THE 4850 cm⁻¹ SPECTRAL REGION OF CO₂: CONSTRAINED MULTISPECTRUM NONLINEAR LEAST SQUARES FITTING INCLUDING LINE MIXING, SPEED DEPENDENT LINE PROFILES AND FERMI RESONANCE

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Room temperature spectra of carbon dioxide were obtained with the Fourier transform spectrometers at the National Solar Observatory's McMath-Pierce telescope and at the Jet Propulsion Laboratory. The multispectrum nonlinear least squares fitting technique^b is being used to derive accurate spectral line parameters for the strongest CO_2 bands in the 4700-4930 cm⁻¹ spectral region. Positions of the spectral lines were constrained to their quantum mechanical relationships, and the rovibrational constants were derived directly from the fit. Similarly, the intensities of the lines within each of the rovibrational bands were constrained to their quantum mechanical relationships, and the band strength and Herman-Wallis coefficients were derived directly from the fit. These constraints even include a pair of interacting bands with the interaction coefficient derived directly using both the positions and intensities of the spectral lines. Room temperature self and air Lorentz halfwidth and pressure induced line shift coefficients are measured for most lines. Constraints upon the positions improve measurement of pressure-induced shifts, and constraints on the intensities improve the measurement of the Lorentz halfwidths. Line mixing and speed dependent line shapes are also required and characterized.

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^bD. Chris Benner, C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, and D. Atkins, J. Quant. Spectrosc. Radiat. Transfer 53, 705-721 (1995)