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**Recommended acetylene line list in the 20 – 240 cm⁻¹ and 400 – 630 cm⁻¹
regions: new measurements and global modeling**

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Abstract

A new recommended $^{12}\text{C}_2\text{H}_2$ line list for the $13 - 248 \text{ cm}^{-1}$ and $390 - 634 \text{ cm}^{-1}$ regions is presented. It is based on the results of the global modeling of the line positions and intensities performed in Tomsk within the framework of the method of effective operators. To validate the Tomsk calculations new measurements of both line positions and intensities were performed using acetylene spectra recorded between 25 and 680 cm^{-1} with the AILES-A beamline of SOLEIL synchrotron. Line positions and intensities of 627 transitions belonging to 9 bands have been measured for the first time in this region. Using the results of these new measurements and the published results of the measurements in the $13 - 248 \text{ cm}^{-1}$ and $390 - 634 \text{ cm}^{-1}$ regions performed with the same facilities new fittings of the line intensities for the $\Delta P = 0$ and $\Delta P = 1$ series of transitions have been performed. Here $P = 5v_1 + 3v_2 + 5v_3 + v_4 + v_5$ is a polyad number, where v_1 , v_2 , v_3 , v_4 , and v_5 are the principal quantum numbers of the acetylene harmonic oscillators. These new sets of the effective dipole moment parameters were used to generate the line list which contains the line positions and intensities of 39 and 29 bands, respectively for the $\Delta P = 0$ and $\Delta P = 1$ series of transitions. None of these bands is present in the HITRAN 2012 and GEISA 2015 databases. This paper presents the first part of a global work on the validation of Tomsk calculations.

Keywords : acetylene; calculated line positions and intensities; new measurements; global modelling; line list; spectroscopic databases.

1. Introduction

The infrared spectroscopy of the acetylene molecule C_2H_2 is important for the atmospheric, planetary, astrophysical, and industrial applications. This molecule is present and detected as a trace constituent in the troposphere [1] and in the upper atmosphere of the giant planets where it comes from methane photodissociation, but also in the circumstellar shell of cool carbon stars [2] and in the interstellar clouds [3]. The knowledge of accurate line positions and intensities is crucial to perform accurate detection of acetylene. Recent and future instruments such as e.g. SPITZER [4,5], ALMA [6], or HERSCHEL [7] are operating in the FIR spectral region where only very few line intensities of acetylene have been measured. The 20- μm spectral region has never been studied at high resolution to retrieve absolute line intensities. Below 600 cm^{-1} , atmospheric databases such as HITRAN 2012 [8] and GEISA 2015 [9] do not contain any line parameters. Above 600 cm^{-1} the line positions and intensities have come from experimental measurements and their interpolations and extrapolations. This paper is devoted to the extension of the acetylene line list for the new 2016 edition of the HITRAN database. The presented line list covers the $13 - 248\text{ cm}^{-1}$ and $390 - 634\text{ cm}^{-1}$ spectral regions. These spectral regions include transitions of the $\Delta P = 0$ and 1 series of bands, where P is a pseudo-quantum number equals to $5v_1 + 3v_2 + 5v_3 + v_4 + v_5$, where v_1, v_2, v_3, v_4 , and v_5 are the principal quantum numbers of the $^{12}C_2H_2$ harmonic oscillators. The corresponding line list is based on the global calculation performed in Tomsk (updated from the new measurements presented in this work) and on the Jet Propulsion Laboratory (JPL, Pasadena) line list [10] for the line positions when available. The JPL line list is based on the global modeling of the vibration-rotation energy levels of the bending vibrations [11] and on the estimates of the line intensities using the vibrational transition dipole moment 0.051 D for the difference $v_5 - v_4$ band from Ref. [12]. The Tomsk line list is based on the global modeling of the line positions and intensities within the framework of the method of effective operators [13-15] applied to various ΔP series [15-20].

The $\Delta P = 0$ region (around $100\text{ }\mu m$) has been recently studied using the AILES-A (Advanced Infrared Line Exploited for Spectroscopy) beamline of SOLEIL synchrotron [21,22] in France and using the far-infrared beamline of Canadian Light Source (Saskatoon) [23]. The lower frequency part of the $\Delta P = 1$ region (around $20\text{ }\mu m$) where bands are weaker than the strongest bands in this region (especially the v_5^1 band) was never studied to our knowledge in terms of accurate determination of the line positions or intensities.

One of the goals of the present work was to assess the Tomsk calculated line list in the lower part of the $\Delta P = 1$ spectral region where no intensity measurements have been performed before. For these purposes the measurements of the absolute line positions and intensities between the 400 and 600 cm^{-1} have been performed using the spectra recorded in SOLEIL [21,22]. These measurements have been compared to the Tomsk predicted line parameters. The effective dipole moment parameters for the $\Delta P = 1$ spectral region were then improved through a global fit including newly measured line intensities.

The SOLEIL experimental spectra and their analysis between the 400 and 680 cm^{-1} will be presented in Section 2. In Section 3, the line intensity fits for the $\Delta P = 0$ and 1 series of bands will be described. The comparisons of Tomsk predictions/calculations with the measurements and the JPL line list will be given in Section 4, whereas Section 5 will be devoted to the description of the recommended $^{12}\text{C}_2\text{H}_2$ line list in the 13 – 248 cm^{-1} and 390 – 634 cm^{-1} regions which are available as supplementary data.

2. New measurements in the 400 – 680 cm^{-1} spectral region

In Ref. [21], six spectra were recorded with the rapid scan Bruker IFS 125 HR interferometer coupled to the far infrared beamline AILES of the SOLEIL synchrotron. This beamline utilizes infrared synchrotron radiation from both edge emission and constant field synchrotron source. The far infrared synchrotron emission is extracted and transported under vacuum in AILES beamline and is focused on the entrance aperture of the high resolution interferometer. The Bruker IFS 125 was equipped with a 6 μm Mylar beam splitter, and a 4.2 K Si-bolometer detector. Experimental conditions are shown in Table 1 (the same as Table 1 of Ref. [21], except the erroneous resolution for the spectrum #5 that has been corrected here).

Table 1: Experimental conditions and characteristics of the spectra recorded using the rapid-scan interferometer of SOLEIL-AILES beamline.

Commercial sample (Air Liquide Alphagaz)

Natural C ₂ H ₂	97.760% of ¹² C ₂ H ₂
Stated purity	99.55%
Total absorption path	151,75(1) m
Collimator focal length	418 mm
Beam size at focal point	1.1 mm

Spectrum number	Total pressure (mbar)	Temperature (K)	Bruker-resolution ^a (cm ⁻¹)	Number of co-added scans
1	0.2532	294.85	0.002	360
2	0.6031	295.05	0.002	520
3	1.943	294.95	0.002	400
4	4.947	295.05	0.003	820
5	9.709	296.85	0.002	482

^a Bruker-resolution = $0.9/\Delta_{max}$, Δ_{max} being the maximum optical path difference.

An optical filter covering the spectral region between 50 and 600 cm⁻¹ was employed. The whole optical path was under vacuum and a metal multipass White-type cell (2.5-m base length) was aligned to provide a 151.75 ± 0.01 m absorption path length. More details concerning the experimental spectra and their preliminary analysis to study the apparatus function can be found in Ref. [21]. Based on that study, an average effective radius of the beam equal to (1.1 ± 0.1) mm was used for optical weighting of the boxcar delimiting the maximal optical path difference [21]. The portions of the spectra #2, #3 and #5 between 440 and 580 cm⁻¹ are plotted in Fig. 1. One can clearly see the acetone unresolved absorption band between 500 and 550 cm⁻¹ growing with the pressure. Acetone traces (not quantified but smaller than 0.1% of the total pressure of our experimental spectra) are due to the conditioning of acetylene gas inside commercial bottles for safety reasons. This band, centered at 520-530 cm⁻¹, is quite strong and is almost saturated in the spectrum #5 at the highest acetylene pressure.

Fig. 1. Overview of the spectra #2 (black line), #3 (red line) and #5 (blue line) (see Table 1 for the experimental conditions).

Figure 2 shows the Q -branch of the ν_4^1 band of $^{12}\text{C}_2\text{HD}$, present as a natural constituent in the commercial bottles of acetylene. In the upper panel of this figure the intensity diagram is plotted using the $^{12}\text{C}_2\text{HD}$ data from HITRAN [8] and $^{12}\text{C}_2\text{H}_2$ data from the Tomsk calculations [15]. Both HITRAN and GEISA [9] databases include the $^{12}\text{C}_2\text{HD}$ data of Jolly et al. [24]. In the lower panel of Fig. 2 the experimental spectrum #2 at a sample pressure of 0.6031 mbar is presented. Note that in the various experimental spectra, the $^{12}\text{C}_2\text{HD}$ transitions linearly increase with the growing of the pressure of C_2H_2 introduced into the cell, which suggest that this isotopologue comes from the commercial sample and that its abundance is stable and equal to natural abundance (0.00030455). The ν_4^1 band of $^{12}\text{C}^{13}\text{CH}_2$ has also been observed in our spectra, and as for $^{12}\text{C}_2\text{HD}$, this isotopologue of acetylene is stable and present in natural abundance in the commercial sample of acetylene used in this work.

Fig. 2. Overview of the Q -branch of the ν_4^1 band of C_2HD . Upper panel is a stick plot of HITRAN 2012 [8] for $^{12}C_2HD$ (red sticks) and Toms calculations for $^{12}C_2H_2$ (black sticks). The line intensities are given in $cm^{-1}/(molecule.cm^{-2})$ at 296K in natural abundances. In the lower panel the spectrum #2 recorded with 0.6031 mbar of acetylene is plotted. The star symbol stands for the water transition due to the water impurity inside the tank of the interferometer.

The signal to noise ratio of the spectra depends on the wavenumber and is about 60 around 425 cm^{-1} , 50 around 480 cm^{-1} , 45 around 520 cm^{-1} , and 50 around 560 cm^{-1} . The decreasing signal to noise ratio is mainly due to the acetone absorption feature between 510 and 550 cm^{-1} (see Fig. 1). Because of this absorption, spectrum #5 was not used between 499 and 550 cm^{-1} to retrieve the line parameters. For this spectral range, only spectra #1-4 were retained for line parameters retrieval. As it can be observed in Fig.1, an irregular multiplicative channel spectrum is present on the spectra. This channel spectrum was modelled locally as a background adjusted in a small spectral domain of around 0.050 cm^{-1} with a second order polynomial function.

Using the preliminary study of Ref. [21] (wavenumber calibration and determination of the apparatus function for this given set of spectra), the multispectrum fitting procedure of Ref. [25] based on Ref. [26] was used fixing the self-broadening coefficients at the values of Ref. [27] and using the Voigt profile.

Fig. 3. Overview of the simultaneous fit of Q_{ef} and Q_{fe} branches of the $2v_4^2 - v_5^1$ band of $^{12}\text{C}_2\text{H}_2$. The upper panel is a stick plot of Tomsk calculations for $^{12}\text{C}_2\text{H}_2$ with rotational assignment. In the middle panel are plotted the experimental spectra #1-5 (in black) and the respective fitted spectra (red for spectrum #1, blue for #2, green for #3, cyan for #4 and orange for #5) using the multispectrum fitting procedure [25]. In the lower panel the residuals of the fit for the experimental spectra #1-5 (the same set colors as for the fitted spectra have been used) are given.

An example of the result of the multispectrum fit is given in Fig. 3 for the Q_{ef} and Q_{fe} branches of the $2v_4^2 - v_5^1$ band of $^{12}\text{C}_2\text{H}_2$ between 499.5 and 499.9 cm^{-1} . Taking into account the signal to-noise ratio (which is close to 50), the residuals of the fit do not show any strong characteristic signature.

Absolute line positions and intensities have been retrieved for 627 transitions involving 9 vibration-rotation bands. A sample of the results for the two Q branches of the $2v_4^2 - v_5^1$ band is given in Table 2 (the whole set of the measurements is given as supplementary material). A summary of the measurements performed in this work is presented in Table 3 for the 9 studied bands.

Table 2. Line positions (in cm^{-1}) and intensities (in $\text{cm}^{-1}/(\text{molecule} \cdot \text{cm}^{-2})$ at 296K in natural abundance) measured for the two Q branches of the $2\nu_4^2 - \nu_5^1$ band.

Rotational assignment	Vibrational assignment		Line position	Line intensity
	Upper	Lower		
Qf 33	00020 2 0	00001 0 1	492.40345	3.38E-25
Qf 31	00020 2 0	00001 0 1	493.31787	7.18E-25
Qf 30	00020 2 0	00001 0 1	493.75334	3.09E-25
Qf 28	00020 2 0	00001 0 1	494.58109	5.88E-25
Qf 27	00020 2 0	00001 0 1	494.97310	2.37E-24
Qf 26	00020 2 0	00001 0 1	495.35041	1.02E-24
Qf 25	00020 2 0	00001 0 1	495.71299	4.07E-24
Qf 24	00020 2 0	00001 0 1	496.06067	1.69E-24
Qf 23	00020 2 0	00001 0 1	496.39331	6.64E-24
Qf 22	00020 2 0	00001 0 1	496.71077	2.69E-24
Qf 21	00020 2 0	00001 0 1	497.01295	1.01E-23
Qf 20	00020 2 0	00001 0 1	497.29953	3.97E-24
Qf 19	00020 2 0	00001 0 1	497.57033	1.48E-23
Qf 18	00020 2 0	00001 0 1	497.82511	5.34E-24
Qf 17	00020 2 0	00001 0 1	498.06343	1.97E-23
Qf 16	00020 2 0	00001 0 1	498.28505	7.06E-24
Qf 15	00020 2 0	00001 0 1	498.48953	2.32E-23
Qf 14	00020 2 0	00001 0 1	498.67647	8.27E-24
Qf 13	00020 2 0	00001 0 1	498.84547	2.67E-23
Qf 12	00020 2 0	00001 0 1	498.99623	8.38E-24
Qf 11	00020 2 0	00001 0 1	499.12863	2.53E-23
Qf 10	00020 2 0	00001 0 1	499.24272	7.98E-24
Qf 9	00020 2 0	00001 0 1	499.33906	2.22E-23
Qf 8	00020 2 0	00001 0 1	499.41849	6.40E-24
Qf 7	00020 2 0	00001 0 1	499.48242	1.71E-23
Qf 6	00020 2 0	00001 0 1	499.53253	4.66E-24
Qf 5	00020 2 0	00001 0 1	499.57079	1.11E-23
Qf 4	00020 2 0	00001 0 1	499.59917	2.64E-24
Qf 3	00020 2 0	00001 0 1	499.61952	5.55E-24
Qf 2	00020 2 0	00001 0 1	499.63333	9.64E-25
Qe 2	00020 2 0	00001 0 1	499.66190	2.88E-24
Qe 3	00020 2 0	00001 0 1	499.67796	1.48E-24
Qe 4	00020 2 0	00001 0 1	499.69923	6.37E-24
Qe 5	00020 2 0	00001 0 1	499.72587	2.44E-24
Qe 6	00020 2 0	00001 0 1	499.75781	8.84E-24
Qe 7	00020 2 0	00001 0 1	499.79504	3.05E-24
Qe 8	00020 2 0	00001 0 1	499.83758	9.81E-24
Qe 9	00020 2 0	00001 0 1	499.88539	3.21E-24
Qe 10	00020 2 0	00001 0 1	499.93846	9.80E-24
Qe 11	00020 2 0	00001 0 1	499.99680	3.13E-24
Qe 13	00020 2 0	00001 0 1	500.12917	2.77E-24
Qe 14	00020 2 0	00001 0 1	500.20321	7.83E-24
Qe 15	00020 2 0	00001 0 1	500.28241	2.24E-24
Qe 16	00020 2 0	00001 0 1	500.36675	6.00E-24
Qe 17	00020 2 0	00001 0 1	500.45628	1.76E-24
Qe 18	00020 2 0	00001 0 1	500.55092	4.58E-24
Qe 19	00020 2 0	00001 0 1	500.65059	1.26E-24
Qe 20	00020 2 0	00001 0 1	500.75539	3.24E-24
Qe 21	00020 2 0	00001 0 1	500.86526	8.68E-25
Qe 22	00020 2 0	00001 0 1	500.98008	2.20E-24

Qe 23	00020 2 0	00001 0 1	501.09987	5.64E-25
Qe 25	00020 2 0	00001 0 1	501.35436	3.47E-25
Qe 26	00020 2 0	00001 0 1	501.48897	7.90E-25
Qe 28	00020 2 0	00001 0 1	501.77261	4.93E-25

Note: The vibrational assignment for the upper and lower states refers to the $V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5$ quantum numbers (see Section 3.3 for more details). Concerning the rotational assignment, the branch type is first given, then the e/f character of the lower state, and finally the rotational quantum number J of the lower state.

Table 3. Statistics for the measurements performed in the 429 – 593 cm^{-1} spectral region.

Studied band		Number of measurements	Positions		Line intensities	
			min	max	min	max
00020 2 0	00001 0 1	120	429.6	572.8	0.634E-25	0.267E-22
00020 0 0	00001 0 1	94	429.6	592.5	0.139E-24	0.338E-22
00030 1 0	00011 1 1	106	449.6	583.9	0.858E-25	0.207E-23
00030 1 0	00011 1-1	59	478.8	580.5	0.121E-24	0.583E-23
00030 3 0	00011 1 1	71	468.2	559.8	0.884E-25	0.238E-23
00021 0 1	00002 0 0	56	457.4	568.3	0.912E-25	0.191E-23
00021 0 1	00002 0 2	71	458.5	536.5	0.106E-24	0.153E-23
00021 2 1	00002 0 2	47	456.8	563.5	0.732E-25	0.828E-24
00021 2 1	00002 0 0	3	555.6	565.6	0.752E-25	0.115E-24

Note: The band notation refers to the upper and lower vibrational state, see note of Table 2. The line positions are given in cm^{-1} and the line intensities are in $\text{cm}^{-1}/(\text{molecule} \cdot \text{cm}^{-2})$ at 296K in natural abundance.

3. Tomsk calculated line lists

As we have already mentioned in the Introduction a cluster (polyad) model of the effective Hamiltonian has been used by Tomsk group for global modeling of the acetylene line positions and intensities [13-15]. The matrix of this Hamiltonian was written in the basis of the products of the eigenfunctions of the harmonic oscillators and rigid symmetric top. The fit of the 237 effective Hamiltonian parameters was performed to about 25000 line positions collected from the literature. The global RMS of the fit was 0.00265 cm^{-1} .

The line intensities were calculated using the eigenfunctions of the effective Hamiltonian. In this case one has to use the effective dipole moment operator which is obtained from the dipole moment operator by the same unitary transformation as one applied to the vibration-rotation Hamiltonian to generate the effective Hamiltonian. Within the framework of the polyad model of the effective Hamiltonian all transitions could be distributed among the series of transitions determined by the values of $\Delta P = P_{\text{up}} - P_{\text{low}}$. Each series of transitions is described by its own set of the effective dipole moment parameters. This approach applied to the acetylene molecule was originally presented in our papers [14,15]. The effective dipole moment parameters of 16 series of transitions $\Delta P=0,1,2,\dots,15$ were fitted to the observed line intensities collected from the literature [15,20]. The result of the new refined fit for $\Delta P=0$ and 1 are given in the following sub-sections. Note that for these two spectral regions, the fitted effective dipole moment parameters reproduce the observed line intensities practically within their experimental uncertainties.

In the present paper we will compare the C_2H_2 line positions and intensities calculated within the framework of the method of effective operators to those measured in this work. In the case of the line intensities two calculations will be considered. The first one is based on the published effective dipole moment parameters [15], and the second one is based on the effective dipole moment parameters fitted in this paper. Note that the calculated line intensities for a band for which no measurement is available are considered as predictions. The recently published sets of the effective Hamiltonian and effective dipole moment parameters [15] were used to generate the acetylene line list in the $20\text{-}10000 \text{ cm}^{-1}$ region. This line list contains more than 400 000 transitions using an intensity cutoff of $10^{-27} \text{ cm molecule}^{-1}$ at 296 K. The graphical overview of this line list is presented in Fig. 4 together with the data from HITRAN 2012 or GEISA 2015. The majority of the calculated line positions and intensities in the region under study in this work ($20\text{-}600 \text{ cm}^{-1}$) are predictions. In the $\Delta P = 0$ region only the measurements of Ref. [22] for the strongest $\nu_5 - \nu_4$ band were used in the fittings of the

effective Hamiltonian and the effective dipole moment parameters [15], so that for all 15 additional bands measured in Ref. [21], the calculated line parameters could be considered as predictions. In the $\Delta P = 1$ region, the line intensities are measured only in the present work (Section 2), so the respective calculated line intensities could be considered as predicted ones. The new refined effective dipole moment parameters lead to the improved calculated values of the line intensities especially in the $400 - 630 \text{ cm}^{-1}$ region. The new calculation for $\Delta P = 0$ and $\Delta P = 1$ will be presented respectively in sub-sections 3.1 and 3.2 together with comparisons to the predictions and measurements. Since vibrational labeling of the current HITRAN [8] and GEISA [9] databases is not sufficient anymore to describe all bands, an alternative vibrational labeling is described in sub-section 3.3.

Fig. 4. Overview of the line positions and intensities available for $^{12}\text{C}_2\text{H}_2$ in the atmospheric HITRAN and GEISA databases (red symbols), calculated using the parameters determined in Ref. [15] (black solid squares) and calculated in this work (open blue triangles).

3.1 Line intensity fit ($\Delta P = 0$ series of transitions)

In the recent calculations [15] the effective dipole moment parameters for the $\Delta P=0$ series of transitions were determined by fitting to the line intensities of only one difference

band $\nu_5\text{-}\nu_4$ observed in Ref. [22]. In the present paper we have performed a new fit of the effective dipole moment parameters for this series of transitions involving the observed line intensities of 15 additional bands published in Ref. [21]. The equation for the transition dipole moment squared published in our papers [14,15] and the eigenfunctions of our global effective Hamiltonian [15] were used in the fit. The partition sum $Q=414.03$ at 296 K was taken from Ref. [28]. The aim of the fitting procedure was to minimize the value of the dimensionless weighted standard deviation

$$\chi = \sqrt{\frac{\sum_{i=1}^N ((S_i^{obs} - S_i^{calc}) / \delta_i)^2}{N - n}}, \quad (1)$$

where S_i^{obs} and S_i^{calc} are, respectively, the observed and calculated values of the intensity for the i^{th} line, $\delta_i = (S_i^{obs} \sigma_i) / 100\%$ is the absolute measurement error of i^{th} line, σ_i is the measurement error in %, N is the number of the fitted line intensities, and n is the number of the adjusted effective dipole moment parameters. We used the same value $\sigma_i = 5\%$ for all observed line intensities. With 5 effective dipole moment parameters we reached $\chi = 0.8$ and global RMS=4.2%. The set of the effective dipole moment parameters is presented in Table 4 and the statistics of the fit is given in Table 5. Note that some measurements were removed from the fit of the effective dipole moment parameters that explains why the number of the measured transitions in Table 5 is not always equal to those given in Refs. [21,22]. As observed in this table, the statistics for the strongest $\nu_5^1\text{-}\nu_4^1$ band measured in both Refs. [21,22] is slightly improved in our new calculations (second line of Table 5) compared to the previous ones [15]. In Table 4 we give both the new set of the effective dipole moment parameters and that obtained in Ref. [15] using the line intensities of only one difference $\nu_5^1\text{-}\nu_4^1$ band. In Ref. [15] only two effective dipole moment parameters for $\Delta P = 0$ series were determined. They are not considerably changed in the new fit. Figures 5-8 show rotational dependences of the transition dipole moments squared for four bands of the $\Delta P = 0$ series deduced from measurements, from prediction and from the calculations using the new fitted set of the effective dipole moment parameters. Figures 5-8 show that the predictions are practically as good as the new calculations for the bands measured for the first time in Ref. [21].

Table 4. Effective dipole moment parameters for the $\Delta P=0$ series of transitions.

Parameter ^a	ΔV_1	ΔV_2	ΔV_3	ΔV_4	ΔV_5	$\Delta \ell_4$	$\Delta \ell_5$	Value ^b	Ref. [15]
M	0	0	0	1	-1	1	-1	$0.2674(7) \times 10^{-1}$	$0.2562(5) \times 10^{-1}$
κ_4	0	0	0	1	-1	1	-1	$-0.209(1) \times 10^{-1}$	
κ_5	0	0	0	1	-1	1	-1	$-0.125(1) \times 10^{-1}$	
b_{JO}	0	0	0	1	-1	1	-1	$-0.2474(3) \times 10^{-2}$	$-0.247(7) \times 10^{-2}$
M	0	0	0	1	-1	1	1	$-0.128(1) \times 10^{-4}$	

^a Parameters M are given in Debye while the other parameters are dimensionless. For the definition of the parameters see Refs. [15,16].

^b Confidence intervals (1 SD, in unit of the last quoted digit) are given between parenthesis.

Table 5. Statistics of the fitted bands of $\Delta P=0$ series.

Observed band	Spectral range in cm^{-1}	$J_{\max}$ ^a	N ^b	MR ^c in %	RMS ^d in %
00001 0 1 - 00010 1 0	65.9 - 191.3	30	117	0.18	4.25
00001 0 1 - 00010 1 0	54.3 - 214.8	40	122	0.60	2.98
00011 1 1 - 00020 2 0	62.5 - 202.0	36	100	1.28	4.24
00002 0 2 - 00011 1 1	64.1 - 206.1	37	72	0.35	3.33
00012 1 2 - 00021 2 1	74.5 - 178.1	27	66	-0.90	4.23
00003 0 3 - 00012 1 2	82.7 - 170.6	23	54	-1.26	4.77
00002 0 0 - 00011 1-1	64.8 - 201.2	33	50	0.61	2.82
00021 2 1 - 00030 3 0	75.9 - 177.1	26	48	1.49	4.07
00012 1 0 - 00021 2-1	65.6 - 170.8	25	47	2.24	4.56
00003 0 1 - 00012 1 0	86.1 - 182.8	25	39	2.16	4.49
00011 1-1 - 00020 0 0	61.8 - 168.1	31	39	-4.51	5.30
00021 2-1 - 00030 1 0	64.4 - 143.0	24	33	-1.89	4.20
00011 1 1 - 00020 0 0	64.2 - 190.2	33	30	-1.11	3.13
00011 1-1 - 00020 2 0	64.8 - 188.6	35	27	-1.85	3.41
00012 1 0 - 00021 0 1	95.2 - 154.7	25	11	-1.49	7.35
00021 2 1 - 00030 1 0	141.2 - 165.5	24	10	1.36	6.03
00021 0 1 - 00030 1 0	80.8 - 134.7	12	8	3.87	5.62
00021 0 1 - 00030 3 0	148.5 - 172.3	26	8	4.45	9.78

Note: The statistics for the ν_5^1 - ν_4^1 band (first two lines) are given twice. The first line corresponds to the old set of parameters [15] obtained using intensity data only from Ref. [22]. The second line corresponds to the new set of parameters, which are fitted to the line intensities of 17 bands measured in Ref. [21].

^a Maximum value of the angular momentum quantum number for a given band.

^b N is the number of the measured line intensities included in the fit

^c Mean residuals.

^d Root mean squares of the residuals.

Fig. 5. Transition dipole moment squared deduced from the measurements [21], old calculations [15] and new calculations (this work) for the strong ν_5^1 - ν_4^1 band of $\Delta P = 0$ region. Solid symbols stands for the measurements [21], black symbols correspond to the transitions with a lower state symmetry e and red symbols correspond to the transitions with f -symmetry for the lower state. The same colors are used for both old (dot lines) and new calculations (continuous lines).

Fig. 6. Transition dipole moment squared deduced from the measurements [21], prediction [15] and new calculation (this work) for the “forbidden” $(\nu_4^1 + \nu_5^{-1}) - 2\nu_4^2$ band (P_{ee} and R_{ee} sub-branches, see legend of Fig. 5 for symbols and lines).

Fig. 7 Transition dipole moment squared deduced from the measurements [21], prediction [15] and new calculation (this work) for the “forbidden” $(v_4^1 + v_5^1) - 2v_4^0$ band (P_{ee} and R_{ee} sub-branches, see legend of Fig. 5 for symbols and lines).

Fig. 8 Transition dipole moment squared deduced from the measurements [21], prediction [15] and new calculation (this work) for the $(2v_4^2 + v_5^1) - 3v_4^3$ band (P_{ee} , P_{ff} , R_{ee} and R_{ff} sub branches, see legend of Fig. 5 for symbols and lines). Note that the half-open symbols correspond to measurements that have not been retained for the fit of the effective dipole moment parameters of the $\Delta P=0$ series.

Very strong dependence on the rotational quantum number J of the transition dipole moment squared in the Q -branches of the bands with $\Delta K=0$ and $K \neq 0$ in C_2H_2 was experimentally observed in Refs. [21,22]. Here K is the quantum number of the projection of the total angular momentum on the molecular axis. This effect was theoretically predicted in our papers [14,15]. The Herman-Wallis type function responsible for the influence of the vibration-rotation interaction on the line intensity in this particular case is given by equation [14,15].

$$F_{\Delta J=0 \Delta K=0}^{\Delta V \Delta \ell_4 \Delta \ell_5}(J, K) = \left(\frac{b_{JQ}^{\Delta V \Delta \ell_4 \Delta \ell_5}}{K} + d_J^{\Delta V \Delta \ell_4 \Delta \ell_5} \right) [J(J+1) - K^2]. \quad (2)$$

Here $b_{JQ}^{\Delta V \Delta \ell_4 \Delta \ell_5}$ and $d_J^{\Delta V \Delta \ell_4 \Delta \ell_5}$ are the parameters of the matrix element of the effective dipole moment operator, ℓ_4 and ℓ_5 are the vibrational angular momentum quantum numbers associated with the degenerate normal modes with the harmonic frequencies ω_4 and ω_5 , respectively, ($\ell_4 + \ell_5 = K$). The strong rotational dependence of the transition dipole moment squared is connected with the parameter $b_{JQ}^{\Delta V \Delta \ell_4 \Delta \ell_5}$ which appears only in this particular case in the first order of the perturbation theory and its value is at least two orders of magnitude larger than the value of the parameter $d_J^{\Delta V \Delta \ell_4 \Delta \ell_5}$ appearing in the second order of the perturbation theory. In the usual case of a band with $\Delta K=0$ and $K=0$, the parameter $b_{JQ}^{\Delta V \Delta \ell_4 \Delta \ell_5}$ is absent and the rotational dependence of the line intensities of the Q -branch is described by $d_J^{\Delta V \Delta \ell_4 \Delta \ell_5}$ parameter. The fitted sets of the effective dipole moment parameters reproduce this effect very well.

3.2. Line intensity fit ($\Delta P=1$ series of transitions)

In this section we present the results of the fit of the line intensities for the bands belonging to the $\Delta P=1$ series of transitions. Basing on the new measurements performed in this work (Section 2) and on the measurements published earlier [29,30] we have fitted 14 effective dipole moment parameters for the $\Delta P=1$ series of transitions to 874 measured line intensities of 14 bands. The set of the effective dipole moment parameters for $\Delta P = 1$ is presented in Table 6 and the statistics of the fit is given in Table 7. The intensities of 185 blended lines were excluded from the fit. For the weighting we used the mean experimental uncertainties for each band which are presented in column “Error” of Table 7. As in the case of the $\Delta P=0$ series of

transitions the eigenfunctions of our global effective Hamiltonian [15] and the partition sum from Ref. [28] were used in the fit. The fit reached the value $\chi = 0.75$ for the weighted dimensionless standard deviation and the value RMS=4.4% for the global root mean squares of the residuals. Note that some measurements were removed from the fit of the effective dipole moment parameters that explains why the number of measured transitions in Table 7 is not always equal to those of Table 3. Figures 9-12 show the rotational dependences of the transition dipole moments squared deduced from the measurements, prediction [15] and new calculation for four bands of the $\Delta P = 1$ region. These figures show that the prediction is not as good as for the $\Delta P = 0$ region. For example, in the case of the $3\nu_4^1 - (\nu_4^1 + \nu_5^1)$ band (see Fig. 11), the prediction are strongly underestimated compared to the measurements (especially for the P_{ff} , R_{ff} and Q_{ef} sub-branches), whereas for the Q_{fe} sub-branch the prediction is strongly overestimated (Section 2). The reason for this is the absence of some important parameters for the respective bands in the old set of the effective dipole moment parameters [15] (see Table 6). For example, in the case of the $3\nu_4^1 - (\nu_4^1 + \nu_5^1)$ band the parameters of the effective dipole moment matrix element with $\Delta V_4=2$, $\Delta V_5=-1$, $\Delta \ell_4=0$, $\Delta \ell_5=1$ are very important but they were absent in the old set of parameters [15]. The absent parameters could not be determined using the line intensity data from Refs. [29,30]. The new measurements performed in this work allowed determining additional parameters compared to the old set [15] that improved significantly the line intensity calculation.

Table 6. Effective dipole moment parameters for the $\Delta P=1$ series of transitions.

Parameter ^a	ΔV_1	ΔV_2	ΔV_3	ΔV_4	ΔV_5	$\Delta \ell_4$	$\Delta \ell_5$	Value ^b	Ref. [15]
M	0	0	0	0	1	0	1	-0.1578(2)	-0.1579(2)
κ_5	0	0	0	0	1	0	1	-0.017(2)	-0.013(2)
b_J	0	0	0	0	1	0	1	$-0.76(5) \times 10^{-3}$	$-0.72(5) \times 10^{-3}$
d_J	0	0	0	0	1	0	1	$0.45(3) \times 10^{-4}$	$0.47(3) \times 10^{-4}$
M	0	0	0	2	-1	2	-1	$-0.3343(5) \times 10^{-2}$	
κ_4	0	0	0	2	-1	2	-1	0.020(3)	
b_J	0	0	0	2	-1	2	-1	$-0.244(9) \times 10^{-2}$	
d_J	0	0	0	2	-1	2	-1	$-0.63(6) \times 10^{-4}$	
M	0	0	0	2	-1	0	1	$0.665(2) \times 10^{-2}$	
κ_4	0	0	0	2	-1	0	1	0.059(2)	
a_5	0	0	0	2	-1	0	1	0.026(2)	
b_J	0	0	0	2	-1	0	1	$-0.119(8) \times 10^{-2}$	
d_J	0	0	0	2	-1	0	1	$-0.61(4) \times 10^{-4}$	
M	0	0	0	2	-1	-2	3	$-0.30(3) \times 10^{-3}$	

^a Parameters M are given in Debye while the other parameters are dimensionless. For the definition of the parameters see Refs. [15,16].

^b Confidence intervals (1 SD, in unit of the last quoted digit) are given between parentheses.

Table 7. Statistics of the fitted bands of the $\Delta P = 1$ series.

Observed band	Spectral range in cm^{-1}	J_{max}^a	N^b	Error ^c	MR ^d in %	RMS ^e in %
Bands measured in this work						
00020 2 0 - 00001 0 1	429.6 - 564.0	33	102	7	-0.79	3.86
00020 0 0 - 00001 0 1	429.6 - 586.8	34	86	7	0.98	3.96
00030 1 0 - 00011 1 1	449.7 - 583.9	27	79	7	-0.65	5.18
00030 1 0 - 00011 1-1	478.9 - 580.6	25	41	10	2.72	6.99
00030 3 0 - 00011 1 1	475.3 - 555.3	25	31	7	1.35	7.50
00021 0 1 - 00002 0 0	457.4 - 568.3	23	33	7	0.20	5.94
00021 0 1 - 00002 0 2	458.6 - 527.2	25	53	7	-0.26	3.74
00021 2 1 - 00002 0 2	456.8 - 563.6	24	20	10	2.95	7.47
00021 2 1 - 00002 0 0	555.7 - 565.6	21	2	10	6.69	6.73
Bands measured in the previous works [29,30]						
00001 0 1 - 00000 0 0	644.5 - 820.2	38	77	3	-0.22	3.36
00002 0 0 - 00001 0 1	661.0 - 800.2	32	64	5	0.21	3.64
00002 0 2 - 00001 0 1	674.7 - 794.8	30	79	5	0.35	2.66
00011 1-1 - 00010 1 0	655.8 - 787.5	31	109	5	0.31	3.29
00011 1 1 - 00010 1 0	669.4 - 798.8	28	98	5	0.45	4.37

Note: The band notation refers to the upper and lower vibrational states.

^a Maximum value of the angular momentum quantum number for a given band.

^b Number of the fitted line intensities for a given band.

^c Experimental uncertainty used in the fit for a given band.

^d Mean residuals.

^e Root mean squares of the residuals.

Fig. 9 Transition dipole moments squared deduced from the measurements (this work, Section 2), prediction [15] and from the new calculation (this work) for the $2v_4^2 - v_5^1$ band (P_{ee} , P_{ff} , R_{ee} and R_{ff} sub branches are in the left panel, Q_{ef} and Q_{ee} sub branches are in the right panel, see legend of Fig. 5 for symbols and lines). Note that the half-open symbols correspond to the measurements that have not been retained for the fit of the effective dipole moment parameters of the $\Delta P=1$ series.

Fig. 10 Transition dipole moments squared deduced from the measurements (this work, Section 2), prediction [15] and from the new calculation (this work) for the $2v_4^0 - v_5^1$ band (P_{ee} , R_{ee} and Q_{ef} sub-, see legend of Fig. 5 for symbols and lines). Note that the half-open symbols correspond to the measurements that have not been retained for the fit of the effective dipole moment parameters of the $\Delta P=1$ series.

Fig. 11 Transition dipole moment squared deduced from the measurements (this work, Section 2), prediction [15] and from the new calculation (this work) for the $3v_4^1 - (v_4^1 + v_5^1)$ band (P_{ee} , P_{ff} , R_{ee} and R_{ff} sub branches are in the left panel, Q_{ef} and Q_{fe} sub branches are in the right panel, see legend of Fig. 5 for symbols and lines). Note that the half-open symbols correspond to the measurements that have not been retained for the fit of the effective dipole moment parameters of the $\Delta P=1$ series.

Fig. 12 Transition dipole moments squared deduced from the measurements (this work, Section 2), prediction [15] and from the new calculation (this work) for the $3v_4^3 - (v_4^1 + v_5^1)$ band (P_{ee} , R_{ee} and Q_{ef} sub branches in left panel, P_{ff} , R_{ff} and Q_{fe} sub branches in right panel, see legend of Fig. 5 for symbols and lines). Note that the half-open symbols correspond to the measurements that have not been retained for the fit of the effective dipole moment parameters of the $\Delta P=1$ series.

3.3. Vibrational labeling

Within the framework of the method of effective operators the eigenfunction of the vibration-rotation state is given by equation

$$\Psi_{PNJq\varepsilon}^{eff} = \sum_{\substack{5V_1+3V_2+5V_3+V_4+V_5=P \\ \ell_4 \ell_5}}^J C_{PNJq\varepsilon}^{V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5} |V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5 J K \varepsilon\rangle, \quad (3)$$

where $C_{PNJq\varepsilon}^{V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5}$ is the expansion coefficient of an eigenfunction, P is the polyad number and N is the ranking index of an eigenvalue in a (P, q, ε, J) block. As the basis functions we use the Wang combinations of the products of the harmonic oscillators and rigid symmetric top eigenfunctions [13,15]

$$|V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5 J M K \varepsilon\rangle = \frac{1}{\sqrt{2}} |V_1 V_2 V_3 V_4^{\ell_4} V_5^{\ell_5}\rangle |J M K = \ell_4 + \ell_5\rangle \\ + \varepsilon |V_1 V_2 V_3 V_4^{-\ell_4} V_5^{-\ell_5}\rangle |J M - K = -\ell_4 - \ell_5\rangle, \quad (4)$$

with $\varepsilon=1$ or -1 and

$$|V_1 V_2 V_3 V_4 V_5 0 0 J M \varepsilon = 1\rangle = |V_1 V_2 V_3 V_4^0 V_5^0\rangle |JM0\rangle. \quad (5)$$

Taking into account the symmetry properties of the basis functions each P block can be split into four isolated subblocks $\{P, q, \varepsilon\}$. Here

$$q = \begin{cases} g & V_3 + V_5 \text{ even} \\ u & V_3 + V_5 \text{ odd}, \end{cases} \quad (6)$$

where g and u stand for the states symmetric and antisymmetric with respect to the point group inversion operation.

As it follows from the Eq.(3) the indexes ($JPNq\varepsilon$) give an unambiguous labeling of the vibration-rotation states of the acetylene molecule. However, from the physical point of view this labeling is not convenient, because labeling in terms of the quantum numbers of the harmonic oscillators and the rigid symmetric top gives a clearer physical picture in the case of low lying vibrational states where the energy level crossing takes place very seldom. In the case of tetratomic linear molecule there exists the condition

$$K = \ell_4 + \ell_5, \quad (7)$$

and a band is defined by the changing of the principal vibrational quantum numbers $\Delta V_1, \Delta V_2, \Delta V_3, \Delta V_4, \Delta V_5$ and by ΔK value. In the literature the labeling of the vibrational states in terms of $V_1 V_2 V_3 V_4 V_5 K$ quantum numbers is widely used. However, this labeling is ambiguous because for the given principal vibrational quantum numbers V_4 and V_5 , K could be composed by different combinations of the vibrational angular momentum quantum numbers ℓ_4 and ℓ_5 (see Eq.(7)). For example, there exist three vibrational states with $V_4=2, V_5=3$ and $K=1$: $\ell_4=0$ and $\ell_5=1, \ell_4=2$ and $\ell_5=-1, \ell_4=-2$ and $\ell_5=3$. To avoid this ambiguity Pliva [31,32] has suggested utilizing the ranking number r for such group of vibrational states ($r = 1$ for the highest energy level). To apply this vibrational labeling to the vibration-rotation states with high J values, the energy level prediction is used with the following polynomial equation:

$$E_{VK\pm}(J) = E_{VK} + B_{VK}J(J+1) - D_{VK}[J(J+1)]^2 + H_{VK}[J(J+1)]^3 \pm q_{VK}J(J+1). \quad (8)$$

In this equation E_{VK} is the vibrational term value, B_{VK}, D_{VK}, H_{VK} are the centrifugal distortion constants q_{VK} is the constant of the rotational ℓ -doubling. This kind of assignment could have a problem in the regions of the energy level crossing. The number of the crossings increases with the growth of the values of the rotational and vibrational quantum numbers.

In the HITRAN [8] and GEISA [9] databases the vibrational assignment defined in Ref. [33] is used:

$$V_1 V_2 V_3 V_4 V_5 \ell = K \pm r \text{ sym}, \quad (9)$$

where “ $\pm$ ” being the symmetry type for Σ vibrational states ($\ell = 0$), the *sym* field is used for the vibrational symmetry *g* or *u*.

The Tomsk group uses unambiguous (*JPNqe*) labeling when they deal with the global modeling of the vibration-rotation spectra of the acetylene molecule. However, for the generation of the C₂H₂ line list, it was decided to use the labels of the basis function corresponding to the principal expansion coefficient. In the majority of cases this labeling is the same as the traditional one, but for strong interacting bands this labeling can change within a band and be different from the traditional one. As an example, in the $\Delta P = 0$ region the largest contributor of the lower state of the transitions belonging to the sub-branch R_{ff} of the 00003 0 1 – 00012-1 2 band changes from $J = 12$. For J values greater than 11, the largest contributor of the lower state becomes 00012 1 0 instead of 00012-1 2. Not only the $\ell_4 + \ell_5$ value used up to now needs to be replaced by ℓ_4 and ℓ_5 in order to distinguish levels, but the largest contributor of the lower or upper states can change inside a series of transitions (a vibrational band). No rigorous algorithm has yet been found to resolve this problem of notation so that for some bands with strong interacted levels the vibrational labeling has been changed by hand in order to keep one unique vibrational labeling for a series of transitions. In some cases, the largest contributor to the eigenfunction can change several times inside a series of transitions. There is such a case, for example, in the $\Delta P = 1$ region, where the sub-branch Q_{ef} of the 00031 1 1 – 00012-1 2 band has different largest contributors depending on J values. From $J = 2$ to 11, the largest contributors are 00031 1 1 – 00012-1 2. From $J = 12$ to 26, the largest contributors are 00031 1 1 – 00012 1 0 (the largest contributor of the lower state changed). Finally, from $J = 27$ to 34, the largest contributors are 00031 3 1 – 00012 1 0 (the largest contributor of the upper state changed). In such cases, the vibrational labeling obtained for the lowest J value has been retained for all transitions belonging to the band. All bands affected by similar changes have been modified carefully by hand and are marked with a star in the last columns of Tables 8 and 9 for the $\Delta P = 0$ and 1 regions respectively.

4. Comparisons of the Tomsk line lists to the JPL catalog and the experimental measurements

The whole set of the measured line positions and intensities (816 transitions belonging to 19 bands between 51 and 215 cm^{-1}) from Ref. [21], and from this work (627 transitions belonging to 9 bands between 429 and 593 cm^{-1} , see Section 2) are compared in Fig. 13 with the Tomsk (see Sections 3.1 and 3.2) and JPL calculated line parameters. The average difference of the positions for common transitions (1231) between the Tomsk calculation and JPL line list is equal to $(0.02 \pm 1.05) \times 10^{-3} \text{ cm}^{-1}$. The average difference of the positions for the common transitions (1443) between the Tomsk calculation and the measurements performed in Ref. [21] and in this work (Section 2) is equal to $(-0.06 \pm 0.75) \times 10^{-3} \text{ cm}^{-1}$. The maximum differences do not exceed 0.01 cm^{-1} for both comparisons. The comparison of the JPL line positions to the measurements gives the mean residuals equal to $(-0.03 \pm 0.32) \times 10^{-3} \text{ cm}^{-1}$ (JPL - measurements). It does mean that the JPL line positions are slightly closer to the measurements than Tomsk line positions. As far as the line intensities are concerned, the JPL calculation has been performed using the vibrational transition dipole moment 0.051 D [12] for the line intensity calculations of all bands. The accuracy of the line intensities for the strongest $\nu_5^1 - \nu_4^1$ band is estimated to be 40% whereas for the other bands, accuracy of the line intensities calculation “should be viewed with more cautious since there might be systematic errors”. Indeed, whereas the JPL calculated line positions have been found very accurate (as expected), for most of the bands the JPL calculated line intensities have to be corrected by a constant scaling factor depending on the sub-branch of the bands. Moreover, many bands are missing in the JPL catalog, and for some calculated bands only a few transitions are given. The missing bands are due to the fact that the JPL calculation includes only the transitions involving the ground state and the upper vibrational states of the bands ν_4 , $2\nu_4$, ν_5 , $2\nu_5$, and $\nu_4 + \nu_5$.

The average relative intensity difference between our new calculations and the measurements (Ref. [21] and Section 2 of this paper) is equal to $(0.6 \pm 12.4)\%$ for 1443 common transitions. This average value has been obtained by taking into account all measurements of Ref. [21] and Section 2 of this paper, even those that do not follow the smooth rotation dependence for a band (measurements removed from the fit of the effective dipole moment parameters, see Figs. 8-12, half-open symbols). Removing these measurements, the average relative discrepancy equal to $(0.5 \pm 4.5)\%$ is obtained for 1197 common transitions.

Fig. 13. Comparisons of the line positions (left panel) and intensities (right panel) for all common transitions between our new calculation and the JPL line list (solid squares), and between our new calculation and measurements of Ref. [21] and of Section 2 of this work (open triangles).

In Figs. 14-18 the band-by-band comparisons are presented for 5 different types of bands having various ΔK and K values. The band-by-band analysis plotted in Figs. 14-18 allows observing both the erroneous scaling factors for the JPL calculated line intensities and effects of ignoring the rotational dependences. In Fig. 14 one can observe the large deviations of the JPL line intensities from the observed ones around 120 cm⁻¹ (see the right panel of Fig. 14), resulting from ignoring the strong rotational dependence exhibited by the two Q branches (see Fig. 5). In Fig. 15, the JPL calculation has clearly an erroneous factor 2 for the line intensities of the $2\nu_5^0 - (\nu_4^1 + \nu_5^{-1})$ band. In Figs. 16-17, it is more complicated to understand what happened to the JPL calculation, but the line intensities from the JPL calculation have to be updated.

Fig. 14. Comparisons of the line positions (left panel) and intensities (right panel) for the $\nu_5^1 - \nu_4^1$ band. In the left panel, the black solid square stands for the difference between the line positions from the Tomsk and JPL calculations, whereas in the right panel, it stands for the ratio of the line intensities (our new calculation / JPL). In the left panel, the red open triangle stands for the difference between the line positions from the Tomsk calculation and measurements [21], whereas in the right panel, it stands for the ratio of the line intensities (our new calculation / measurements of Ref. [21]).

Fig. 15. Comparisons of the line positions (left panel) and intensities (right panel) for the $2\nu_5^0 - (\nu_4^1 + \nu_5^1)$ band. See Fig. 14 for legend.

Fig. 16. Comparisons of the line positions (left panel) and intensities (right panel) for the $2v_5^2 - (v_4^1 + v_5^1)$ band. See Fig. 14 for legend.

Fig. 17. Comparisons of the line positions (left panel) and intensities (right panel) for the $2v_4^2 - v_5^1$ band. See Fig. 14 for legend. Note that the open triangles (in the right panel) that are not close to 1 correspond to the measurements removed from the fit because of the blending of the respective lines.

Fig. 18. Comparisons of the line positions (left panel) and intensities (right panel) for the $3v_4^1 - (v_4^1 + v_5^1)$ band. See Fig. 14 for legend. Note that this band is absent in the JPL line list.

5. Acetylene ($^{12}\text{C}_2\text{H}_2$) line list for databases

The results of this work allow building an accurate line list of positions and intensities in the 13 - 634 cm⁻¹ spectral range of acetylene ($^{12}\text{C}_2\text{H}_2$) corresponding to the $\Delta P = 0$ and lower part of $\Delta P = 1$ absorption regions. The Tomsk calculated line list, generated as described in section 3, was taken as the basis of the line list for databases. The line positions and intensities can be calculated with a quite good accuracy (better than 0.001 cm⁻¹ and 5%, respectively, for most of the bands). For a better accuracy of line positions, the JPL calculation of the line positions was used when available (except for the beginning, up to $J = 9$, of the Q branch of the $2v_4^0 - v_5^1$ band), in other cases the Tomsk calculations [15] were used. The new sets of the effective dipole moment parameters (Tables 4 and 6) were used to generate all line intensities. Tables 8 and 9 summarize the statistics on the bands for $\Delta P = 0$ and lower part of $\Delta P = 1$ regions that constitute our final line list for acetylene $^{12}\text{C}_2\text{H}_2$ between 13 and 634 cm⁻¹ for 10208 transitions. Instead of choosing an intensity cutoff, we chose to add 20 complete bands that are the most intense after the ones observed in Ref. [21] for $\Delta P = 0$ region and in Section 2 of this paper for the $\Delta P = 1$ region. The line list generated in this work between 13 to 634 cm⁻¹ is available as supplementary data in the HITRAN format.

The line list was completed with other parameters (broadening coefficients, temperature dependence and shifting coefficients) as described in Section 4 of Ref. [34]. As for the references and the error codes in the HITRAN format, the following rules were used:

- Error codes 4 ($(0.1-1) \times 10^{-3} \text{ cm}^{-1}$) and 5 (5-10%) were used for the line positions and intensities, respectively, when the band was measured (noted “Obs” in Tables 8 and 9). When a band was predicted (noted “Cal” in Tables 8 and 9), the error codes 3 ($(1-10) \times 10^{-3} \text{ cm}^{-1}$) and 4 ($\geq 10\%$ and $< 20\%$) were used for the line positions and intensities, respectively. The references numbers added in the supplementary line list are “21” and “18” (*this work*) for the line positions and intensities respectively.
- When the JPL line positions were used instead of our calculated positions, the error code 5 ($(0.01-0.1) \times 10^{-3} \text{ cm}^{-1}$) was used. In this case, the reference number of line positions has been changed to “20” (referring to the JPL calculation).

The Tomsk labeling $V_1 V_2 V_3 V_4 \ell_4 \ell_5 J \epsilon$ of the rovibrational states was used in this list (see Section 3.3).

Table 8. Statistics of the bands of the $\Delta P = 0$ series included in our line list. The line intensities are given in natural abundances in $\text{cm}^{-1}/(\text{molecule} \cdot \text{cm}^{-2})$ at 296 K.

Vibrational assignment			Number of transitions	Spectral range (cm^{-1})		Line intensities at 296 K		$J_{\min}$	$J_{\max}$
Upper	Lower			Min	Max	Sum	Min		
00001 0 1	00010 1 0		277	14.5	248.1	5.3E-21	1.0E-28	1	54
00011 1 1	00020 2 0		211	21.3	239.0	4.0E-22	1.1E-28	2	48
00002 0 2	00011 1 1		215	23.3	233.8	2.9E-22	1.2E-28	2	48
00011 1-1	00020 0 0		79	14.6	192.4	1.6E-22	1.1E-28	0	45
00002 0 0	00011 1-1		89	27.8	236.5	1.5E-22	1.5E-28	0	48
00011 1 1	00020 0 0		107	17.7	227.0	4.3E-23	1.1E-28	2	49
00011 1-1	00020 2 0		147	13.6	223.7	4.0E-23	1.1E-28	2	49
00012 1 2	00021 2 1		187	31.5	214.5	2.3E-23	1.2E-28	3	43
00021 2 1	00030 3 0		179	36.3	217.0	2.3E-23	1.0E-28	3	40
00012 1 0	00021 2-1		159	37.7	210.5	1.9E-23	1.4E-28	1	41
00021 2-1	00030 1 0		179	14.4	174.8	1.7E-23	1.1E-28	1	40
00003 0 1	00012 1 0		189	40.0	220.8	1.3E-23	1.0E-28	1	43
00003 0 3	00012 1 2		185	34.5	217.6	1.2E-23	1.0E-28	3	43
00021 0 1	00030 1 0		164	32.4	204.5	3.6E-24	1.1E-28	1	34
00012-1 2	00021 0 1		137	38.7	192.3	3.5E-24	1.1E-28	1	35
00012-1 2	00021 2-1		166	43.6	223.1	3.4E-24	1.0E-28	1	41
00021 2 1	00030 1 0		165	26.9	208.9	3.4E-24	1.1E-28	3	42
00021 0 1	00030 3 0		157	33.9	214.3	2.1E-24	1.0E-28	4	42
00012 1 0	00021 0 1		148	22.3	182.3	4.9E-24	1.1E-28	1	35
00021 2-1	00030 3 0		144	18.0	195.9	1.9E-24	1.0E-28	4	43
00022 2 2	00031 3 1		133	46.3	186.0	1.3E-24	1.5E-28	4	33

00031	3	1	00040	4	0	126	54.1	194.9	1.1E-24	1.1E-28	4.1E-26	4	34	Cal*
00013	1	3	00022	2	2	145	44.7	196.0	9.7E-25	1.0E-28	3.2E-26	4	35	Cal
00022	2	0	00031	3	-1	123	46.5	187.1	9.5E-25	1.6E-28	3.6E-26	2	30	Cal
00013	1	1	00022	2	0	127	50.5	194.9	8.7E-25	1.1E-28	3.2E-26	2	35	Cal*
00012	1	2	00021	0	1	143	44.7	215.6	8.1E-25	1.1E-28	4.5E-26	5	39	Cal
00013	1	-1	00022	2	-2	120	46.4	199.9	7.1E-25	1.2E-28	3.6E-26	0	35	Cal*
00022	2	-2	00031	1	-1	107	27.5	164.1	6.7E-25	1.1E-28	4.4E-26	0	33	Cal
00031	3	-1	00040	2	0	122	19.9	163.6	6.3E-25	1.1E-28	2.5E-26	2	35	Cal*
00031	1	-1	00040	0	0	57	18.5	151.5	4.9E-25	1.1E-28	3.8E-26	0	33	Cal
00004	0	2	00013	1	1	135	59.7	201.8	4.8E-25	1.1E-28	1.6E-26	2	33	Cal
00002	0	2	00011	1	-1	147	45.4	229.8	4.7E-25	1.3E-28	3.3E-26	2	41	Cal*
01001	0	1	01010	1	0	127	67.8	209.0	4.4E-25	1.0E-28	1.4E-26	1	33	Cal
00003	0	1	00012	-1	2	134	45.9	199.0	4.2E-25	1.0E-28	5.8E-26	1	36	Cal*
00004	0	4	00013	1	3	129	52.4	192.5	4.2E-25	1.2E-28	1.4E-26	4	33	Cal*
00022	0	2	00031	1	1	115	47.6	170.3	4.0E-25	1.0E-28	1.6E-26	2	29	Cal
00002	0	0	00011	1	1	68	33.9	192.7	2.9E-25	1.0E-28	2.7E-26	4	38	Cal
00031	1	1	00040	2	0	78	60.6	147.0	2.8E-25	1.1E-28	1.4E-26	2	18	Cal
00004	0	0	00013	1	-1	59	61.5	200.3	2.7E-25	1.4E-28	1.8E-26	0	32	Cal

Note: The vibrational labeling for the upper and lower state corresponds to $V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5$ (see Section 3.3). In the last column "Obs" means that the band was measured in Ref. [21], otherwise the band was predicted and this is noted "Cal". A star means that a band is affected by strong resonance interactions. Because of this the vibrational labeling from the Toms line list was changed for the transitions affected by strong resonance interactions (see Section 3.3).

Table 9. Statistics of the bands of the $\Delta P = 1$ series included in our line list. The line intensities are given in natural abundances in $\text{cm}^{-1}/(\text{molecule} \cdot \text{cm}^{-2})$ at 296 K.

Vibrational assignment		Number of transitions	Spectral range (cm^{-1})		Line intensities at 296 K		$J_{\min}$	$J_{\max}$
Upper	Lower		Min	Max	Sum	Min		
00020	0 0	141	405.8	634.0	7.7E-22	1.4E-28	1	48
00020	2 0	265	389.8	603.2	4.9E-22	1.3E-28	1	49
00030	1 0	243	430.4	634.1	1.2E-22	1.0E-28	0	42
00030	1 0	231	411.5	630.6	9.4E-23	1.1E-28	2	43
00030	3 0	188	424.3	590.9	6.4E-23	1.2E-28	2	44
00021	0 1	96	442.2	580.9	3.8E-23	1.3E-28	0	39
00021	0 1	191	414.3	585.7	3.7E-23	1.3E-28	2	43
00021	2 1	210	414.3	605.6	2.3E-23	1.2E-28	2	42
00021	2 1	112	424.2	619.7	2.5E-24	1.5E-28	3	41
00040	2 0	189	436.1	600.4	1.0E-23	1.0E-28	1	38
00040	0 0	88	464.9	605.2	8.9E-24	1.0E-28	1	31
00030	3 0	215	416.3	612.4	8.8E-24	1.0E-28	3	45
00040	2 0	180	437.0	614.3	6.5E-24	1.7E-28	3	37
00031	1-1	155	446.2	580.3	5.9E-24	1.3E-28	1	34
00040	4 0	141	461.6	581.1	5.5E-24	1.4E-28	3	34
00031	1 1	197	437.1	605.7	5.2E-24	1.1E-28	1	37
00031	1 1	136	450.9	557.6	3.9E-24	1.2E-28	3	38
00031	3 1	155	436.1	599.4	3.5E-24	1.3E-28	3	34
00021	2-1	173	397.5	547.3	2.9E-24	1.0E-28	2	38
00040	2 0	192	462.8	630.7	2.7E-24	1.0E-28	1	35
00031	1-1	137	443.0	610.9	2.2E-24	1.1E-28	1	35
00040	0 0	91	452.9	611.0	2.0E-24	3.4E-28	3	34
00022	0 0	103	441.5	604.3	1.8E-24	1.3E-28	1	35
00040	2 0	189	436.1	600.4	1.0E-23	1.0E-28	1	38
00040	0 0	88	464.9	605.2	8.9E-24	1.0E-28	1	31
00030	3 0	215	416.3	612.4	8.8E-24	1.0E-28	3	45
00040	2 0	180	437.0	614.3	6.5E-24	1.7E-28	3	37
00031	1-1	155	446.2	580.3	5.9E-24	1.3E-28	1	34
00040	4 0	141	461.6	581.1	5.5E-24	1.4E-28	3	34
00031	1 1	197	437.1	605.7	5.2E-24	1.1E-28	1	37
00031	1 1	136	450.9	557.6	3.9E-24	1.2E-28	3	38
00031	3 1	155	436.1	599.4	3.5E-24	1.3E-28	3	34
00021	2-1	173	397.5	547.3	2.9E-24	1.0E-28	2	38
00040	2 0	192	462.8	630.7	2.7E-24	1.0E-28	1	35
00031	1-1	137	443.0	610.9	2.2E-24	1.1E-28	1	35
00040	0 0	91	452.9	611.0	2.0E-24	3.4E-28	3	34
00022	0 0	103	441.5	604.3	1.8E-24	1.3E-28	1	35

00022	0	2	00003	0	1	187	437.5	601.7	1.6E-24	1.1E-28	3.9E-26	1	33	Cal
00040	4	0	00021	0	1	164	441.1	598.2	1.3E-24	1.0E-28	7.7E-26	4	41	Cal*
00022	0	2	00003	0	3	171	429.3	568.6	1.3E-24	1.1E-28	3.3E-26	3	35	Cal
00022	2	2	00003	0	3	167	434.3	585.9	9.7E-25	1.0E-28	2.9E-26	3	32	Cal
00031	1	1	00012	1	0	127	480.1	600.3	5.3E-25	1.0E-28	1.6E-26	1	26	Cal*
00021	2	-1	00002	0	0	85	411.1	572.6	1.4E-25	1.1E-28	6.2E-27	5	37	Cal

Note: The vibrational labeling for upper and lower state corresponds to $V_1 V_2 V_3 V_4 V_5 \ell_4 \ell_5$ (see Section 3.3). In the last column “Obs” means that the band was measured in this work (Section 2), otherwise the band was predicted and this is noted “Cal”. A star means that a band is affected by strong resonance interactions. Because of this the vibrational labeling from the Toms line list was changed for the transitions affected by strong resonance interactions (see Section 3.3).

6. Conclusion

New measurements of the line positions and intensities of the acetylene molecule have been performed in the 429-593 cm^{-1} region. Based on these measurements and those of Ref. [21], new effective dipole moment parameters have been obtained for $\Delta P = 0$ and $\Delta P = 1$ series of bands which together with the effective Hamiltonian parameters published in our paper [15] were used for the line intensities calculations. Comparisons of the Tomsk and the JPL calculated line positions to the experiment showed that the JPL line positions are in better agreement with the experiments for the high J values. The line list of line positions and intensities for $^{12}\text{C}_2\text{H}_2$ has been generated between 13 and 634 cm^{-1} for 10208 transitions belonging to 68 bands. Where it was possible the Tomsk calculated line positions were substituted by the JPL values. Vibrational labeling has been changed compared to HITRAN 2012 or GEISA 2015: the $\ell_4 + \ell_5$ value used up to now needs to be replaced by ℓ_4 and ℓ_5 . The present line list is suggested to be directly added to the HITRAN 2012 line list for the HITRAN 2016 edition, since all the bands presented in this work are missing in the HITRAN 2012 line list.

Aknowlegment

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Highlights:

- Fourier transform spectroscopy of acetylene using SOLEIL synchrotron beam.
- First measurements of the positions and intensities for 627 acetylene lines in the 429 – 593 cm^{-1} region.
- New fitted sets of the effective dipole moment parameters for the $\Delta P = 0$ and $\Delta P = 1$ series of the acetylene transitions.
- C_2H_2 line list of 10165 transitions between 13 and 634 cm^{-1} .

Graphical abstract