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The spectrum of acetylene in the 5- μm region from new line-parameter measurements

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Abstract

Using Fourier Transform spectra (unapodized FWHM: 0.002 cm^{-1}) of acetylene $^{12}\text{C}_2\text{H}_2$, absolute line positions have been obtained in the 5- μm region for about 490 lines belonging to 15 hot bands arising from the $v_4 = 1$ or $v_5 = 1$ lower vibrational level, improving the data available in this spectral region. Absolute line intensities have been measured for about 410 lines, from which vibrational transition dipole moments squared could be determined, as well as empirical Herman-Wallis coefficients when it was possible. The self-broadening coefficients of more than 370 lines have been measured at room temperature, showing that no vibrational dependence exists for the bands of acetylene already studied, and allowing a significant determination of their rotational dependence. Furthermore, about 120 measured values of self-shifting coefficients are tentatively proposed. Combining results published for other bands, and using the smoothed line-parameter values obtained in this work, a HITRAN-format line list of the acetylene molecule has been set up in this spectral region. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: Acetylene; Infrared; Vibro-rotational transitions; Fourier transform spectroscopy; Transition dipole moment; Line parameters

1. Introduction

The present paper is dedicated to the study of acetylene FT spectra recorded with the Reims interferometer [1,2]. It is the continuation of a previous study [3] in which numerous absolute line

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parameters, i.e., line positions, self-shifting coefficients, intensities, and self-broadening coefficients, were measured for the cold bands of $^{12}\text{C}_2\text{H}_2$ absorbing in the 5- μm spectral region. This region was first studied by Plíva [4,5]. The set of bands arising in this region are important for theoretical calculations [6,7], since they involve energy levels affected by numerous anharmonic, Coriolis, and ℓ -type resonances. The goal of this effort was to complete the experimental quantitative spectroscopic information in this region, mainly as far as line intensities are concerned. A maximum of line parameters were measured for the 15 remaining hot bands, not studied in Ref. [3]. As a result, 406 intensities were obtained for lines belonging to 9 bands of $^{12}\text{C}_2\text{H}_2$ arising from the $v_4 = 1$ lower vibrational level, and to 6 bands arising from the $v_5 = 1$ level, allowing the determination of vibrational transition dipole moments squared and band intensities. As no significant vibrational dependence was observed for the self-broadening coefficients, the 371 new values obtained in this work were included in the set of values given in Ref. [3], in order to deduce a polynomial expansion describing the rotational dependence. A synthetic spectrum of the studied bands was generated, combining the line positions calculated by Plíva [4] and those smoothed in this work when it was possible. Line intensities were calculated from our measured values. To make these data more easily usable, we chose to put them in a HITRAN format line list. For that, the best available experimental data were chosen to update the air-broadening and air-shifting coefficients.

2. Experimental procedure and line-parameter measurements

The step-by-step interferometer [1,2] built at GSMA (Reims) was used under the experimental conditions described in Ref. [3]. The characteristics of the 15 recorded spectra can be found in Table 1. A portion of one of the spectra is given in Fig. 1. Let us recall that two filters were used to cover the whole 1800–2260 cm^{-1} spectral region, and that the middle of the region was inaccessible to study, being on the edge of the two filters. A commercial gas sample, furnished by Air Liquide Alphagaz, with a stated purity of 99.55% in natural abundances, was used without further purification. Cross comparisons [3] with line intensities obtained by other authors in a different spectral region led to the conclusion that the amount of $^{12}\text{C}_2\text{H}_2$ in our cell is known with an uncertainty smaller than 2%.

As in Ref. [3], a multispectrum fitting procedure [8] (hereafter denoted as MSF) was used to retrieve line parameters from the spectra. This procedure was found very efficient to complete the previous results [3] when treating weak bands, or lines located in complicated regions of the spectrum. In this work, the MSF method was used in the same conditions as in Ref. [3]. First, the phase error and the effective iris radius needed to calculate an accurate apparatus function were determined for each spectrum. Second, an average self-collisional narrowing coefficient was obtained [3] to calculate an absorption coefficient that takes into account the collisional narrowing, this value being fixed in the final run of the MSF code. An absolute calibration of the wavenumber scales was also performed [3].

3. Results

The results of this work are given in Table 2. The wavenumber calibration allowed the determination of 486 absolute line positions, with a mean accuracy of $\pm 0.0002 \text{ cm}^{-1}$. As in Ref. [3],

Table 1
Experimental conditions and characteristics of the recorded spectra

Commercial sample (Air Liquide Alphagaz)				
Natural C ₂ H ₂ :		97.760% of ¹² C ₂ H ₂		
Stated purity of natural C ₂ H ₂ :		99.55%		
		Region 1	Region 2	
Maximum path difference (cm)		301	261	
Unapodized FWHM resolution limit (10 ⁻³ cm ⁻¹)		1.7	1.9	
Collimator focal length (mm)		1040	1040	
Useful spectral domain (cm ⁻¹)		1800–1950	1940–2260	
Spectrum No. (Region)	Iris radius (mm)	Total pressure ±0.5% (Torr) ^a	Absorbing path (cm)	Temperature ±0.5 K
1 (2) ^b	2.0	20.68	31.19	295.7 ₅
2 (2)	2.05	4.007	816.6	294.4 ₅
3 (1)	2.02	4.004	816.6	294.3 ₅
4 (1)	2.17	4.013	1616.6	294.9 ₅
5 (2) ^c	2.0	4.016	1616.6	294.9 ₅
6 (2)	2.17	10.14	816.6	295.1 ₅
7 (1)	2.16	10.13	816.6	295.0 ₅
8 (1)	2.25	4.043	2416.6	295.6 ₅
9 (2)	2.26	4.043	2416.6	295.6 ₅
10 (2)	2.17	10.20	1616.6	294.9 ₅
11 (1)	2.25	10.20	1616.6	294.9 ₅
12 (1)	2.2 ^d	49.9	416.6	295.4 ₅
13 (2)	2.2 ^d	49.9	416.6	292.2 ₅
14 (2)	2.29	10.12	2416.6	294.9 ₅
15 (1)	2.30	10.11	2416.6	294.8 ₅

^a 1 Torr = 1.333 hPa.

^b This preliminary spectrum, recorded with a weak optical depth, was not used in the final treatment.

^c This spectrum could not be used in the final treatment, because of a small experimental defect.

^d Average effective iris radius.

the line positions of each sub-band were adjusted, each time that it was possible, by polynomial expansions in order to check the assignments. For that, the *P* and *R* branches of each sub-band were fitted simultaneously, and the *Q* branch separately. (As they are effective, the coefficients obtained for these polynomial expansions are not given here.) Note that the line positions of the *Pee* and *Ree* sub-branches of the $(3\nu_4 + \nu_5)^2\Pi - \nu_4^1$ band cannot be adjusted simultaneously, because of strong interactions already pointed out by Plíva [4]. On the whole, the comparison with Plíva's experimental line positions [4] is quite good, and his extrapolations allowed the assignment of new lines for some of the bands.

Absolute line intensities were measured for 406 lines (see Table 2). The precision is between about ±3 to ±5%, and the accuracy in absolute values is on the average ±5% [3]. The formalism and the relation used to calculate the transition dipole moment squared from the line intensity are the same as those used in previous works (see Eqs. (1)–(6) of Ref. [9]), and the partition function was calculated using the polynomial expansion given by Gamache et al. [10]. The transition dipole

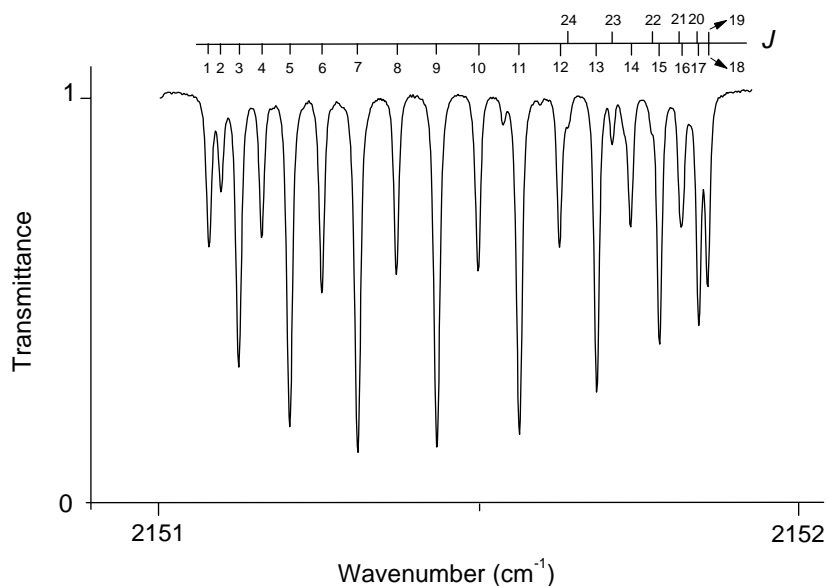


Fig. 1. Portion of spectrum 14 of Table 1, showing the Q branch of the $4\nu_5^0 - \nu_5^1$ band, exhibiting a branch head at $J = 19$, around 2151.9 cm^{-1} . Note the intensity alternation of the $^{12}\text{C}_2\text{H}_2$ lines, and the presence of a few $^{12}\text{C}^{13}\text{CH}_2$ lines.

moments squared have been plotted in Figs. 2–11 for some bands. When it was possible, significant empirical Herman-Wallis coefficients were deduced, without taking into account the resonances. The Herman-Wallis factors were expanded as

$$F^{RP}(m) = [1 + A_1^{RP}m + A_2^{RP}m^2] \quad (1)$$

for P and R branches, m being equal to $J + 1$ in the R branch, and $-J$ in the P branch; and for a Q branch, with m equal to J

$$F^Q(m) = [1 + A_2^Q m(m + 1)]. \quad (2)$$

Note that the terms between brackets are not squared. The band centers and Herman-Wallis coefficients are given in Table 3, together with the vibrational dipole moments squared, and band intensities calculated using Eq. (10) of Ref. [9]. In Table 3, the results obtained in Ref. [3] for the 3 cold bands have also been recalled. Note that for one band with ℓ -type doubling, the two sub-bands could be treated separately. For a few bands, the number of measured line intensities was too weak to allow the determination of Herman-Wallis coefficients, but we thought it useful to deduce, tentatively, values of vibrational transition dipole moments in order to perform predictive calculations of transition dipole moment squared values.

As can be seen in Fig. 10, the simultaneous adjustment of the Pee , Ree , and Qef branches of the $4\nu_5^0 - \nu_5^1$ band (see Fig. 1) is difficult, the Qef low- J lines leading to a vibrational transition dipole moment squared noticeably smaller than for Pee and Ree branches. We checked carefully that for

Table 2
Line parameters obtained for 15 hot bands of $^{12}\text{C}_2\text{H}_2$ in the 5- μm spectral region^a

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
$(3\nu_4 + \nu_5)_+ - \nu_4^1$ <i>Qef</i> 20	1951.49101	1.03D-23	1.02D-23	0.97	1.85D-05	0.1340
$(3\nu_4 + \nu_5)_- - \nu_4^1$ <i>Qfe</i> 4	1972.30691	1.74D-24	1.67D-24	4.02	4.26D-06	—
<i>Qfe</i> 5	1972.37238	5.69D-24	5.87D-24	-3.16	4.02D-06	0.1611
<i>Qfe</i> 6	1972.44668	2.28D-24	2.19D-24	3.95	4.38D-06	0.1605
<i>Qfe</i> 7	1972.52825	6.65D-24	7.13D-24	-7.22	4.00D-06	0.1471
<i>Qfe</i> 9	1972.70409	8.08D-24	7.74D-24	4.21	4.66D-06	0.1537
<i>Qfe</i> 10	1972.79556	2.79D-24	2.60D-24	6.81	4.90D-06	0.1411
<i>Qfe</i> 11	1972.88785	8.31D-24	7.73D-24	6.98	5.03D-06	0.155
<i>Qfe</i> 12	1972.97936	2.24D-24	2.51D-24	-12.05	4.29D-06	—
<i>Qfe</i> 13	1973.07157	6.97D-24	7.20D-24	-3.30	4.78D-06	0.1391
<i>Rff</i> 6	1988.76038	1.77D-24	2.09D-24	-18.08	2.44D-06	0.1547
<i>Rff</i> 10	1998.16100	1.17D-24	1.02D-24	12.82	1.42D-06	0.1450
$(3\nu_4 + \nu_5)^2\text{II} - \nu_4^1$ <i>Pee</i> 9	1924.43559	1.01D-23	1.13D-23	-11.88	3.65D-05	0.1438
<i>Pee</i> 11	1919.93952	1.15D-23	1.21D-23	-5.22	4.04D-05	0.1538
<i>Pee</i> 13	1915.44460	1.17D-23	1.18D-23	-0.85	4.41D-05	0.1505
<i>Pee</i> 15	1910.93702	1.08D-23	1.06D-23	1.85	4.74D-05	0.1441
<i>Pee</i> 17	1906.40816	9.19D-24	8.78D-24	4.46	5.06D-05	0.1390
<i>Pee</i> 19	1901.85420	7.14D-24	6.85D-24	4.06	5.27D-05	0.1283
<i>Pee</i> 21	1897.27439	5.17D-24	5.03D-24	2.71	5.44D-05	0.1196
<i>Pee</i> 23	1892.66951	3.55D-24	3.49D-24	1.69	5.63D-05	0.1143
<i>Pee</i> 27	1883.38747	1.37D-24	1.42D-24	-3.65	5.83D-05	0.1021
<i>Ree</i> 3	1954.65251	1.45D-23	1.69D-23	-16.55	2.74D-05	0.1888
<i>Ree</i> 5	1959.50405	1.62D-23	1.84D-23	-13.58	2.72D-05	0.1740
<i>Ree</i> 9	1969.28797	1.82D-23	1.76D-23	3.30	3.02D-05	0.1758
<i>Ree</i> 13	1979.06574	1.33D-23	1.31D-23	1.50	2.87D-05	0.1457
<i>Ree</i> 17	1988.74504	7.83D-24	7.76D-24	0.89	2.77D-05	0.1305
<i>Ree</i> 19	1993.53792	5.57D-24	5.54D-24	0.54	2.74D-05	0.1288
<i>Ree</i> 21	1998.29918	3.60D-24	3.77D-24	-4.72	2.59D-05	0.1185
<i>Ree</i> 22	2000.66805	9.80D-25	1.02D-24	-4.08	2.62D-05	0.1213
<i>Ree</i> 23	2003.02909	2.34D-24	2.44D-24	-4.27	2.61D-05	0.1133
<i>Ree</i> 24	2005.38241	5.71D-25	6.44D-25	-12.78	2.41D-05	0.1023
<i>Pff</i> 8	1926.35236	7.54D-24	7.72D-24	-2.39	2.91D-05	0.1647
<i>Pff</i> 12	1917.09168	8.67D-24	8.59D-24	0.92	3.12D-05	0.1547
<i>Pff</i> 14	1912.48543	7.83D-24	7.78D-24	0.64	3.17D-05	0.1492
<i>Pff</i> 18	1903.31092	5.26D-24	5.08D-24	3.42	3.36D-05	0.1355
<i>Pff</i> 20	1898.73723	3.72D-24	3.72D-24	0.00	3.29D-05	0.1194
<i>Pff</i> 26	1885.03289	1.01D-24	1.03D-24	-1.98	3.35D-05	0.1043
<i>Rff</i> 4	1956.97997	1.43D-23	1.46D-23	-2.10	2.52D-05	0.1730
<i>Rff</i> 9	1968.96809	4.77D-24	4.77D-24	0.00	2.39D-05	0.1587

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Rff</i> 10	1971.37664	1.35D–23	1.35D–23	0.00	2.35D–05	0.1500
<i>Rff</i> 12	1976.20223	1.15D–23	1.15D–23	0.00	2.29D–05	0.1433
<i>Rff</i> 14	1981.03696	8.96D–24	9.12D–24	–1.79	2.15D–05	0.1397
<i>Rff</i> 16	1985.87757	7.05D–24	6.85D–24	2.84	2.17D–05	0.1332
<i>Rff</i> 18	1990.72098	4.85D–24	4.85D–24	0.00	2.02D–05	0.1267
<i>Rff</i> 20	1995.56303	3.21D–24	3.24D–24	–0.93	1.92D–05	0.1224
<i>Rff</i> 21	1997.98229	8.66D–25	8.67D–25	–0.12	1.89D–05	0.1218
<i>Rff</i> 22	2000.39978	2.01D–24	2.05D–24	–1.99	1.81D–05	0.1095
<i>Rff</i> 24	2005.22692	1.26D–24	1.23D–24	2.38	1.81D–05	0.1173
$(3v_4 + v_5)^2I - v_4^1$						
<i>Ree</i> 9	1997.49134	1.76D–24	1.66D–24	5.68	2.88D–06	0.1547
<i>Ree</i> 10	1999.97071	4.19D–25	4.47D–25	–6.68	2.15D–06	—
<i>Rff</i> 9	1997.18193	1.10D–24	1.13D–24	–2.73	5.43D–06	0.1623
<i>Rff</i> 10	1999.61650	3.34D–24	3.36D–24	–0.60	5.73D–06	0.1511
<i>Rff</i> 11	2002.05801	1.09D–24	1.09D–24	0.00	5.95D–06	0.1470
$v_2 + v_5^1 - v_4^1$						
<i>Pee</i> 2	2085.50461	5.93D–25	5.60D–25	5.56	7.61D–06	0.2030
<i>Pee</i> 3	2083.13324	2.90D–24	2.89D–24	0.34	7.22D–06	0.1896
<i>Pee</i> 4	2080.75264	1.30D–24	1.30D–24	0.00	7.25D–06	0.1838
<i>Pee</i> 5	2078.36110	4.89D–24	4.70D–24	3.89	7.51D–06	0.1866
<i>Pee</i> 6	2075.95998	1.75D–24	1.78D–24	–1.71	7.11D–06	0.1553
<i>Pee</i> 8	2071.12740	2.05D–24	2.03D–24	0.98	7.37D–06	0.1546
<i>Pee</i> 9	2068.69628	6.21D–24	6.20D–24	0.16	7.30D–06	0.1563
<i>Pee</i> 10	2066.25520	2.04D–24	2.05D–24	–0.49	7.26D–06	0.1509
<i>Pee</i> 11	2063.80453	6.01D–24	5.99D–24	0.33	7.33D–06	0.1463
<i>Pee</i> 12	2061.34402	1.93D–24	1.90D–24	1.55	7.44D–06	0.1481
<i>Pee</i> 13	2058.87347	5.36D–24	5.34D–24	0.37	7.36D–06	0.1452
<i>Pee</i> 14	2056.39336	1.70D–24	1.64D–24	3.53	7.64D–06	0.1422
<i>Pee</i> 15	2053.90375	4.41D–24	4.44D–24	–0.68	7.31D–06	0.1375
<i>Pee</i> 16	2051.40431	1.28D–24	1.32D–24	–3.13	7.17D–06	0.1314
<i>Pee</i> 17	2048.89545	3.36D–24	3.46D–24	–2.98	7.19D–06	0.1287
<i>Pee</i> 18	2046.37692	9.92D–25	9.95D–25	–0.30	7.39D–06	0.1346
<i>Pee</i> 19	2043.84896	2.53D–24	2.54D–24	–0.40	7.38D–06	0.1245
<i>Pee</i> 21	2038.76448	1.71D–24	1.76D–24	–2.92	7.23D–06	0.1133
<i>Ree</i> 2	2097.20612	—	9.92D–25	—	—	—
<i>Ree</i> 13	2122.03232	5.68D–24	5.63D–24	0.88	7.02D–06	0.1407
<i>Ree</i> 14	2124.22547	—	1.71D–24	—	—	—
<i>Ree</i> 15	2126.40764	4.67D–24	4.62D–24	1.07	7.01D–06	0.1335
<i>Ree</i> 16	2128.57914	1.35D–24	1.36D–24	–0.74	6.87D–06	0.1330
<i>Ree</i> 18	2132.88897	1.05D–24	1.02D–24	2.86	7.08D–06	—
<i>Pff</i> 2	2085.48245	1.69D–24	1.68D–24	0.59	7.21D–06	0.1987
<i>Pff</i> 3	2083.09866	9.37D–25	9.64D–25	–2.88	7.01D–06	0.1851
<i>Pff</i> 4	2080.70395	3.88D–24	3.89D–24	–0.26	7.20D–06	0.1786

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Pff</i> 6	2075.88097	5.29D–24	5.35D–24	–1.13	7.19D–06	0.1623
<i>Pff</i> 7	2073.45290	1.93D–24	1.94D–24	–0.52	7.26D–06	0.1595
<i>Pff</i> 8	2071.01380	6.12D–24	6.09D–24	0.49	7.33D–06	0.1580
<i>Pff</i> 9	2068.56370	2.09D–24	2.07D–24	0.96	7.40D–06	0.1560
<i>Pff</i> 10	2066.10263	6.27D–24	6.17D–24	1.59	7.45D–06	0.1561
<i>Pff</i> 11	2063.63080	1.97D–24	2.00D–24	–1.52	7.25D–06	0.1455
<i>Pff</i> 12	2061.14798	5.74D–24	5.72D–24	0.35	7.39D–06	0.1476
<i>Pff</i> 14	2056.15000	4.92D–24	4.92D–24	0.00	7.40D–06	0.1414
<i>Pff</i> 15	2053.63583	—	1.48D–24	—	—	—
<i>Pff</i> 16	2051.10914	3.93D–24	3.95D–24	–0.51	7.40D–06	0.1355
<i>Pff</i> 17	2048.57299	—	1.15D–24	—	—	—
<i>Pff</i> 18	2046.02567	2.96D–24	2.98D–24	–0.68	7.41D–06	0.1296
<i>Pff</i> 19	2043.46785	8.54D–25	8.46D–25	0.94	7.56D–06	0.1248
<i>Pff</i> 20	2040.90001	2.11D–24	2.13D–24	–0.95	7.44D–06	0.1221
<i>Pff</i> 21	2038.32139	—	5.86D–25	—	—	—
<i>Rff</i> 2	2097.23112	3.04D–24	2.97D–24	2.30	7.28D–06	0.1940
<i>Rff</i> 4	2101.85096	4.90D–24	4.92D–24	–0.41	7.04D–06	0.1700
<i>Rff</i> 7	2108.69426	2.21D–24	2.18D–24	1.36	7.11D–06	0.1554
<i>Rff</i> 13	2122.06591	1.83D–24	1.86D–24	–1.64	6.83D–06	0.1379
<i>Rff</i> 14	2124.25333	5.09D–24	5.08D–24	0.20	6.91D–06	0.1408
<i>Rff</i> 15	2126.42868	1.52D–24	1.52D–24	0.00	6.89D–06	0.1301
<i>Rff</i> 16	2128.59227	3.98D–24	4.02D–24	–1.01	6.78D–06	0.1320
<i>Rff</i> 18	2132.88475	—	3.00D–24	—	—	—
$(\nu_4 + 3\nu_5)_+^0 - \nu_4^1$						
<i>Pee</i> 1	2143.75278	—	1.35D–24	—	—	—
<i>Pee</i> 11	2121.26792	4.34D–24	4.43D–24	–2.07	4.68D–06	0.1427
<i>Pee</i> 12	2119.10248	—	1.43D–24	—	—	—
<i>Pee</i> 13	2116.94732	3.98D–24	4.08D–24	–2.51	4.91D–06	0.1402
<i>Pee</i> 14	2114.80007	—	1.27D–24	—	—	—
<i>Pee</i> 15	2112.65948	3.52D–24	3.53D–24	–0.28	5.30D–06	0.1373
<i>Pee</i> 16	2110.52345	1.07D–24	1.07D–24	0.00	5.45D–06	0.1336
<i>Pee</i> 17	2108.39073	2.89D–24	2.89D–24	0.00	5.65D–06	0.1338
<i>Qef</i> 1	2146.11288	—	6.74D–25	—	—	—
<i>Qef</i> 2	2146.13234	3.20D–24	3.28D–24	–2.50	3.99D–06	0.1898
<i>Qef</i> 3	2146.15979	1.46D–24	1.46D–24	0.00	4.02D–06	0.1793
<i>Qef</i> 4	2146.19594	5.24D–24	5.34D–24	–1.91	3.93D–06	0.1678
<i>Qef</i> 5	2146.24009	—	2.02D–24	—	—	—
<i>Qef</i> 6	2146.29050	6.51D–24	6.59D–24	–1.23	3.83D–06	0.1584
<i>Qef</i> 8	2146.40888	6.93D–24	6.94D–24	–0.14	3.71D–06	0.1520
<i>Qef</i> 9	2146.47400	2.37D–24	2.27D–24	4.22	3.77D–06	0.1652
<i>Qef</i> 10	2146.54134	6.56D–24	6.50D–24	0.91	3.53D–06	0.1521
<i>Qef</i> 11	2146.60920	1.99D–24	2.02D–24	–1.51	3.33D–06	0.1462
<i>Qef</i> 12	2146.67628	5.34D–24	5.50D–24	–3.00	3.14D–06	0.1383
<i>Qef</i> 13	2146.74032	—	1.63D–24	—	—	—
<i>Qef</i> 15	2146.85428	—	1.20D–24	—	—	—

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Qef</i> 16	2146.89942	3.04D–24	2.99D–24	1.64	2.64D–06	0.1510
<i>Qef</i> 17	2146.93422	—	8.05D–25	—	—	—
<i>Qef</i> 18	2146.96058	—	1.90D–24	—	—	—
<i>Ree</i> 3	2155.70253	—	1.95D–24	—	—	—
<i>Ree</i> 4	2158.14893	—	8.36D–25	—	—	—
<i>Ree</i> 7	2165.58698	3.84D–24	3.73D–24	2.86	4.51D–06	0.1573
<i>Ree</i> 8	2168.09412	—	1.32D–24	—	—	—
<i>Ree</i> 10	2173.14717	—	1.39D–24	—	—	—
<i>Ree</i> 13	2180.78805	3.87D–24	3.87D–24	0.00	4.98D–06	0.1319
<i>Ree</i> 15	2185.90288	3.52D–24	3.39D–24	3.69	5.47D–06	0.1371
<i>Ree</i> 17	2191.01849	2.68D–24	2.81D–24	–4.85	5.33D–06	0.1113
<i>Ree</i> 18	2193.57284	8.46D–25	8.32D–25	1.65	5.85D–06	0.1246
<i>Ree</i> 19	2196.12315	2.30D–24	2.19D–24	4.78	6.23D–06	0.1080
<i>Ree</i> 20	2198.66847	6.04D–25	6.33D–25	–4.80	5.86D–06	0.1186
$(v_4 + 3v_5)_- - v_4^1$						
<i>Pff</i> 7	2155.58657	2.15D–24	2.27D–24	–5.58	6.66D–06	—
<i>Pff</i> 9	2150.97231	2.39D–24	2.40D–24	–0.42	7.21D–06	0.1476
<i>Pff</i> 14	2139.52538	6.54D–24	5.86D–24	10.40	8.78D–06	0.1524
<i>Pff</i> 18	2130.41564	3.79D–24	3.77D–24	0.53	8.61D–06	0.1265
<i>Pff</i> 19	2128.13883	1.10D–24	1.09D–24	0.91	8.83D–06	0.1260
<i>Pff</i> 20	2125.86112	2.79D–24	2.78D–24	0.36	8.98D–06	0.1379
<i>Pff</i> 21	2123.58147	7.62D–25	7.82D–25	–2.62	8.94D–06	0.1140
<i>Pff</i> 22	2121.29928	1.96D–24	1.95D–24	0.51	9.44D–06	0.1007
<i>Pff</i> 24	2116.72697	1.27D–24	1.30D–24	–2.36	9.69D–06	0.1074
<i>Pff</i> 26	2112.14035	8.15D–25	8.21D–25	–0.74	1.03D–05	0.1114
<i>Qfe</i> 4	2172.13684	3.25D–24	2.96D–24	8.92	7.23D–06	—
<i>Qfe</i> 6	2172.33160	3.63D–24	3.68D–24	–1.38	6.33D–06	0.1606
<i>Qfe</i> 7	2172.45459	1.14D–23	1.16D–23	–1.75	6.24D–06	0.1547
<i>Qfe</i> 9	2172.74866	1.19D–23	1.17D–23	1.68	6.20D–06	0.1708
<i>Qfe</i> 10	2172.91866	3.99D–24	3.74D–24	6.27	6.36D–06	0.1694
<i>Qfe</i> 11	2173.10322	1.01D–23	1.06D–23	–4.95	5.55D–06	0.1410
<i>Qfe</i> 14	2173.73697	—	2.59D–24	—	—	—
<i>Qfe</i> 15	2173.97157	6.37D–24	6.73D–24	–5.65	4.81D–06	0.1230
<i>Qfe</i> 18	2174.73790	1.25D–24	1.29D–24	–3.20	4.24D–06	0.1166
<i>Qfe</i> 19	2175.01153	3.20D–24	3.10D–24	3.13	4.26D–06	0.1332
<i>Qfe</i> 20	2175.29265	7.31D–25	8.08D–25	–10.53	3.49D–06	0.0974
<i>Qfe</i> 21	2175.58083	—	2.00D–24	—	—	—
<i>Qfe</i> 22	2175.87561	5.27D–25	5.43D–25	–3.04	3.75D–06	0.1225
<i>Rff</i> 3	2181.47562	9.94D–25	1.06D–24	–6.64	6.31D–06	0.1646
<i>Rff</i> 4	2183.87312	3.99D–24	4.07D–24	–2.01	6.63D–06	0.1731
<i>Rff</i> 5	2186.27704	1.58D–24	1.61D–24	–1.90	6.67D–06	0.1594
<i>Rff</i> 6	2188.68727	5.33D–24	5.47D–24	–2.63	6.68D–06	0.1510
<i>Rff</i> 8	2193.52333	6.46D–24	6.27D–24	2.94	7.18D–06	0.1609
<i>Rff</i> 9	2195.94818	2.27D–24	2.15D–24	5.29	7.47D–06	0.1620

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Rff</i> 10	2198.37662	6.54D-24	6.47D-24	1.07	7.23D-06	0.1549
<i>Rff</i> 12	2203.24185	6.25D-24	6.15D-24	1.60	7.47D-06	0.1437
<i>Rff</i> 13	2205.67688	1.94D-24	1.95D-24	-0.52	7.43D-06	0.1351
<i>Rff</i> 14	2208.11250	5.63D-24	5.45D-24	3.20	7.85D-06	0.1388
<i>Rff</i> 15	2210.54797	1.68D-24	1.67D-24	0.60	7.77D-06	0.1386
<i>Rff</i> 17	2215.41442	1.37D-24	1.35D-24	1.46	8.18D-06	0.1296
<i>Rff</i> 19	2220.27109	1.02D-24	1.03D-24	-0.98	8.29D-06	0.1178
<i>Rff</i> 20	2222.69356	2.65D-24	2.65D-24	0.00	8.55D-06	0.1179
<i>Rff</i> 21	2225.11162	7.21D-25	7.48D-25	-3.74	8.47D-06	0.1082
<i>Rff</i> 22	2227.52454	1.81D-24	1.87D-24	-3.31	8.69D-06	0.1108
<i>Rff</i> 23	2229.93214	5.34D-25	5.14D-25	3.75	9.56D-06	0.1139
<i>Rff</i> 24	2232.33222	—	1.25D-24	—	—	—
$(v_4 + 3v_5)^2\Pi - v_4^1$						
<i>Pee</i> 5	2145.19522	8.47D-25	9.30D-25	-9.80	5.05D-06	0.1719
<i>Pee</i> 7	2140.71162	1.42D-24	1.36D-24	4.23	5.50D-06	—
<i>Pee</i> 9	2136.31818	1.58D-24	1.52D-24	3.80	5.12D-06	—
<i>Pee</i> 15	2123.75708	7.88D-25	8.56D-25	-8.63	3.11D-06	0.1427
<i>Qfe</i>						
<i>Qfe</i> 3	2156.86984	2.60D-24	2.64D-24	-1.54	5.72D-06	0.1985
<i>Qfe</i> 5	2157.03975	4.08D-24	4.20D-24	-2.94	5.66D-06	0.1781
<i>Qfe</i> 6	2157.15237	—	1.58D-24	—	—	—
<i>Qfe</i> 9	2157.60177	5.29D-24	5.39D-24	-1.89	5.70D-06	0.1618
<i>Qfe</i> 10	2157.78734	1.85D-24	1.78D-24	3.78	6.06D-06	0.1508
<i>Qfe</i> 11	2157.99124	4.92D-24	5.17D-24	-5.08	5.53D-06	0.1430
<i>Qfe</i> 12	2158.21234	1.55D-24	1.64D-24	-5.81	5.52D-06	0.1336
<i>Qfe</i> 13	2158.45079	4.87D-24	4.59D-24	5.75	6.18D-06	0.1354
<i>Qfe</i> 14	2158.70606	—	1.40D-24	—	—	—
<i>Qfe</i> 15	2158.97866	3.70D-24	3.79D-24	-2.43	5.68D-06	0.1325
<i>Qfe</i> 16	2159.26748	—	1.12D-24	—	—	—
<i>Qfe</i> 20	2160.57872	6.68D-25	6.01D-25	10.03	6.46D-06	0.1420
<i>Qfe</i> 21	2160.94237	—	1.49D-24	—	—	—
<i>Ree</i>						
<i>Ree</i> 9	2181.36715	3.02D-24	3.15D-24	-4.30	4.53D-06	0.1561
<i>Ree</i> 10	2183.95424	9.65D-25	9.60D-25	0.52	4.53D-06	0.1694
<i>Ree</i> 11	2186.56900	2.35D-24	2.57D-24	-9.36	3.89D-06	0.1475
<i>Ree</i> 13	2191.88594	1.86D-24	1.90D-24	-2.15	3.62D-06	0.1516
<i>Ree</i> 14	2194.59014	—	5.23D-25	—	—	—
<i>Ree</i> 15	2197.32838	1.23D-24	1.26D-24	-2.44	2.97D-06	0.1449
<i>Ree</i> 16	2200.10029	3.30D-25	3.25D-25	1.52	2.73D-06	0.1285
<i>Ree</i> 17	2202.90701	8.67D-25	7.24D-25	16.49	2.76D-06	0.1486
<i>Ree</i> 18	2205.74827	—	1.70D-25	—	—	—
<i>Ree</i> 21	2214.49958	—	8.92D-26	—	—	—
<i>Pff</i>						
<i>Pff</i> 8	2138.10390	—	1.60D-24	—	—	—
<i>Pff</i> 10	2133.52691	1.89D-24	1.72D-24	8.99	5.96D-06	0.1704
<i>Pff</i> 12	2128.98000	1.62D-24	1.63D-24	-0.62	5.24D-06	0.1386
<i>Pff</i> 14	2124.46331	1.45D-24	1.40D-24	3.45	5.27D-06	0.1404

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Pff</i> 20	2111.07756	—	5.49D–25	—	—	—
<i>Qef</i> 2	2156.78218	1.58D–24	1.58D–24	0.00	5.88D–06	0.1956
<i>Qef</i> 4	2156.84337	3.47D–24	3.61D–24	–4.03	5.75D–06	0.1840
<i>Qef</i> 5	2156.88868	1.50D–24	1.46D–24	2.67	6.24D–06	0.1899
<i>Qef</i> 8	2157.09123	5.74D–24	5.89D–24	–2.61	6.29D–06	0.1559
<i>Qef</i> 9	2157.18433	—	2.04D–24	—	—	—
<i>Qef</i> 10	2157.29236	6.04D–24	6.23D–24	–3.15	6.60D–06	0.1376
<i>Qef</i> 12	2157.55739	6.00D–24	6.07D–24	–1.17	7.13D–06	0.1451
<i>Qef</i> 13	2157.71763	—	1.95D–24	—	—	—
<i>Qef</i> 15	2158.10016	1.65D–24	1.72D–24	–4.24	7.66D–06	0.1278
<i>Qef</i> 16	2158.32514	4.79D–24	4.74D–24	1.04	8.33D–06	0.1380
<i>Qef</i> 17	2158.57523	—	1.43D–24	—	—	—
<i>Qef</i> 18	2158.84953	3.65D–24	3.84D–24	–5.21	8.43D–06	0.1253
<i>Qef</i> 19	2159.15019	1.15D–24	1.13D–24	1.74	9.38D–06	0.1296
<i>Rff</i> 3	2166.28463	—	1.13D–24	—	—	—
<i>Rff</i> 7	2175.94330	1.38D–24	1.28D–24	7.25	6.04D–06	0.1850
<i>Rff</i> 8	2178.37623	3.47D–24	3.76D–24	–8.36	5.08D–06	0.1579
<i>Rff</i> 9	2180.81719	1.14D–24	1.21D–24	–6.14	5.16D–06	0.1540
<i>Rff</i> 13	2190.64703	8.06D–25	8.71D–25	–8.06	4.73D–06	0.1419
<i>Rff</i> 14	2193.11961	2.31D–24	2.31D–24	0.00	5.01D–06	0.1445
<i>Rff</i> 15	2195.59698	—	6.69D–25	—	—	—
<i>Rff</i> 16	2198.08092	1.75D–24	1.72D–24	1.71	4.87D–06	0.1447
<i>Rff</i> 17	2200.56769	4.88D–25	4.81D–25	1.43	4.71D–06	—
<i>Rff</i> 19	2205.55717	3.20D–25	3.25D–25	–1.56	4.30D–06	—
<i>Rff</i> 21	2210.56865	—	2.06D–25	—	—	—
$(v_4 + 3v_5)^2\text{I} - v_4^1$						
<i>Pee</i> 7	2162.98253	1.51D–24	1.52D–24	–0.66	5.81D–06	0.1795
<i>Pee</i> 9	2158.54474	—	1.79D–24	—	—	—
<i>Pee</i> 11	2154.17754	—	1.82D–24	—	—	—
<i>Pee</i> 13	2149.88209	1.67D–24	1.66D–24	0.60	5.58D–06	0.1433
<i>Pee</i> 15	2145.65806	1.50D–24	1.39D–24	7.33	5.86D–06	—
<i>Qfe</i> 2	2179.12336	—	5.42D–25	—	—	—
<i>Qfe</i> 4	2179.24463	—	1.24D–24	—	—	—
<i>Qfe</i> 5	2179.33262	4.47D–24	4.54D–24	–1.57	6.12D–06	0.1714
<i>Qfe</i> 6	2179.43912	1.84D–24	1.74D–24	5.43	6.72D–06	—
<i>Qfe</i> 7	2179.56449	5.61D–24	5.73D–24	–2.14	6.33D–06	0.1590
<i>Qfe</i> 8	2179.70894	2.00D–24	2.04D–24	–2.00	6.48D–06	0.1510
<i>Qfe</i> 9	2179.87306	6.25D–24	6.37D–24	–1.92	6.67D–06	0.1515
<i>Qfe</i> 13	2180.73866	—	6.12D–24	—	—	—
<i>Qfe</i> 15	2181.30591	5.52D–24	5.43D–24	1.63	8.37D–06	0.1446
<i>Qfe</i> 16	2181.62628	1.68D–24	1.67D–24	0.60	8.60D–06	0.1341
<i>Qfe</i> 17	2181.97148	4.78D–24	4.54D–24	5.02	9.35D–06	0.1418
<i>Qfe</i> 18	2182.34272	—	1.35D–24	—	—	—

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Qfe</i> 19	2182.74079	3.67D–24	3.59D–24	2.18	9.80D–06	0.1292
<i>Qfe</i> 20	2183.16673	—	1.04D–24	—	—	—
<i>Qfe</i> 21	2183.61912	2.73D–24	2.68D–24	1.83	1.05D–05	0.1261
<i>Qfe</i> 22	2184.10089	—	7.59D–25	—	—	—
<i>Qfe</i> 23	2184.61067	1.86D–24	1.90D–24	–2.15	1.10D–05	0.1185
<i>Qfe</i> 24	2185.14992	5.10D–25	5.24D–25	–2.75	1.14D–05	0.1182
<i>Ree</i> 4	2191.08281	—	1.24D–24	—	—	—
<i>Ree</i> 5	2193.53756	—	3.91D–24	—	—	—
<i>Ree</i> 6	2196.00879	—	1.33D–24	—	—	—
<i>Ree</i> 7	2198.49740	3.86D–24	4.02D–24	–4.15	5.55D–06	0.1620
<i>Ree</i> 8	2201.00310	1.26D–24	1.32D–24	–4.76	5.49D–06	0.1582
<i>Ree</i> 9	2203.52593	3.71D–24	3.84D–24	–3.50	5.51D–06	0.1561
<i>Ree</i> 10	2206.06560	1.18D–24	1.22D–24	–3.39	5.47D–06	0.1546
<i>Ree</i> 12	2211.19617	1.03D–24	1.05D–24	–1.94	5.44D–06	0.1499
<i>Ree</i> 13	2213.78692	—	2.85D–24	—	—	—
<i>Ree</i> 15	2219.01833	2.21D–24	2.23D–24	–0.90	5.30D–06	0.1388
<i>Ree</i> 21	2235.08707	—	7.52D–25	—	—	—
<i>Pff</i> 8	2160.38525	—	1.79D–24	—	—	—
<i>Pff</i> 9	2158.08737	6.18D–25	6.36D–25	–2.91	5.98D–06	—
<i>Pff</i> 10	2155.79874	1.95D–24	1.96D–24	–0.51	6.11D–06	—
<i>Pff</i> 14	2146.75086	—	1.64D–24	—	—	—
<i>Qef</i> 3	2179.11103	—	9.08D–25	—	—	—
<i>Qef</i> 4	2179.13882	3.49D–24	3.61D–24	–3.44	5.72D–06	—
<i>Qef</i> 6	2179.21514	4.90D–24	4.87D–24	0.61	5.98D–06	0.1696
<i>Qef</i> 7	2179.26351	—	1.75D–24	—	—	—
<i>Qef</i> 8	2179.31925	—	5.47D–24	—	—	—
<i>Qef</i> 9	2179.38164	1.81D–24	1.85D–24	–2.21	5.80D–06	—
<i>Qef</i> 10	2179.45104	5.42D–24	5.49D–24	–1.29	5.86D–06	—
<i>Qef</i> 11	2179.52752	1.78D–24	1.77D–24	0.56	5.96D–06	0.1489
<i>Qef</i> 12	2179.61091	5.01D–24	5.05D–24	–0.80	5.89D–06	0.1452
<i>Qef</i> 13	2179.70135	—	1.57D–24	—	—	—
<i>Qef</i> 14	2179.79877	4.48D–24	4.31D–24	3.79	6.17D–06	—
<i>Qef</i> 15	2179.90330	1.27D–24	1.29D–24	–1.57	5.81D–06	—
<i>Qef</i> 16	2180.01500	3.51D–24	3.44D–24	1.99	6.05D–06	0.1346
<i>Qef</i> 17	2180.13359	1.04D–24	1.00D–24	3.85	6.16D–06	—
<i>Qef</i> 20	2180.53273	—	1.84D–24	—	—	—
<i>Qef</i> 22	2180.83519	—	1.23D–24	—	—	—
<i>Qef</i> 24	2181.16509	—	7.84D–25	—	—	—
<i>Qef</i> 25	2181.34158	—	2.04D–25	—	—	—
<i>Qef</i> 26	2181.52519	5.15D–25	4.73D–25	8.16	6.46D–06	—
<i>Qef</i> 27	2181.71774	1.22D–25	1.20D–25	1.64	6.02D–06	—
<i>Rff</i> 2	2186.19459	3.11D–24	3.10D–24	0.32	5.70D–06	0.1965
<i>Rff</i> 3	2188.58454	9.86D–25	1.10D–24	–11.56	4.99D–06	0.1911

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Rff</i> 4	2190.98043	3.45D–24	3.47D–24	–0.58	5.43D–06	0.1735
<i>Rff</i> 6	2195.79712	3.62D–24	3.57D–24	1.38	5.26D–06	0.1651
<i>Rff</i> 7	2198.21814	1.19D–24	1.17D–24	1.68	5.13D–06	0.1682
<i>Rff</i> 8	2200.64772	3.41D–24	3.37D–24	1.17	4.95D–06	0.1591
<i>Rff</i> 10	2205.53626	2.83D–24	2.94D–24	–3.89	4.40D–06	0.1493
<i>Rff</i> 11	2207.99600	8.67D–25	8.86D–25	–2.19	4.28D–06	—
<i>Rff</i> 14	2215.44683	1.65D–24	1.75D–24	–6.06	3.55D–06	0.1475
<i>Rff</i> 17	2223.01882	3.49D–25	3.19D–25	8.60	3.33D–06	—
$v_2 + v_4^1 - v_5^1$						
<i>Pee</i> 2	1839.66051	3.55D–24	3.32D–24	6.48	3.04D–05	0.2213
<i>Pee</i> 3	1837.27846	1.99D–24	1.90D–24	4.52	2.99D–05	0.2022
<i>Pee</i> 4	1834.88150	7.70D–24	7.64D–24	0.78	2.87D–05	0.1827
<i>Pee</i> 5	1832.47013	2.85D–24	3.08D–24	–8.07	2.64D–05	0.1536
<i>Pee</i> 7	1827.60323	3.76D–24	3.78D–24	–0.53	2.83D–05	0.1643
<i>Pee</i> 9	1822.67889	4.06D–24	4.02D–24	0.99	2.88D–05	0.1811
<i>Pee</i> 10	1820.19458	1.20D–23	1.20D–23	0.00	2.86D–05	0.1578
<i>Pee</i> 11	1817.69636	3.86D–24	3.87D–24	–0.26	2.84D–05	0.1577
<i>Pee</i> 12	1815.18338	1.07D–23	1.10D–23	–2.80	2.77D–05	0.1477
<i>Pee</i> 13	1812.65647	3.04D–24	3.44D–24	–13.16	2.52D–05	0.1265
<i>Pee</i> 14	1810.11495	9.20D–24	9.45D–24	–2.72	2.77D–05	0.1408
<i>Ree</i> 2	1851.35101	6.01D–24	5.94D–24	1.16	2.88D–05	0.1933
<i>Ree</i> 3	1853.64461	2.68D–24	2.69D–24	–0.37	2.84D–05	0.1792
<i>Ree</i> 4	1855.92328	9.88D–24	9.90D–24	–0.20	2.84D–05	0.1703
<i>Ree</i> 5	1858.18694	3.80D–24	3.79D–24	0.26	2.85D–05	0.1650
<i>Ree</i> 6	1860.43566	1.25D–23	1.25D–23	0.00	2.85D–05	0.1590
<i>Ree</i> 7	1862.66929	4.45D–24	4.42D–24	0.67	2.87D–05	0.1564
<i>Ree</i> 8	1864.88778	1.42D–23	1.37D–23	3.52	2.97D–05	0.1639
<i>Ree</i> 9	1867.09122	4.59D–24	4.59D–24	0.00	2.85D–05	0.1499
<i>Ree</i> 11	1871.45259	4.35D–24	4.35D–24	0.00	2.85D–05	0.1469
<i>Ree</i> 12	1873.61034	1.24D–23	1.24D–23	0.00	2.86D–05	0.1434
<i>Ree</i> 13	1875.75279	3.79D–24	3.83D–24	–1.06	2.82D–05	0.1393
<i>Ree</i> 14	1877.88003	1.06D–23	1.05D–23	0.94	2.88D–05	0.1391
<i>Ree</i> 15	1879.99174	3.15D–24	3.16D–24	–0.32	2.85D–05	0.1340
<i>Ree</i> 16	1882.08813	8.46D–24	8.39D–24	0.83	2.87D–05	0.1315
<i>Ree</i> 18	1886.23440	6.25D–24	6.30D–24	–0.80	2.82D–05	0.1222
<i>Pff</i> 2	1839.64291	1.02D–24	1.11D–24	–8.82	2.62D–05	0.1883
<i>Pff</i> 3	1837.25376	5.54D–24	5.74D–24	–3.61	2.77D–05	0.1862
<i>Pff</i> 4	1834.85060	2.65D–24	2.57D–24	3.02	2.97D–05	0.1912
<i>Pff</i> 5	1832.43413	9.38D–24	9.35D–24	0.32	2.90D–05	0.1759
<i>Pff</i> 7	1827.56090	1.11D–23	1.15D–23	–3.60	2.80D–05	0.1581
<i>Pff</i> 9	1822.63412	1.23D–23	1.23D–23	0.00	2.90D–05	0.1536
<i>Pff</i> 10	1820.15082	4.31D–24	4.09D–24	5.10	3.08D–05	0.1533
<i>Pff</i> 11	1817.65410	1.21D–23	1.19D–23	1.65	2.98D–05	0.1563
<i>Pff</i> 12	1815.14426	3.87D–24	3.79D–24	2.07	3.00D–05	0.1590

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Pff</i> 13	1812.62128	1.04D–23	1.06D–23	–1.92	2.89D–05	0.1443
<i>Pff</i> 14	1810.08489	3.22D–24	3.25D–24	–0.93	2.93D–05	0.1393
<i>Rff</i> 2	1851.38595	1.89D–24	1.96D–24	–3.70	2.73D–05	0.1781
<i>Rff</i> 3	1853.69334	8.03D–24	8.00D–24	0.37	2.83D–05	0.1839
<i>Rff</i> 4	1855.98694	3.31D–24	3.25D–24	1.81	2.86D–05	0.1778
<i>Rff</i> 5	1858.26666	1.12D–23	1.12D–23	0.00	2.80D–05	0.1673
<i>Rff</i> 6	1860.53248	4.03D–24	4.08D–24	–1.24	2.76D–05	0.1603
<i>Rff</i> 8	1865.02235	4.46D–24	4.44D–24	0.45	2.79D–05	0.1545
<i>Rff</i> 9	1867.24626	1.32D–23	1.34D–23	–1.52	2.73D–05	0.1524
<i>Rff</i> 11	1871.65185	1.26D–23	1.26D–23	0.00	2.75D–05	0.1472
<i>Rff</i> 12	1873.83335	4.11D–24	3.96D–24	3.65	2.85D–05	0.1587
<i>Rff</i> 13	1876.00074	1.09D–23	1.10D–23	–0.92	2.72D–05	0.1439
<i>Rff</i> 14	1878.15390	3.26D–24	3.35D–24	–2.76	2.66D–05	0.1364
<i>Rff</i> 15	1880.29274	8.75D–24	9.01D–24	–2.97	2.65D–05	0.1325
<i>Rff</i> 16	1882.41726	2.74D–24	2.65D–24	3.28	2.81D–05	0.1436
<i>Rff</i> 19	1888.70451	4.31D–24	5.02D–24	–16.47	2.32D–05	0.0916
<i>Rff</i> 21	1892.82342	3.49D–24	3.44D–24	1.43	2.72D–05	0.1191
$(2v_4 + 2v_5)_+^0 \Pi - v_5^1$						
<i>Pee</i> 6	1904.98093	2.81D–24	3.29D–24	–17.08	6.12D–06	—
<i>Pee</i> 8	1900.47404	3.88D–24	3.74D–24	3.61	7.84D–06	0.1548
<i>Pee</i> 10	1896.01826	3.98D–24	3.88D–24	2.51	8.18D–06	0.1519
<i>Pee</i> 14	1887.22406	3.45D–24	3.38D–24	2.03	9.25D–06	0.1403
<i>Pee</i> 15	1885.04210	1.05D–24	1.05D–24	0.00	9.45D–06	0.1316
<i>Pee</i> 16	1882.86408	2.94D–24	2.87D–24	2.38	9.94D–06	0.1343
<i>Pee</i> 18	1878.51283	2.32D–24	2.31D–24	0.43	1.05D–05	0.1264
<i>Pee</i> 20	1874.15802	1.69D–24	1.75D–24	–3.55	1.08D–05	0.1158
<i>Qef</i> 5	1918.95566	5.32D–24	4.85D–24	8.83	6.85D–06	—
<i>Qef</i> 7	1919.03095	5.45D–24	5.54D–24	–1.65	5.97D–06	—
<i>Qef</i> 9	1919.11811	5.17D–24	5.56D–24	–7.54	5.44D–06	—
<i>Qef</i> 11	1919.20882	4.54D–24	5.04D–24	–11.01	5.02D–06	—
<i>Qef</i> 12	1919.25256	1.37D–24	1.54D–24	–12.41	4.81D–06	—
<i>Qef</i> 13	1919.29273	4.39D–24	4.17D–24	5.01	5.51D–06	—
<i>Qef</i> 21	1919.31952	9.74D–25	8.61D–25	11.60	3.82D–06	—
$(2v_4 + 2v_5)_-^0 - v_5^1$						
<i>Pff</i> 9	1910.96858	4.24D–24	4.26D–24	–0.47	8.51D–06	0.1527
$(2v_4 + 2v_5)^2 \Pi - v_5^1$						
<i>Pff</i> 17	1892.95282	3.02D–24	3.28D–24	–8.61	2.99D–05	0.1221
<i>Pff</i> 21	1883.95462	1.63D–24	1.71D–24	–4.91	3.10D–05	0.1157
<i>Pff</i> 23	1879.47637	1.21D–24	1.13D–24	6.61	3.47D–05	—
$4v_5^0 - v_5^1$						
<i>Pee</i> 1	2148.71309	—	1.43D–24	—	—	—

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Pee</i> 2	2146.37971	—	6.32D–24	—	—	—
<i>Pee</i> 5	2139.48877	3.73D–24	3.75D–24	–0.54	2.37D–05	0.1858
<i>Pee</i> 9	2130.53558	4.35D–24	4.65D–24	–6.90	2.34D–05	0.1504
<i>Pee</i> 11	2126.14004	4.55D–24	4.53D–24	0.44	2.60D–05	0.1618
<i>Pee</i> 21	2104.45773	1.62D–24	1.57D–24	3.09	3.36D–05	0.1216
<i>Pee</i> 22	2102.28038	4.01D–24	3.92D–24	2.24	3.42D–05	0.1232
<i>Pee</i> 23	2100.09761	1.08D–24	1.07D–24	0.93	3.44D–05	0.1124
<i>Pee</i> 24	2097.90888	2.60D–24	2.62D–24	–0.77	3.49D–05	0.1045
<i>Pee</i> 25	2095.71381	7.09D–25	7.01D–25	1.13	3.66D–05	0.1151
<i>Pee</i> 28	2089.09248	—	9.28D–25	—	—	—
<i>Qef</i> 1	2151.07562	5.92D–24	6.40D–24	–8.11	2.12D–05	0.1880
<i>Qef</i> 2	2151.09436	3.23D–24	3.45D–24	–6.81	2.14D–05	0.1861
<i>Qef</i> 3	2151.12206	1.29D–23	1.38D–23	–6.98	2.11D–05	0.1773
<i>Qef</i> 5	2151.20178	1.76D–23	1.89D–23	–7.39	2.02D–05	0.1630
<i>Qef</i> 8	2151.36853	6.68D–24	6.97D–24	–4.34	1.89D–05	0.1504
<i>Qef</i> 11	2151.56090	1.83D–23	1.73D–23	5.46	1.80D–05	0.1540
<i>Qef</i> 24	2151.63712	—	5.97D–25	—	—	—
<i>Ree</i> 2	2158.23697	4.25D–24	4.20D–24	1.18	2.33D–05	0.1932
<i>Ree</i> 5	2165.56530	3.05D–24	3.11D–24	–1.97	2.30D–05	0.1616
<i>Ree</i> 6	2168.03917	1.03D–23	1.05D–23	–1.94	2.31D–05	0.1593
<i>Ree</i> 7	2170.52633	3.87D–24	3.82D–24	1.29	2.41D–05	0.1562
<i>Ree</i> 9	2175.53532	4.27D–24	4.15D–24	2.81	2.50D–05	0.1502
<i>Ree</i> 11	2180.57846	4.38D–24	4.12D–24	5.94	2.66D–05	0.1414
<i>Ree</i> 12	2183.10886	1.27D–23	1.20D–23	5.51	2.71D–05	0.1464
<i>Ree</i> 16	2193.24267	9.68D–24	8.90D–24	8.06	2.99D–05	0.1329
<i>Ree</i> 17	2195.77111	2.90D–24	2.66D–24	8.28	3.07D–05	0.1315
<i>Ree</i> 20	2203.32428	5.59D–24	5.26D–24	5.90	3.20D–05	0.1183
<i>Ree</i> 21	2205.82828	1.47D–24	1.49D–24	–1.36	3.06D–05	0.1045
<i>Ree</i> 22	2208.32469	3.82D–24	3.73D–24	2.36	3.24D–05	0.1096
<i>Ree</i> 23	2210.81323	1.01D–24	1.03D–24	–1.98	3.18D–05	0.1047
<i>Ree</i> 24	2213.29368	2.45D–24	2.51D–24	–2.45	3.25D–05	0.1192
<i>Ree</i> 25	2215.76663	6.65D–25	6.74D–25	–1.35	3.38D–05	0.1182
<i>Ree</i> 26	2218.22924	1.57D–24	1.61D–24	–2.55	3.44D–05	0.1001
<i>Ree</i> 27	2220.68531	4.02D–25	4.20D–25	–4.48	3.46D–05	0.1045
$4v_5^2 - v_5^1$						
<i>Pee</i> 6	2146.32946	3.66D–24	3.80D–24	–3.83	2.98D–05	0.1743
<i>Pee</i> 9	2139.68063	1.56D–24	1.62D–24	–3.85	2.69D–05	0.1556
<i>Pee</i> 10	2137.51066	4.71D–24	4.81D–24	–2.12	2.63D–05	0.1574
<i>Pee</i> 11	2135.36597	1.42D–24	1.52D–24	–7.04	2.37D–05	0.1547
<i>Pee</i> 13	2131.15930	1.22D–24	1.25D–24	–2.46	2.19D–05	0.1467
<i>Pee</i> 14	2129.09999	3.19D–24	3.23D–24	–1.25	2.04D–05	0.1533
<i>Pee</i> 15	2127.07214	8.87D–25	8.98D–25	–1.24	1.86D–05	0.1520
<i>Pee</i> 18	2121.19211	1.42D–24	1.24D–24	12.68	1.43D–05	0.1400
<i>Pee</i> 23	2112.12098	—	1.65D–25	—	—	—

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma}^N_{\text{obs}}$	$k_{\sigma}^N_{\text{calc}}$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Qfe</i> 3	2160.27763	2.94D–24	2.84D–24	3.40	3.43D–05	0.2140
<i>Qfe</i> 4	2160.34950	1.09D–23	1.13D–23	–3.67	3.20D–05	0.1798
<i>Qfe</i> 6	2160.54644	1.48D–23	1.53D–23	–3.38	3.22D–05	0.1692
<i>Qfe</i> 9	2160.97255	—	5.80D–24	—	—	—
<i>Qfe</i> 11	2161.34274	5.48D–24	5.56D–24	–1.46	3.27D–05	0.1552
<i>Qfe</i> 13	2161.77859	4.68D–24	4.93D–24	–5.34	3.15D–05	0.1389
<i>Qfe</i> 14	2162.02059	1.38D–23	1.36D–23	1.45	3.37D–05	—
<i>Qfe</i> 15	2162.27829	3.91D–24	4.07D–24	–4.09	3.18D–05	0.1406
<i>Qfe</i> 17	2162.83916	3.12D–24	3.16D–24	–1.28	3.27D–05	0.1390
<i>Qfe</i> 18	2163.14167	7.49D–24	8.17D–24	–9.08	3.04D–05	0.1106
<i>Qfe</i> 21	2164.13252	1.56D–24	1.60D–24	–2.56	3.25D–05	0.1251
<i>Qfe</i> 25	2165.63063	6.66D–25	6.49D–25	2.55	3.40D–05	0.1172
<i>Qfe</i> 26	2166.03385	—	1.50D–24	—	—	—
<i>Ree</i> 5	2174.67493	4.05D–24	3.85D–24	4.94	3.25D–05	0.1915
<i>Ree</i> 8	2182.20411	1.03D–23	1.08D–23	–4.85	2.66D–05	0.1604
<i>Ree</i> 9	2184.76203	—	3.37D–24	—	—	—
<i>Ree</i> 10	2187.34484	8.77D–24	9.20D–24	–4.90	2.43D–05	0.1560
<i>Ree</i> 11	2189.95568	2.52D–24	2.73D–24	–8.33	2.22D–05	0.1490
<i>Ree</i> 12	2192.59562	6.71D–24	7.11D–24	–5.96	2.11D–05	0.1494
<i>Ree</i> 13	2195.26632	1.93D–24	2.00D–24	–3.63	1.99D–05	0.1308
<i>Ree</i> 14	2197.96816	4.73D–24	4.94D–24	–4.44	1.80D–05	0.1443
<i>Ree</i> 15	2200.70350	1.28D–24	1.31D–24	–2.34	1.64D–05	0.1350
<i>Ree</i> 17	2206.27761	7.92D–25	7.40D–25	6.57	1.34D–05	0.1294
<i>Ree</i> 18	2209.11776	1.81D–24	1.54D–24	14.92	1.20D–05	0.1312
<i>Ree</i> 20	2214.90738	—	1.11D–24	—	—	—
<i>Ree</i> 21	2217.85844	—	3.02D–25	—	—	—
<i>Pff</i> 5	2148.44490	—	3.22D–24	—	—	—
<i>Pff</i> 6	2146.12499	—	1.39D–24	—	—	—
<i>Pff</i> 11	2134.65687	5.96D–24	6.22D–24	–4.36	3.33D–05	0.1550
<i>Pff</i> 13	2130.12554	5.60D–24	5.83D–24	–4.11	3.37D–05	0.1505
<i>Pff</i> 17	2121.14959	—	4.03D–24	—	—	—
<i>Pff</i> 19	2116.70179	3.23D–24	3.03D–24	6.19	3.84D–05	0.1404
<i>Pff</i> 22	2110.07123	—	5.86D–25	—	—	—
<i>Pff</i> 25	2103.48010	—	8.98D–25	—	—	—
<i>Qef</i> 2	2160.19570	—	1.70D–24	—	—	—
<i>Qef</i> 4	2160.25817	4.03D–24	3.88D–24	3.72	3.55D–05	0.1911
<i>Qef</i> 5	2160.30456	1.40D–23	1.41D–23	–0.71	3.42D–05	0.1748
<i>Qef</i> 6	2160.36191	5.89D–24	5.39D–24	8.49	3.84D–05	0.1896
<i>Qef</i> 8	2160.51367	6.19D–24	6.31D–24	–1.94	3.60D–05	0.1551
<i>Qef</i> 12	2161.00038	7.11D–24	6.47D–24	9.00	4.48D–05	0.1575
<i>Qef</i> 14	2161.35851	6.44D–24	5.88D–24	8.70	4.75D–05	0.1502
<i>Qef</i> 15	2161.57148	1.76D–23	1.64D–23	6.82	4.80D–05	0.1449
<i>Qef</i> 16	2161.80887	5.30D–24	5.03D–24	5.09	4.89D–05	0.1365

(continued on next page)

Table 2 (continued)

Line	σ_{obs}	$k_{\sigma \text{ obs}}^N$	$k_{\sigma \text{ calc}}^N$	o-c%	$ R _{\text{obs}}^2$	$\gamma_{\text{self obs}}^0$
<i>Qef</i> 20	2163.02239	3.26D–24	3.10D–24	4.91	5.63D–05	0.1330
<i>Qef</i> 21	2163.39486	8.17D–24	7.96D–24	2.57	5.72D–05	0.1260
<i>Qef</i> 23	2164.22392	5.54D–24	5.61D–24	–1.26	5.93D–05	0.1218
<i>Qef</i> 24	2164.67925	1.41D–24	1.54D–24	–9.22	5.72D–05	—
<i>Qef</i> 25	2165.16218	3.62D–24	3.75D–24	–3.59	6.27D–05	0.0938
<i>Qef</i> 26	2165.67057	9.79D–25	1.00D–24	–2.15	6.58D–05	0.1093
<i>Rff</i> 4	2172.10875	3.61D–24	3.84D–24	–6.37	3.04D–05	0.1685
<i>Rff</i> 5	2174.52138	1.13D–23	1.21D–23	–7.08	3.02D–05	0.1633
<i>Rff</i> 6	2176.94173	3.92D–24	4.12D–24	–5.10	3.06D–05	0.1571
<i>Rff</i> 7	2179.37028	1.21D–23	1.24D–23	–2.48	3.11D–05	0.1601
<i>Rff</i> 9	2184.24923	1.18D–23	1.19D–23	–0.85	3.15D–05	0.1588
<i>Rff</i> 10	2186.69935	3.70D–24	3.79D–24	–2.43	3.08D–05	0.1572
<i>Rff</i> 11	2189.15630	1.07D–23	1.07D–23	0.00	3.16D–05	0.1615
<i>Rff</i> 12	2191.61990	3.27D–24	3.29D–24	–0.61	3.11D–05	0.1486
<i>Rff</i> 14	2196.56353	—	2.69D–24	—	—	—
<i>Rff</i> 15	2199.04526	6.90D–24	7.15D–24	–3.62	2.98D–05	0.1376
<i>Rff</i> 16	2201.53102	2.03D–24	2.08D–24	–2.46	2.99D–05	0.1362
<i>Rff</i> 17	2204.02143	5.28D–24	5.36D–24	–1.52	3.00D–05	0.1347
<i>Rff</i> 18	2206.51619	1.50D–24	1.52D–24	–1.33	3.00D–05	0.1317
<i>Rff</i> 19	2209.01440	3.76D–24	3.81D–24	–1.33	2.98D–05	0.1296
<i>Rff</i> 20	2211.51604	1.06D–24	1.05D–24	0.94	3.03D–05	0.1302
<i>Rff</i> 21	2214.02056	2.57D–24	2.57D–24	0.00	3.00D–05	0.1222
<i>Rff</i> 22	2216.52761	—	6.89D–25	—	—	—
<i>Rff</i> 23	2219.03592	—	1.64D–24	—	—	—
<i>Rff</i> 24	2221.54600	—	4.29D–25	—	—	—

^aOnly lines whose position at least could be significantly determined by the multispectrum fitting procedure have been reported; for other lines, the adjustment could not converge, e.g., because of blendings. The lines are given band per band, and by increasing J values inside each branch. In the assignment, the first quoted e or f character concerns the upper level, and the second concerns the lower level. σ_{obs} is the measured zero pressure line position in cm^{-1} . $k_{\sigma \text{ obs}}^N$ is the measured line intensity in cm molecule^{-1} , for pure $^{12}\text{C}_2\text{H}_2$ at 296 K. $k_{\sigma \text{ calc}}^N$ is the calculated line intensity in the same units. o-c% is the percentage ratio $100 \times (k_{\sigma \text{ obs}}^N - k_{\sigma \text{ calc}}^N)/k_{\sigma \text{ obs}}^N$. $|R|_{\text{obs}}^2$ is the transition dipole moment squared in D^2 ($1\text{D} = 3.33546 \times 10^{-30} \text{C m}$) deduced from $k_{\sigma \text{ obs}}^N$. $\gamma_{\text{self obs}}^0$ is the measured self-broadening coefficient in $\text{cm}^{-1} \text{atm}^{-1}$ at 296 K.

this band our multispectrum fitting procedure led to correct line parameters and adjustment of the experimental spectra, so that we do not suspect systematic errors due to the measurement process. This effect could be explained by Coriolis interactions affecting differently the e and f sub-levels of the $v_5 = 1$ vibrational level, but it is difficult to confirm, considering the set of experimental data available at the present time, as far as intensities of transitions involving the $v_5 = 1$ vibrational level are concerned. Note that, despite very regular rotational dependences, the line intensities of the Pee and Ree sub-branches of the $(3v_4 + v_5)^2\Pi - v_4^1$ band (see Fig. 2) cannot be adjusted by Eq. (1), because of strong interactions which also perturb the line positions as stated above.

Self-broadening coefficients γ_{self}^0 have been measured for 371 lines. In Ref. [3], we saw that there does not exist any significant vibrational dependence. In Fig. 12, we have gathered all the self-broadening coefficients obtained in this work and in Ref. [3]. Adjusting these values by a

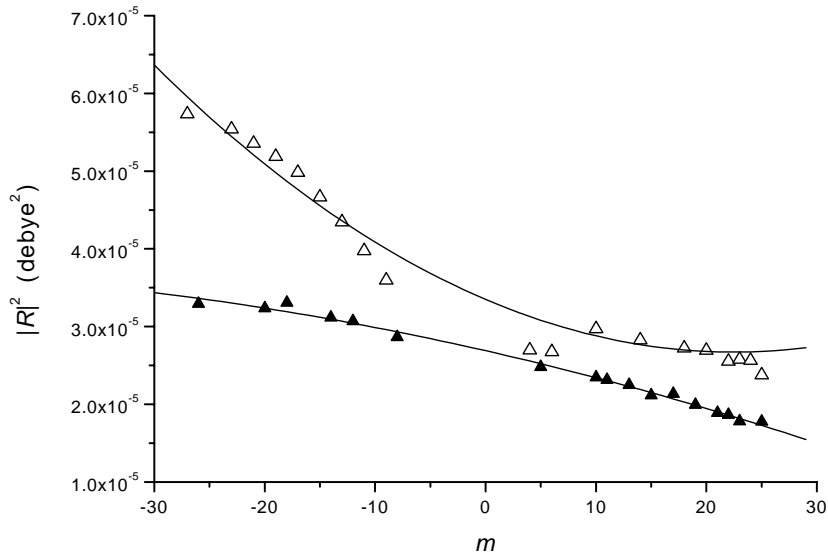


Fig. 2. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(3\nu_4 + \nu_5)^2\Pi - \nu_4^1$ band of $^{12}\text{C}_2\text{H}_2$. Open triangles are for *Pee* and *Ree* lines, and black triangles for *Pff* and *Rff* lines. The curves have been calculated using the constants found in this work (see Table 3).

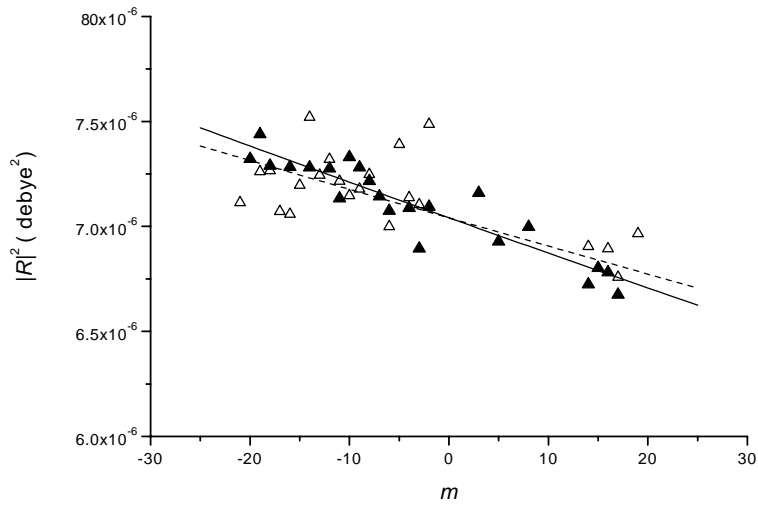


Fig. 3. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $\nu_2 + \nu_5^1 - \nu_4^1$ band of $^{12}\text{C}_2\text{H}_2$. Open triangles are for *Pee* and *Ree* lines, and black triangles for *Pff* and *Rff* lines. The curves have been calculated using the constants found in this work (see Table 3): the dashed straight line is for the *ee* sub-band, and the continuous straight line for the *ff* sub-band.

polynomial expansion vs. $|m|$, we found

$$\gamma_{\text{self}}^0(T) = [0.2031(19) - 0.00642(45)|m| + 0.000181(29)m^2 - 2.93(58) \times 10^{-6}|m|^3] \times (T_0/T)^{0.75} \quad (3)$$

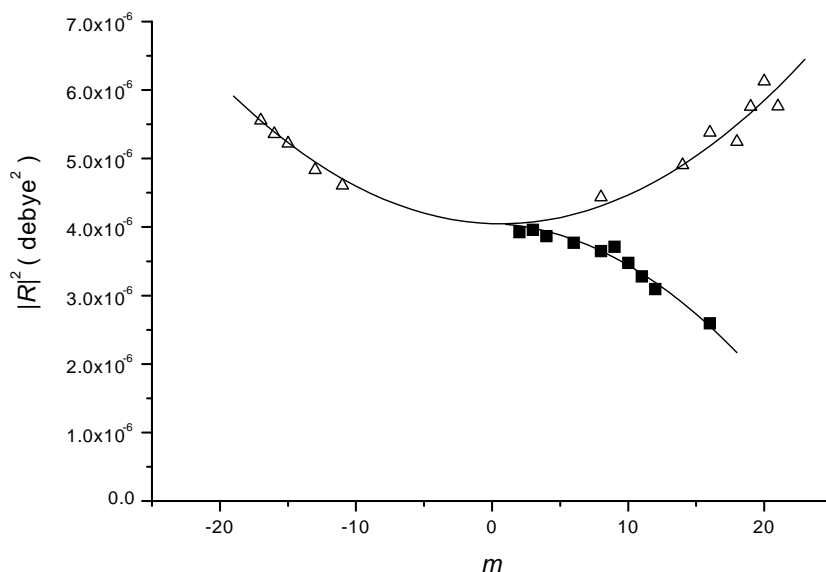


Fig. 4. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(\nu_4 + 3\nu_5)_+^0 - \nu_4^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

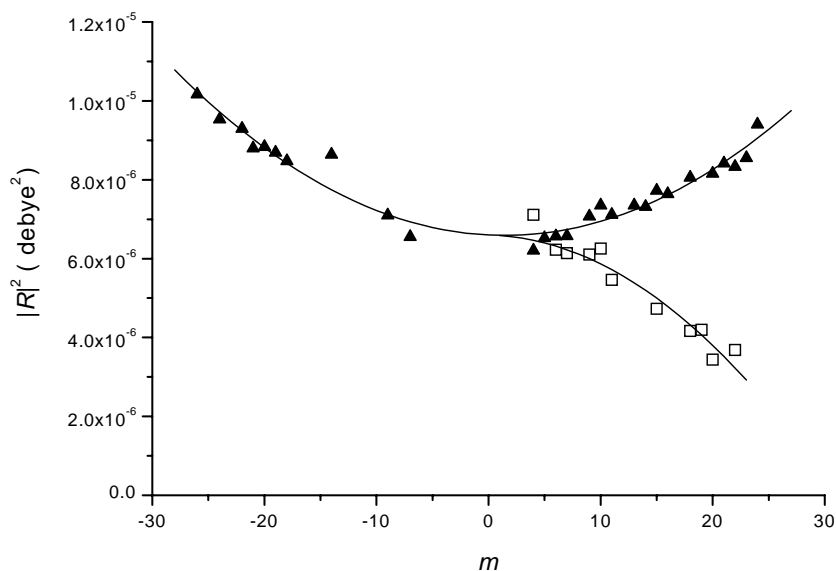


Fig. 5. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(\nu_4 + 3\nu_5)_-^0 - \nu_4^1$ band of $^{12}C_2H_2$. Black triangles are for *Pff* and *Rff* lines, and open squares for *Qfe* lines. The curves have been calculated using the constants found in this work (see Table 3).

with, between parenthesis, 1 SD in unit of the last digit, T_0 being equal to 296 K. The exponent 0.75 comes from Varanasi et al. [11]. Note that Eq. (5) of Ref. [3], obtained from a set of data smaller than in the present work, leads to very similar results. Thus, we propose

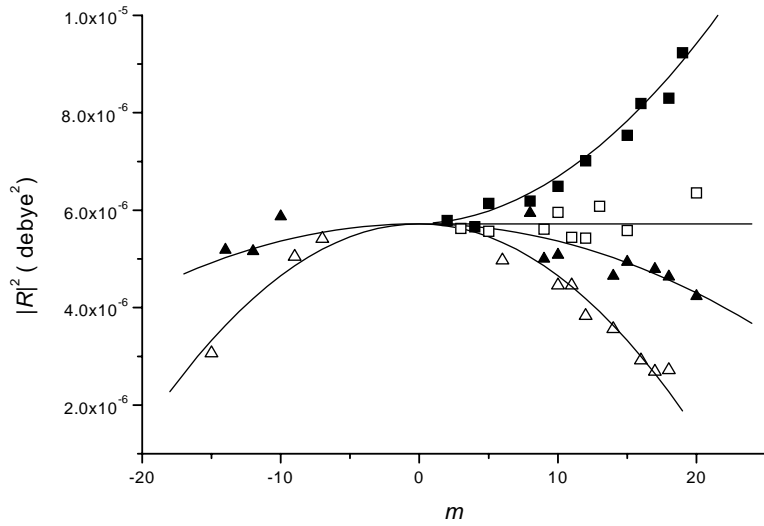


Fig. 6. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(\nu_4 + 3\nu_5)^2II - \nu_4^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, black triangles for *Pff* and *Rff* lines, open squares for *Qfe* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

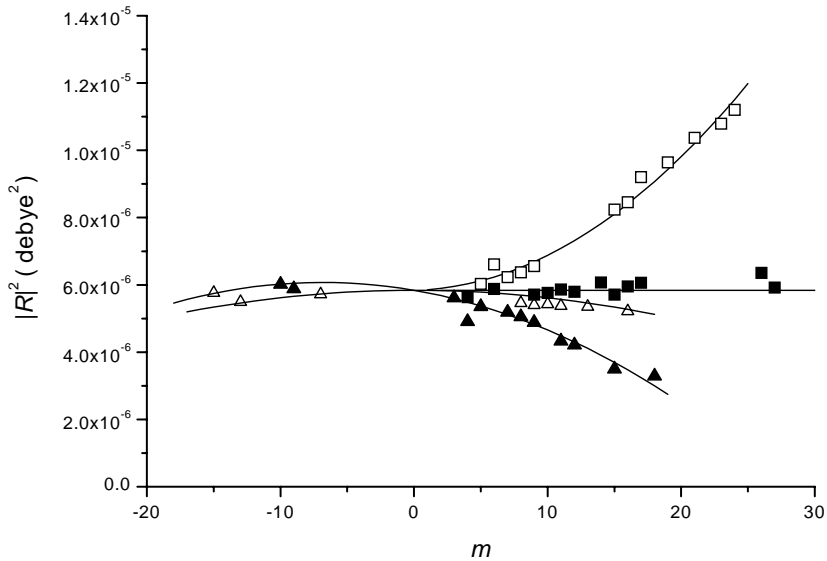


Fig. 7. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(\nu_4 + 3\nu_5)^2I - \nu_4^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, black triangles for *Pff* and *Rff* lines, open squares for *Qfe* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

Eq. (3) for calculating the self-broadening coefficient of all lines in all bands of acetylene, up to $|m|$ equal to 33, and with $\gamma_{self}^0 = 0.0812 \text{ cm}^{-1} \text{ atm}^{-1}$ for $|m|$ greater than or equal to 34. The rotational dependence of γ_{self}^0 given by this formula can be considered as

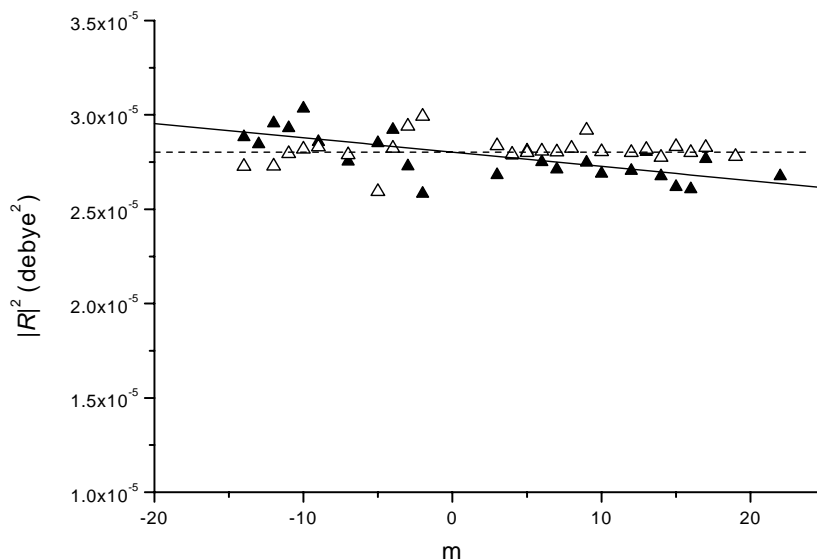


Fig. 8. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D=3.33546 \times 10^{-30}$ C m), vs. m , for the $v_2 + v_4^1 - v_5^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, and black triangles for *Pff* and *Rff* lines. The curves have been calculated using the constants found in this work (see Table 3): the dashed straight line is for the *ee* sub-band, and the continuous straight line for the *ff* sub-band.

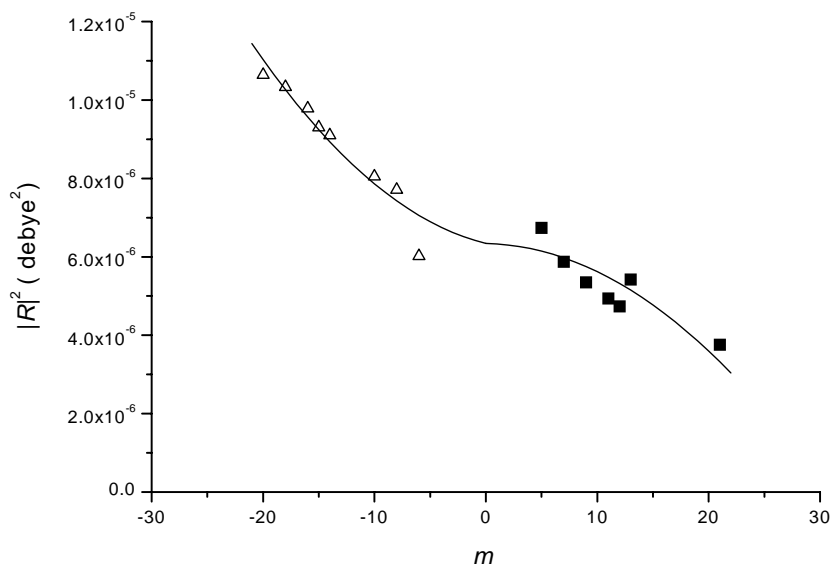


Fig. 9. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D = 3.33546 \times 10^{-30}$ C m), vs. m , for the $(2v_4 + 2v_5)^0_+ - v_5^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

accurate within an uncertainty of $\pm 3\%$, with the assumption that it is applied to bands for which there is no vibrational dependence, not too high J lines, and inside a temperature range close to room temperature.

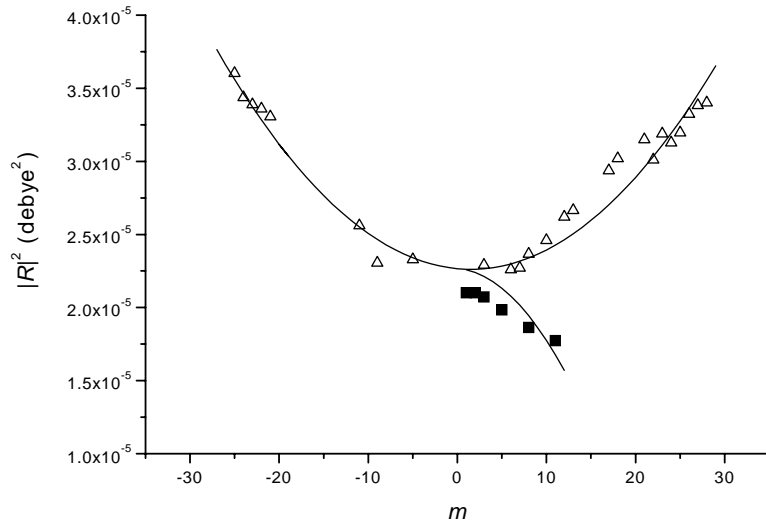


Fig. 10. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D=3.33546 \times 10^{-30}$ C m), vs. m , for the $4v_5^0 - v_5^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

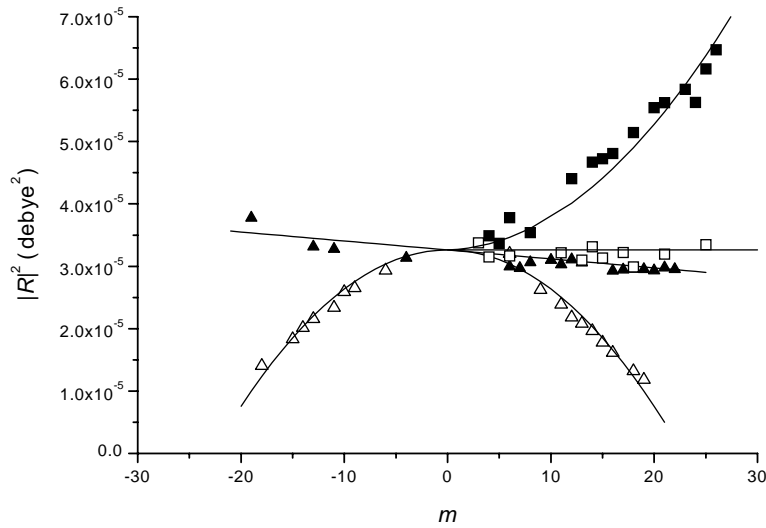


Fig. 11. Variation of the transition dipole moment squared $|R|^2$ (in D^2 , $1D=3.33546 \times 10^{-30}$ C m), vs. m , for the $4v_5^2 - v_5^1$ band of $^{12}C_2H_2$. Open triangles are for *Pee* and *Ree* lines, black triangles for *Pff* and *Rff* lines, open squares for *Qfe* lines, and black squares for *Qef* lines. The curves have been calculated using the constants found in this work (see Table 3).

Self-shifting coefficients δ_{self}^0 are tentatively given for 122 lines (see Table 4). They have been plotted in Figs. 13–15 for some interesting bands. The confidence intervals (1 SD) of the retained δ_{self}^0 values are around $\pm 0.002 \text{ cm}^{-1} \text{ atm}^{-1}$, but they can attain about $\pm 0.006 \text{ cm}^{-1} \text{ atm}^{-1}$ for some

Table 3

Summary of $^{12}\text{C}_2\text{H}_2$ vibrational transition dipole moments squared, Herman-Wallis coefficients, and band intensities, obtained for 3 cold bands [3] and 15 hot bands in the 5- μm spectral region (this work)^a

Band	Center	$ R_0 ^2$	A_1^{RP}	A_2^{RP}	A_2^O	S_V
$3\nu_5^1$	2169.166	10.828(67)	-3.54(19)	-0.29(10)		810
$(2\nu_4 + \nu_5)^1\text{II}$	1940.003	7.685(69)	-15.11(35)	-0.53(19)		514
$(2\nu_4 + \nu_5)^1\text{I}$	1959.697	2.060(34)	-2.60(70)	2.66(59)		142
$(3\nu_4 + \nu_5)_+^0 - \nu_4^1$	1948.906	18 ₃ (—) ^b		—	—	61.9
$(3\nu_4 + \nu_5)_-^0 - \nu_4^1$	1972.151	3.99(47)	0	-57(14)		13.9
$(3\nu_4 + \nu_5)^2\text{II} - \nu_4^1$	<i>ee</i> 1945.126	34.0(34)	-18.0(34)	4.0(28)		58.5
	<i>ff</i> 1945.126	27.36(47)	-11.96(57)	-0.91(47)		46.9
$(3\nu_4 + \nu_5)^2\text{I} - \nu_4^1$	<i>ee</i> 1973.283	4.7 ₈ (12 ₀)	0	-43(13)		16.7
	<i>ff</i>		0	17(26)		
$\nu_2 + \nu_5^1 - \nu_4^1$	<i>ee</i> 2090.213	7.157(51)	-1.92(73)	0		26.4
	<i>ff</i>		-2.41(81)	0		
$(\nu_4 + 3\nu_5)_+^0 - \nu_4^1$	2146.104	4.12(12)	-1.6(14)	11.9(16)		15.6
$(\nu_4 + 3\nu_5)_-^0 - \nu_4^1$	2171.957	6.71(17)	-2.11(99)	7.33(92)		25.7
$(\nu_4 + 3\nu_5)^2\text{II} - \nu_4^1$	<i>ee</i> 2156.792	5.81(14)	0	-18.6(19)	<i>fe</i>	0
	<i>ff</i>		0	-6.2(17)	<i>ef</i>	15.4(20)
$(\nu_4 + 3\nu_5)^2\text{I} - \nu_4^1$	<i>ee</i> 2179.100	5.934(96)	0	-3.8(19)	<i>fe</i>	16.19(94)
	<i>ff</i>		-11.7(33)	-8.5(26)	<i>ef</i>	0
$\nu_2 + \nu_4^1 - \nu_5^1$	<i>ee</i> 1844.372	28.49(23)	0	0		52.4
	<i>ff</i>		-2.7(10)	0		
$(2\nu_4 + 2\nu_5)_+^0\text{II} - \nu_5^1$	1918.863	6.44(82)	-11(37)	13(19)		-10.3(60)
$(2\nu_4 + 2\nu_5)_-^0 - \nu_5^1$	1932.033	8.5 ₄ (—) ^b	—	—		16.47
$(2\nu_4 + 2\nu_5)^2\text{II} - \nu_5^1$	<i>ff</i> ^c 1932.289	32.5(25) ^c	—	—		62.6 ^c
$4\nu_5^0 - \nu_5^1$	2151.065	23.03(74)	-2.5(12)	8.14(98)		-19.7(77)
$4\nu_5^2 - \nu_5^1$	<i>ee</i> 2160.208	33.15(68)	0	-19.2(15)	<i>fe</i>	0
	<i>ff</i>		-4.4(19)	0	<i>ef</i>	14.7(11)

^aThe quoted band centers, in cm^{-1} , are from Plíva [4]. The vibrational transition dipole moments squared $|R_0|^2$ are in 10^{-6}D^2 ($1\text{D} = 3.33546 \times 10^{-30} \text{C m}$). The Herman-Wallis coefficients are defined by Eqs. (1) and (2). The A_1^{RP} coefficients have to be multiplied by 10^{-3} , and the A_2^{RP} and A_2^O coefficients have to be multiplied by 10^{-4} ; when a zero value is reported, the corresponding coefficient was fixed to zero in the fit. Between parentheses, the quoted 95% statistical confidence intervals are 2 SD in units of the last digit. The band intensities S_V are in $10^{-23} \text{cm}^{-1}/(\text{molecule cm}^{-2})$ at 296 K and in natural abundances. In case of ℓ -type doubling, and if the two sub-bands were fitted simultaneously, $|R_0|^2$ is reported once, and the quoted S_V value is the whole intensity of the band (not to be confused with the intensities reported for each sub-band, when the two sub-bands could be fitted separately).

^bValue of $|R_0|^2$ obtained from only one line.

^cValue of $|R_0|^2$ obtained from only three *Pff* lines. S_V is the total band intensity.

lines. Note that the measurement of pressure-shifts is particularly difficult when the lines are weak because of the noise level (as is the case for many lines in the present work), and taking into account the fact that the maximum pressure of our spectra is only 50 Torr (our spectra were not especially recorded with the aim of deducing pressure-shifting coefficients). A discussion is necessary about the effect of the uncertainty of the pressure-shifting coefficient determination, on the deduced zero-pressure line position. In the “general” version [8] of the multispectrum fitting procedure (MSF), in which all the line parameters (including the zero-pressure line position and the

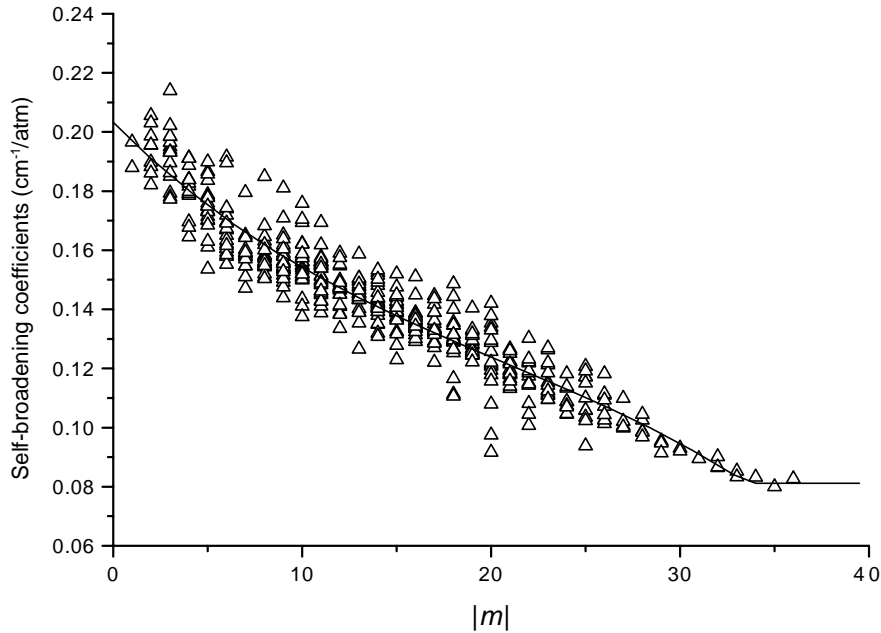


Fig. 12. Self-broadening coefficients γ_{self}^0 of $^{12}\text{C}_2\text{H}_2$ vs. $|m|$, in $\text{cm}^{-1} \text{atm}^{-1}$ at 296 K. Plotted are all our results concerning the 3 cold bands studied in Ref. [3] and the 15 hot bands studied in the present work: one sees that these values are well gathered around an adjusted polynomial expansion (continuous line); cf. Eq. (3).

self-shifting coefficient) are common to all spectra, the information allowing the determination of the zero-pressure line position comes from the low-pressure spectra, whereas the information leading to the pressure-shifting coefficient comes from the high-pressure spectra. In our case, an accurate adjustment of the zero-pressure line position is forced by the numerous low-pressure spectra taken into account, since even a noticeable error in the pressure-shifting coefficient, for which the information comes mainly from the 50-Torr spectrum, has a totally negligible consequence in the final zero-pressure line position. The previous conclusion would no longer be valid if our set of spectra contained much more high-pressure spectra than low-pressure spectra (by “high” pressure, we mean a pressure high enough to induce non-negligible pressure-shifts, but too low to lead to a very accurate determination of these pressure-shifts). However, even in this case, this drawback can be avoided by using a “reduced” version [8] of the MSF procedure, in which the line positions are not constrained in each spectrum (consequently, pressure-shifting coefficients cannot be deduced), other line parameters remaining common to all spectra. Then, zero-pressure line positions can be obtained considering only the line positions adjusted for the low-pressure spectra. Let us discuss a typical example. The tests we performed on a weak line (poor SNR), for which a significant and relatively large self-shifting coefficient of $0.012 \text{ cm}^{-1} \text{atm}^{-1}$ was found (confidence interval: $0.014 \text{ cm}^{-1} \text{atm}^{-1}$), led to conclusions that we checked with other similar lines:

- First, the “general” MSF procedure applied to all spectra (i.e., including the 50-Torr spectrum) gave a zero-pressure line position identical to that obtained by the same method, but disregarding

Table 4

Self-shifting coefficients measured at room temperature, for hot bands of $^{12}\text{C}_2\text{H}_2$ in the 5- μm spectral region^a

Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD	Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD
$(3\nu_4 + \nu_5)_+^0 - \nu_4^1$ <i>Qef</i> 20	1951.49101	-5.49	3.38				
$(3\nu_4 + \nu_5)_-^0 - \nu_4^1$ <i>Qfe</i> 9	1972.70409	-2.55	2.21	<i>Qfe</i> 11	1972.88785	-1.08	2.57
$(3\nu_4 + \nu_5)^2\text{II} - \nu_4^1$ <i>Pee</i> 11	1919.93952	-2.24	0.90	<i>Pff</i> 8	1926.35236	-2.23	2.92
<i>Pee</i> 13	1915.44460	-2.19	0.93	<i>Pff</i> 12	1917.09168	1.05	0.89
<i>Pee</i> 15	1910.93702	-0.54	0.55	<i>Pff</i> 14	1912.48543	-1.08	0.81
<i>Pee</i> 19	1901.85420	-1.35	0.74	<i>Pff</i> 18	1903.31092	1.93	0.81
<i>Pee</i> 21	1897.27439	0.74	0.97				
<i>Pee</i> 23	1892.66951	-1.35	1.59				
<i>Ree</i> 3	1954.65251	-4.70	4.17	<i>Rff</i> 9	1968.96809	-6.25	5.16
<i>Ree</i> 5	1959.50405	-6.73	2.56	<i>Rff</i> 14	1981.03696	-8.62	2.59
<i>Ree</i> 9	1969.28797	-5.25	3.82	<i>Rff</i> 16	1985.87757	-6.30	3.20
<i>Ree</i> 13	1979.06574	-8.60	2.17	<i>Rff</i> 18	1990.72098	-8.38	2.19
<i>Ree</i> 17	1988.74504	-7.93	2.21	<i>Rff</i> 20	1995.56303	-6.57	2.30
<i>Ree</i> 19	1993.53792	-6.56	2.82				
<i>Ree</i> 21	1998.29918	-6.34	2.10				
<i>Ree</i> 23	2003.02909	-4.92	2.37				
$(3\nu_4 + \nu_5)^2\text{I} - \nu_4^1$ <i>Rff</i> 10	1999.61650	-1.65	2.02				
$\nu_2 + \nu_5^1 - \nu_4^1$ <i>Pee</i> 11	2063.80453	-2.60	0.91	<i>Pff</i> 4	2080.70395	-1.60	1.48
<i>Pee</i> 12	2061.34402	-2.37	1.94	<i>Pff</i> 6	2075.88097	0.84	2.14
<i>Pee</i> 15	2053.90375	0.20	0.84	<i>Pff</i> 7	2073.45290	-2.25	2.19
<i>Pee</i> 17	2048.89545	-3.66	3.04	<i>Pff</i> 8	2071.01380	-2.83	0.78
<i>Pee</i> 19	2043.84896	-4.19	6.40	<i>Pff</i> 9	2068.56370	0.68	1.79
<i>Pee</i> 21	2038.76448	-0.96	1.73	<i>Pff</i> 12	2061.14798	-0.94	0.71
				<i>Pff</i> 14	2056.15000	0.97	1.12
				<i>Pff</i> 16	2051.10914	0.91	0.84
				<i>Pff</i> 20	2040.90001	-0.17	1.36
<i>Ree</i> 13	2122.03232	0.02	1.26	<i>Rff</i> 4	2101.85096	-4.13	1.85
<i>Ree</i> 15	2126.40764	-1.00	0.87	<i>Rff</i> 13	2122.06591	-0.42	3.15
				<i>Rff</i> 15	2126.42868	-0.77	2.56
				<i>Rff</i> 16	2128.59227	-2.32	1.56
$(\nu_4 + 3\nu_5)_+^0 - \nu_4^1$ <i>Pee</i> 11	2121.26792	0.68	0.90	<i>Ree</i> 15	2185.90288	-0.13	1.70
<i>Pee</i> 13	2116.94732	1.63	1.17				
<i>Pee</i> 15	2112.65948	0.89	1.12				
<i>Pee</i> 17	2108.39073	-0.96	1.29				

Table 4 (continued)

Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD	Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD
$(v_4 + 3v_5)^0_- - v_4^1$							
<i>Pff</i> 18	2130.41564	-1.45	1.32	<i>Rff</i> 10	2198.37662	-2.90	1.08
				<i>Rff</i> 12	2203.24185	-4.71	0.86
<i>Rff</i> 4	2183.87312	-1.22	2.15	<i>Rff</i> 14	2208.11250	-3.53	1.27
<i>Rff</i> 6	2188.68727	-2.90	5.34	<i>Rff</i> 20	2222.69356	-1.71	2.15
<i>Rff</i> 9	2195.94818	-3.95	4.13	<i>Rff</i> 22	2227.52454	-1.94	2.82
$(v_4 + 3v_5)^2_{\text{II}} - v_4^1$							
<i>Ree</i> 9	2181.36715	-4.19	1.61	<i>Rff</i> 8	2178.37623	-7.73	2.49
<i>Ree</i> 11	2186.56900	-5.80	4.50	<i>Rff</i> 14	2193.11961	-3.79	1.70
				<i>Rff</i> 16	2198.08092	-0.41	3.59
<i>Pff</i> 14	2124.46331	-3.12	3.58				
$(v_4 + 3v_5)^2_{\text{I}} - v_4^1$							
<i>Qfe</i> 19	2182.74079	-1.64	1.16	<i>Ree</i> 7	2198.49740	-1.67	1.11
				<i>Ree</i> 15	2219.01833	0.91	2.09
$v_2 + v_4^1 - v_5^1$							
<i>Ree</i> 4	1855.92328	5.27	0.93	<i>Rff</i> 3	1853.69334	3.55	1.19
<i>Ree</i> 6	1860.43566	4.01	0.62	<i>Rff</i> 5	1858.26666	4.88	0.87
<i>Ree</i> 7	1862.66929	0.72	1.27	<i>Rff</i> 9	1867.24626	2.64	0.55
<i>Ree</i> 8	1864.88778	-3.68	1.32	<i>Rff</i> 11	1871.65185	-0.45	0.60
<i>Ree</i> 9	1867.09122	4.67	1.26	<i>Rff</i> 13	1876.00074	-0.78	0.63
<i>Ree</i> 11	1871.45259	-1.29	1.00	<i>Rff</i> 14	1878.15390	0.39	1.62
<i>Ree</i> 12	1873.61034	-1.27	0.42	<i>Rff</i> 15	1880.29274	-2.79	0.78
<i>Ree</i> 13	1875.75279	0.85	1.16	<i>Rff</i> 16	1882.41726	-0.82	4.20
<i>Ree</i> 14	1877.88003	-4.14	0.41				
<i>Ree</i> 15	1879.99174	0.10	1.29				
<i>Ree</i> 16	1882.08813	-3.54	0.51				
<i>Ree</i> 18	1886.23440	-6.68	0.83				
$(2v_4 + 2v_5)^0_{\text{II}} - v_5^1$							
<i>Pee</i> 10	1896.01826	0.84	1.70	<i>Pee</i> 14	1887.22406	-1.47	1.17
$(2v_4 + 2v_5)^0_- - v_5^1$							
<i>Pff</i> 9	1910.96858	-3.08	1.75				
$4v_5^0 - v_5^1$							
<i>Pee</i> 24	2097.90888	-1.55	1.43	<i>Ree</i> 16	2193.24267	-4.00	0.52
				<i>Ree</i> 20	2203.32428	-3.19	0.70
<i>Ree</i> 6	2168.03917	-1.93	1.05	<i>Ree</i> 22	2208.32469	-2.49	2.86
<i>Ree</i> 12	2183.10886	-3.91	0.61	<i>Ree</i> 26	2218.22924	-3.04	1.92

(continued on next page)

Table 4 (continued)

Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD	Line	σ_{obs}	$\delta_{\text{self obs}}^0$	SD
$4\nu_5^2 - \nu_5^1$							
<i>Pee</i> 10	2137.51066	-1.76	1.24	<i>Pff</i> 13	2130.12554	1.94	1.71
<i>Pee</i> 13	2131.15930	-1.40	3.97	<i>Pff</i> 19	2116.70179	0.04	0.79
<i>Pee</i> 14	2129.09999	6.19	2.11	<i>Qef</i> 23	2164.22392	-0.42	1.46
<i>Qfe</i> 21	2164.13252	-2.90	3.93	<i>Rff</i> 9	2184.24923	-0.29	0.54
<i>Ree</i> 8	2182.20411	-3.44	0.73	<i>Rff</i> 10	2186.69935	-2.45	1.09
<i>Ree</i> 10	2187.34484	-1.99	1.53	<i>Rff</i> 11	2189.15630	-3.43	1.54
<i>Ree</i> 11	2189.95568	1.05	2.02	<i>Rff</i> 15	2199.04526	-5.34	0.95
<i>Ree</i> 12	2192.59562	-2.26	1.47	<i>Rff</i> 16	2201.53102	-3.78	1.76
<i>Ree</i> 14	2197.96816	-4.43	0.82	<i>Rff</i> 17	2204.02143	-5.76	0.78
<i>Ree</i> 18	2209.11776	2.58	2.34	<i>Rff</i> 19	2209.01440	-2.50	1.02
				<i>Rff</i> 21	2214.02056	-3.96	1.66

^aThe lines are given band per band, and by increasing J values inside each branch. In the assignment, the first quoted e or f character concerns the upper level, and the second concerns the lower level. σ_{obs} is the measured zero-pressure line position in cm^{-1} . $\delta_{\text{self obs}}^0$ is the measured self-shifting coefficient in $10^{-3} \text{cm}^{-1} \text{atm}^{-1}$ at about 296 K. SD, is the 68% confidence interval, i.e., 1 SD, of $\delta_{\text{self obs}}^0$ in $10^{-3} \text{cm}^{-1} \text{atm}^{-1}$.

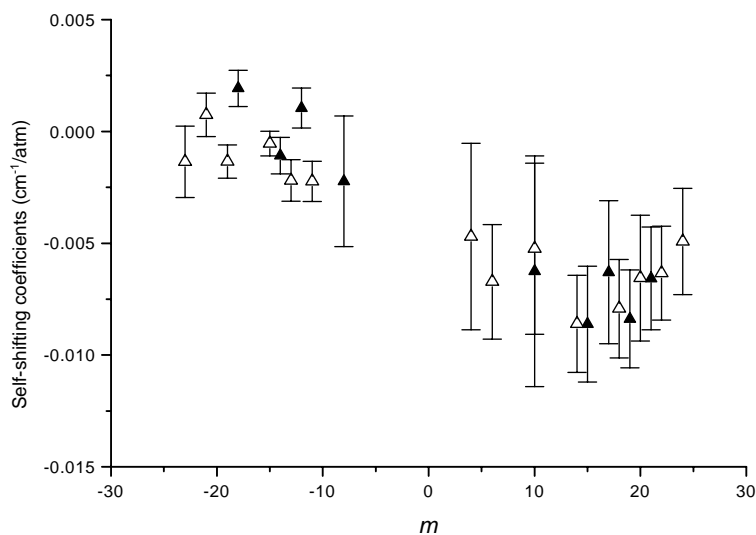


Fig. 13. Self-shifting coefficients δ_{self}^0 of $^{12}\text{C}_2\text{H}_2$ vs. m in $\text{cm}^{-1} \text{atm}^{-1}$ at about 296 K, for the $(3\nu_4 + \nu_5)^2\Pi - \nu_4^1$ band. Open triangles are for *Pee* and *Ree* lines, and black triangles for *Pff* and *Rff* lines. The error bars are a ± 1 SD statistical uncertainty.

the 50-Torr spectrum (discrepancy smaller than 10^{-6}cm^{-1}), showing that taking into account the 50-Torr spectrum does not worsen the zero-pressure line position, even in the case where the retrieved self-shifting coefficient has an anomalously large value.

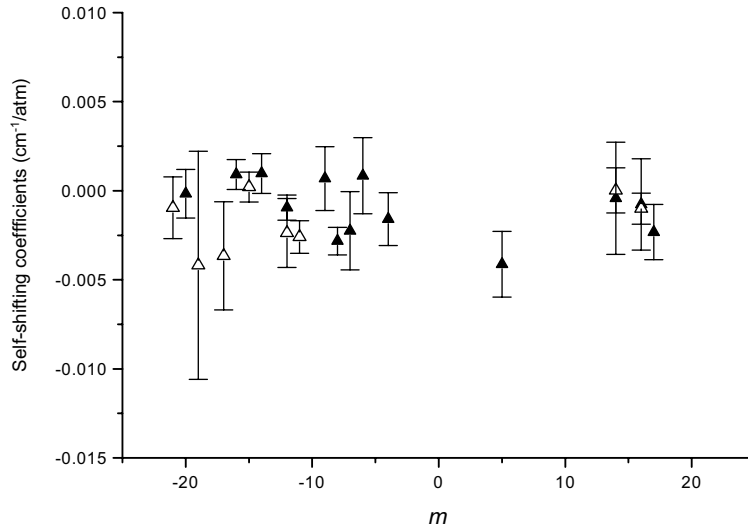


Fig. 14. Self-shifting coefficients δ_{self}^0 of $^{12}\text{C}_2\text{H}_2$ vs. m in $\text{cm}^{-1} \text{atm}^{-1}$ at about 296 K, for the $v_2 + v_3^1 - v_4^1$ band. Open triangles are for *Pee* and *Ree* lines, and black triangles for *Pff* and *Rff* lines. The error bars are a ± 1 SD statistical uncertainty.

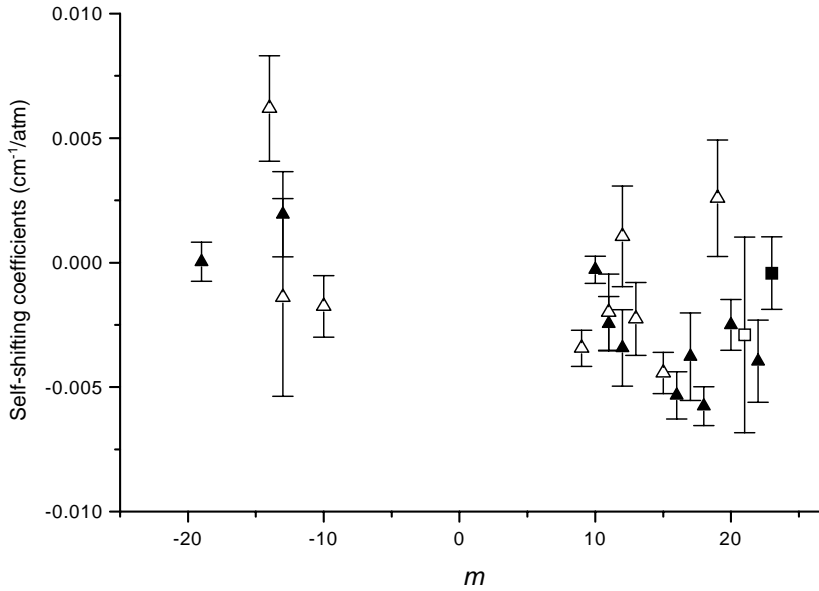


Fig. 15. Self-shifting coefficients δ_{self}^0 of $^{12}\text{C}_2\text{H}_2$ vs. m in $\text{cm}^{-1} \text{atm}^{-1}$ at about 296 K, for the $4v_5^2 - v_5^1$ band. Open triangles are for *Pee* and *Ree* lines, black triangles for *Pff* and *Rff* lines, the black square for a *Qef* line, and the open square for a *Qfe* line. The error bars are a ± 1 SD statistical uncertainty.

- Second, the “reduced” MSF procedure (with or without the 50-Torr spectrum) gave line positions in low-pressure spectra very close together (discrepancies smaller than $5 \times 10^{-5} \text{ cm}^{-1}$), showing that the relative calibration of the wavenumber scales of the involved spectra is correct.

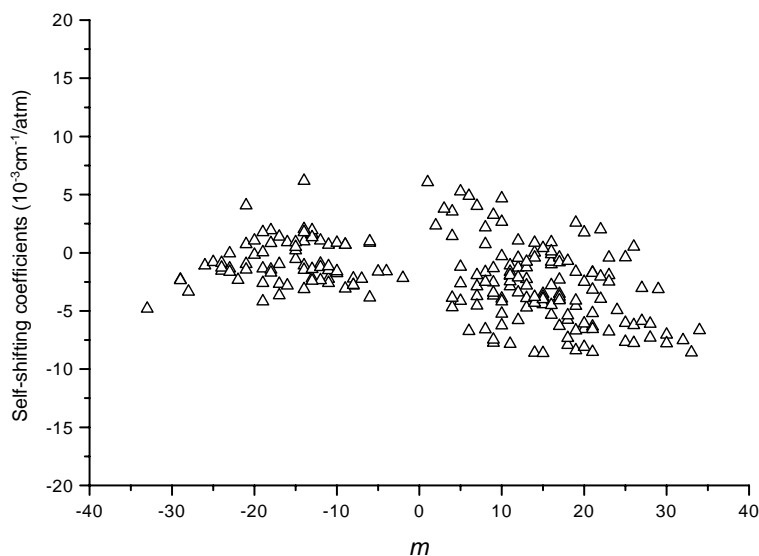


Fig. 16. Self-shifting coefficients δ_{self}^0 of $^{12}\text{C}_2\text{H}_2$ vs. m in $\text{cm}^{-1}\text{atm}^{-1}$ at about 296 K, for all the 5- μm region bands studied in Ref. [3] and in the present work.

- Third, these line positions obtained by the “reduced” MSF procedure do not differ from the zero-pressure line positions obtained from the “general” MSF procedure by more than 10^4cm^{-1} , a discrepancy well inside our stated $2 \times 10^{-4}\text{cm}^{-1}$ mean accuracy.
- Fourth, the self-shifting coefficient determined from the “reduced” MSF line positions in the low-pressure spectra and in the 50-Torr spectrum is very close to the value deduced by the “general” MSF procedure (0.011 vs. $0.012\text{cm}^{-1}\text{atm}^{-1}$). This shows the coherence of the method: the information allowing the determination of δ_{self}^0 comes from the 50-Torr spectrum and leads to very similar results whatever the method is, but, as this information is very poor, those results can be erroneous, showing that the uncertainty in the absolute values of δ_{self}^0 is certainly larger than the confidence intervals.

For all these reasons, few significant values were finally retained (see Table 4). Fig. 16 contains all the results obtained in the present work, together with the results obtained in Ref. [3]. Taking into account the uncertainties, neither vibrational dependence nor rotational dependence could be observed. As estimations of self-shifting coefficients can be useful for wavenumber calibration purposes, it is interesting to give the average value calculated from our results: $-0.0022\text{cm}^{-1}\text{atm}^{-1}$ at about 296 K.

4. Synthetic spectrum

The bands occurring in the studied spectral region involve energy levels coupled by anharmonic resonances, and vibrational or rotational essential ℓ -type resonances, so that they are interesting for further theoretical calculations, using effective operator models enabling the calculation of the whole

spectrum of acetylene [6,7]. The concerned anharmonic interactions are due to the 44/55 and ⁶44/55 accidental vibrational resonances (see, e.g., Refs. [5,6]), i.e., the so-called bending–bending second order Darling–Dennison type interactions, which occur between levels with $\Delta v_1 = \Delta v_2 = \Delta v_3 = 0$, $\Delta v_4 = \pm 2, \Delta v_5 = \mp 2$. Thus we thought it useful to gather all the data concerning this region, and available at the present time, in a HITRAN-format line list. This file¹ is of course evolving and will be updated as soon as new computations become available. Between 1810 and 2255 cm⁻¹, the ¹²C₂H₂ bands taken into account to set up this file are the 3 cold bands studied in Ref. [3] and the 15 hot bands studied in the present paper. At the present time, no resonance was taken into account in the calculation of the line positions and line intensities.

The line positions have been calculated as explained in Section 3, and no extrapolation was performed for the final list: the last line in each branch corresponds to the larger J value observed either by Plíva or by us. In the case where the maximum J value observed by Plíva is greater than ours, Plíva's calculated line positions (possibly slightly shifted) have sometimes been chosen rather than ours for the lines we could not analyze. For the bands for which no adjustment was possible, Plíva's calculated line positions were chosen. Note that because of strong interactions mentioned in Ref. [4], only the *Pff* and *Rff* sub-branches of the $(2v_4 + 2v_5)^2\Pi - v_5^1$ band are observable and consequently were calculated. Conversely, it is worth noticing that we observed many *P* lines in the $v_2 + v_5^1 - v_4^1$ and $v_2 + v_4^1 - v_5^1$ bands, whereas none of them is present in Ref. [4]. The lower-state energy values, E'' , were taken from HITRAN [12].

The line intensities have been calculated, in cm molecule⁻¹ at 296 K, and in natural abundances as is usual for HITRAN (97.760% for ¹²C₂H₂), using the constants listed in Table 3. For J greater than the J value corresponding to our last measured intensity, namely J_{\max} , the line intensities were calculated extrapolating Eqs. (1) and (2), but for some bands, they were calculated fixing the transition dipole moment squared at its value calculated for J_{\max} . The self-broadening coefficients have been calculated using Eq. (3). Among the experimental results available for air-broadening effects (see bibliography in Table 1 of Ref. [3]), we have chosen the results of Lambot et al. [13] and Bouanich et al. [14] concerning v_5^1 lines. The temperature-dependence exponent, $n = 0.75$, of the air-broadening coefficient is a mean value obtained from Refs. [14–16] which showed that n is noticeably J -dependent, since its experimental values vary from about 0.85 to 0.60 according to J between 1 and 30. Despite this variation, the same rough mean value 0.75 was incorporated for all the lines involved in the 5- μ m region. The air-broadening coefficients are smoothed values obtained from Refs. [13,14] for $|m|$ between 1 and 34; they are given in Table 5, at $T_0 = 296$ K. For $|m|$ greater or equal to 34, γ_{air}^0 is fixed to 0.0450 cm⁻¹ atm⁻¹ at 296 K. The value of γ_{air}^0 for $m=0$ was extrapolated. Note that recent measurements from Sun and Varanasi [17] should allow the improvement of these data. As far as air-shifting coefficients are concerned, we are only aware of the N₂-shifting coefficients measured by Babay et al. [18] for v_5^1 lines at room temperature (between 290 and 295 K). Although these values are noticeably J -dependent, we chose a rough mean value -0.001 cm⁻¹ atm⁻¹ for all lines.

The accuracy codes follow the HITRAN convention and are: 3 for calculated line positions (error range between 0.001 and 0.01 cm⁻¹), 6 for calculated line intensities and broadening coefficients (between 2% and 5%). Note that the intensity accuracy code has been degraded (code 4, i.e.,

¹ Available upon request to the authors. This file can be down-loaded from the web-site <http://CfA-www.Harvard.edu/HITRAN/updates.html>.

Table 5

Air-broadening coefficients γ_{air}^0 of $^{12}\text{C}_2\text{H}_2$ lines, obtained from the smoothed values published by Lambot et al. [13] and Bouanich et al. [14]. The unit is $10^{-3} \text{ cm}^{-1} \text{ atm}^{-1}$ at 296 K

$ m $	γ_{air}^0	$ m $	γ_{air}^0
0	117.7	18	71.9
1	111.4	19	70.4
2	104.3	20	68.8
3	98.5	21	67.1
4	94.0	22	65.3
5	90.3	23	63.5
6	87.5	24	61.6
7	85.2	25	59.7
8	83.4	26	57.8
9	82.0	27	56.0
10	80.8	28	54.1
11	79.6	29	52.4
12	78.7	30	50.7
13	77.7	31	49.1
14	76.8	32	47.7
15	75.6	33	46.3
16	74.6	34	45.0
17	73.3		

between 10% and 20%, or code 5, i.e., between 5% and 10%) for a strongly perturbed sub-band (*Pee*, *Ree*, and *Qfe* sub-branches of the $(3\nu_4 + \nu_5)^2\Pi - \nu_4^1$ band), and for some bands ($(3\nu_4 + \nu_5)_+^0 - \nu_4^1$, $(3\nu_4 + \nu_5)_-^0 - \nu_4^1$, $(3\nu_4 + \nu_5)^2\Pi - \nu_4^1$, $(2\nu_4 + 2\nu_5)_-^0 - \nu_5^1$, and $(2\nu_4 + 2\nu_5)^2\Pi - \nu_5^1$), whose intensity is known only from a few individual line intensities.

To conclude this paper, let us recall that a large number of line parameters have been obtained in this work for 18 bands of acetylene in the 5- μm region, using a multispectrum fitting procedure. Particularly, together with improved absolute line positions, absolute intensities have been measured for 540 lines (mean accuracy $\pm 5\%$). These data will be useful for further theoretical calculations. Numerous self-broadening and self-shifting coefficients have also been measured, and an approximate value of the self-collisional narrowing coefficient, namely $\beta^0 = 0.064 \pm 0.015$ (1SD) $\text{cm}^{-1} \text{ atm}^{-1}$ at about 296 K [3], has been determined, improving noticeably the knowledge of pressure effects on C_2H_2 lines belonging to various bands.

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