Research Article

Line Intensity Measurements of the $\nu_7 + \nu_8$ Band of Ethylene ($^{12}\text{C}_2\text{H}_4$)

G. B. Lebron and T. L. Tan

Natural Sciences and Science Education, National Institute of Education, Nanyang Technological University,
1 Nanyang Walk, Singapore 637616

Correspondence should be addressed to T. L. Tan; augustine.tan@nie.edu.sg

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From the four high-resolution FTIR absorbance spectra recorded at a spectral resolution of 0.0063 cm^{-1} , 123 line intensities belonging to the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$ were measured and fit. The upper $\nu_7 + \nu_8 = 1$ state rovibrational constants up to sextic terms determined using a Watson's *A*-reduced Hamiltonian model in I' representation were used to calculate the line intensities of the band. Results of the experimental fit of the line intensities agree well with those obtained by calculations.

1. Introduction

Spectroscopists take special interest in ethylene ($^{12}\text{C}_2\text{H}_4$) for its atmospheric and astrophysical importance. Ethylene is naturally present in the atmosphere and is one of several precursors for the formation of tropospheric ozone, a pollutant that has adverse effects on human health. It also has been detected in the atmospheres of the Jovian planets Jupiter, Saturn, Neptune [1–4] and the satellite Titan [5]. Since accurate rotation-vibration parameters and knowledge of line positions and intensities are needed in the detection and monitoring of ethylene in the atmosphere, there have been a number of ethylene studies on the subject in the literature (e.g., [6–10]). As part of our ongoing FTIR investigation of ethylene and its isotopic variants [11–21], determination of the upper state rovibrational constants and line intensity measurements of the *A*-type $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$ in the $1820\text{--}1950\text{ cm}^{-1}$ region were performed. The present study aims to contribute to the limited but growing body of knowledge on ethylene line positions and intensities.

Previous studies on the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$ include [22–25] which all considered the Coriolis interactions between the band and the $\nu_4 + \nu_8$ and $\nu_8 + \nu_{10}$ states. Ben Hassen and coworkers [6] measured the absolute line intensities of ethylene in the $1800\text{--}2350\text{ cm}^{-1}$ region. According

to a previous paper [25], 39 of the 264 line intensities they measured belonged to the $\nu_7 + \nu_8$ band.

In the present study, the upper $\nu_7 + \nu_8 = 1$ state rovibrational constants up to sextic centrifugal distortion terms were determined first using a standard Watson's Hamiltonian model. The derived parameters were then used to calculate line intensities and positions of the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$. From the high-resolution FTIR spectra collected in the laboratory, 123 ethylene line positions and intensities were measured using a peak fitting analysis that implemented the Levenberg-Marquardt algorithm. We found the fit to be satisfactory falling within 6% error when compared to the calculated line intensities.

2. Experimental Details

A Bruker 125HR Fourier transform spectrometer located at the FTIR laboratory of the National Institute of Education, Nanyang Technological University, in Singapore was used to record all high-resolution infrared spectra used for the present study. It was equipped with a Global mid-infrared source, a high sensitivity liquid nitrogen-cooled Hg-Cd-Te detector, and a KBr beamsplitter. By adjusting for four passes in the multiple absorption gas cell with a 20 cm base length, an absorption length of 80 cm was attained. The background spectra and the infrared spectra of the 99.99%

FIGURE 1: The four high-resolution FTIR spectra showing the $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ in the 1820–1950 cm^{-1} region collected at different pressures (see Table 1).

pure ethylene gas samples purchased from Sigma-Aldrich, USA, were recorded at a spectral resolution of 0.0063 cm^{-1} and at an ambient temperature of 296 K in the 1.628×10^{-4} – 8.954×10^{-4} atm vapor pressure range. A capacitance pressure gauge was installed on the gas cell.

The sample spectra were coadded, and the resultant average spectrum was ratioed against the background spectrum to generate a transmittance spectrum with a smooth baseline and high signal-to-noise ratio. The gas samples contained water vapor as impurities and the unblended water absorption lines recorded in the 1607–1831 cm^{-1} region along with the standard water wavenumber values taken from Guelachvili and Rao [26] were used to calibrate the transmittance spectrum. From the least-square fitting of 62 water frequencies, a relative precision of 0.00012 cm^{-1} for all measured frequencies was achieved. The correction factor applied to the measured spectrum was 1.000000343. The frequencies from the corrected spectrum were used in the determination of the rotation-vibration constants of the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$.

Four of the seven sample spectra recorded were also used to measure line intensities of the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$. Each of the four sample spectra which are shown in Figure 1 were calibrated using water absorption lines as discussed above. Table 1 presents these spectra and the calibration results for each spectrum. After calibration, each of the spectra was converted to an absorbance spectrum.

3. Rovibrational Analysis of the $\nu_7 + \nu_8$ Band of Ethylene

In Figure 2, the 1820–1950 cm^{-1} region of the transmittance spectrum where the $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ is located is shown. As evident in Figure 2, the band exhibits

FIGURE 2: An overview of the FTIR absorption spectrum of the $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ in the 1820–1950 cm^{-1} region collected at a resolution of 0.0063 cm^{-1} .

the characteristic contour features of an A-type band: moderate P- and R-branches on opposite ends and a strong Q-branch in the middle. A rather straightforward rovibrational analysis of the unperturbed lines of the band was carried out using a standard A-reduced Watson's Hamiltonian in I' representation [27]. For this, the nonlinear least-squares fitting program originally written by Maki [28] was used. For the initial assignments and calculations, we used the line list provided by Herman [29] and the ground state constants from [30]. As more lines were assigned and fitted, the upper $\nu_7 + \nu_8 = 1$ state rovibrational constants were calculated and improved. A weighting equivalent to the inverse square of the estimated uncertainty (0.0006 cm^{-1}) assigned to each infrared transition was applied to the fitting procedure. The final fit with a root mean square (rms) deviation of 0.000653 cm^{-1} included a total of 391 infrared transitions. The rovibrational constants determined for the excited state consisted of the three rotational constants, the band center, all five quartic, and two sextic centrifugal distortion parameters. Table 2 presents the results of the rotational analysis.

4. Line Intensity Measurements and Calculations

Extraction of the line positions and intensities in the 1820–1950 cm^{-1} spectral region of all four high-resolution absorbance spectra of $^{12}\text{C}_2\text{H}_4$ (see Table 1) was done using a peak fitting analysis that implemented the Levenberg-Marquardt algorithm. Although the vapor pressure range may be considered to be on the low side, each peak was fitted to a Voigt profile which accounts for the effects of both Doppler and collisional broadening. Figure 3 illustrates the quality of the peak fitting analysis that was performed in Spectrum no. 2 (see Table 1). The blue circles are actual data points extracted from Spectrum no. 2, and the red line traces the Voigt profile fit. The bottom panel of Figure 3 gives the residual plot (observed – calculated).

TABLE 1: Infrared spectra collected for this study and wavenumber calibration results.

Spectrum no.	No. of scans	Pressure ($\times 10^{-4}$ atm)	Calibration results	
			RMS error $\times 10^{-4}$ (cm^{-1})	Correction factor
1	200	1.628	1.6	1.000000360
2	200	4.569	1.5	1.000000353
3	150	6.409	1.8	1.000000336
4	60	8.954	1.6	1.000000339

TABLE 2: Ground state and upper $\nu_7 + \nu_8 = 1$ state rovibrational constants (cm^{-1}) for the $\nu_7 + \nu_8$ combination band of $^{12}\text{C}_2\text{H}_4$ (A-reduction and I' representation).

	Ground state [30]	$\nu_7 + \nu_8 = 1$ state
A	4.8646201954 (464) ^a	4.870611 (24) ^a
B	1.0010565039 (119)	0.9895253 (22)
C	0.8280459778 (117)	0.8303283 (11)
$\Delta_J \times 10^6$	1.4702286 (406)	1.3957 (37)
$\Delta_{JK} \times 10^4$	0.102319954 (3678)	0.2836 (27)
$\Delta_K \times 10^4$	0.86486844 (1953)	1.17094 (85)
$\delta_J \times 10^6$	0.2816829 (149)	0.2361 (14)
$\delta_K \times 10^4$	0.10161652 (1391)	0.2155 (11)
$\Phi_J \times 10^9$	0.0024347 (503)	[0.0024347] ^b
$\Phi_{JK} \times 10^9$	0.194771 (3364)	0.428 (60)
$\Phi_{KJ} \times 10^6$	-0.00045941 (1185)	-0.4229 (54)
$\Phi_K \times 10^9$	6.24752 (1300)	[6.24752] ^b
$\varphi_J \times 10^9$	0.00112776 (1669)	[0.00112776] ^b
$\varphi_{JK} \times 10^9$	0.110854 (2077)	[0.110854] ^b
$\varphi_K \times 10^9$	3.7555 (1030)	[3.7555] ^b
ν_0	—	1888.978834 (92)
no. of IR transitions	—	391
rms deviation (cm^{-1})	—	0.000653

^aThe uncertainty in the last digits (twice the estimated standard error) is given in parentheses.

^bFixed to ground state value (see column 2).

Beer's law could be expressed as [31]:

$$S' = \frac{1}{pl} \int \ln \frac{I_0}{I} d\nu. \quad (1)$$

In the above equation, S' is the experimental line intensity given in $\text{cm}^{-1}/(\text{cm atm})$, p is vapor pressure in atm, l is the path length which for this study was 80 cm (see Section 2), and I_0 and I are the incident and transmitted intensities of light, respectively, at frequency ν . From the peak fitting analysis that has just been described, $\ln A = \int \ln(I_0/I) d\nu$ (in cm^{-1}) was obtained for each peak. To determine the experimental line intensity, $\ln A = \int \ln(I_0/I) d\nu$ was plotted against p , and the gradient of the best fit line passing through the origin gives the experimental line intensity. An example of this pressure dependence plot is shown in Figure 4 for line positions $1880.27874 \text{ cm}^{-1}$ in the P-branch and $1904.99430 \text{ cm}^{-1}$ in the R-branch.

FIGURE 3: Part of peak fitting analysis performed in observed Spectrum no. 2 ($P = 4.569 \times 10^{-4}$ atm) with the corresponding residuals in the lower panel (peak nos. 40–43 in Table 3).

FIGURE 4: Beer's law plot showing pressure dependence for two lines.

TABLE 3: Line positions, assignments, and intensities of the $\nu_7 + \nu_8$ band of $^{12}\text{C}_2\text{H}_4$.

Peak no.	J'	K'_a	K'_c	J''	K''_a	K''_c	Measured wavenumber (cm^{-1})	O – C (cm^{-1})	Line intensities [$\text{cm}^{-1}/(\text{cm atm})$]		% Error
									Expt'l	Calc'd	
1	19	3	16	20	3	17	1848.10619	0.00069	0.01606	0.01560	–2.971
2	21	1	20	22	1	21	1848.64789	–0.00055	0.01446	0.01426	–1.444
3	16	2	14	17	2	15	1854.62328	–0.00084	0.02340	0.02448	4.416
4	19	0	19	20	0	20	1855.23843	–0.00074	0.05011	0.05116	2.047
5	19	1	19	20	1	20	1855.28243	–0.00065	0.02256	0.02266	0.440
6	16	4	13	17	4	14	1856.28998	–0.00058	0.04276	0.04532	5.650
7	15	2	13	16	2	14	1856.70408	–0.00090	0.06124	0.06292	2.675
8	16	1	15	17	1	16	1856.76313	–0.00044	0.02648	0.02639	–0.325
9	18	0	18	19	0	19	1856.82825	–0.00067	0.02456	0.02458	0.076
10	15	3	12	16	3	13	1857.35152	–0.00017	0.02509	0.02532	0.902
11	15	4	12	16	4	13	1858.33672	–0.00039	0.02055	0.02115	2.876
12	14	2	12	15	2	13	1858.81149	–0.00096	0.02864	0.02930	2.245
13	16	0	16	17	0	17	1860.01569	–0.00065	0.03085	0.02989	–3.240
14	16	1	16	17	1	17	1860.11702	–0.00073	0.02960	0.02988	0.934
15	14	1	13	15	1	14	1860.18831	–0.00043	0.03299	0.03133	–5.310
16	14	4	11	15	4	12	1860.37046	–0.00024	0.05120	0.05299	3.380
17	13	2	11	14	2	12	1860.93859	–0.00086	0.06963	0.07323	4.921
18	15	1	15	16	1	16	1861.74391	–0.00072	0.03209	0.03239	0.927
19	13	6	7	14	6	8	1862.56749	0.00067	0.04786	0.04859	1.513
20	12	2	10	13	2	11	1863.07805	–0.00085	0.03328	0.03311	–0.510
21	13	2	12	14	2	13	1863.15373	–0.00080	0.03355	0.03254	–3.104
22	14	0	14	15	0	15	1863.21161	–0.00058	0.03543	0.03471	–2.079
23	14	1	14	15	1	15	1863.37938	–0.00069	0.03465	0.03469	0.123
24	12	1	11	13	1	12	1863.78464	–0.00054	0.03439	0.03536	2.747
25	12	3	9	13	3	10	1863.94266	–0.00074	0.02858	0.02960	3.440
26	11	3	8	12	3	9	1866.04610	–0.00088	0.03105	0.03049	–1.836
27	12	1	12	13	1	13	1866.67826	–0.00071	0.03791	0.03828	0.963
28	11	2	10	12	2	11	1866.80502	–0.00078	0.03435	0.03516	2.313
29	10	2	8	11	2	9	1867.36336	–0.00095	0.03383	0.03504	3.444
30	10	1	9	11	1	10	1867.54113	–0.00063	0.03787	0.03765	–0.588
31	10	3	7	11	3	8	1868.10596	–0.00077	0.03138	0.03081	–1.853
32	10	3	8	11	3	9	1868.28975	–0.00089	0.03255	0.03089	–5.360
33	9	1	8	10	1	9	1869.46527	–0.00067	0.03780	0.03786	0.176
34	9	2	7	10	2	8	1869.49207	–0.00081	0.07921	0.08174	3.103
35	10	1	10	11	1	11	1870.01782	–0.00067	0.03948	0.03990	1.037
36	9	3	6	10	3	7	1870.12636	–0.00092	0.03106	0.03045	–2.017
37	9	3	7	10	3	8	1870.23830	–0.00100	0.03038	0.03050	0.379
38	9	4	6	10	4	7	1870.31021	–0.00038	0.08089	0.08210	1.470
39	9	5	5	10	5	6	1870.40586	0.00016	0.03628	0.03704	2.035
40	9	0	9	10	0	10	1871.28500	–0.00062	0.08776	0.09346	6.102
41	8	1	7	9	1	8	1871.41065	–0.00066	0.03654	0.03734	2.132
42	8	2	6	9	2	7	1871.59872	–0.00082	0.03386	0.03427	1.192
43	9	1	9	10	1	10	1871.70380	–0.00041	0.04055	0.03974	–2.031
44	8	0	8	9	0	9	1872.94192	–0.00074	0.03965	0.03931	–0.865
45	8	1	8	9	1	9	1873.39988	–0.00066	0.03836	0.03885	1.264
46	7	2	5	8	2	6	1873.67558	0.00003	0.07336	0.07621	3.739
47	7	3	4	8	3	5	1874.07039	–0.00074	0.02819	0.02735	–3.083
48	7	4	4	8	4	5	1874.18383	–0.00073	0.06605	0.06964	5.155

TABLE 3: Continued.

Peak no.	J'	K'_a	K'_c	J''	K''_a	K''_c	Measured wavenumber (cm^{-1})	O – C (cm^{-1})	Line intensities [$\text{cm}^{-1}/(\text{cm atm})$]		% Error
									Expt'l	Calc'd	
49	7	2	6	8	2	7	1874.2107	-0.00061	0.03404	0.03289	-3.484
50	7	5	3	8	5	4	1874.27146	-0.00066	0.02911	0.02857	-1.869
51	7	0	7	8	0	8	1874.62617	-0.00062	0.08373	0.08825	5.122
52	6	5	2	7	5	3	1876.18440	-0.00072	0.02076	0.02160	3.899
53	6	0	6	7	0	7	1876.34147	-0.00057	0.03586	0.03554	-0.909
54	6	1	6	7	1	7	1876.82250	-0.00061	0.03563	0.03465	-2.824
55	5	1	4	6	1	5	1877.30902	-0.00069	0.03059	0.03073	0.458
56	5	2	3	6	2	4	1877.71216	-0.00056	0.06023	0.06230	3.326
57	5	1	5	6	1	6	1878.54707	-0.00056	0.03122	0.03130	0.256
58	4	2	2	5	2	3	1879.67047	-0.00048	0.02164	0.02223	2.661
59	4	1	4	5	1	5	1880.27874	-0.00061	0.02718	0.02713	-0.200
60	3	1	2	4	1	3	1881.2420	-0.00060	0.02281	0.02194	-3.970
61	3	2	1	4	2	2	1881.59210	-0.00029	0.03805	0.03881	1.951
62	3	1	3	4	1	4	1882.01624	-0.00051	0.02253	0.02213	-1.780
63	2	1	2	3	1	3	1883.75761	-0.00057	0.01734	0.01630	-6.386
64	4	1	4	3	1	3	1895.92667	-0.00056	0.02389	0.02306	-3.592
65	4	0	4	3	0	3	1896.15857	-0.00065	0.02545	0.02499	-1.835
66	4	2	3	3	2	2	1896.23848	-0.00044	0.04011	0.04055	1.083
67	4	2	2	3	2	1	1896.28176	-0.00034	0.01777	0.01738	-2.226
68	4	1	3	3	1	2	1896.47926	-0.00063	0.02295	0.02295	0.008
69	5	1	5	4	1	4	1897.64824	-0.00057	0.02920	0.02856	-2.219
70	5	0	5	4	0	4	1897.90300	-0.00069	0.06879	0.07038	2.260
71	6	1	6	5	1	5	1899.36413	-0.00061	0.03363	0.03330	-0.981
72	6	0	6	5	0	5	1899.62494	-0.00064	0.03432	0.03465	0.955
73	6	2	5	5	2	4	1899.77723	-0.00054	0.06549	0.06667	1.769
74	6	1	5	5	1	4	1900.10630	-0.00061	0.03410	0.03289	-3.656
75	7	1	7	6	1	6	1901.07464	-0.00064	0.03734	0.03724	-0.261
76	7	0	7	6	0	6	1901.32589	-0.00069	0.08671	0.08953	3.142
77	7	4	3	6	4	2	1901.67885	-0.00084	0.06004	0.06347	5.407
78	7	2	5	6	2	4	1901.72320	-0.00076	0.07384	0.07622	3.127
79	7	5	2	6	5	1	1901.74327	-0.00048	0.02443	0.02331	-4.805
80	8	1	8	7	1	7	1902.78030	-0.00068	0.04118	0.04035	-2.046
81	8	0	8	7	0	7	1903.00952	-0.00067	0.04122	0.04128	0.131
82	8	2	7	7	2	6	1903.26718	-0.00069	0.07925	0.08368	5.293
83	8	3	6	7	3	5	1903.38554	-0.00083	0.03151	0.02986	-5.501
84	8	3	5	7	3	4	1903.40236	-0.00088	0.02999	0.02986	-0.408
85	8	5	4	7	5	3	1903.48914	-0.00039	0.02967	0.03117	4.811
86	8	2	6	7	2	5	1903.53266	-0.00072	0.03610	0.03582	-0.796
87	8	1	7	7	1	6	1903.64766	-0.00060	0.03873	0.03942	1.754
88	9	1	9	8	1	8	1904.48187	-0.00069	0.04269	0.04261	-0.181
89	9	0	9	8	0	8	1904.68064	-0.00068	0.09736	0.10117	3.759
90	9	2	8	8	2	7	1904.99430	-0.00073	0.03804	0.03814	0.258
91	9	3	7	8	3	6	1905.13308	-0.00097	0.03196	0.03239	1.312
92	9	5	5	8	5	4	1905.22533	0.00033	0.03566	0.03708	3.823
93	9	2	7	8	2	6	1905.33298	-0.00080	0.08518	0.08876	4.041
94	9	1	8	8	1	7	1905.38538	-0.00066	0.04257	0.04135	-2.948
95	10	1	10	9	1	9	1906.18023	-0.00068	0.04431	0.04404	-0.606
96	10	0	10	9	0	9	1906.34476	-0.00062	0.04372	0.04462	2.022
97	10	2	9	9	2	8	1906.71002	-0.00079	0.08937	0.09230	3.178

TABLE 3: Continued.

Peak no.	J'	K'_a	K'_c	J''	K''_a	K''_c	Measured wavenumber (cm ⁻¹)	O – C (cm ⁻¹)	Line intensities [cm ⁻¹ /(cm atm)]		% Error
									Expt'l	Calc'd	
98	10	1	9	9	1	8	1907.10144	-0.00056	0.04345	0.04241	-2.436
99	10	2	8	9	2	7	1907.11905	-0.00094	0.03971	0.03936	-0.868
100	12	1	12	11	1	11	1909.57111	-0.00073	0.04447	0.04453	0.149
101	12	0	12	11	0	11	1909.67100	-0.00035	0.04414	0.04486	1.608
102	12	3	9	11	3	8	1910.40373	-0.00068	0.03404	0.03492	2.519
103	12	1	11	11	1	10	1910.47072	-0.00054	0.04105	0.04215	2.613
104	13	1	13	12	1	12	1911.26574	-0.00064	0.04612	0.04373	-5.480
105	13	2	12	12	2	11	1911.79607	-0.00068	0.03899	0.03920	0.539
106	14	0	14	13	0	13	1913.01332	-0.00060	0.04431	0.04249	-4.279
107	14	2	13	13	2	12	1913.47402	-0.00060	0.08445	0.08824	4.298
108	14	3	11	13	3	10	1913.85956	-0.00042	0.03315	0.03317	0.039
109	14	2	12	13	2	11	1914.04936	-0.00093	0.03640	0.03694	1.465
110	15	2	14	14	2	13	1915.14502	-0.00055	0.03635	0.03597	-1.073
111	15	3	12	14	3	11	1915.57036	0.00013	0.03122	0.03153	0.977
112	15	2	13	14	2	12	1915.72204	-0.00072	0.07749	0.08138	4.779
113	16	2	15	15	2	14	1916.81050	-0.00032	0.07632	0.07876	3.102
114	16	3	13	15	3	12	1917.26494	0.00018	0.02985	0.02953	-1.094
115	16	2	14	15	2	13	1917.37156	-0.00090	0.03252	0.03247	-0.157
116	17	1	16	16	1	15	1918.63389	-0.00040	0.03193	0.03197	0.117
117	17	3	14	16	3	13	1918.94100	0.00062	0.02739	0.02725	-0.515
118	18	1	18	17	1	17	1919.76121	-0.00056	0.03258	0.03271	0.389
119	18	0	18	17	0	17	1919.77121	-0.00077	0.03172	0.03274	3.106
120	18	1	17	17	1	16	1920.25070	-0.00056	0.03080	0.02914	-5.706
121	20	3	17	19	3	16	1923.83142	0.00046	0.02002	0.01974	-1.386
122	21	3	18	20	3	17	1925.41296	-0.00049	0.01821	0.01728	-5.359
123	22	1	21	21	1	20	1926.76828	-0.00060	0.01859	0.01809	-2.752

The intensity S_A^B in cm⁻¹/(cm atm) of an individual absorption line with frequency ν_{AB} in cm⁻¹ is given by [7]:

$$S_A^B = \left(\frac{8\pi^3}{3hc} \right) \left(\frac{N}{a} \right) \left(\frac{h\nu_{AB}g_A}{Q_T} \right) (e^{-E_A/hckT}) \times [1 - e^{-h\nu_{AB}/kT}] |\langle A|\mu|B \rangle|^2. \quad (2)$$

In (2), h is Planck's constant in erg·s; c is the speed of light in cm/s; $a = 0.9773$ [32] is the isotopic abundance of ¹²C₂H₄; Q_T is the total partition function; E_A is the energy of the lower state in erg; k is Boltzmann constant in erg/K; T is the temperature in K; and $|\langle A|\mu|B \rangle|$ is the dipole moment operator. For ¹²C₂H₄, the nuclear spin factor g_A has a value of 7 if K_a and K_c of the transition are both even and 3 if otherwise. The total population $N = T_0 L_0 / pT$ where $L_0 = 2.6868 \times 10^{19}$ molecules/cm³ at standard temperature and pressure and $T_0 = 273.15$ K [7]. Using the upper $\nu_7 + \nu_8 = 1$ rovibrational constants we determined (see Table 2), line positions and assignments were generated which in turn were used in (2) for the line intensity calculations. Calculations were made at the same experimental conditions when the high-resolution FTIR spectra were recorded. The calculated dipole moment was 0.0175 D. Table 3 lists the 123 measured and calculated

line intensities along with the observed frequencies and the assignments. The experimental fit was satisfactory with the % error between measured and calculated line intensities within $\pm 6\%$ for all 123 lines. Also, the measured and calculated frequencies agree very closely (see O – C column in Table 3).

5. Conclusion

In the present study, 123 line intensities of the $\nu_7 + \nu_8$ band of ¹²C₂H₄ were measured by carrying out a peak fitting analysis based on Levenberg-Marquardt algorithm. Results of the experimental fit agree well when compared with the line intensities calculated using the upper $\nu_7 + \nu_8 = 1$ rovibrational constants determined for this study.

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