Comparing the limiting resolution of the Agilent Cary 5000 and Cary 6000i UVVis-NIR spectrophotometers using the transmission spectrum of water vapor

Application Note

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Introduction

The NIR spectral characteristics of many gases and solids exhibit narrow bands containing vibrational fine structure. Being able to resolve these peaks, which are on the order of < 1 nm FWHM, on traditional UV-Vis-NIR absorption spectrophotometers have been a challenge over the years, however, with the release of the new generation UV-Vis-NIR absorption spectrophotometers from Agilent, the measurements of even the most difficult of samples is now possible. This application note demonstrates one aspect of these improvements by showing the ability of the Agilent Cary 5000 and Cary 6000i instruments to resolve the transmission peaks of water vapor in the NIR spectral region.

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Theory

The resolving power of an absorption spectrophotometer depends on a number of different mechanical instrument parameters which influence resolution. These include the grating resolution (lines per mm), focal length of the monochromator, the minimum slit width and the minimum stepping interval. These parameters, along with the detector sensitivity across the wavelength range of interest, dictate the minimum resolution. A common, but incorrect, assumption often made is that the minimum resolution is only dependent on the SBW, however, if there are not enough data points collected, or the S/N is extremely low, then the fine spectral characteristics of the sample will not be resolved.

To resolve a peak, it is a general requirement to set the SBW to 1/3rd the natural peak width, and the data interval to 1/10th the natural peak width. However, the narrower the SBW setting, the lower the amount of light hitting the detector, hence, the sensitivity of the detector becomes a very important factor if good S/N spectra are to be collected. Agilent has typically made high performance spectrophotometers that can measure the most demanding samples and, with the release of its new generation Cary 5000 and Cary 6000i UV-Vis-NIR absorption spectrophotometers, has raised the bar to a new level. In theory, the Cary 6000i can resolve a peak of between 0.06 – 0.1 nm natural bandwidth in a relatively short time. It is without a doubt that the new generation Cary range are the best UV-Vis-NIR instruments available on the market today.

Method

To demonstrate the NIR resolving power of the Cary 5000 and 6000i, the transmission spectrum of water vapor was measured from 1200 – 1800 nm. The difference between these instruments is that the Cary 6000i has a more sensitive InGaAs detector (~100 times), better grating resolution in the NIR (600 lines/mm vs 300 lines/mm) and a smaller minimum SBW and data interval setting. The Agilent Cary 5000 and 6000i were both run in Fixed SBW mode. The other settings are listed below.

Instrument Parameter	Cary 5000	Cary 6000i
SBW (nm)	0.05	0.02
Data Interval (nm)	0.02	0.01
Averaging time (s)	10	2
Beam mode	Single front	Single front
Slit height	Reduced	Reduced

Results

Wavelength scans were performed from 1370 – 1390 nm. Figures 1 and 2 show the transmission spectrum of water vapor collected on the Cary 5000 and Cary 6000i UV-Vis-NIR spectrophotometers respectively. Figure 3 shows the resolution between the Cary 5000 and Cary 6000i by comparing the peak at 1380 nm.

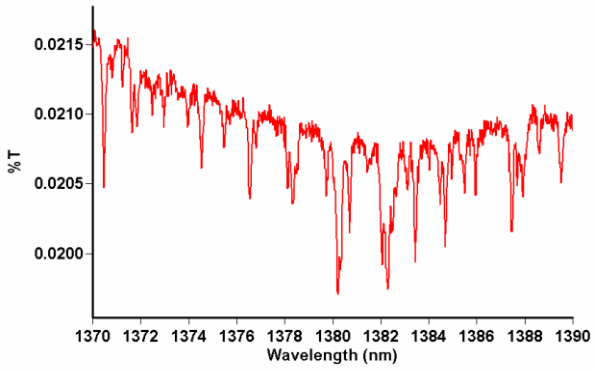

Figure 1. Water vapor transmission spectrum collected on a Cary 5000 spectrophotomer

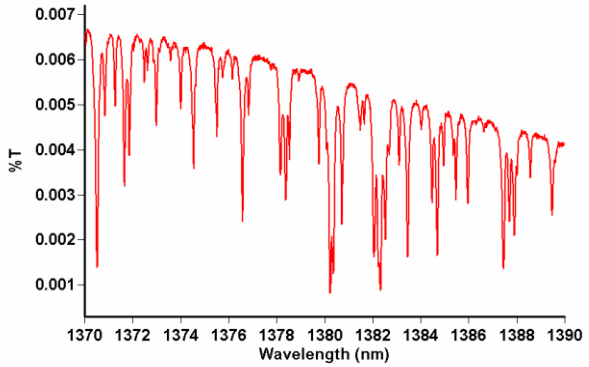

Figure 2: Water vapor transmission spectrum collected on a Cary 6000i spectrophotometer

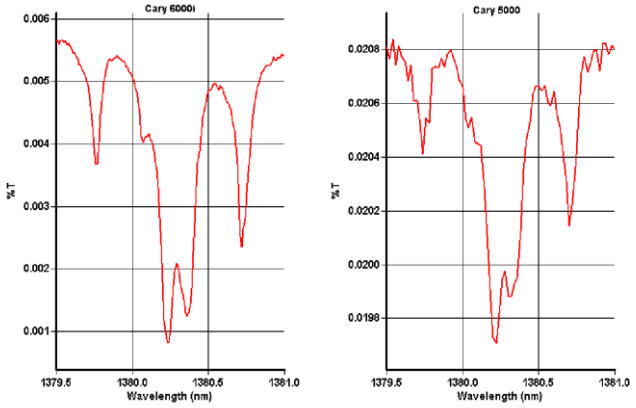

Figure 3: Resolution of the 1380 nm water vapor peak collected on a Cary 6000i and a Cary 5000 spectrophotometer

Discussion

The difference between the Agilent Cary 5000 and 6000i is the minimum resolution and sensitivity. As mentioned earlier, the narrower the SBW setting, the less light hits the detector, which results in poorer S/N or requires a much longer averaging time. The Cary 6000i has a minimum SBW of 0.02 nm and uses an InGaAs detector, which has approximately 100 times greater sensitivity over the traditional PbS detectors used in most NIR measurements.

This is evident in Figure 2, where a signal averaging of 2 seconds was only required to achieve excellent S/N compared to 10 seconds being used for the Cary 5000 instrument, as shown in Figure 1. Also, the SBW setting on the Cary 5000 was 0.05 nm compared to 0.02 nm on the Cary 6000i. This difference in resolution results in the peak at 1380 nm being better resolved into a doublet on the 6000i compared to the 5000, as shown in Figure 3. For comparison, this 1380 nm peak cannot be resolved into a doublet on other UV-Vis-NIR absorption spectrophotometers.

Conclusion

The Agilent Cary 5000 and 6000i instruments are by far the best spectrophotometers on the market today if high sensitivity and fine spectral resolution is required. Both instruments can resolve a peak of <0.5 nm bandwidth, with the additional sensitivity of the Cary 6000i InGaAs detector providing an order of magnitude increase in speed and throughput. Both instruments have provided new technology that will benefit customers in all areas of research.

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Published March, 2011
Publication Number SI-A-1203

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