GAS Analysis 2026 PARIS

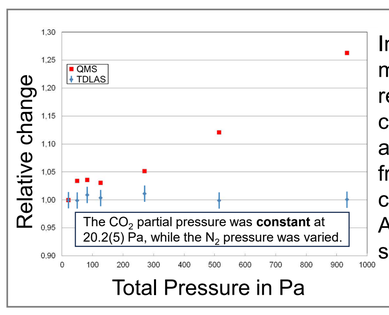
Molecular Line Parameters, Impact on Climate Models and the Quantum-Pascal

PTB Physikalisch-Technische Bundesanstalt
Germany's metrology institute

Traceability

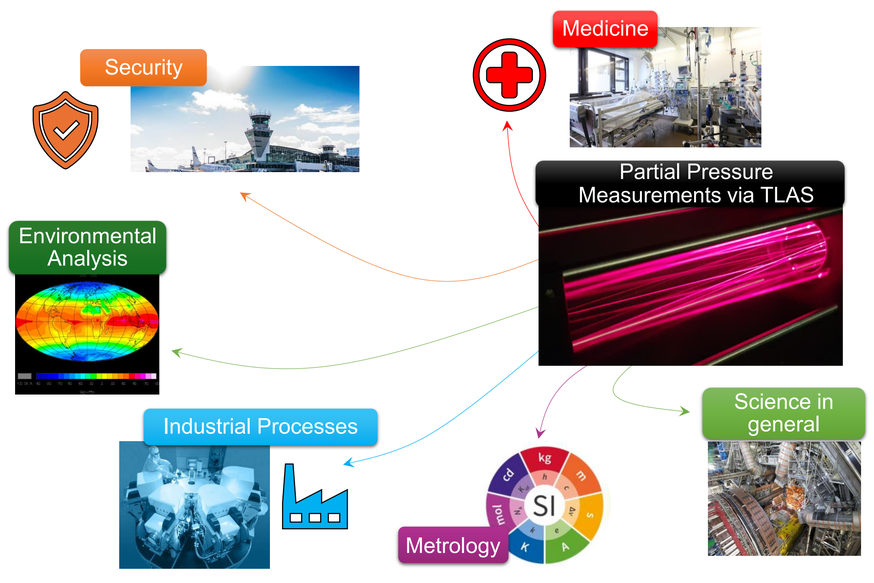
Absorption spectroscopy is well-suited for metrological gas analysis in the context of the redefined SI (2019).

Measurement results - such as partial pressures and temperatures - are directly traceable to fundamental gas properties, which are physical constants. (No recalibrations needed.)

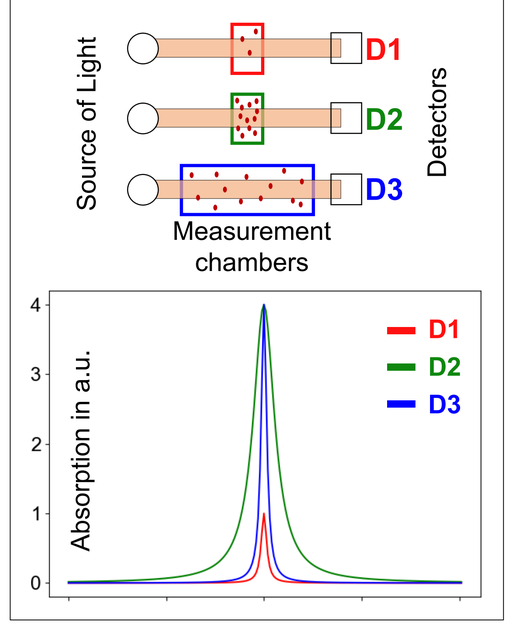


In contrast, e.g., mass spectrometry requires frequent calibrations and additionally suffers from significant cross-sensitivities. An example is shown in the figure.

Need



Principle



Beer-Lambert

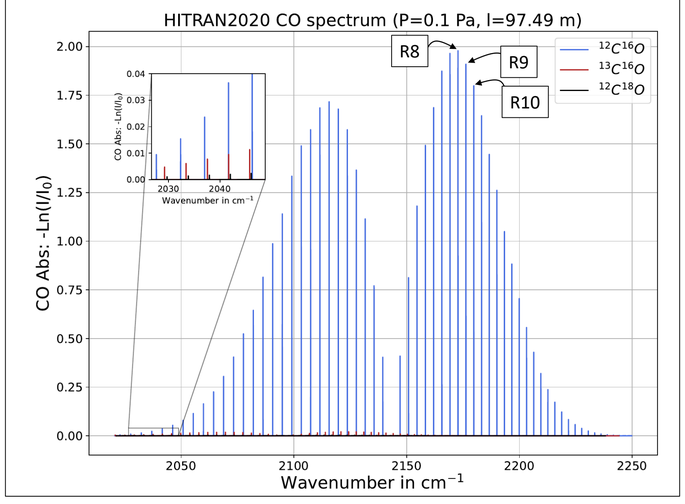
Beer-Lambert's Law enables precise calculation of the gas density from frequency-resolved transmission spectra:

$$I = I_0 e^{-\alpha_\rho \rho L} \Rightarrow \rho = -ln\left(\frac{I}{I_0}\right)/(\alpha_\rho L)$$

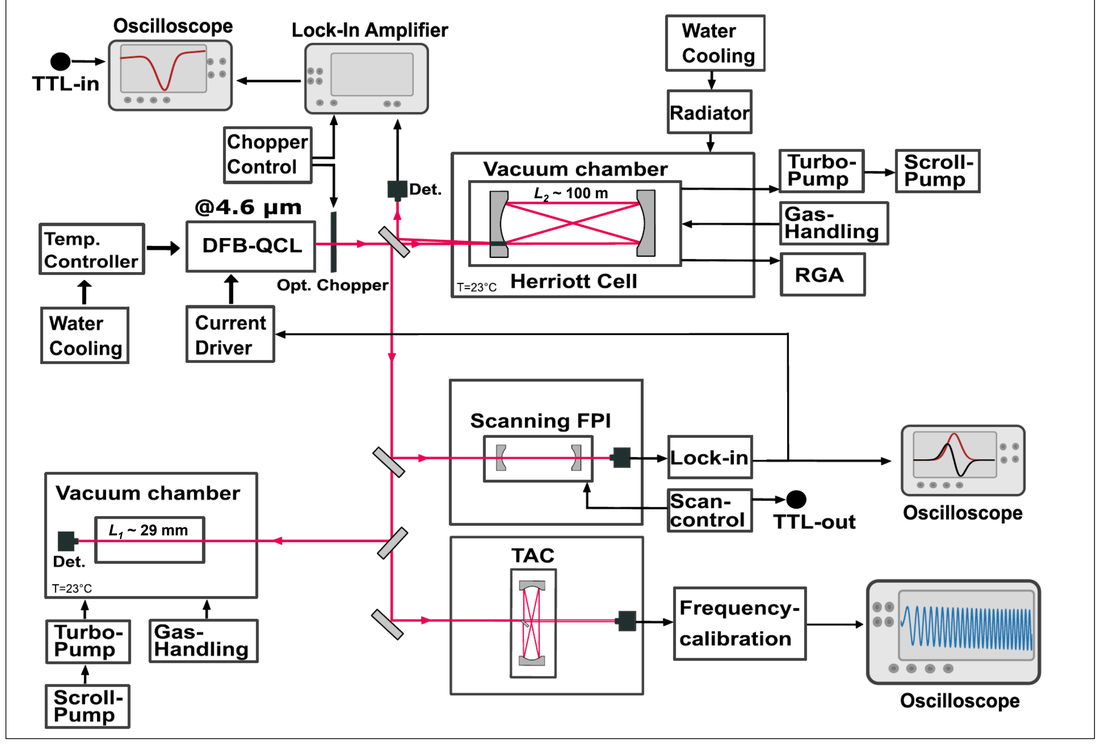
At a known temperature, the partial pressure can then be derived directly from the corresponding gas density:

$$p = \rho_n k_B T(1 + \rho_n B(T) + ...)$$

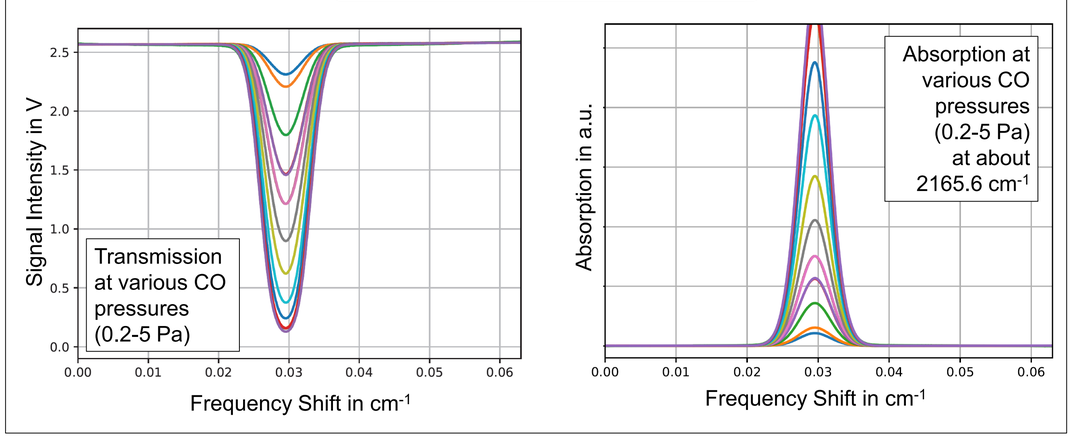
Simulations



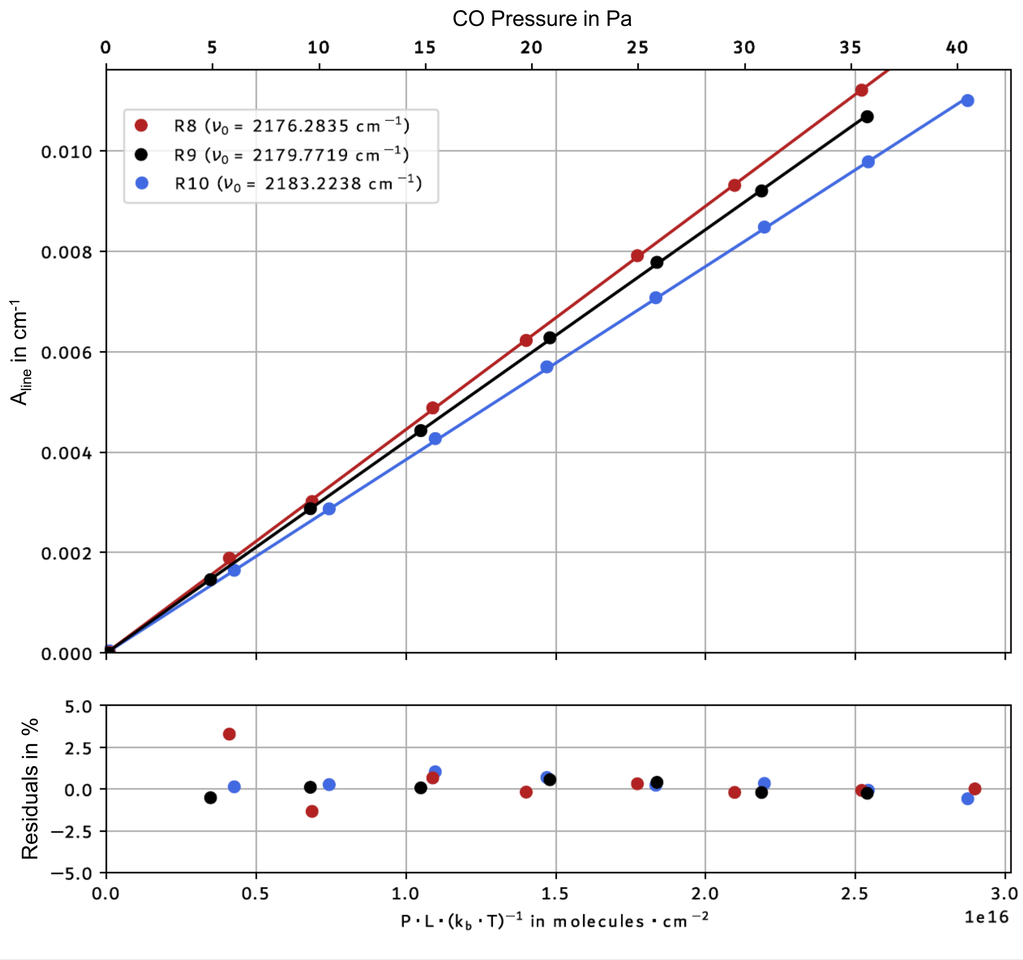
Experimental Setup



Measured CO Absorptions



Assessed Line Strengths for Key Absorption Transitions



Results and Recent Theoretical Values for CO at T = 296 K

Line center in cm^{-1}	S_{PTB} in 10^{-19} cm/molecule	u_{rel} (S_{PTB}) in %	S_{Calc} in 10^{-19} cm/molecule	S_{PTB}/S_{Calc} -1 in %
2176.2835	4.452(16)	0.335	4.468	-0.353
2179.7719	4.217(16)	0.372	4.205	0.278
2183.2238	3.851(15)	0.372	3.845	0.143

Measured results show excellent agreement with recent theoretical predictions!
(Theoretical values were provided by Dr. Oleg Polyansky, Uni. College London)

Uncertainty Budget

The table provides the details for the expanded uncertainties with respect to the measured line strengths.

It is exemplary for the CO absorption line at 2176.2835 cm^{-1}, corresponding to the R8 line of the fundamental (0-1) band as shown in the simulations (in blue) for the main isotope $^{12}C^{16}O$.

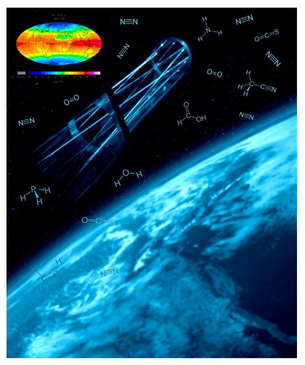
Quantity	Rel. uncertainty in % (k=2)	Type
Linear fit (S)	0.284	A
Pressure	0.120	B
Frequency	0.126	B
Gas purity	0.030	B
Temperature	0.008	A
Laser linewidth	0.006	A
Optical pathlength	0.004	B
Isotopologue	0.004	B
Sum	**0.335**	**-**

Summary and Outlook

The line strengths of the most dominant carbon monoxide (CO) absorption lines were measured with improved uncertainties. The results agree with recent theoretical values, which is also a validation of the corresponding models. This also helps improving the theoretical calculations for other gases, like the greenhouse gas CO_2.

Improved uncertainties are possible and planned for the future through an automated measurement process, as well as lower uncertainties in pressure and temperature, as enabled by the so-called Quantum-Pascal.

MQB Pascal UANTUM follow-up



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