{-1}$

End wavelength
$\lambda = 1259\ cm^{-1}$

Molecules: C_3H_2



Observed spectrum of the C_3H_2 ν_3 band (P branch). The spectral lines marked by an asterisk are assigned to the C_4H_2 (diacetylene) $\nu_6 + \nu_3$ band and its vibrational hot bands.

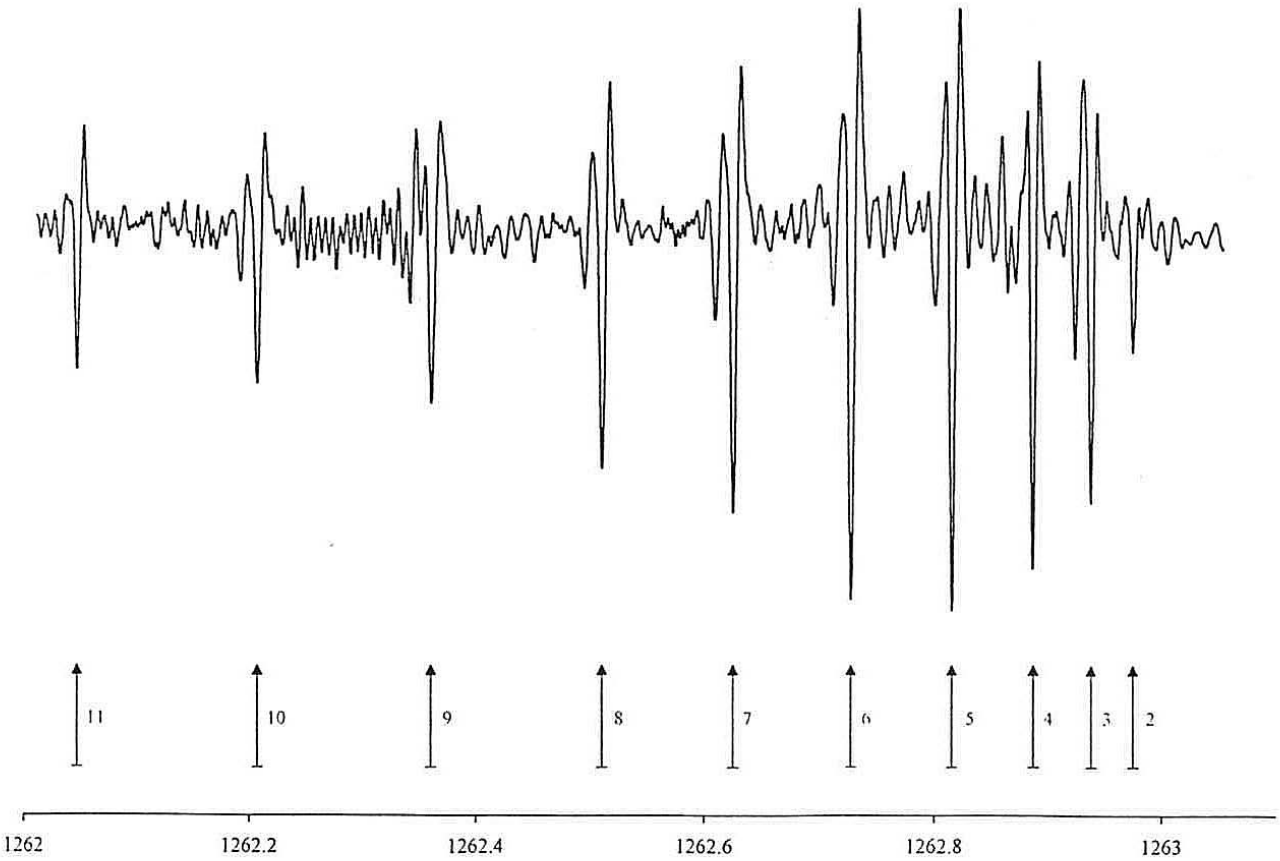
Reference:
Y. Hirahara, A. Masuda, K. Kawaguchi, *Chem.Phys.* **95** (6), (1991).

SPECTRUM 1262

Start wavelength
$\lambda = 1262\ cm^{-1}$

End wavelength
$\lambda = 1263\ cm^{-1}$

Molecules: CIPO



Diode laser absorption spectrum of the a-type Q-branch of the P-O stretch in ClPO. The lines are labelled according to the value of K_a and consist of unresolved *J* components.

Reference:
P. B. Davies, *Spectrochimica Acta Part A* **55**, 1987 – 1997 (1999).

SPECTRUM 500

Start wavelength
$\lambda = 500\ cm^{-1}$

End wavelength
$\lambda = 4000\ cm^{-1}$

Molecules: CO, CO_2, H_2O, CH_4

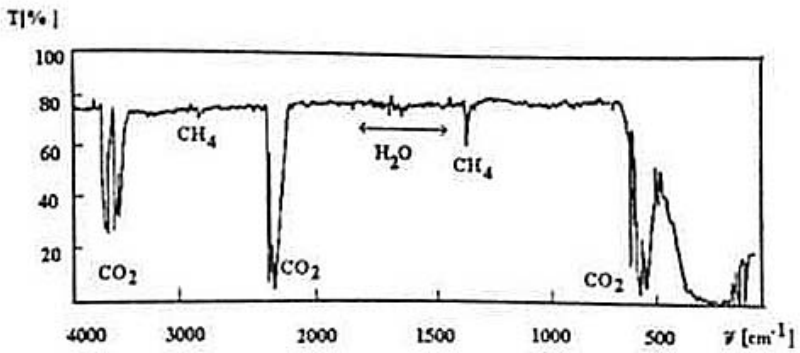
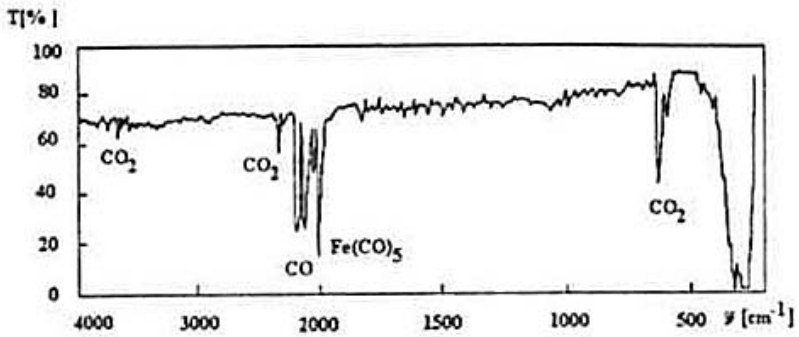


Figure 3. The IR absorption spectrum of CO_2.



(a)

The IR absorption spectrum of CO_2.

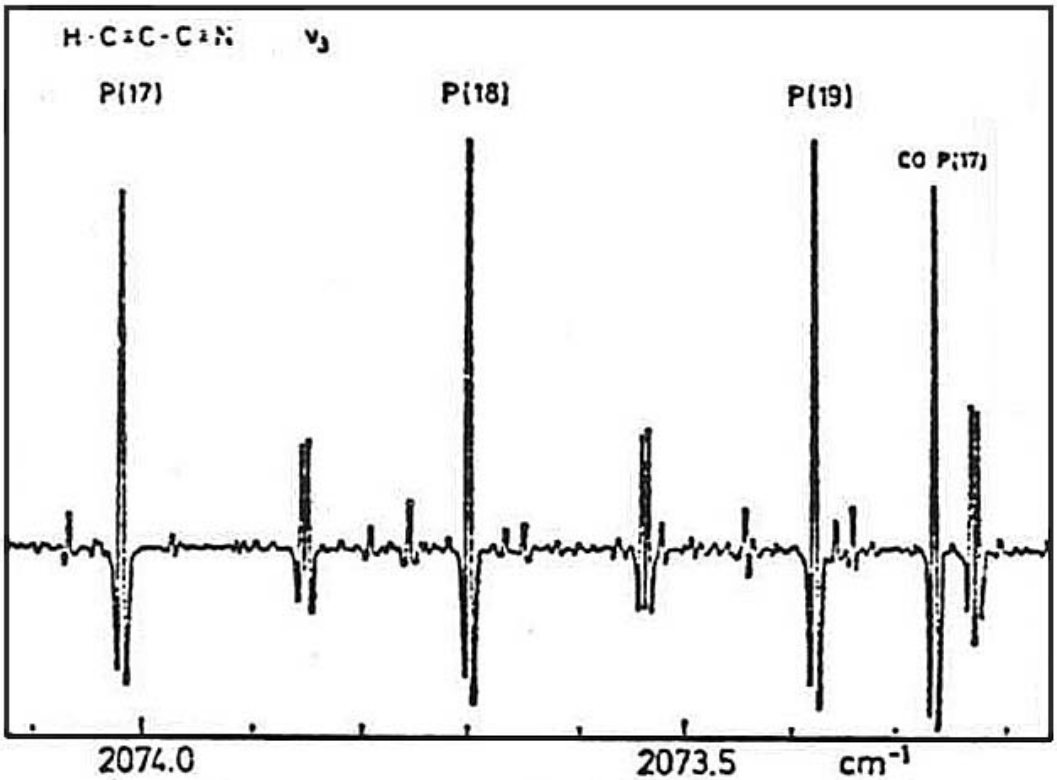
Reference:
M. Morvová, *Czechoslovak Journal of Physics*, ***47*** (2), (1997).

SPECTRUM 2073.5

Start wavelength
$\lambda = 2073.5\ cm^{-1}$

End wavelength
$\lambda = 2074\ cm^{-1}$

Molecules: HC_3N, CO



High resolution diode laser spectrum of the ν_3 vibration-rotation spectrum of HC_3N. Three successive *J* lines of the P branch are displayed. The P (17) CO line (CO appears as an impurity in the sample) is used as a calibration standard in this section of the spectrum. The weaker doublet lines in the spectrum are hot band transitions and exhibit *l*-type splitting. The spectrum was recorded by using frequency modulation and is displayed in second derivative form. It may be noted that reflection of laser power back into the laser causes weak energy modulation which produces errors in the baseline.

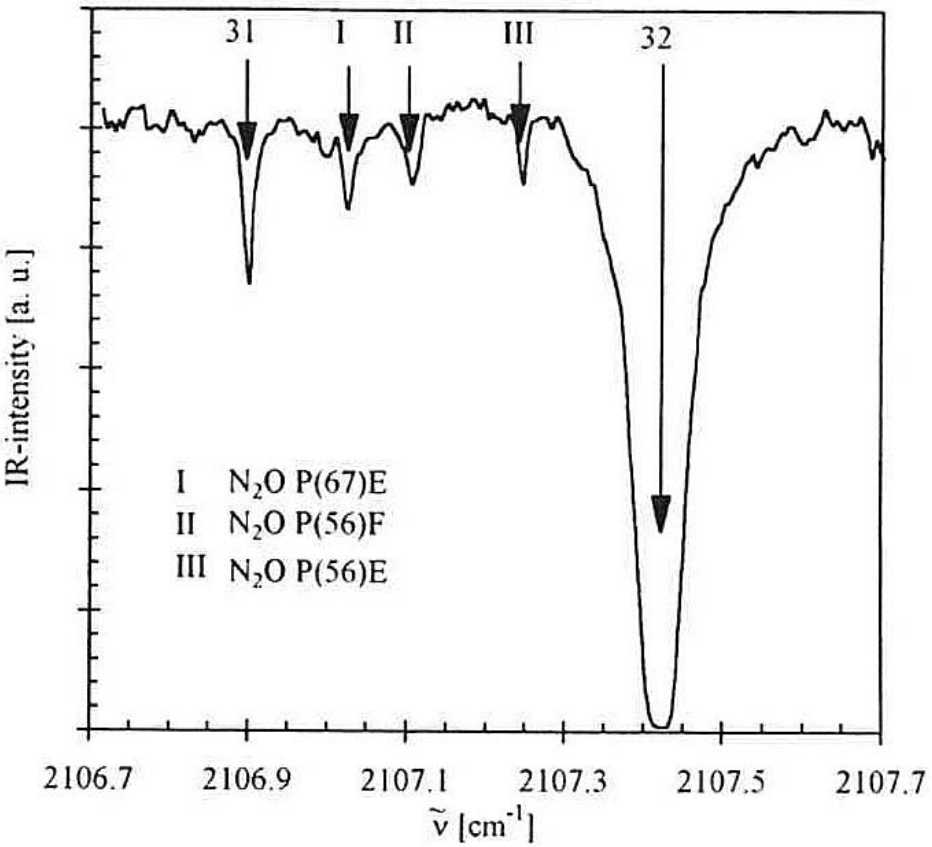
Reference:
K. Yamada, R. Schieder, G. Winnewisser, *Physikalisches Institut Universität zu Köln, Z. Naturforsch.* **35a**, 690-693 (1980).

SPECTRUM 2106.7

Start wavelength
$\lambda = 2106.7\ cm^{-1}$

End wavelength
$\lambda = 2107.7\ cm^{-1}$

Molecules: CO, N_2O



Example for a multi-component can with CO and N_2O, multireflection cell with 9.5 m optical pathlength, $p_{N2O} = 35$ Torr, $p_{CO} = 0.007$ Torr.

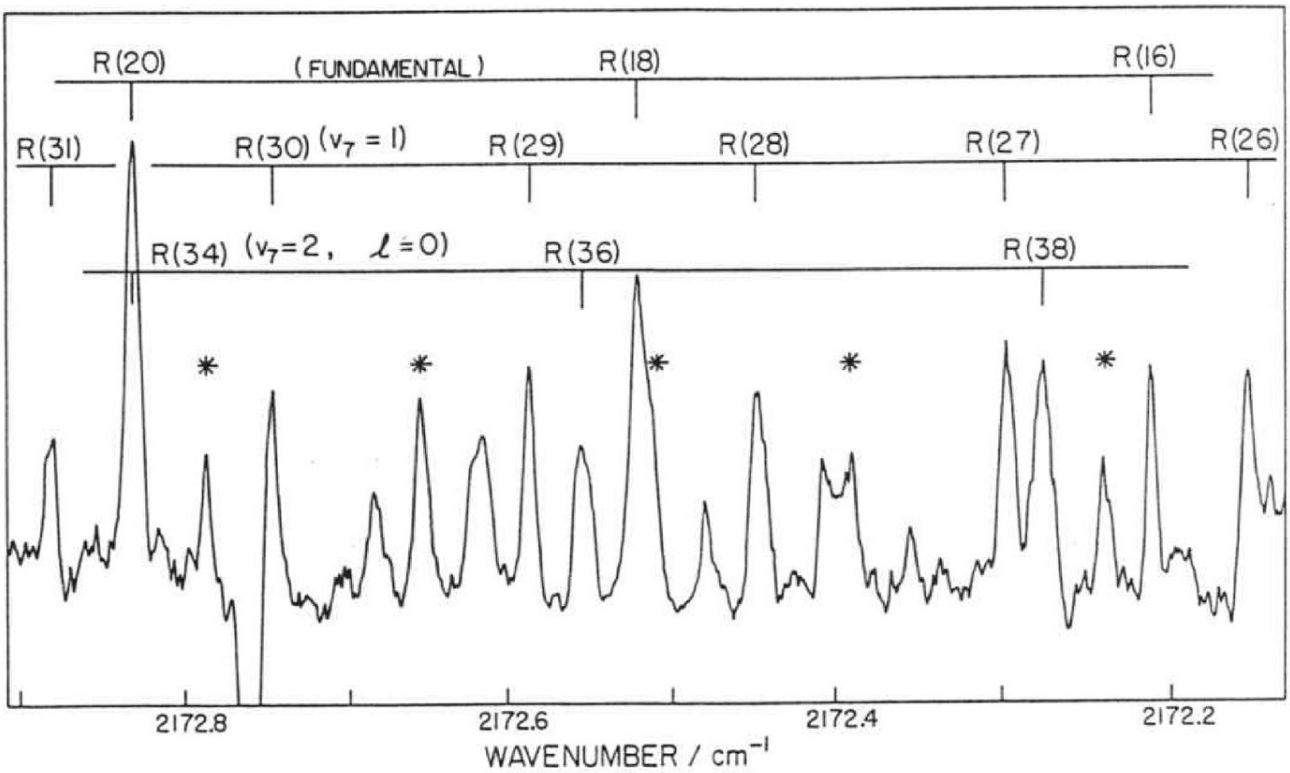
Reference:
T. Kelz et al., *Journal of Quantitative Spectroscopy and Radiative Transfer*, **61** (5), 591-601 (1999).

SPECTRUM 2172.2

Start wavelength
$\lambda = 2172.2\ cm^{-1}$

End wavelength
$\lambda = 2172.8\ cm^{-1}$

Molecules: C_5, CO



A portion of the spectrum of C_5, as recorded using a tunable diode laser source. The three most prominent bands analyzed in this paper are shown directly, while lines belonging to the $\nu_5 = 1$ hot band, whose assignment is somewhat less certain, are indicated with asterisks. Note that the intensity scale is not uniform due to laser power variations and also that the wave number scale is not necessarily exactly linear. The negative feature at 2172.76 cm^{-1} is due to CO, present as an impurity in the discharge.

Reference:
N. Moazzen-Ahmadi, A. R. W. Mc Kellar, T. Amano, *J. Chem.Phys.*, **91** (4), (1989).

SPECTRUM 500

Start wavelength
$\lambda = 500\ cm^{-1}$

End wavelength
$\lambda = 4000\ cm^{-1}$

Molecules: CO, CO_2, H_2O, CH_4

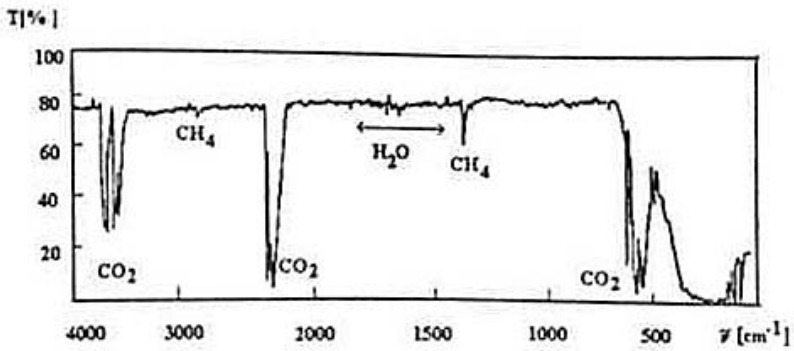
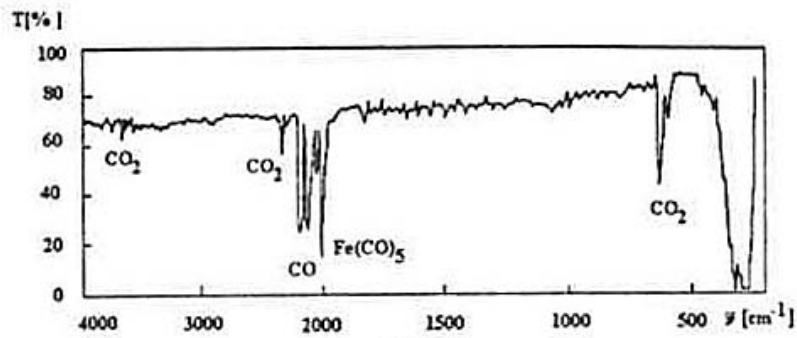


Figure 3. The IR absorption spectrum of CO_2.



(a)

The IR absorption spectrum of CO_2.

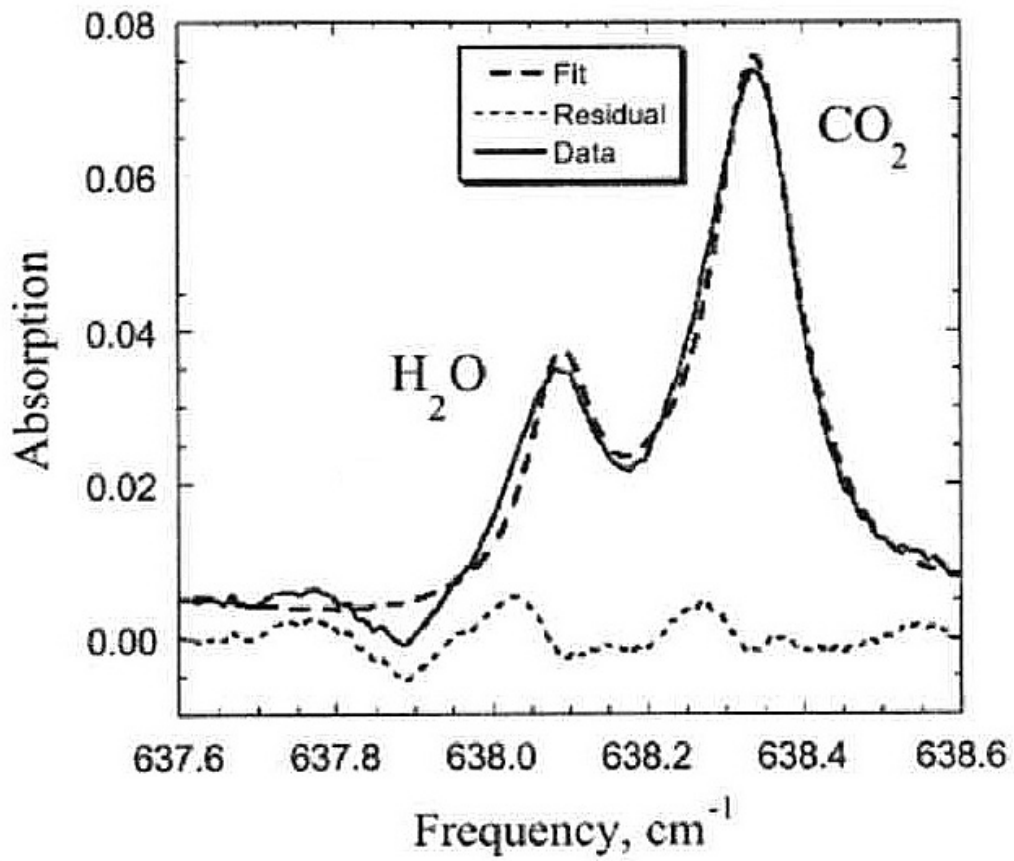
Reference:
M. Morvová, *Czechoslovak Journal of Physics*, ***47*** (2), (1997).

SPECTRUM 637.6

Start wavelength
$\lambda = 637.6\ cm^{-1}$

End wavelength
$\lambda = 638.6\ cm^{-1}$

Molecules: CO_2, H_2O



CO_2 and H_2O absorption.

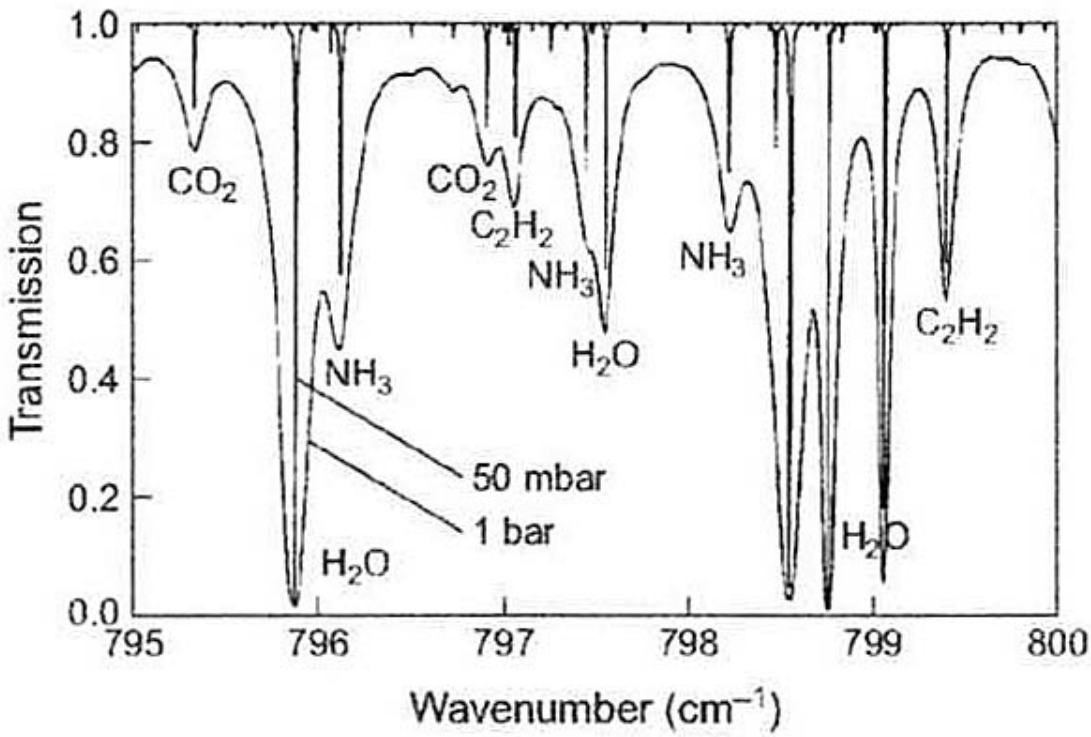
Reference:
A. A. Kosterev, R. F. Curl, F. K. Tittel, M. Rochat, M. Beck, D. Hofstetter, J. Faist, *Applied Physics B, Laser and Optics* (2002).

SPECTRUM 795

Start wavelength
$\lambda = 795\ cm^{-1}$

End wavelength
$\lambda = 800\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4, NH_3



Transmission spectrum of a gas mixture typical for emissions of technical combustion containing H_2O, CO_2, NH_3 and C_2H_2 in N_2 at 470 K and 1 m optical path. (Taken from Ref. 2). Such a mixture can be found in combustion exhaust to the atmosphere. While at atmospheric pressure the absorption lines merge, at low pressure (50 mbar) lines are only Doppler broadened and well isolated.

Reference 1:
M. Tacke, F. Wienhold, R. Grisar, H. Fischer, F. - J. Lübken, *Encyclopedia of Analytical Chemistry R.A. Meyers (Ed.) © John Wiley & Sons Ltd*, 2033-2065 (2000).

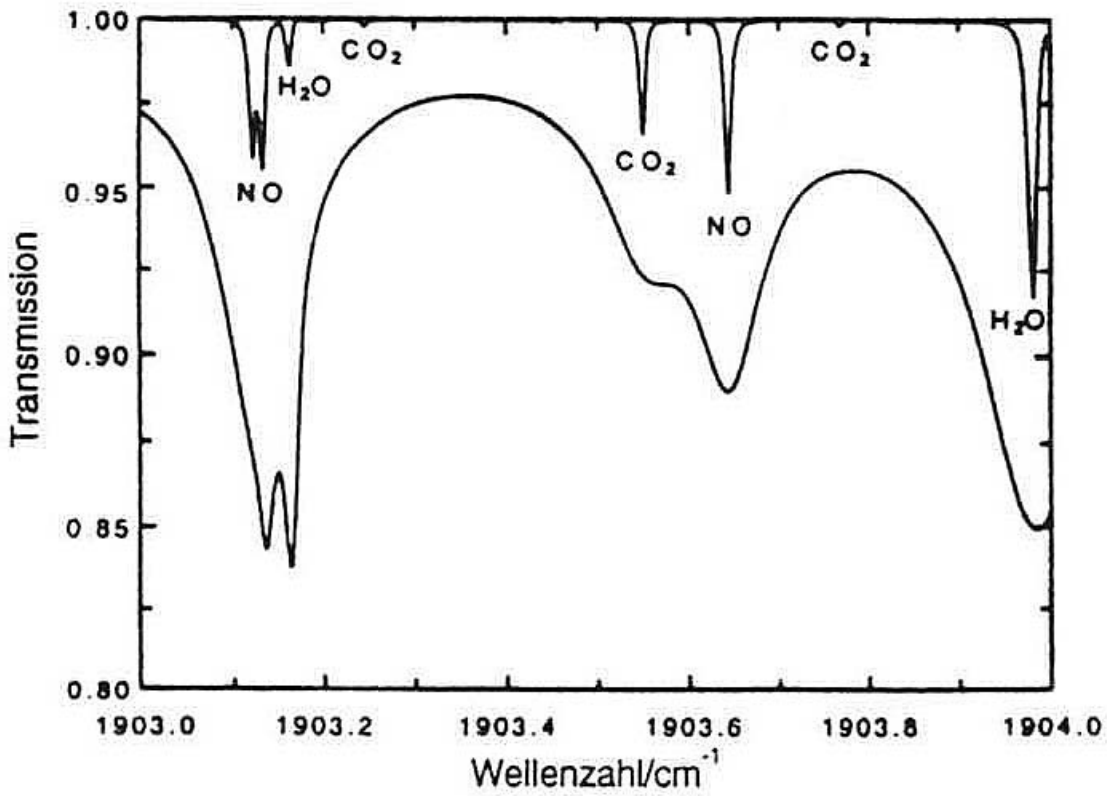
Reference 2:
U. von Zahn et al., *J. Geophys. Res.*, 102, 7443-7456 (1990).

SPECTRUM 1903

Start wavelength
$\lambda = 1903\ cm^{-1}$

End wavelength
$\lambda = 1904\ cm^{-1}$

Molecules: CO_2, NO, H_2O



Transmission spectrum of a gas mixture consisting of 100 ppm NO, 15% CO_2 and 15% H_2O in N_2 at 470 K and 1 m optical path. At atmospheric pressure (lower curve) the NO lines appear on the background of the other gases, at 30 mbar (needle-shaped minima) the NO lines can be traced nearly free of interference by other gases.

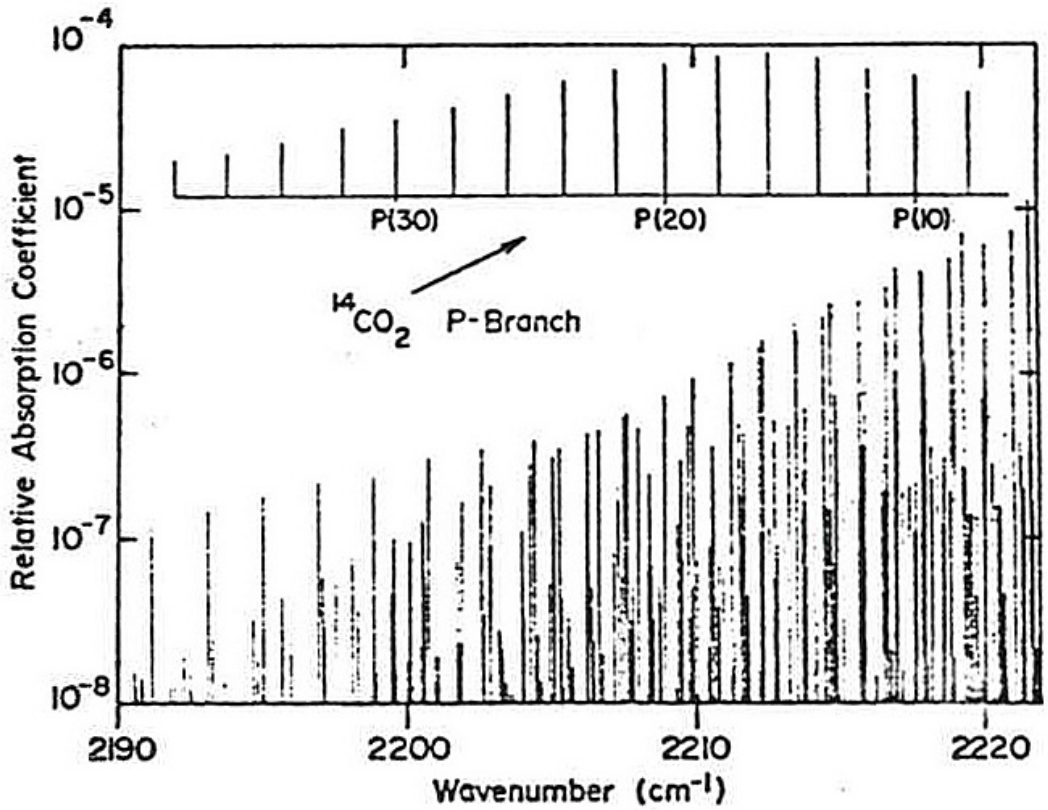
Reference:
M. Tacke, R. Grisar, *Laser und Optoelektronik*, 51-56 (1995).

SPECTRUM 2190

Start wavelength
$\lambda = 2190\ cm^{-1}$

End wavelength
$\lambda = 2220\ cm^{-1}$

Molecules: CO_2



Detailed CO_2 spectrum, including hot bands in the region of the *P*-branch of $^{14}CO_2$. All lines are normalised to the strong lines in the fundamental of $^{12}C^{16}O_2$.

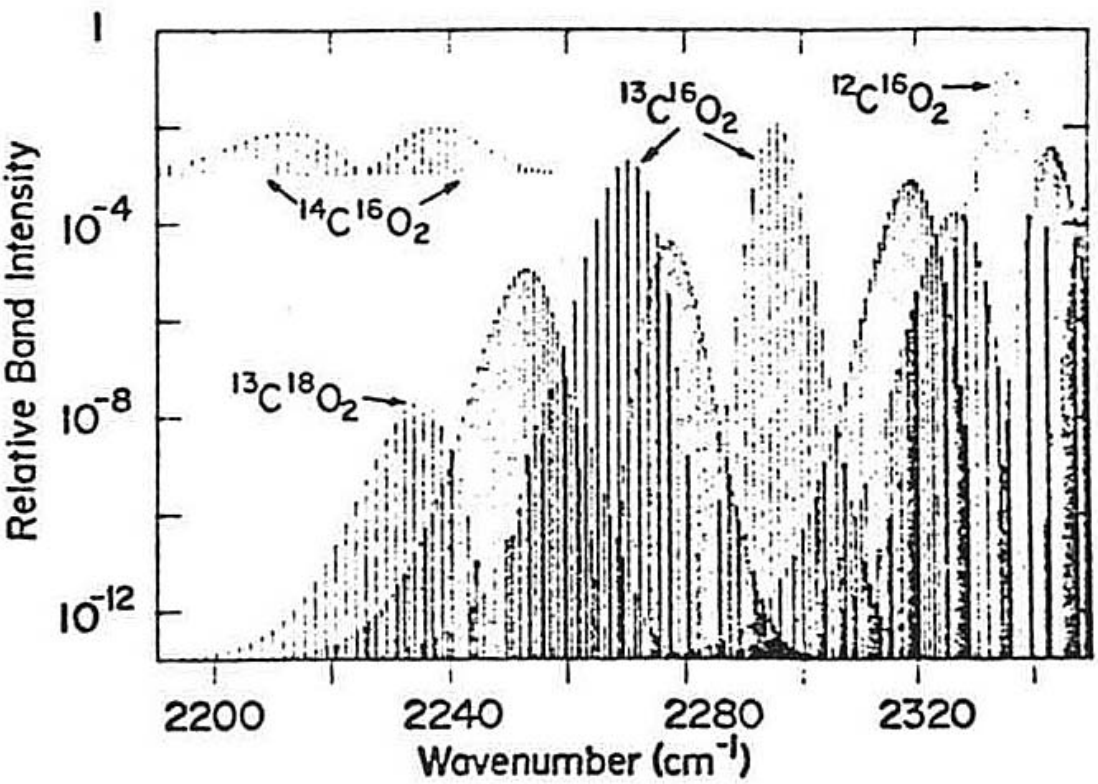
Reference:
D. Labrie, J. Reid, *Appl. Phys.* **24**, 381-386 (1981).

SPECTRUM 2200

Start wavelength
$\lambda = 2200\ cm^{-1}$

End wavelength
$\lambda = 2340\ cm^{-1}$

Molecules: CO_2



Calculated spectrum of CO_2 in the 4.4 μm region. The ν_3 fundamental bands of most of the relevant isotopic species are included. The relative strength of each band is normalised to the $^{12}C^{16}O_2$ bandstrength on a logarithmic scale, but the individual lines in each band are plotted in a linear fashion. The $^{14}CO_2$ ν_3 band is offset for clarity and is displayed with an intensity corresponding to a modern carbon sample ($^{14}C/^{12}C \sim 10^{-12}$).

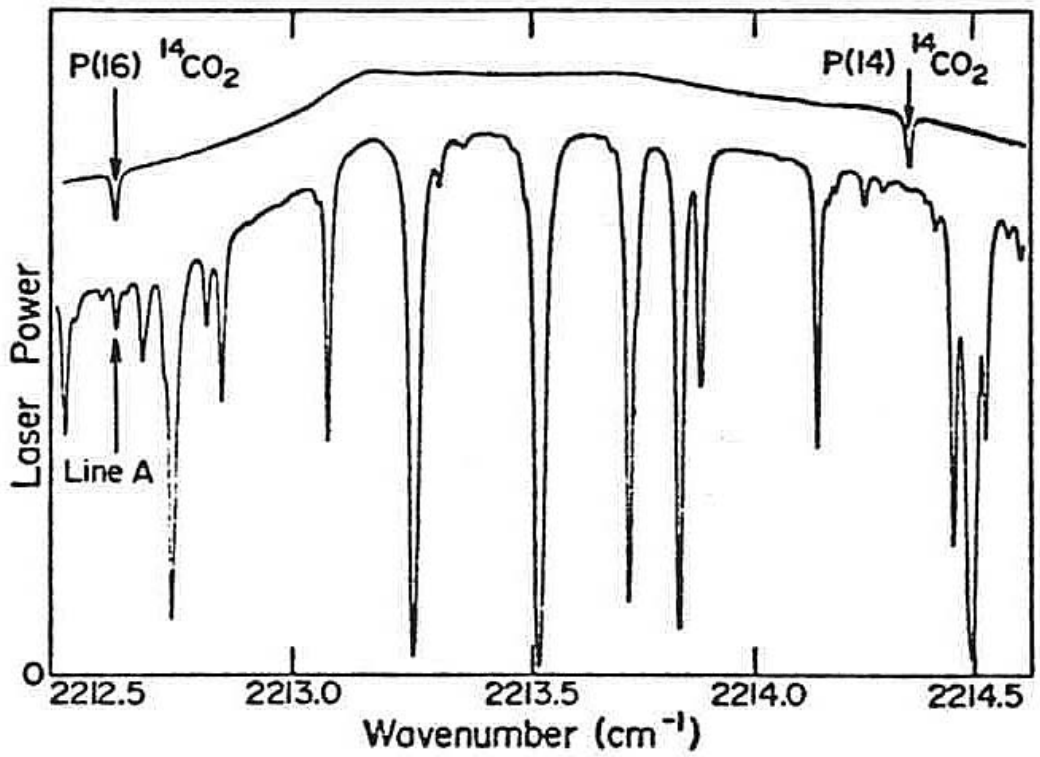
Reference:
D. Labrie, J. Reid, *Appl. Phys.* **24**, 381-386 (1981).

SPECTRUM 2212.5

Start wavelength
$\lambda = 2212.5\ cm^{-1}$

End wavelength
$\lambda = 2214.5\ cm^{-1}$

Molecules: CO_2



Results of diode scans over the *P*(16) and *P*(14) lines of $^{14}CO_2$. The lower trace was taken with a pathlength of 200 m trough CO_2 at a pressure of 30 Torr. For the upper trace the multipass cell was evacuated and a small cell of $^{14}CO_2$ inserted in the laser beam. Note that the *P*(16) line is overlapped by line A, while the *P*(14) line is relatively free from interference. All the strong absorption lines observed in the lower trace were identified using the date of [4-11]. However, there was insufficient spectral data available to identify many of the weaker lines, including line A.

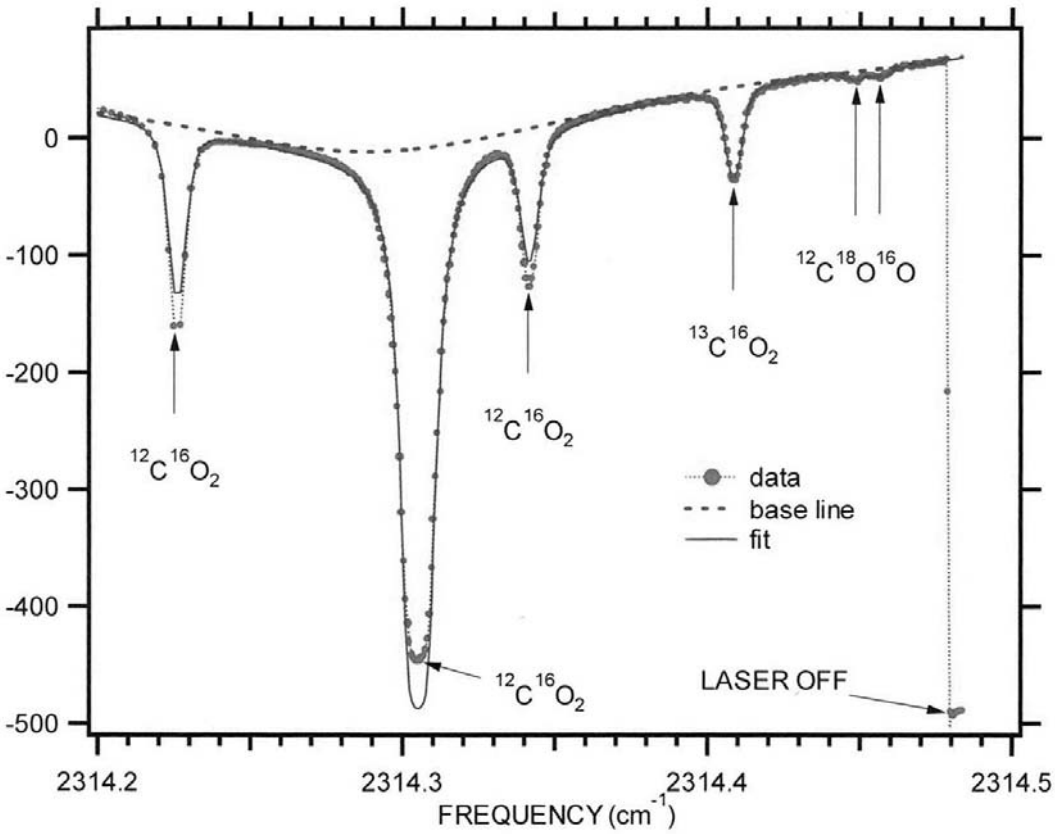
Reference:
D. Labrie and J. Reid, *Appl. Phys.* **24**, 381-386 (1981).

SPECTRUM 2314.2

Start wavelength
$\lambda = 2314.2\ cm^{-1}$

End wavelength
$\lambda = 2314.5\ cm^{-1}$

Molecules: CO_2



TDL spectrometer scan near 2314 cm^{-1}, showing CO_2 isotopomere lines for ($^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{13}C^{16}O^{18}O$), using the long pathlength of 36.51 m, at 16 Torr and ambient CO_2 mixing ratio of 380 ppm.

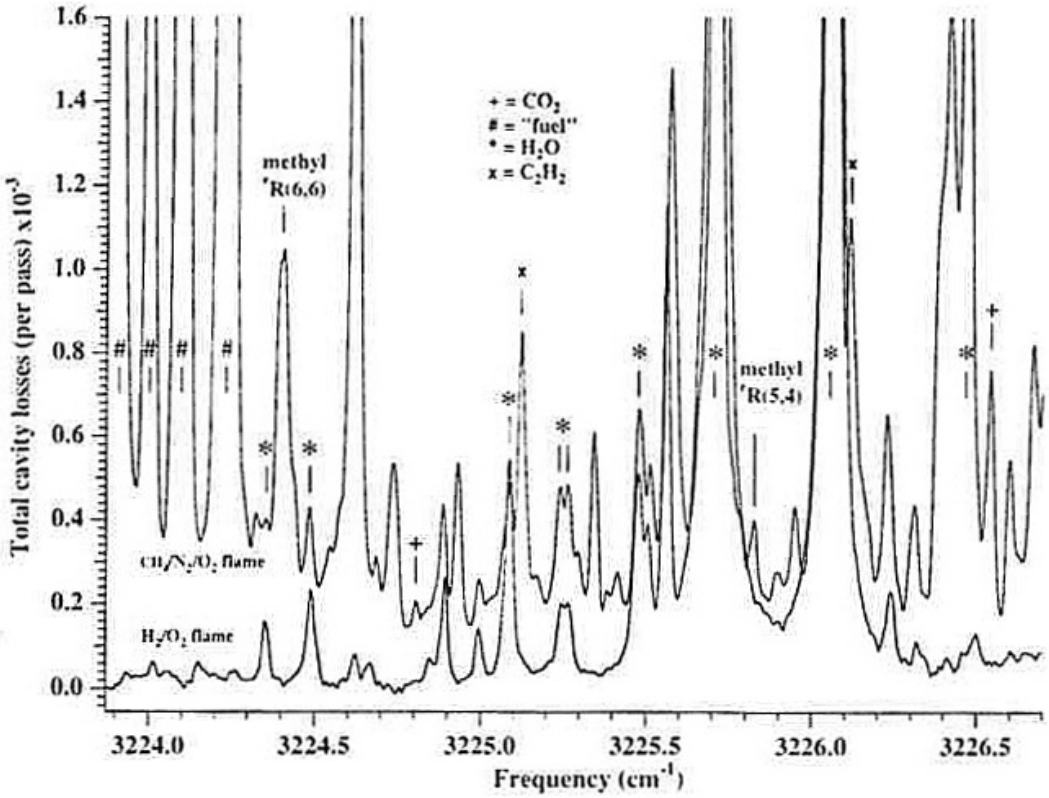
Reference:
J. B. McManus, M. S. Zahniser, D. D. Nelson, L. R. William, C. E. Kolb, *Spectrochim. Acta* **58**, 2465-2479 (2002).

SPECTRUM 3324.4

Start wavelength
$\lambda = 3324.4\ cm^{-1}$

End wavelength
$\lambda = 3226.5\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4



High resolution IR-CRLAS spectra obtained in the 3 micron region in a 37.5 Torr $CH_4/N_2/O_2$ (upper trace) and $H_2/N_2/O_2$ (lower trace) flame. Comparison of the two scans readily identifies likely H_2O features, which frequently overlap methyl transitions. In these data, the unique ability to obtain data for reactants (# = fuel and x = C_2H_2), Intermediates (CH_3) and products (* = H_2O and + = CO_2) in the infrared spectral region is demonstrated.

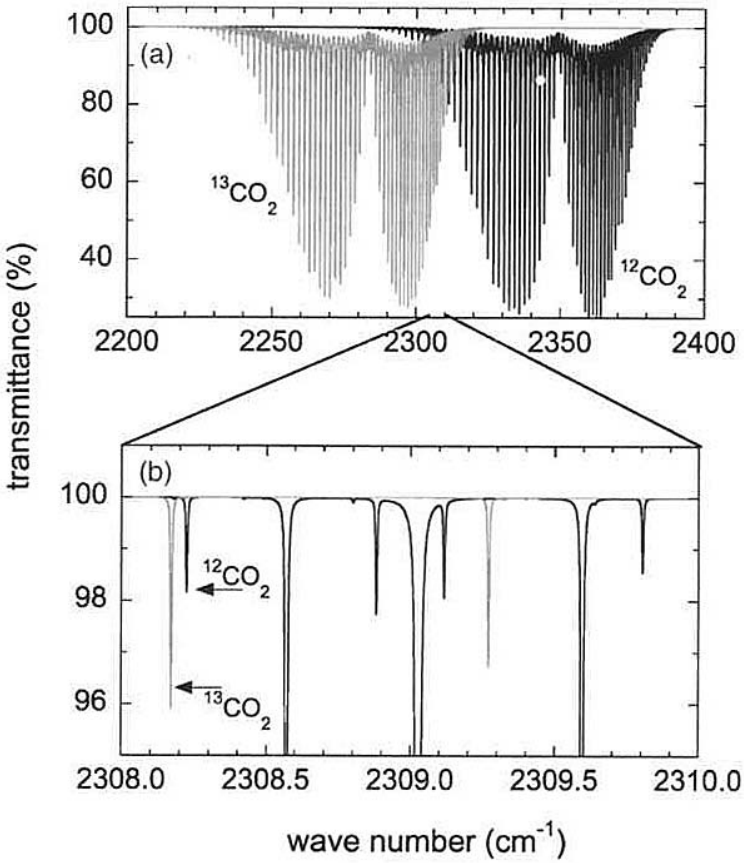
Reference:
J. J. Scherer et al., *J. Chem. Phys.* **107** (16), (1997).

SPECTRUM 2308

Start wavelength
$\lambda = 2308\ cm^{-1}$

End wavelength
$\lambda = 2310\ cm^{-1}$

Molecules: $^{13}CO_2$, $^{12}CO_2$



Transmission spectra for $^{12}CO_2$ and $^{13}CO_2$. Shown in (a) are spectra over a broad wave number range; the two right-most lobes are the spectra for $^{12}CO_2$ and the left ones are $^{13}CO_2$. The individual absorption lines used by the TDL for each isotope are shown in (b).

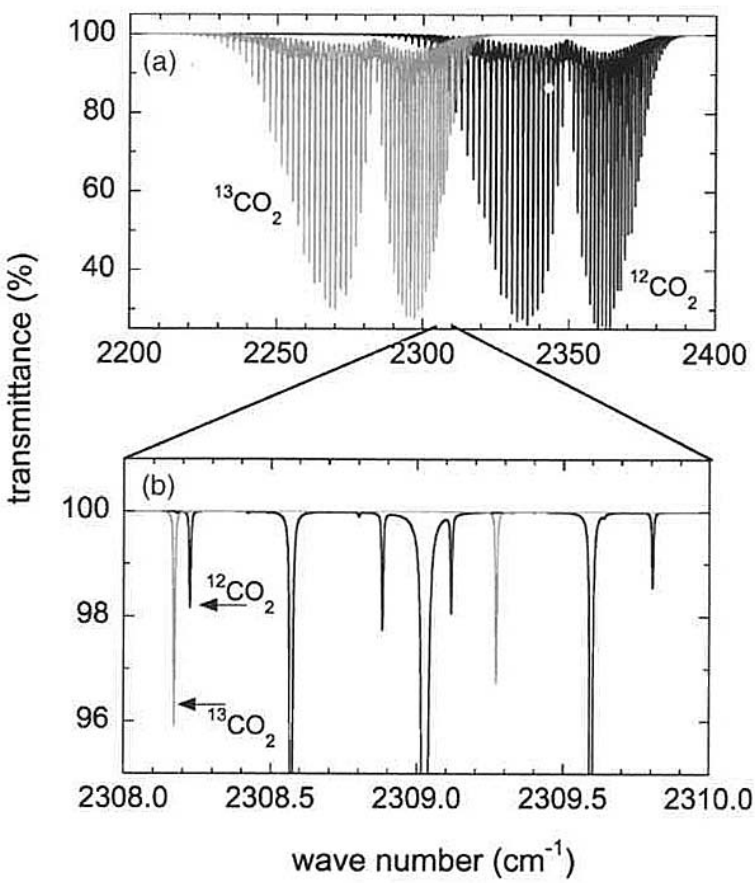
Reference:
D. R. Bowling, S. D. Sargent, B. D. Tanner, J. R. Ehleringer, *Science direct, Agricultural and Forest Meteorology* **118**, 1-19 (2003).

SPECTRUM 2308

Start wavelength
$\lambda = 2308\ cm^{-1}$

End wavelength
$\lambda = 2310\ cm^{-1}$

Molecules: $^{13}CO_2$, $^{12}CO_2$



Transmission spectra for $^{12}CO_2$ and $^{13}CO_2$. Shown in (a) are spectra over a broad wave number range; the two right-most lobes are the spectra for $^{12}CO_2$ and the left ones are $^{13}CO_2$. The individual absorption lines used by the TDL for each isotope are shown in (b).

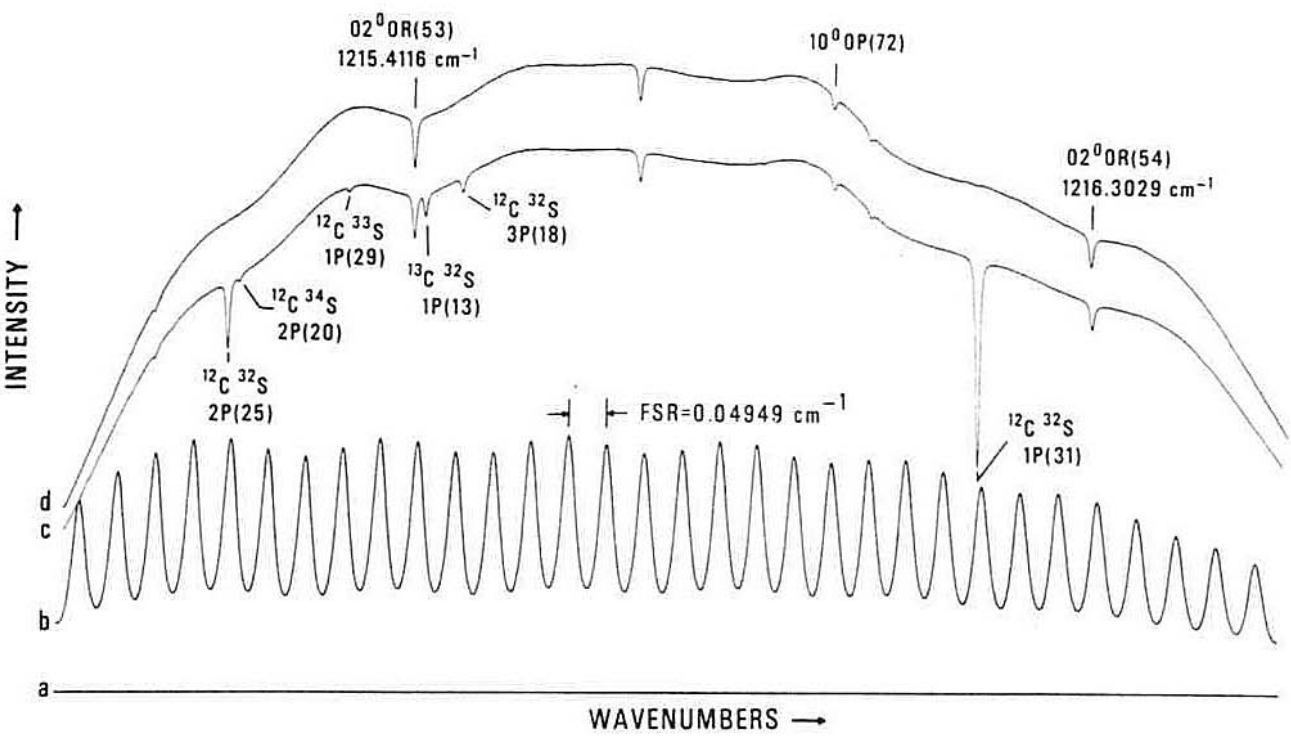
Reference:
D. R. Bowling, S. D. Sargent, B. D. Tanner, J. R. Ehleringer, *Science direct, Agricultural and Forest Meteorology* **118**, 1-19 (2003).

SPECTRUM 1215

Start wavelength
$\lambda = 1215\ cm^{-1}$

End wavelength
$\lambda = 1216\ cm^{-1}$

Molecules: CS, N_2O



A diode laser spectrum of CS and N_2O. Traces a-d are, respectively, zero transmittance, etalon fringes, CS + N_2O spectra. N_2O spectrum. Traces b and c were recorded simultaneously while trace d was recorded later with slightly increased gain and the CS_2 discharge turned off. The N_2O pressure-path length product was 660 Pa · 50 cm. Line identifications are by $\nu\ '\Delta J(J'')$. The vibrational designations for N_2O, 10^00, and 02^00 refer, respectively, to $[10^00, 02^00]_{I,II}$ states.

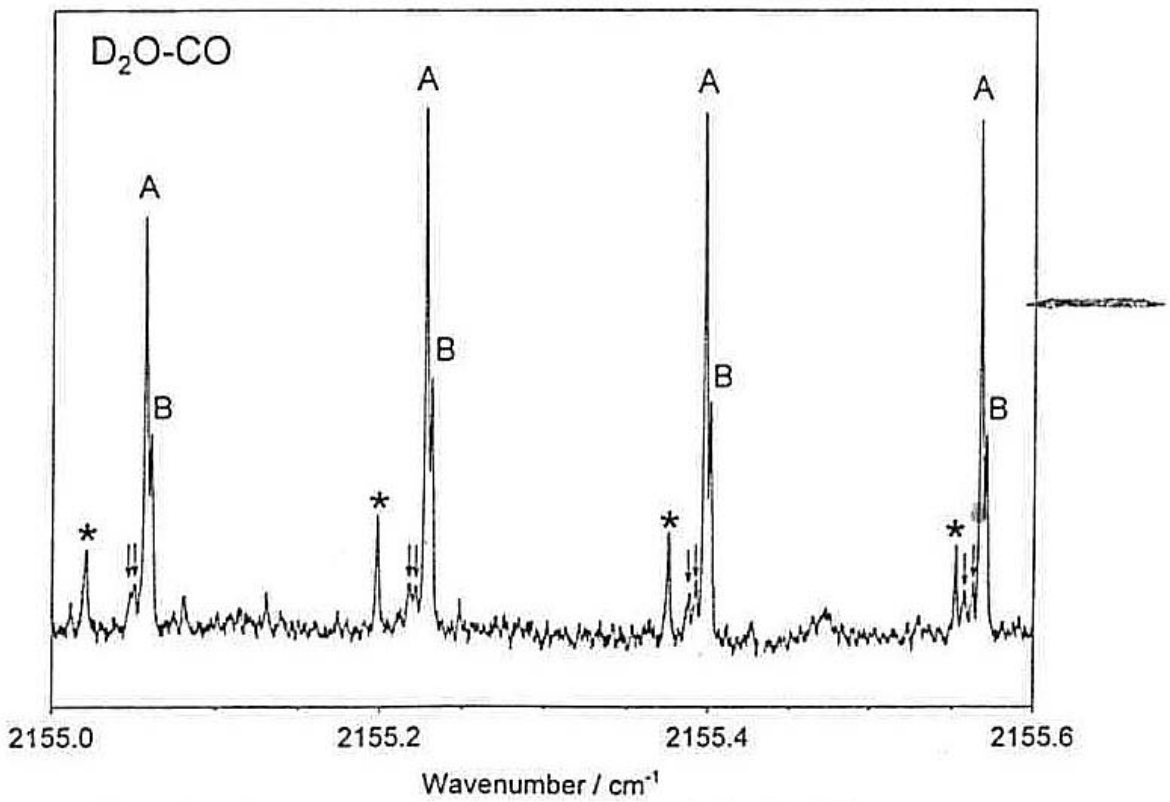
Reference:
T. Todd and B. Olsen, *Journal of Molecular Spectroscopy*, **74** (2), 190-202 (1979).

SPECTRUM 2155

Start wavelength
$\lambda = 2155\ cm^{-1}$

End wavelength
$\lambda = 2155.6\ cm^{-1}$

Molecules: D_2O-CO



Close-up view of part of the R-branch of D_2O-CO, showing the splitting of each line into A and B tunnelling components; the magnitude of this splitting is about 0.003 cm^{-1}. The lines marked with asterisks are due to HOD-CO and the pairs of lines marked with arrows are due to the K = 1 - 1 transitions of D_2O-CO.

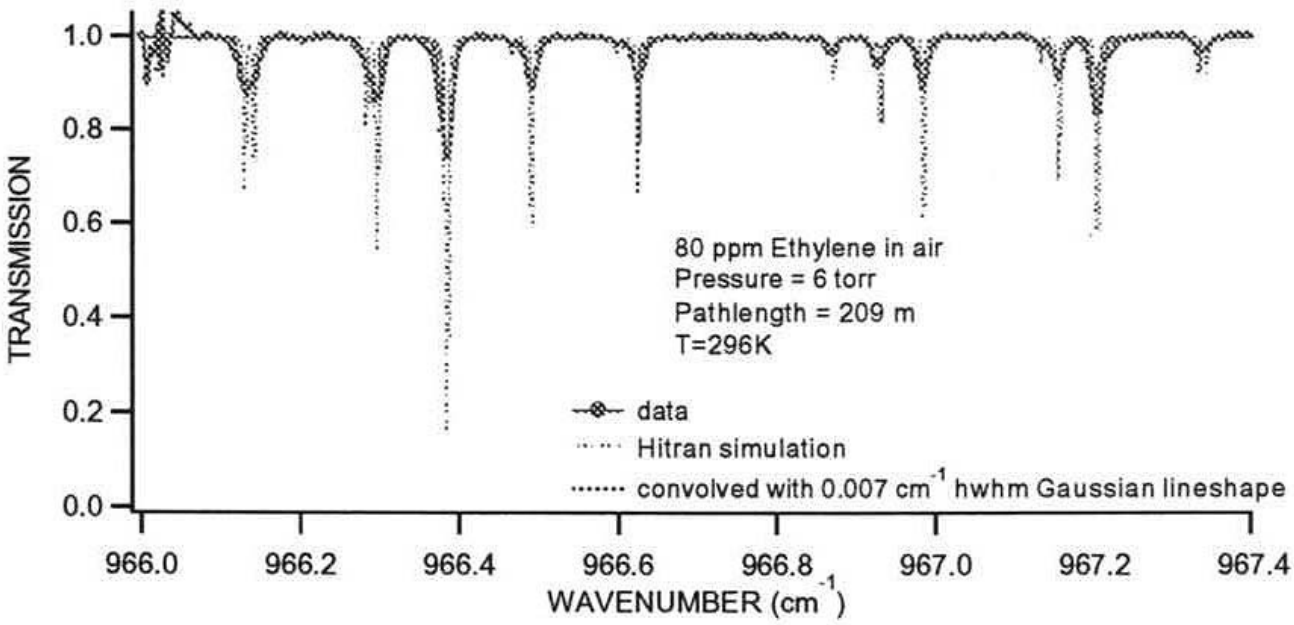
Reference:
D. Matthew, A. R. W. Mc Kellar et al., *The Journal of Chemical Physics* **109** (14), 5823-5829, (1998).

SPECTRUM 966

Start wavelength
$\lambda = 966\ cm^{-1}$

End wavelength
$\lambda = 967.4\ cm^{-1}$

Molecules: Ethylen



Comparison of data and fit for transmission spectra. The best fit is obtained by convolving a 0.007 cm^{-1} laser linewidth (Gaussian HWHM) with the calculated transmission spectrum based on the HITRAN database.

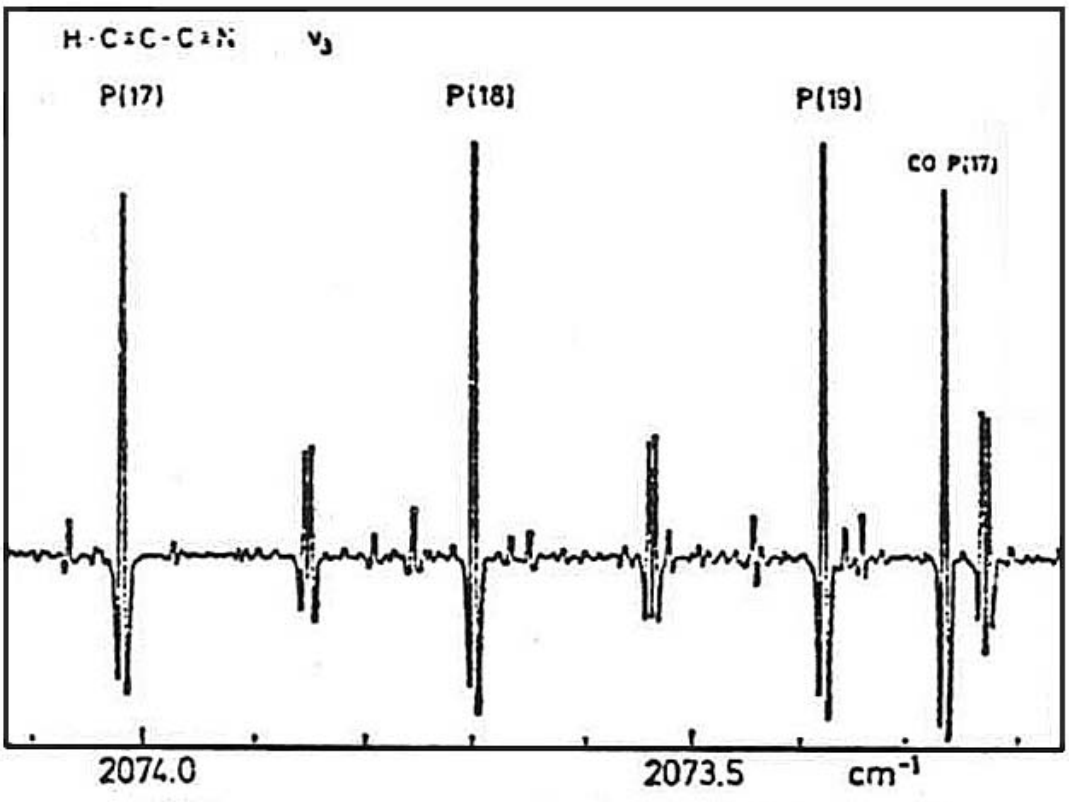
Reference:
J. B. McManus, D. D. Nelson Jr., J. Shorter, M. Zahniser, A. Mueller, Y. Bonetti, M. Beck, D. Hofstetter, J. Faist, *Diode Lasers and Applications in Atmospheric Sensing, SPIE Proceedings,* **4817**, 22-33 (2002).

SPECTRUM 2073.5

Start wavelength
$\lambda = 2073.5\ cm^{-1}$

End wavelength
$\lambda = 2074\ cm^{-1}$

Molecules: HC_3N, CO



High resolution diode laser spectrum of the ν_3 vibration-rotation spectrum of HC_3N. Three successive *J* lines of the P branch are displayed. The P (17) CO line (CO appears as an impurity in the sample) is used as a calibration standard in this section of the spectrum. The weaker doublet lines in the spectrum are hot band transitions and exhibit *l*-type splitting. The spectrum was recorded by using frequency modulation and is displayed in second derivative form. It may be noted that reflection of laser power back into the laser causes weak energy modulation which produces errors in the baseline.

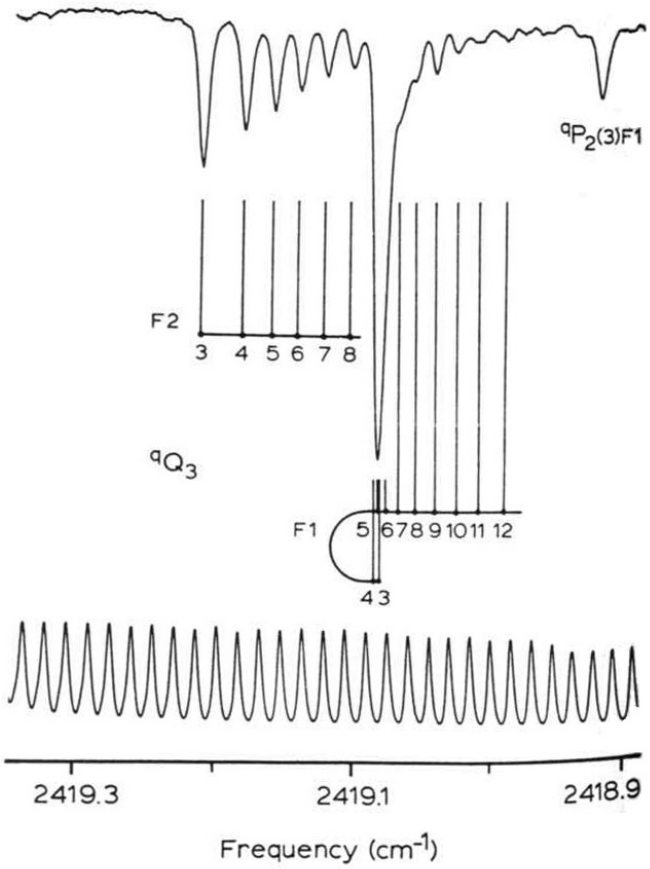
Reference:
K. Yamada, R. Schieder, G. Winnewisser, *Physikalisches Institut Universität zu Köln, Z. Naturforsch.* **35a**, 690-693 (1980).

SPECTRUM 2419.1

Start wavelength
$\lambda = 2419.1\ cm^{-1}$

End wavelength
$\lambda = 2419.3\ cm^{-1}$

Molecules: HCO



K = 3 parallel Q branches of the CH stretching fundamental of HCO. 50 transient digitizer points each of 500 ns duration are averaged immediately before and after each excimer shot and subtracted. The laser is stepped 20 MHz in scanning with 30 shots averaged per step. The asymmetry splittings are not resolved. Conditions: He pressure = 5 Torr, acetaldehyde pressure = 2.5 Torr, XeCl pulse energy = 75 mJ, repetition rate = 20 Hz. Pictured as well are the 500 MHz etalon fringes used in laser scanning and calibration.

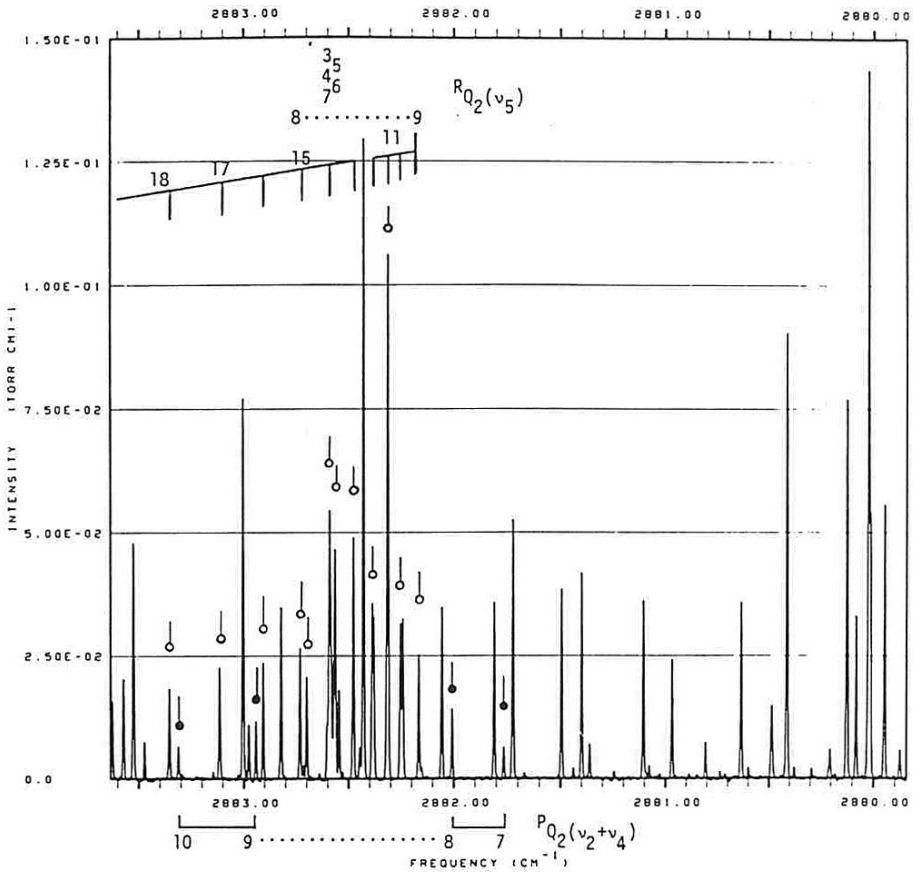
Reference:
C. B. Dane, D. R. Lander, R. F. Curl, F. K. Tittel, *J.Chem.Phys.* **88** (4), (1988).

SPECTRUM 2880

Start wavelength
$\lambda = 2880\ cm^{-1}$

End wavelength
$\lambda = 2883\ cm^{-1}$

Molecules: H_2CO



The effect of the ν_5, $\nu_2 + \nu_4$ interaction of Fig. 3 as observed in the H_2CO spectrum at 2882 cm^{-1} where ${}^{P}Q_2$ of $\nu_2 + \nu_4$ and ${}^{R}Q_2$ of ν_5 overlap. The $J = 9$ transition of ν_5 is displaced toward lower frequency while the $J = 9$ line of $\nu_2 + \nu_4$ is displaced toward higher frequency. The intensity enhancement of $\nu_2 + \nu_4$ is greatest for $J = 8$ and 9.

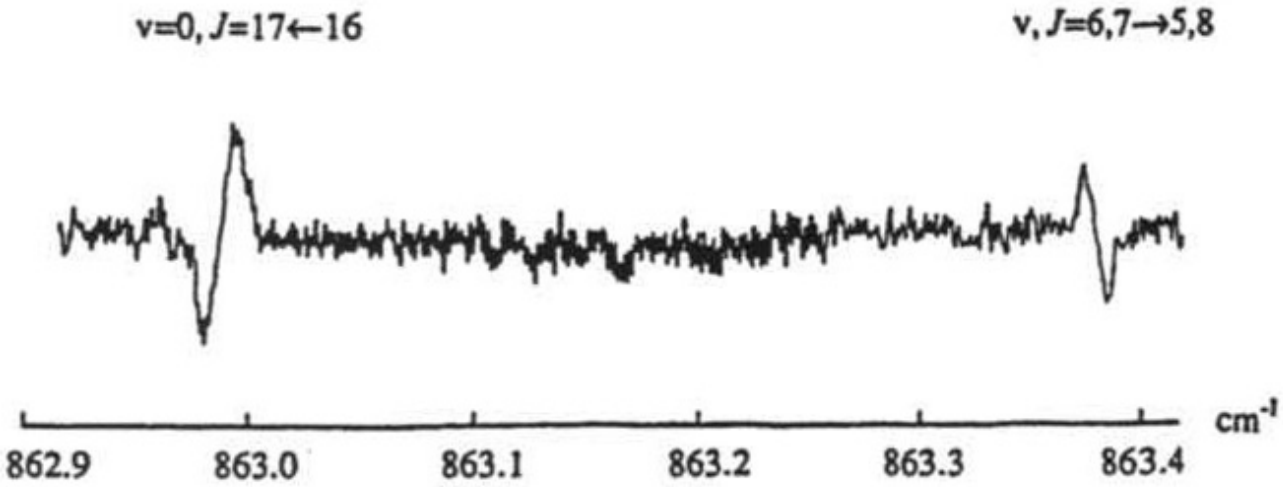
Reference:
L. Brown, R. Hunt, A. Pine, *Journal of Molecular Spectroscopy* ***75*** (3), 406-4

SPECTRUM 862.9

Start wavelength
$\lambda = 862.9\ cm^{-1}$

End wavelength
$\lambda = 863.4\ cm^{-1}$

Molecules: HeH^+



A pair of HeH^+ lines one observed in absorption ($J = 17 \leftarrow 16$, $\nu = 0$) and the other ($J = 7$, $\nu = 6 \rightarrow J = 8$, $\nu = 5$) in emission.

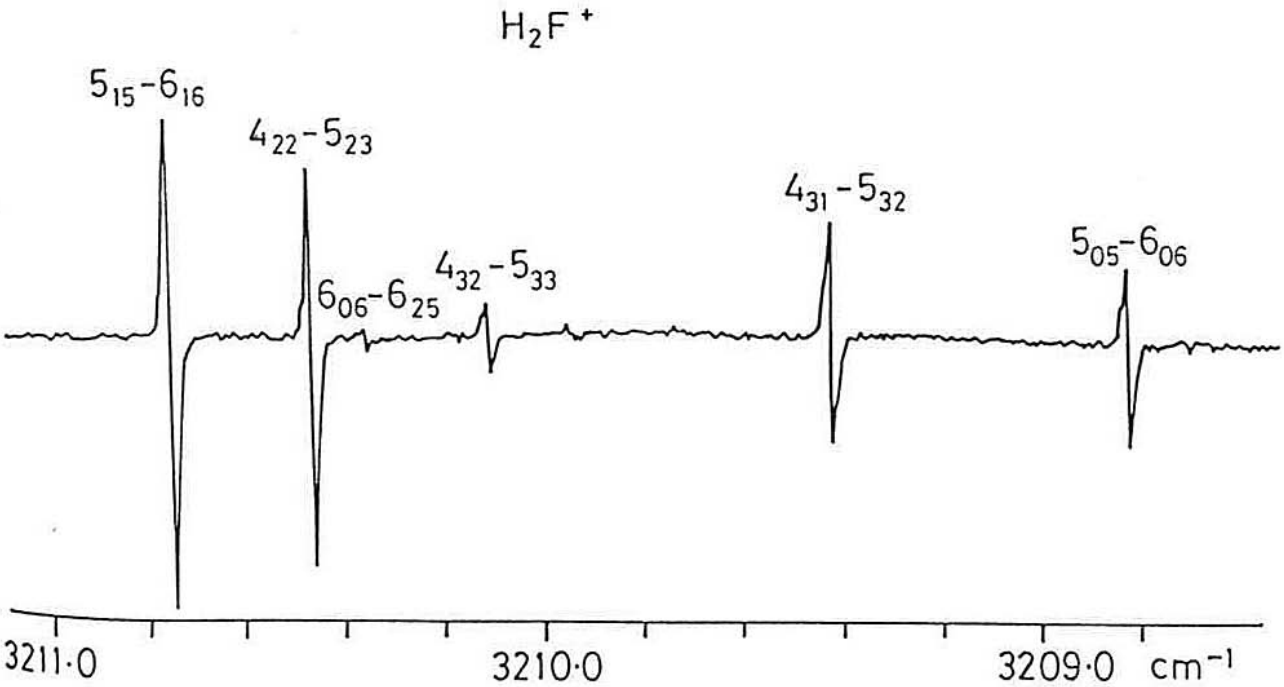
Reference:
Z. Liu, P. B. Davies, *J.Chem. Phys.* **107** (2), (1997).

SPECTRUM 3209

Start wavelength
$\lambda = 3209\ cm^{-1}$

End wavelength
$\lambda = 3211\ cm^{-1}$

Molecules: H_2F^+



A portion of the P-branch of the ν_3 band of H_2F^+, recorded with a colour-centre laser[33]. Note the 3:1 relative intensity of the 4_3-5_3 asymmetry doublet.

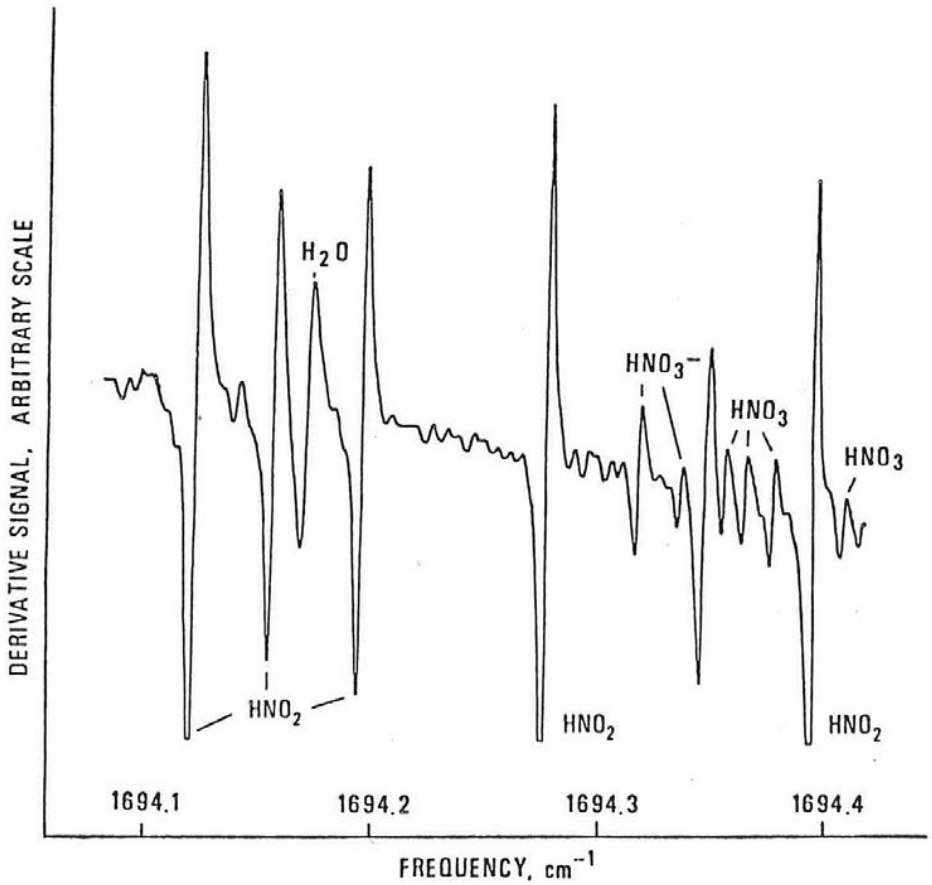
Reference:
W. Demtroeder, M. Inguscio, Proceedings of a NATO ASI held in San Miniato (Pisa) Italy, (1989).

SPECTRUM 1694.1

Start wavelength
$\lambda = 1694.1\ cm^{-1}$

End wavelength
$\lambda = 1694.4\ cm^{-1}$

Molecules: HNO_2, HNO_3, H_2O



Derivatives of spectra of both nitric and nitrous acids when the laser is simultaneously swept and frequency modulated (8 KHz) at low amplitude corresponding to less than 0.1 linewidth. The amplitudes of the derivative signals are used as an indicator of relative changes in concentrations of the molecules. Several regions of similar overlap of the ν_2 band of HNO_2 and the ν_2 band of HNO_2, existed in the 1690–1700 cm^{-1} region covered by this particular diode laser.

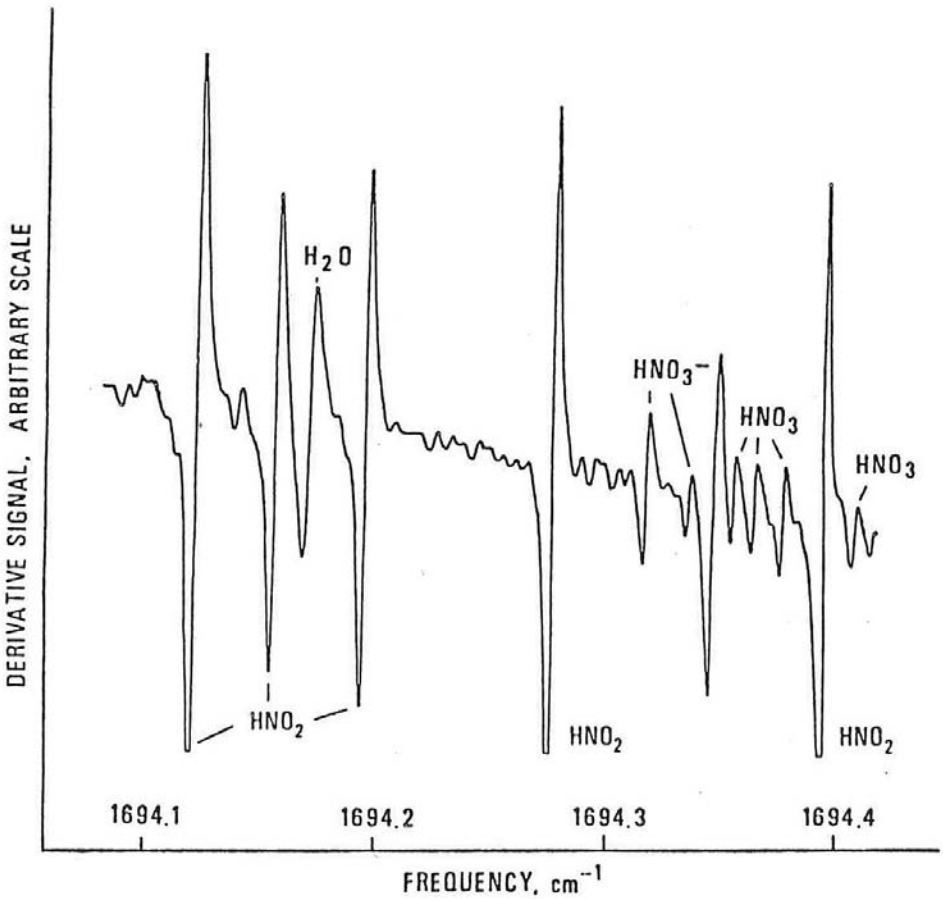
Reference:
J. S. Wells, *Tunable Semiconductor Laser Applications to air pollution measurements, Division 524, Final Report, Part one.*

SPECTRUM 1694.1

Start wavelength
$\lambda = 1694.1\ cm^{-1}$

End wavelength
$\lambda = 1694.4\ cm^{-1}$

Molecules: HNO_2, HNO_3, H_2O



Derivatives of spectra of both nitric and nitrous acids when the laser is simultaneously swept and frequency modulated (8 KHz) at low amplitude corresponding to less than 0.1 linewidth. The amplitudes of the derivative signals are used as an indicator of relative changes in concentrations of the molecules. Several regions of similar overlap of the ν_2 band of HNO_2 and the ν_2 band of HNO_2, existed in the 1690–1700 cm^{-1} region covered by this particular diode laser.

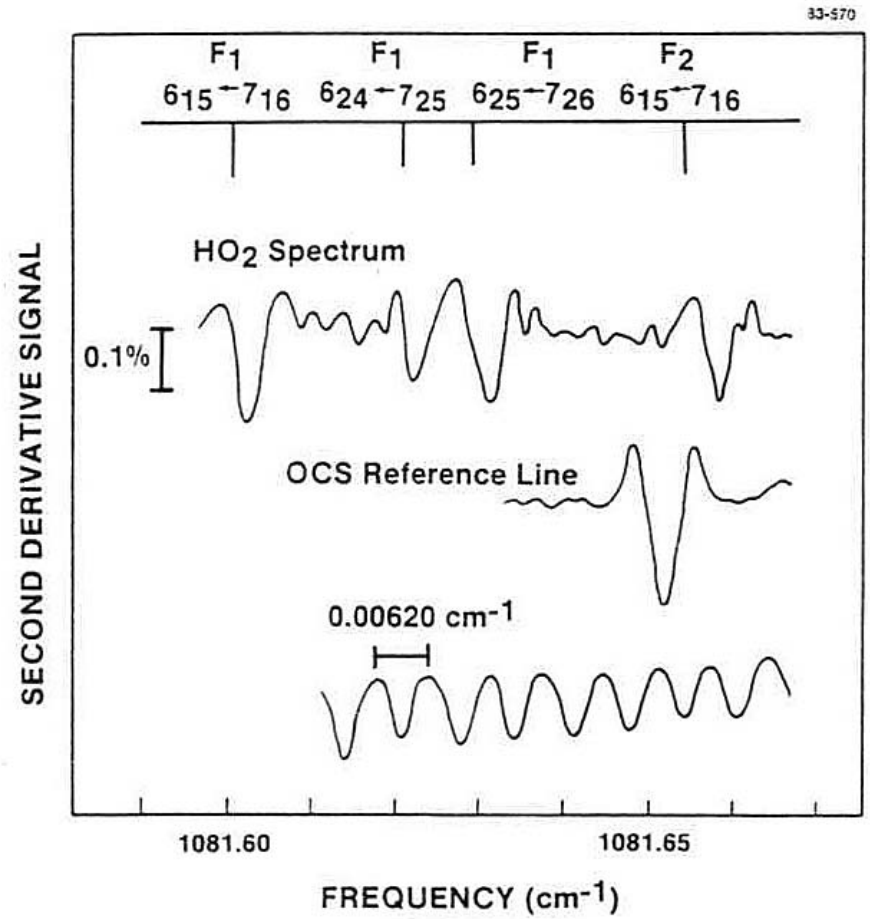
Reference:
J. S. Wells, *Tunable Semiconductor Laser Applications to air pollution measurements, Division 524, Final Report, Part one.*

SPECTRUM 1081.5

Start wavelength
$\lambda = 1081.5\ cm^{-1}$

End wavelength
$\lambda = 1081.7\ cm^{-1}$

Molecules: HO_2



HO_2 absorption lines (second derivate) from the *P* branch of the ν_3 band. Predicted positions are from Johns *et al.* (Ref. 5). The middle trace shows the OCS reference line whose frequency of 1081.6522(5) cm^{-1} is determined from Maki *et al.* (Ref.20) The frequency scale is determined by the etalon fringes from the multipass cell. The fringe spacing is $6.20 \times 10^{-3}\ cm^{-1}$.

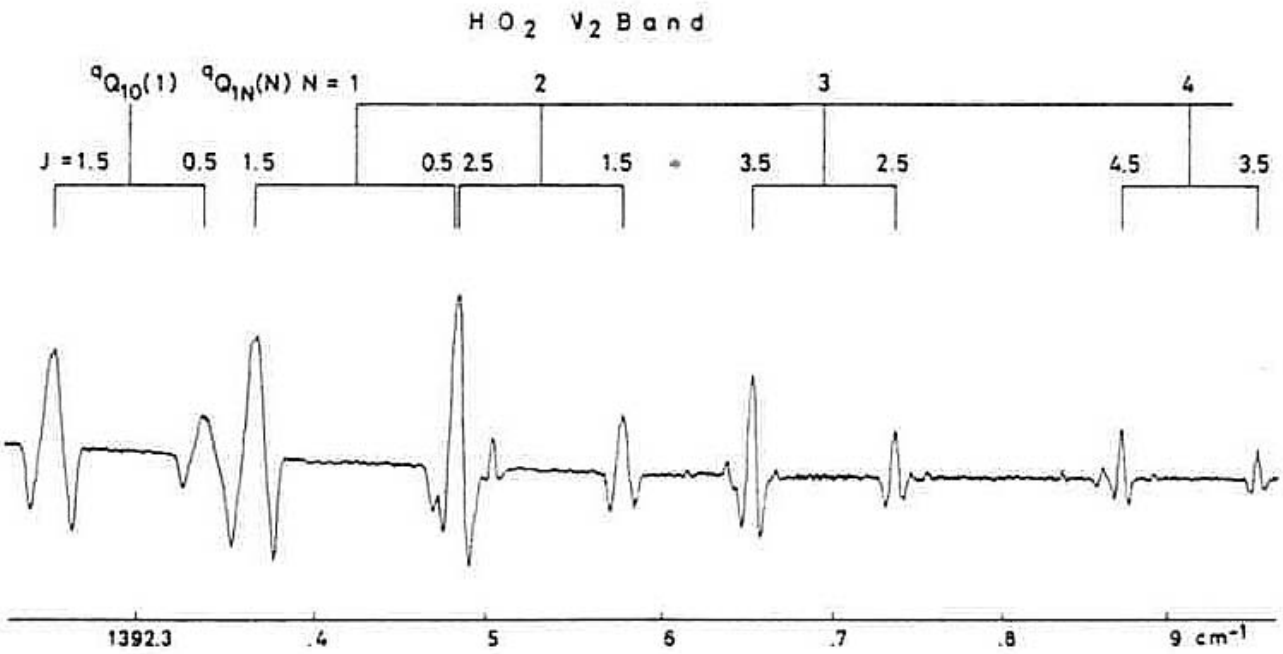
Reference:
M. S. Zahniser and A. C. Stanton, *J. Chem. Phys.* **80** (10), (1984).

SPECTRUM 1392

Start wavelength
$\lambda = 1392\ cm^{-1}$

End wavelength
$\lambda = 1393\ cm^{-1}$

Molecules: HO_2



Q-branch transitions with $K_a = 1$ of the $HO_2\nu_2$ band, recorded by Zeeman modulation.

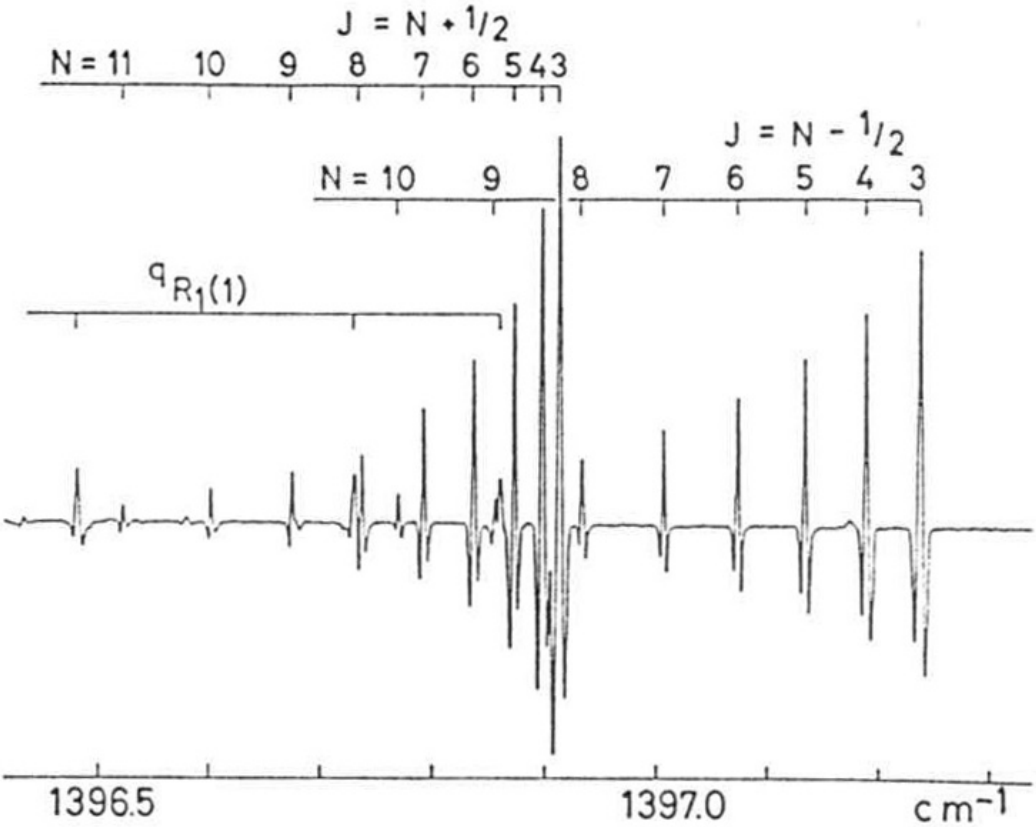
Reference:
K. Nagai et al., *Journal of Molecular Spectroscopy*, **89** (2), 520-527 (1981).

SPECTRUM 1396.5

Start wavelength
$\lambda = 1396.5\ cm^{-1}$

End wavelength
$\lambda = 1397.5\ cm^{-1}$

Molecules: HO_2



Part of the ν_2 band of the HO_2 radical recorded with a diode laser[27]. The lineshape arises from the use of Zeeman modulation. The two Q-branches shown arise from the effects of spin doubling.

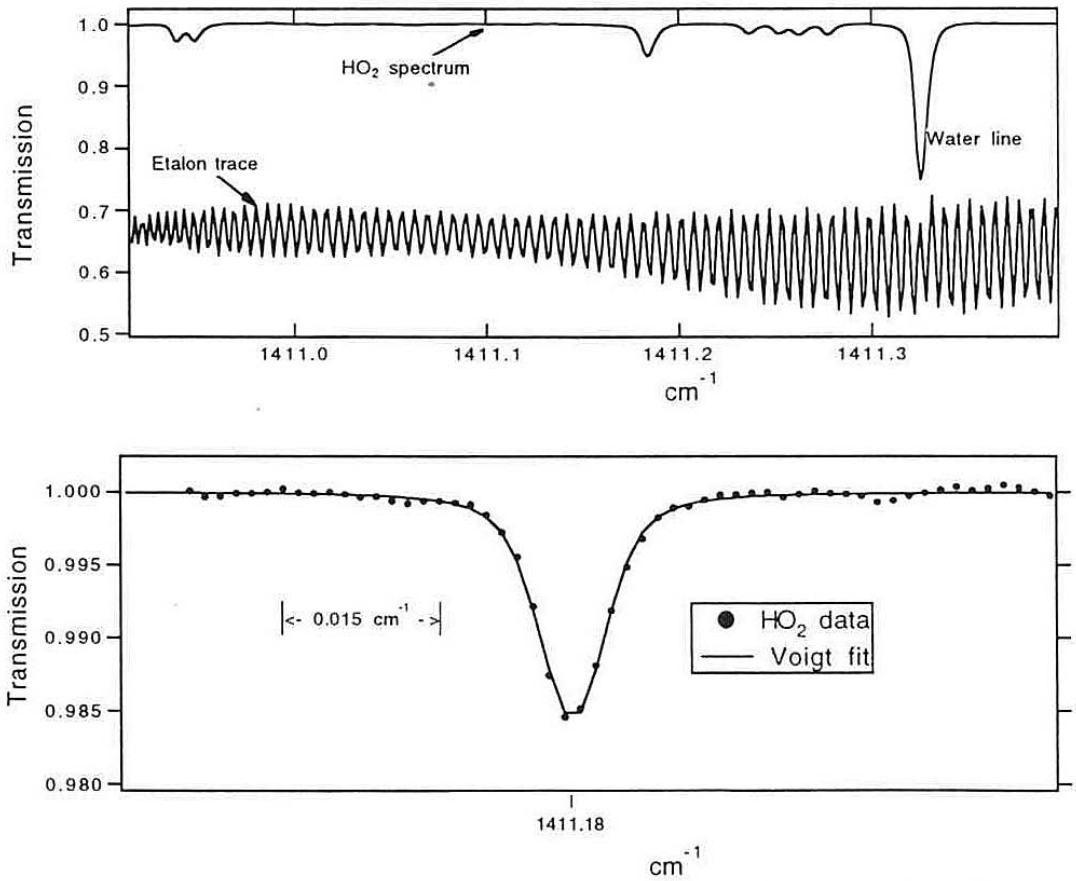
Reference:
W. Demtroeder, M. Inguscio, *Proceedings of a NATO ASI held in San Miniato (Pisa) Italy, (1989).*

SPECTRUM 1410.9

Start wavelength
$\lambda = 1410.9\ cm^{-1}$

End wavelength
$\lambda = 1411.3\ cm^{-1}$

Molecules: HO_2



HO_2 absorption spectra obtained in the 100-m path length fast-response flow cell.

Reference:
D. D. Nelson and M. S. Zahniser, *Nasa CR 18935, Laboratory, Studies of chemical and photochemical processes relevant to stratospheric Ozone annual report* **2** (1994).

SPECTRUM 500

Start wavelength
$\lambda = 500\ cm^{-1}$

End wavelength
$\lambda = 4000\ cm^{-1}$

Molecules: CO, CO_2, H_2O, CH_4

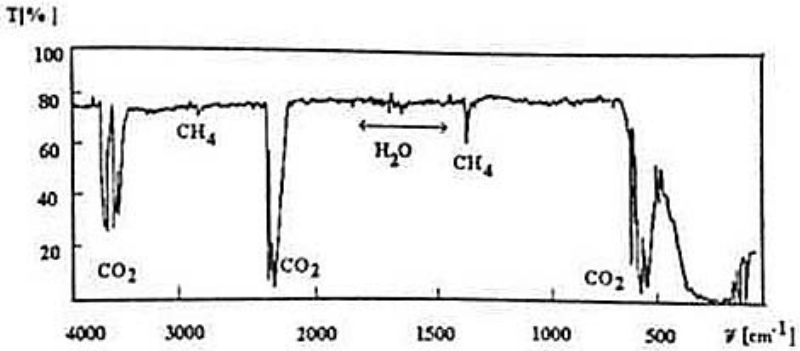
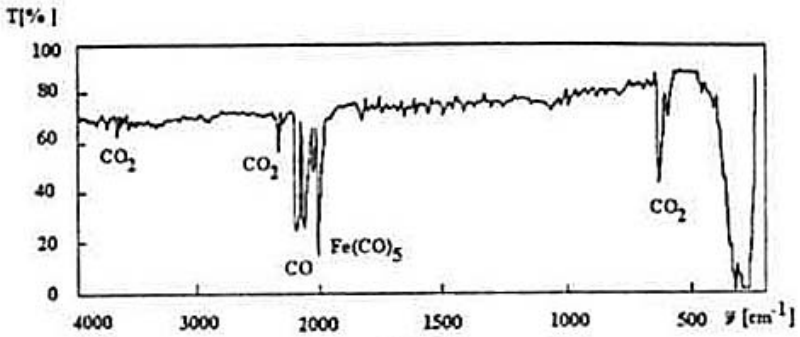


Figure 3. The IR absorption spectrum of CO_2.



(a)

The IR absorption spectrum of CO_2.

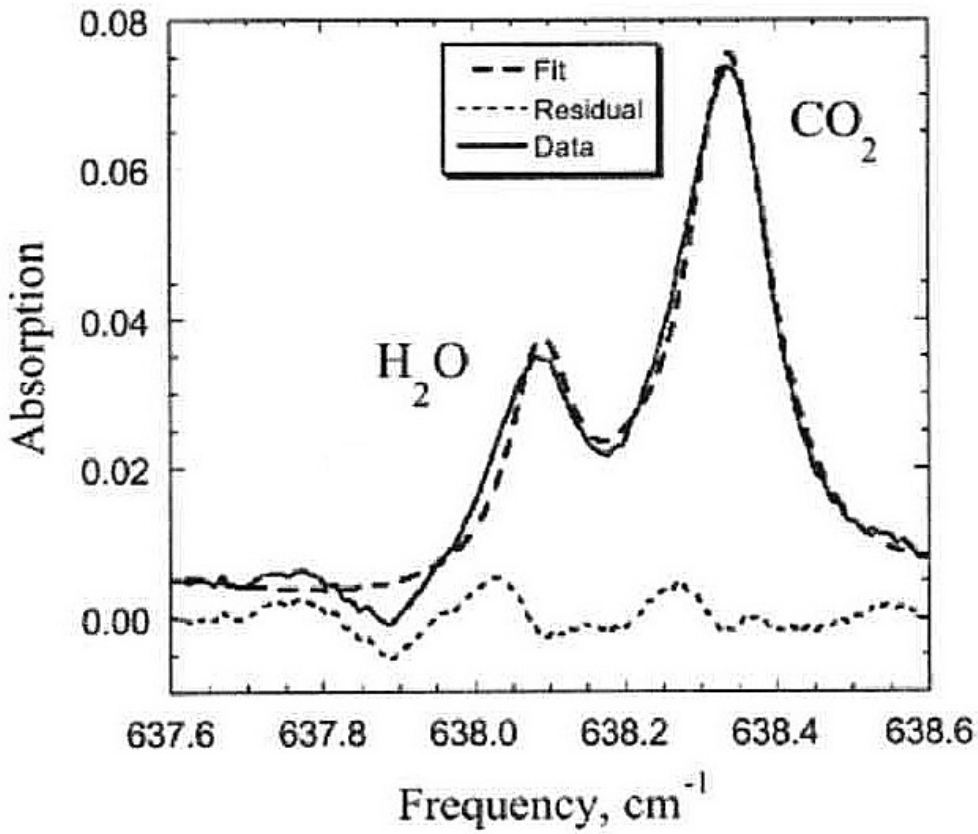
Reference:
M. Morvová, *Czechoslovak Journal of Physics*, ***47*** (2), (1997).

SPECTRUM 637.6

Start wavelength
$\lambda = 637.6\ cm^{-1}$

End wavelength
$\lambda = 638.6\ cm^{-1}$

Molecules: H_2O, CO_2



CO_2 and H_2O absorption.

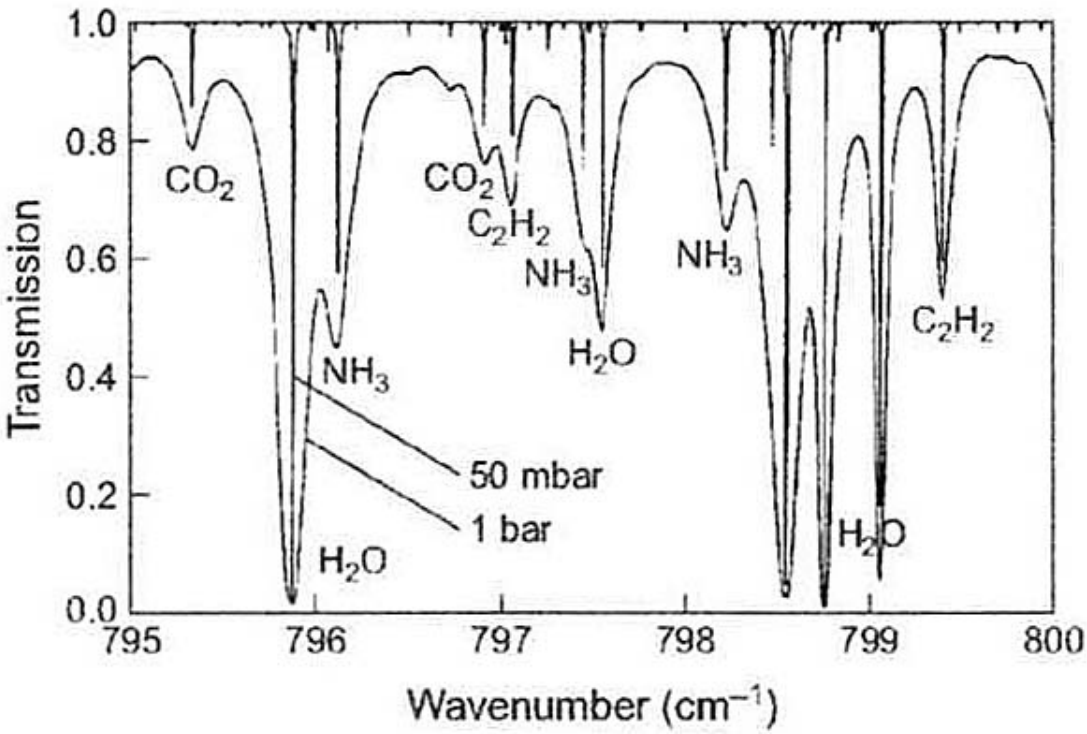
Reference:
A. A. Kosterev, R. F. Curl, F. K. Tittel, M. Rochat, M. Beck, D. Hofstetter, J. Faist, *Applied Physics B, Laser and Optics* (2002).

SPECTRUM 795

Start wavelength
$\lambda = 795\ cm^{-1}$

End wavelength
$\lambda = 800\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4, NH_3



Transmission spectrum of a gas mixture typical for emissions of technical combustion containing H_2O, CO_2, NH_3 and C_2H_2 in N_2 at 470 K and 1 m optical path. (Taken from ref. 2). Such a mixture can be found in combustion exhaust to the atmosphere. While at atmospheric pressure the absorption lines merge, at low pressure (50 mbar) lines are only Doppler broadened and well isolated.

Reference 1:
M. Tacke, F. Wienhold, R. Grisar, H. Fischer, F. - J. Lübken, *Encyclopedia of Analytical Chemistry R.A. Meyers (Ed.) © John Wiley & Sons Ltd*, 2033-2065 (2000).

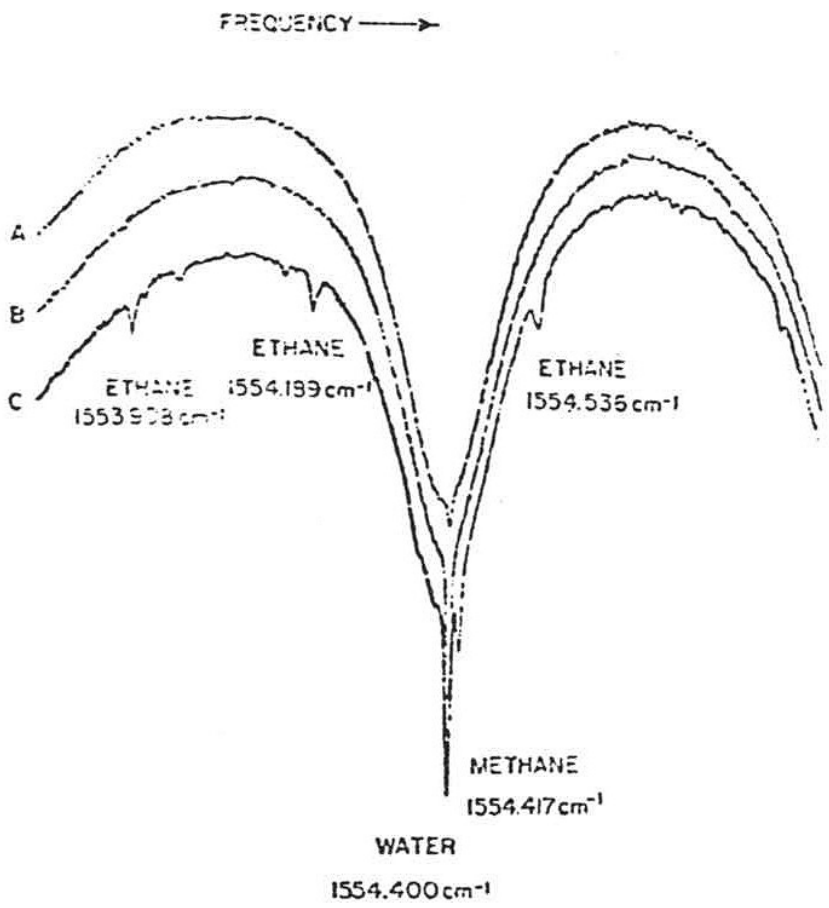
Reference 2-:
U. von Zahn et al., *J. Geophys. Res.*, 102, 7443-7456 (1990).

SPECTRUM 1553.97

Start wavelength
$\lambda = 1553.97\ cm^{-1}$

End wavelength
$\lambda = 1554.54\ cm^{-1}$

Molecules: H_2O, CH_4, C_2H_4



Transmission spectra in the 1553 cm^{-1} region. The 50 cm^2 samples of either cigarette smoke (C) or room air containing 11.73 mm H_2O (B) were examined at a cell pressure of 12 Torr. Lock-in amplifier gain was 25 mV with a 0.3-sec time constant. Scan rate was 0.0077 cm^{-1} sec^{-1}. The background (A) and etalon calibration spectra (D) are also shown.

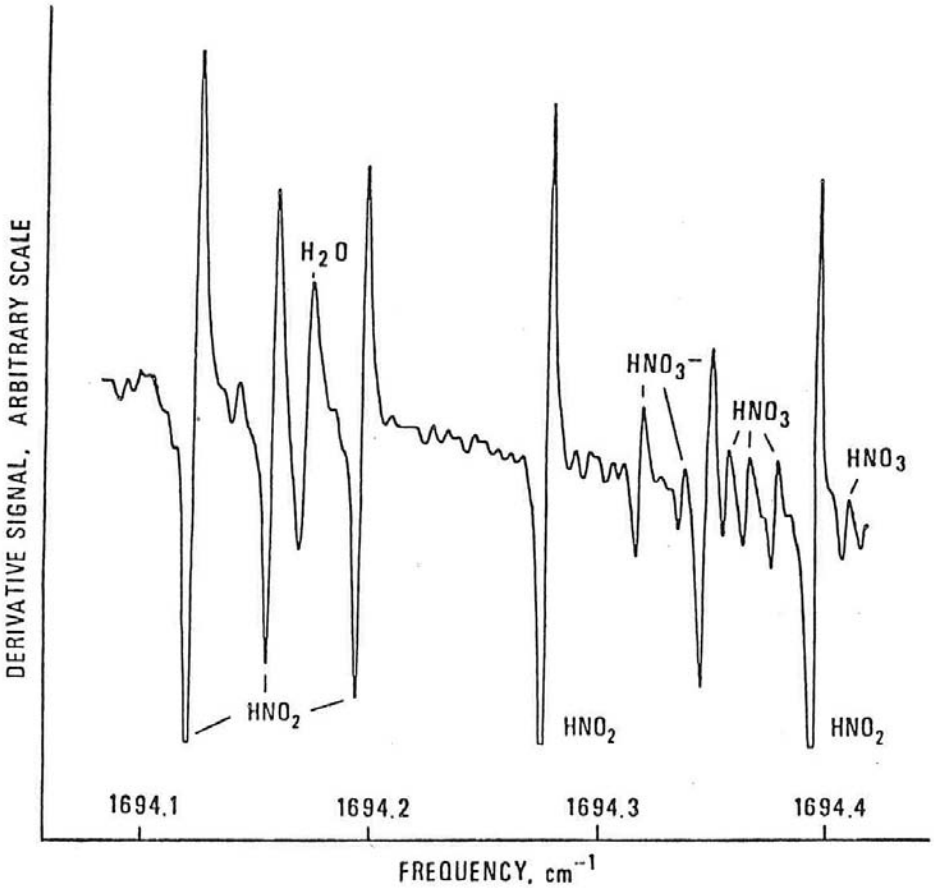
Reference:
G. T. Forrest, *APPLIED OPTICS* **19** (13), (1990).

SPECTRUM 1694.1

Start wavelength
$\lambda = 1694.1\ cm^{-1}$

End wavelength
$\lambda = 1694.4\ cm^{-1}$

Molecules: HNO_2, HNO_3, H_2O



Derivatives of spectra of both nitric and nitrous acids when the laser is simultaneously swept and frequency modulated (8 KHz) at low amplitude corresponding to less than 0.1 linewidth. The amplitudes of the derivative signals are used as an indicator of relative changes in concentrations of the molecules. Several regions of similar overlap of the ν_2 band of HNO_2 and the ν_2 band of HNO_2, existed in the 1690–1700 cm^{-1} region covered by this particular diode laser.

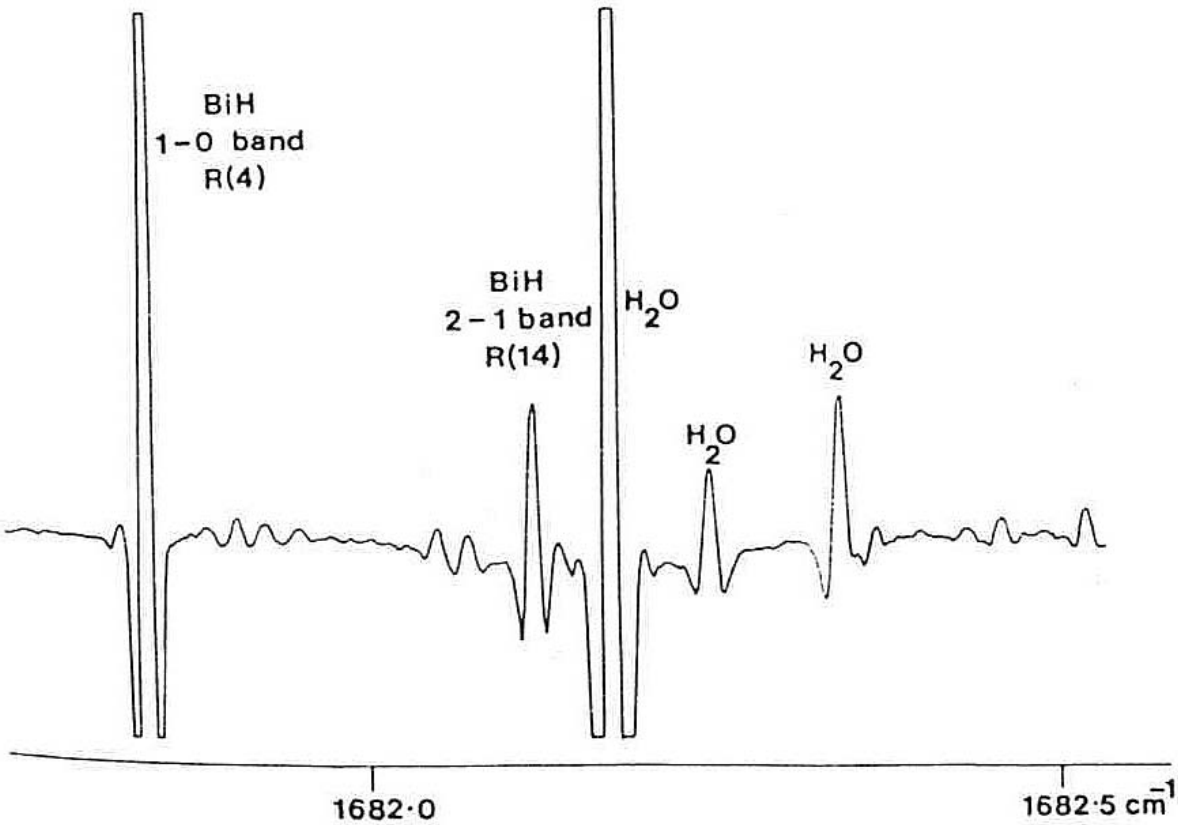
Reference:
J. S. Wells, *Tunable Semiconductor Laser Applications to air pollution measurements, Division 524, Final Report, Part one.*

SPECTRUM 1681.8

Start wavelength
$\lambda = 1681.8\ cm^{-1}$

End wavelength
$\lambda = 1682.5\ cm^{-1}$

Molecules: H_2O, BiH



A "typical" spectrum from the diode laser study of BiH (91). The BiH was made in a hot cell by the reaction of Bi vapour with 25 Torr of hydrogen at 1000 °C. The molecular lineshape is a second derivative because the technique of frequency modulation with lock-in detection at twice the modulation frequency was used. This modulation scheme gives a flatter baseline than lock-in detection at the modulation frequency.

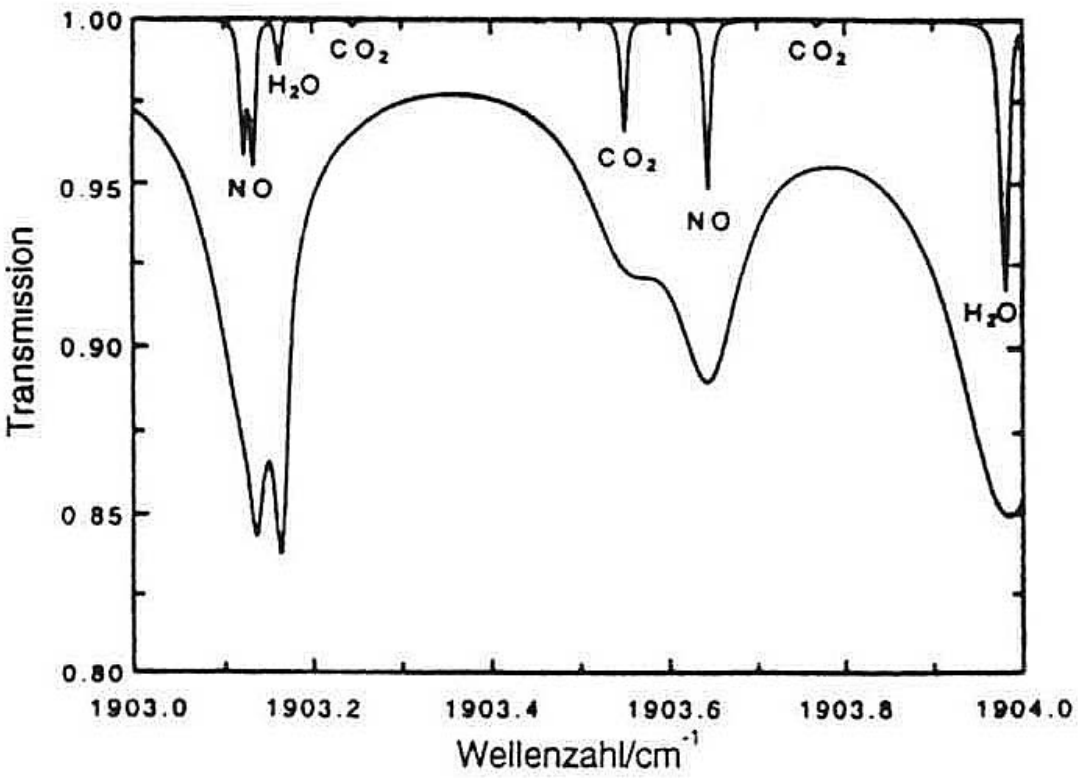
Reference:
Peter F. Bernath, *Annual Review of Physical Chemistry* **41**, 91-122 (1990).

SPECTRUM 1903

Start wavelength
$\lambda = 1903\ cm^{-1}$

End wavelength
$\lambda = 1904\ cm^{-1}$

Molecules: CO_2, NO, H_2O



Transmission spectrum of a gas mixture consisting of 100 ppm NO, 15 % CO_2 and 15 % H_2O in N_2 at 470 K and 1 m optical path. At atmospheric pressure (lower curve) the NO lines appear on the background of the other gases, at 30 mbar (needle-shaped minima) the NO lines can be traced nearly free of interference by other gases.

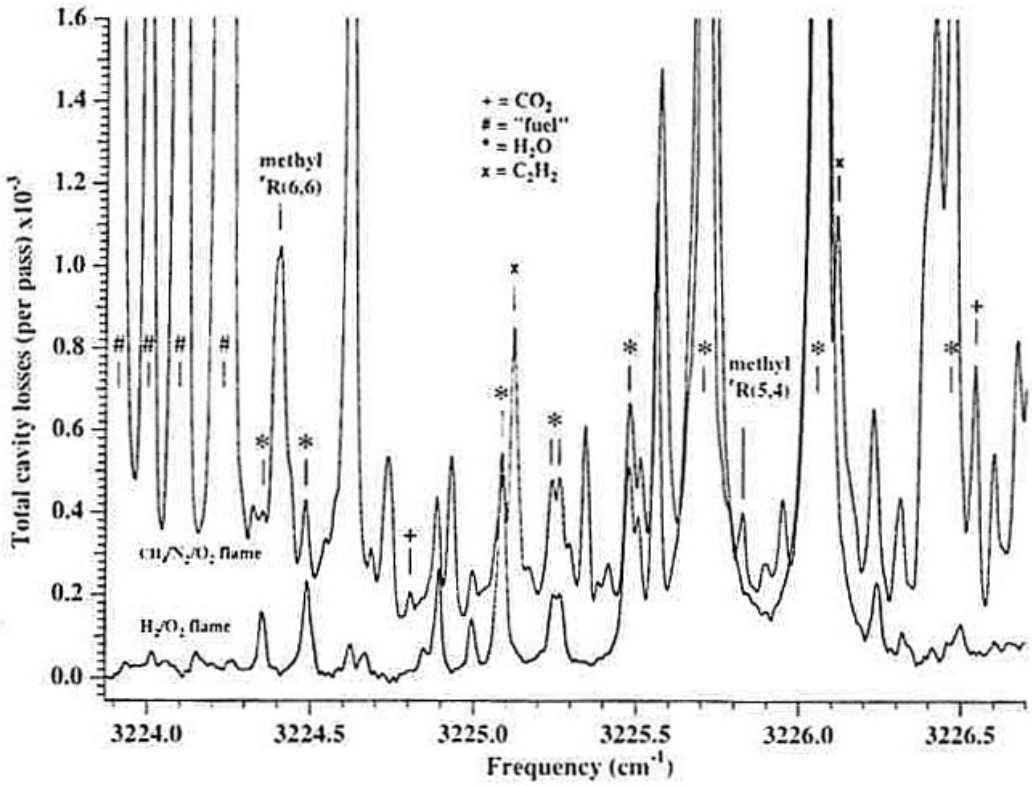
Reference:
M. Tacke, R. Grisar, *Laser und Optoelektronik*, 51-56 (1995).

SPECTRUM 3224.4

Start wavelength
$\lambda = 3224.4\ cm^{-1}$

End wavelength
$\lambda = 3226.5\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4



High resolution IR-CRLAS spectra obtained in the 3 micron region in a 37.5 Torr $CH_4/N_2/O_2$ (upper trace) and $H_2/N_2/O_2$ (lower trace) flame. Comparison of the two scans readily identifies likely H_2O features, which frequently overlap methyl transitions. In these data, the unique ability to obtain data for reactants (# = fuel and x = C_2H_2), Intermediates (CH_3) and products (* = H_2O and + = CO_2) in the infrared spectral region is demonstrated.

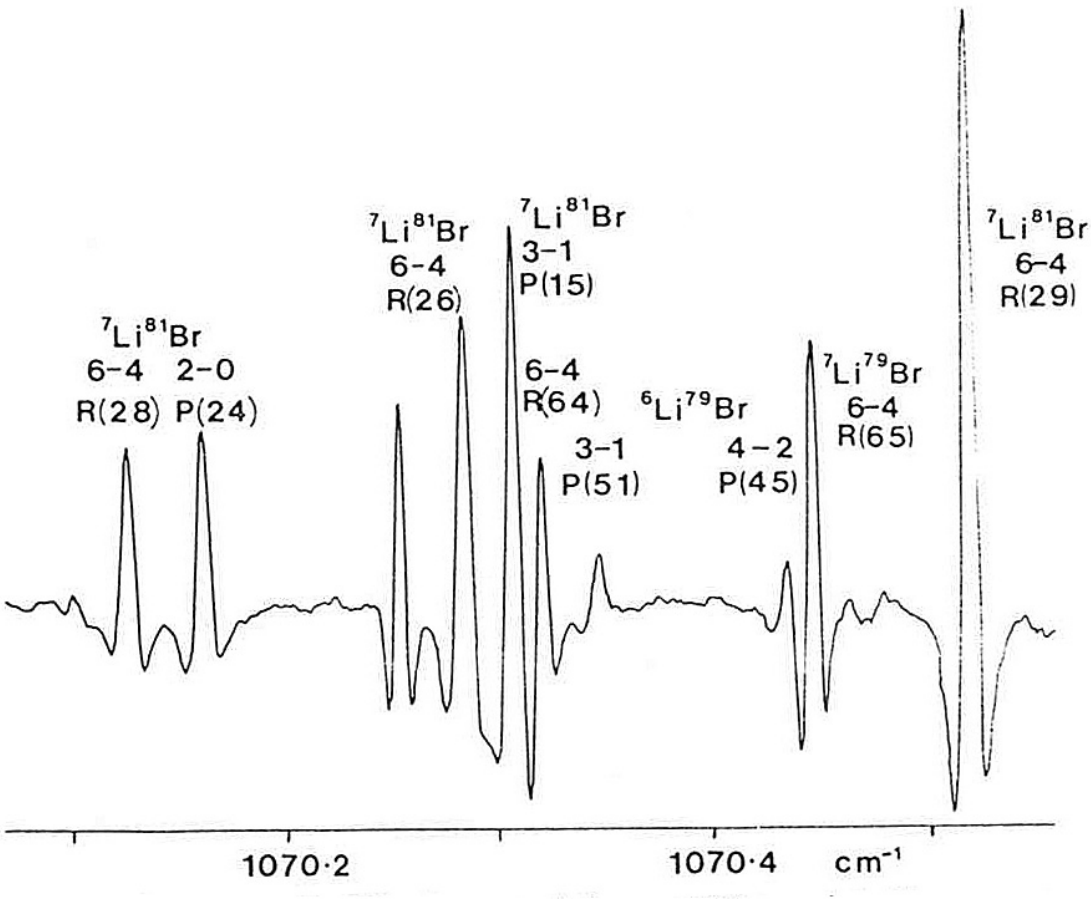
Reference:
J. J. Scherer et al., *J. Chem. Phys.* **107** (16), (1997).

SPECTRUM 1070.1

Start wavelength
$\lambda = 1070.1\ cm^{-1}$

End wavelength
$\lambda = 1070.5\ cm^{-1}$

Molecules: LiBr



A portion of the LiBr vibration-rotation spectrum recorded with a diode laser spectrometer (104). The LiBr molecule was made by simply heating the salt to 800 °C. The spectrum was very dense because at this high temperature many vibrational and rotational levels are populated and because there are four isomeric forms of LiBr, $^6Li^{81}Br$, $^7Li^{81}Br$, $^6Li^{79}Br$, and $^7Li^{79}Br$.

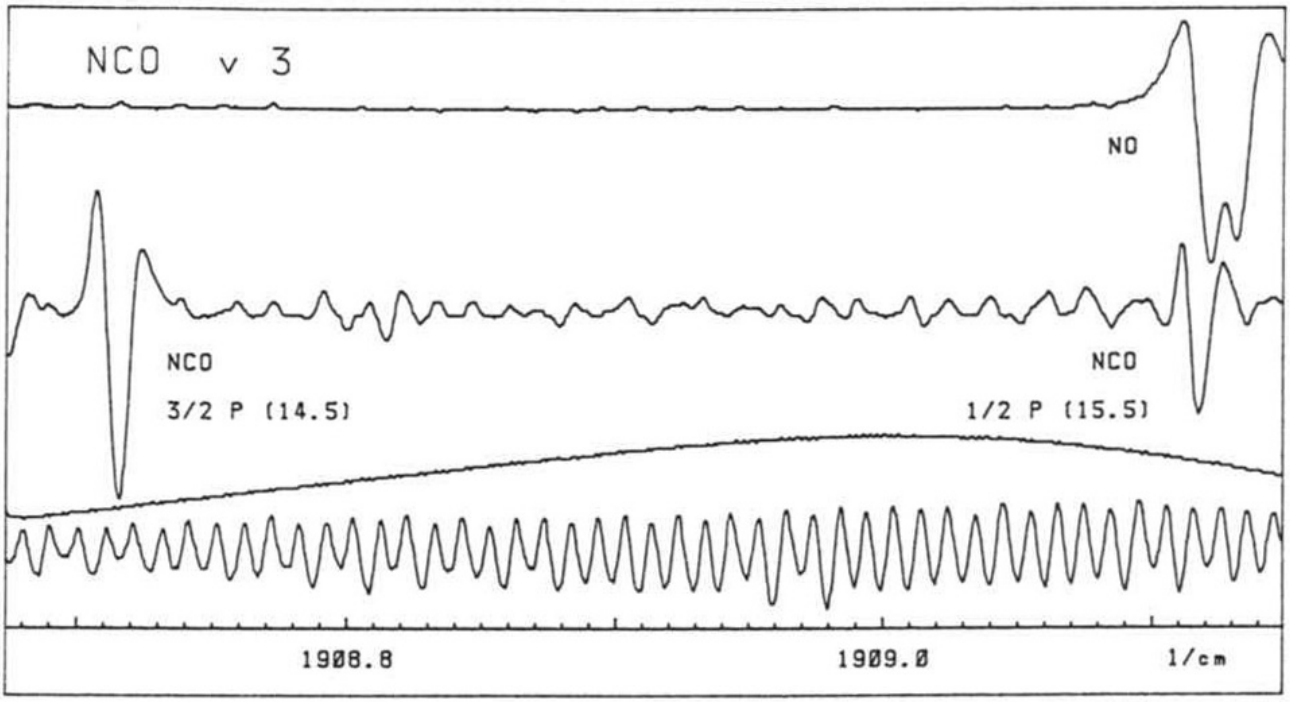
Reference:
P. F. Bernath, *Annual Review of Physical Chemistry* **41**, 91-122 (1990).

SPECTRUM 1908.6

Start wavelength
$\lambda = 1908.6\ cm^{-1}$

End wavelength
$\lambda = 1909\ cm^{-1}$

Molecules: NCO



Spectrum with reference gas, two NCO absorption lines [P3/2(14.5), P1/2(15.5)], intensity, and marker channel.

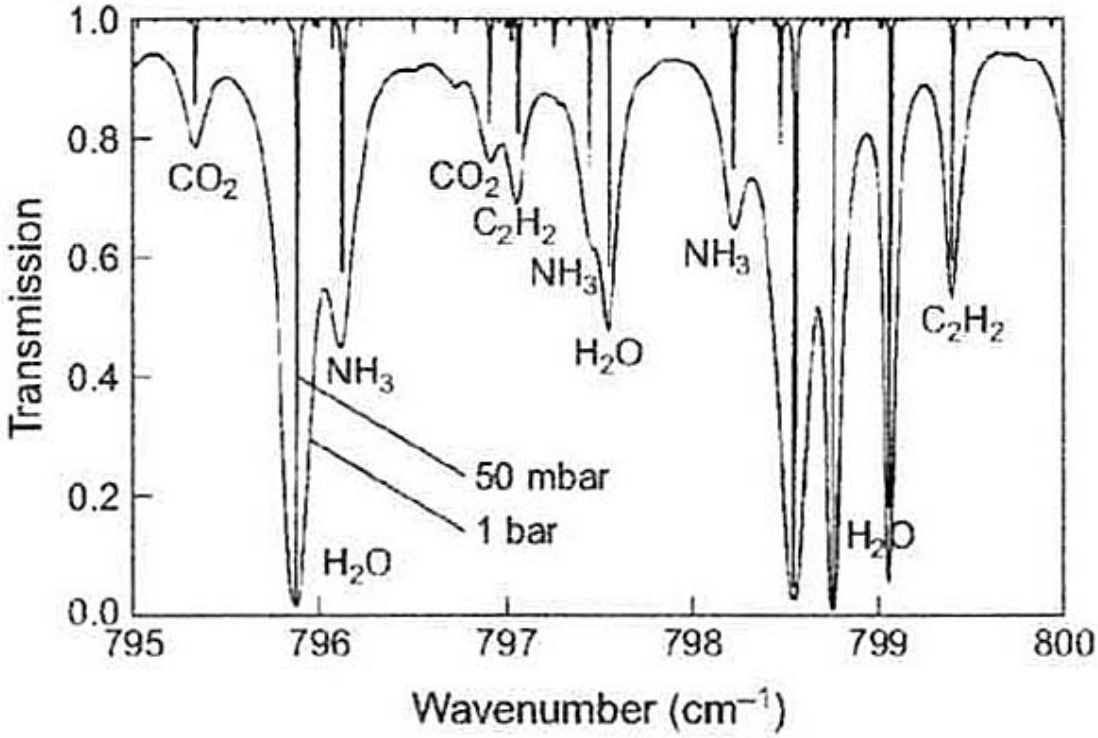
Reference:
R. Brüggemann, M. Petri, H. Fischer, D. Mauer, D. Reinert, W. Urban, *Applied Physics B* **48** (2), 105-110 (1989).

SPECTRUM 795

Start wavelength
$\lambda = 795\ cm^{-1}$

End wavelength
$\lambda = 800\ cm^{-1}$

Molecules: CO_2, H_2O, C_2H_4, NH_3



Transmission spectrum of a gas mixture typical for emissions of technical combustion containing H_2O, CO_2, NH_3 and C_2H_2 in N_2 at 470 K and 1 m optical path. (Taken from ref. 2). Such a mixture can be found in combustion exhaust to the atmosphere. While at atmospheric pressure the absorption lines merge, at low pressure (50 mbar) lines are only Doppler broadened and well isolated.

Reference 1:
M. Tacke, F. Wienhold, R. Grisar, H. Fischer, F. - J. Lübken, *Encyclopedia of Analytical Chemistry R.A. Meyers (Ed.) © John Wiley & Sons Ltd*, 2033-2065 (2000).

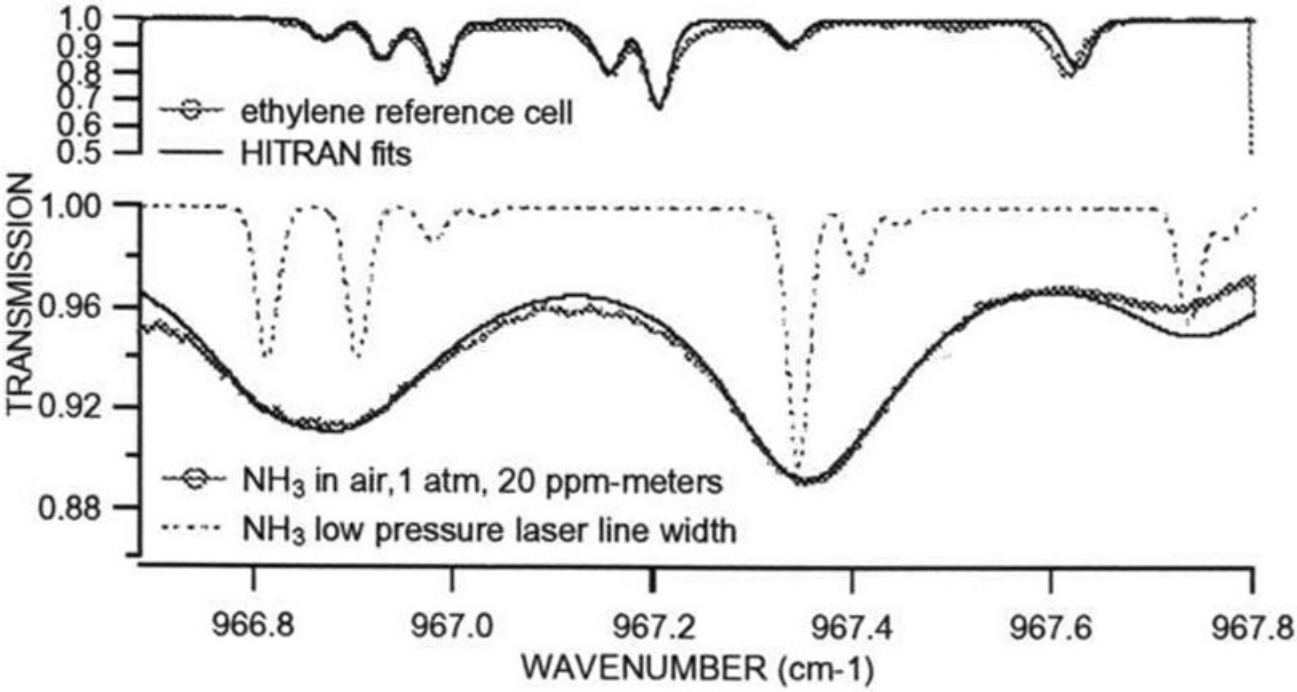
Reference 2:
U. von Zahn et al., *J. Geophys. Res.*, 102, 7443-7456 (1990).

SPECTRUM 966

Start wavelength
$\lambda = 966\ cm^{-1}$

End wavelength
$\lambda = 967.4\ cm^{-1}$

Molecules: NH_3



Observation of atmospheric pressure NH_3 lines. An experimental ammonia spectrum at 1 atm in air is compared to s simulated spectrum of low pressure NH_3 assuming a laser linewidth of 0.007 cm^{-1}. The frequency scale is determined from the ethylene reference cell shown in the top panel.

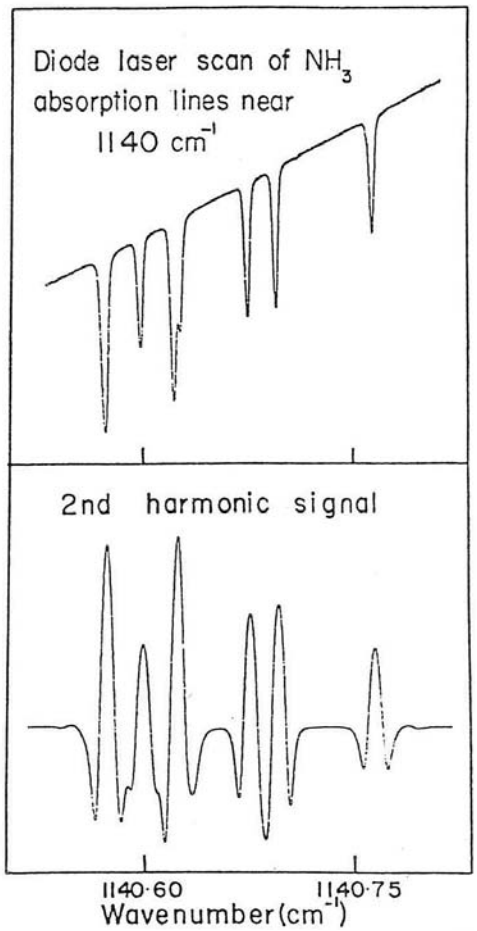
Reference:
J. B. McManus, D. D. Nelson Jr., J. Shorter, M. Zahniser, A. Mueller, Y. Bonetti, M. Beck, D. Hofstetter, J. Faist, *Diode Lasers and Applications in Atmospheric Sensing, SPIE Proceedings* **4817**, 22-33 (2002)

SPECTRUM 1140.6

Start wavelength
$\lambda = 1140.6\ cm^{-1}$

End wavelength
$\lambda = 1140.75\ cm^{-1}$

Molecules: NH_3



High resolution diode spectra of NH_3 lines near 1140 cm^{-1}. The upper trace was taken with conventional amplitude detection using a 10 cm sample cell containing < 1 Torr NH_3. For the lower trace, the lines were broadened by adding 20 Torr N_2 to the cell and second harmonic detection was employed.

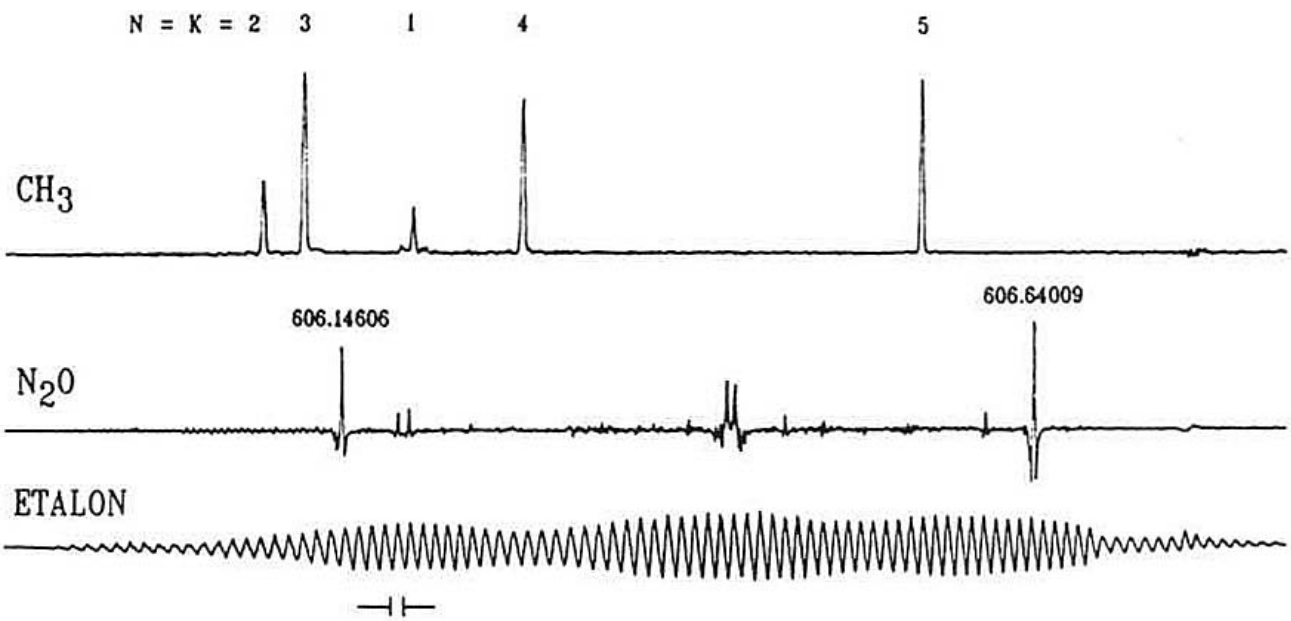
Reference:
J. Reid, J. Shewchun, B. K. Garside, E. A. Ballik, *OPTICAL ENGINEERING* **17** (1), (1978).

SPECTRUM 606.1

Start wavelength
$\lambda = 606.1\ cm^{-1}$

End wavelength
$\lambda = 606.4\ cm^{-1}$

Molecules: CH_3, N_2O



A portion of the CH_3 spectrum of the ν_2, out-of-plane bending mode, $N = K$ Q branch head. Depicted, left to right, are the $N = K = 2,3,1,4,5$ transitions. Also shown is the N_2O absorptions used to calibrate the wavenumber of the CH_3 transitions and the etalon interference pattern used to interpolate between the upper two traces.

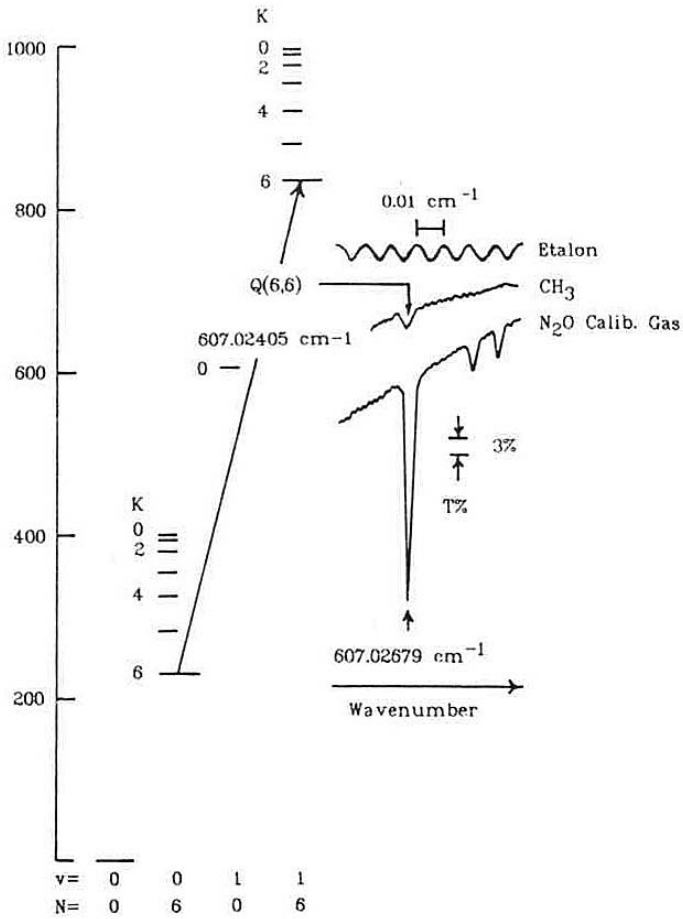
Reference:
D. K. Gaskill, V. Kolubatev, N. Bottka, R. S. Sillmon and J. E. Butler, *J. Crystal Growth* **77**, (1986).

SPECTRUM 607.02

Start wavelength
$\lambda = 607.02\ cm^{-1}$

End wavelength
$\lambda = 607.03\ cm^{-1}$

Molecules: CH_3, N_2O



The Q(6,6) rotational feature of the ν_2 fundamental vibrational mode of the CH_3 radical is presented as the middle trace in the right hand portion of the figure. A portion of the N_2O reference spectrum is shown on the lower trace. The left side of the figure displays the relevant energy levels involved in this transition. The methyl radical was formed by the decomposition of the TMG over the susceptor at 600 °C.

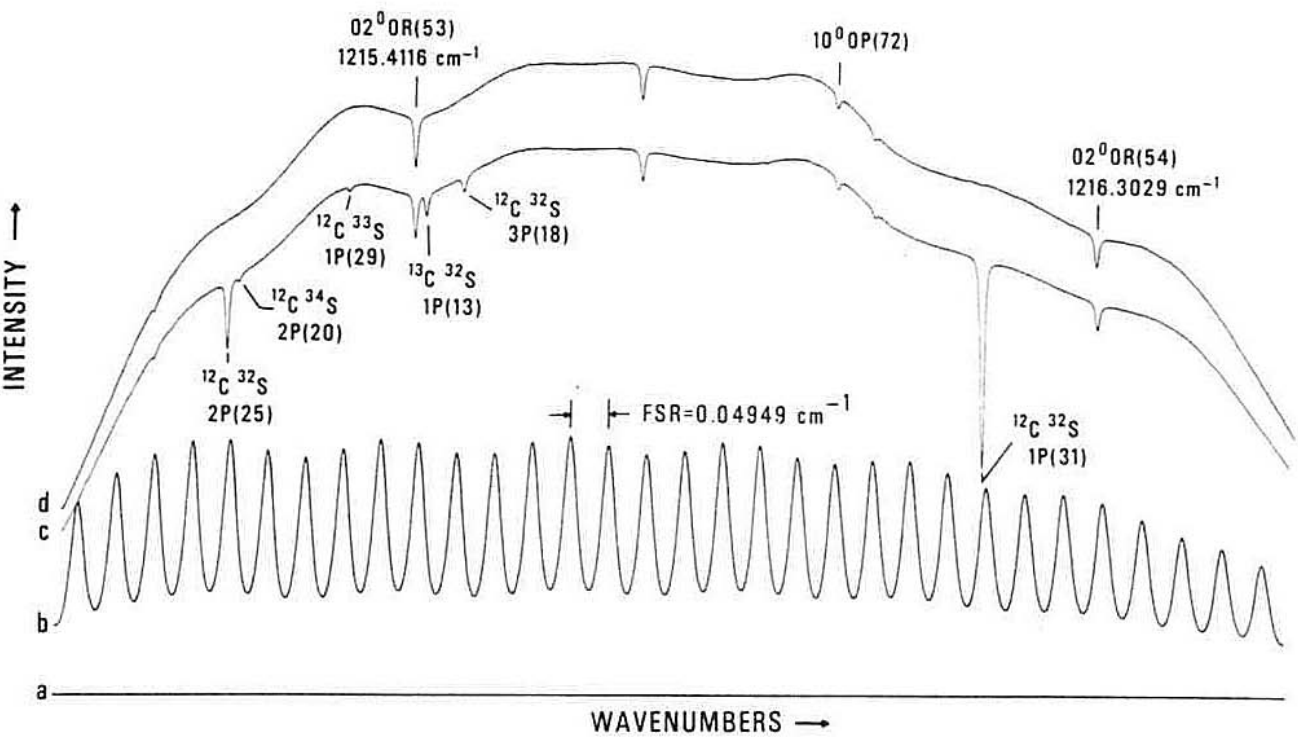
Reference:
J. E. Butler, N. Bottka, R. S. Sillmon, D. K. Gaskill, *Crystal Growth* **77**, 163 (1986).

SPECTRUM 1215

Start wavelength
$\lambda = 1215\ cm^{-1}$

End wavelength
$\lambda = 1216\ cm^{-1}$

Molecules: CS, N_2O



A diode laser spectrum of CS and N_2O. Traces a-d are, respectively, zero transmittance, etalon fringes, CS + N_2O spectra. N_2O spectrum. Traces b and c were recorded simultaneously while trace d was recorded later with slightly increased gain and the CS_2 discharge turned off. The N_2O pressure-path length product was 660 Pa · 50 cm. Line identifications are by $\nu\ '\Delta J(J'')$. The vibrational designations for N_2O, 10^00, and 02^00 refer, respectively, to $[10^00, 02^00]_{I,II}$ states.

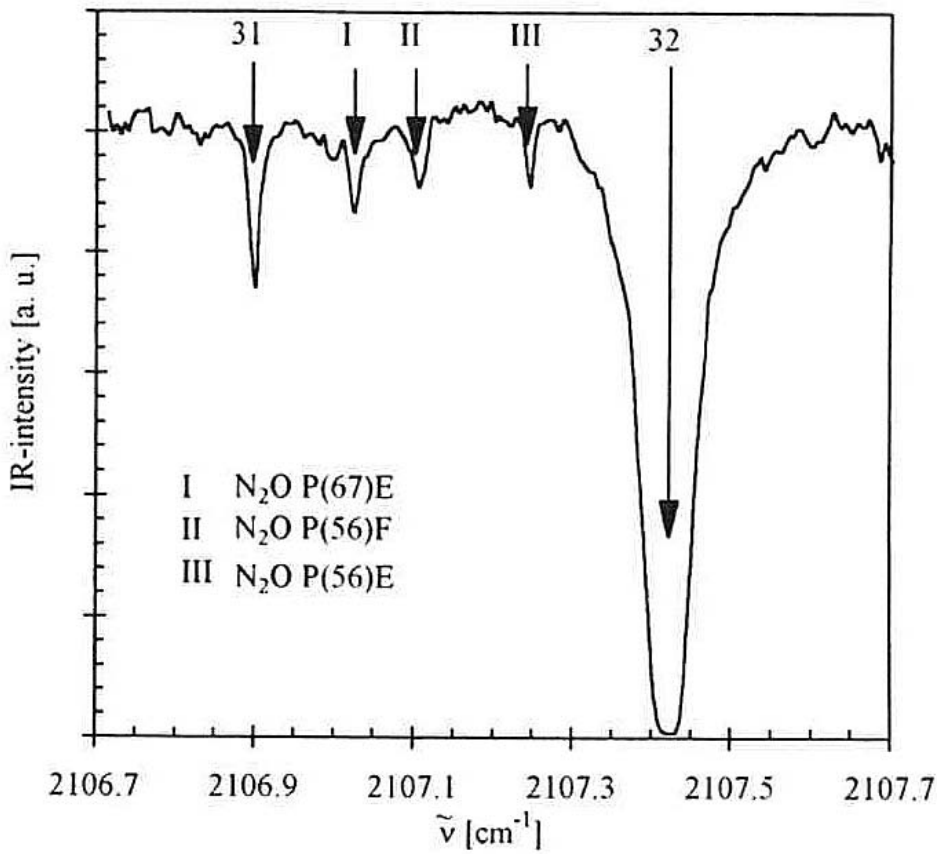
Reference:
T. Todd and B. Olsen, *Journal of Molecular Spectroscopy*, **74** (2), 190-202 (1979).

SPECTRUM 2106.7

Start wavelength
$\lambda = 2106.7\ cm^{-1}$

End wavelength
$\lambda = 2107.7\ cm^{-1}$

Molecules: CO, N_2O



Example for a multi-component can with CO and N_2O, multireflection cell with 9.5 m optical pathlength, $p_{N2O} = 35$ Torr, $p_{CO} = 0.007$ Torr.

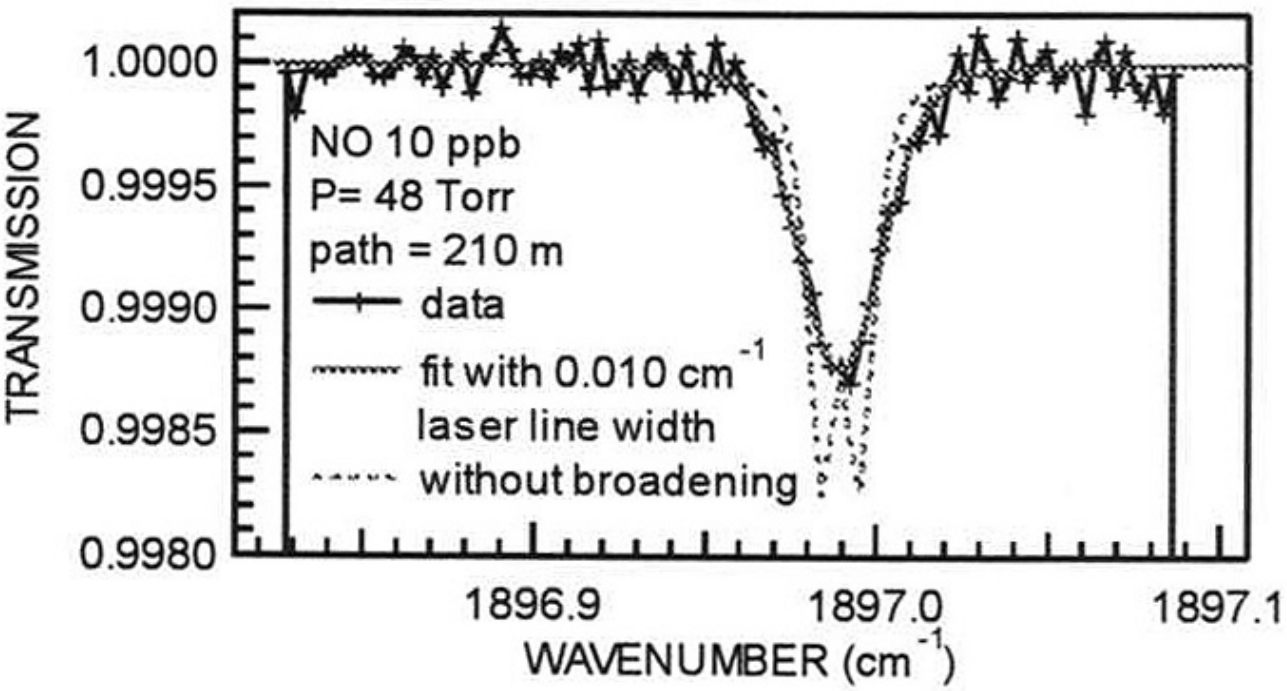
Reference:
T. Kelz et al., *Journal of Quantitative Spectroscopy and Radiative Transfer*, **61** (5), 591-601 (1999).

SPECTRUM 1896.9

Start wavelength
$\lambda = 1896.9\ cm^{-1}$

End wavelength
$\lambda = 1897.1\ cm^{-1}$

Molecules: NO



Nitric oxide transmission spectrum with 1-second averaging time using TE-cooled laser and detector. The fit is obtained with a laser linewidth of 0.010 cm^{-1} HWHM. The simulation without laser broadening for the NO doublet is shown by the dashed line.

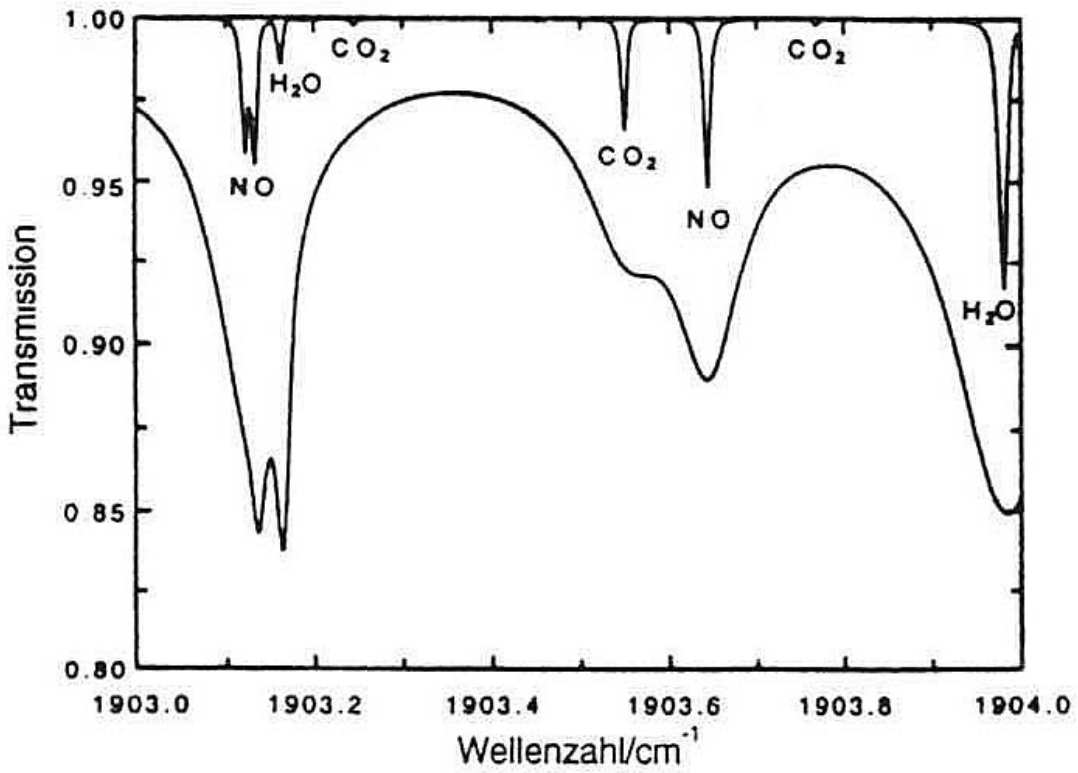
Reference:
D. D. Nelson, J. H. Shorter, J. B. McManus, M. S. Zahniser, *Appl. Phys. B.*, ***75***, 343-350 (2002).

SPECTRUM 1903

Start wavelength
$\lambda = 1903\ cm^{-1}$

End wavelength
$\lambda = 1904\ cm^{-1}$

Molecules: CO_2, NO, H_2O



Transmission spectrum of a gas mixture consisting of 100 ppm NO, 15% CO_2 and 15% H_2O in N_2 at 470 K and 1 m optical path. At atmospheric pressure (lower curve) the NO lines appear on the background of the other gases, at 30 mbar (needle-shaped minima) the NO lines can be traced nearly free of interference by other gases.

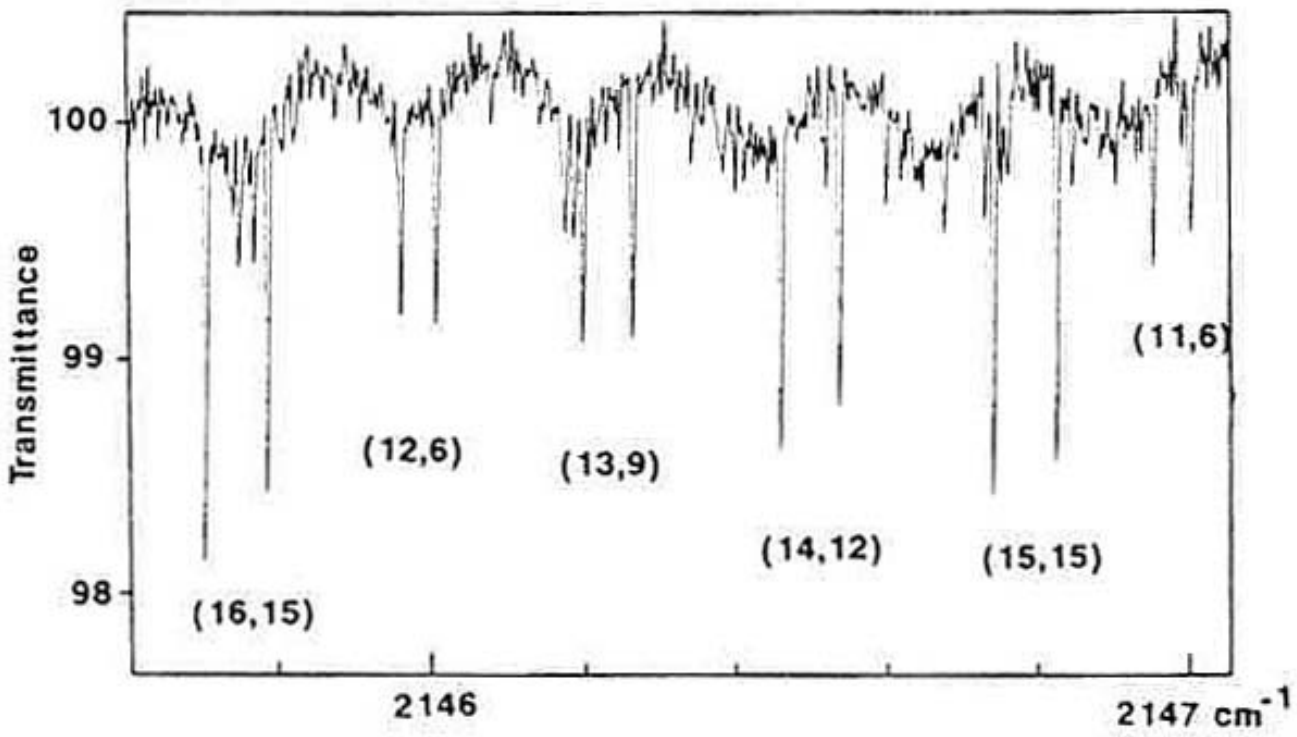
Reference:
M. Tacke, R. Grisar, *Laser und Optoelektronik*, 51-56 (1995).

SPECTRUM 2145.8

Start wavelength
$\lambda = 2145.8\ cm^{-1}$

End wavelength
$\lambda = 2147\ cm^{-1}$

Molecules: NO_3



Observed spectrum of the NO_3 2155 cm^{-1} band. Numbers in parentheses denote *N* and *K* values in ^{P}P branch transitions.

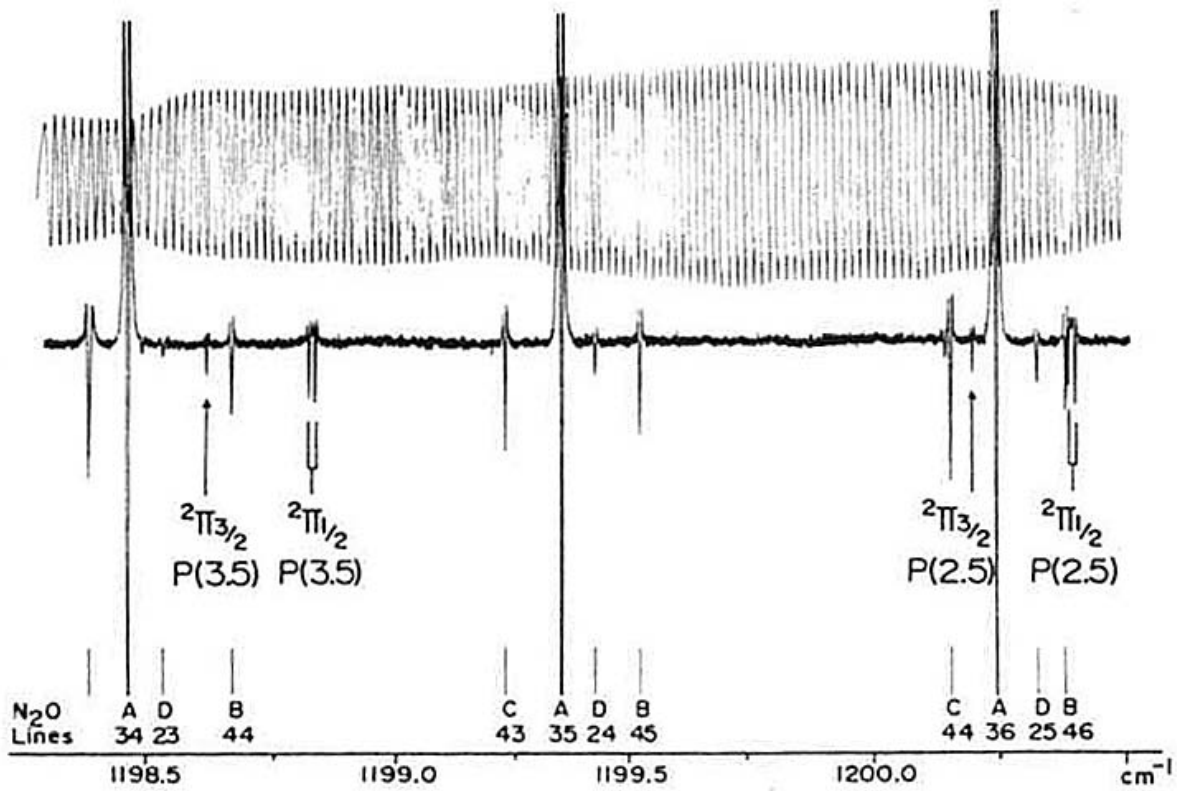
Reference:
K. Kawaguchi, T. Ishiwata, I. Tanka and E. Hirota, *Chemical physics letters* **180** (5), (1991).

SPECTRUM 1198.5

Start wavelength
$\lambda = 1198.5\ cm^{-1}$

End wavelength
$\lambda = 1200\ cm^{-1}$

Molecules: NS



A portion of the observed spectra. Source modulation was used with 2*f* detection. The *P*(2.5) und *P*(3.5) transitions of the NS fundamental band appear along with N_2O lines. The upper trace shows fringes produced by a Ge etalon; the fringe spacing is about 0.016 cm^{-1}. All N_2O lines used as standards are *R* branches of the following bands: A for $2\nu_2$, B for $3\nu_2$ (1e) – ν_2 (1e), C for $3\nu_2$ (1*f*) – ν_2 (1*f*) and D for $2\nu_2$ (2e). The numbers attached denote the *J* values.

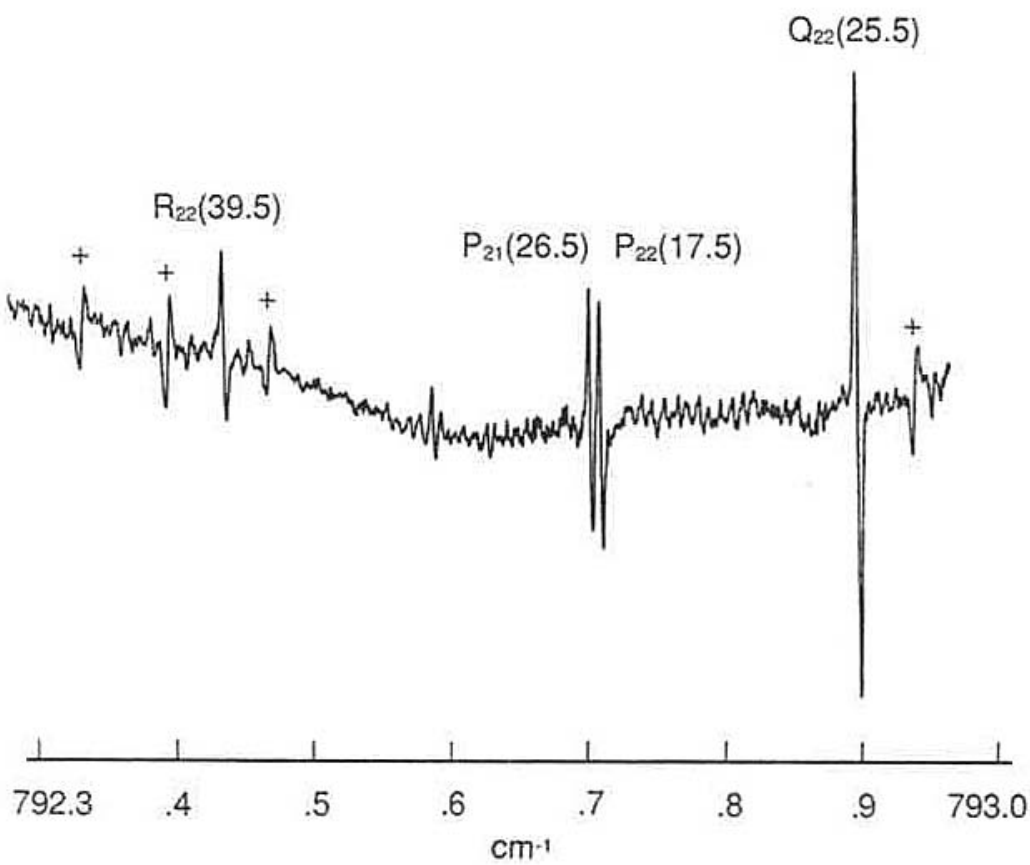
Reference:
K. Matsumura et al., *Journal of molecular spectroscopy* **84** (1), 68-71 (1980).

SPECTRUM 792.3

Start wavelength
$\lambda = 792.3\ cm^{-1}$

End wavelength
$\lambda = 793.0\ cm^{-1}$

Molecules: Si_2



Assigned lines forming part of the $A^2{}_{u1/2}(\nu = 1) \leftarrow \Pi\ X^2\ \Sigma^+_g\ (\nu = 0)$ subband of Si_2^- recorded in a silane plasma using infrared laser velocity modulation spectroscopy. Lines indicated by (+) are cation lines appearing with opposite phase to the anion lines.

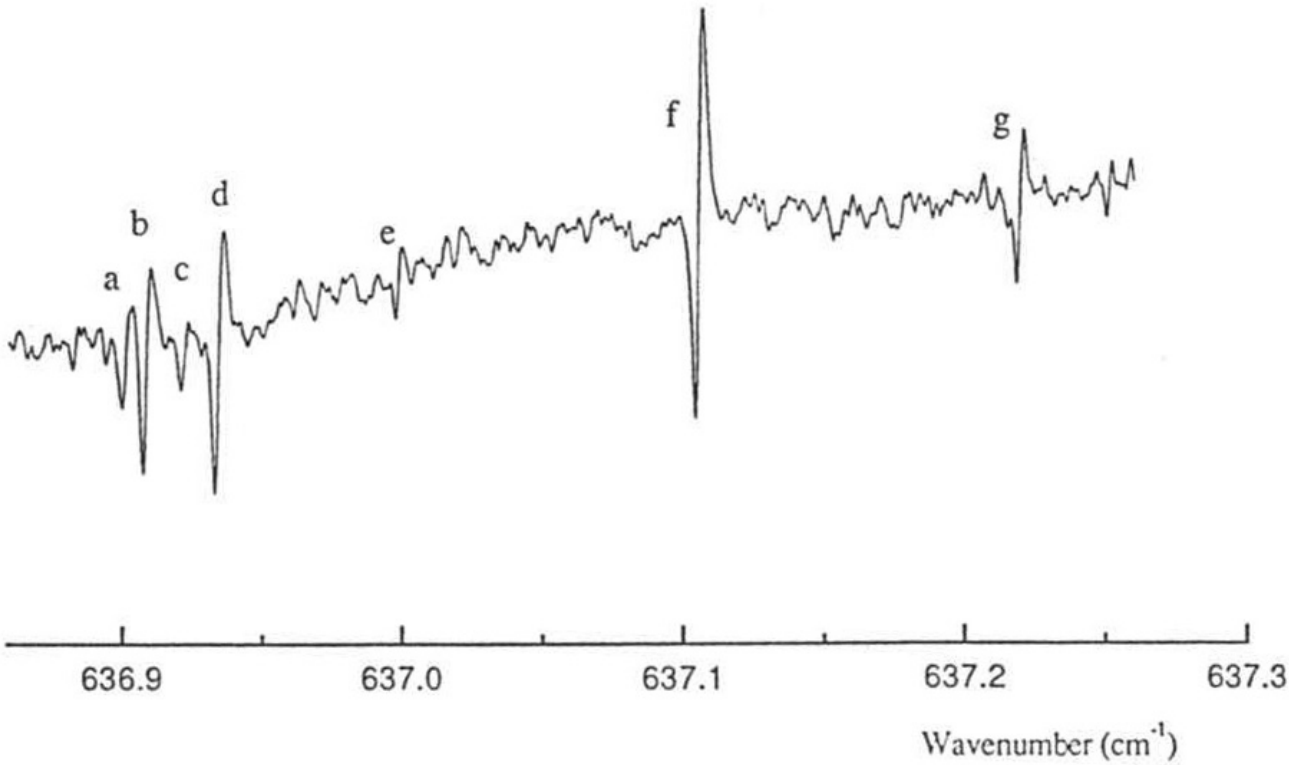
Reference:
Z. Liu, P. B. Davies, *Physical Review Letters* **76** (4), (1996).

SPECTRUM 636.9

Start wavelength
$\lambda = 636.9\ cm^{-1}$

End wavelength
$\lambda = 637.3\ cm^{-1}$

Molecules: $SICL^+$



Fundamental and hot band transitions of $^{28}Si^{35}Cl+$ (1) and $^{28}Si^{37}Cl+$ (2) near 637 cm^{-1}: (a) 1 (4, 36)← (3, 37); (b) 2 (1, 45) ← (0, 46); (c) 1 (6, 22) ← (5, 23); (d) 1 (2, 49) ← (1, 50); (e) 1 (5, 29) ← (4, 30); (f) 1 (1, 55) ← (0, 56); and (g) 2 (2, 38) ← (1, 39)

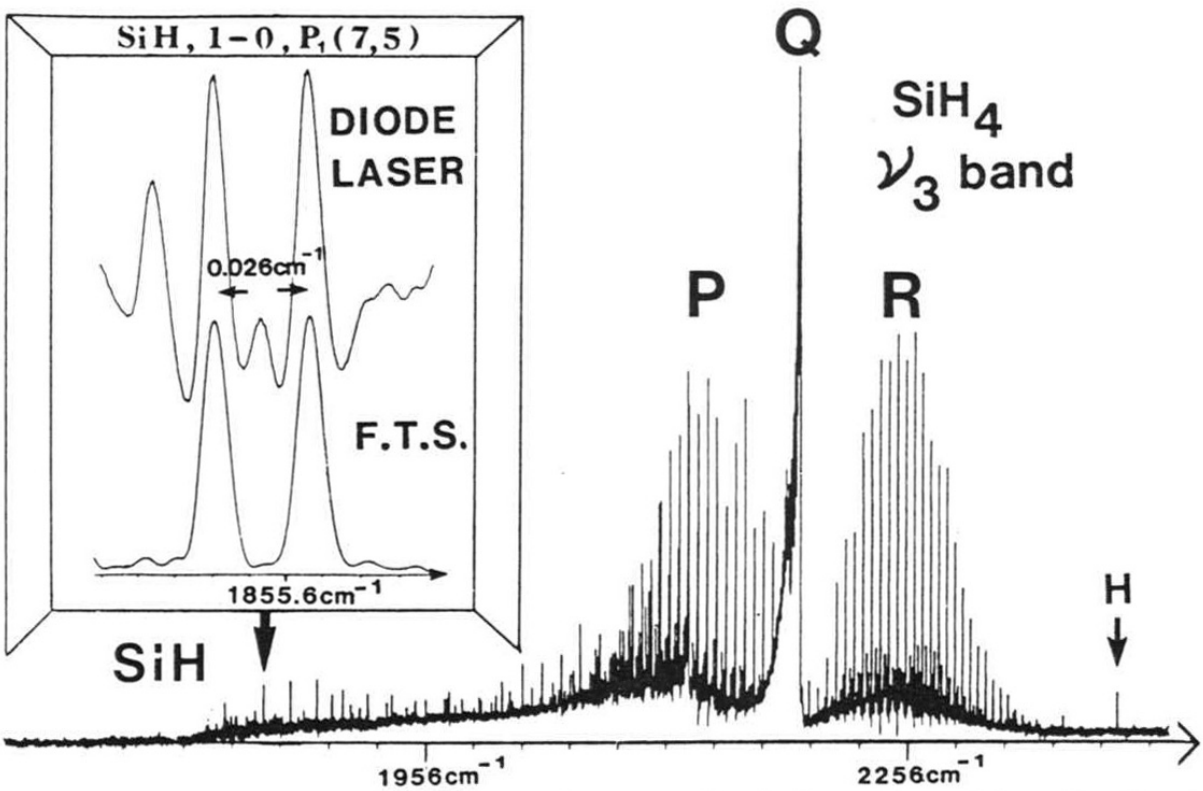
Reference:
P. B. Davies, *Spectrochimica Acta Part A* **55**, 1987-1997 (1999).

SPECTRUM 1855

Start wavelength
$\lambda = 1855\ cm^{-1}$

End wavelength
$\lambda = 2256\ cm^{-1}$

Molecules: SiH_4, SiH



The silane-plasma emission recorded with the Fourier interferometer and partly shown at low resolution. Boxed insert: upper trace, the same doublet from the diode laser as in Fig. 4. Lower trace, very small portion with full resolution of the Fourier-transform spectrum.

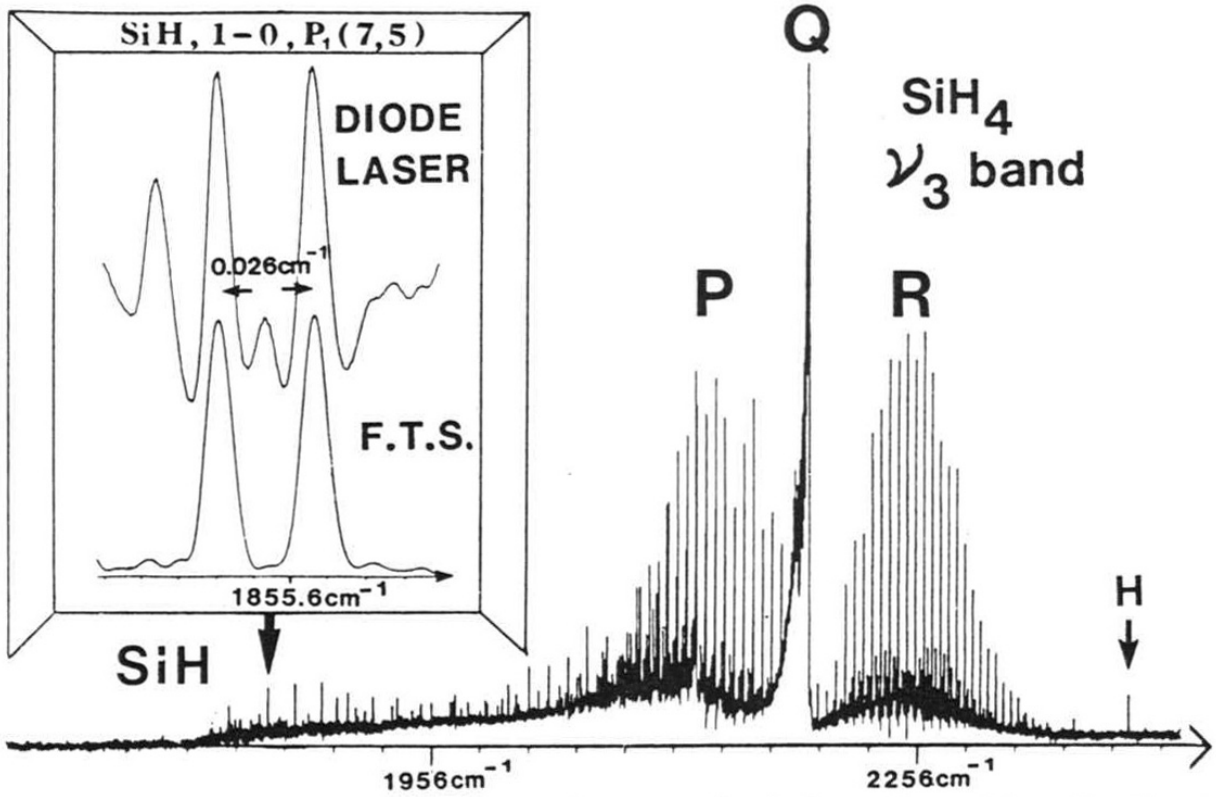
Reference:
P. Chollet, G. Guelachvili, M. Morillon-Chapey, *J. Opt. Soc. Am. B.* **3** (5), (1986).

SPECTRUM 1855

Start wavelength
$\lambda = 1855\ cm^{-1}$

End wavelength
$\lambda = 2256\ cm^{-1}$

Molecules: SiH_4, SiH



The silane-plasma emission recorded with the Fourier interferometer and partly shown at low resolution. Boxed insert: upper trace, the same doublet from the diode laser as in Fig. 4. Lower trace, very small portion with full resolution of the Fourier-transform spectrum.

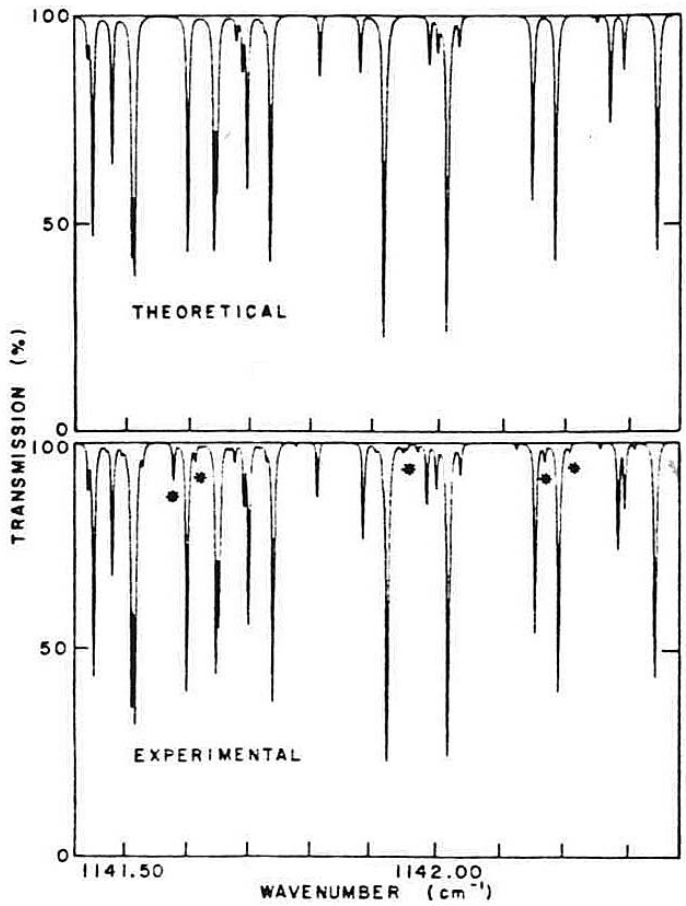
Reference:
P. Chollet, G. Guelachvili, M. Morillon-Chapey, *J. Opt. Soc. Am. B.* **3** (5), (1986).

SPECTRUM 1141.5

Start wavelength
$\lambda = 1141.5\ cm^{-1}$

End wavelength
$\lambda = 1142.5\ cm^{-1}$

Molecules: SO_2



Experimental and theoretical transmission spectra for SO_2 in the 1142 cm^{-1} region. A pathlength of 60 m is used, with a 1000 ppm mixture of SO_2 in N_2 at a total pressure of 10 Torr. Many weak SO_2 absorption lines which are obtained experimentally are not predicted by the theoretical compilation of Clough[19], a few of these are indicated by an asterisk.

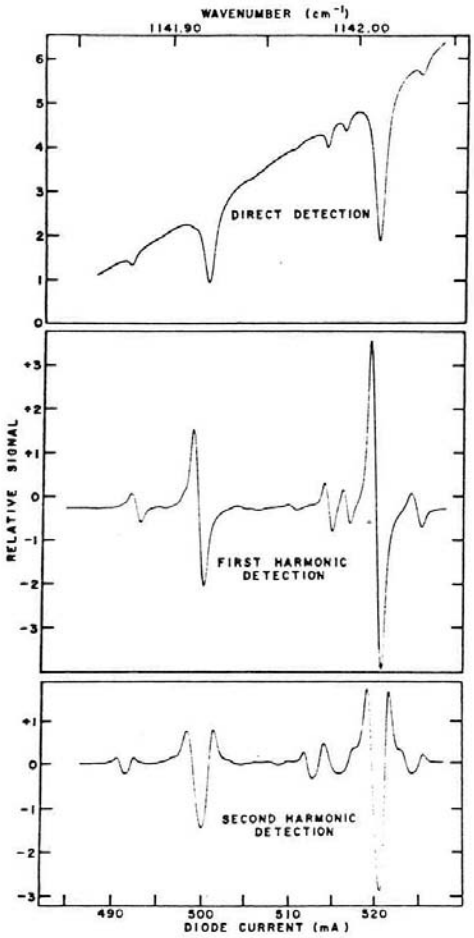
Reference:
J. Reid, J. Shewchun, B. K. Garside, E. A. Ballik, *APPLIED OPTICS* **17** (2), (1978)

SPECTRUM 1141.8

Start wavelength
$\lambda = 1141.8\ cm^{-1}$

End wavelength
$\lambda = 1142.4\ cm^{-1}$

Molecules: SO_2



Three different SO_2 detection schemes. Upper trace: direct absorption detection: middle trace: first harmonic detection: lower trace: second harmonic detection. A 1 - kHz diode modulation is used for the harmonic detection. Conditions are 1000-ppm SO_2 in N_2 10-Torr total pressure, 40 m path.

Reference:
J. Reid, J. Shewchun, B. K. Garside, E. A. Ballik, *APPLIED OPTICS* **17** (2), (1978).

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