C2

"LINE-by-LINE" SOFTWARE FOR SPECTRA SIMULATION

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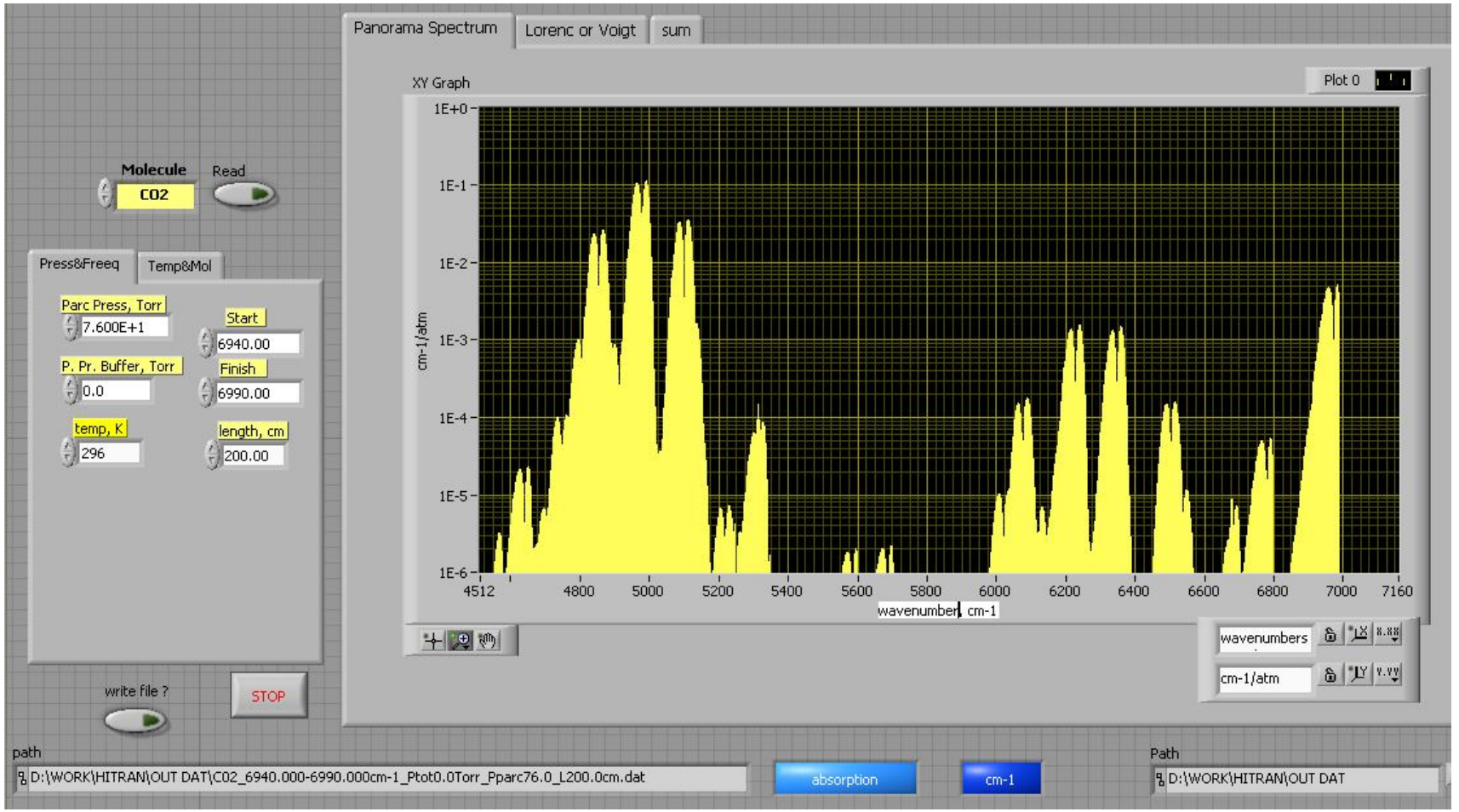
Introduction

TDLS analytical applications frequently need operative optimization of DL and analytical spectral line choice. Analysis has to be done taking into account absorption of other molecules in gas mixture under investigation. For atmosphere: H_2O, CO_2, CH_4, O_2, etc. To solve this problem, software "***Line-by-line***" was developed based on "LabView 8.6", spectral database "HITRAN-2008" [1], [2] and Voigt line shape. Additional software option is recorded TDLS spectra comparison with simulation to identify recorded lines.

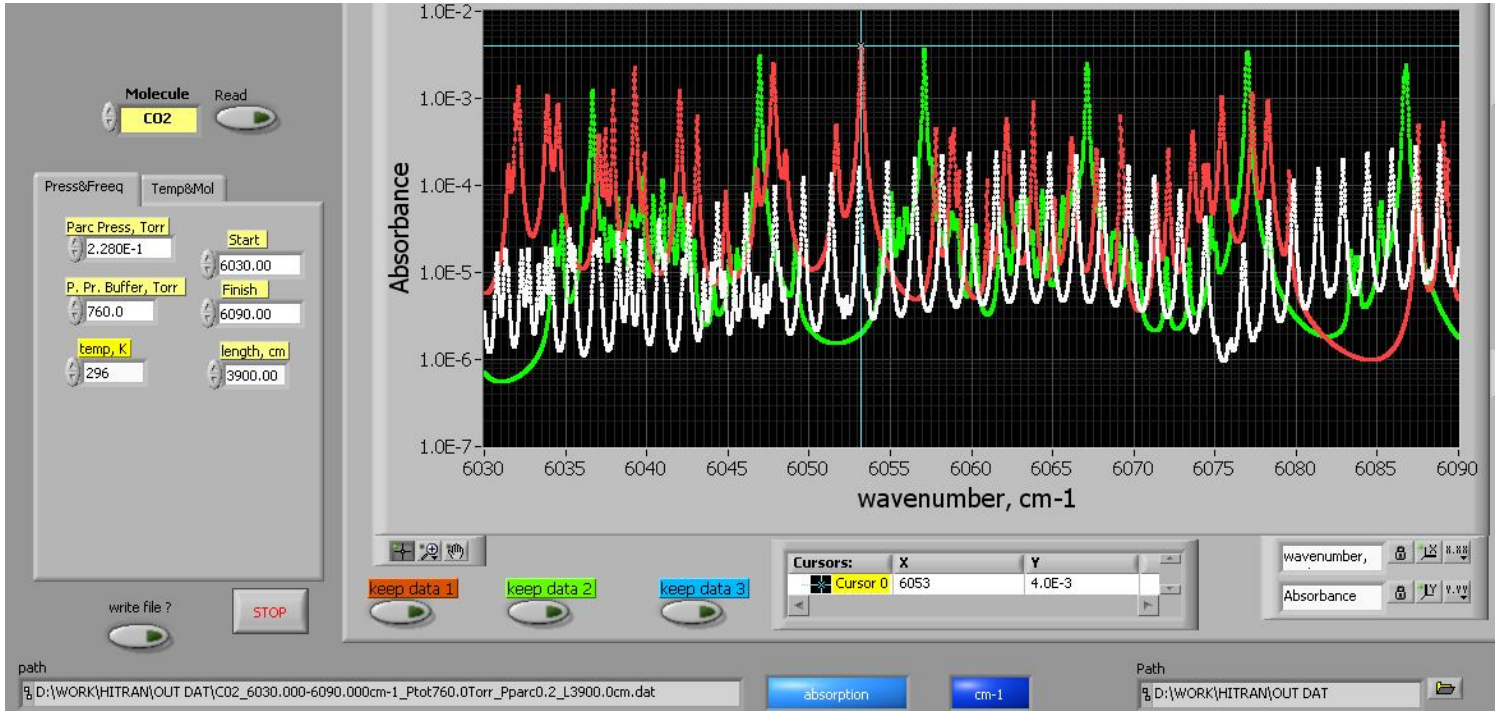
[1] http://www.cfa.harvard.edu/HITRAN/
[2] L.S. Rothman, I.E. Gordon, A. Barbe, D.Chris Benner, P.F. Bernath, M. Birk, V. Boudon, L.R. Brown, A. Campargue, J.-P. Champion, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, S. Fally, J.-M. Flaud, R.R. Gamache, A. Goldmanm, D. Jacquemart, I. Kleiner, N. Lacome, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, S.N. Mikhailenko, C.E. Miller, N. Moazzen-Ahmadi, O.V. Naumenko, A.V. Nikitin, J. Orphal, V.I. Perevalov, A. Perrin, A. Predoi-Cross, C.P. Rinsland, M. Rotger, M.Simeckova, M.A.H. Smith, K. Sung, S.A. Tashkun, J. Tennyson, R.A. Toth, A.C. Vandaele, J. Vander Auwera, "The HITRAN 2008 molecular spectroscopic database", JQRST, 110, pages 533-572 (2009).

HITRAN data



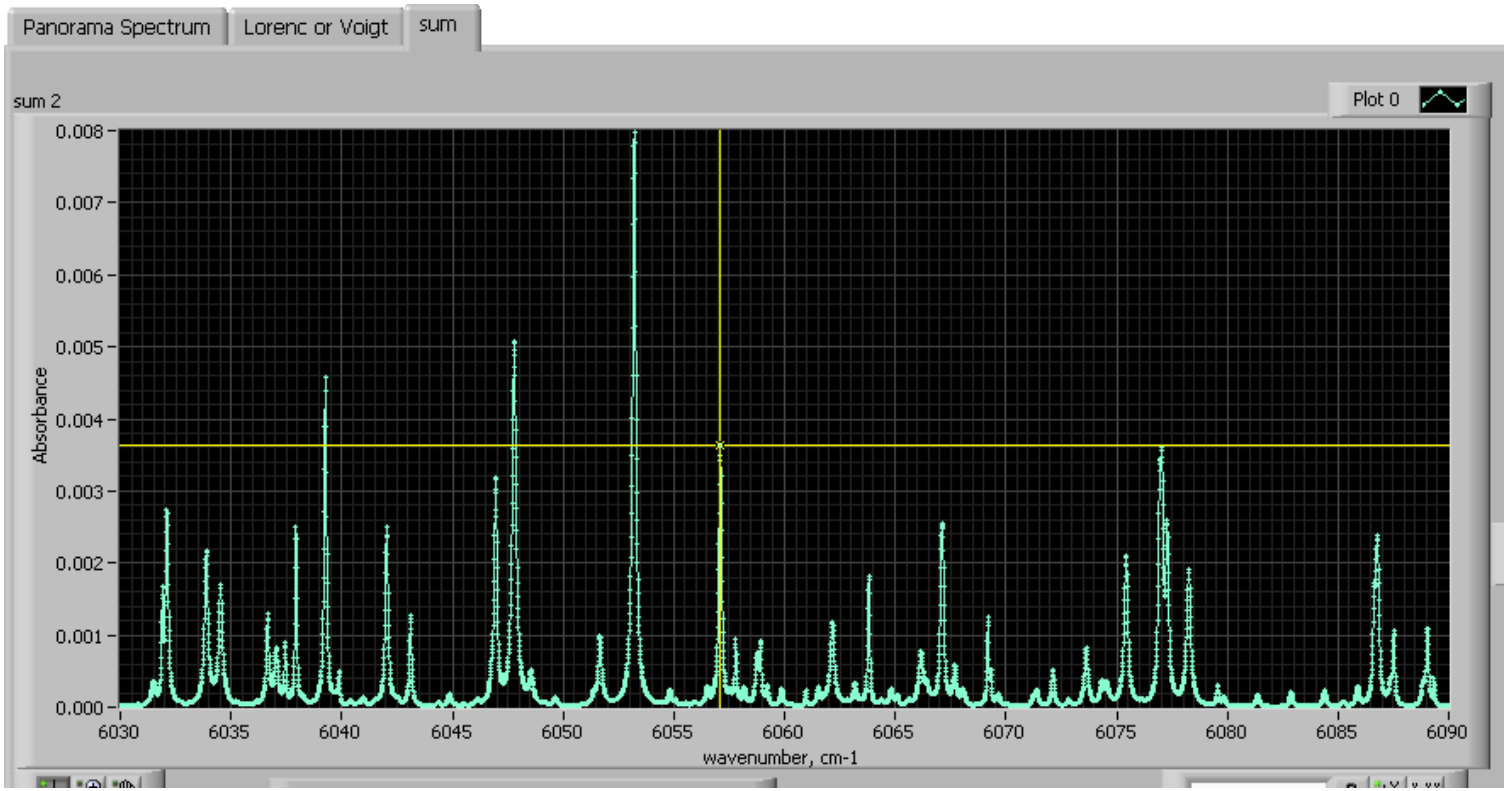
Preliminary data review

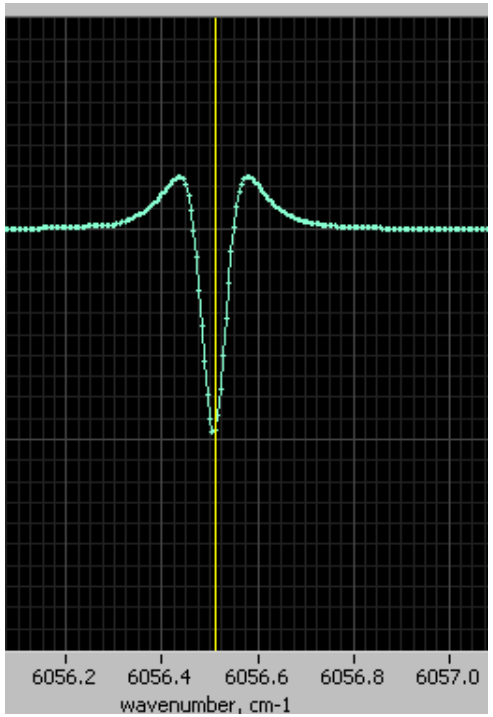
Software interface



User can select molecules from HITRAN 2008, their partial pressures, total gas mixture pressure, temperature, optical length, and spectral range of interest. There are options to present result as absorbance or transmission vs wave number or wave length. Data calculated can be stored in computer. In present case CO_2 (white), H_2O (green), and CH_4 (red) were considered. Cursors (blue) can determine line position and its absorbance.

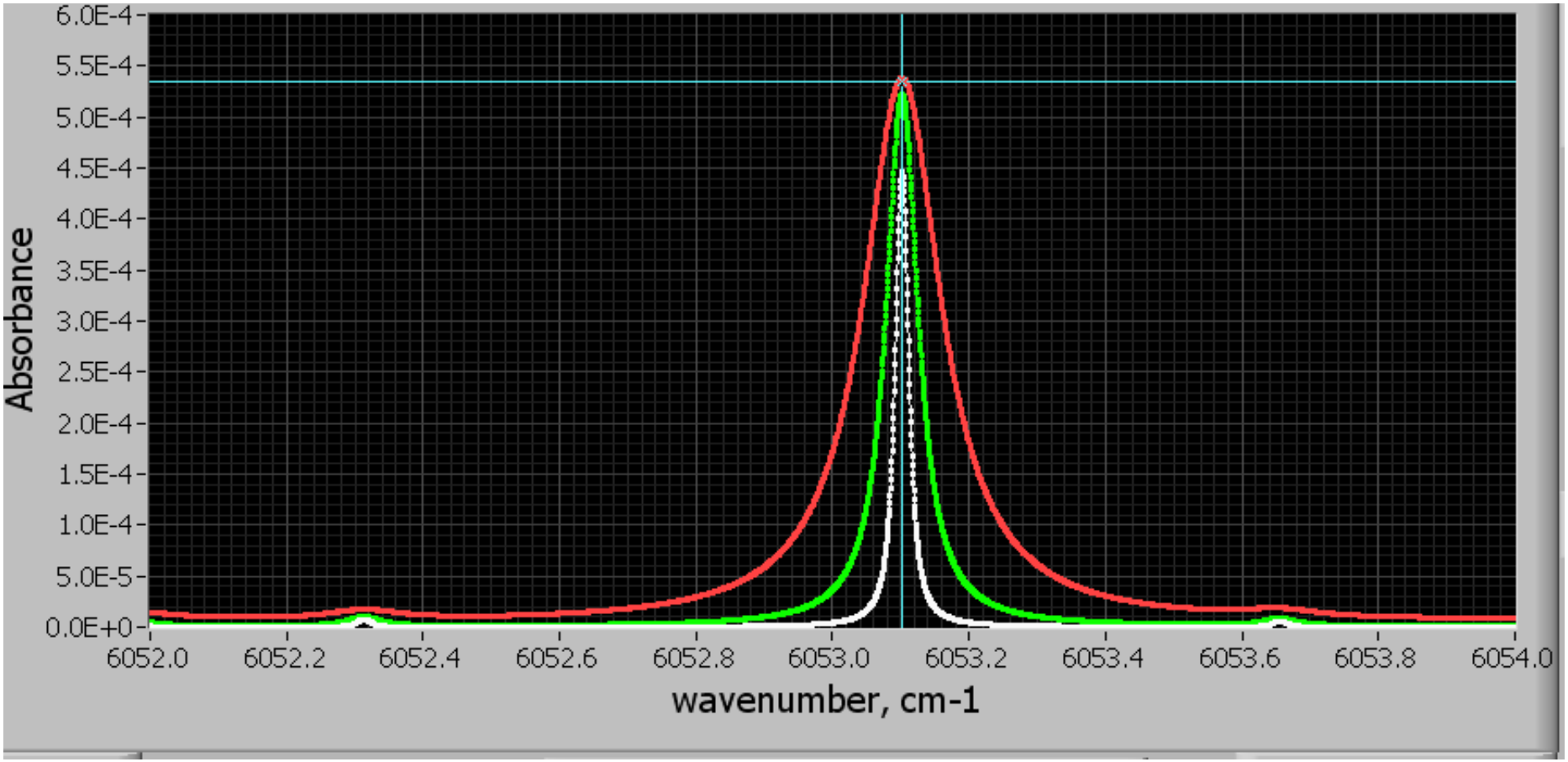
Complex gas mixture spectrum





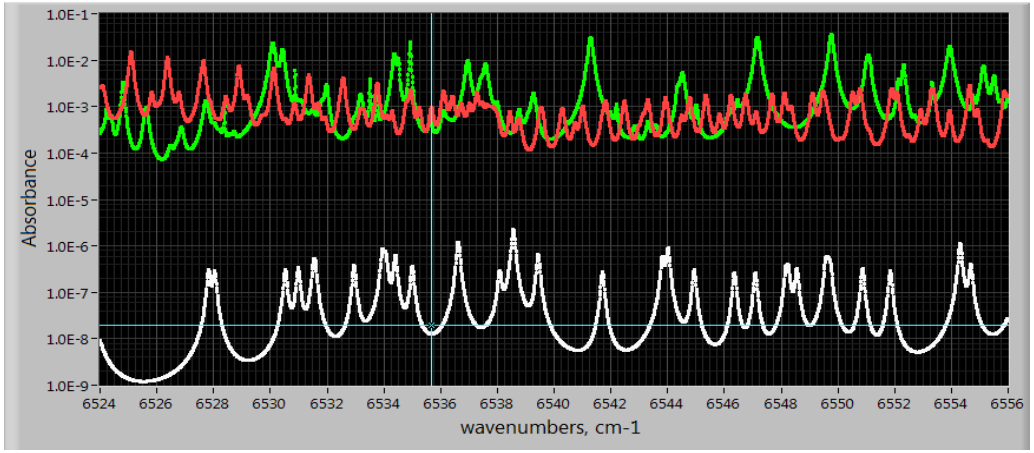
As option total absorbance of complex gas mixture under consideration (similar as on previous slide) and its derivatives can be calculated to be compared with data obtained by TDLS.

Pressure dependence

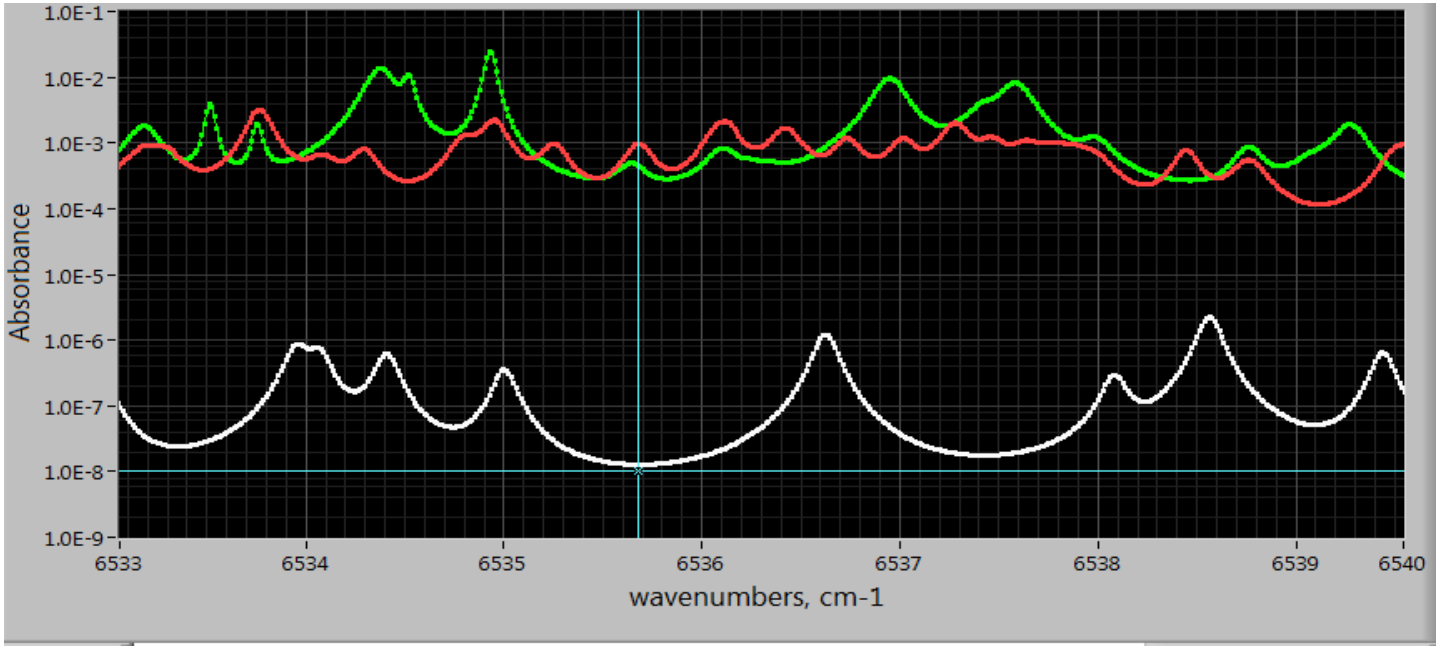


CO_2:air = 1:1000 absorbance spectrum simulation: L = 39 m, P = 760 (red), 300 (green), 100 (white) Torr.

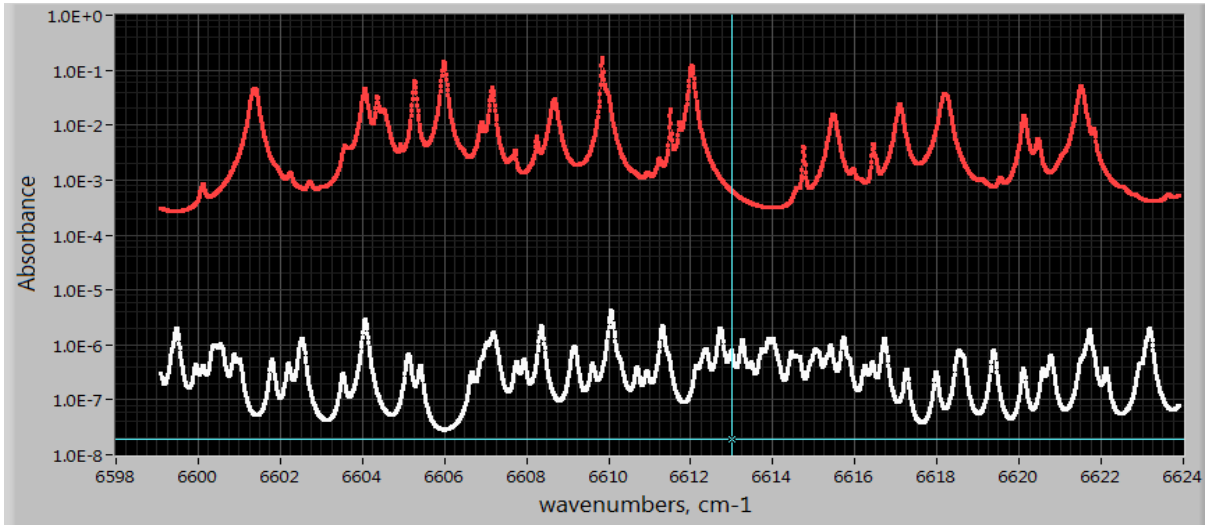
NH_3 detection in human breath in 1.53 μ



CH_4 =10.0 ppm (white),
H_2O =2 % (green),
CO_2 =3% (red) ,L=39 m,
P=1 atm, T=296 ^{0}K

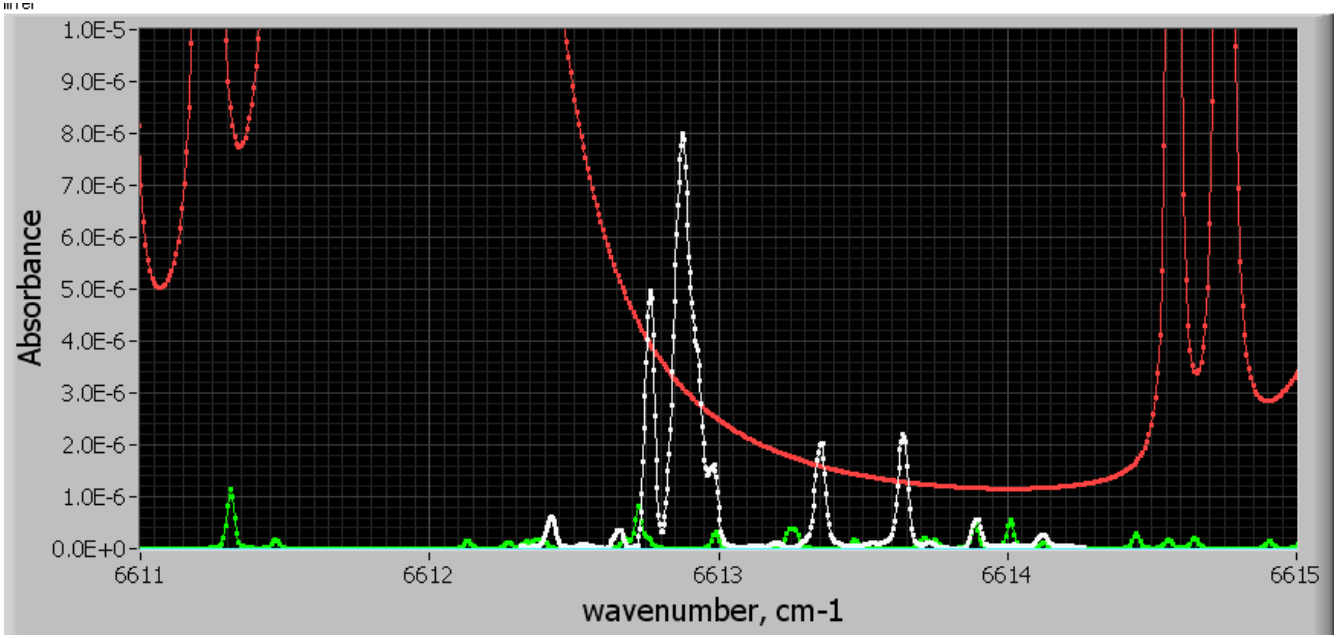


NH_3 detection in human breath in 1.51 μ

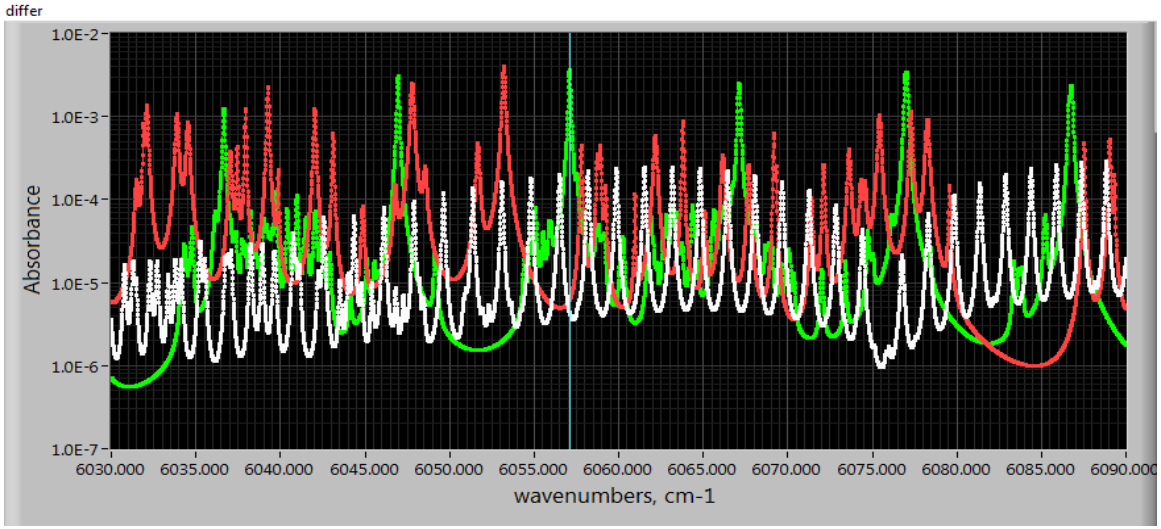


CH_4 =10.0 ppm (white),
H_2O =2 % (red),
L=39 m, P=1 atm,
T=296 ^{0}K

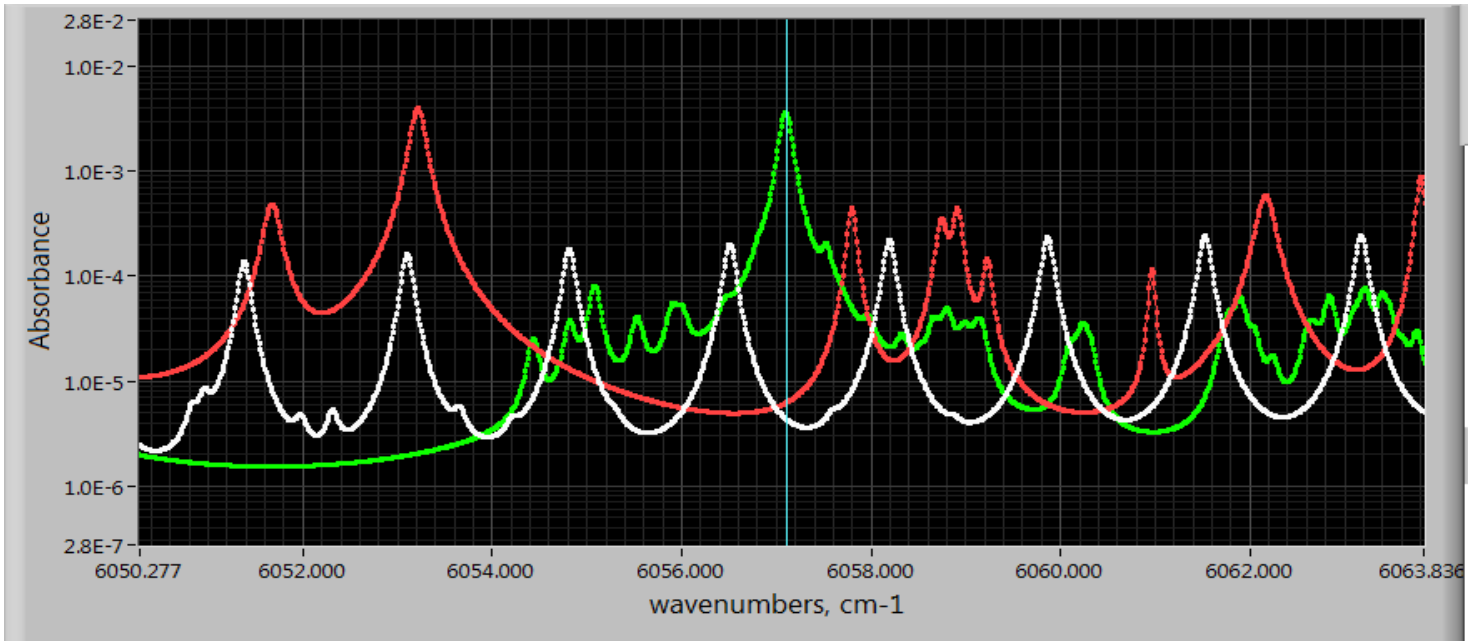
TDLS spectrum of
NH_3=1.5 ppb (white)
CH_4 =10.0 ppm (green),
H_2O =2 % (red),
L=39 m, P=0.1 atm,
T=296 ^{0}K



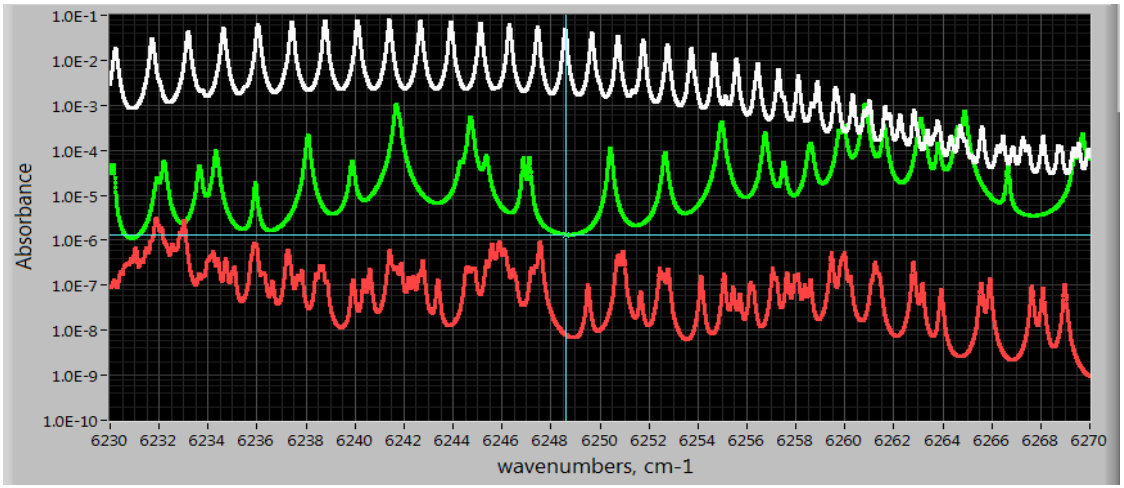
Trace CH_4 detection in 1.65 μ



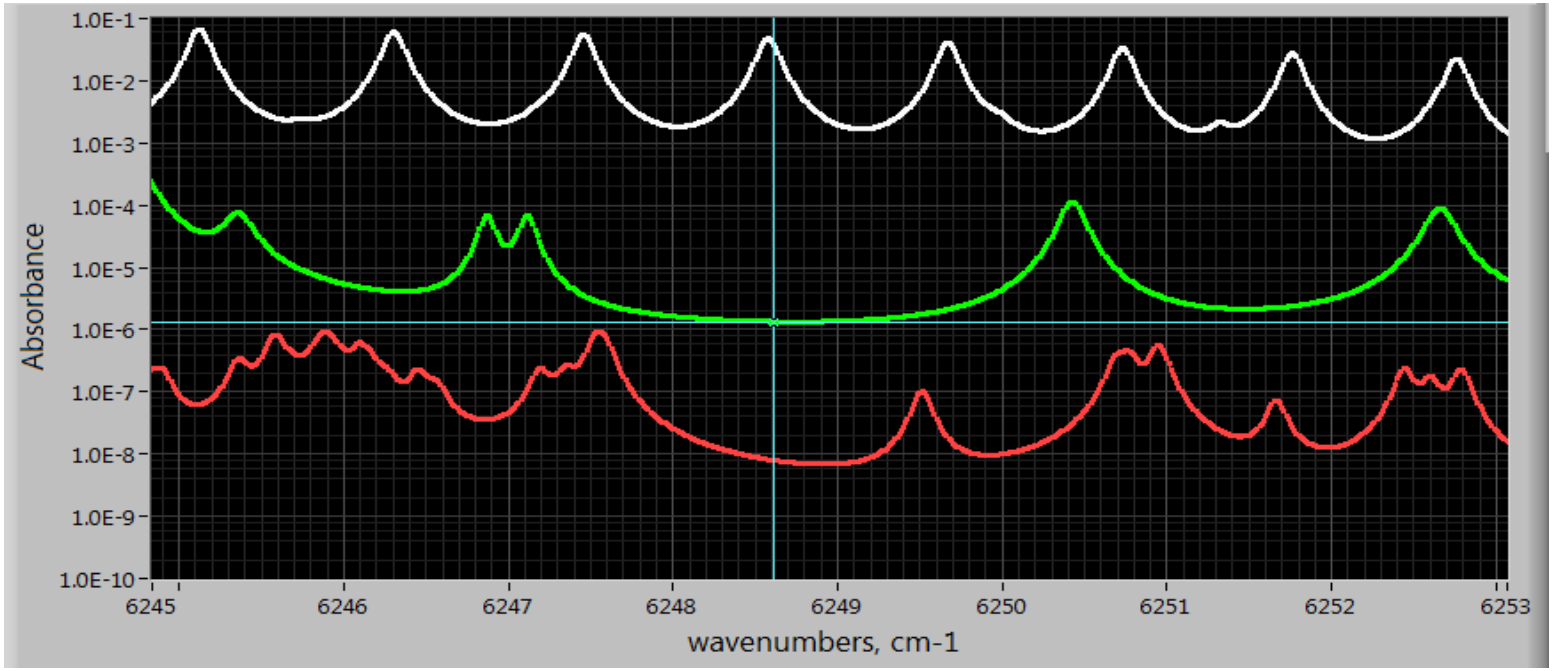
CH_4 =2.0 ppm (green),
CO_2 =300 ppm (white),
H_2O =1 % (red), L=39 m,
P=1 atm, T=296 ^{0}K



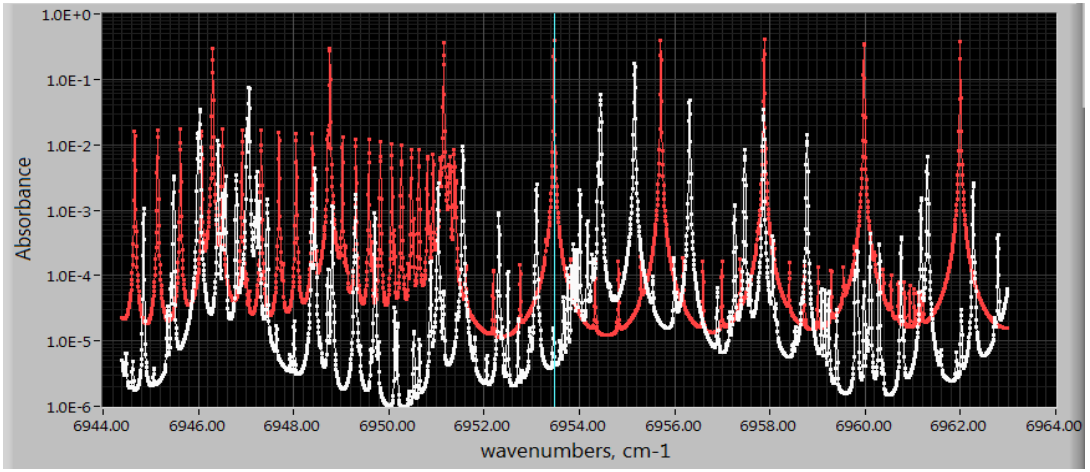
Trace CO_2 detection in 1.60 μ



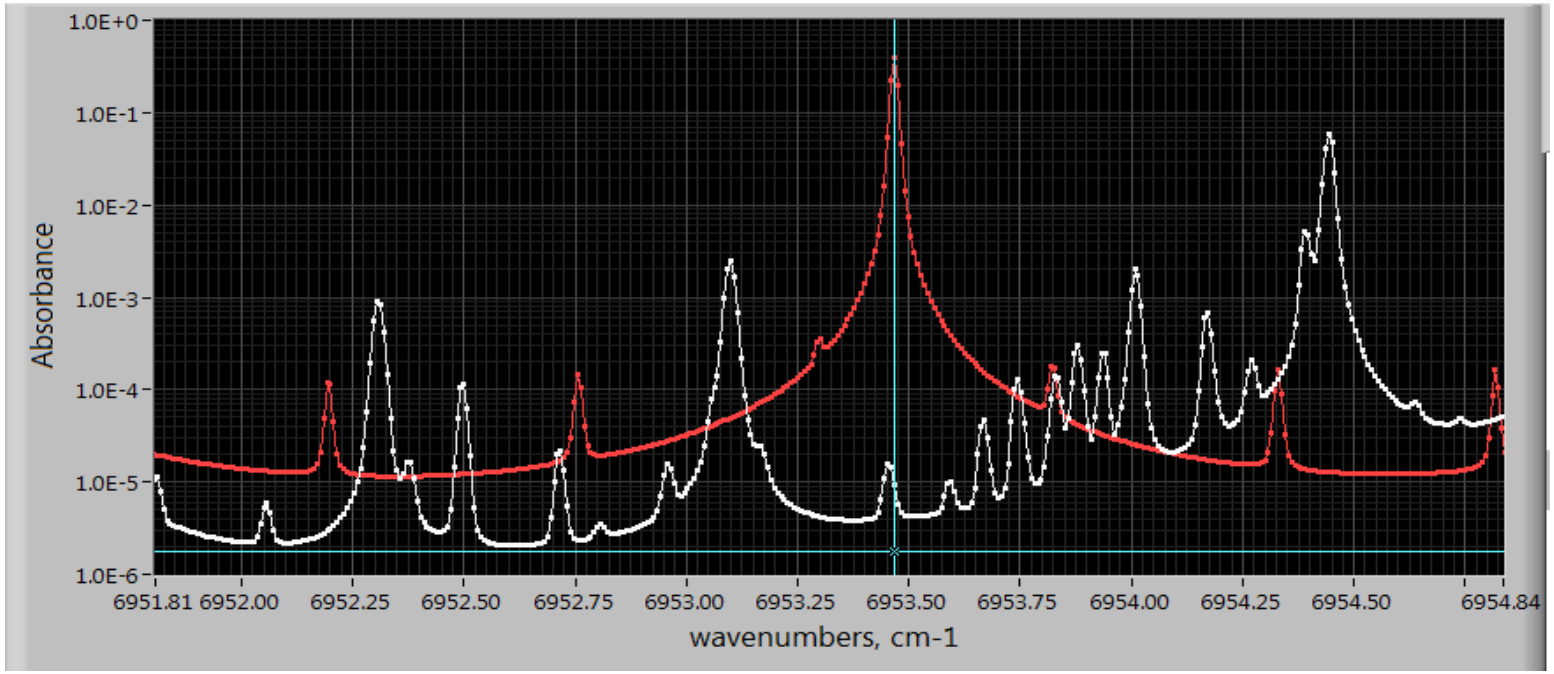
CO_2 =300 ppm (white), H_2O =1 % (green), CH_4 =2.0 ppm (red), L=39 m, P=1 atm, T=296 ^{0}K



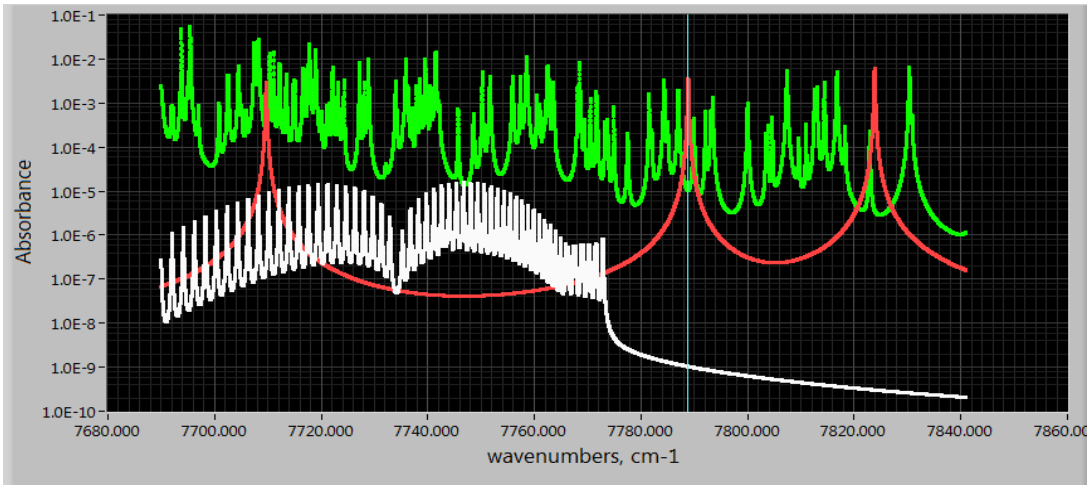
Precision measurement of contour line CO_2 in 1.44 μ



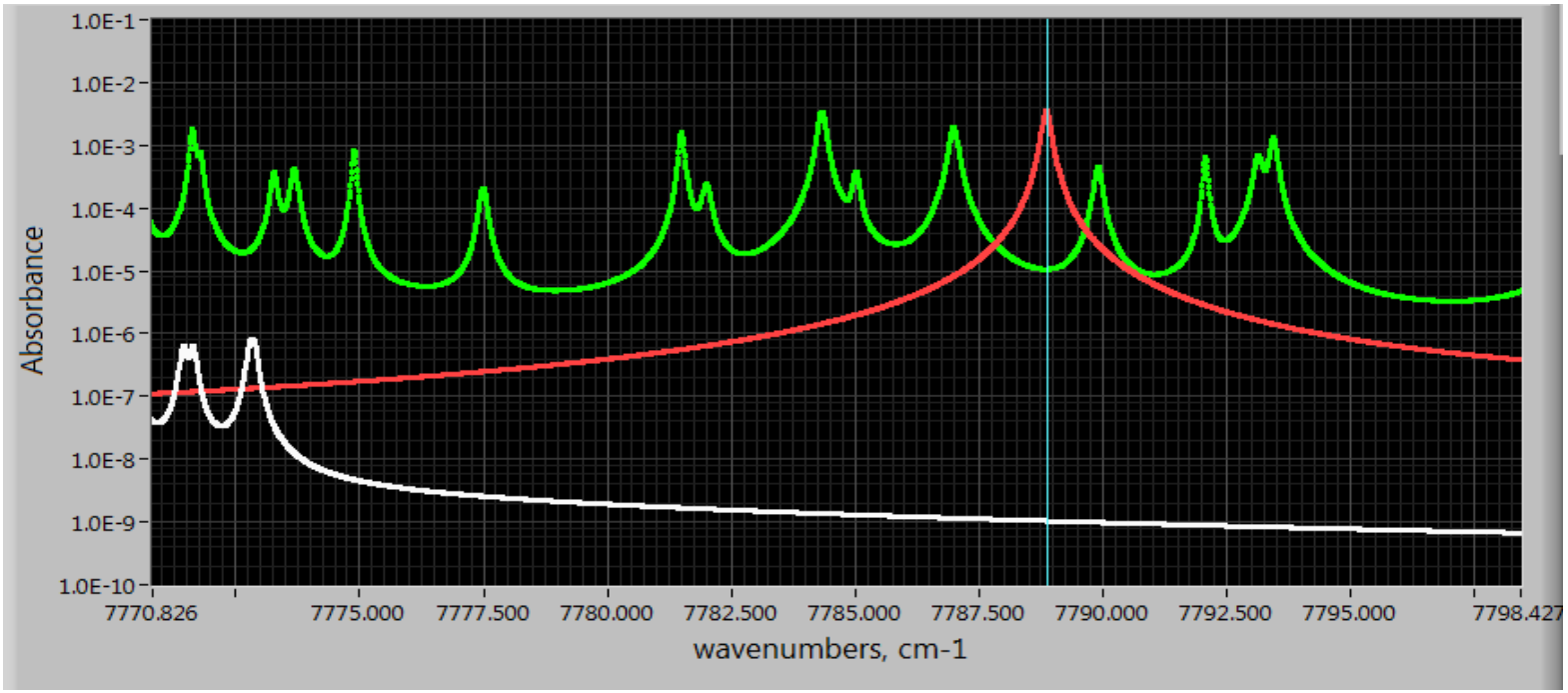
CO_2 =2.63 kPa(red), H_2O =0.065 kPa(white) in 2.63 kPA N_2, L=200 cm, T=296 ^{0}K



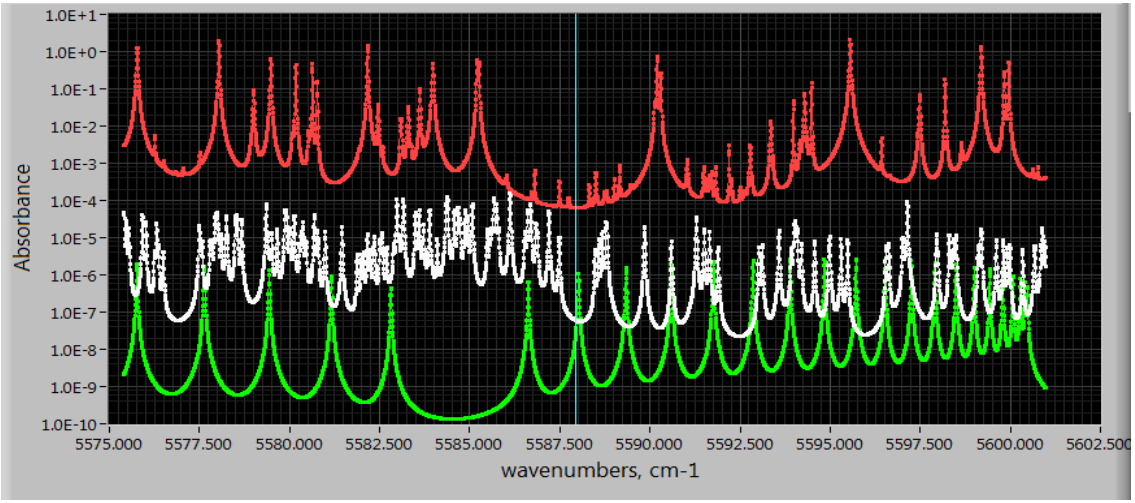
HF detection in 1.3 μ



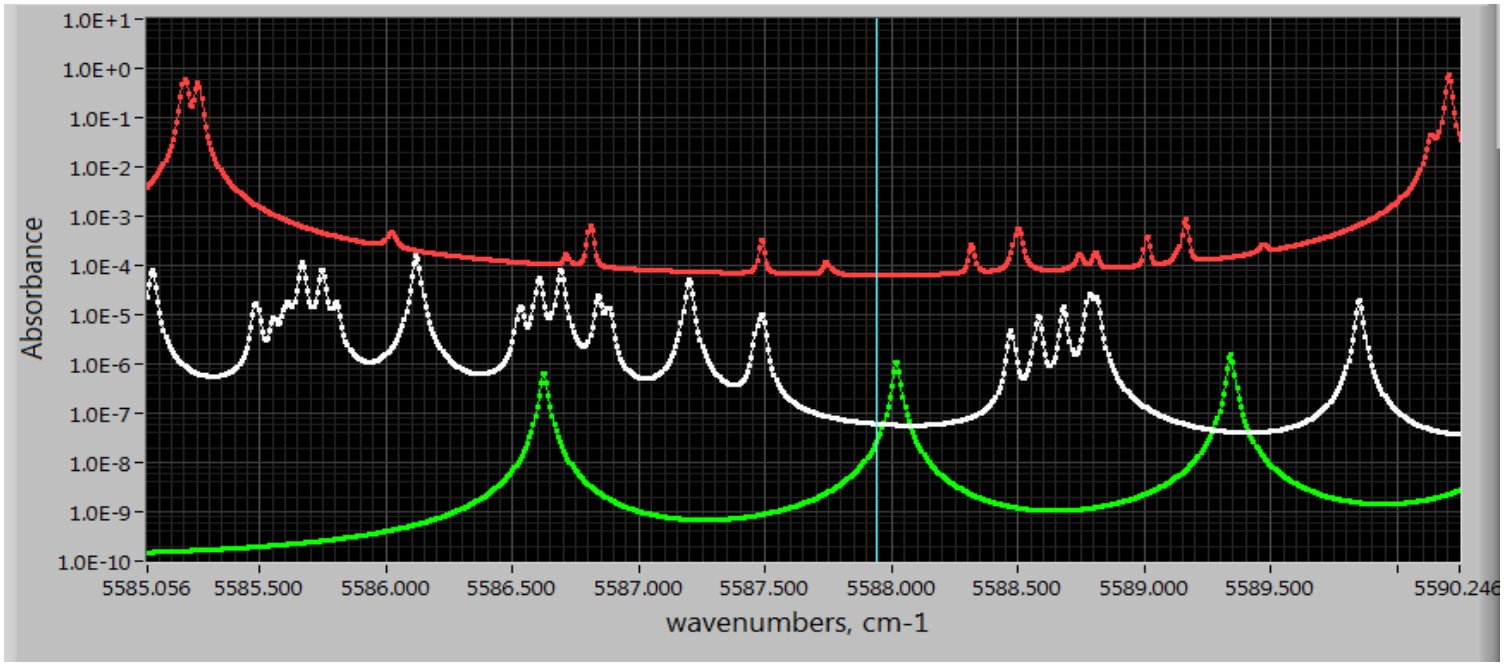
HF =200 ppp (red), CO_2 =300 ppm (white), H_2O =1 % (green), L=39 m, P=1 atm, T=296 ^{0}K



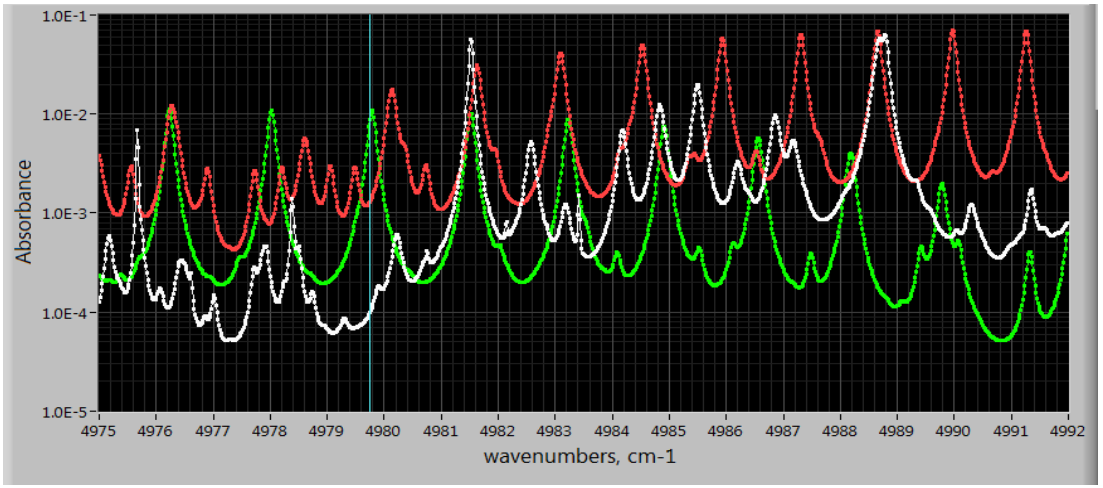
H_2CO detection in 1.79 μ



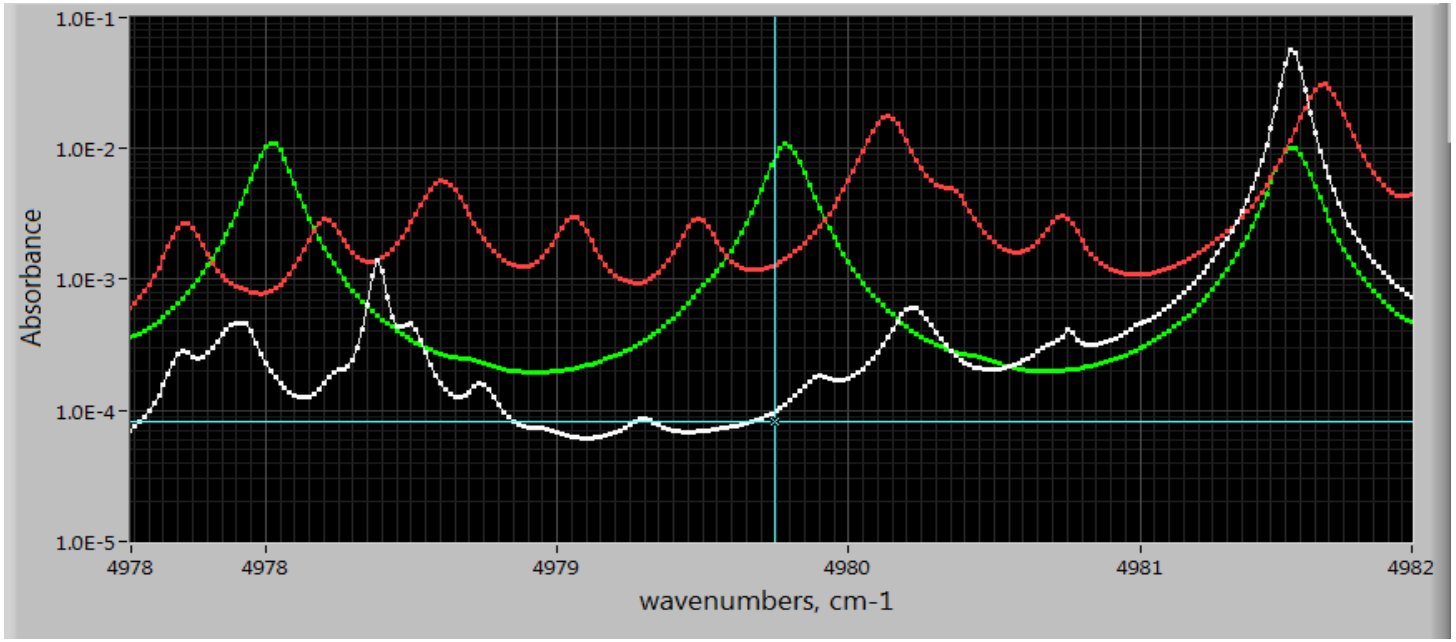
Analytical region for detection H_2CO. H_2O=1% (red), CH_4 =2 ppm (white), CO_2 =300 ppm (green)



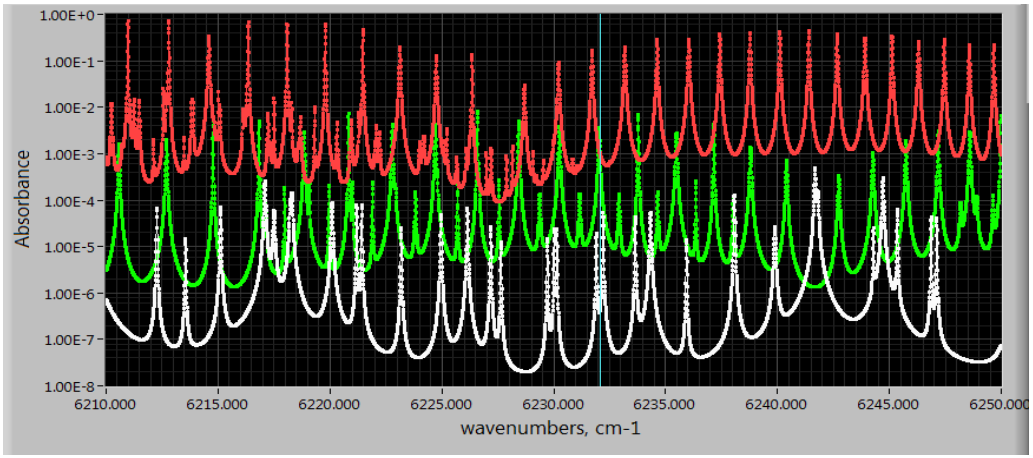
$^{13}CO_2$ /$^{12}CO_2$ -ratio measurements in 2.0 μ



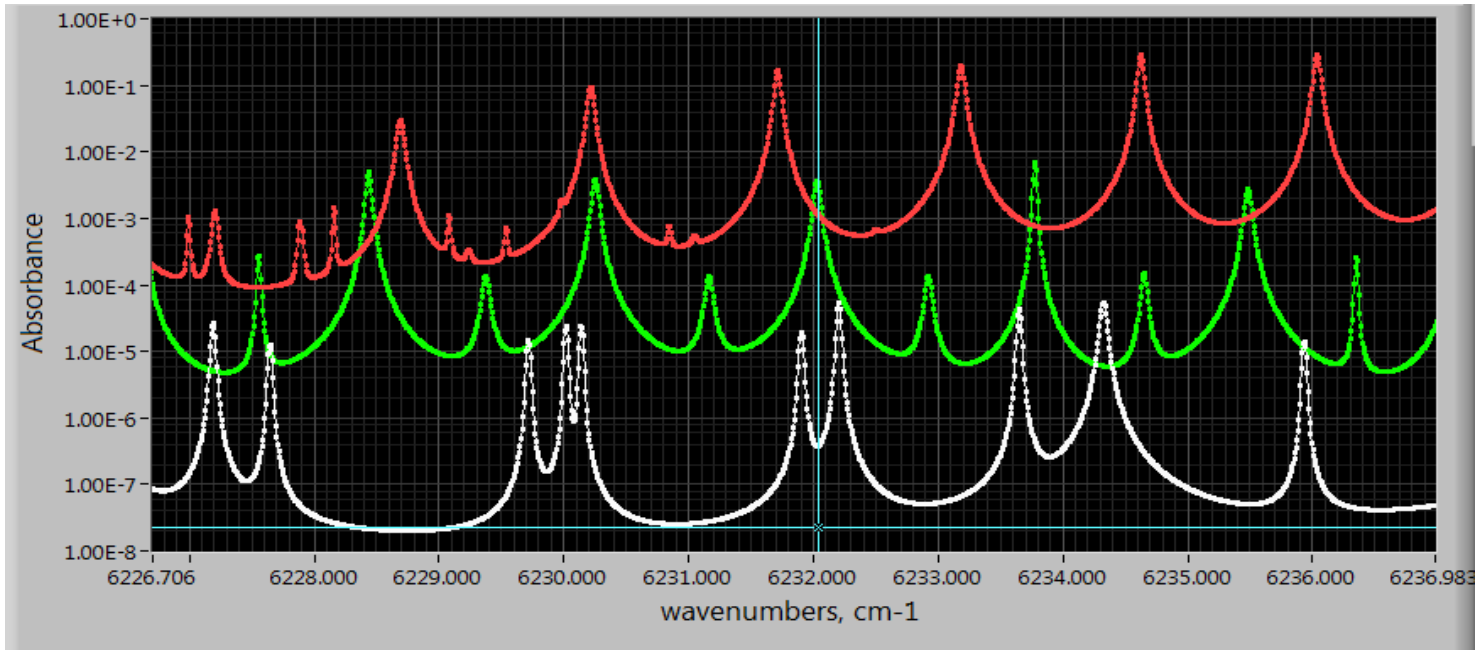
$^{12}CO_2$ =300 ppm (red), $^{13}CO_2$ =30 ppm (green), H_2O =1% (white), L=15 m, P=1 atm.



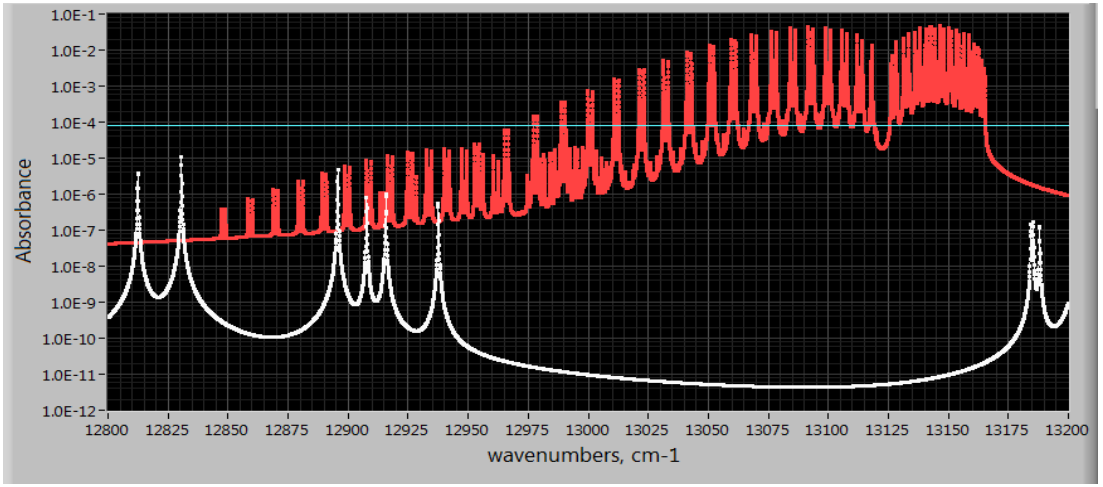
$^{13}CO_2$ /$^{12}CO_2$ -ratio measurements in 1.6 μ



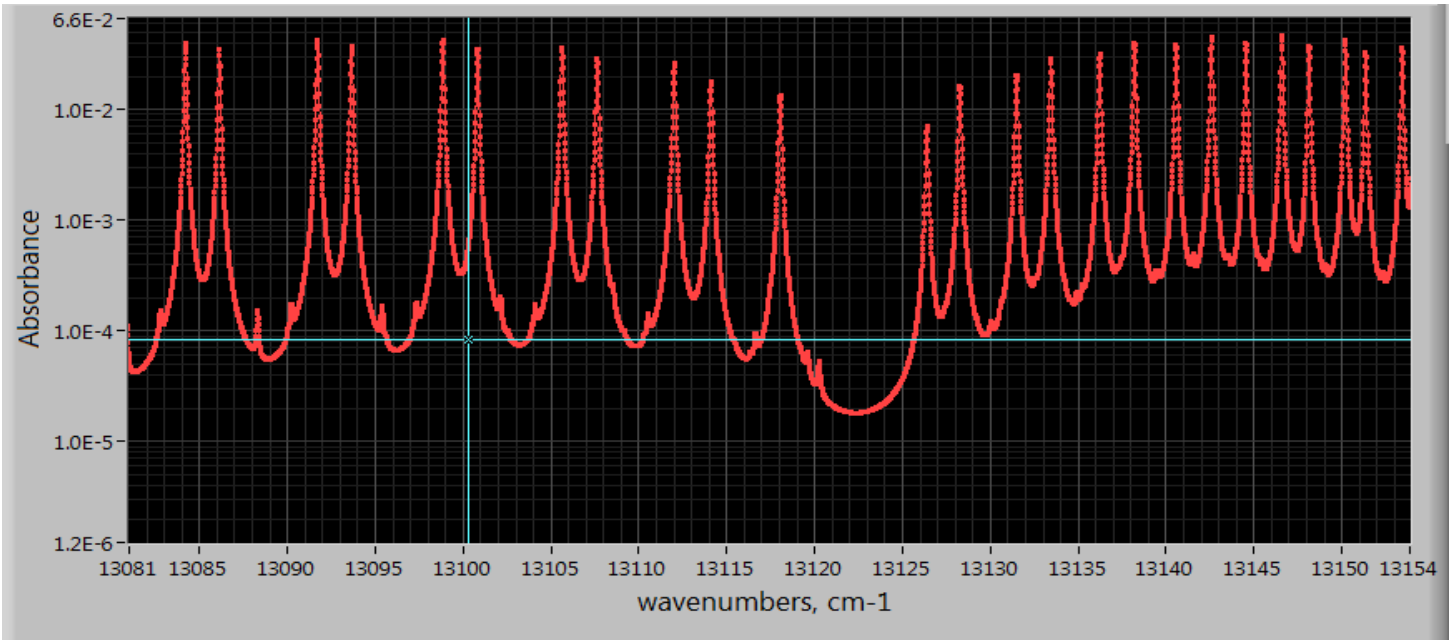
$^{12}CO_2$ =4% (red), $^{13}CO_2$ =0.4% (green), H_2O =3% (white), L=39 m, P=0.13 atm.



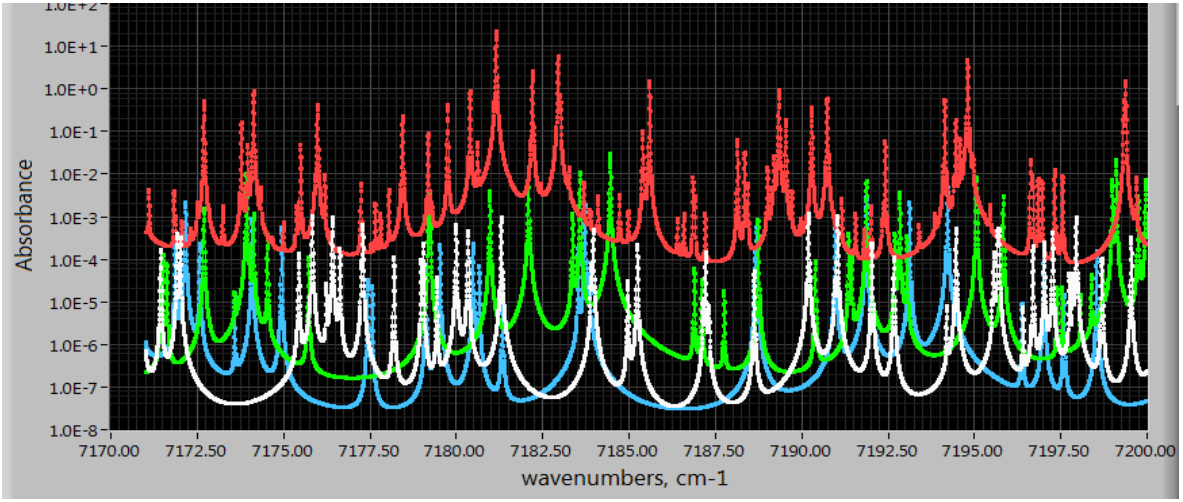
O_2 detection in 0.76 μ



O_2 =20 % (red) , H_2O =1 % (white), L=2 m, P=1 atm.

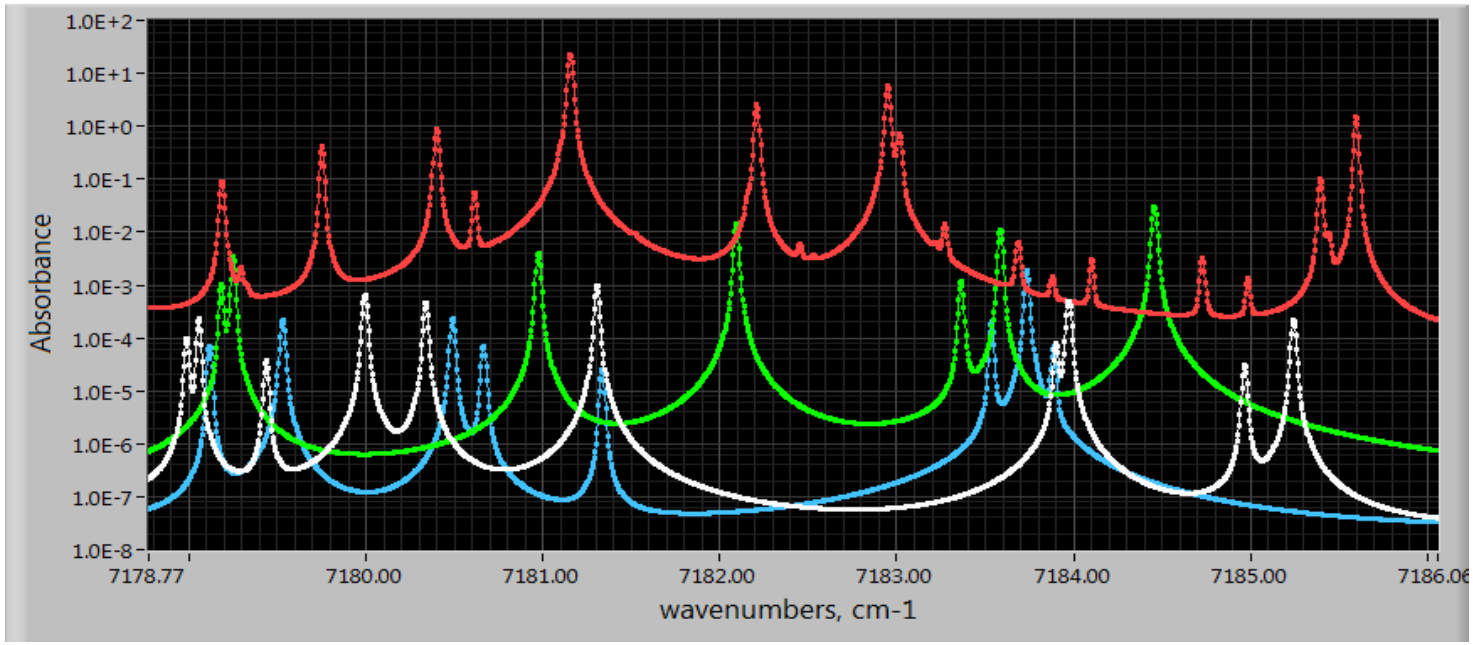


Accurate H_2O isotope analysis in 1.39 μ



$H_2{}^{16}O$ - red , $H_2{}^{18}O$ - green, $H_2{}^{17}O$ – blue, HDO – white.

P_{H2O} =7 Torr, L=200 cm



Conclusion

Software “Line-by-line” was develop to simulate spectra of different molecules in near and mid IR spectral ranges where commercially available diode lasers operate. Simulation takes less than 1 min. Some examples are presented. Simulation was performed for spectral ranges of operation for more than 50 NEL, Anritsu, Vertilas, Laser Components, and Nano Plus DLs available at GPI. Simulation results are using to select analytical line for particular DL for different applications. Some examples will be presented in poster.

Now similar simulation and analysis are performing before DL ordering.

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