UNCERTAINTIES IN THE FITTING OF SPECTRA

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Fitting spectra produces uncertainties in derived parameters which are known to be deceptive at times. Sometimes results must be quoted to much higher precision than the formal uncertainties or the original spectra cannot be reproduced adequately, while the same parameters reported by various groups may differ by several times the formal uncertainties. For least squares fits to a spectrum, several subtle factors influence the formal uncertainties. The solution is assumed to be linear near the final fit. There is not a straightforward way to incorporate uncertainties associated with physical parameters such as pressure and temperature. Modeling of the spectral line formation and the line shape of the spectrometer are assumed to be known without any uncertainty. The continuum and zero level uncertainties are prone to induce systematic errors that are often not negligible. The correlation between derived parameters in the solution may contribute uncertainty to individual parameters much larger than the uncertainty of certain functions of the same parameters. There is not any satisfactory way of dealing with all of these problems, but some can be minimized. It is possible to extract from a least squares solution the correlation between each pair of derived parameters. Although these correlations point out where problems are, they do not solve them. The correlations may be decreased by including in a single fit several spectra[a] which are recorded with physical conditions that correlate the derived parameters in different ways. This method is considerably more effective than fitting one spectrum at a time, then combining the results. This simultaneous fitting technique points out many of the systematic problems since a combined solution generally has considerably fewer free parameters than the sum of free parameters in the corresponding single spectrum fits.

[a] D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Atkins, *JQSRT* **53**, 705-721 (1995).