LA-UR-12-25548
Approved for public release; distribution is unlimited.

Title: Remote Detection of NO2 Stable Isotopes

Author(s): Clegg, Samuel M.
Nowak-Lovato, Kristy Lynne
Fessenden-Rahn, Julianna E.
Obrey, Stephen J.
Currier, Robert P.

Intended for: Program Meeting at PNNL

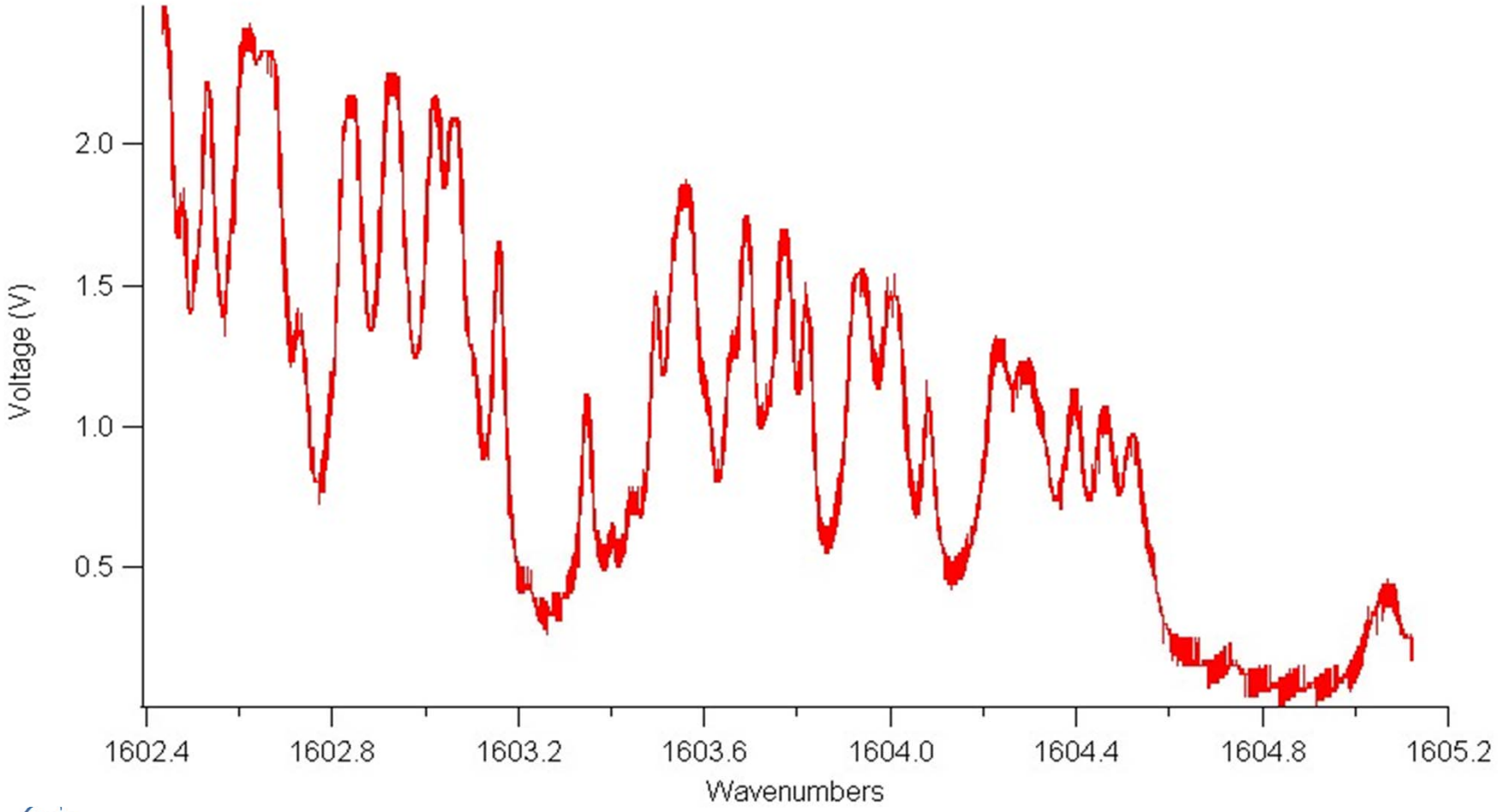
Remote Detection of NO_2 Stable Isotopes

Sam Clegg, Kristy Nowak-Lovato, Julianna Fessenden, Robert Currier and Steven Obrey

Los Alamos National Laboratory

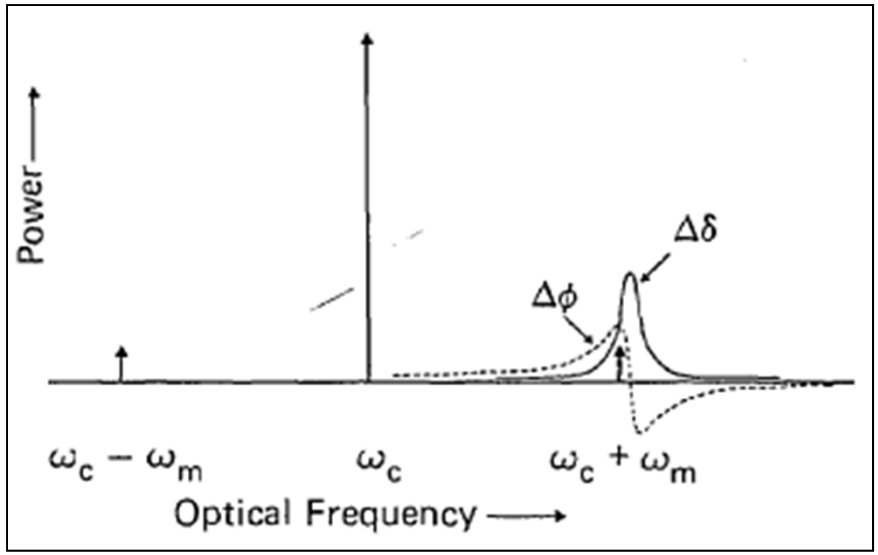
October 17-18, 2012

$^{15}NO_2$ Spectrum

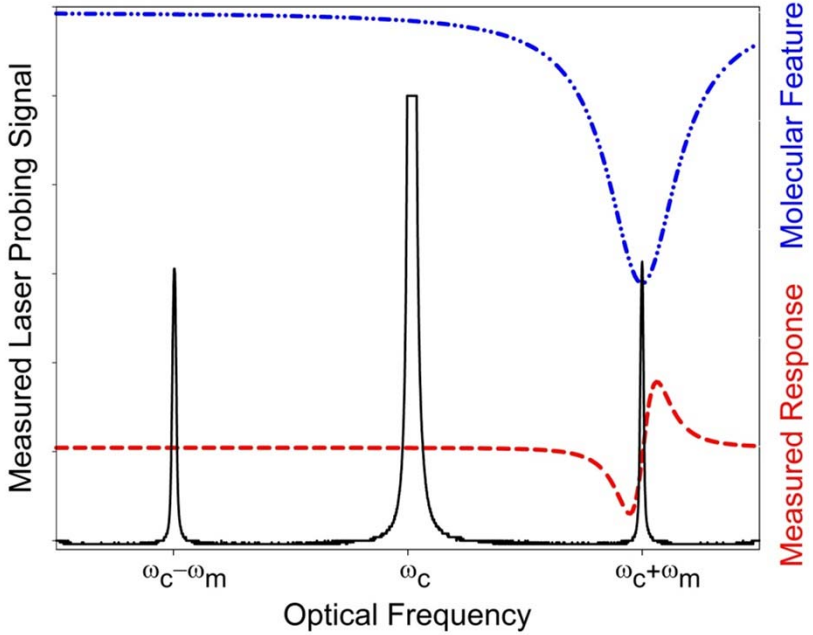


Fundamental FMS

From G.C. Bjorklund Optics Letters, 5, 15, 1980



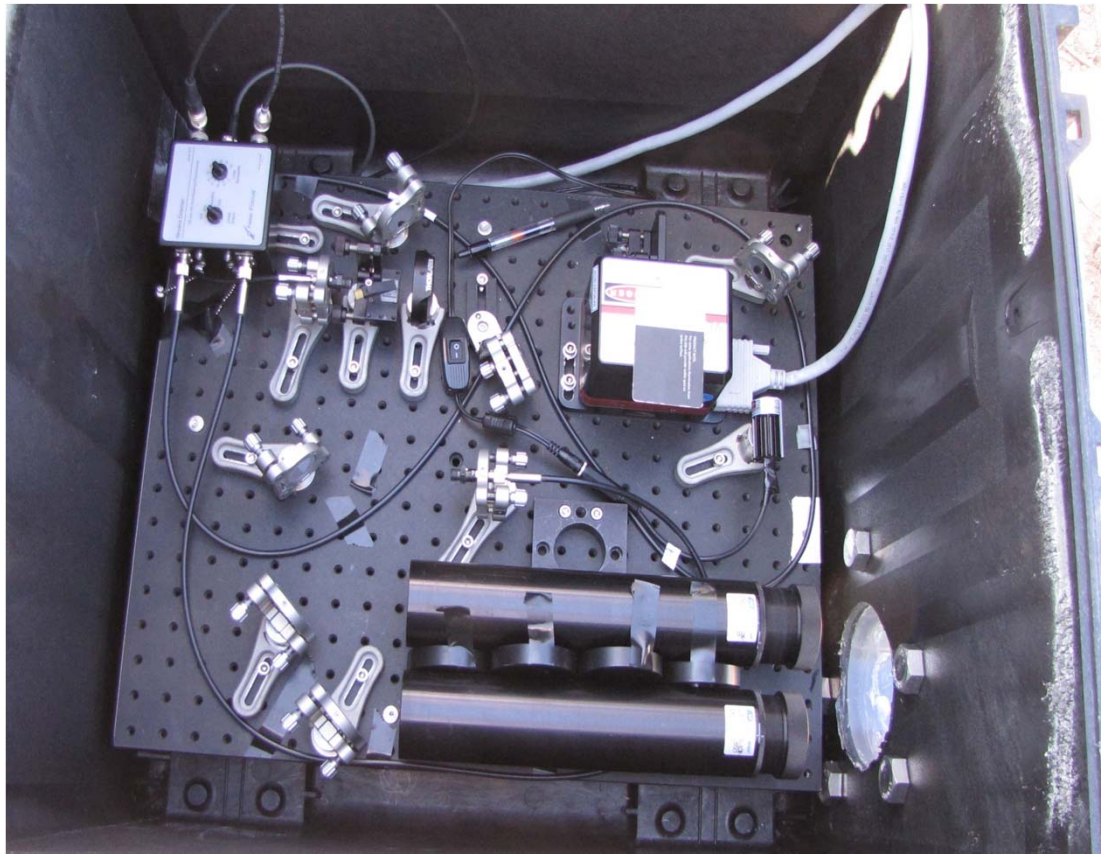
From LANL in situ instrument

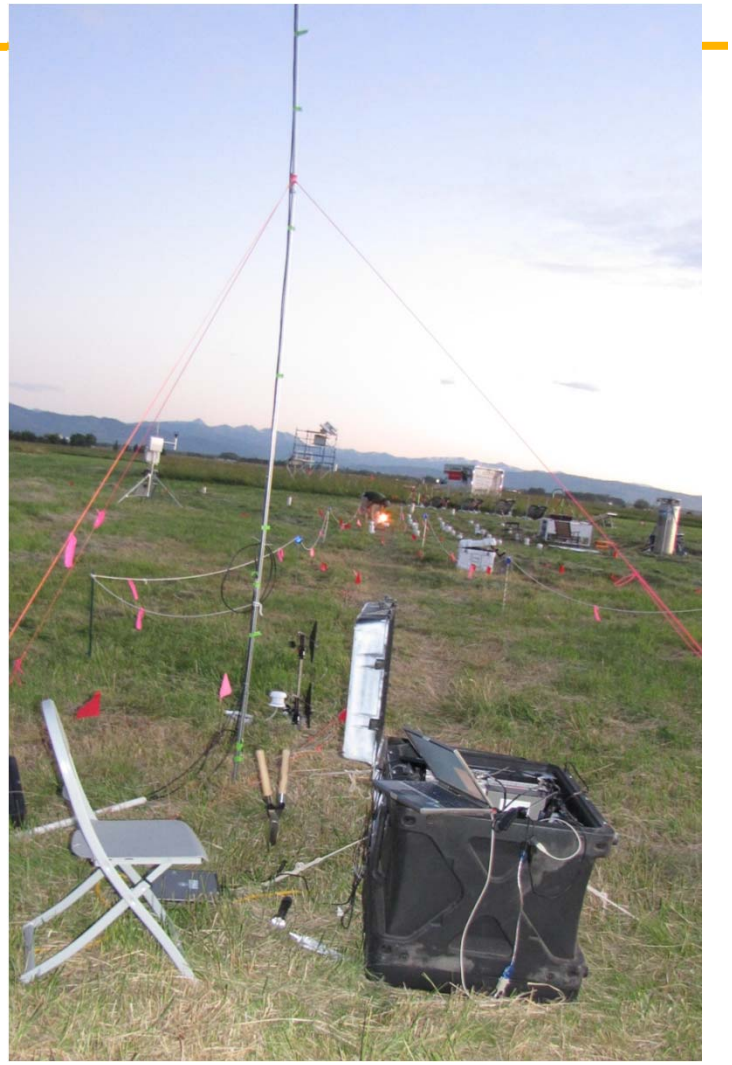


ω_c = 1607 nm

ω_m = ±2 GHz

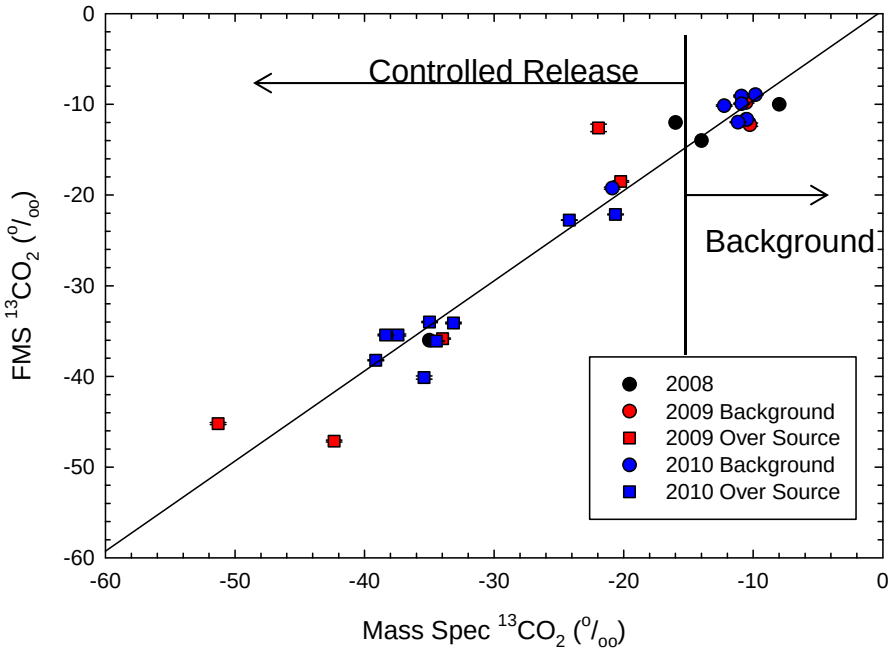
LANL – FMS Program





CO_2 FMS Field Results

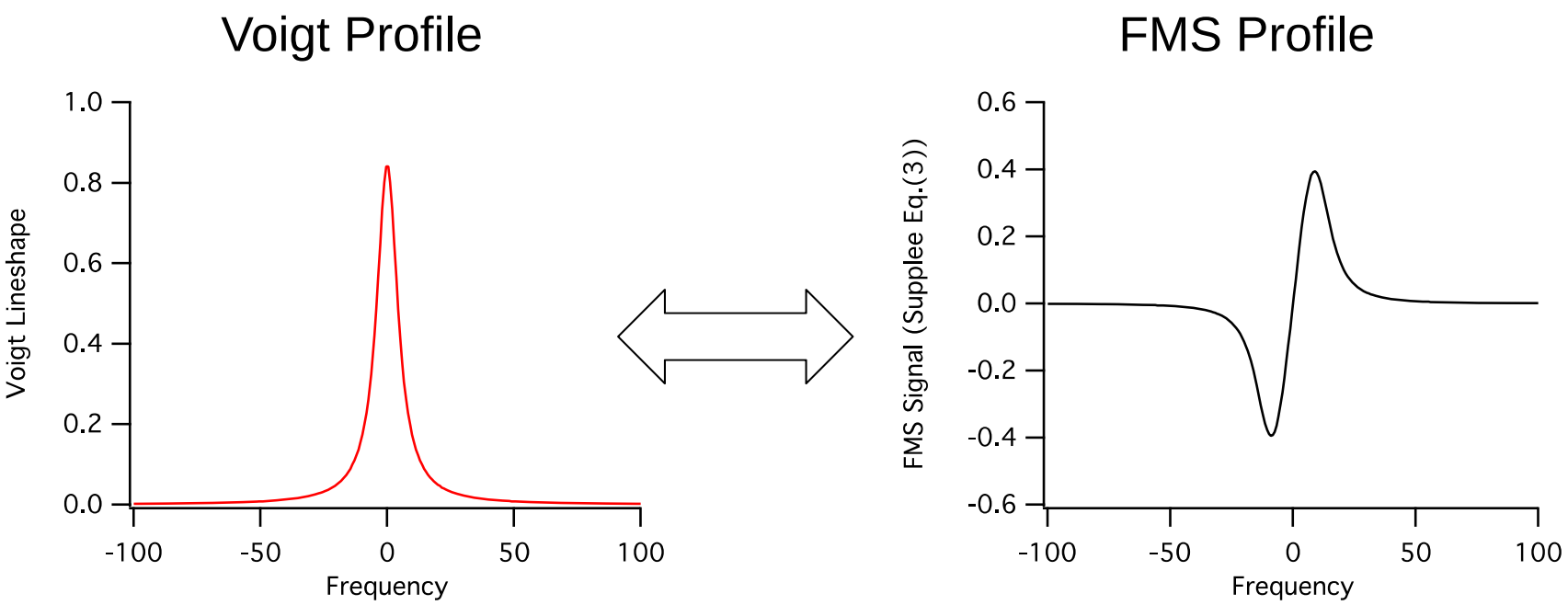
In Situ Field Results



Background = -8 to -11$^o/_{oo}$

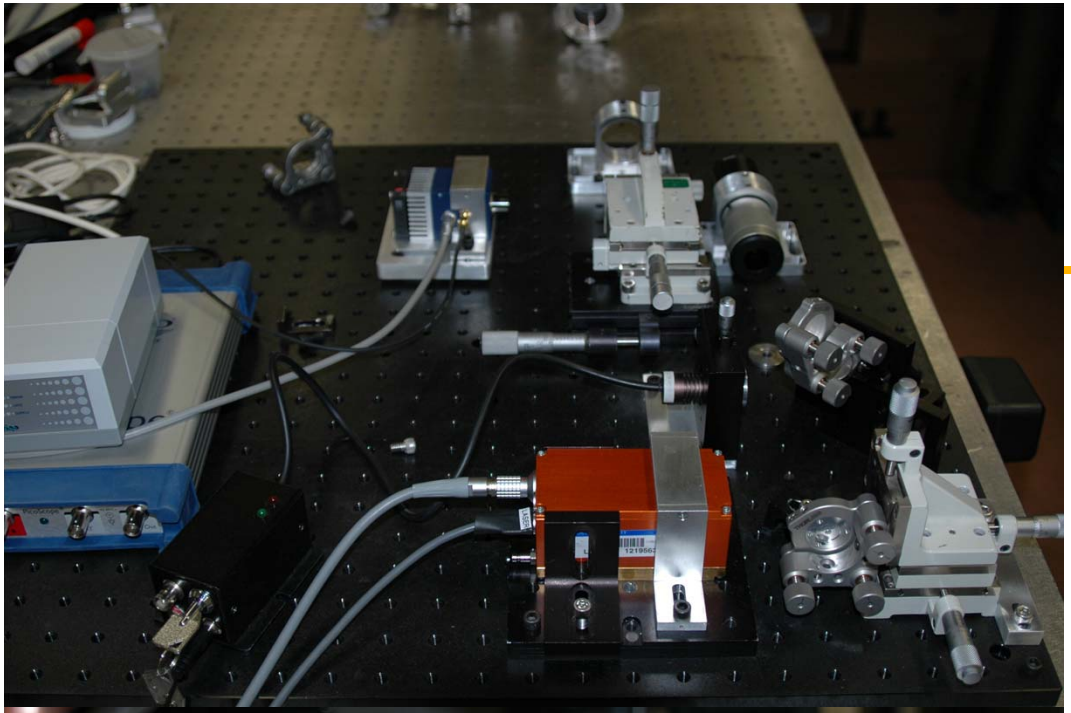
Seepage < -15$^o/_{oo}$

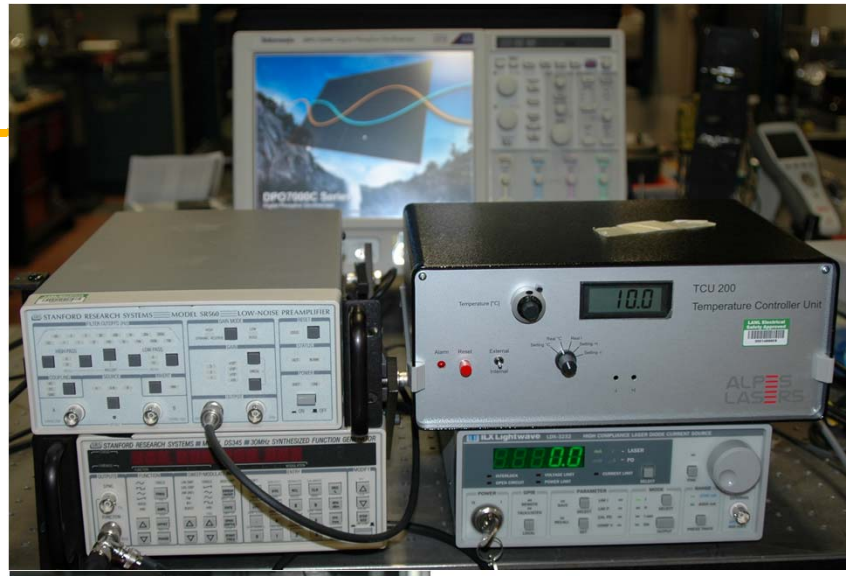
FMS Forward-Backward Modeling

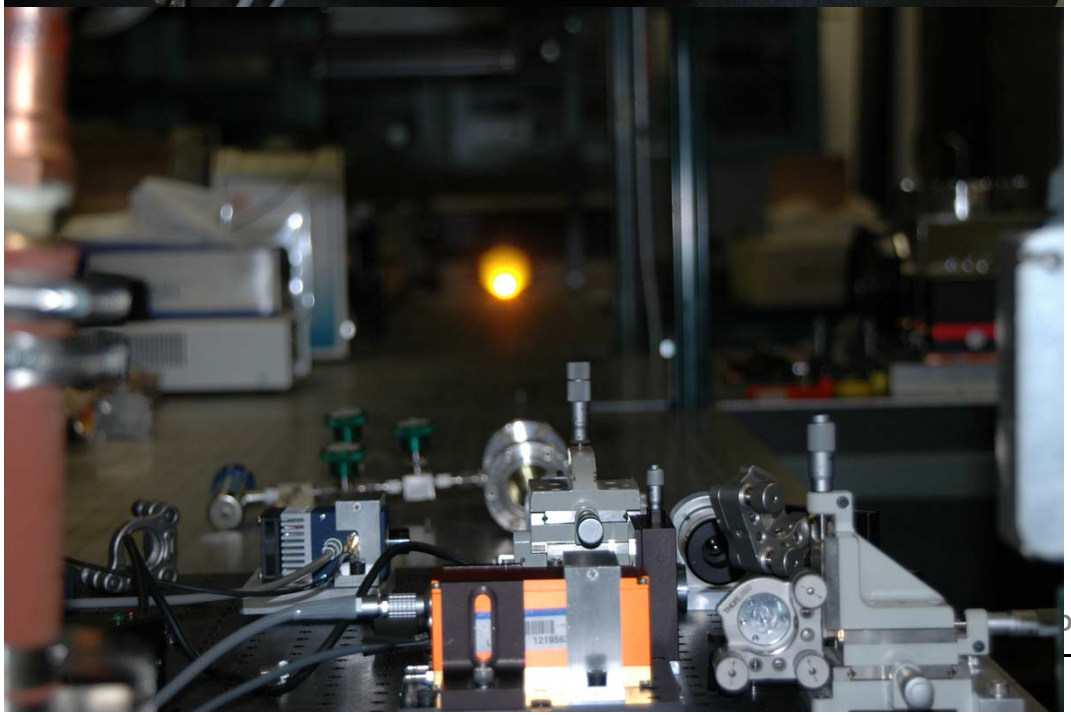


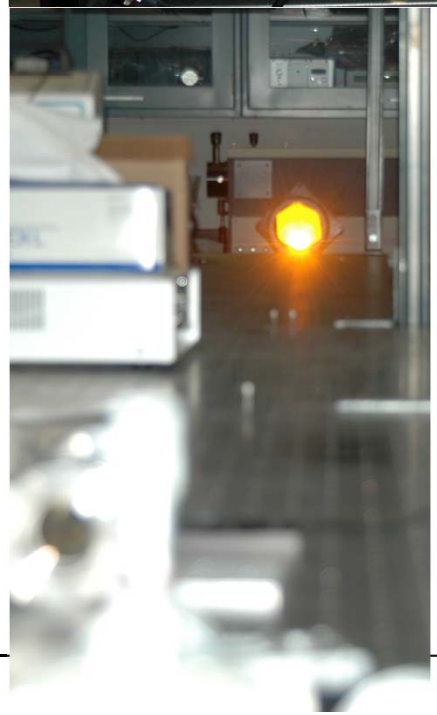
Voigt Profile accounts for both Temperature and Pressure Line Width

The Model Code was included in the 4th Quarter Report




STANFORD RESEARCH SYSTEMS MODEL SR560 LOW-NOISE PREAMPLIFIER
10.0
TCU 200
Temperature Controller Unit





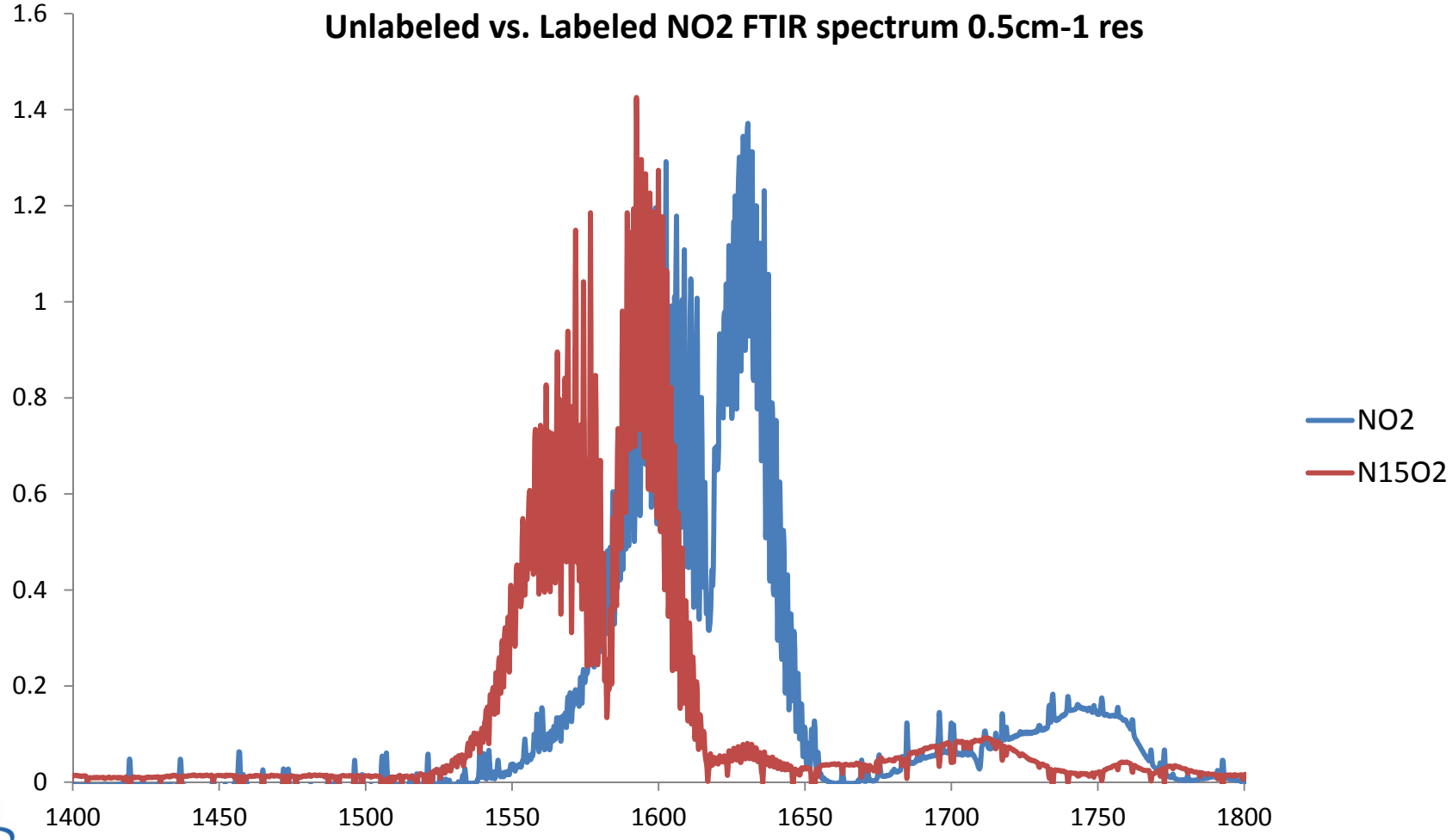
$^{14}NO_2$ and $^{15}NO_2$ Synthesis

$^{x}HNO_3 + HgO \rightarrow Hg(^{x}NO_3)_2$ Eq. 1

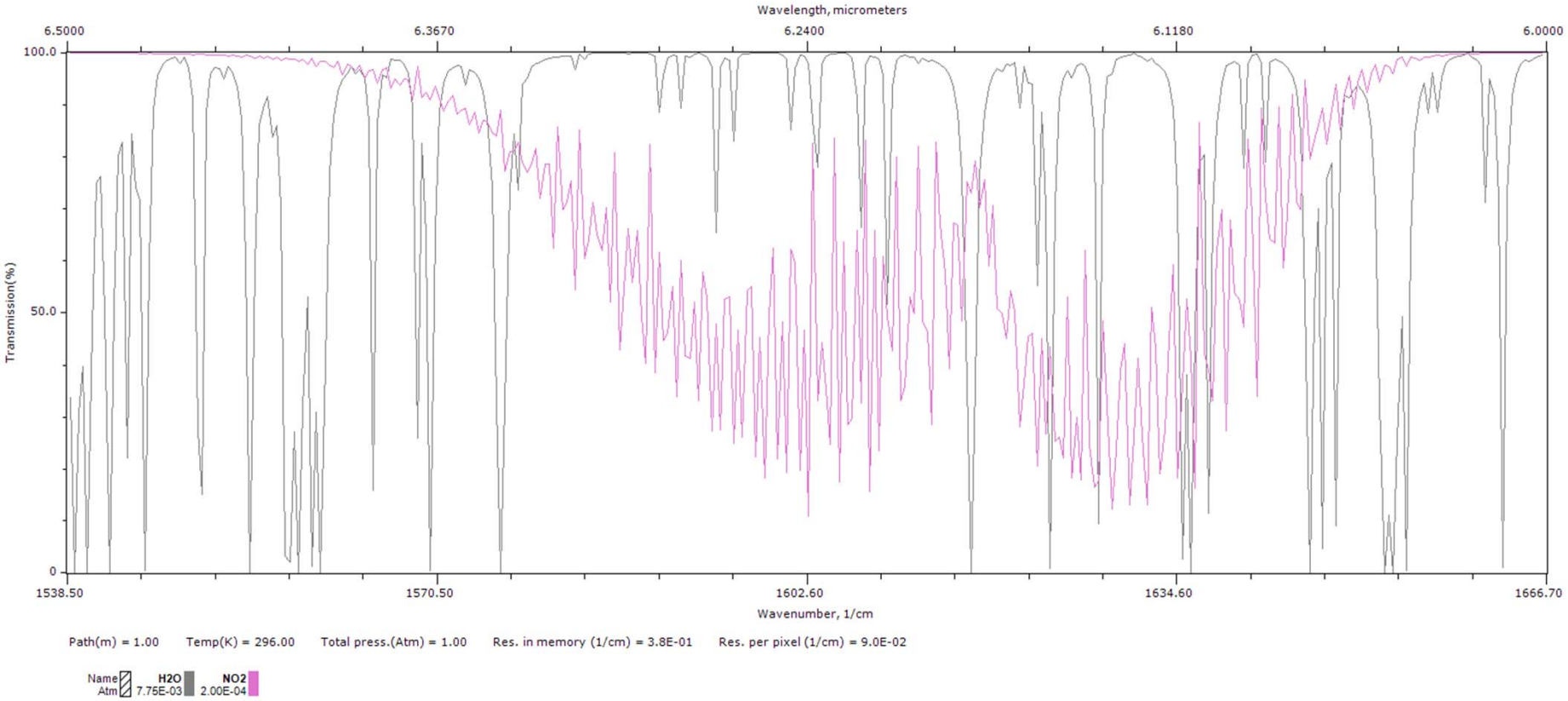
$Hg(^{x}NO_3)_2 + \text{heat} \rightarrow HgO + {}^{x}NO_2 + O_2$ Eq. 2

x = 14 or 15

FTIR Validation of Synthesized NO2



NO_2, H_2O Transmission Spectrum



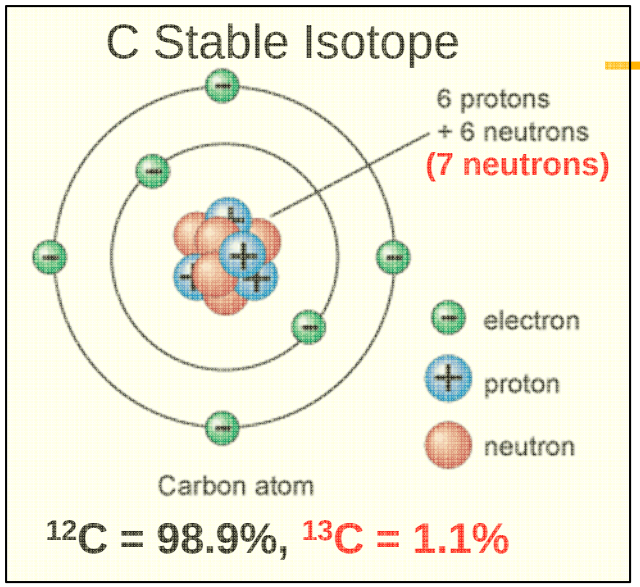
H_2O here is NOT a Problem!

Summary

- **Built and Tested a FMS Instrument**
  - Ready for Field Tests
- **Completed FMS Backward – Forward Model**
  - Determine the Concentration of a Species given the FMS Trace
  - Predict FMS Signal from a Sample for a given Instrument Setup
- **Successfully Synthesized $^{14}NO_2$ and $^{15}NO_2$.**
- **Obtained FMS and Absorption Spectra of neat and mixtures of $^{14}NO_2$ and $^{15}NO_2$.**
- **Determined that Atmospheric Water will not Interfere with the $^{14}NO_2$ and $^{15}NO_2$ Measurement.**

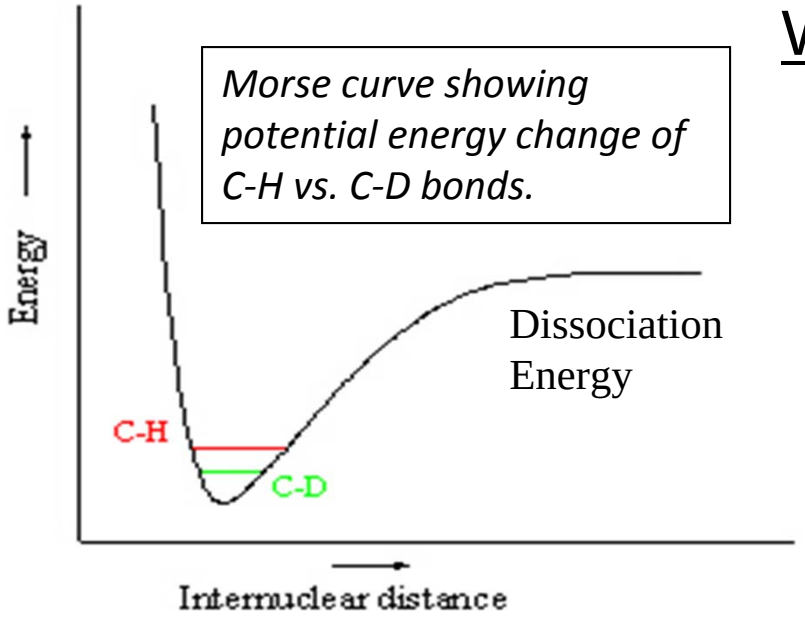
Backup

Stable Isotopes – Theory of Signature



Stable Isotopes:

- exist in all molecules
- exist as ratio of heavy/light: R = $^{15}N/^{14}N$
- chemical fingerprint (unique)
- not radiogenic/long lived



Morse curve showing potential energy change of C-H vs. C-D bonds.

Why Signature Exists?:

- fractionation in chemical reactions
- partition into reactants/products
- due to bond strength differences