SPECTRAL LINE PARAMETERS IN THE ν_4 BAND OF CH₃CN

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To support remote sensing of the atmosphere of Titan, we are analyzing CH₃CN, a predicted constituent with spectral signatures in the mid- and far infrared that are candidates for detection in the emission spectra recorded by the Composite Infrared Spectrometer (CIRS). The parallel ν_4 band of CH₃CN near 920 cm⁻¹ has been analyzed in high resolution (0.0016 cm⁻¹) laboratory spectra of pure and N₂-broadened CH₃CN recorded at room temperature using the Bruker 125 HR Fourier transform spectrometer located at the Pacific Northwest National Laboratory (PNNL). These data have been fitted simultaneously with the multispectrum nonlinear least squares technique^{*a*} in order to maximize the accuracy of the retrieved parameters. Short spectral intervals containing manifolds of transitions from the same value of *J* are fitted together. In all, we have obtained accurate line positions, absolute line intensities, self- and N₂-broadening coefficients for the P(44) through P(3) and R(0) through R(46) manifolds. Pressure-induced shifts were also determined where possible. Variation of the width and shift coefficients with the *J* and *K* quantum numbers will be discussed. Intensities will be analyzed and compared to the integrated absorption coefficients reported by Rinsland et al.^{*b*} The status of the assignments for CH₃CN in the mid- and far infrared regions is discussed.

^{*a*}D. Chris Benner et al. *JQSRT* <u>53</u>, 705-721, 1995. ^{*b*}Curtis P. Rinsland et al. *JQSRT* <u>96</u>, 271-280, 2005.