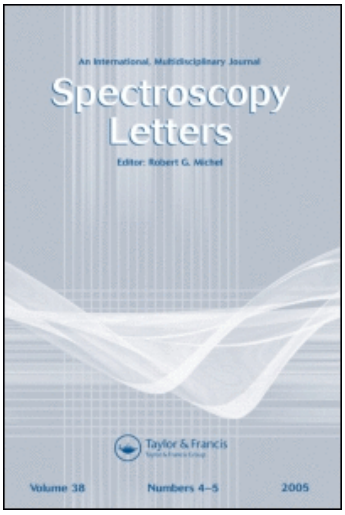

Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

Self-Broadening Coefficients of CH_3D Spectral Lines in the P-Branch of the v_2 Band at 2200 cm^{-1}

Carlos B. Suárez[a]; Charles Chackerian Jr[b]; Francisco Valero[b]
[a] Programa Quinor and CONICET, La Plata, Argentina [b] NASA-Ames Research Center, Moffett Field, California

To cite this Article Suárez, Carlos B. , Chackerian Jr, Charles and Valero, Francisco(1993) 'Self-Broadening Coefficients of CH_3D Spectral Lines in the P-Branch of the v_2 Band at 2200 cm^{-1}', Spectroscopy Letters, 26: 8, 1523 — 1527
To link to this Article: DOI: 10.1080/00387019308011630
URL: http://dx.doi.org/10.1080/00387019308011630

SPECTROSCOPY LETTERS, 26(8), 1523-1527 (1993)

Self-Broadening Coefficients of CH_3D Spectral Lines in the P-Branch of the ν_2 Band at 2200 cm^{-1}.

Keywords: Spectroscopy-Infrared Spectra-Half-Widths-Fourier Spectroscopy.

Carlos B. Suárez,
Programa Quinor and CONICET, C.C. 962, 1900 La Plata, Argentina

Charles Chackerian, Jr. and Francisco Valero,
NASA-Ames Research Center, Moffett Field, California.

ABSTRACT: We report the pressure broadening coefficients of 18 lines of the P-branch of the ν_2 band of CH_3D near 2200 cm^{-1}, obtained at room temperature, using a Fourier Transform spectrometer with a resolution of 0.006 cm^{-1}.

INTRODUCTION

We have measured the half-width at half-height of 18 individual lines of the P branch in the ν_2 band of CH_3D near 2200 cm^{-1} at room temperature, obtaining the pressure broadening coefficients.

Together with line intensities, half-widths are essential parameters for modeling band spectra which is a powerful tool to estimate abundances and to understand the dynamical structures of planetary atmospheres. In fact, CH_3D has been detected in the atmospheres of Jupiter, Saturn and Titan, as a minor component but showing strong spectroscopic features in the vecinity of the 5μm observation window.

Chackerian Jr. et al[1] have studied this interesting species from several points of view, determining spectroscopic constants and line modeling

parameters. In the case of the ν_2 band they reported absolute intensities using Fourier Transform spectroscopy at high resolution for all three P, Q and R branches. However, for broadening coefficients they report values for only five P lines.

In our present case, we report self-broadening coefficients for 18 lines in the P branch, with the added value that each one has been obtained after reducing data from 7 different experiments, with the corresponding improved statistics.

EXPERIMENTAL CONDITIONS

The spectra analyzed here were recorded with a Bomem DA 3.002 Fourier Transform spectrometer with actual resolution of 0.006 cm^{-1}, in the spectral region of 2000-2220 cm^{-1}, using an InSb detector cooled at liquid Nitrogen temperatures and scanning typically 30 times. The absorption cells were made of stainless steel with Sapphire windows and Indium gaskets. The temperature (293.6 K) was measured by means of a calibrated thermocouple and was simultaneously monitored on a strip chart recorder. The pressure was measured with a MKS Baratron capacitance manometer. We recorded spectra at seven different pressures: 50.9 and 149.9 torr using a cell of 2 mm in length; and at 59.85, 77.5, 100.0; 143.1 and 213.9 torr, using a 5 mm cell in these cases.

The spectral intensities, half-widths and wavenumbers were obtained by means of non-linear least-squares fitting techniques applied to each individual lines or multiplets, as needed, according to the procedure explained in ref. 1. However, to determine intensities we think that the

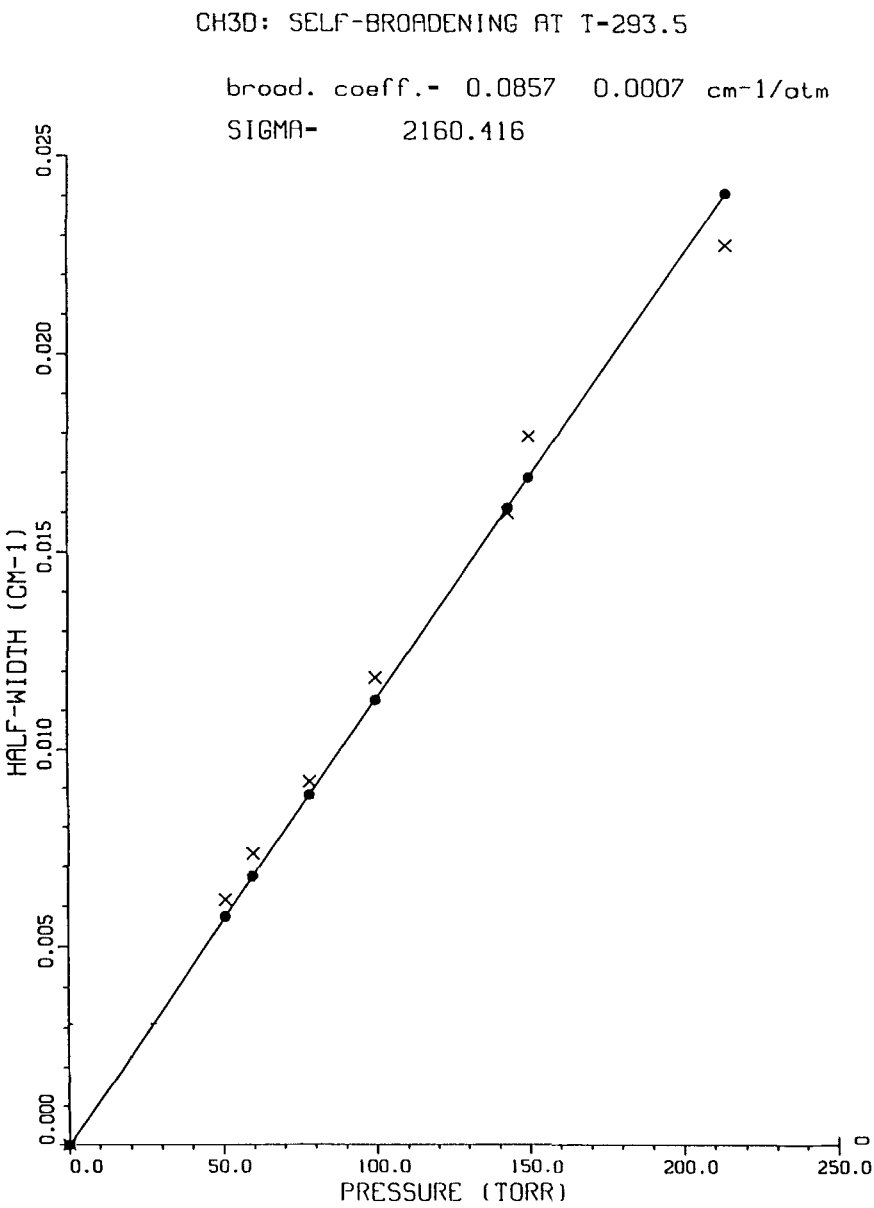

Fig.1-Typical case of a plot of Half-Widths against pressure. A cross indicates the measured value. A straight line has been drawn through the dots which correspond to the recalculated values. The slope provides the broadening coefficient.

Table 1: Self-Broadening Coefficients for the P-Branch of the ν_2 Band of CH_3D

J,K	wavenumber cm^{-1}	broadening coefficient cm^{-1}/atm
7,0	2144.007	0.0846 ±0.0006
7,1	2144.046	0.0766 ±0.0005
7,2	2144.165	0.0767 ±0.0007
7,3	2144.364	0.0758 ±0.0005
7,4	2144.643	0.0814 ±0.0010
7,5	2144.999	0.0817 ±0.0007
7,6	2145.431	0.0817 ±0.0006
6,0	2152.251	0.0868 ±0.0010
6,1	2152.290	0.0770 ±0.0008
6,2	2152.408	0.0772 ±0.0009
6,3	2152.605	0.0766 ±0.0007
6,4	2152.880	0.0762 ±0.0009
6,5	2153.233	0.0793 ±0.0018
5,0	2160.416	0.0857 ±0.0007
5,1	2160.455	0.0770 ±0.0007
5,2	2160.572	0.0785 ±0.0011
5,3	2160.768	0.0797 ±0.0006
5,4	2161.040	0.0809 ±0.0008

measurements at the lower pressures are more convenients. At higher pressures, overlapping and wing corrections make the constants obtained less reliable. For that reason we do not average those values with data obtained at lower pressures where we find agreement with the values reported in ref. 1 so we do not need to reproduce them here again.

To reduce the experimental measured half-widths for the seven different pressures we plotted these values against the corresponding pressure for each spectral line, as shown in Fig. 1. These points, together with the origin, should line up in a straight line. We fitted by means of least-squares routines and obtained the slope and its related error. This slope is the self-broadening coefficient for the particular line we plot. Fig. 1 shows a

typical example with the experimental values scattered closely to the theoretical fitting line.

The values obtained are reported in Table 1 in cm^{-1}/atm, together with the corresponding error brackets.

RESULTS AND CONCLUSION

With the experimental setup described we recorded the whole region specified, but we report only the broadening coefficients of 18 individual lines of the P branch at room temperature, as shown in Table 1. In our model we can reproduce the whole spectrum using the line intensities and the half-widths, besides the wavenumbers. We compared point by point the recalculated values with the experimental data, showing that the goodness of the fit is much better than one percent.

Summarizing, we have completely resolved the spectrum in the vecinity of 2200 cm^{-1} which is an important observational window, obtaining accurateself-broadening coefficients of representative individual lines of the P branch of CH_3D at room temperature.

ACKNOWLEDGMENT

One of us (CBS) is greatly indebted to the National Research Council for economic support.

REFERENCE

1. Chackerian Jr. C. and Guelachvili, G. Direct Retrieval of Lineshape Parameters: Absolute Line Intensities for the ν_2 Band of CH_3D. J.Molec.Spectr. 1983; **97**: 316-332.

Date Received: March 23, 1993
Date Accepted: May 7, 1993