Rotational Raman scattering

(Air, breath, H_2, D_2)

Date: 04-21-2016

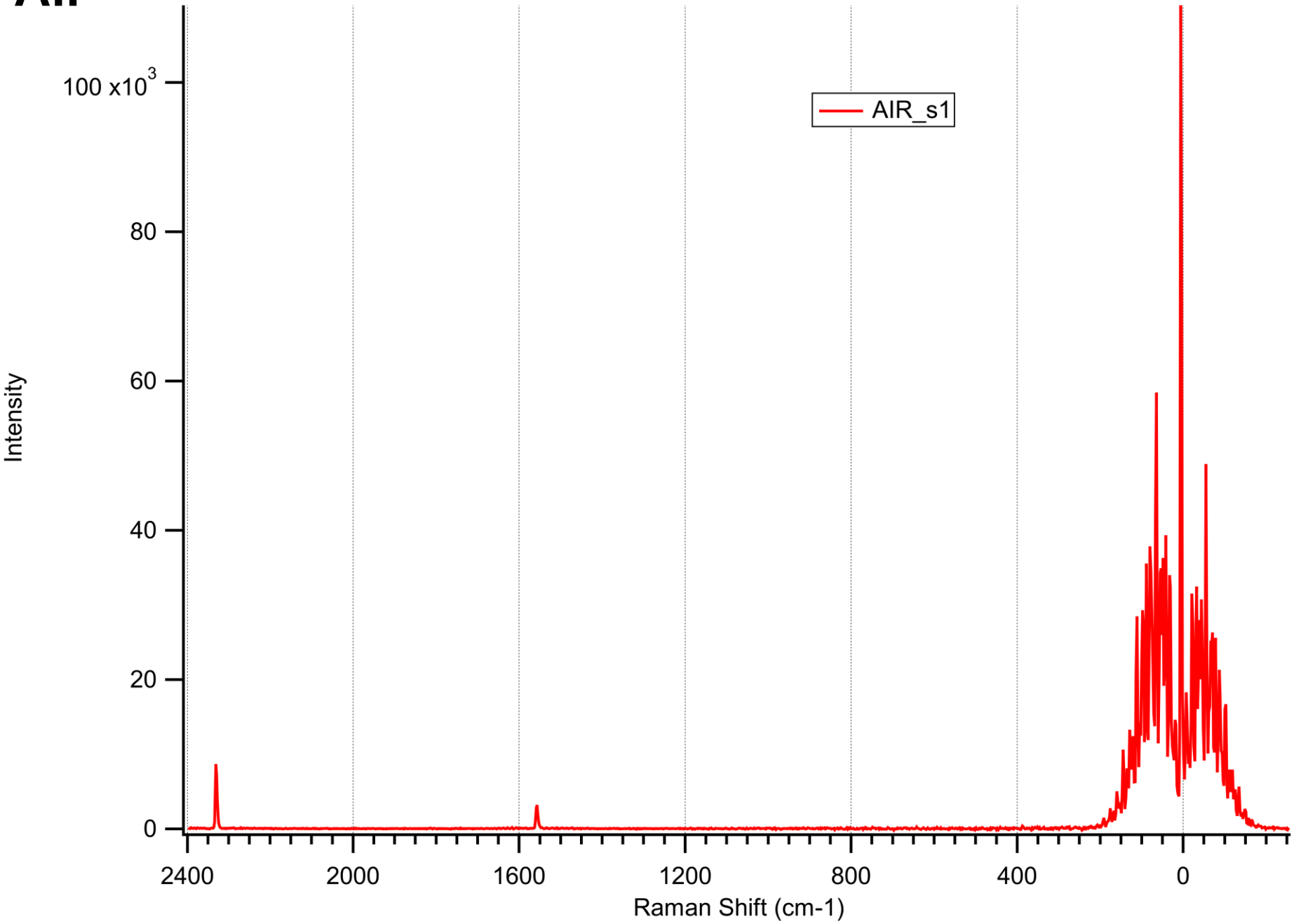
Experimental details

Measurements using gas-cell
(cell was evacuated before each measurement)

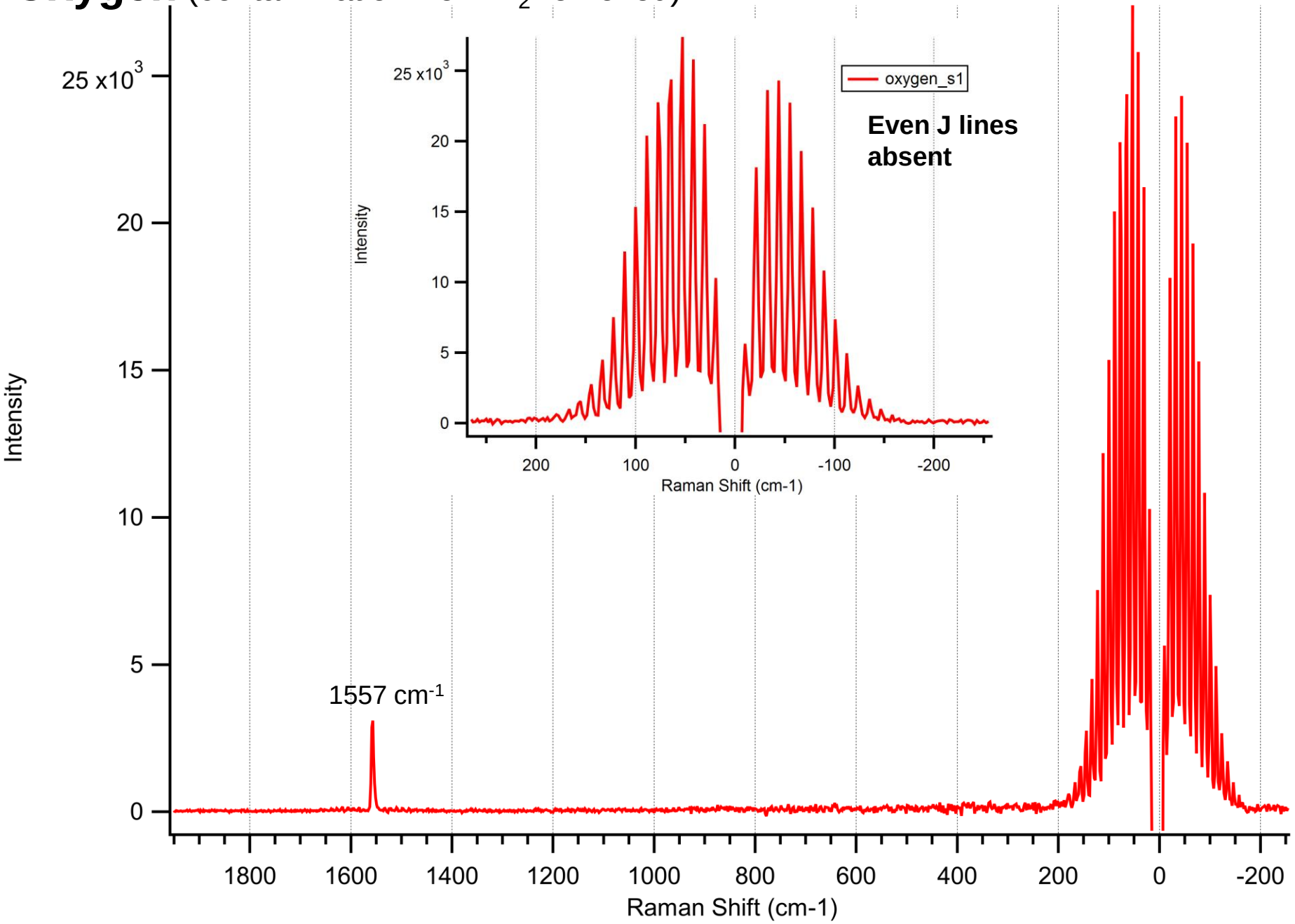
532 nm, 225 mW at sample point
Objective: 20x, 25mm Working distance
600 grooves/mm grating , Slit: 120µm
(spectral range : -250 cm^{-1} to 2400 cm^{-1})

Samples:
Air
Oxygen
Breath (all students)
Hydrogen
Deuterium

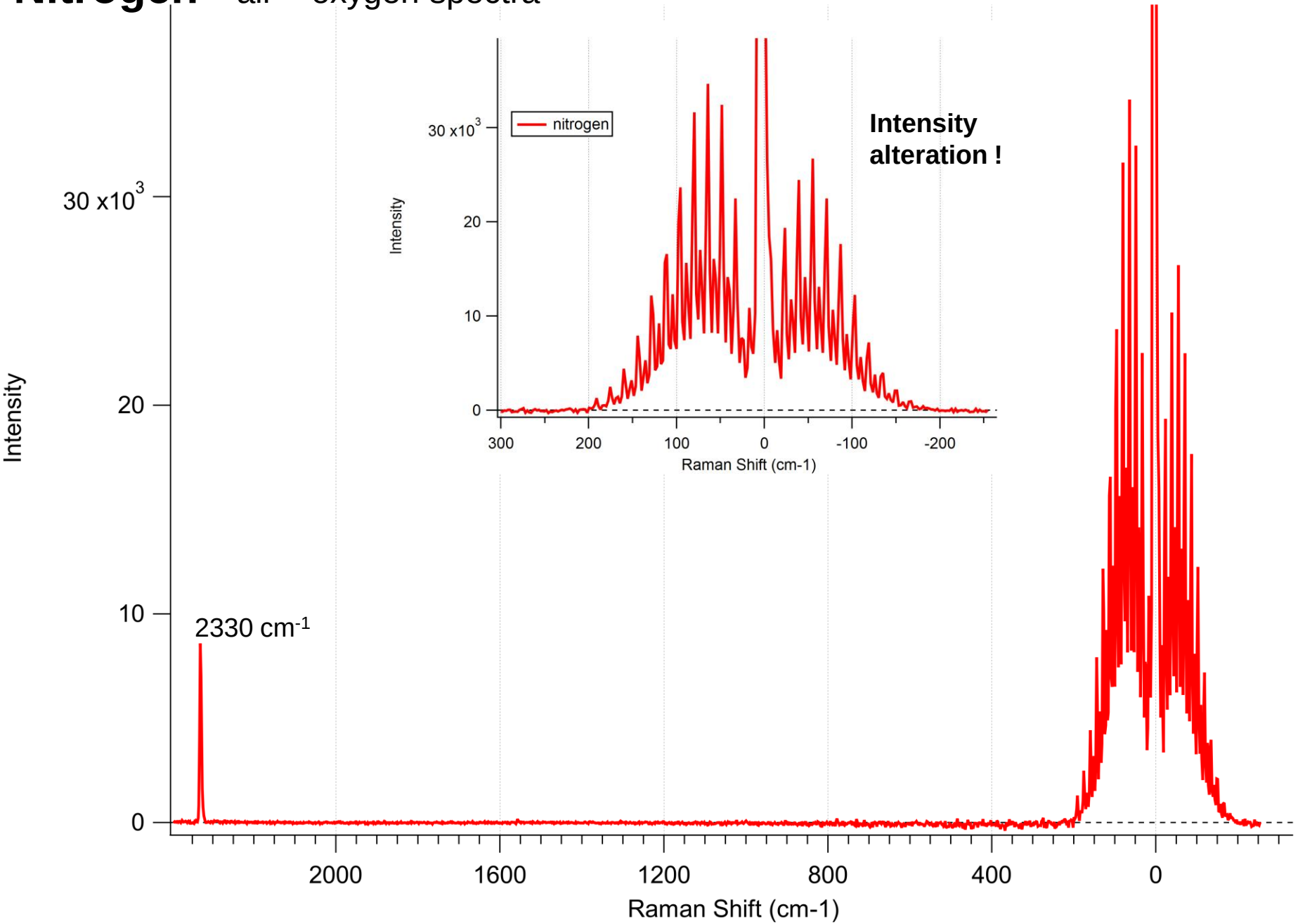
Air


100 x10^3
80
60
40
20
0
Intensity
AIR_s1
2400
2000
1600
1200
800
400
0
Raman Shift (cm-1)

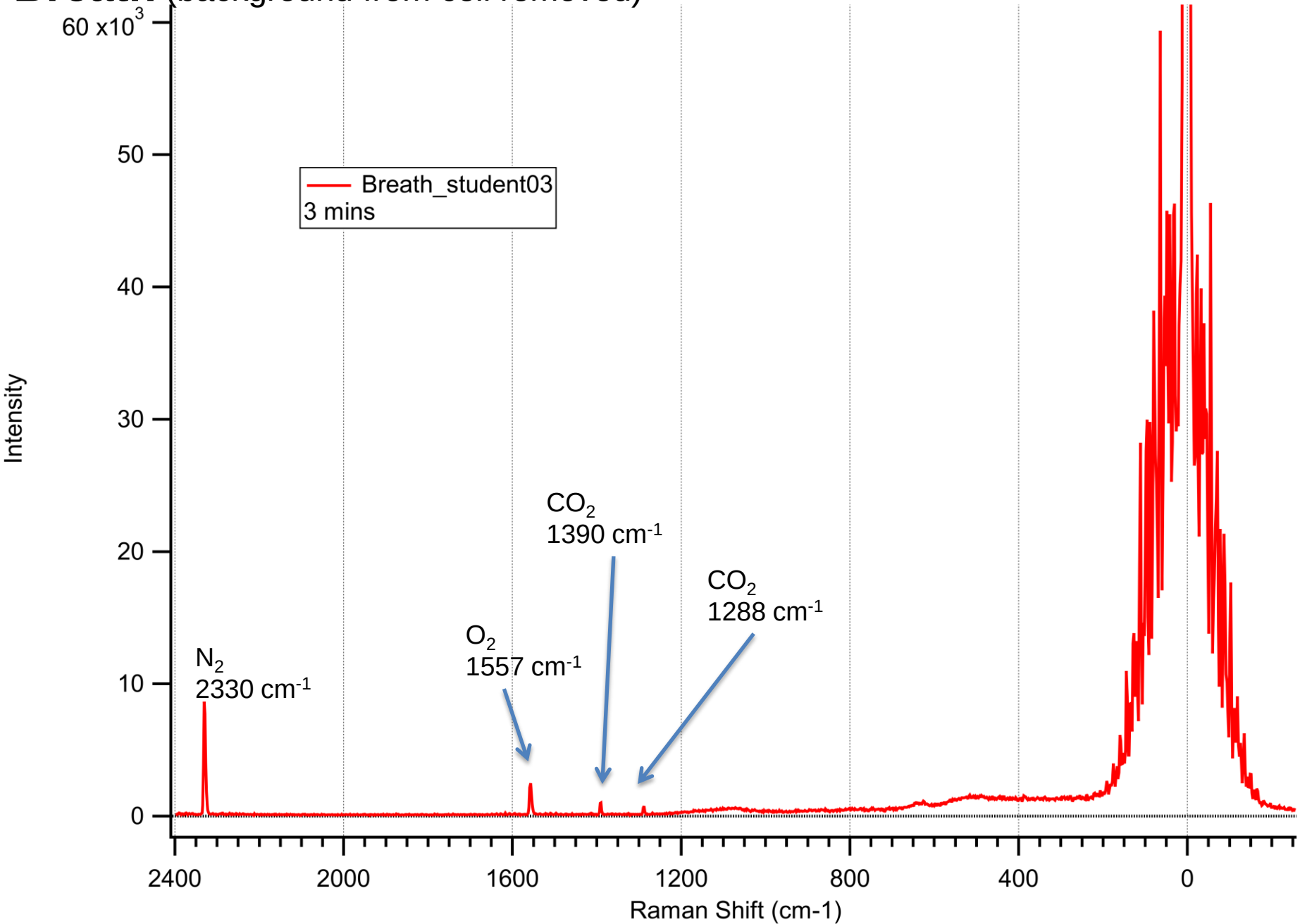
Oxygen (contamination from N_2 removed)



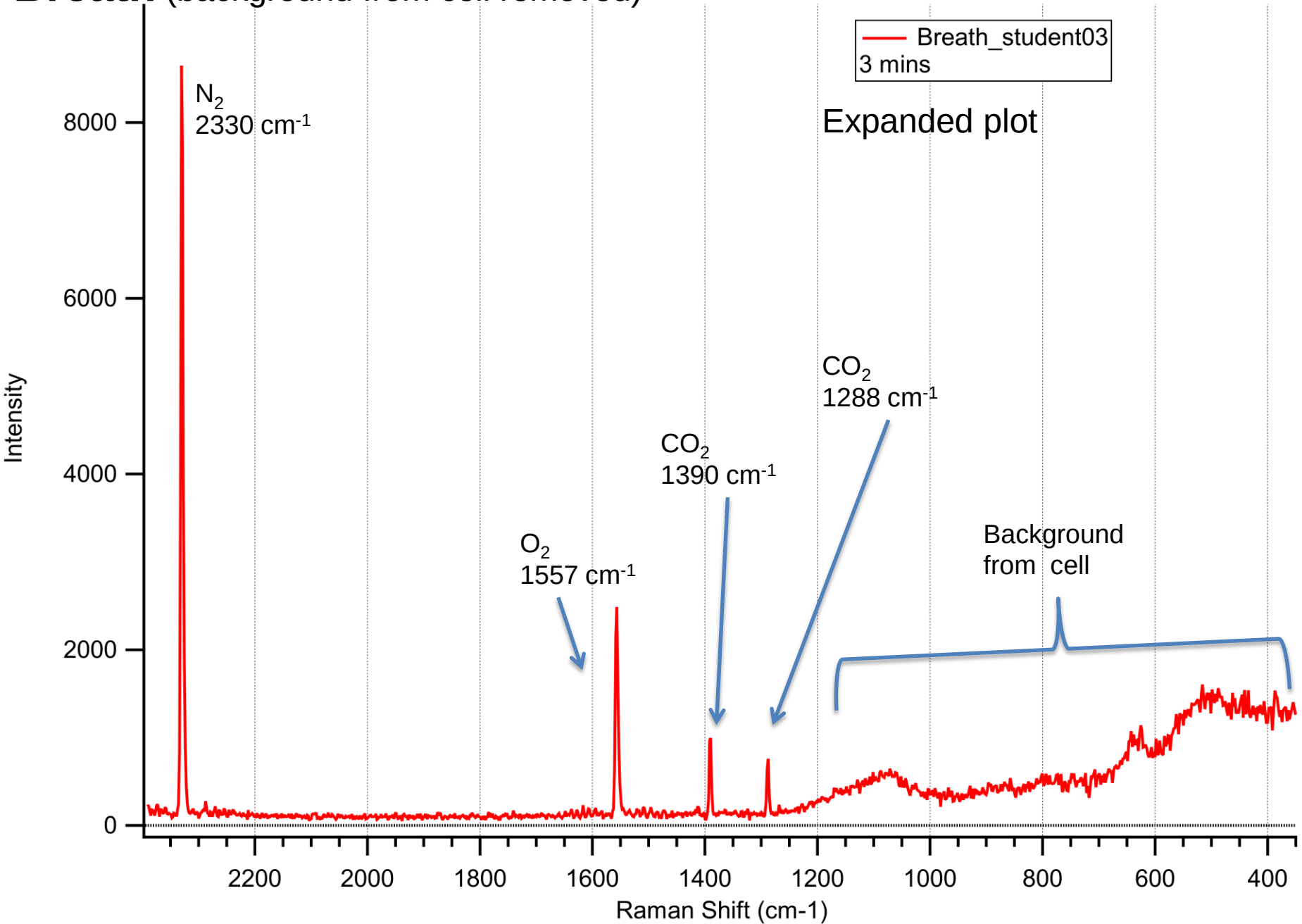
Nitrogen = air – oxygen spectra



Breath (background from cell removed)



Breath (background from cell removed)



Breath analysis

Vibrational-Raman peaks used for analysis

We observe oxygen, nitrogen and
CO_2 peaks simultaneously

Inhaled air
N_2 fraction = 78.08 %
O_2 fraction = 20.95 %
CO_2 fraction = 0.04%

Exhaled air
N_2 fraction = 78.08 % (stays constant)
O_2 fraction = decreases
CO_2 fraction = increases

Amount of nitrogen stays constant
All breath spectra normalized to the nitrogen peak (air).

Breath analysis

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From pure air;

$$\frac{I_{O_2}}{I_{N_2}} = \frac{\sigma_{O_2}}{\sigma_{N_2}} * \frac{(Concentration)_{O_2}}{(Concentration)_{N_2}} * \frac{[Population factor]}{[Population factor]} * \frac{D}{D}$$

From spectra

We need this

known

=1 (good approximation*)

$$\frac{\sigma_{O_2}}{\sigma_{N_2}} = 2.232 \text{ (fundamental vibration compared)}$$

* = Intensity correction using white light

In exhaled air

$$\frac{I_{O_2}}{I_{N_2}} = \frac{\sigma_{O_2}}{\sigma_{N_2}} * \frac{(Concentration)_{O_2}}{(Concentration)_{N_2}} * \frac{[Population factor]}{[Population factor]} * \frac{D}{D}$$

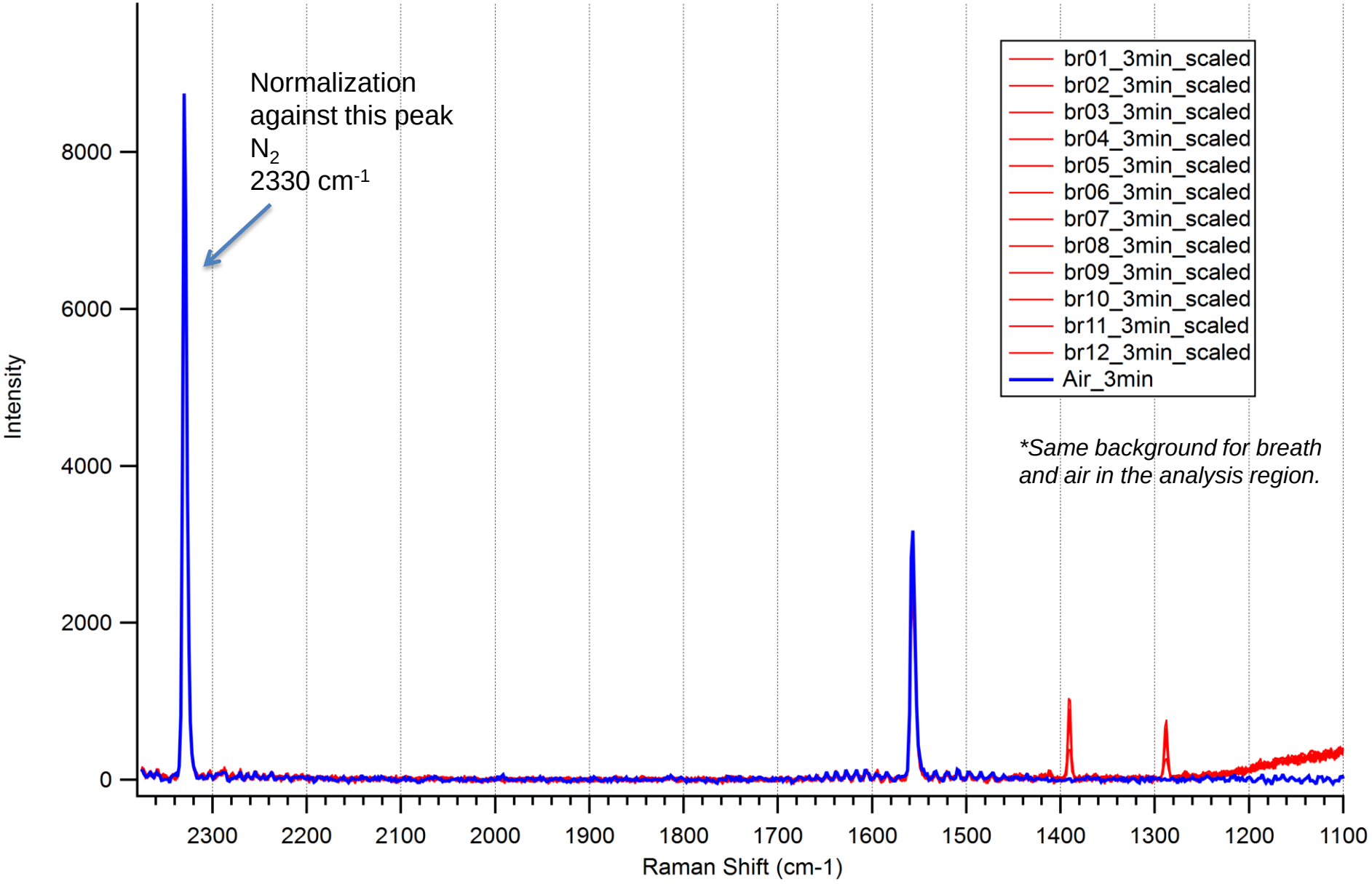
Calculated (from air spectra)

We can now find in exhaled air

=1 (good approximation*)

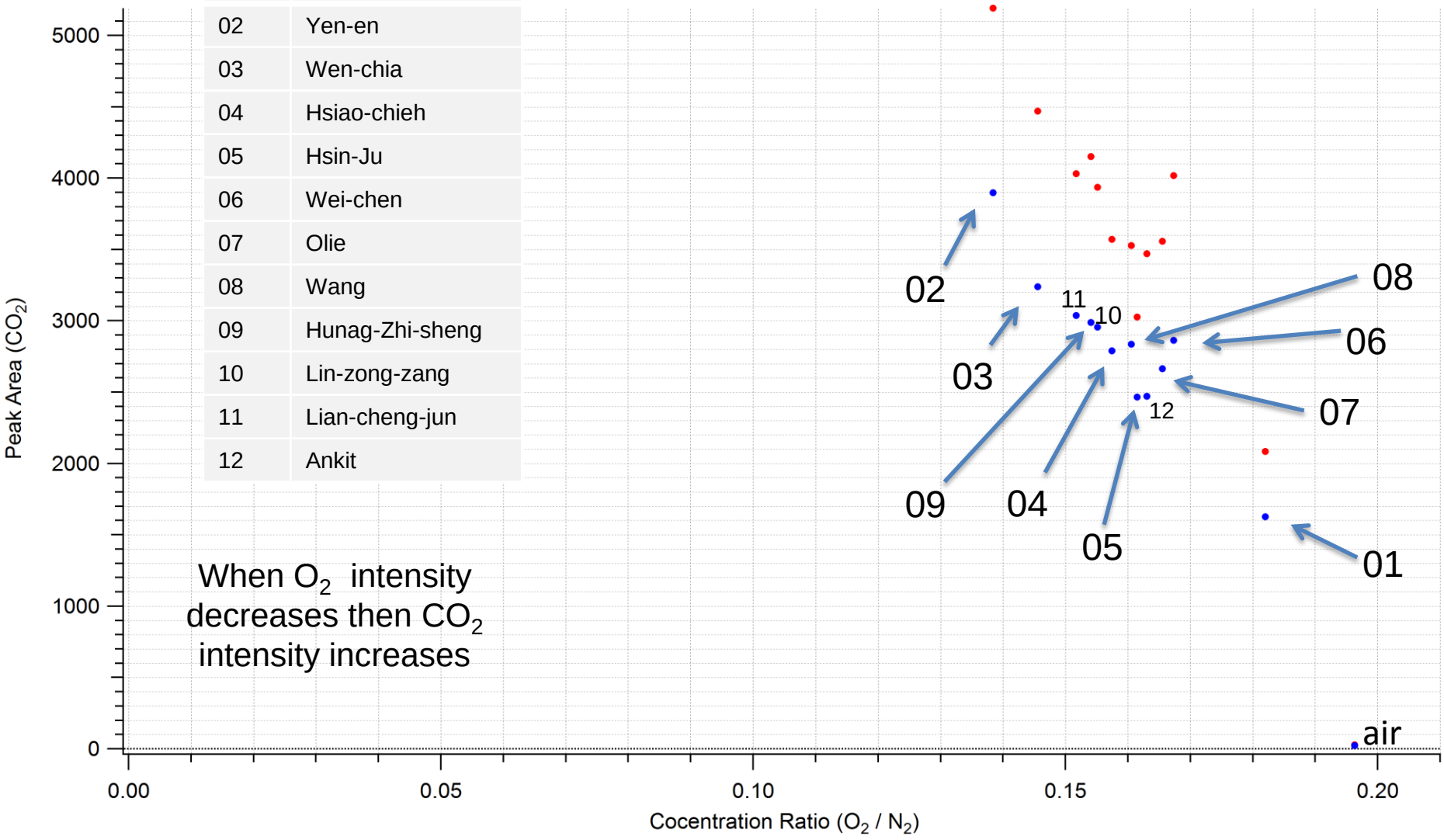
* = Intensity correction using white light

Breath = ($Breath_{raw}$) – (evacuated cell spectra) * (1.13695)



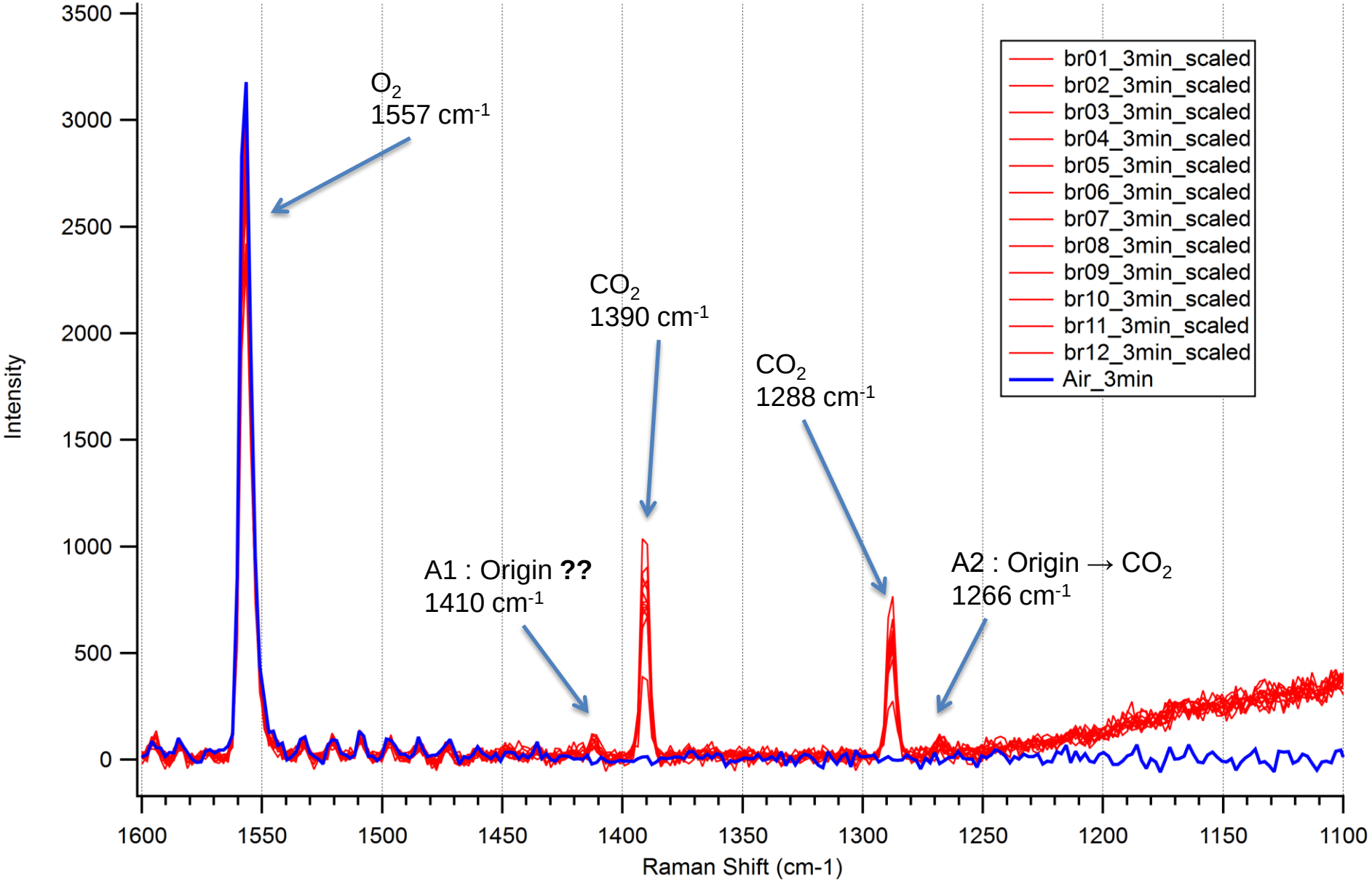
CO_2 peak area vs (O_2/N_2) concentration ratio

01	Chih-lin
02	Yen-en
03	Wen-chia
04	Hsiao-chieh
05	Hsin-Ju
06	Wei-chen
07	Olie
08	Wang
09	Hunag-Zhi-sheng
10	Lin-zong-zang
11	Lian-cheng-jun
12	Ankit

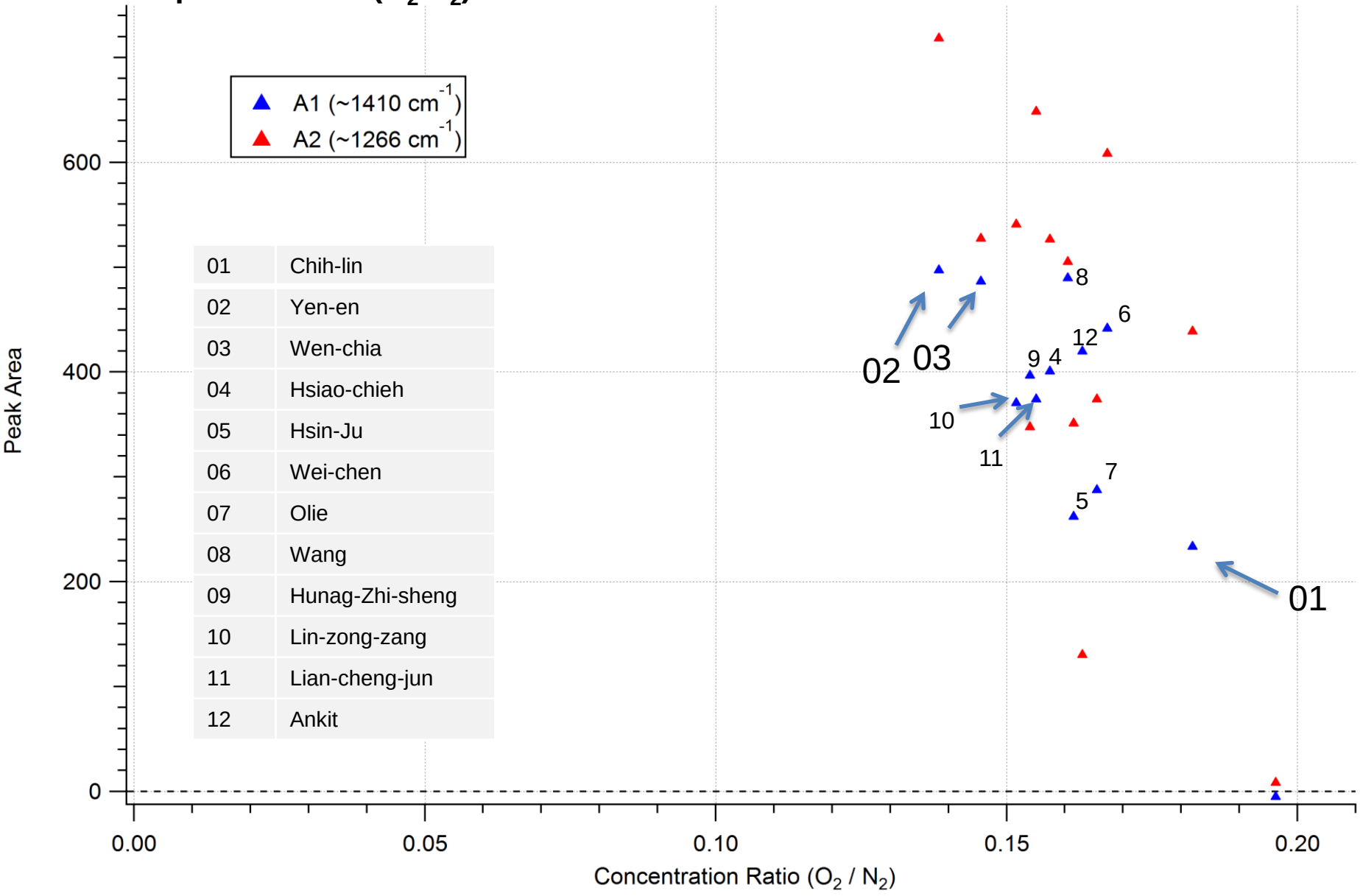


When O_2 intensity decreases then CO_2 intensity increases

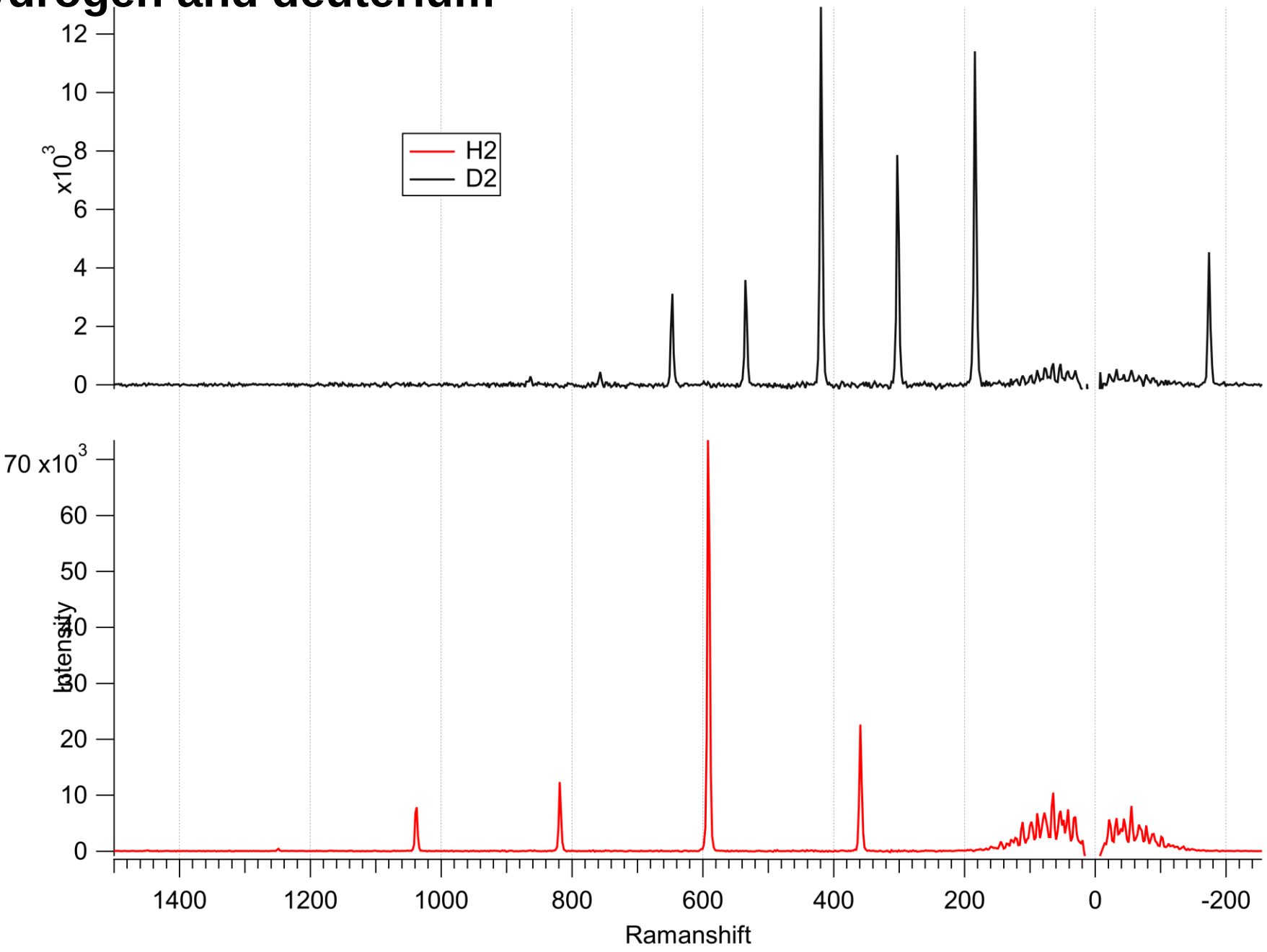
Zoomed-up spectra : fingerprint region



A1 and A2 peak area vs (O_2/N_2) concentration ratio



Hydrogen and deuterium



Bond length from rotational Raman spectra

Hydrogen

$$\text{Rotational Constant from spectra} = 59.8367 cm^{-1}$$

$$I_{H_2} = \frac{\hbar}{2B} = \frac{(1.0545 \times 10^{-34})^2 [J.s]^2}{2 * (59.8367 \times 1.9863 \times 10^{-23})[J]}$$

$$I_{H_2} = \frac{\hbar}{2B} = 4.678534 \times 10^{-48} [J.s^2] = 4.678534 \times 10^{-48} [kg.m^2]$$

$$r_{H_2} = \sqrt{\frac{I}{\mu}} = 74.794 \times 10^{-12} m$$

Similarly deuterium,

$$\text{Rotational Constant from spectra} = 30.683 cm^{-1}$$

$$r_{D_2} = \sqrt{\frac{I}{\mu}} = 73.875 \times 10^{-12} m$$