LINE PARAMETERS OF ETHANE ($^{12}C_2H_6$) AT 12 μm WITH CONSTRAINED MULTISPECTRUM FITTING

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A multispectrum nonlinear least squares technique[a] was applied to simultaneously fit 43 infrared absorption spectra of C_2H_6 between 795 and 850 cm^{-1}. The high resolution (0.0016-0.005 cm^{-1}) spectra were recorded with two different Bruker Fourier transform spectrometers at PNNL and JPL to support Earth and planetary atmosphere studies, e.g. Titan's cold stratosphere. Accurate line positions and absolute intensities at room temperature were retrieved for over 1750 transitions of ν_9. N_2- and self-broadened halfwidth coefficients with their temperature dependences were obtained for over 1330 lines using sample temperatures between $\sim$150 and 298 K. Constraints to intensity ratios, torsional splittings, halfwidth coefficients and their temperature dependence exponents were incorporated in the analysis to determine these parameters for both torsional split components. The variations of the observed halfwidth coefficients and their temperature dependences with respect to J, K quanta are discussed. No pressure-induced shifts were measured or even required to fit the spectra to their noise levels. Present results are compared with previously reported measurements and predictions.[b]

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

[b] Part of the research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, the College of William and Mary, Connecticut College, and NASA Langley Research Center under contracts and cooperative agreements with the National Aeronautics and Space Administration.