LEAST SQUARES FIT OF LINE PROFILES IN TRANSMITTANCE AND ABSORBANCE SPECTRA WITH DETECTOR OR SOURCE NOISE

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When an observed profile of a spectral line is analyzed using an equally weighted least squares method, the noise property of the spectrum determines whether transmittance or absorbance spectrum is appropriate for the analysis. To verify this, we simulate transmittance spectra (TS) of Lorentz profiles with three simulation parameters of absorption strength, center frequency, and width and add either detector noise (DN) or source noise (SN) to the simulated TS. The TSs with DN or SN and absorbance spectra (AS), negative logarithms of them, are fitted to the Lorentz profile using least squares methods. Equally weighted fits of TS with DN and AS with SN, as statistic mathematics predicts, reproduce the noise magnitude and the parameters well and give the expected uncertainties close to the standard deviations of a thousand simulated spectra regardless of the absorption intensity and the noise magnitude. In contrast, equally weighted fits of TS with SN and AS with DN reproduce the simulation parameters but not the noise magnitude and do not predict the uncertainties of the parameters. Properly weighted fits of TS with SN and AS with DN reproduce the noise magnitude and give the expected uncertainties like those given from equally weighted fits of AS with SN and TS with DN but do not always reproduce the absorption strength and width.