

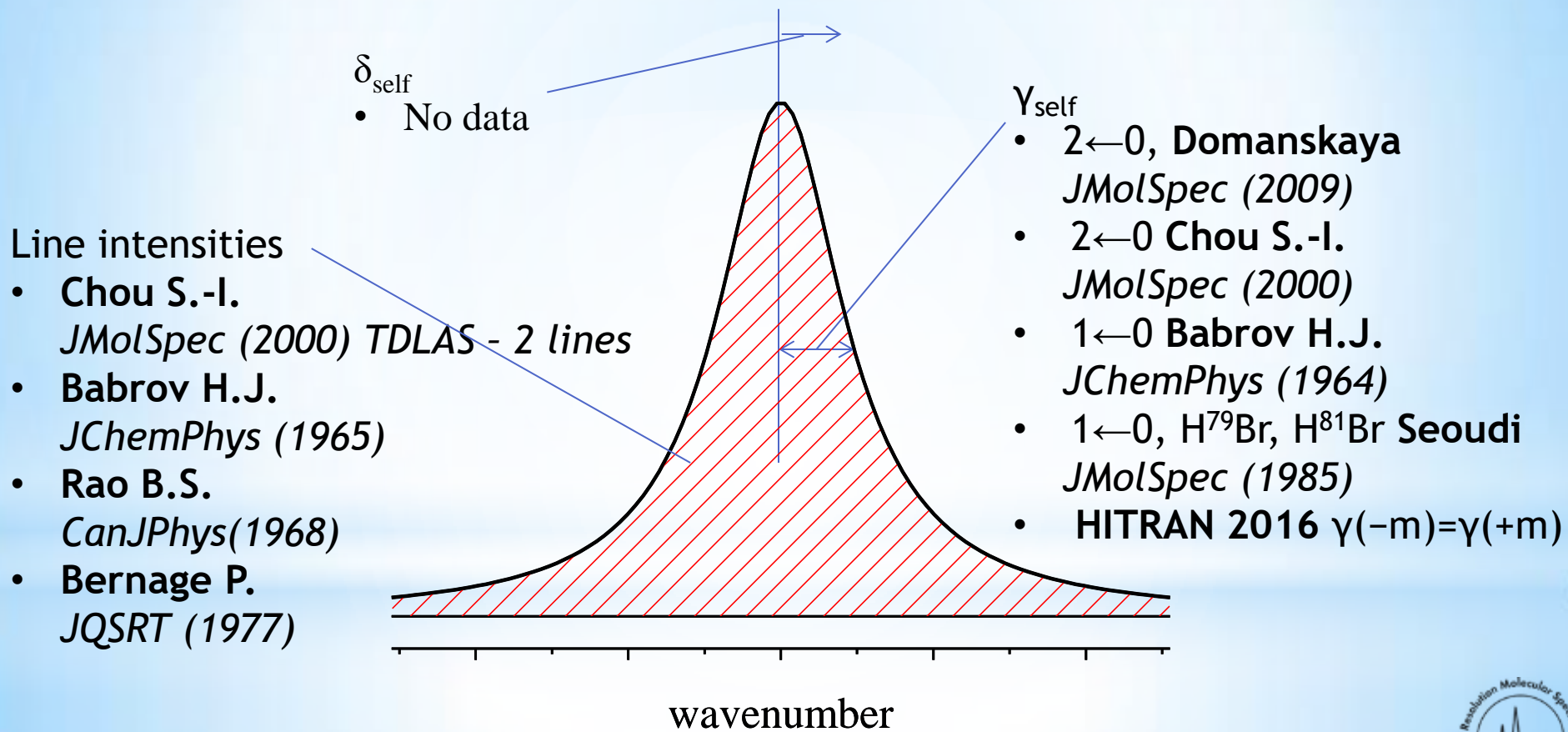
Self-perturbed rovibrational lines in the region of the first overtone of HBr. What I have learned from my mistakes

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HBr: molecule from HITRAN. The first overtone



Setup

An Instrument: Bruker IFS-120HR

$T = 24 \pm 1 \text{ } ^\circ\text{C}$

- Si/CaF₂ beamsplitter
- LN InSb detector
- tungsten lamp

A Resolution:

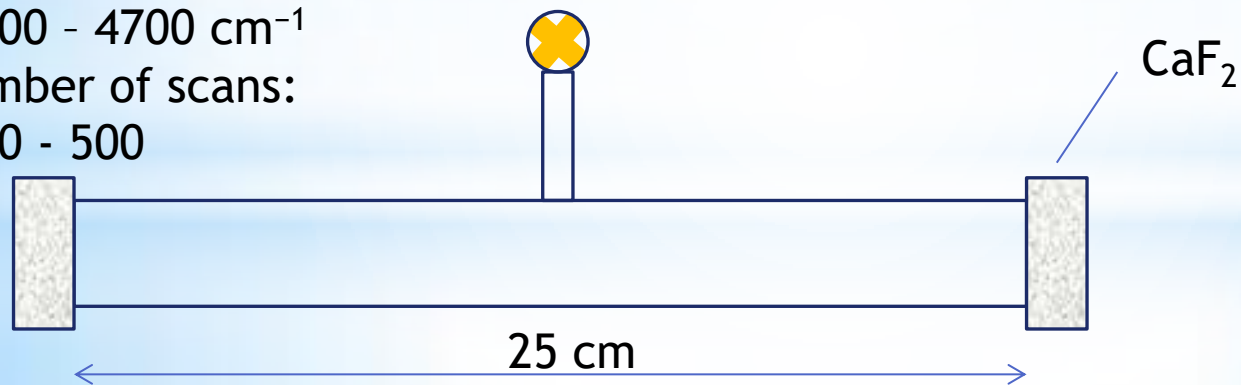
- 0.003 cm^{-1} (Aperture 0.8 mm) $p = 42 - 405 \text{ mbar}$
- 0.005 cm^{-1} (Aperture 1.0 mm) $p = 606 - 870 \text{ mbar}$

A Filter:

- $5100 - 4700 \text{ cm}^{-1}$

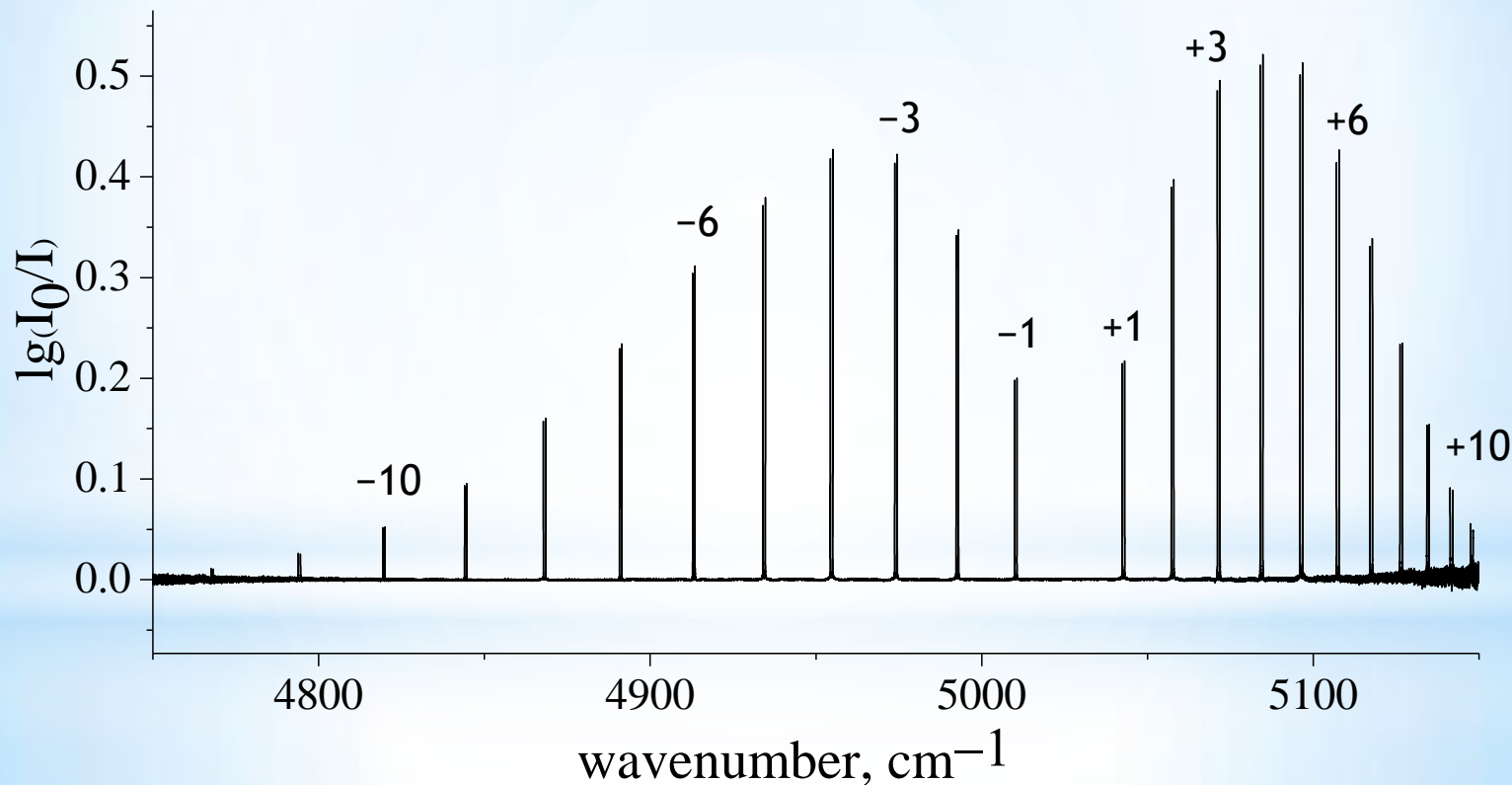
A Number of scans:

- 250 - 500

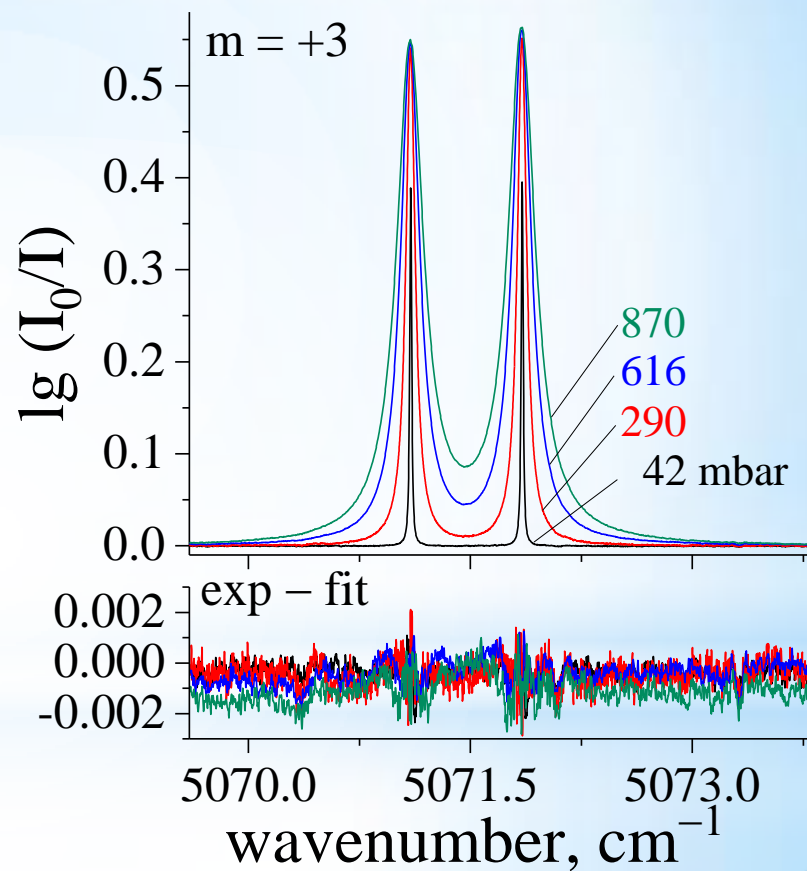
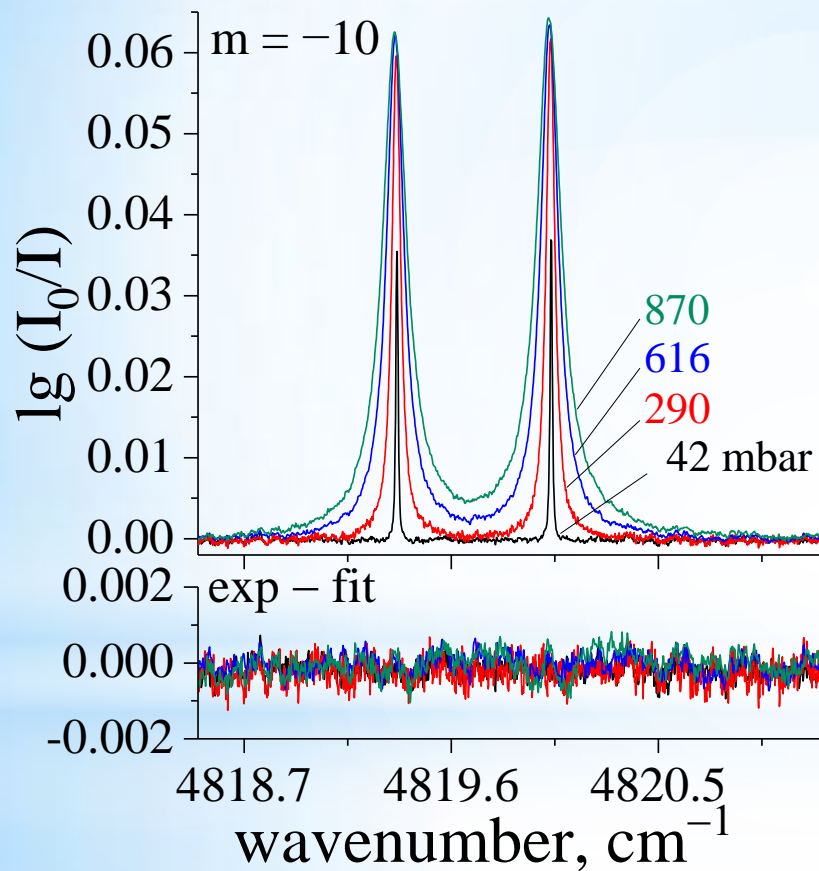


MKS Baratron
0.1 - 1000 mbar

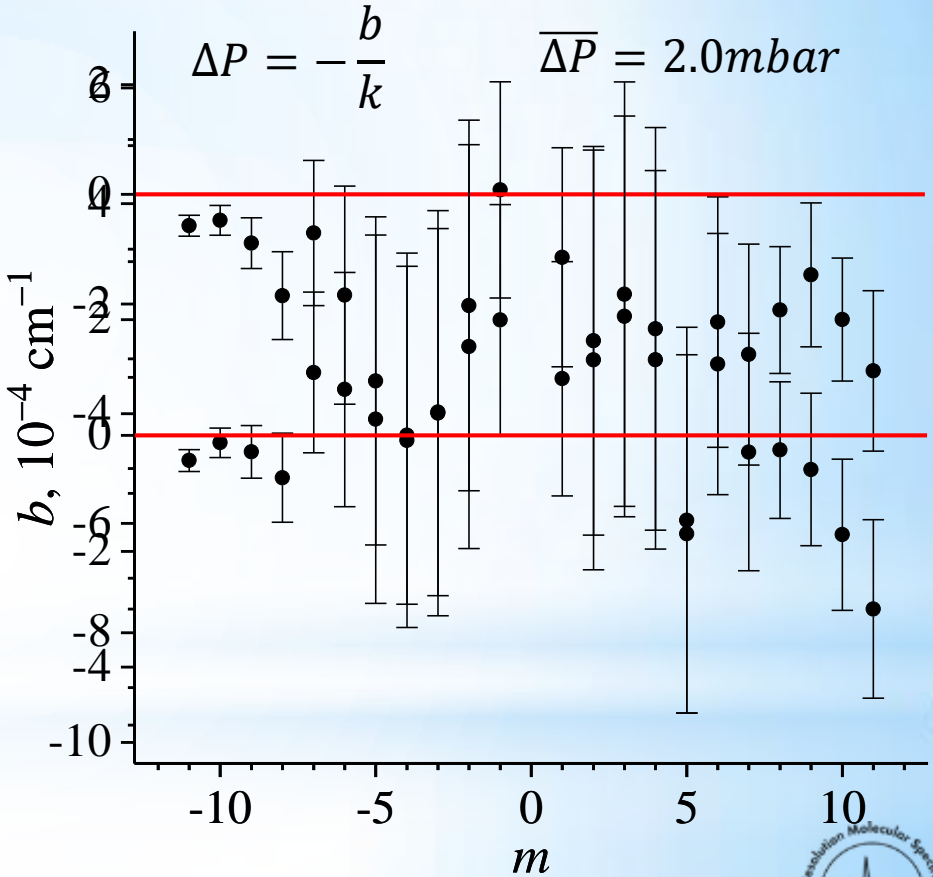
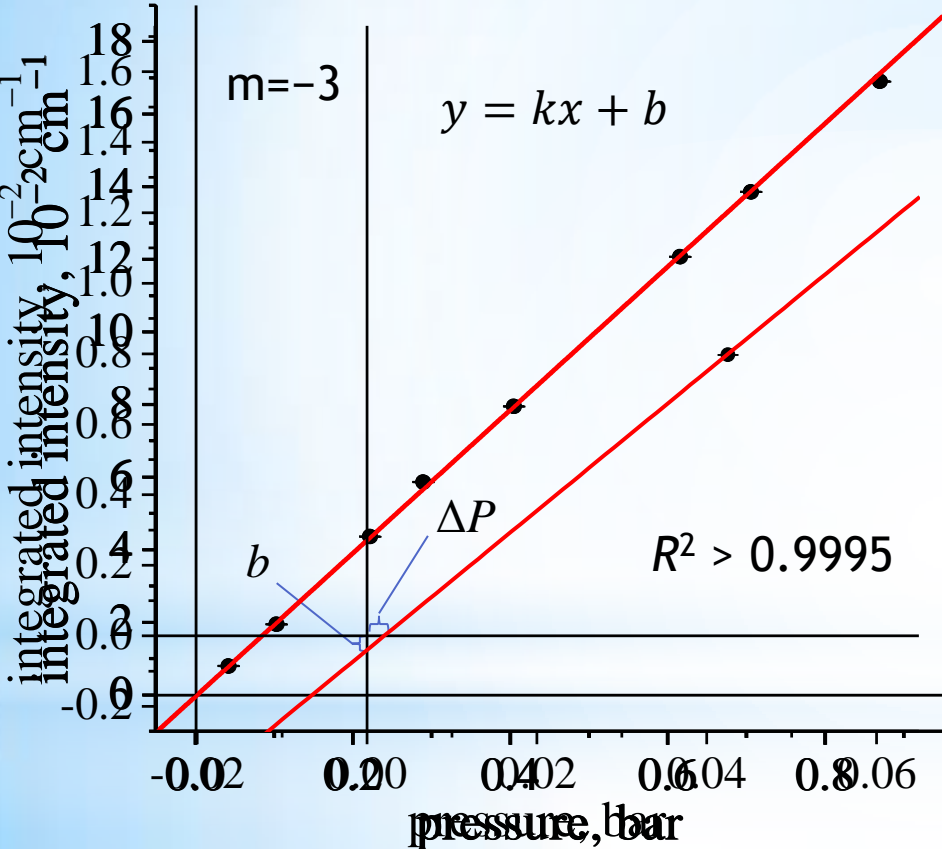
HBr, the first overtone



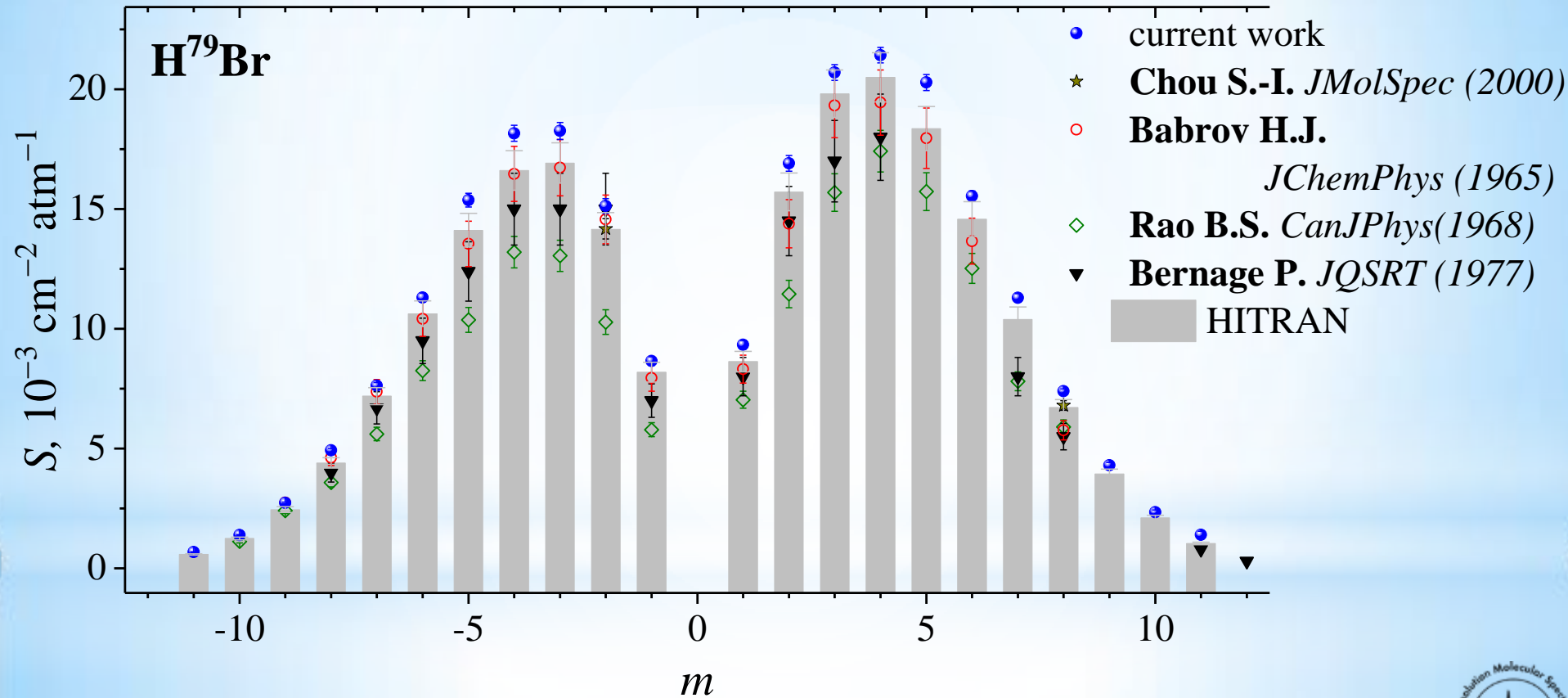
Fitting with Voigt profiles



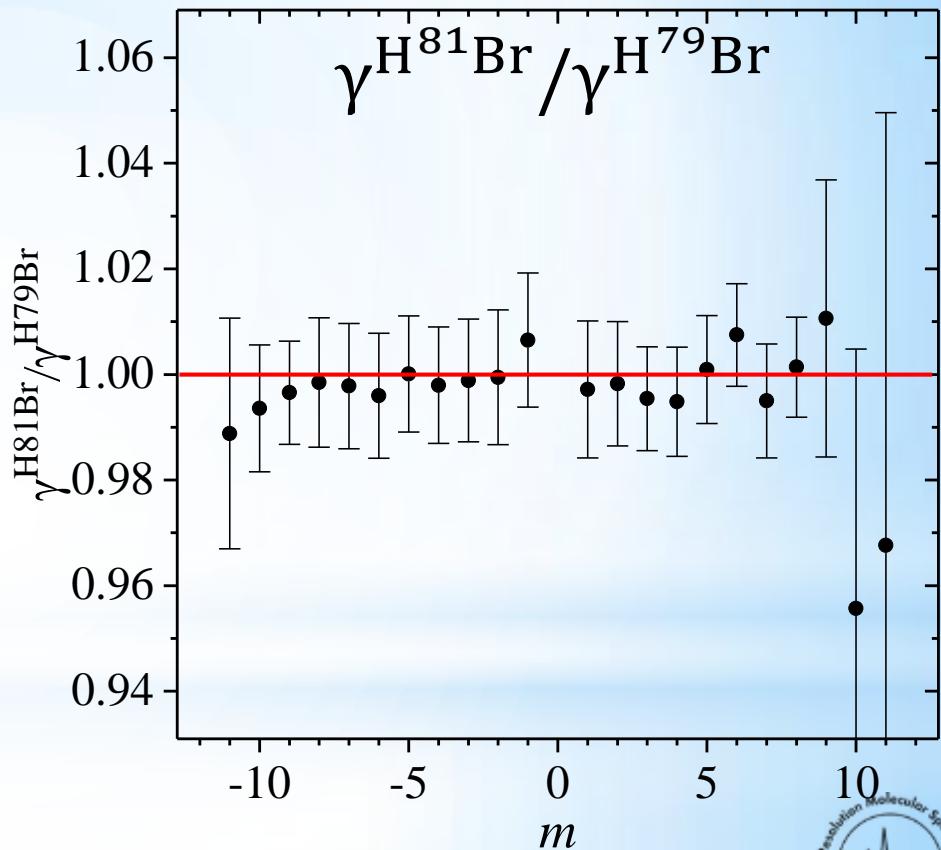
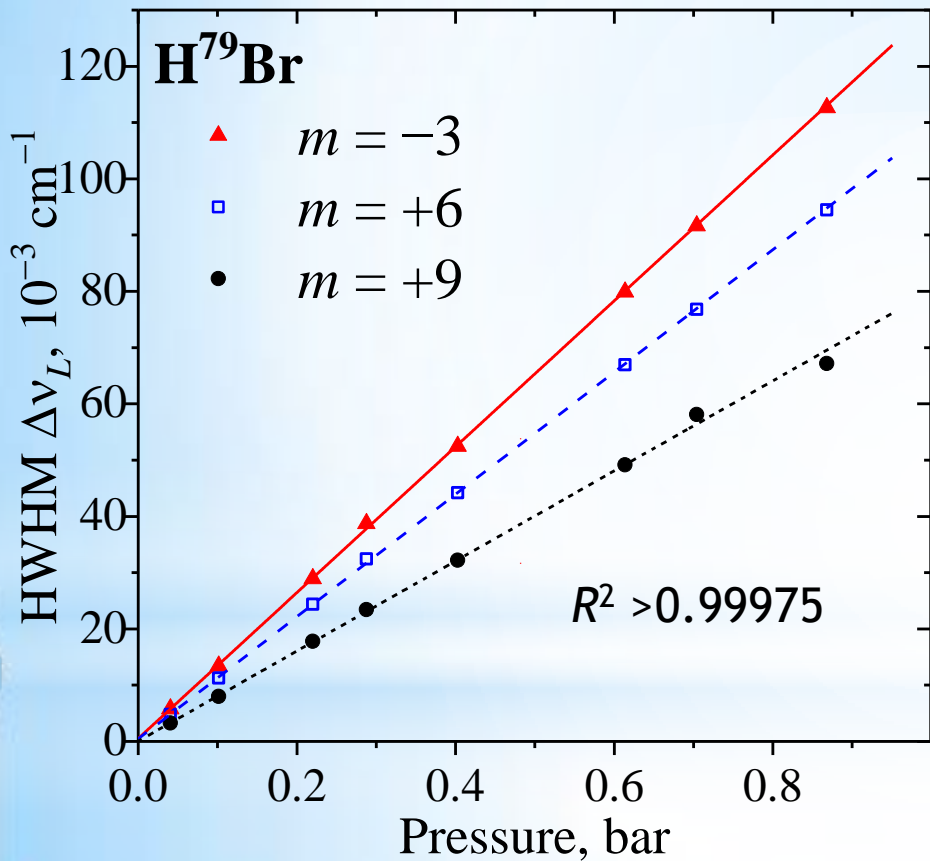
Intensities



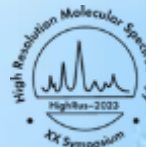
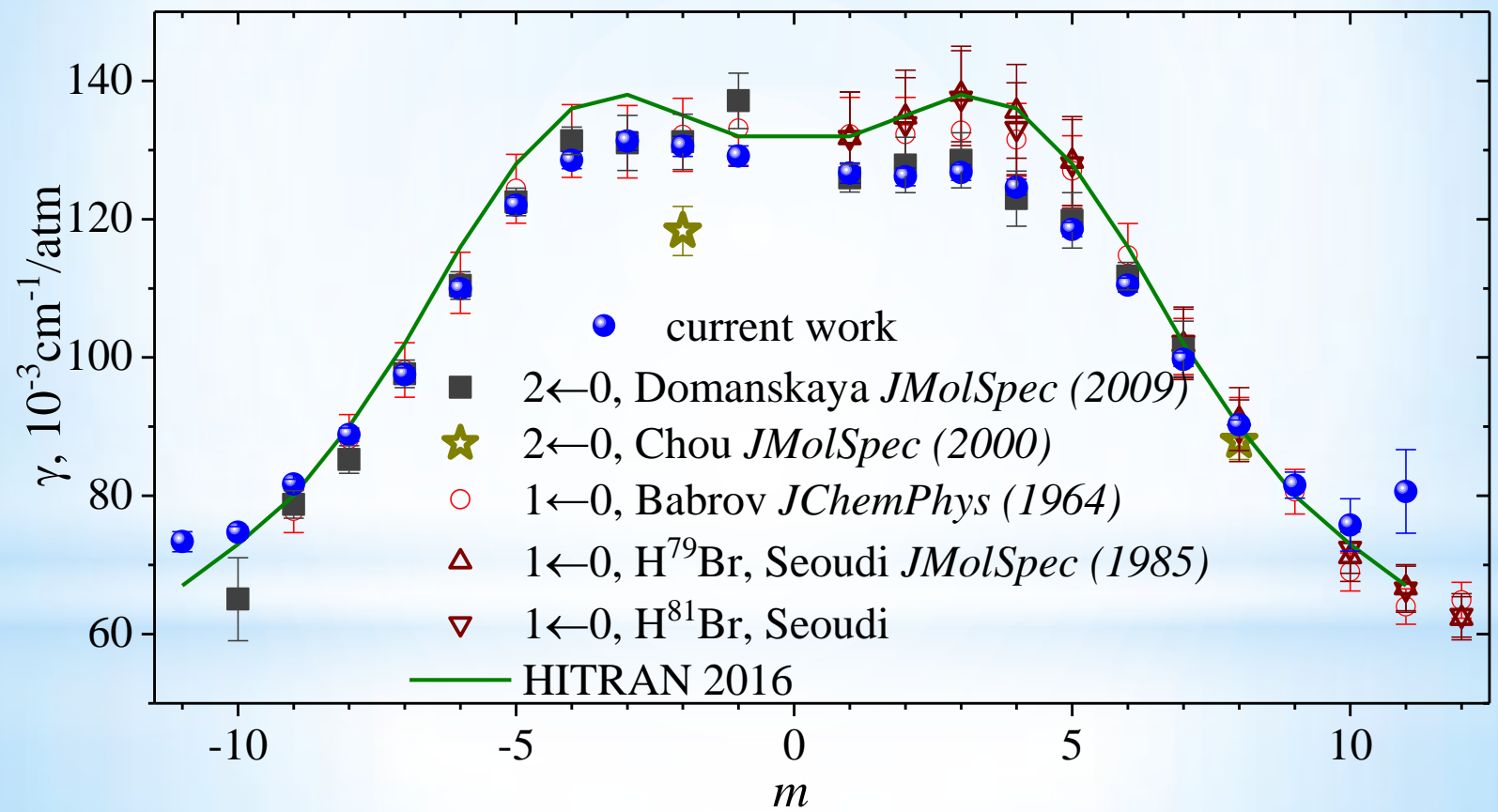
Intensities



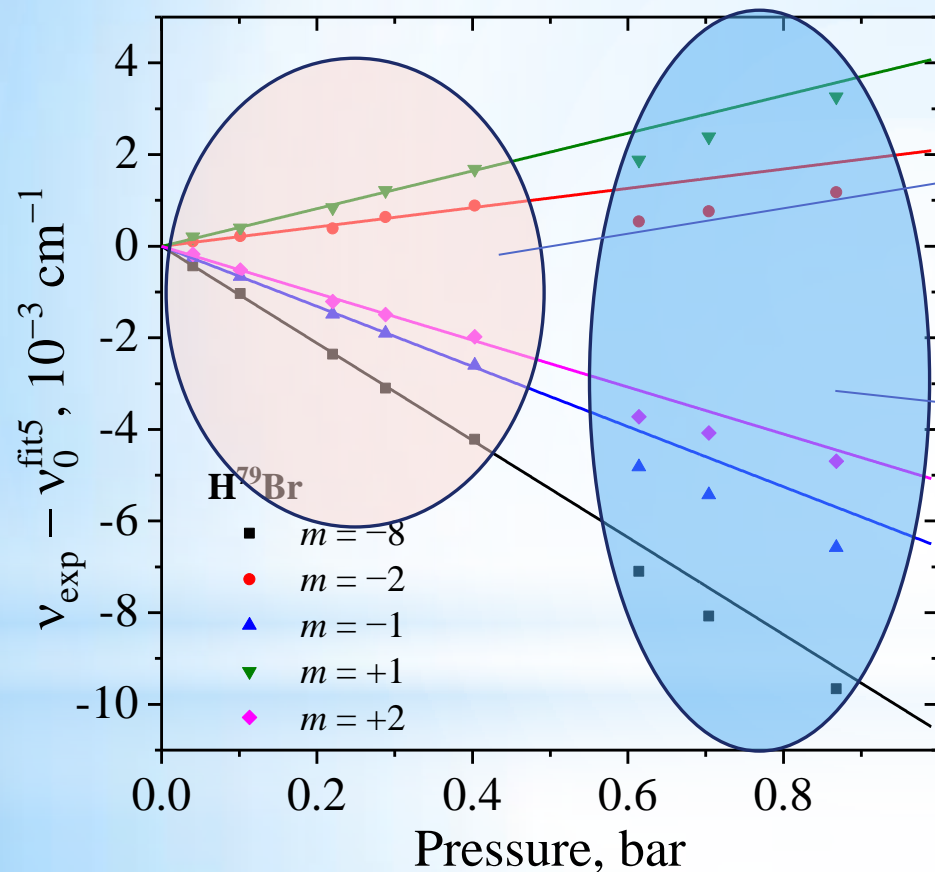
Broadening coefficients γ



Broadening coefficients γ

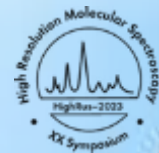


Shifting coefficients δ



Aperture 0.8 mm
Res 0.003 cm^{-1}

Aperture 1.0 mm
Res 0.005 cm^{-1}



Measurement [X]

Basic Advanced **Optic** Acquisition FT Display Background Check Signal

External synchronisation: Off

Source setting: MIR

Beamsplitter: KBr

Optical Filter setting: Open

Aperture setting: 1.7 mm

Warning: Aperture limits resolution at 3385 cm⁻¹

Measurement channel: Front sample compartment

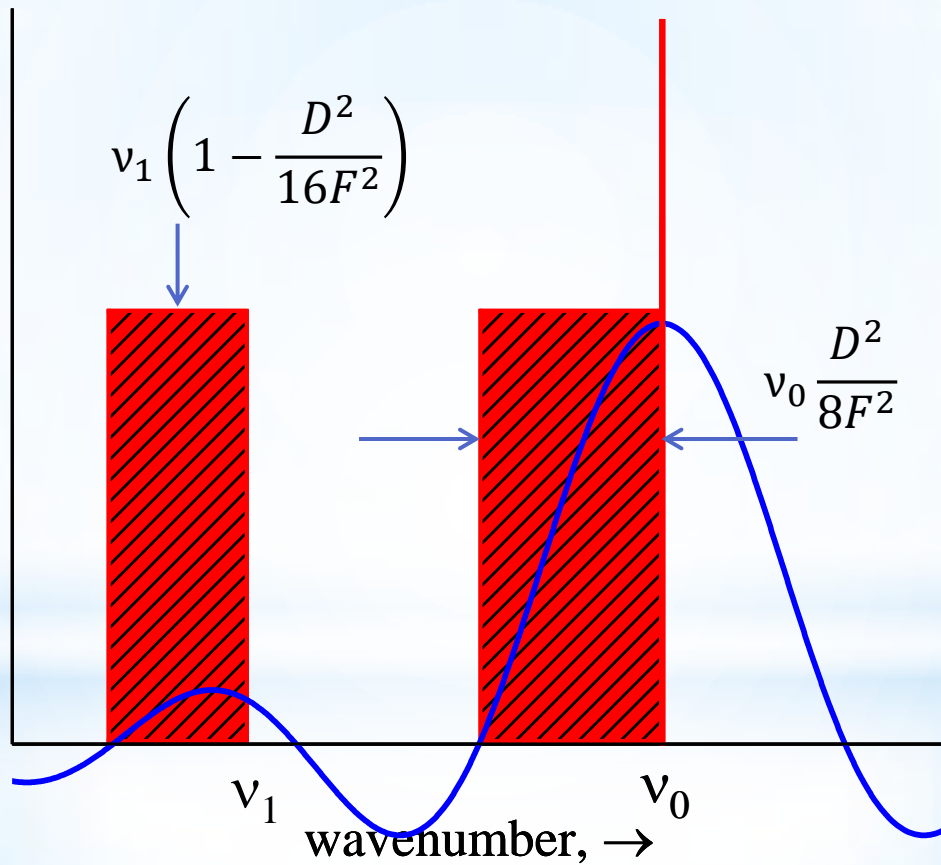
Background meas. channel: Back sample compartment

Detector setting: LN-MCT Mid FOV=30° [Internal Pos.1]

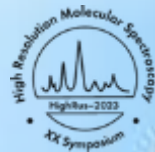
Scanner velocity: 40 kHz

Sample signal gain: x1

Preamp gain: Ref

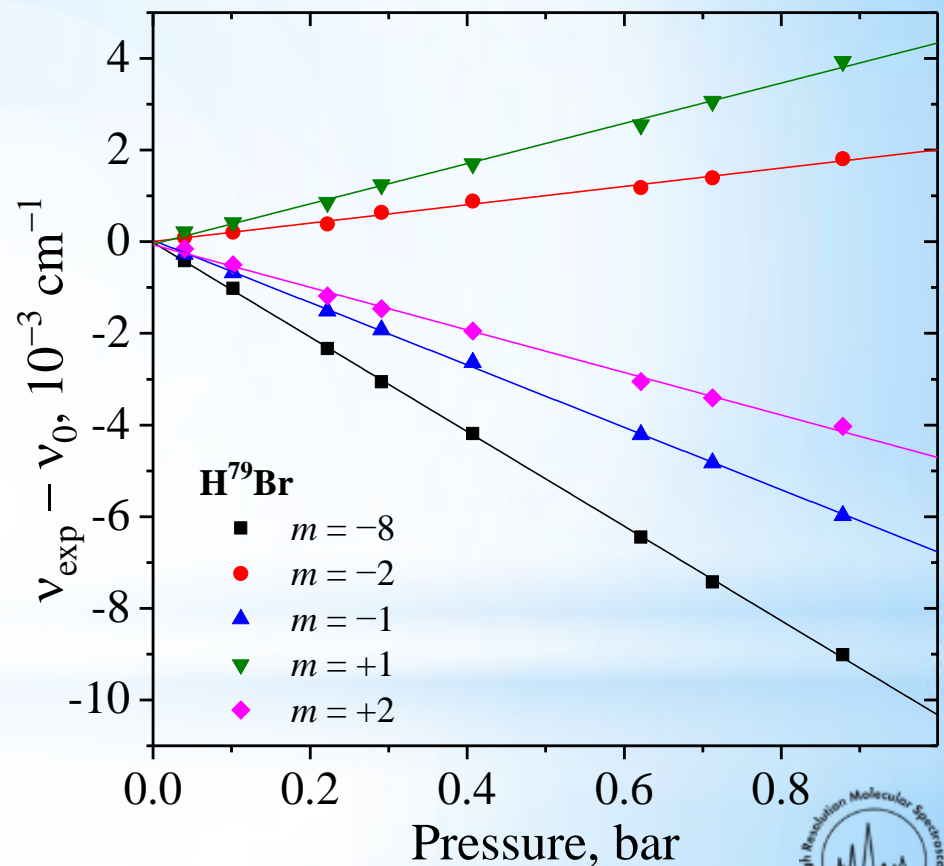
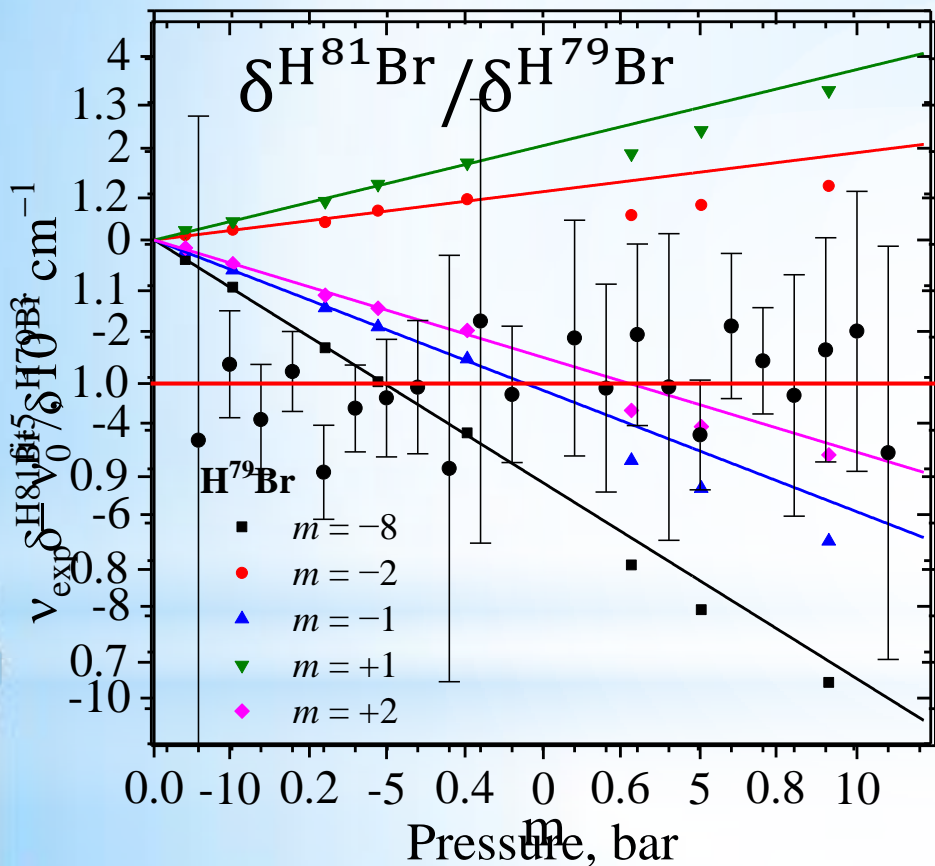


R.J.Bell "Introductory Fourier Transform Spectroscopy" 1972

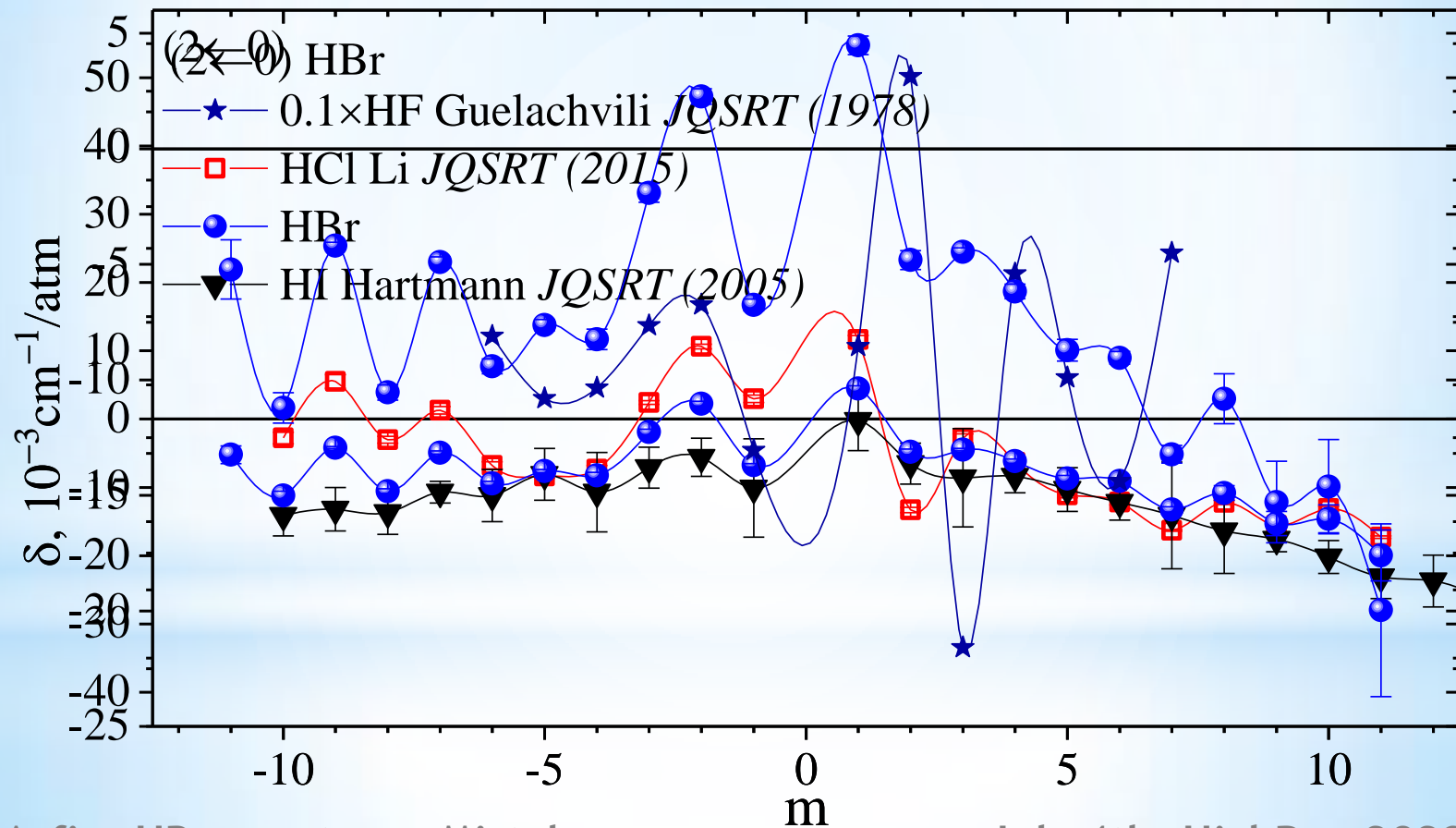


- ✓ $\delta v = v \frac{D^2}{16F^2} < \frac{1}{2} \text{ Res}$
- ✓ $\Delta_{\text{std}} v \approx 10^{-1} - 10^{-2} \text{ Res}$ for symmetric profiles
- ✓ $\delta v \propto v \Rightarrow$ calibration by tuning of v_{las} value
- ✓ Calibration only for one aperture
- ✓ One knows the reason, one knows the solution

Shifting coefficients δ



Shifting coefficients δ



Conclusions

- ✓ The spectra of HBr at different subatmospheric pressures in the first overtone were recorded
- ✓ The intensity of lines was determined. They are in satisfactory agreement with literature and HITRAN data
- ✓ The self-broadening coefficients are essentially differ from HITRAN data
- ✓ The self-shifting coefficients have been measurement for the first time
- ✓ Use one aperture in the series
- ✓ Calibrate your instrument with an aperture you used
- ✓ Read textbooks and manuals



Self-broadening and Shifting Coefficients for the Spectral Lines in the First Overtone Band of HBr

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Abstract—Spectra of HBr with a natural abundance of isotopologues were recorded in the region of the first overtone at room temperature at various sub-atmospheric pressures. The coefficients of self-broadening and shifting were found for two isotopologues of HBr. Both broadening and shifting coefficients for different isotopologues coincide within the error margins. The broadening coefficients are in good agreement with those reported previously, however they have a smaller error, about 1%. The shifting coefficients are reported for the first time. The obtained line intensities of both isotopologues are in reasonable agreement with values published earlier.

Keywords: self-shifting, self-broadening, overtone, hydrogen halides, diatomic

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Michael Bulanin
(1931-2015)

R.E. Asfin, A. Domanskaya, C. Maul, *Opt. Spectr.* **130**, 1 (2022)



Konstantin Tokhadze
(1944 - 1923)

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Thank you for your attention

Спасибо за внимание

感谢您的关注