WAVELENGTH ANOMALIES IN UV-Vis SPECTROPHOTOMETRY

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Commercial spectrophotometers are great tools for recording absorption spectra of low-to-moderate resolution and high photometic quality. However, in the case of at least one such instrument, the Shimadzu UV-2101PC (and by assumption, similar Shimadzu models), the wavelength accuracy may not match the photometric accuracy. In fact the wavelength varies with slit width, spectral sampling interval, and even the specified range, with a smoothing algorithm invoked any time the spectrum includes more than 65 sampled wavelengths. This behavior appears not to be documented anywhere, but it has been present for at least 20 years and persists even in the latest software available to run the instrument. The wavelength shifts can be as large as 1 nm, so for applications where wavelength accuracy better than this is important, wavelength calibration must be done with care to ensure that the results are valid for the parameters used to record the target spectra.