GAS ANALYSIS

Quantitative FT-IR based Gas Analysis Without Calibration Measurements

Innovation with Integrity

Quantitative FT-IR based Gas Analysis

FT-IR spectroscopy is a powerful tool for the unambiguous identification of IR-active gases due to the unique IR fingerprint of each compound. The resultant high selectivity and sensitivity of FT-IR permits the detection of gases present at low concentrations even in complex mixtures featuring many IR-active compounds across a wide range of concentrations. In addition to excelling at identifying gas species, FT-IR can also accurately quantify gas concentrations in real time by employing quantitative reference spectra and by considering the spectral signatures of interfering gases in case of a gas mixture.

Traditionally, calibration measurements are necessary to be able to quantify gas concentrations. In principle, calibrations are carried out by collecting IR spectra of pure gases or calibration mixtures with known mixing ratios. These calibrations are typically performed by the manufacturer of the gas analyzer and are provided with each system.

This method of calibration presents some issues, however. If the analyte is a liquid under ambient conditions, for example ethanol, the generation of a calibration mixture is complex and involves the evaporation of the analyte using a syringe pump, valves, flow controllers, and heated injection needles. Furthermore, if the application changes causing an alteration in the gaseous compounds to be quantified or compensated for, additional calibration measurements need to be conducted. Hence, calibration measurements are costly, time-consuming, require additional equipment and chemicals, and limit the uptime of the instrument.

Quantitative and Accurate Analysis Without Calibration Measurements

Bruker's Gas Analysis FT-IR systems of the MATRIX II-MG series and OMEGA 5 bypass this expensive and time-consuming calibration process by offering the gas analysis software OPUS GA in combination with the spectral database B-GAS-LIBRARY. This unique combination enables calibration-free quantification through automatic real-time comparison of spectral data to universal reference spectra of more than 350 compounds that are part of the spectral library. Quantification for a given compound is achieved solely via selections in the software, such as selecting the appropriate spectral region for its IR absorbance and identifying interfering compounds absorbing nearby.

In the case where a gas compound of interest is not in the spectral database, it can be added to the library via a one-time traditional calibration curve, permitting subsequent quantification.

Verification of OPUS GA Results

Measurements with a gas standard were performed to verify the OPUS GA analysis results and the calibration-free quantification algorithm. The spectra were collected on a MATRIX II-MG5 Gas Analyzer operated with OPUS GA using a spectral resolution of 0.5 cm^{-1} and an effective measurement time of 1 second per spectrum. The retrieved results are in accordance with the values provided by the supplier of the gas standard (Table 1).

Compound (matrix N_2)	Mixing ration according to supplier [ppm]	OPUS GA Results [ppm]	Rel. Deviation [%]
CH_4	998.0 ± 0.2 % (rel.)	1002 ± 3 (stat.)	0.4
CO	99.9 ± 0.2 % (rel.)	100.6 ± 0.1 (stat.)	0.7
N_2O	10.02 ± 0.2 % (rel.)	9.98 ± 0.01 (stat.)	0.4

Table. 1
Comparison of OPUS GA quantification results to the concentration specified by the gas supplier.

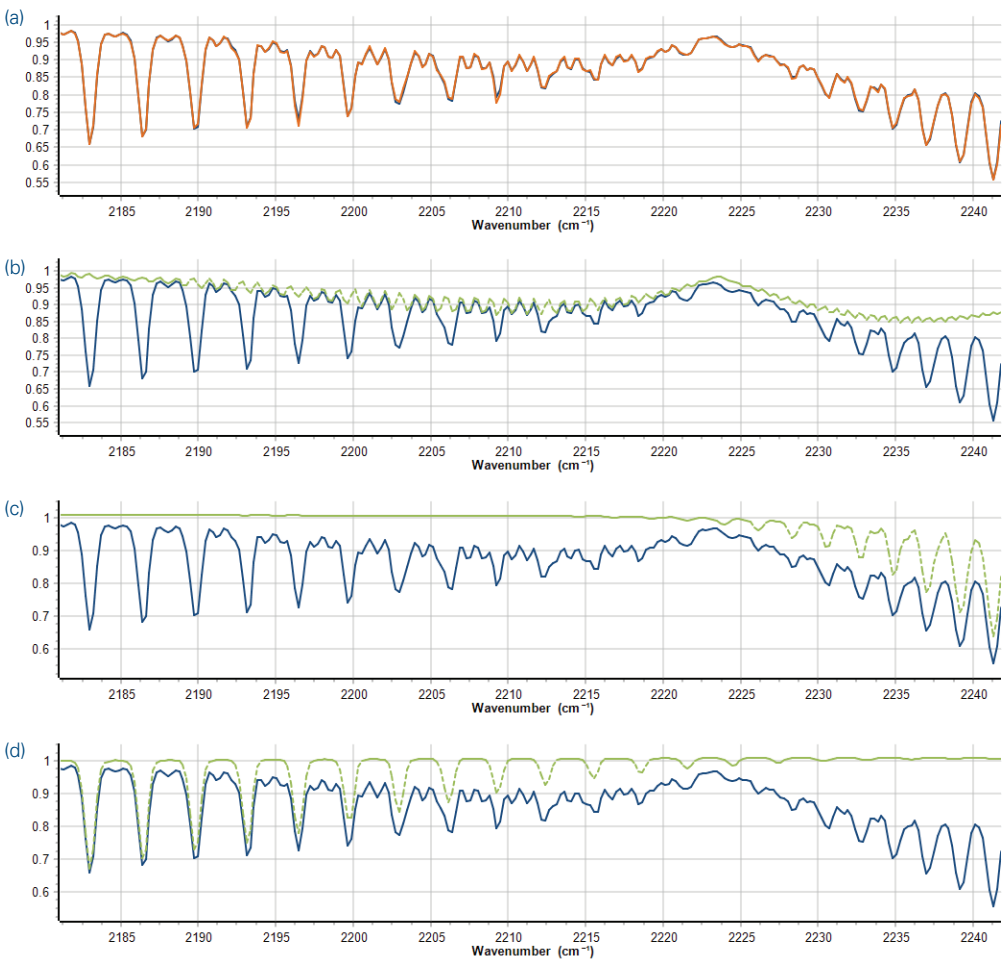

Fig. 1
Quantification of N_2O. (a) Selected region of the measured IR transmission spectrum of the gas standard (blue) and fit to the measurement (orange) overlaid with the measured spectrum. Individual contributions (green) of (b) N_2O, (c) CO_2 and (d) CO to the measured spectrum (blue).

Accurate quantification of N_2O was possible without performing any time-consuming calibration measurements even despite spectral interference. In fact, the analyte N_2O contributes even less to the overall IR spectrum than the relevant interfering gases CO_2 and CO. The contribution of the target compound N_2O as well as of the interfering compounds to the overall IR spectrum can be displayed in OPUS GA (Figure 1) such that the user gets a detailed understanding of the retrieved results.

Benefits of Gas Analysis without Calibration Measurements

- **Defining new quantification methods**
  Evolving applications and gas mixtures are effortlessly managed by creating new methods in OPUS GA. Defining a quantification method for a new gas or application takes only a few minutes and clicks in the software.

- **Extension of the spectral database**
  Reference spectra for new gases are regularly added to the spectral library, including those specially requested by users. This ongoing expansion of the database makes the OMEGA 5 and MATRIX II-MG Gas Analyzers even more versatile year after year.

- **Transfer of quantification methods**
  As quantification methods and universal reference spectra are not device specific, they can be easily transferred by the user to other Bruker Gas Analyzers operated by OPUS GA without sustaining any loss of accuracy or precision.

Gas Analyzers MATRIX II-MG5 and OMEGA 5

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