MULTISPECTRUM FITTING OF FTS AND CRDS SPECTRA SIMULTANEOUSLY

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Various types of spectra contain different sorts of spectral line information. An FTS spectrum provides broad coverage of an identical sample at all parts of the spectrum, but a cavity ring down spectrometer provides higher resolution, more information about line shapes and greater dynamic range in spectral line intensity. In order to use all of the information available, one should put all the spectra available into a single solution. The multispectrum nonlinear least squares fitting technique has proven successful in doing this with transmission spectra from various spectrometers. However, fitting data from cavity ring down spectrometers that produce cross sections is a problem when combined with transmission spectrometers. The solution is to choose a path length for the CRDS data to produce transmissions and use the uncertainty of each cross section as a means of weighting the transmission in the multispectrum solution. This has been incorporated into our fitting technique[a]. Sample oxygen A band fits of CRDS data from NIST combined with FTS data from a high resolution Fourier transform spectrometer in the Infrared, Bruker IFS125-HR, at JPL, equipped with two multipass White cells (absorption path length extendible to 32.5 m and 148 m, respectively) will be shown[b].

[a] D. Chris Benner, C. P. Rinsland, V. M. Devi, M. A. H. Smith, and D. A. Atkins, JQSRT 1995;53:705-21.

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