

A MULTISPECTRUM NONLINEAR LEAST SQUARES FITTING TECHNIQUE: INCLUSION OF LINE MIXING

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An extension to the multispectrum nonlinear least squares fitting technique^a provides the capability to solve for line mixing coefficients without resort to approximations such as that of Rosenkrantz.^b Lorentz, Doppler and instrumental broadening are supported. In general, it is very difficult to obtain unique coefficients for solutions that contain only a single spectrum when the line shape is as complex as that required by line mixing. The fitting of numerous spectra obtained with different physical conditions in the optical path can allow a unique solution. Mathematical techniques have been incorporated which make the calculation of the line profiles and their derivatives not greatly longer than the equivalent spectral lines without line mixing.

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

^bP. W. Rosenkrantz, *IEEE Trans. Antennas Propag.* **AP-23**, 498 (1975).