A MULTISPECTRUM NONLINEAR LEAST SQUARES FITTING TECHNIQUE: VOIGT CALCULATIONS

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Calculation of the Voigt profile is a time consuming process in any spectrum nonlinear least squares fitting technique. This calculation may be accomplished faster by the use of highly optimized algorithms, but much more gain is possible by carefully minimizing the number of calls to the Voigt algorithm. Storage of some critical calculations in order to eliminate repeated calculation of the same quantities is one such way to minimize the calls. Yet another technique is to find ways to calculate derivatives without recalculation of the spectrum. Truncation of the wings of spectral lines when they are so weak as to not be significant in the calculation is another. Criteria are derived to simplify and reliably choose how far into the wings of a spectral line calculations need be carried.