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Application News

IRXross™ Fourier Transform Infrared Spectrophotometer

High Resolution Analysis of Gases Related to Air Pollution and Global Warming

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User Benefits

- The IRXross FTIR enables accurate measurement of the vibrational-rotational spectra of low molecular gases by measurement with a maximum resolution of 0.25 cm^{-1}.
- Infrared spectra of gases can be acquired with the standard DLATGS detector by using a short-path gas cell.

■ Introduction

The IRXross, a new FTIR which Shimadzu Corporation recently released, has best-in-class sensitivity and resolution in its class and supports high speed scanning at a maximum of 20 spectra/sec. The IRXross also includes the original Shimadzu software IR Pilot™ for analysis navigation as a standard feature, and thus provides excellent operability in addition to outstanding performance.

Among the features mentioned above, this article introduces application to the gas analysis, focusing on the high resolution of the IRXross.

■ Gases with Harmful Impacts on Global Environment and Analysis by FTIR

Various gas species with harmful impacts on the global environment were analyzed using the new IRXross Fourier transform infrared spectrophotometer (FTIR). The four gases used here were NO, N_2O, SO_2, and CH_4. NO and SO_2 form fine acidic particles by a chemical reaction when released into the atmosphere, and it is known to be a cause of acid rain. Although CO_2 is the best-known greenhouse gas (GHG), N_2O and CH_4 are also classified as GHGs, and efforts to suppress emissions in order to prevent global warming have already begun (the target of "zero emissions" is carbon neutrality).

The infrared (IR) spectra of gases are affected by vibration and rotation, and show the IR absorption of narrow bands called vibrational-rotational spectra. In order to acquire vibrational-rotational spectra accurately, high resolution is necessary in the FTIR. Therefore, an IRXross (see Fig. 1), which enables measurement with the highest resolution of 0.25 cm^{-1}, was used in this experiment.

Fig. 1 Appearance of IRXross

■ Measurement

In a measurement of gases, it is necessary to select a gas cell with an appropriate light-path length for the sample concentration. Here, two short-path gas cells (10 cm, 5 cm) were used. Gas cells in which light is transmitted in a straight line from the inlet to the outlet are also called single path gas cells. Since there is no significant attenuation of infrared light in a single path gas cell, measurement is possible using the DLATGS, which is the standard detector for FTIR. Fig. 2 shows the 5 cm gas cell mounted on the sample chamber of the IRXross.

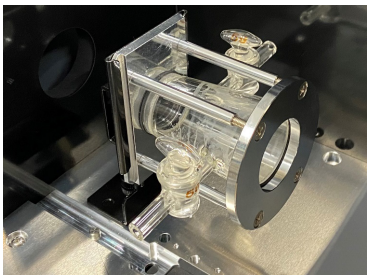

Fig. 2 Appearance of 5 cm Gas Cell

Table 1 shows the measurement conditions. Fig. 3 shows the IR spectra of N_2O gas when measured with resolutions of 0.25 cm^{-1}, 0.5 cm^{-1}, and 1.0 cm^{-1} to investigate the effect of differences in resolution on the measured IR spectrum. In terms of the peaks around 2230 cm^{-1}, the result at the resolution of 1.0 cm^{-1} shows only double-peak but the result at the resolution of 0.25 cm^{-1} shows many narrow bands on the double-peak. Therefore, the vibrational-rotational spectrum was accurately obtained by the high resolution measurement.

Table 1 Measurement Conditions

Instruments	:	IRXross Fourier transform infrared spectrophotometer (KBr window) 10 cm gas cell (KBr window) [N_2O] 5 cm gas cell (KBr window) [NO, SO_2, CH_4]
Resolution	:	0.25, 0.5, 1.0 cm^{-1}
Accumulation	:	30 times
Apodization function	:	SqrTriangle
Detector	:	DLATGS

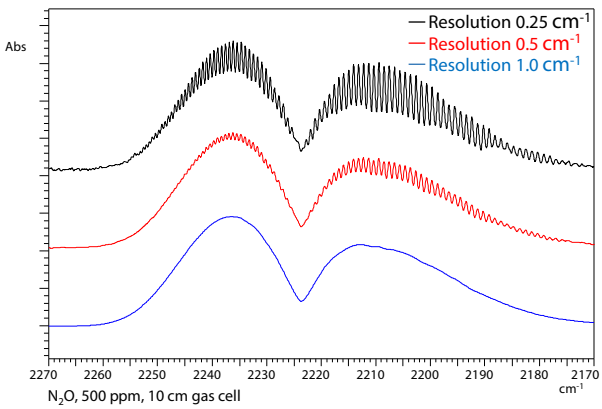

Fig. 3 Comparison of IR Spectra of N_2O Gas Measured at Different Resolutions

■ Infrared Spectra of Gas Species

The IR spectra of the gas species (N_2O, NO, SO_2, CH_4) were measured at a resolution of 0.25 cm^{-1}. Fig. 4 to Fig. 7 show the regions where characteristic IR absorption was detected in the spectra of each gas. The distinctive comb-shaped spectrum of low molecular gases was confirmed in all cases.

■ Conclusion

High resolution measurement of various species of gases with harmful impacts on the global environment was carried out using the IRXross FTIR. The comb-shaped spectrum originating from molecular vibration and rotation, which is a characteristic of low molecular gases, could be measured with high accuracy. It may also be noted that high sensitivity measurement of gases with low concentrations is also possible by using a long-path gas cell and MCT detector. Appropriate selection of the instrument configuration according to the target gas concentration is recommended.

The next article in this series will introduce an example of quantitative analysis of gases using a long-path gas cell.

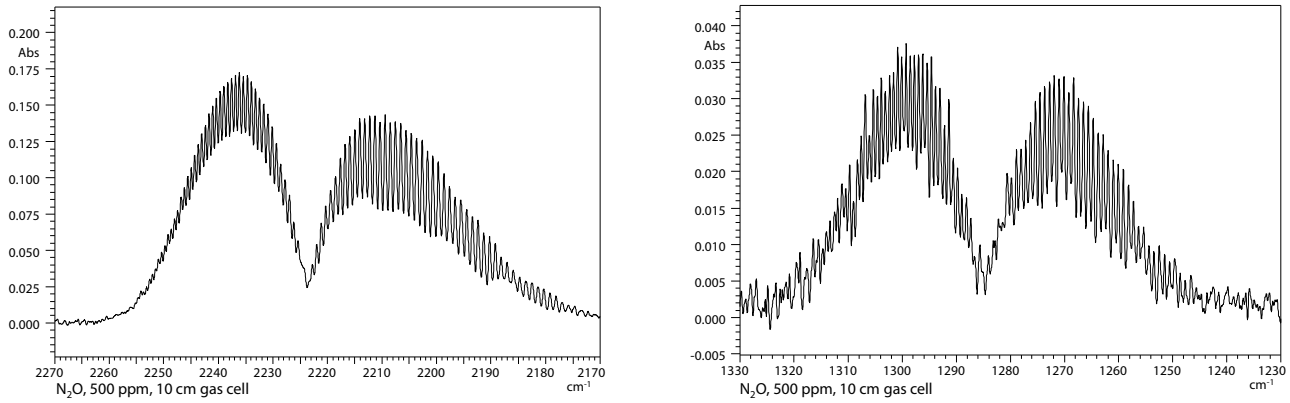

Fig.4 IR Spectra of N_2O Gas (Left: Around 2230 cm^{-1}, Right: Around 1290 cm^{-1})

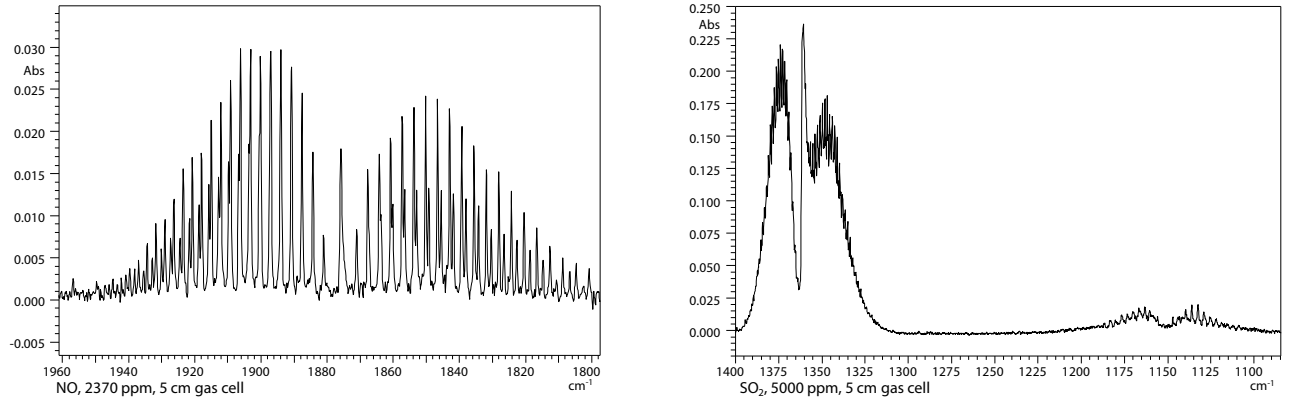

Fig. 5 IR Spectrum of NO Gas

Fig.6 IR Spectrum of SO_2 Gas

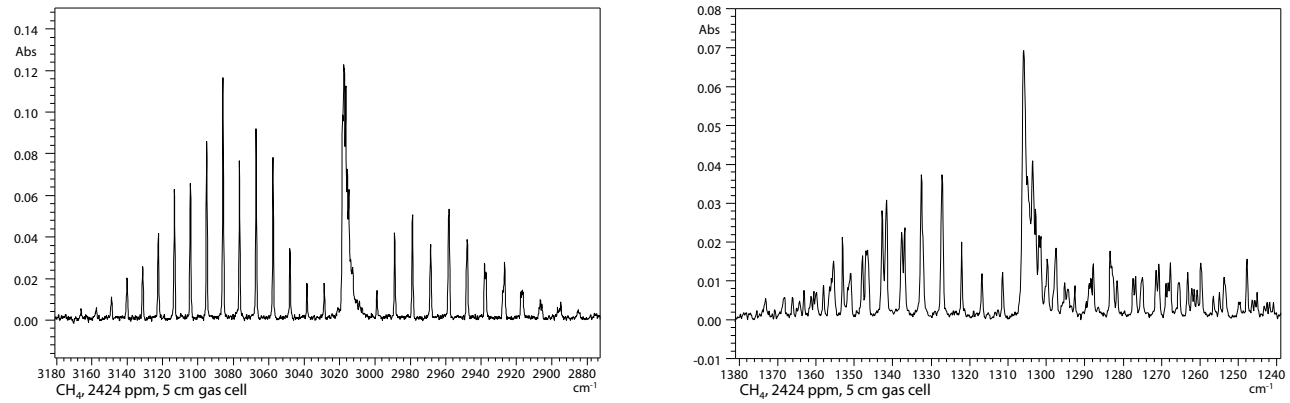

Fig.7 IR Spectra of CH_4 Gas (Left: Around 3000 cm^{-1}, Right: Around 1300 cm^{-1})

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