



Acetylene, $^{12}\text{C}_2\text{H}_2$: new CRDS data and global vibration-rotation analysis up to 8600 cm $^{-1}$

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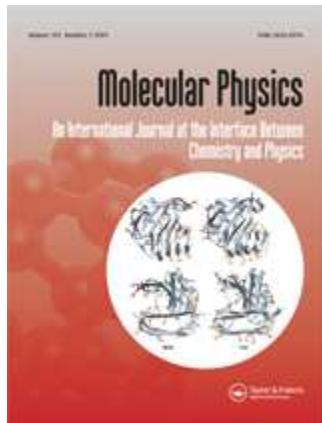
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Acetylene, $^{12}\text{C}_2\text{H}_2$: new CRDS data and global vibration-rotation analysis up to 8600 cm^{-1}

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6 **Acetylene, $^{12}\text{C}_2\text{H}_2$: new CRDS data and global vibration-**
7 **rotation analysis up to 8600 cm^{-1}**

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Abstract

The absorption spectrum of $^{12}\text{C}_2\text{H}_2$ has been recorded using cavity ringdown spectroscopy and analyzed in the ranges $6000\text{--}6356\text{ cm}^{-1}$ and $6667\text{--}7015\text{ cm}^{-1}$. Fourteen new bands have been identified and additional J -lines were assigned in 10 already known bands. These new data, together with the published vibration-rotation absorption lines of $^{12}\text{C}_2\text{H}_2$ accessing vibrational states up to 8600 cm^{-1} have been gathered in a database. The resulting set includes 12137 transitions involving 186 different $k = l_4 + l_5$ sub-states, with l_4 the angular momentum quantum number associated to the j degenerate bending vibration. These lines have been fitted simultaneously to spectroscopic parameters through J -dependent Hamiltonian matrices exploiting the vibrational polyad or cluster block-diagonalization, in terms of the pseudo quantum numbers $N_r = 5v_1 + 3v_2 + 5v_{3^+} v_{4^+} v_5$ and $N_s = v_1 + v_2 + v_3$, also accounting for k and e/f parities and u/g symmetry. Modes 1 and 2 correspond to the symmetric CH and CC stretchings, mode 3 to the antisymmetric CH stretch, and modes 4 and 5 to the *trans*- and *cis*-degenerate bendings, respectively. The fit was successfully achieved, with a dimensionless standard deviation of 0.92, leading to the determination of 266 effective vibration-rotation parameters.

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1 2 1. Introduction 3

4 The high resolution spectrum of acetylene, $^{12}\text{C}_2\text{H}_2$, has been already
5 investigated in the 1.5 μm spectral range using Fourier transform infrared
6 spectroscopy (FTIR)^{1–4}. The strong $\nu_1 + \nu_3$ band, of metrological relevance, is
7 observed in this range, together with various combination and hot bands.
8

9 Nowadays, cavity ~~ringdown~~ spectroscopy (CRDS) (e.g.^{5,6}) allows the
10 experimental sensitivity to be significantly increased with respect to FTIR
11 measurements. We have ~~used CW-CRDS~~^{7,8} to record the acetylene spectrum
12 around 1.5 μm , in Grenoble. Experimental details are provided in section 2
13 and the results of the band-by-band analyses performed in Bologna, between
14 6000–6356 cm^{-1} and 6667–7015 cm^{-1} , are listed in section 3.
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28 The new spectra revealed very weak bands compared to the existing
29 literature data. Their analysis was facilitated by unpublished global
30 constants obtained in Brussels from the simultaneous fit of many sets of
31 already known vibration-rotation lines. Such a procedure, which was already
32 achieved for $^{13}\text{CH}^{12}\text{CH}$ up to 6750 cm^{-1} using a set of programs developed in
33 Louvain⁹, exploits the very regular vibrational energy pattern in acetylene,
34 as recently reviewed in¹⁰. The present investigation stimulated an update of
35 the still unpublished results of our $^{12}\text{C}_2\text{H}_2$ global fit, to include the new CRDS
36 data reported here. The data base gathering the published vibration-rotation
37 lines in $^{12}\text{C}_2\text{H}_2$ involving vibrational states up to 8600 cm^{-1} , is summarized in
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2 section 4. This range was selected to include all states observed through cold
3 and hot bands in the present CRDS spectra. The global model is presented in
4 section 5. The results, also updating a previously published global analysis by
5 Perevalov *et al.*¹¹, are detailed in section 6 and discussed in section 7, before
6 concluding in section 8.
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15 The conventional normal mode numbering in acetylene is used
16 throughout this paper, with 1 to 5 corresponding to the symmetric CH σ_g^+ (ν_1)
17 and CC σ_g^+ (ν_2) stretchings, the antisymmetric CH stretch σ_u^+ (ν_3), and the
18 *trans*- π_g (ν_4) and *cis*- π_u (ν_5) degenerate bendings. The latter are characterized
19 by the usual bending angular momentum quantum numbers, l_4 and l_5 , with k
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2. Experimental details

36 The CW-CRDS spectra of acetylene were recorded with the same
37 spectrometer used in studies of species of atmospheric relevance such as H₂O
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39 and ¹²CO₂¹³⁻¹⁵ or O₃¹⁶. The fibered CW-CRDS spectrometer and the
40 procedure adopted for an accurate calibration of the wavenumber scale of the
41 recorded spectra were described in Refs. ^{12 14 17}. Fig. 1 shows an overview of
42 the acetylene absorption spectrum recorded by FTS at ULB, highlighting the
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two spectral sections presently investigated. The 6000–6356 cm⁻¹ and 6667–7015 cm⁻¹ regions were selected for the present CRDS recordings as they correspond to transparency windows located between strong absorption bands. These two regions were covered by using a set of 18 and 12 Distributed Feed-Back (DFB) diode lasers, respectively. Only the range 6122–6130 cm⁻¹ could not be recorded due to the lack of diode.

[Insert figure 1 about here]

The tuning range of each DFB laser is about 7 nm (~ 30 cm⁻¹) by temperature variation from -10 to 65°C. The typical sensitivity (noise equivalent absorption $\alpha_{min} \sim 2-5 \times 10^{-10}$ cm⁻¹), wide spectral coverage and the four to five decades linear dynamic range, make it an ideal tool for high sensitivity absorption spectroscopy in the important atmospheric window of transparency around 1.5 μm. The CRDS cell fitted by the super mirrors is 1.40 m long. The typical ringdown times were of the order of 60 μs. A few hundred ringdown events were averaged for each spectral data point, taking some 220 ms per averaged point, and the duration of a temperature scan was about 70 minutes for each DFB laser. The pressure, measured by a capacitance gauge, as well as the ringdown cell temperature, were monitored during the spectrum recording. Different series of recordings were performed

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for pressure values of 667, 1333 and 2666 Pa depending on the spectral region. The DFB line width is much smaller than the Doppler width and the observed resolution is mostly Doppler limited in the adopted pressure conditions. In cases of overlapped lines, whenever it was possible, a deconvolution by means of Voigt profile was performed, keeping the full width at half maximum at a value observed for close $^{12}\text{C}_2\text{H}_2$ isolated lines.

The wavenumber calibration of the spectrum is based on the wavelength values measured by a wavemeter (Burleigh WA1640) during the DFB frequency scan. When necessary, it was further refined by simply stretching the frequency scale (with an origin at 0) in agreement with highly accurate positions of reference lines due to impurities. H_2^{16}O line positions as provided by the HITRAN database¹⁸ were used as reference lines. The obtained absolute wavenumber calibration is estimated accurate within better than $\pm 2 \times 10^{-3} \text{ cm}^{-1}$.

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The achieved sensitivity and dynamics are illustrated in Fig. 2 on a small section of the spectrum near 6235 cm^{-1} . It is significantly improved compared to the previous investigation by Keppler *et al.*³, based on FTIR and up to 352.5 m long absorption path. The improvement is best demonstrated by the analysis of 14 additional, new bands in the present spectra.

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The spectrum analysis is complicated by the presence of absorption lines due to several impurities: H₂O, CH₄ and C₂H₄. Methane transitions, as reported in the HITRAN database ¹⁸, were observed in the region of the strong 2v₃ band near 6000 cm⁻¹, while C₂H₄ lines belonging to the v₅+v₉ band at 6151 cm⁻¹ were identified between 6095 and 6210 cm⁻¹ ¹⁹. However, the main problem was the presence of acetone, which is added to stabilize acetylene when it is compressed. On the overview FTIR spectrum of Fig. 1, the broad absorption features of acetone are clearly observed below 6050 cm⁻¹. They induced additional losses which strongly decreased the ringdown times and therefore the sensitivity near 6000 cm⁻¹. In this range, the noise equivalent absorption increased up to •_{min}~3×10⁻⁹ cm⁻¹, to be compared to 2–5×10⁻¹⁰ cm⁻¹, typically.

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3. Description of the spectra and band-by-band analyses

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Fourteen new vibrational bands have been identified in the CRDS spectra, arising from the ground state or from excited bending states with v₄₊ v₅ ≤ 2. They altogether involve 23 different upper vibrational states. These bands are gathered in Table 1 together with 10 bands already reported by Keppler

et al.³ whose rotational assignments have been extended. Band centres and vibrational term values are also reported in Table 1. The states are identified using the vibrational quantum numbers in acetylene, defined in the introduction. The assignments correspond, as usual, to the dominant zero order at the lowest existing J -value for the k sub-state in the corresponding polyad as resulting from the global fit.

In the 6000–6356 cm^{−1} range, the most prominent features are the $R(J)$ lines of the $2v_1(\Sigma_g^+) \leftarrow v_5(\Pi_u)$ hot band extending from 6000 to 6050 cm^{−1} (see Fig. 1). At 6011 cm^{−1} the red degraded Q branch of the $v_1+v_2+v_4+v_5(\Sigma_u^+) \leftarrow v_4(\Pi_g)$ is observed together with the corresponding R branch up to 6068 cm^{−1}.

Other weaker Q branches centred at 6030, 6052 and 6093.5 cm^{−1} are present, corresponding to the $v_1+v_2+2v_5(\Sigma_g^+) \leftarrow v_5(\Pi_u)$, $v_1+v_2+v_5(\Pi_u) \leftarrow$ G.S. and $2v_2+3v_5(\Pi_u) \leftarrow$ G.S. newly observed bands. The corresponding P and R transitions have also been identified, with the exception of the $P(J)$ lines of the 6052 cm^{−1} band, despite their position can be precisely calculated. This intensity perturbation, probably due to a high order Coriolis type vibration-rotation interaction, is not fully understood. Fig. 3 illustrates the very weak Q branch of the $v_1+v_2+2v_5(\Sigma_g^+) \leftarrow v_5(\Pi_u)$ band superimposed with the R branch of the $2v_1(\Sigma_g^+) \leftarrow v_5(\Pi_u)$ band, while the very weak Q branch of the $2v_2+3v_5(\Pi_u) \leftarrow$ G.S. band is presented in Fig. 4. A parallel band centred at 6079.7 cm^{−1}

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2 has been assigned to $v_1 + v_4 + 3v_5 (\Sigma_u^+) \leftarrow$ G.S.. Between 6095 and 6210 cm⁻¹ the
3 spectrum is dominated by the strong lines of the C₂H₄ impurity, which
4 overlap the weaker C₂H₂ transitions, making the assignment very difficult. In
5 fact, only a few transitions have been added to previously observed bands³.
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18 At both ends of the region between 6667 and 7015 cm⁻¹ the wings of
19 the strong $v_1 + v_3$ and $v_1 + v_3 + v_4$ band systems, centred at 6556 and 7141 cm⁻¹,
20 respectively, are visible. In the FTIR spectrum only the $2v_1 + v_5 (\Pi_u) \leftarrow v_4 (\Pi_g)$
21 and $v_2 + v_3 + 2v_5 (\Sigma_u^+) \leftarrow$ G.S. assigned in Keppler *et al.*³ at 6804.7 and 6690 cm⁻¹,
22 respectively, have been identified. Most of the bands observed in the CRDS
23 spectrum are of parallel type, $\Sigma_{g/u}^+ \leftarrow \Sigma_{u/g}^+$, $\Pi_{g/u} \leftarrow \Pi_{u/g}$ and $\Delta_{g/u} \leftarrow \Delta_{u/g}$. In a few
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The spectral analysis was made difficult by the superposition of the
different bands of ¹²C₂H₂ with lines due to impurities (in particular H₂O and
C₂H₄) or to the ¹³CH¹²CH isotopologue. In fact, lines without intensity

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2 alternation due to transitions already reported⁶ in twelve bands for this
3 molecule have been observed mainly in the 6667–7015 cm⁻¹ range.
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10 The rotational analysis of the bands listed in Table 1 was performed
11 using standard procedures. The energy of the rovibrational levels of the Σ^+ , Π ,
12 and Δ states was calculated according to the expression:
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$$T(v, J) = G_c + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3 \\ \pm \frac{1}{2} \{ q_v [J(J+1)] + q_v' [J(J+1)]^2 + q_v^{JJ} [J(J+1)]^3 \} \quad (1)$$

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24 with $q_v, q_v', q_v^{JJ} = 0$ for $l=0$, Σ states, and the centre term value defined as
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$$G_c = G_v - B_v k^2 - D_v k^4 \quad (2)$$

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33 and G_v the vibrational term value. In Eq. (1) upper signs refer to
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35 e -symmetry states, lower signs to f -symmetry states.
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40 The constants resulting from the band-by-band analysis are listed in
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42 Table 1. The term values of the lower states of the transitions were calculated
43 from literature data²⁰. The number of lines assigned in the branches and the
44 number of fitted lines are also indicated for each band.
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Transitions whose wavenumbers differed from the corresponding calculated values by more than a chosen limit, ranging from 0.001 to 0.003 cm^{-1} , were excluded from the final cycle of the least-squares procedure. Most of these excluded line positions correspond to high J values which cannot be reproduced by using Eq. (1), in which the number of fitted constants is limited to the sextic coefficient H' . Actually, for many bands, additional coefficients in the $J(J+1)$ expansion could as well be fitted and statistically determined. This behaviour is typical whenever resonances occur, which are not accounted for in the band-by-band rotational model of Eq. (1). For the same reason, some of the distortion constants listed in Table 1 are anomalously large or negative. One can notice that the same upper state $v_1+v_2+v_4+v_5 (\Sigma_u^+)$ is involved in both cold and hot bands. Upper state rotational constants slightly differ for these bands reaching the same upper state, because of the different number and measurement precision of the rotational lines included in the fitting procedure.

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Additional, weaker lines remain to be identified in the range presently studied. Some can tentatively be assigned to impurities in the sample, others probably arise from the studied species. In fact, a few sequences of lines with the appropriate intensity alternation have been observed which cannot be assigned for several reasons. They are probably R (or P) branches whose

1 corresponding P (or R) counterpart is outside the investigated spectral region.
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4 With the help of the predicted line positions by means of the parameters of
5 the global fit three R branches of this kind have been assigned to the $\Pi \leftarrow \Pi$
6 bands centred at 6662, 6672 and 6674 cm^{-1} (see Table 1). Unassigned series
7 could also correspond to hot bands from states with vibrational excitation
8 higher than those considered in the predictions, limited to $v_{4^+} v_5 \bullet 2$. Another
9 possibility, which has not been exploited, is represented by zero-order
10 forbidden transitions with $|\Delta k| = 2$. These additional structures will be
11 considered at a later stage of the global analysis.
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14 All line wavenumbers from the rotational analyses reported in Table 1,
15 together with their assignments, are attached as Supplementary Material.
16 Observed-calculated values obtained from the global procedure described in
17 section 6, rather than from the band-by-band parameters listed in Table 1,
18 are also provided.

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40 4. Data base

41 The data base consists of the assigned line wavenumbers from the
42 literature, within the upper vibrational state energy limit of 8600 cm^{-1} . This
43 limit was selected to include all new states from the present CRDS data.
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2 The bands involved in the data base are identified in Table 2. All data,
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4 except for the Raman ones by Bermejo *et al.*^{21,22}, come from various
5 absorption techniques. It is interesting to notice that, besides the bending
6 range investigated using FTIR^{20,23,24}, some low energy bands were only
7 reported in the early literature, investigated using high resolution
8 spectrographs, by Rao and coworkers²⁵⁻²⁸. The quality of these data, although
9 optimal at the time of their publication, may possibly be improved nowadays.
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12 Some more recent data recorded using FTIR have actually since been
13 published but the related list of assigned lines could unfortunately not be
14 made available by the authors²⁹.
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17 The data base includes the vibration-rotation wavenumbers from the
18 systematic investigation by Jacquemart and co-workers, using FTIR^{23,30-37}.
19
20 Additional conventional FTIR results around 1.5^{2,3} and 1.17 μm³⁸, as well as
21 lines around 2.5 μm reported from very sensitive FTIR experiments using a
22 femto laser as absorption source³⁹, are included. Finally, 14 new bands
23 presently observed by CW-CRDS are also part of the data base, together with
24 additional lines in 10 previously reported ones.
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[Insert Table 2 about here]

Data concerning very highly excited bending states in the range considered were reported by Field and co-workers using resolved laser

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2 induced fluorescence from the \tilde{A} excited electronic state⁴⁰. They were,
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4 however, not considered because of the required extension in the size of the
5 Hamiltonian matrices, further detailed in section 6.
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11 When two published sets of lines were available for the same band, the
12 information has been merged in various ways, depending on the quality of
13 the measurements. For instance, in several cases FTIR data were selected for
14 the lower J -lines and complemented with the higher J -line wavenumbers
15 reported from more sensitive laser-based techniques. In few cases, the latter
16 data have been included for some of the lower J values. However, only one
17 line position was selected in cases where several appear in the literature.
18 These finer details are not reported in Table 2. Each data set is then
19 separately treated in the fitting procedure in terms of weighting factors, as
20 further detailed in section 6.
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34 The data base amounts to 12137 vibration-rotation lines accessing
35 states up to 8600 cm⁻¹. They arise from bands linking 186 different l -
36 substates (counting e and f components separately). All states involved in the
37 data base are gathered in Table 3, together with their centre term value G_c ,
38 calculated from the global constants resulting from the procedure detailed in
39 the next sections. It is interesting to notice that, because of the u/g selection
40 rule, this data set is significantly reduced compared to ¹³CH¹²CH, for which
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about the same number of lines was gathered from the literature, up to the limit of 6750 cm^{-1} as compared to 8600 cm^{-1} in the present case.

[Insert Table 3 about here]

It must be emphasized that, as the same states are observed from spectra recorded in different wavelength ranges and using various experimental conditions, spectral calibration is a critical issue when performing global fitting. We satisfactorily checked that the line measurement accuracy, described in the references just mentioned, was comparable to the quality of the standard deviation of the final fit.

5. Vibration-rotation Hamiltonian

For several isotopologues of acetylene, the vibrational state energies could be gathered into so-called polyads or vibrational clusters up to high excitation, block-diagonalizing the global vibrational Hamiltonian⁴¹⁻⁴⁶. Each of these blocks within the Hamiltonian matrix image of the molecule (MIME) shows a similar structure, accounting for the same set of anharmonic resonances, all characterized by well-defined interaction matrix elements. As a consequence of this regularity, new constants of the motion, N_r and N_s , can be defined in $^{12}\text{C}_2\text{H}_2$ and also in $^{13}\text{CH}^{12}\text{CH}$ and $^{13}\text{C}_2\text{H}_2$ ^{47,48}:

$$N_r = 5v_1 + 3v_2 + 5v_3 + v_4 + v_5 \quad (3)$$

$$N_s = v_1 + v_2 + v_3 \quad (4)$$

Interesting issues of dynamical and statistical natures support this very specific vibrational MIME structure (e.g. ^{40,49-53}).

Inclusion of rotation in the global picture has been already achieved for ¹²C₂H₂ by Perevalov and coworkers ^{11,54,55}, simultaneously considering 7290 lines involving states up to 9700 cm⁻¹. No detailed related discussion was, however, ever published to complement the limited information provided in a symposium proceeding^s ⁵⁴. Concerning ¹³CH¹²CH, the 12703 vibration-rotation lines reported in the literature up to 6750 cm⁻¹ could be simultaneously fitted and all reproduced within experimental precision (3σ), by Fayt and co-workers ⁹. Since the vibrational structure in ¹²C₂H₂ is very close to the one in ¹³CH¹²CH, apart for restrictive u/g selection rules, the vibrational energy patterns and MIME are almost identical for both species and the same strategy and programs adopted for ¹³CH¹²CH ^{9,46} were applied here to ¹²C₂H₂.

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The vibrational interactions active in ¹²C₂H₂ are known to be 3/245, 14/35, 15/34, 1/244, 1/255, 44/55 and 11/33 ⁴³. The notation i/jkk (ii/jj) refers to anharmonic resonance interaction terms of the type

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 2 $\Delta v_i = \pm 1$, $\Delta v_j = \mp 1$, $\Delta v_k = \mp 2$ ($\Delta v_i = \pm 2$, $\Delta v_j = \mp 2$) characterized by the
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 4 interaction constant $K_{i/jkk}$ ($K_{ii/jj}$). The related main coupling terms fulfill the
 5
 6 $\Delta k = 0$ selection rule in various possible ways, thus with either $\Delta l_4 = \Delta l_5 = 0$,
 7
 8 or $\Delta l_4 = -\Delta l_5 \neq 0$. Higher order terms, labeled $O_{ij/mn}$, apply for $\Delta k = \pm 2$
 9
 10 coupling schemes. For completeness, vibrational and rotational interaction
 11 terms in the global Hamiltonian are defined in Table 4. Only some of the
 12 anharmonic resonance terms are explicitly provided in this Table, namely
 13 those relevant to the 3/245 and 44/55 anharmonic couplings in eqs. (13-16)
 14 and (17-19), respectively. The selection of higher order terms was adapted to
 15 the results of the global fit presented in the next section.
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31 As detailed in ⁹, vibration-rotation polyads include states with different
 32 values of $k = l_4 + l_5$, either even or odd. The *e* and *f* partition defined in ⁵⁶ is
 33 also included, with the symmetrized basis as defined in ⁵⁷ for pentatomic
 34 molecules. Also, *g* and *u* symmetry is used to classify the total wavefunction
 35 and to further block-diagonalize the Hamiltonian. Finally, the resulting
 36 vibration-rotation matrices are diagonal in *J*. Each block is characterized by
 37 the pseudo-quantum numbers N_r and N_s defined in Eqs (3) and (4), the total
 38 angular momentum quantum number *J*, and the symmetry properties *e/f* and
 39 *u/g*. Each block is therefore labeled using the $\{N_r, N_s, J, e/f, u/g\}$ notation.
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6. Fitting procedure and results

The package of computer programs developed in Louvain-La-Neuve and described in^{57,58} was used for the fitting procedure. The matrices were set to include states up to $v_b = 7$ ($b = 4$ or 5) and $k_{\max} = 7$, with the constraint $v_4 + v_5 \leq 8$. In this way, the most relevant data were accounted for without significantly increasing computer time. This limit, however, prevented data concerning highly excited bending states⁴⁰ to be considered, as mentioned in section 4. Polyads were nevertheless built to include levels up to 16000 cm^{-1} , to allow for later developments.

We used a weighted fitting procedure (weights inversely proportional to the square of the experimental uncertainties) initially accounting for the estimated accuracy (3σ) mentioned by the authors, which is mainly dependent on the used technique and spectral range investigated. For each set of data, the uncertainty was later reduced in order to agree with the corresponding mean (obs.– calc.) value from the global fit, whenever this value was better than the stated experimental accuracy.

The final selection of parameters, although not expected to be unique, results from a careful fitting strategy. Higher order parameters were added one at a time, depending on both the nature of the specific problem to be solved and on the size and precision of the corresponding lower order parameters. In the end, the number of parameters was systematically reduced removing those statistically undetermined, taking care of not degrading the standard deviation of the fit.

The final global fit included 10750 lines out of 12137 assigned ones. It produced 266 parameters, listed in Table 5. The dimensionless standard deviation of the fit is 0.92, ~~this is~~ defined as:

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$$\hat{\sigma} = \sqrt{\frac{\sum_i [(\tilde{\nu}_i^{obs.} - \tilde{\nu}_i^{calc.}) / \varepsilon_i]^2}{N - n}} \quad (5)$$

with $\tilde{\nu}_i^{obs.}$ and $\tilde{\nu}_i^{calc.}$ the observed and calculated line wavenumbers, respectively, N the number of fitted transitions, n the number of adjusted parameters and ε_i the uncertainty on the corresponding data. The standard deviation in cm^{-1} for each data set is listed in Table 2.

[Insert Table 5 about here]

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2 A statistical survey of the quality of the vibration-rotation data of $^{12}\text{C}_2\text{H}_2$
3 accounted for in the global fit is presented in Table 6.
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9 A zero weight has been assigned to 1387 lines for which the fit was not
10 satisfactory, meaning all those with observed-calculated value larger than
11 three times the uncertainty ε_i . Since we do not have access to all spectra, we
12 could not systematically check the quality of these rejected lines. About 80%
13 of these correspond to very low or high J -values. They are thus most likely
14 weaker or overlapped lines in different bands, less precisely measured. We
15 could clearly assess this in $^{13}\text{CH}^{12}\text{CH}$ ⁹, as further discussed below. Their
16 rejection, only occurs because they are characterized by the same
17 uncertainties as for the other more accurately measured lines in the same
18 bands and does therefore not affect the global picture.
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33 We identified specific high order Coriolis type vibration-rotation
34 interaction schemes, 14/22 in particular, likely to explain the rejection of the
35 remaining 20%. This coupling sometimes affects many rotational levels
36 within the same vibrational sub-state. It is e.g. the case for $(v_1 v_2 v_3 v_4 v_5, l_4 l_5) =$
37 $(10012, 10) \Pi^f$ sub-state at 5381.56 cm^{-1} , perturbed by the $(02002, 02) \Delta^f$ one.
38 Significant changes in the programs would be required to account for these
39 additional $\Delta k = 1$ couplings, affecting only a very small fraction, about 2%, of
40 the information available in the present data base. Depending on the various
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1
2 | high order Coriolis type vibration-rotation interaction schemes to be
3 | accounted for in acetylene, the block diagonal structure of the Hamiltonian
4 | might even be destroyed, leading to an infinite matrix representation.
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11 The total fraction of the data base which was rejected (11.4%) is
12 actually of the same order of magnitude as in $^{13}\text{CH}^{12}\text{CH}$ (7.6%)⁹. The slight
13 increase might result from more pronounced high order Coriolis type
14 vibration-rotation effects. The better coherence of the data set in $^{13}\text{CH}^{12}\text{CH}$,
15 because a larger fraction of them results from a single series of high quality
16 FTIR spectra, probably also contributes to this comparison. One should
17 furthermore account for the energy ranges considered in both cases, up to
18 8600 cm^{-1} in $^{12}\text{C}_2\text{H}_2$ and 6750 cm^{-1} , only, in $^{13}\text{CH}^{12}\text{CH}$. More complex
19 interaction schemes due to a denser pattern of states at the higher energies
20 considered are thus to be unraveled in the symmetric isotopologue. In
21 addition, since the number of data is almost identical in both data bases, the
22 information content is significantly higher in the asymmetric isotopologue,
23 imposing more efficient constraints on the fitting procedure.
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[Insert Table 6 about here]

7. Global constants

The large number of fitted data (10750) ensures the overall statistical meaning of the procedure, despite the large number of determined parameters (266). However, severe correlation problems can not be avoided when performing global vibration–rotation fits and certainly characterize several of the present effective parameters. The use of constraints in the fitting procedure as explained in ⁵⁷ significantly contributed to the final selection of higher order terms in the model. These terms for ¹²C₂H₂ are different from those determined in the similar fit of ¹³CH¹²CH ⁹. It is interesting to notice that the number of parameters is higher in ¹²C₂H₂ (266), compared to ¹³CH¹²CH (216), due to the inclusion of higher energy vibrational states in the main isotopologue. This involves polyads with larger pseudo-quantum numbers and requires higher order dependences in the equations. Nevertheless, the resulting sets of parameters show very good consistency, as demonstrated by the selection listed in Tables 7 and 8. All higher order parameters present very similar values, a trend probably to be expected given the very similar vibrational and rotational properties of these isotopologues.

[Insert Table 7 about here]

Further comparison of the present results on ¹²C₂H₂, with those in ⁵⁴, is more difficult. Indeed, despite the fact that the basic theoretical models are

1
2 identical, the fitting was neither achieved using the same data base nor
3 adopting the same selection of diagonal and off diagonal interaction terms or
4 the same procedure and constraints. We thus only mention that all leading
5 and higher order rotational terms compare well, but not the vibrational ones.
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9 Actually their constants (absolute values in cm^{-1}) x_{11} (18.96), x_{33} (30.02), x_{13}
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11 (105.29), and $K_{11/33}$ (14.06)⁵⁴ do not fit the so-called x - K relations, *i.e.*
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$$x_{11} = x_{33} = \frac{1}{4}x_{13} = \frac{1}{4}K_{11/33} \quad (6)$$

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22 predicted to apply in all symmetric isotopologues of acetylene⁵⁹. These
23 relations are reasonably well fulfilled by the present values, listed in the first
24 column of Table 8.
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28 [Insert Table 8 about here]
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35 It is interesting to notice that the values of the vibrational parameters
36 for $^{12}\text{C}_2\text{H}_2$ derived from a fit of the vibrational energies only⁴³ are very similar
37 to those presently obtained considering vibration-rotation data. This previous
38 set, listed in the second column of Table 8, was derived from vibrational data
39 covering a much broader spectral range, up to the visible region. This
40 agreement gives some feeling about the effective character of the parameters.
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47 The same comment applies to the parameters of $^{13}\text{CH}^{12}\text{CH}$, also reported in
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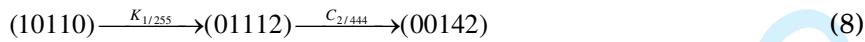
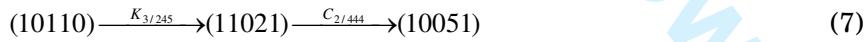
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2 Table 8, from ^{9,46}. Values for the same parameters in ¹³C₂H₂ ⁴⁴ and ¹²C₂D₂ ⁴²,
3 resulting from a vibrational fit, are also listed for completeness.
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Another test of the reliability of the present set of parameters comes from their predictive efficiency. As already mentioned, the global approach significantly facilitated the assignment of the new weaker bands on the CW-CRDS spectrum discussed in section 3. Also, as demonstrated in a preliminary report ⁶⁰, the global parameters are presently being used with success to assign new emission spectra from very hot acetylene.

[Insert figure 5 about here]

As another example, Fig. 5 details the vibration–rotation states around 7135 cm⁻¹ from data reported in ^{3,38}, with their reduced energy plotted as function of $J(J+1)$. Only *u*-symmetry vibrational states existing in the range appear on Fig. 5, with those relevant assigned. We have selected the zero-order state with the largest weight in the eigenvector at the lowest *J*-value to label these eigenstates, as everywhere else in the text. The state of interest, (10110,10) $\Pi^{e,f}$, appears to be perturbed for *J*-values from 21 to 23 for the *f*-symmetry, and from 18 to 21 and 28-29 for the *e*-symmetry. As shown in Fig. 5, level crossings can be identified from the predictions. Predicted crossings agree within no more than a fraction of a wavenumber from the observed

1 perturbations, allowing them to be unraveled. The coupling schemes are very
2 complicated. Indeed, the (10110,10) $\Pi^{e,f}$ zero order state is actually strongly
3 coupled to many other zero order states in the $\{N_r, N_s, u\} = \{11, 2, u\}$ polyad, all
4 with odd k values, such as (11021), through $K_{3/245}$, and (01112), through $K_{1/255}$.
5 The resulting eigenstate at 7141.5 cm^{-1} thus shares these various zero-order
6 assignments in the eigenvector composition. On the other hand, several zero
7 order states in the $\{11, 1, u\}$ polyad, now all with even k values and involving
8 states such as (01053), (10051) and (00142) also happen to be highly coupled
9 by anharmonic and ℓ -type resonances. High order Coriolis type vibration-
10 rotation coupling schemes involving e.g. the $C_{2/444}$ interaction constant may
11 occur between these sets of states belonging to the $\{11, 2, u\}$ and $\{11, 1, u\}$
12 polyads which are very close in energy, explaining the observed
13 perturbations. For instance, two of the many interaction schemes
14 contributing to the perturbations illustrated in Fig. 5, using the zero-order
15 labels indicated on the figure, are:
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44 The composition of the eigenvectors of interest is very complicated and not
45 detailed here.
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8. Conclusion

Thanks to the ultra high sensitivity of CW-CRDS, various new combination and hot bands could be recorded and analyzed, while additional J -lines were assigned in known bands, in the ranges $6000\text{--}6356\text{ cm}^{-1}$ and $6667\text{--}7015\text{ cm}^{-1}$ for $^{12}\text{C}_2\text{H}_2$. These data were merged into a data base with all absorption and Raman vibration-rotation lines available from the literature accessing vibrational states up to 8600 cm^{-1} . This data base amounts to 12137 transitions involving 186 different k sub-states, counting e and f parities separately. All transitions were simultaneously fitted to $\{N_r, N_s, J, e/f, u/g\}$ Hamiltonian matrices, exploiting the vibrational polyad or cluster block-diagonalization in acetylene. The dimensionless standard deviation of the fit was 0.92, and 266 effective vibration-rotation parameters have been determined. Their quality has been assessed by various predictions and comparisons.

The present results strongly confirm the validity of the global approach to deal with the vibration-rotation structure in acetylene. The results also confirm the role of high order Coriolis type vibration-rotation interaction, probably affecting less than 2% of the data, not accounted for in the model and computer programs, yet.

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The next steps in the acetylene saga⁷, will consist in additional spectral assignments in the range presently considered and resulting updates

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2 of the global constants. Higher excited ranges need also to be included in the
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4 fitting procedure. Finally, high order Coriolis type vibration-rotation
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6 interaction should be considered in more details.
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13 **Acknowledgments**
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Figure captions

Figure 1: Overview of the acetylene spectrum between 5850 and 7200 cm⁻¹.

The spectrum was recorded by Fourier Transform Spectroscopy at ULB (Experimental conditions: Pressure = 120 hPa, Pathlength: 48 m). The two spectral intervals presently studied by CW-CRDS are indicated. Note the broad absorption features due to acetone below 6050 cm⁻¹.

Figure 2: CW-CRDS spectrum of acetylene showing very weak absorption lines near 6235 cm⁻¹. The sample pressure was 667 Pa. Three successive enlargements show the typical sensitivity achieved by CW-CRDS: the noise level corresponding to the minimum value of the absorption coefficient which can be detected is about 5×10^{-10} cm⁻¹.

Figure 3: CW-CRDS spectrum of acetylene near 6028 cm⁻¹ showing the very weak Q branch of the $v_1 + v_2 + 2v_5 (\Sigma_g^+) \leftarrow v_5 (\Pi_u)$ band centred at 6030.084 cm⁻¹, superimposed with the R branch of the $2v_1 (\Sigma_g^+) \leftarrow v_5 (\Pi_u)$ band. The sample pressure was 2666 Pa.

Figure 4: Q branch of the $2v_2 + 3v_5 (\Pi_u) \leftarrow$ G.S band newly observed by CW-CRDS near 6093 cm⁻¹. The sample pressure was 2666 Pa.

Figure 5: Reduced energy graph (in cm^{-1}) defined as $E(v,r) - 1.162540 J(J+1) + 1.6265 \cdot 10^{-6} J^2(J+1)^2$, presenting vibration-rotation states of u -symmetry in $^{12}\text{C}_2\text{H}_2$, in a selected energy range. Only those relevant to the perturbation affecting the $(v_1 v_2 v_3 v_4 v_5, l_4 l_5) = (10110, 10)$ sub-state are assigned, using the dominant zero order state in the eigenvector composition at low J -values. Full and empty dots indicate unperturbed and perturbed observed levels, respectively. Full and dashed lines indicate e - and f - parity states, respectively. The color code is adapted to the sub-state symmetry: in red, Σ ; in blue, Π ; in pink, Δ ; in green Γ .

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Table legends

Table 1: Band centres ($\tilde{\nu}_c$), vibrational term values (G_v), rotational constants (in cm^{-1}), number of fitted and assigned lines, and standard deviation of the fit (σ_{lines} in cm^{-1}) in $^{12}\text{C}_2\text{H}_2$ from the band-by-band analysis^a.

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Table 2: Summary of vibration-rotation bands in the $^{12}\text{C}_2\text{H}_2$ database used for the global fit.

Table 3: Calculated term value G_c , in cm^{-1} , of all states included in the data base of $^{12}\text{C}_2\text{H}_2$ used for the global fit.

Table 4: Terms in the Hamiltonian used to perform the global vibration-rotation fit in $^{12}\text{C}_2\text{H}_2$ ^a.

Table 5: Vibration-rotation parameters (in cm^{-1}) with their uncertainties (1σ) for the global fit of $^{12}\text{C}_2\text{H}_2$.

Table 6: Statistical survey of the quality of the vibration-rotation data of $^{12}\text{C}_2\text{H}_2$ accounted for in the global fit.

Table 7: Comparison of selected parameters (in cm^{-1}) determined for two acetylene isotopologues using similar procedures (see text).

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4 | *Table 8:* Check of x - K relations in acetylene isotopologues (all parameters in
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Table 1

$v_1 v_2 v_3 v_4 v_5, l_4 l_5$	Transition	\tilde{v}_c	G_v	B_v	$D_v \times 10^6$	$H_v \times 10^9$	$q_v \times 10^3$ $q_J \times 10^6$ $q_{JJ} \times 10^9$	$P, Q, R \{J_{\min}, J_{\max}\}$	n. of fitted/ass. lines $\sigma_{\text{lines}} \times 10^3$
11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34	$\Sigma_g^+ \leftarrow \Pi_u (v_5)$ $\Sigma_u^+ \leftarrow \Pi_g (v_4)$ $\Sigma_g^+ \leftarrow \Pi_u (v_5)$ $\Pi_u \leftarrow \text{G.S.}$ $\Sigma_u^+ \leftarrow \text{G.S.}$ $\Pi_u \leftarrow \text{G.S.}$ $\Delta_g \leftarrow \Delta_u (v_4+v_5)$	5979.867032(61) 6011.44215(27) 6030.08441(25) 6052.07472(14) 6079.69351(40) 6093.51086(27) 6342.66832(39)	6709.0212 6623.1360 6759.2386 6053.2406 6079.6935 6094.6814 7690.1434	1.16309389(29) 1.1679733(39) 1.1684360(34) 1.1659268(12) 1.179181(12) 1.1705347(53) 1.168212(14)	1.60165(24) 3.995(14) 4.647(11) 1.6755(20) 9.803(81) 2.454(27) 17.22(16)	0.361(13) 	 	$P_e\{1,34\}; R_e\{2,36\}$ $Q_f\{1,33\}$ $P_e\{1,23\}; R_e\{1,26\}$ $Q_f\{1,22\}$ $P_e\{2,10\}; R_e\{1,28\}$ $Q_f\{1,25\}$ $R_e\{2,29\}; Q_e\{1,23\}$ $P_e\{1,20\}; R_e\{0,17\}$ $P_e\{2,15\}; R_e\{0,12\}$ $Q_e\{3,29\}$ $P_e\{4,16\}; R_e\{4,12\}$ $P_f\{3,29\}; R_f\{3,19\}$	93/99 0.32 59/66 0.78 49/61 0.77 39/50 0.40 35/38 1.02 46/53 0.80 42/60 0.87

$\Sigma_u^+ \leftarrow \Sigma_g^+(2v_5)$	6355.89158(33)	7805.0040	1.170123(24)	4.48(10)	1.31(16)		$P_e\{1,19\} ; R_e\{3,13\}$	21/28 0.61
$\Pi_g \leftarrow \Pi_u(v_5)$	6362.12705(20)	7092.4489	1.1676643(19)	2.6110(42)	0.1899(23)	-7.2812(22) 0.6875(61) -0.1307(37)	$P_e\{2,36\} ; R_e\{1,26\}$ $P_f\{3,37\} ; R_f\{1,28\}$	86/115 0.76
$\Pi_u \leftarrow \Pi_g(v_4)$	6606.50704(20)	7219.3685	1.1676694(16)	2.3259(30)	0.1270(15)	-2.3916(19) -0.5588(43) 0.1431(24)	$P_e\{3,29\} ; R_e\{1,39\}$ $P_f\{4,18\} ; R_f\{4,37\}$	79/93 0.75
$\Pi_u \leftarrow \Pi_g(v_4)$	6616.57126(86)	7229.4356	1.170534(18)	2.111(10)	-0.46(15)	-4.062(13) 7.38(10) -8.94(18)	$P_e\{4,17\} ; R_e\{1,27\}$ $P_f\{3,25\} ; R_f\{1,27\}$	43/85 1.13
$\Sigma_u^+ \leftarrow G.S.$	6623.13568(23)	6623.1357	1.1679887(17)	4.0647(29)	0.4330(13)		$P_e\{1,32\} ; R_e\{0,43\}$	64/72 0.86
$\Sigma_u^+ \leftarrow G.S.$	6654.25168(29)	6654.2517	1.1718021(44)	8.233(15)	2.121(13)		$P_e\{2,20\} ; R_e\{1,31\}$	37/44 0.81
$\Pi_u \leftarrow \Pi_g(v_4)$	6662.07839(26)	7274.9429	1.1706463(32)	2.6856(98)	0.0323(80)	-10.3624(37) 0.111(15) 0.456(13)	$R_e\{2,29\} ; R_f\{2,27\}$	41/54 0.59
$\Pi_g \leftarrow \Pi_u(v_5)$	6672.23153(17)	7402.5573	1.1716056(35)	2.088(19)	2.223(31)	-8.1878(50) 0.095(35)	$P_e\{2\} ; R_e\{1,20\}$ $P_f\{2\} ; R_f\{1,27\}$	39/49 0.46

$\Pi_u \leftarrow \Pi_g(v_4)$	6674.42955(40)	7287.2938	1.170452(13)	4.48(10)	0.994(24)	6.683(59)	$P_e\{2,3\} ; R_e\{1,10\}$	25/41
$\Sigma_u^+ \leftarrow \Sigma_g^+(2v_4)$	6764.00626(27)	7994.3967	1.167236(11)	3.25(11)	-1.50(28)	-6.35(19)	$P_f\{2,3\} ; R_f\{1,27\}$	1.01
$\Delta_u \leftarrow \Delta_g(2v_4)$	6779.43633(10)	8012.9029	1.1666208(12)	0.7283(28)		-0.0074(16)	$P_e\{3,21\} ; R_e\{2,19\}$	93/114
						1.8309(51)	$P_f\{3,28\} ; R_f\{2,29\}$	0.49
							$Q_e\{2,13\} ; Q_f\{2,12\}$	
$\Delta_g \leftarrow \Delta_u(v_4+v_5)$	6780.95991(14)	8128.4317	1.1673700(19)	0.1343(58)	-0.4731(43)	-0.0577(24)	$P_e\{3,24\} ; R_e\{2,30\}$	70/116
						3.0252(89)	$P_f\{3,23\} ; R_f\{2,29\}$	0.53
						-0.9367(70)	$Q_e\{2,10\} ; Q_f\{2,10\}$	
$\Sigma_g^+ \leftarrow \Sigma_u^+(v_4+v_5)$	6786.28975(25)	8114.3630	1.1679559(26)	4.5797(62)	0.7045(38)		$P_e\{1,26\} ; R_e\{0,34\}$	48/61
								0.83
$\Pi_u \leftarrow \Pi_g(v_4)$	6804.706648(65)	7417.5658	1.16534366(30)	1.63375(23)		-4.87823(38)	$P_e\{2,32\} ; R_e\{1,37\}$	142/172
						0.05701(36)	$P_f\{2,35\} ; R_f\{1,37\}$	0.42
							$Q_e\{1,16\} ; Q_f\{1,18\}$	
$\Pi_u \leftarrow \Pi_g(v_4)$	6854.75979(17)	7467.6243	1.1706494(26)	2.7275(89)	-0.0453(82)	-9.9510(30)	$P_e\{2,27\} ; R_e\{1,26\}$	99/117
						0.189(13)	$P_f\{2,29\} ; R_f\{1,26\}$	0.68
						0.468(13)	$Q_e\{1\} ; Q_f\{1,10\}$	

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4	0 0 2 2 0, 2 0	$\Delta_g \leftarrow \Pi_u(v_5)$	6956.31619(42)	7690.1436	1.168317(17)	18.96 (19)	37.12(59)	-1.474(23) -33.49(33) 75.3(11)	P _e {3,19} ; R _e {1,17} P _f {3,21} ; R _f {1,19} Q _e {2,15}	36/86 0.72
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9	0 0 2 2 0, 0 0	$\Sigma_g^+ \leftarrow \Pi_u(v_5)$	6956.92295(59)	7686.0771	1.169304(58)	-61.2(13)	-227.5(67)		P _e {1,16} ; R _e {1,14} Q _f {1,27}	25/57 1.21
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 13 ^a The vibrational assignments correspond to those of the dominant zero order state in the eigenvector composition at low J -
 14 values. The standard deviation (1σ) is indicated in parentheses in the unit of the last quoted digit. The assigned lines are listed for each branch.
 15 The last column gives the number of lines included in the fit and the corresponding standard deviation. The band centre is
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 17 $\tilde{v}_c = G_v' - B_v' k'^2 - D_v' k'^4 - G_v'' + B_v'' k''^2 + D_v'' k''^4$.

18 ^b Band previously observed by Keppler et al.³. The range of J values has been extended.
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Table 2

	v'	v''	lines	Jmin	Jmax	ref	$\sigma \times 10^3$	ΔG_c
5	0 0 0 0 1, 0 1e	0 0 0 1 0, 1 0f	10	1	10	rob07	0.052	117.46038
6	0 0 0 0 1, 0 1f	0 0 0 1 0, 1 0e	9	1	11	rob07	0.094	117.46038
7	0 0 0 0 1, 0 1f	0 0 0 1 0, 1 0f	56	1	31	rob07	0.052	117.46038
8	0 0 0 0 1, 0 1f	0 0 0 0 0, 0 0e	40	1	41	rob07	0.053	729.15416
9	0 0 0 0 1, 0 1e	0 0 0 0 0, 0 0e	76	1	40	rob07	0.054	729.15416
10	0 0 0 0 1, 0 1e	0 0 0 0 1, 1 0e	54	1	31	rob07	0.045	117.46038
11	0 0 0 2 0, 2 0f	0 0 0 0 1, 0 1f	23	2	24	rob07	0.119	499.64591
12	0 0 0 2 0, 2 0f	0 0 0 0 1, 0 1e	57	2	32	rob07	0.118	499.64591
13	0 0 0 2 0, 2 0e	0 0 0 0 1, 0 1e	21	2	13	rob07	0.174	499.65410
14	0 0 0 2 0, 2 0e	0 0 0 0 1, 0 1f	35	2	37	rob07	0.089	499.65410
15	0 0 0 2 0, 0 0e	0 0 0 0 1, 0 1f	30	1	31	rob07	0.216	501.22835
16	0 0 0 2 0, 0 0e	0 0 0 0 1, 0 1e	61	0	31	rob07	0.089	501.22835
17	0 0 0 1 1, 1-1e	0 0 0 2 0, 0 0e	36	0	22	rob07	0.094	97.69080
18	0 0 0 1 1, 1-1e	0 0 0 0 0, 0 0e	84	0	42	rob07	0.086	1328.07331
19	0 0 0 1 1, 1-1e	0 0 0 1 0, 1 0e	61	0	32	rob07	0.113	716.37953
20	0 0 0 1 1, 1-1e	0 0 0 1 0, 1 0f	25	6	32	rob07	0.094	716.37953
21	0 0 0 1 1, 1-1f	0 0 0 1 0, 1 0f	54	0	29	rob07	0.078	728.85705
22	0 0 0 1 1, 1-1f	0 0 0 1 0, 1 0e	29	1	31	rob07	0.198	728.85705
23	0 0 0 1 1, 1 le	0 0 0 1 0, 1 0e	50	2	28	rob07	0.094	731.10839
24	0 0 0 1 1, 1 le	0 0 0 1 0, 1 0f	28	2	34	rob07	0.223	731.10839
25	0 0 0 1 1, 1 le	0 0 0 2 0, 2 0e	35	3	22	rob07	0.190	113.99391
26	0 0 0 1 1, 1 le	0 0 0 0 0, 0 0e	62	6	40	rob07	0.290	1342.80217
27	0 0 0 1 1, 1 1f	0 0 0 2 0, 2 0f	38	2	25	rob07	0.098	114.00211
28	0 0 0 1 1, 1 1f	0 0 0 1 0, 1 0f	54	2	29	rob07	0.088	731.10840
29	0 0 0 1 1, 1 1f	0 0 0 1 0, 1 0e	29	2	31	rob07	0.062	731.10840
30	0 0 0 0 2, 0 0e	0 0 0 0 1, 0 1f	23	7	29	rob07	0.082	719.95812
31	0 0 0 0 2, 0 0e	0 0 0 1 1, 1-1e	34	1	21	rob07	0.169	121.03897
32	0 0 0 0 2, 0 0e	0 0 0 0 1, 0 1e	59	0	31	rob07	0.080	719.95812
33	0 0 0 0 2, 0 2f	0 0 0 1 1, 1 1f	27	2	20	rob07	0.180	115.49149
34	0 0 0 0 2, 0 2f	0 0 0 0 1, 0 1f	54	2	30	rob07	0.096	729.13951
35	0 0 0 0 2, 0 2f	0 0 0 0 1, 0 1e	26	3	32	rob07	0.061	729.13951
36	0 0 0 0 2, 0 2e	0 0 0 0 1, 0 1f	28	2	34	rob07	0.275	729.13954
37	0 0 0 0 2, 0 2e	0 0 0 0 1, 0 1e	50	2	27	rob07	0.103	729.13954
38	0 0 0 0 2, 0 2e	0 0 0 1 1, 1 1e	28	3	21	rob07	0.245	115.49153
39	0 0 0 3 0, 3 0e	0 0 0 1 1, 1 1e	28	3	22	rob07	0.263	508.55633
40	0 0 0 3 0, 3 0e	0 0 0 1 1, 1 1f	24	6	29	rob07	0.230	508.55632
41	0 0 0 3 0, 3 0f	0 0 0 1 1, 1 1f	33	3	22	rob07	0.290	508.57212
42	0 0 0 3 0, 3 0f	0 0 0 1 1, 1 1e	23	7	30	rob07	0.207	508.57213
43	0 0 0 3 0, 1 0f	0 0 0 1 1, 1-1e	21	1	22	rob07	0.232	526.52204
44	0 0 0 3 0, 1 0f	0 0 0 1 1, 1 1e	16	2	18	rob07	0.089	511.79318
45	0 0 0 3 0, 1 0f	0 0 0 1 1, 1 1f	49	1	26	rob07	0.105	511.79317
46	0 0 0 3 0, 1 0f	0 0 0 1 1, 1-1f	50	1	26	rob07	0.104	514.04452
47	0 0 0 3 0, 1 0e	0 0 0 1 1, 1 1e	52	1	29	rob07	0.125	511.80612
48	0 0 0 3 0, 1 0e	0 0 0 1 1, 1-1e	36	2	22	rob07	0.198	526.53498
49	0 0 0 3 0, 1 0e	0 0 0 1 1, 1-1f	26	1	26	rob07	0.230	514.05746
50	0 0 0 3 0, 1 0e	0 0 0 1 1, 1 1f	16	2	18	rob07	0.084	511.80611
51	0 0 0 2 1, 2-1e	0 0 0 1 0, 1 0e	75	1	38	rob07	0.176	1328.30621
52	0 0 0 2 1, 2-1e	0 0 0 2 0, 2 0f	10	2	20	rob07	0.132	711.19992
53	0 0 0 2 1, 2-1e	0 0 0 0 2, 0 2e	16	1	14	rob07	0.277	481.70629
54	0 0 0 2 1, 2-1e	0 0 0 0 2, 0 2f	13	2	15	rob07	0.293	481.70632
55	0 0 0 2 1, 2-1e	0 0 0 0 0, 0 0e	41	2	33	jac02	0.153	1939.99999
56	0 0 0 2 1, 2-1e	0 0 0 2 0, 2 0e	14	4	20	rob07	0.106	711.19173
57	0 0 0 2 1, 2-1f	0 0 0 0 2, 0 2e	18	2	19	rob07	0.296	481.70630
58	0 0 0 2 1, 2-1f	0 0 0 0 2, 0 2f	23	1	15	rob07	0.419	481.70633
59	0 0 0 2 1, 2-1f	0 0 0 2 0, 0 0e	13	3	19	rob07	0.180	709.61749
60	0 0 0 2 1, 2-1f	0 0 0 2 0, 2 0e	8	3	17	rob07	0.148	711.19174
61	0 0 0 2 1, 2-1f	0 0 0 2 0, 2 0f	10	1	21	rob07	0.194	711.19993
62	0 0 0 2 1, 2-1f	0 0 0 1 0, 1 0f	73	1	37	rob07	0.156	1328.30622
63	0 0 0 2 1, 2-1f	0 0 0 0 2, 0 0e	8	3	13	rob07	0.510	490.88772
64	0 0 0 2 1, 2-1f	0 0 0 0 0, 0 0e	19	1	21	jac02	0.059	1940.00000
65	0 0 0 2 1, 0 1e	0 0 0 0 2, 0 0e	48	1	24	rob07	0.163	510.57930
66	0 0 0 2 1, 0 1e	0 0 0 2 0, 2 0f	4	10	16	rob07	0.225	730.89151
67	0 0 0 2 1, 0 1e	0 0 0 0 2, 0 2f	24	2	26	rob07	0.199	501.39791
68	0 0 0 2 1, 0 1e	0 0 0 0 0, 0 0e	24	2	18	rob07	0.193	729.30907
69	0 0 0 2 1, 0 1e	0 0 0 0 0, 0 0e	22	4	26	jac02	0.146	1959.69158
70	0 0 0 2 1, 0 1e	0 0 0 0 2, 0 2e	33	1	18	rob07	0.322	501.39788
71	0 0 0 2 1, 0 1e	0 0 0 1 0, 1 0e	23	1	16	rob07	0.408	1347.99780

1	0 0 0 2 1, 0 1f	0 0 0 0 2, 0 2f	29	1	19	rob07	0.126	501.39830
2	0 0 0 2 1, 0 1f	0 0 0 0 2, 0 2e	19	2	23	rob07	0.170	501.39827
3	0 0 0 2 1, 0 1f	0 0 0 2 0, 2 0e	2	13	15	rob07	0.000	730.88371
4	0 0 0 2 1, 0 1f	0 0 0 1 0, 1 0f	43	1	27	rob07	0.385	1347.99819
5	0 0 0 2 1, 0 1f	0 0 0 0 0, 0 0e	9	10	18	jac02	0.052	1959.69197
6	0 0 0 2 1, 0 1f	0 0 0 2 0, 0 0e	1	14	14	kab91	0.000	729.30946
7	0 0 0 2 1, 0 1f	0 0 0 0 2, 0 0e	22	1	22	rob07	0.066	510.57969
8	0 0 0 2 1, 2 1f	0 0 0 1 0, 1 0f	28	13	29	rob07	0.284	1350.23834
9	0 0 0 2 1, 2 1f	0 0 0 2 0, 2 0e	7	3	15	rob07	0.150	733.12386
10	0 0 0 2 1, 2 1f	0 0 0 2 0, 2 0f	17	3	17	rob07	0.130	733.13205
11	0 0 0 2 1, 2 1f	0 0 0 0 2, 0 2e	10	3	12	rob07	0.472	503.63842
12	0 0 0 2 1, 2 1f	0 0 0 0 2, 0 2f	43	3	27	rob07	0.196	503.63845
13	0 0 0 2 1, 2 1e	0 0 0 0 2, 0 2e	44	3	26	rob07	0.251	503.63882
14	0 0 0 2 1, 2 1e	0 0 0 2 0, 2 0e	12	3	16	rob07	0.246	733.12426
15	0 0 0 2 1, 2 1e	0 0 0 2 0, 2 0f	8	4	20	rob07	0.168	733.13245
16	0 0 0 2 1, 2 1e	0 0 0 0 2, 0 2f	15	3	20	rob07	0.263	503.63885
17	0 1 0 0 0, 0 0e	0 0 0 0 1, 0 1f	27	1	27	rob07	0.123	1245.16186
18	0 1 0 0 0, 0 0e	0 0 0 0 1, 0 1e	44	0	25	rob07	0.312	1245.16186
19	0 0 0 1 2, 1 0f	0 0 0 1 1, 1-1e	18	2	24	rob07	0.149	719.80291
20	0 0 0 1 2, 1 0f	0 0 0 0 1, 0 1f	71	1	38	rob07	0.206	1318.72206
21	0 0 0 1 2, 1 0e	0 0 0 1 1, 1-1e	23	3	21	rob07	0.111	719.80291
22	0 0 0 1 2, 1 0e	0 0 0 0 1, 0 1e	65	1	37	rob07	0.111	1318.72206
23	0 0 0 1 2, -1 2e	0 0 0 1 1, 1-1f	20	1	23	rob07	0.184	725.24214
24	0 0 0 1 2, -1 2e	0 0 0 0 1, 0 1e	49	1	29	rob07	0.327	1336.63881
25	0 0 0 1 2, -1 2f	0 0 0 0 1, 0 1f	48	1	28	rob07	0.308	1336.63882
26	0 0 0 1 2, -1 2f	0 0 0 1 1, 1-1f	22	4	20	rob07	0.188	725.24215
27	0 0 0 1 2, 1 2e	0 0 0 1 1, 1 1e	17	3	19	rob07	0.238	731.37801
28	0 0 0 1 2, 1 2e	0 0 0 1 1, 1 1f	12	3	23	rob07	0.123	731.37800
29	0 0 0 1 2, 1 2f	0 0 0 1 1, 1 1f	15	4	20	rob07	0.164	731.37806
30	0 0 0 1 2, 1 2f	0 0 0 1 1, 1 1e	12	4	18	rob07	0.225	731.37807
31	0 0 0 0 3, 0 1f	0 0 0 0 2, 0 2f	1	7	7	rob07	0.127	710.86340
32	0 0 0 0 3, 0 1f	0 0 0 0 2, 0 2e	5	7	17	rob07	0.214	710.86337
33	0 0 0 0 3, 0 1f	0 0 0 0 2, 0 0e	17	1	21	rob07	0.153	720.04479
34	0 0 0 0 3, 0 1f	0 0 0 0 0, 0 0e	16	1	35	jac02	0.111	2169.15707
35	0 0 0 0 3, 0 1e	0 0 0 0 2, 0 2f	2	10	12	rob07	0.065	710.86342
36	0 0 0 0 3, 0 1e	0 0 0 0 2, 0 2e	1	8	8	rob07	0.092	710.86339
37	0 0 0 0 3, 0 1e	0 0 0 0 2, 0 0e	24	1	20	rob07	0.200	720.04481
38	0 0 0 0 3, 0 1e	0 0 0 0 0, 0 0e	45	1	36	jac02	0.061	2169.15709
39	0 0 0 0 3, 0 3e	0 0 0 0 2, 0 2e	14	3	22	rob07	0.237	729.15730
40	0 0 0 0 3, 0 3f	0 0 0 0 2, 0 2f	15	5	21	rob07	0.248	729.15737
41	0 0 0 0 3 1, 3-1f	0 0 0 1 0, 1 0f	17	5	25	jac03	0.133	1945.10106
42	0 0 0 0 3 1, 3-1f	0 0 0 2 0, 2 0f	37	2	31	rob07	0.314	1327.99477
43	0 0 0 0 3 1, 3-1e	0 0 0 1 0, 1 0e	19	4	26	jac03	0.090	1945.10127
44	0 0 0 0 3 1, 3-1e	0 0 0 2 0, 2 0e	37	3	32	rob07	0.351	1327.98679
45	0 0 0 0 3 1, 1-1e	0 0 0 0 0, 0 0e	33	0	20	jac07	0.076	2560.59503
46	0 0 0 0 3 1, 1-1e	0 0 0 0 2 0, 0 0e	59	0	30	rob07	0.189	1330.21252
47	0 0 0 0 3 1, 1-1e	0 0 0 0 1 0, 1 0f	1	20	20	jac03	0.113	1948.90125
48	0 0 0 0 3 1, 1-1e	0 0 0 0 1 0, 1 0f	26	1	19	jac03	0.159	1844.38129
49	0 1 0 1 0, 1 0e	0 0 0 0 1, 0 1e	26	1	22	jac03	0.100	1844.38129
50	0 1 0 1 0, 1 0f	0 0 0 0 1, 0 1f	26	7	11	jac03	0.263	1972.17337
51	0 0 0 0 3 1, 1-1f	0 0 0 1 0, 1 0f	2	7	11	jac03	0.198	1972.17337
52	0 0 0 0 3 1, 1-1f	0 0 0 1 0, 1 0e	9	4	13	jac03	0.138	1973.25428
53	0 0 0 0 3 1, 1-1e	0 0 0 0 1 0, 1 0f	3	10	12	jac03	0.082	1973.26647
54	0 0 0 0 3 1, 1 1e	0 0 0 1 0, 1 0e	2	10	11	jac03	0.186	1918.85990
55	0 0 0 0 2 2, 2-2e	0 0 0 0 1, 0 1f	7	5	21	jac03	0.075	1918.85990
56	0 0 0 0 2 2, 2-2e	0 0 0 0 1, 0 1e	8	5	19	jac03	0.289	1319.94075
57	0 0 0 0 2 2, 2-2e	0 0 0 1 1, 1-1e	59	0	31	rob07	0.242	1320.63955
58	0 0 0 0 2 2, 2-2f	0 0 0 1 1, 1-1f	38	0	24	rob07	0.333	1318.38820
59	0 0 0 0 2 2, 2-2f	0 0 0 1 1, 1 1f	14	10	24	rob07	0.133	1932.03622
60	0 0 0 0 2 2, 2 0f	0 0 0 0 1, 0 1f	1	8	8	jac03	0.484	1932.27378
61	0 0 0 0 2 2, 2 0f	0 0 0 1 1, 1 1f	40	4	28	rob07	0.271	1318.62576
62	0 0 0 0 2 2, 2 0f	0 0 0 1 1, 1-1f	28	12	27	rob07	0.331	1320.87711
63	0 0 0 0 2 2, 2 0e	0 0 0 1 1, 1 1e	42	4	29	rob07	0.279	1318.62710
64	0 1 0 0 1, 0 1e	0 0 0 0 0, 0 0e	36	1	23	jac07	0.053	2701.90945
65	0 1 0 0 1, 0 1f	0 0 0 0 0, 0 0e	25	1	25	jac07	0.092	2701.90945
66	0 1 0 0 1, 0 1e	0 0 0 0 1 0, 1 0e	24	1	20	jac03	0.204	2090.21567
67	0 1 0 0 1, 0 1f	0 0 0 0 1 0, 1 0f	26	1	20	jac03	0.148	2090.21567
68	0 0 0 1 3, 1-1e	0 0 0 0 2, 0 0e	37	0	26	rob07	0.236	1308.68464
69	0 0 0 1 3, 1-1e	0 0 0 1 0, 1 0f	16	1	18	jac03	0.197	2146.10314
70	0 0 0 1 3, 1-1e	0 0 0 1 0, 1 0e	19	0	21	jac03	0.153	2146.10314
71	0 0 0 1 3, 1 1f	0 0 0 1 0, 1 0f	16	4	22	jac03	0.201	2156.75654

0	0	1	2	0,	2	0f	0	0	0	1	0,	1	0e	18	2	19	sar95	0.388	3892.84332
0	0	1	2	0,	2	0f	0	0	0	2	0,	2	0f	47	2	26	sar95	1.114	3275.73703
0	0	1	2	0,	0	0e	0	0	0	0	0,	0	0e	57	0	30	lyu7b	0.415	4508.01322
0	0	1	2	0,	0	0e	0	0	0	2	0,	0	0e	50	0	25	sar95	1.774	3277.63071
0	0	1	2	0,	0	0e	0	0	0	1	0,	1	0e	46	0	25	sar95	0.435	3896.31944
																gir06			
0	0	1	2	0,	0	0e	0	0	0	1	0,	1	0f	20	1	20	sar95	0.307	3896.31944
0	1	0	2	2,	2	-2f	0	0	0	1	1,	1	-1f	54	0	32	rin82	1.297	3259.22329
0	1	0	2	2,	2	0f	0	0	0	1	1,	1	1f	50	2	36	lyu06		
0	1	0	2	2,	2	0e	0	0	0	1	1,	1	1e	39	2	30	rin82	3.837	3260.47068
0	1	0	2	2,	2	1-1e	0	0	0	1	1,	1	1-1e	50	0	25	lyu06		
0	0	1	1	1,	1	1-1e	0	0	0	0	1,	0	1e	42	0	26	sar95	1.551	3281.21743
0	0	1	1	1,	1	1-1e	0	0	0	0	1,	0	1e	42	0	26	sar95	0.509	3880.13658
0	0	1	1	1,	1	1-1e	0	0	0	0	1,	0	1f	19	1	19	sar95	0.316	3880.13658
0	0	1	1	1,	1	1-1f	0	0	0	0	1,	0	1e	20	1	20	sar95	0.338	3888.77236
0	0	1	1	1,	1	1-1f	0	0	0	0	1,	0	1f	39	0	25	sar95	0.447	3888.77236
																gir06			
0	0	1	1	1,	1	1-1f	0	0	0	1	1,	1	1-1f	51	0	26	sar95	1.952	3277.37569
0	0	1	1	1,	1	1e	0	0	0	1	1,	1	1e	47	2	26	sar95	0.708	3277.25526
0	0	1	1	1,	1	1f	0	0	0	1	1,	1	1f	47	2	26	sar95	0.975	3277.25525
0	0	1	1	1,	1	1e	0	0	0	0	1,	0	1e	46	2	31	sar95	0.402	3890.90327
																gir06			
0	0	1	1	1,	1	1e	0	0	0	0	1,	0	1f	20	2	21	sar95	0.417	3890.90327
0	0	1	1	1,	1	1f	0	0	0	0	1,	0	1f	54	2	36	sar95	0.530	3890.90327
																gir06			
0	0	1	1	1,	1	1f	0	0	0	0	1,	0	1e	20	2	21	sar95	0.244	3890.90327
1	0	0	1	1,	1	-1e	0	0	0	0	0,	0	0e	53	0	30	lyu7b	0.338	4620.05743
1	0	0	1	1,	1	-1e	0	0	0	1	0,	1	0e	66	0	38	dcu91	1.098	4008.36365
																gir06			
1	0	0	1	1,	1	-1e	0	0	0	1	0,	1	0f	28	1	28	dcu91	1.037	4008.36365
1	0	0	1	1,	1	1e	0	0	0	1	0,	1	0f	24	2	25	lyu07		
1	0	0	1	1,	1	1e	0	0	0	1	0,	1	0e	46	2	26	dcu91	0.543	4075.66942
1	0	0	1	1,	1	1f	0	0	0	1	0,	1	0f	61	2	36	lyu07		
																gir06			
1	0	0	1	1,	1	1f	0	0	0	1	0,	1	0e	29	2	30	dcu91	0.421	4075.66946
1	0	0	1	1,	1	-1f	0	0	0	1	0,	1	0e	26	1	26	lyu07		
1	0	0	1	1,	1	-1f	0	0	0	1	0,	1	0f	61	0	35	dcu91	0.317	4077.14564
1	0	0	1	1,	1	-1f	0	0	0	1	0,	1	0f	61	0	35	lyu07	0.446	4077.14564
0	1	0	1	3,	1	-1e	0	0	0	0	2,	0	0e	26	0	21	rin82	1.785	3261.62186
0	1	0	1	3,	-1	3f	0	0	0	0	2,	0	2f	38	3	31	rin82	2.622	3262.82770
0	1	0	1	3,	-1	3e	0	0	0	0	2,	0	2e	36	3	26	lyu06		
																rin82	3.606	3262.84803	
0	0	1	0	2,	0	0e	0	0	0	0	2,	0	0e	45	0	24	sar95	1.313	3277.93741
0	0	1	0	2,	0	0e	0	0	0	0	0,	0	0e	52	0	26	lyu7b	0.117	4727.04969
0	0	1	0	2,	0	2f	0	0	0	0	2,	0	2f	43	2	24	sar95	1.397	3278.02121
0	0	1	0	2,	0	2e	0	0	0	0	2,	0	2e	43	2	24	sar95	1.377	3278.02133
1	0	0	0	2,	0	0e	0	0	0	0	1,	0	1e	72	0	41	dcu91	0.394	4070.98191
																gir06			
1	0	0	0	2,	0	0e	0	0	0	0	1,	0	1f	27	1	27	dcu91	0.359	4070.98191
1	0	0	0	2,	0	2f	0	0	0	0	1,	0	1f	62	2	34	lyu07		
1	0	0	0	2,	0	2f	0	0	0	0	1,	0	1e	26	2	27	dcu91	0.253	4080.35545
1	0	0	0	2,	0	2e	0	0	0	0	1,	0	1f	29	2	30	lyu07		
1	0	0	0	2,	0	2e	0	0	0	0	1,	0	1f	29	2	30	dcu91	1.375	4080.35549

1	0	0	0	2,	0	2e	0	0	0	0	1,	0	1e	58	2	33	lyu07	0.439	4080.35549
0	0	1	3	0,	1	0e*	0	0	0	1	0,	1	0e	15	3	10	lyu7b	0.995	4489.85560
0	0	1	3	0,	1	0e*	0	0	0	0	0,	0	0e	34	2	24	lyu08	2.390	5101.54938
0	0	1	3	0,	1	0f*	0	0	0	0	0,	0	0e	15	1	21	lyu08	1.547	5101.62936
0	0	1	3	0,	1	0f*	0	0	0	1	0,	1	0f	26	3	19	lyu7b	1.233	4489.93558
0	0	1	3	0,	1	0f*	0	0	0	1	0,	1	0f	26	2	19	lyu7b	0.575	4511.70173
0	0	1	3	0,	1	0f*	0	0	0	0	0,	0	0e	16	5	25	lyu08	0.661	5123.39551
0	0	1	3	0,	1	0e*	0	0	0	1	0,	1	0e	29	2	20	lyu7b	0.538	4511.70581
0	0	1	3	0,	1	0e*	0	0	0	0	0,	0	0e	31	1	24	lyu08	1.107	5123.39959
0	2	0	1	1,	1	-1e	0	0	0	0	0,	0	0e	51	0	28	pa172	0.890	5230.22853
																lyu08			
0	1	1	0	0,	0	0e	0	0	0	0	0,	0	0e	52	0	28	pa172	1.024	5260.02212
																lyu08			
1	0	0	2	1,	2	-1e*	0	0	0	1	0,	1	0e	32	2	22	lyu7b	0.738	4656.85217
1	0	0	2	1,	2	-1f*	0	0	0	1	0,	1	0f	34	3	23	lyu7b	0.529	4656.85217
1	0	0	2	1,	2	-1e*	0	0	0	0	0,	0	0e	29	2	22	lyu08	0.774	5289.09956
1	0	0	2	1,	2	-1f*	0	0	0	0	0,	0	0e	14	7	27	lyu08	1.587	5289.10486
1	0	0	2	1,	0	1e	0	0	0	0	0,	0	0e	30	2	26	lyu08	1.020	5301.13135
1	0	0	2	1,	0	1f	0	0	0	0	0,	0	0e	15	3	23	lyu08	2.112	5301.13155
1	1	0	0	0,	0	0e	0	1	0	0	0,	0	0e	20	1	23	ber99	0.870	3361.23286
1	0	0	1	2,	1	0f	0	0	0	0	1,	0	1f	33	3	23	lyu7b	0.821	4652.40710
1	0	0	1	2,	1	0e	0	0	0	0	1,	0	1e	29	3	21	lyu7b	0.382	4652.40711
1	0	0	0	3,	0	1f	0	0	0	0	0,	0	0e	17	3	25	lyu08	1.134	5509.22211
1	0	0	0	3,	0	1e	0	0	0	0	0,	0	0e	28	2	24	lyu08	0.731	5509.22214
0	2	0	2	1,	2	-1e	0	0	0	0	0,	0	0e	52	1	29	kep96	0.371	5816.86353
0	2	0	2	1,	2	-1f	0	0	0	0	0,	0	0e	21	1	23	kep96	0.242	5816.86354
0	1	1	1	0,	1	0f	0	0	0	0	0,	0	0e	29	1	29	kep96	0.347	5850.64984
0	1	1	1	0,	1	0e	0	0	0	0	0,	0	0e	55	1	28	kep96	0.316	5850.67614
1	1	0	0	1,	0	1f	0	0	0	0	0,	0	0e	22	1	23	rob08	0.699	6052.07572
1	1	0	0	1,	0	1e	0	0	0	0	0,	0	0e	28	3	30	rob08	0.818	6052.07572
1	0	0	1	3,	1	-1e	0	0	0	0	0,	0	0e	38	0	19	rob08	1.881	6079.69072
0	2	0	0	3,	0	1f	0	0	0	0	0,	0	0e	26	3	29	rob08	1.849	6093.51244
0	2	0	0	3,	0	1e	0	0	0	0	0,	0	0e	27	1	14	rob08	1.960	6093.51247
0	2	0	3	1,	1	-1e	0	0	0	0	0,	0	0e	37	1	21	kep96	0.477	6413.90039
																rob08			
0	1	1	2	0,	2	0e	0	0	0	1	0,	1	0e	29	3	21	kep96	0.525	5836.08937
0	1	1	2	0,	2	0f	0	0	0	1	0,	1	0f	24	3	17	kep96	0.583	5836.12016
0	1	1	2	0,	0	0e	0	0	0	0	0,	0	0e	45	0	23	kep96	0.384	6449.09176
0	0	2	0	0,	0	0e	0	0	0	0	1,	0	1f	22	1	25	kep96	0.365	5773.19209
0	0	2	0	0,	0	0e	0	0	0	0	1,	0	1e	52	2	29	kep96	0.331	5773.19209
1	1	0	2	0,	0	0e	0	0	0	0	1,	0	1e	43	0	24	kep96	0.452	5784.83853
1	1	0	2	0,	0	0e	0	0	0	0	1,	0	1f	24	1	25	kep96	0.323	5784.83853
1	0	1	0	0,	0	0e	0	0	0	1	0,	1	0f	33	1	33	kep96	0.469	5944.77095
1	0	1	0	0,	0	0e	0	0	0	0	0,	0	0e	73	1	40	kou94	0.278	6556.46473
1	0	1	0	0,	0	0e	0	0	0	1	0,	1	0e	61	0	33	kep96	0.315	5944.77095
1	1	0	1	1,	1	-1e	0	0	0	0	0,	0	0e	72	0	44	kep96	0.281	6623.13650
																rob08			
1	1	0	1	1,	1	-1e	0	0	0	1	0,	1	0e	45	0	28	kep96	0.617	6011.44272
																rob08			
1	1	0	1	1,	1	-1e	0	0	0	1	0,	1	0f	22	1	22	kep96	0.514	6011.44272
																rob08			
0	2	0	1	3,	1	-1e	0	0	0	0	0,	0	0e	44	1	32	kep96	0.280	6654.25190
																rob08			
0	1	1	0	2,	0	0e	0	0	0	0	0,	0	0e	52	0	34	kep96	0.516	6690.42425
2	0	0	0	0,	0	0e	0	0	0	0	1,	0	1f	32	1	33	kep96	0.268	5979.86697
																rob08			
2	0	0	0	0,	0	0e	0	0	0	0	1,	0	1e	67	0	37	kep96	0.345	5979.86697
																rob08			
1	1	0	0	2,	0	0e	0	0	0	0	1,	0	1f	25	1	25	rob08	0.635	6030.08520
1	1	0	0	2,	0	0e	0	0	0	0	1,	0	1e	36	1	29	kep96	1.307	6030.08520
																rob08			
0	0	2	1	0,	1	0f	0	0	0	0	1,	0	1f	59	2	36	kep96	0.411	6362.12703
																rob08			
0	0	2	1	0,	1	0e	0	0	0	0	1,	0	1e	56	1	35	kep96	0.609	6362.12704
																rob08			
1	0	1	1	0,	1	0f	0	0	0	0	0,	0	0e	28	1	29	vda02	0.534	7141.50298
1	0	1	1	0,	1	0f	0	0	0	1	0,	1	0f	56	1	31	kep96	0.418	6529.80920
1	0	1	1	0,	1	0e	0	0	0	1	0,	1	0e	55	2	32	kep96	0.406	6529.80921

1	1 0 1 1 0, 1 0e	0 0 0 0 0, 0 0e	47	1	28	vda02	0.422	7141.50299
2	1 1 0 2 1, 2-1f*	0 0 0 1 0, 1 0f	39	3	31	kep96	0.437	6594.25916
3	1 1 0 2 1, 2-1e*	0 0 0 1 0, 1 0e	42	2	27	kep96	0.502	6594.25916
4	0 0 2 0 1, 0 1e	0 0 0 1 0, 1 0e	56	2	40	kep96	0.529	6606.50586
5	rob08							
6	0 0 2 0 1, 0 1e	0 0 0 0 0, 0 0e	51	1	28	vda02	0.385	7218.19964
7	0 0 2 0 1, 0 1f	0 0 0 0 0, 0 0e	24	1	24	vda02	0.289	7218.19965
8	0 0 2 0 1, 0 1f	0 0 0 1 0, 1 0f	37	3	38	kep96	0.400	6606.50587
9	rob08							
10	1 1 0 2 1, 2-1e*	0 0 0 0 0, 0 0e	25	1	16	vda02	0.607	7228.27124
11	1 1 0 2 1, 2-1e*	0 0 0 1 0, 1 0e	40	2	28	kep96	0.562	6616.57746
12	rob08							
13	1 1 0 2 1, 2-1f*	0 0 0 0 0, 0 0e	18	1	22	vda02	0.397	7228.27434
14	1 0 1 0 1, 0 1e	0 0 0 0 1, 0 1e	56	1	31	kep96	0.359	6534.74916
15	0 1 0 1 0, 0 1f	0 0 0 0 1, 0 1f	57	2	34	kep96	0.339	6534.74916
16	0 1 1 1 2, 1 0f	0 0 0 1 0, 1 0f	26	3	28	rob08	1.413	6662.07802
17	0 1 1 1 2, 1 0e	0 0 0 1 0, 1 0e	28	3	30	rob08	1.459	6662.07968
18	0 1 1 1 2, -1 2e	0 0 0 1 0, 1 0e	12	1	11	rob08	3.264	6674.41487
19	0 1 1 1 2, -1 2f	0 0 0 1 0, 1 0f	29	1	28	rob08	1.566	6674.53735
20	2 0 0 0 1, 0 1e	0 0 0 0 1, 0 1e	45	1	33	kep96	0.393	6567.22885
21	2 0 0 0 1, 0 1f	0 0 0 0 1, 0 1f	43	2	33	kep96	0.309	6567.22886
22	1 1 0 1 2, 1 0f	0 0 0 0 1, 0 1f	40	2	28	kep96	0.511	6600.19072
23	1 1 0 1 2, 1 0e	0 0 0 0 1, 0 1e	35	1	27	kep96	0.553	6600.19073
24	0 1 1 0 3, 0 1f	0 0 0 0 1, 0 1f	28	1	28	rob08	1.822	6672.10942
25	0 1 1 0 3, 0 1e	0 0 0 0 1, 0 1e	21	1	21	rob08	1.166	6672.26918
26	2 0 0 0 1, 0 1f	0 0 0 0 0, 0 0e	27	1	29	vda02	0.299	7416.40041
27	2 0 0 0 1, 0 1e	0 0 0 0 1, 0 1e	68	1	38	kep96	0.313	6804.70663
28	rob08							
29	2 0 0 0 1, 0 1f	0 0 0 1 0, 1 0f	71	1	38	kep96	0.522	6804.70663
30	rob08							
31	2 0 0 0 1, 0 1f	0 0 0 1 0, 1 0e	16	1	16	rob08	1.307	6804.70663
32	2 0 0 0 1, 0 1e	0 0 0 1 0, 1 0f	17	1	18	rob08	0.979	6804.70663
33	2 0 0 0 1, 0 1e	0 0 0 0 0, 0 0e	51	1	28	vda02	0.312	7416.40041
34	1 1 0 0 3, 0 1f	0 0 0 1 0, 1 0f	54	1	28	rob08	0.900	6854.75932
35	1 1 0 0 3, 0 1f	0 0 0 1 0, 1 0e	1	1	1	rob08	3.345	6854.75932
36	1 1 0 0 3, 0 1e	0 0 0 1 0, 1 0f	10	1	10	rob08	1.369	6854.75935
37	1 1 0 0 3, 0 1e	0 0 0 1 0, 1 0e	52	1	27	rob08	1.437	6854.75935
38	0 0 2 2 0, 2 0f	0 0 0 0 1, 0 1f	38	2	20	rob08	1.319	6956.31575
39	0 0 2 2 0, 2 0f	0 0 0 0 1, 0 1e	14	2	15	rob08	1.495	6956.31575
40	0 0 2 2 0, 2 0f	0 0 0 1 1, 1 1f	38	2	28	kep96	0.577	6342.66773
41	rob08							
42	0 0 2 2 0, 2 0e	0 0 0 1 1, 1 1e	22	3	15	rob08	0.911	6342.70646
43	0 0 2 2 0, 0 0e	0 0 0 0 1, 0 1f	27	1	27	rob08	1.763	6956.89393
44	0 0 2 2 0, 0 0e	0 0 0 0 1, 0 1e	30	0	15	rob08	1.363	6956.89393
45	0 0 2 2 0, 0 0e	0 0 0 0 1, 0 1e	30	0	15	rob08	1.363	6956.89393
46	1 0 1 2 0, 2 0f	0 0 0 2 0, 2 0f	43	2	28	kep96	0.496	6503.55145
47	1 0 1 2 0, 2 0e	0 0 0 2 0, 2 0e	36	2	21	kep96	0.487	6503.57532
48	1 0 1 2 0, 0 0e	0 0 0 0 0, 0 0e	46	0	26	vda02	0.417	7732.76330
49	1 0 1 2 0, 0 0e	0 0 0 0 2, 0 0e	37	2	26	kep96	0.443	6502.38079
50	1 0 1 2 0, 0 1e	0 0 0 0 2, 0 1e	28	0	18	kep96	0.561	6356.08851
51	rob08							
52	1 0 1 1 1, 1 -1e	0 0 0 1 1, 1 -1e	30	1	28	kep96	0.382	6506.91254
53	1 0 1 1 1, 1 1e	0 0 0 1 1, 1 1e	18	2	18	kep96	0.442	6504.94704
54	1 0 1 1 1, 1 1f	0 0 0 1 1, 1 1f	24	2	19	kep96	0.646	6504.94707
55	1 0 1 1 1, 1 -1f	0 0 0 1 1, 1 -1f	51	0	34	kep96	0.565	6512.72508
56	1 0 1 0 2, 0 0e	0 0 0 0 2, 0 0e	33	0	27	kep96	0.490	6512.70665
57	1 0 1 0 2, 0 2f	0 0 0 0 2, 0 2f	24	2	22	kep96	0.627	6513.27206
58	1 0 1 0 2, 0 2e	0 0 0 0 2, 0 2e	33	2	26	kep96	0.578	6513.27204
59	2 0 0 1 1, 1 -1e	0 0 0 2 0, 0 0e	39	0	22	rob08	2.577	6764.01188
60	2 0 0 1 1, 1 1e	0 0 0 2 0, 2 0f	11	2	12	rob08	0.793	6779.43585
61	2 0 0 1 1, 1 1e	0 0 0 2 0, 2 0e	37	2	20	rob08	0.741	6779.42766
62	2 0 0 1 1, 1 1f	0 0 0 2 0, 2 0e	12	2	13	rob08	0.695	6779.42771
63	2 0 0 1 1, 1 1f	0 0 0 2 0, 2 0f	54	2	30	rob08	0.840	6779.43590
64	2 0 0 0 2, 0 0e	0 0 0 1 1, 1 -1e	61	0	35	rob08	1.563	6786.28982
65	2 0 0 0 2, 0 2f	0 0 0 1 1, 1 1e	8	2	10	rob08	1.333	6780.95951
66	2 0 0 0 2, 0 2f	0 0 0 1 1, 1 1f	49	2	30	rob08	1.616	6780.95950
67	2 0 0 0 2, 0 2e	0 0 0 1 1, 1 1e	51	2	31	rob08	1.219	6780.95954
68	2 0 0 0 2, 0 2e	0 0 0 1 1, 1 1f	8	2	10	rob08	1.098	6780.95953
69	1 1 1 0 0, 0 0e	0 0 0 0 0, 0 0e	64	0	34	vda02	0.325	8512.05644

1 2 2 0 1 1, 1-1e 0 0 0 0, 0 0e 34 2 22 vda02 0.449 8556.59101

5 The vibrational states, v' and v'' , are identified using the labels $v_1v_2v_3v_4v_5$, $lJ_s\epsilon/f$. Transitions are listed by order of
6 increasing energy of the upper state. The vibrational assignments correspond to those of the dominant zero order state in
7 the eigenvector composition at low J -values and may differ from some of the previous literature. The σ values
8 correspond to the standard deviation for each band in the global fit, in 10^{-3} cm^{-1} . The ΔG_e value, in cm^{-1} , is $G_e^0 - G_e^{v''}$.
9 ber98: Bermejo *et al.*^{21,22}; ber99: Bermejo *et al.*²²; dcu93: D'Cunha *et al.*²⁷; gir06: Girard *et al.*³⁹; jac02: Jacquemart *et*
10 *al.*²⁷; jac03: Jacquemart *et al.*³³; jac07: Jacquemart *et al.*³⁴; kep96: Keppler *et al.*³; kou94: Kou *et al.*²; lyu06: Lyulin
11 *et al.*³⁸; lyu07: Lyulin *et al.*³⁵; lyu7b: Lyulin *et al.*³⁶; lyu08: Lyulin *et al.*³⁷; man05: Mandin *et al.*³²; pal72: Palmer *et*
12 *al.*²³; rin82: Rinsland *et al.*³⁸; rob07: Robert *et al.*²⁴ and refs listed therein; rob08: present work; sar95: Sarma *et*
13 *al.*²⁸; vda93: Vander Auwera *et al.*⁶¹; vda02: Vander Auwera *et al.*³⁸

Table 3

$v_1 v_2 v_3 v_4 v_5 L_1 L_2 e/f$	Gc	$v_1 v_2 v_3 v_4 v_5 L_1 L_2 e/f$	Gc	$v_1 v_2 v_3 v_4 v_5 L_1 L_2 e/f$	Gc
0 0 0 0 0, 0 oe	0.00000	1 0 0 0 0, 0 oe	3372.84725	1 1 0 0 1, 0 1f	6052.07572
0 0 0 1 0, 1 oe	611.69378	0 1 0 2 1, 2-1e	3881.23331	1 0 0 1 3, 1-1e	6079.69072
0 0 0 1 0, 1 of	611.69378	0 1 0 2 1, 2-1f	3881.23331	0 2 0 0 3, 0 1f	6093.51244
0 0 0 0 1, 0 1f	729.15416	0 0 1 1 0, 1 oe	3897.16263	0 2 0 0 3, 0 1e	6093.51247
0 0 0 0 1, 0 1e	729.15416	0 0 1 1 0, 1 of	3897.16265	0 2 0 3 1, 1-1e	6413.90039
0 0 0 2 0, 2 0f	1228.80007	0 1 0 2 1, 0 1e	3908.13474	0 1 1 2 0, 2 0e	6447.78315
0 0 0 2 0, 2 0e	1228.80826	0 2 0 0 0, 0 oe	3933.89754	0 1 1 2 0, 2 0f	6447.81394
0 0 0 2 0, 0 oe	1230.38251	1 0 0 1 0, 1 oe	3968.88384	0 1 1 2 0, 0 oe	6449.09176
0 0 0 1 1, 1-1e	1328.07331	1 0 0 1 0, 1 of	3968.88384	0 0 2 0 0, 0 oe	6502.34625
0 0 0 1 1, 1-1f	1340.55083	0 0 1 0 1, 0 1e	4001.25976*	1 1 0 2 0, 0 0e	6513.99269
0 0 0 1 1, 1 1e	1342.80217	0 0 1 0 1, 0 1f	4001.25977*	1 0 1 0 0, 0 oe	6556.46473
0 0 0 1 1, 1 1f	1342.80218	0 0 1 0 1, 0 1f	4015.53618*	1 1 0 1 1, 1-1e	6623.13650
0 0 0 0 2, 0 0e	1449.11228	0 0 1 0 1, 0 1e	4015.53619*	0 2 0 1 3, 1-1e	6654.25190
0 0 0 0 2, 0 2f	1458.29367	1 0 0 0 1, 0 1e	4091.17259	0 1 1 0 2, 0 oe	6690.42425
0 0 0 0 2, 0 2e	1458.29370	1 0 0 0 1, 0 1f	4091.17259	2 0 0 0 0, 0 oe	6709.02113
0 0 0 3 0, 3 0e	1851.35850	0 1 0 0 3, 0 1f	4138.87768	1 1 0 2 0, 0 oe	6759.23936
0 0 0 3 0, 3 0f	1851.37430	0 1 0 0 3, 0 1e	4138.87771	0 0 2 1 0, 1 of	7091.28119
0 0 0 3 0, 1 0f	1854.59535	0 1 0 3 1, 3-1f	4486.11686	0 0 2 1 0, 1 0e	7091.28120
0 0 0 3 0, 1 0e	1854.60829	0 1 0 3 1, 3-1e	4486.11992	1 0 1 1 0, 1 0f	7141.50298
0 0 0 2 1, 2-1e	1939.99999	0 1 0 3 1, 1-1e	4488.83815	1 0 1 1 0, 1 oe	7141.50299
0 0 0 2 1, 2-1f	1940.00000	0 0 1 2 0, 2 0e	4504.53643	1 1 0 2 1, 2-1e	7205.95294*
0 0 0 2 1, 0 1e	1959.69158	0 0 1 2 0, 2 0f	4504.53710	1 1 0 2 1, 2-1f	7205.95294*
0 0 0 2 1, 0 1f	1959.69197	0 0 1 2 0, 0 oe	4508.01322	0 0 2 0 1, 0 1e	7218.19964
0 0 0 2 1, 2 1f	1961.93212	0 1 0 2 2, 2-2f	4599.77412	0 0 2 0 1, 0 1f	7218.19965
0 0 0 2 1, 2 1e	1961.93252	0 1 0 2 2, 2 0f	4603.27286	1 1 0 2 1, 2-1e	7228.27124*
0 1 0 0 0, 0 oe	1974.31602	0 1 0 2 2, 2 0e	4603.32430	1 1 0 2 1, 2-1f	7228.27434*
0 0 0 1 2, 1 0f	2047.87622	0 0 1 1 1, 1-1e	4609.29074	1 0 1 0 1, 0 1f	7263.90332
0 0 0 1 2, 1 0e	2047.87622	0 0 1 1 1, 1-1f	4617.92652	1 0 1 0 1, 0 1e	7263.90332
0 0 0 1 2, -1 2e	2065.79297	0 0 1 1 1, 1 1e	4620.05743	0 1 1 1 2, 1 0f	7273.77180
0 0 0 1 2, -1 2f	2065.79298	0 0 1 1 1, 1 1f	4620.05743	0 1 1 1 2, 1 0e	7273.77346
0 0 0 1 2, 1 2e	2074.18018	1 0 0 1 1, 1-1e	4673.63162	0 1 1 1 2, -1 2e	7286.10865
0 0 0 1 2, 1 2f	2074.18024	1 0 0 1 1, 1 1e	4687.36320	0 1 1 1 2, -1 2f	7286.23113
0 0 0 0 3, 0 1f	2169.15707	1 0 0 1 1, 1 1f	4687.36324	2 0 0 1 0, 1 0e	7296.38301
0 0 0 0 3, 0 1e	2169.15709	1 0 0 1 1, 1-1f	4688.83942	2 0 0 1 0, 1 0f	7296.38302
0 0 0 0 3, 0 3e	2187.45100	0 1 0 1 3, 1-1e	4710.73414	1 1 0 1 2, 1 0f	7329.34488
0 0 0 0 3, 0 3f	2187.45104	0 1 0 1 3, -1 3f	4721.12137	1 1 0 1 2, 1 0e	7329.34489
0 0 0 3 1, 3-1f	2556.79484	0 1 0 1 3, -1 3e	4721.14173	0 1 1 0 3, 0 1f	7401.26358
0 0 0 3 1, 3-1e	2556.79505	0 0 1 0 2, 0 0e	4727.04969	0 1 1 0 3, 0 1e	7401.42334
0 0 0 3 1, 1-1e	2560.59503	0 0 1 0 2, 0 2f	4736.31488	2 0 0 0 1, 0 1e	7416.40041
0 1 0 1 0, 1 oe	2573.53545	0 0 1 0 2, 0 2e	4736.31503	2 0 0 0 1, 0 1f	7416.40041
0 1 0 1 0, 1 of	2573.53545	0 0 0 0 2, 0 0e	4800.13607	1 1 0 0 3, 0 1f	7466.45310
0 0 0 3 1, 1-1f	2583.86715	1 0 0 0 2, 0 2f	4809.50961	1 1 0 0 3, 0 1e	7466.45313
0 0 0 3 1, 1 1f	2584.94806	1 0 0 0 2, 0 2e	4809.50965	0 0 2 2 0, 2 0f	7685.46991
0 0 0 3 1, 1 1e	2584.96025	0 0 1 3 0, 1 0e	5101.54938*	0 0 2 2 0, 2 0e	7685.50863
0 0 0 2 2, 2-2e	2648.01406	0 0 1 3 0, 1 0f	5101.62936*	0 0 2 2 0, 0 oe	7686.04809
0 0 0 2 2, 2-2f	2661.19038	0 0 1 3 0, 1 0f	5123.39551*	1 0 1 2 0, 2 0f	7732.35152
0 0 0 2 2, 2 0f	2661.42794	0 0 1 3 0, 1 0e	5123.39959*	1 0 1 2 0, 2 0e	7732.38358
0 0 0 2 2, 2 0e	2661.42927	0 2 0 1 1, 1-1e	5230.22853	1 0 1 2 0, 0 oe	7732.76330
0 1 0 0 1, 0 1e	2701.90945	0 1 0 0 1, 0 0e	5260.02212	0 0 2 1 1, 1-1e	7805.20079
0 1 0 0 1, 0 1f	2701.90945	1 0 0 2 1, 2-1e	5268.54595*	1 0 1 1 1, 1-1e	7834.98585
0 0 0 1 3, 1-1e	2757.79692	1 0 0 2 1, 2-1f	5268.54595*	1 0 1 1 1, 1 1e	7847.74921
0 0 0 1 3, 1 1f	2768.45032	1 0 0 2 1, 2-1e	5289.09956*	1 0 1 1 1, 1 1f	7847.74925
0 0 0 1 3, 1 1e	2768.45123	1 0 0 2 1, 2-1f	5289.10486*	1 0 1 1 1, 1-1f	7853.27591
0 0 0 1 3, -1 3e	2783.65003	1 0 0 2 1, 0 1e	5301.13135	1 0 1 0 2, 0 0e	7961.81893
0 0 0 1 3, -1 3f	2790.76333	1 0 0 2 1, 0 1f	5301.13155	1 0 1 0 2, 0 2f	7971.56573
0 0 0 1 3, -1 3f	2790.76350	1 1 0 0 0, 0 0e	5335.54888	1 0 1 0 2, 0 2e	7971.56574
0 0 0 0 4, 0 oe	2880.21891	1 0 0 1 2, 1 0f	5381.56126	2 0 0 1 1, 1-1e	7994.39439
0 0 0 0 4, 0 2f	2889.32383	1 0 0 1 2, 1 0e	5381.56127	2 0 0 1 1, 1 1e	8008.23592
0 0 0 0 4, 0 2e	2889.32524	1 0 0 0 3, 0 1f	5509.22211	2 0 0 1 1, 1 1f	8008.23597
0 0 1 0 0, 0 0e	3281.89920	1 0 0 0 3, 0 1e	5509.22214	2 0 0 0 2, 0 0e	8114.36313
0 1 0 1 1, 1-1e	3294.83960	0 2 0 2 1, 2-1e	5816.86353	2 0 0 0 2, 0 2f	8123.76168
0 1 0 1 1, 1-1f	3300.63499	0 2 0 2 1, 2-1f	5816.86354	2 0 0 0 2, 0 2e	8123.76171
0 1 0 1 1, 1 1f	3303.01742	0 1 1 1 0, 1 0f	5850.64984	1 1 1 0 0, 0 oe	8512.05644
0 1 0 1 1, 1 1e	3303.01745	0 1 1 1 0, 1 0e	5850.67614	1 2 0 1 1, 1-1e	8556.59101
	1 1 0 0 1, 0 1e	6052.07572			

* These states have the same vibrational label because they share the dominant contribution in their eigenvector composition.

The vibrational assignments correspond to those of the dominant zero order state in the eigenvector composition at low J-values and may differ from some of the previous literature.

Table 4

$$E_{vr} = G(v, l) + B_v [J(J+1) - k^2] - D_v [J(J+1) - k^2]^2 + H_v [J(J+1) - k^2]^3 \quad (1)$$

$$G(v, l) = \sum_{i=1,5} \omega_i^0 v_i + \sum_{i \leq j} x_{ij}^0 v_i v_j + \sum_{b \leq b' = 4,5} x_{lb, l'b}^0 l_b l_{b'} + \sum_{i \leq j \leq m} y_{ijm}^0 v_i v_j v_m + \sum_{i \leq j \leq b} y_{ilb, l'b}^0 v_i l_b l_{b'} + \sum_{i \leq j \leq m \leq n} z_{ijmn} v_i v_j v_m v_n + \sum_{i \leq j, b \leq b'} z_{ijl_b l_{b'}} v_i v_j l_b l_{b'} + \sum_{b \leq b' \leq b'' \leq b'''} z_{l_b l_{b'}, l_{b''} l_{b'''} l_{b''''}} \quad (2)$$

$$B_v = B_0 - \sum_i \alpha_i^0 v_i + \sum_{i \leq j} \gamma_{ij}^0 v_i v_j + \sum_{b \leq b'} \gamma_{lb, l'b}^0 l_b l_{b'} + \sum_{i \leq j \leq m} \varepsilon_{ijm} v_i v_j v_m + \sum_{i, b \leq b'} \varepsilon_{ilb, l'b}^0 v_i l_b l_{b'} \quad (3)$$

$$D_v = D_0 + \sum_i \beta_i^0 v_i + \sum_{i \leq t'} \beta_{l_t l_{t'}} l_t l_{t'} \quad (4)$$

$$H_v = H_0 \quad (5)$$

$$\langle l_4, l_5 | \tilde{H} | l_4 \mp 2, l_5 \pm 2 \rangle = \frac{1}{4} r_{45} [(v_4 \pm l_4)(v_4 \mp l_4 + 2)(v_5 \mp l_5)(v_5 \pm l_5 + 2)]^{1/2} \quad (6)$$

$$r_{45} = r_{45}^0 + \sum_i r_{45i} (v_i - \delta_{i4} - \delta_{i5}) + \sum_{i \leq j} r_{45ij} (v_i - \delta_{i4} - \delta_{i5})(v_j - \delta_{j4} - \delta_{j5}) + \sum_{b \leq b'} r_{45l_b l_{b'}} (l_b \mp 1)(l_{b'} \pm 1) + \left[r_{45J}^0 + \sum_i r_{45Ji} (v_i - \delta_{i4} - \delta_{i5}) + r_{45JJ} J(J+1) \right] J(J+1) \quad (7)$$

$$\langle l_b | \tilde{H} | l_b \pm 2 \rangle = \frac{1}{4} q_b [(v_b \mp l_b)(v_b \pm l_b + 2)]^{1/2} F_{\pm}(J, k) F_{\pm}(J, k \pm 1) \quad (8)$$

$$q_b = q_b^0 + \sum_i q_{bi} (v_i - \delta_{ib}) + \sum_{i \leq j} q_{bij} (v_i - \delta_{ib})(v_j - \delta_{jb}) + \left[q_{bj}^0 + \sum_i q_{bJi} (v_i - \delta_{ib}) \right] (J(J+1)) \quad (9)$$

$$\langle l_b | \tilde{H} | l_b \pm 4 \rangle = \frac{1}{4} u_{bb} [(v_b \mp l_b)(v_b \pm l_b + 2)(v_b \mp l_b - 2)(v_b \pm l_b + 4)]^{1/2} F_{\pm}(J, k) F_{\pm}(J, k \pm 1) F_{\pm}(J, k \pm 2) F_{\pm}(J, k \pm 3) \quad (10)$$

$$\langle l_b l_{b'} | \tilde{H} | l_b \pm 2, l_{b'} \pm 2 \rangle = \frac{1}{4} u_{bb'} [(v_b \mp l_b)(v_b \pm l_b + 2)(v_{b'} \mp l_{b'}) (v_{b'} \pm l_{b'} + 2)]^{1/2} F_{\pm}(J, k) F_{\pm}(J, k \pm 1) F_{\pm}(J, k \pm 2) F_{\pm}(J, k \pm 3) \quad (11)$$

$$F_{\pm}(J, k) = [J(J+1) - k(k \pm 1)]^{1/2} \quad (12)$$

$$\langle v_2, v_3, v_4^{l_4}, v_5^{l_5} | \tilde{H} | v_2 - 1, v_3 + 1, (v_4 - 1)^{l_4 \pm 1}, (v_5 - 1)^{l_5 \mp 1} \rangle = -\frac{1}{8} K_{3/245} [v_2(v_3 + 1)(v_4 \mp l_4)(v_5 \pm l_5)]^{1/2} \quad (13)$$

$$K_{3/245} = K_{3/245}^0 + \sum_i K_{3/245,i} (v_i - \delta_{i2} - \delta_{i4} - \delta_{i5}) + K_{3/245,J} [J(J+1) - k^2] + K_{3/245,JJ} [J(J+1) - k^2]^2 \quad (14)$$

$$\langle v_2, v_3, v_4^{l_4}, v_5^{l_5} | \tilde{H} | v_2 - 1, v_3 + 1, (v_4 - 1)^{l_4 \pm 1}, (v_5 - 1)^{l_5 \pm 1} \rangle = \frac{1}{8} O_{3/245} [v_2(v_3 + 1)(v_4 \mp l_4)(v_5 \mp l_5)]^{\frac{1}{2}} F_{\pm}(J, k) F_{\pm}(J, k \pm 1) \quad (15)$$

$$O_{3/245} = O_{3/245}^0 + \sum_i O_{3/245,i} (v_i - \delta_{i2} - \delta_{i4} - \delta_{i5}) + O_{3/245,J} [J(J+1) - k^2] \quad (16)$$

$$\langle v_4^{l_4}, v_5^{l_5} | \tilde{H} | (v_4 + 2)^{l_4}, (v_5 - 2)^{l_5} \rangle = \frac{1}{4} K_{44/55} [(v_4 - l_4 + 2)(v_4 + l_4 + 2)(v_5 + l_5)(v_5 - l_5)]^{\frac{1}{2}} \quad (17)$$

$$\langle v_4^{l_4}, v_5^{l_5} | \tilde{H} | (v_4 + 2)^{l_4 \pm 2}, (v_5 - 2)^{l_5 \mp 2} \rangle = \frac{1}{8} K'_{44/55} [(v_4 \pm l_4 + 2)(v_4 \pm l_4 + 4)(v_5 \pm l_5)(v_5 \pm l_5 - 2)]^{\frac{1}{2}} \quad (18)$$

$$\langle v_4^{l_4}, v_5^{l_5} | \tilde{H} | (v_4 + 2)^{l_4}, (v_5 - 2)^{l_5 \pm 2} \rangle = -\frac{1}{4} O_{44/55} [(v_4 - l_4 + 2)(v_4 + l_4 + 2)(v_5 \mp l_5)(v_5 \mp l_5 - 2)]^{\frac{1}{2}} F_{\pm}(J, k) F_{\pm}(J, k \pm 1) \quad (19)$$

^a In the terms, i, j, m, n refer to the five modes of vibration, b and b' specifically to the bending ones, and $k = l_4 + l_5$. The notation δ_{ij} is the usual Kronecker symbol.

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2 Table 5 (each column is to be read until the end of next page)

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Vibrational diagonal parameters		Rotational Diagonal Parameters		Vibrational 1-type Resonances	
om1	3400.22612	0.01014	B0	1176.646179	0.000010 E-03
om2	1981.89420	0.00728	alpha1	6.82175	0.00060 E-03
om3	3313.80593	0.01050	alpha2	6.16416	0.00047 E-03
om4	608.90351	0.00126	alpha3	5.88402	0.00028 E-03
om5	729.22355	0.00058	alpha4	-1.35767	0.00013 E-03
x11	-27.28251	0.01011	alpha5	-2.22723	0.00011 E-03
x12	-11.18438	0.00242	gam11	-5.15420	0.04655 E-05
x13	-104.54250	0.00127	gam12	6.32682	0.06129 E-05
x14	-14.08892	0.00479	gam13	-17.37955	0.03505 E-05
x15	-10.29553	0.00666	gam14	12.54482	0.08936 E-05
x22	-7.68364	0.01091	gam15	3.89700	0.05731 E-05
x23	-5.72482	0.00128	gam22	-1.52452	0.04697 E-05
x24	-12.50107	0.00104	gam23	7.34949	0.06735 E-05
x25	-1.44329	0.00057	gam24	-7.36584	0.03077 E-05
x33	-25.42248	0.01032	gam25	-5.74927	0.03510 E-05
x34	-9.32073	0.00210	gam34	4.71773	0.04126 E-05
x35	-9.62852	0.00784	gam35	2.48772	0.04763 E-05
x44	3.17877	0.00123	gam44	-0.51993	0.00458 E-05
x45	-2.41630	0.00034	gam45	-2.10716	0.00827 E-05
x55	-2.44012	0.00030	gam55	2.50468	0.00610 E-05
x1414	0.82187	0.00106	g1414	-6.46863	0.00989 E-05
x1415	6.54721	0.00017	g1415	-22.16748	0.01337 E-05
x1515	3.54235	0.00034	g1515	-10.97365	0.01015 E-05
y115	-0.64570	0.00703	eps114	0.28426	0.04476 E-05
y122	-0.19599	0.00237	eps115	-0.91760	0.02434 E-05
y123	-0.49462	0.00280	eps123	1.19413	0.08972 E-05
y124	0.05701	0.00156	eps124	0.66487	0.05490 E-05
y125	0.22653	0.00100	eps125	-0.52958	0.04393 E-05
y134	-0.46045	0.00279	eps134	0.75996	0.04850 E-05
y135	0.08797	0.00323	eps144	-1.55844	0.02705 E-05
y144	0.23732	0.00584	eps145	0.37142	0.02252 E-05
y145	-0.05915	0.00111	eps155	0.13428	0.01097 E-05
y155	0.06643	0.00110	eps225	0.19719	0.02874 E-05
y222	0.10546	0.00363	eps234	-0.57474	0.06338 E-05
y224	-0.24015	0.00092	eps235	-0.84037	0.05832 E-05
y225	-0.09290	0.00010	eps244	0.16461	0.01264 E-05
y235	0.04984	0.00472	eps245	0.41321	0.02226 E-05
y244	0.40306	0.00054	eps345	0.34370	0.03753 E-05
y245	-0.09189	0.00051	eps355	0.19841	0.02011 E-05
y255	-0.07383	0.00046	eps445	-0.09312	0.00369 E-05
y334	-0.30901	0.00157	eps555	0.01010	0.00097 E-05
y335	0.68490	0.00754	eps1144	0.36360	0.03332 E-05
y344	0.05800	0.00115	eps1155	-0.26861	0.00860 E-05
y345	0.19598	0.00383	eps2144	-0.14300	0.01708 E-05
y355	0.04761	0.00350	eps2145	-0.28981	0.01905 E-05
y444	0.03278	0.00045	eps2155	-0.27376	0.02094 E-05
y445	0.09288	0.00025	eps3144	0.16320	0.02311 E-05
y455	0.03987	0.00029	eps3145	-0.26333	0.03508 E-05
y555	0.01110	0.00003	eps3155	-0.28449	0.01748 E-05
y11414	-0.17993	0.00143	eps4144	0.09026	0.00335 E-05
y11415	-0.23524	0.00082	eps4145	0.11413	0.00867 E-05
y11515	-0.02367	0.00058	eps5144	-0.16342	0.00676 E-05
y21414	-0.14961	0.00059	eps5145	-0.57513	0.00728 E-05
y21415	0.00344	0.00028	eps5155	-0.18770	0.00342 E-05
y21515	0.03983	0.00040	D0	1.626551	0.000010 E-06
y31414	0.02427	0.00054	beta1	-1.41610	0.00891 E-08
y31415	0.02123	0.00062	beta2	0.19777	0.01470 E-08
y31515	0.04506	0.00030	beta3	-1.36722	0.01320 E-08
y41414	-0.07400	0.00086	beta4	3.44008	0.00779 E-08
y41415	0.05956	0.00052	beta5	2.59377	0.00599 E-08
y41515	0.00378	0.00040	beta44	-17.23166	0.58604 E-10
y51414	-0.00159	0.00039	beta45	-39.49707	0.73611 E-10
y51415	-0.00265	0.00057	beta55	-14.88397	0.55211 E-10
y51515	-0.00385	0.00006	H0	1.18184	0.03950 E-12
Rotational 1-type Resonances		Anharmonic Resonances			
z1244	0.01718	0.00110	k1244	11.85007	0.01332
z1444	-0.02094	0.00213	k1244v1	2.92736	0.01602
z1555	-0.002651	0.000056	k1244v2	0.20432	0.01661
z2244	0.01417	0.00033	k1244v3	0.98797	0.02337
z2245	0.01109	0.00043	k1244v4	-0.25193	0.00492
z2355	0.04697	0.00246	k1244v5	-0.35600	0.00672
z2444	-0.00400	0.00016	k1244J	-15.23256	0.29161 E-05
z2445	0.01064	0.00039	k1245	7.82628	0.00571
z2455	-0.01171	0.00024	k1255	0.14456	0.00689
z2555	0.00321	0.00010	k1255v1	-0.10118	0.00337
z1155	-0.03310	0.00065	k1255v5	-0.08315	0.00163
z1244	0.01718	0.00110	k1255J	-4.32646	0.16747 E-05
z1444	-0.02094	0.00213	k3245	-18.30048	0.00007
z1555	-0.002651	0.000056	k3245v1	-1.02383	0.02115
z2244	0.01417	0.00033	k3245v2	0.24411	0.00538
z2245	0.01109	0.00043	k3245v3	-0.35927	0.01186
z2355	0.04697	0.00246	k3245v4	0.13263	0.00060
z2444	-0.00400	0.00016	k3245v5	0.20802	0.00034
z2445	0.01064	0.00039	k1133	23.93258	0.09290 E-05
z2455	-0.01171	0.00024	k1133v4	4.1016	0.01175
z2555	0.00321	0.00010	k1133v5	-3.21907	0.04358
z1155	-0.03310	0.00065	k1133J	-21.00477	0.28080 E-05
z1244	0.01718	0.00110	k1435	31.73793	0.01461
z1444	-0.02094	0.00213	k1435v1	3.06397	0.02510
z1555	-0.002651	0.000056	k1435v2	-2.14201	0.01660
q4	-5.230424	0.000066	k1435v3	-4.02053	0.01907
q4v1	-0.02074	0.00030	k1435v5	0.11023	0.00735
q4v2	-0.02406	0.00025	k1435J	-36.03201	0.26893 E-05
q4v3	-0.02557	0.00107	k1435	-9.05463	0.04030 E-05
q4v4	0.01140	0.00012	k1534	35.06790	0.04141
q4v5	-0.06441	0.00022	k1534v1	2.35087	0.04264
q4v14	-3.62033	0.04919	k1534v2	-2.13781	0.02610
q4v23	-1.46612	0.05679	k1534v3	-4.98501	0.04034

z3344	-0.01993	0.00046	q4v24	0.64660	0.02781	E-05	k1534v4	0.08935	0.01338
z3444	-0.00503	0.00031	q4v25	0.34237	0.04928	E-05	k1534v5	-0.78033	0.02186
z3455	-0.08792	0.00316	q4v33	0.46485	0.09164	E-05	k1534J	-37.16915	0.71311 E-05
z3555	-0.03107	0.00111	q4v44	-0.01907	0.00458	E-05	o1534	-9.82520	0.09458 E-05
z4444	-0.003576	0.000060	q4v55	-0.39319	0.01280	E-05	k4455	-8.57758	0.00378
z4445	-0.002867	0.000015	q4J	3.87785	0.00855	E-08	k4455v1	-1.27134	0.02881
z4455	-0.00566	0.00015	q4v1	-0.14985	0.03279	E-08	k4455v2	-0.35485	0.00707
z121515	-0.02480	0.00043	q4Jv4	0.04438	0.00840	E-08	k4455v3	-1.46397	0.00975
z221414	-0.00570	0.00031	q4Jv5	0.010182	0.01411	E-08	k4455v5	0.09946	0.00130
z2241414	0.00269	0.00022	q5	-4.698406	0.000055	E-03	k4455J	18.01478	0.13423 E-05
z341414	-0.02841	0.00026	q5v1	-0.04409	0.00037	E-03	kp4455	4.88246	0.02540
z441414	0.00938	0.00020	q5v2	0.003368	0.000095	E-03	kp4455v1	-0.29289	0.01767
z451414	0.002008	0.000074	q5v4	-0.11244	0.00021	E-03	kp4455v3	0.50071	0.01716
z14444	0.002975	0.000068	q5v5	-0.04289	0.00011	E-03	kp4455v5	-0.03025	0.00379
z14555	0.000605	0.000031	q5v11	-0.48343	0.02039	E-05	kp4455J	-6.80235	0.19095 E-05
z15555	-0.000081	0.000002	q5v14	-1.14897	0.04477	E-05	o4455	3.92494	0.09334 E-05

The parameters are labeled in agreement with the model defined in the text. They are listed as printed by the program.

Table 6

Accuracy	$\leq 4 \times 10^{-4} \text{ cm}^{-1}$	$\leq 9 \times 10^{-4} \text{ cm}^{-1}$	$\leq 2 \times 10^{-3} \text{ cm}^{-1}$	$\leq 10^{-2} \text{ cm}^{-1}$	Total
Lines fitted	6513	1699	1525	1013	10750
Fraction	60.59%	15.80%	14.19%	9.42%	100%

Table 7

	$^{12}\text{C}_2\text{H}_2$	$^{13}\text{CH}^{12}\text{CH}$		$^{12}\text{C}_2\text{H}_2$	$^{13}\text{CH}^{12}\text{CH}$
x14	-14.09	-13.50	Alpha1 (E-03)	6.82	6.52
x15	-10.29	-10.88	Alpha2 (E-03)	6.16	5.98
x22	-7.68	-7.15	Alpha3 (E-03)	5.88	5.55
x23	-5.72	-5.21	Alpha4 (E-03)	-1.36	-1.19
x24	-12.50	-12.45	Alpha5 (E-03)	-2.23	-2.07
x25	-1.44	-1.54	K1244	11.85	10.92
x33	-25.42	-26.99	K1255	7.83	7.00
x34	-9.32	-9.61	K3245	-18.30	-17.24
x35	-9.63	-8.89	O3245 (E-05)	6.55	6.46
x44	3.18	3.11	K1435	31.74	30.79
x45	-2.42	-2.35	O1435 (E-05)	-9.05	-20.73
x55	-2.44	-2.42	K1534	35.07	36.07
xI4I4	0.82	0.76	K4455	-8.58	-8.61
xI4I5	6.55	6.54	O4455 (E-05)	3.92	16.35
xI5I5	3.54	3.53	Kp4455	4.88	4.70

Table 8

	$^{12}\text{C}_2\text{H}_2^{\text{VR}}$	$^{12}\text{C}_2\text{H}_2^{\text{V}}$	$^{13}\text{CH}^{12}\text{CH}^{\text{VR}}$	$^{13}\text{CH}^{12}\text{CH}^{\text{V}}$	$^{13}\text{C}_2\text{H}_2^{\text{V}}$	$^{12}\text{C}_2\text{D}_2^{\text{V}}$
x_{11}	-27.2	-24.8	-27.3	-27.0	-25.4	-12.3
x_{33}	-25.4	-27.6	-27.0	-27.6	-26.7	-15.4
x_{13}	-104.5	-107.5	-101.3	-105.8	-104.3	-47.5
$K_{11/33}$	-113.5	-105.7	-111.4	-111.4	-103.4	-47.2

Constants are from: $^{12}\text{C}_2\text{H}_2^{\text{VR}}$, this work; $^{12}\text{C}_2\text{H}_2^{\text{V}}$, Idrissi *et al.*⁴³; $^{13}\text{CH}^{12}\text{CH}^{\text{VR}}$, Fayt *et al.*⁹; $^{13}\text{CH}^{12}\text{CH}^{\text{V}}$, Robert *et al.*⁴⁶; $^{13}\text{C}_2\text{H}_2^{\text{V}}$, Di Lonardo *et al.*⁴⁴; $^{12}\text{C}_2\text{D}_2^{\text{V}}$, Herman *et al.*⁴².

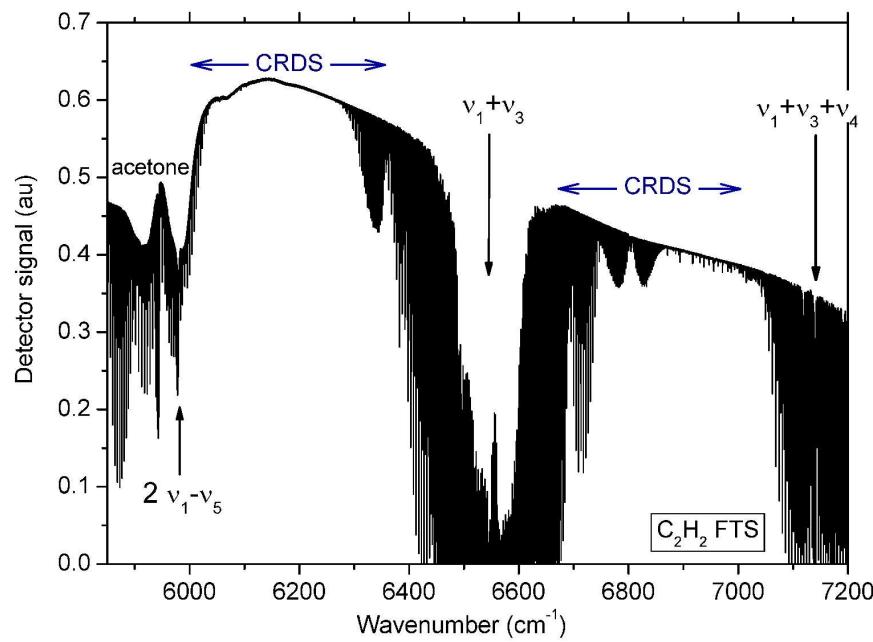


Fig. 1

297x209mm (300 x 300 DPI)

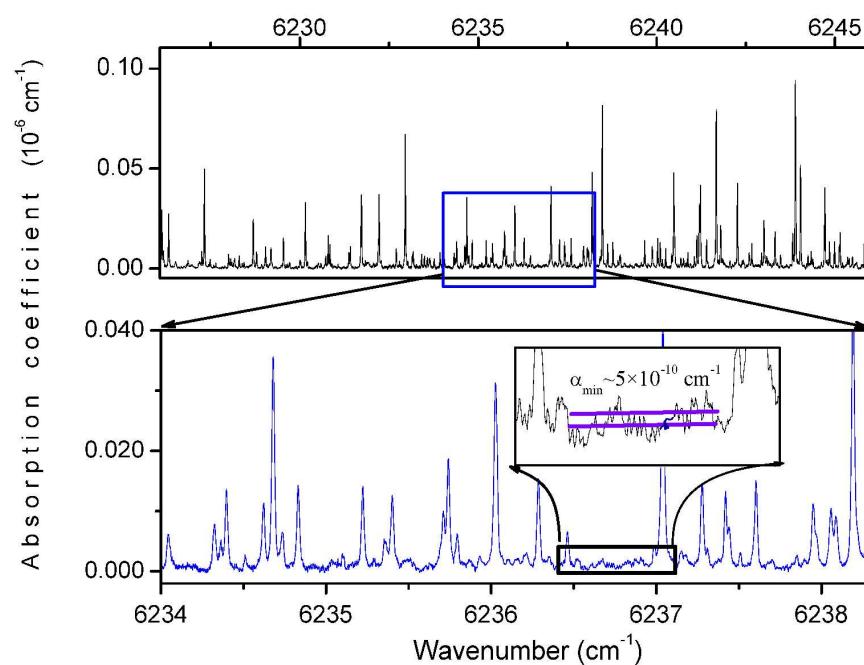
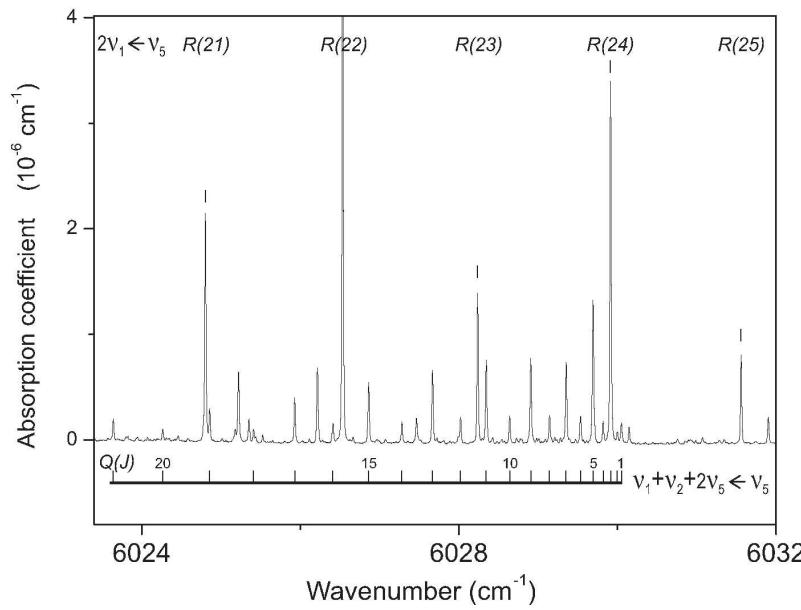
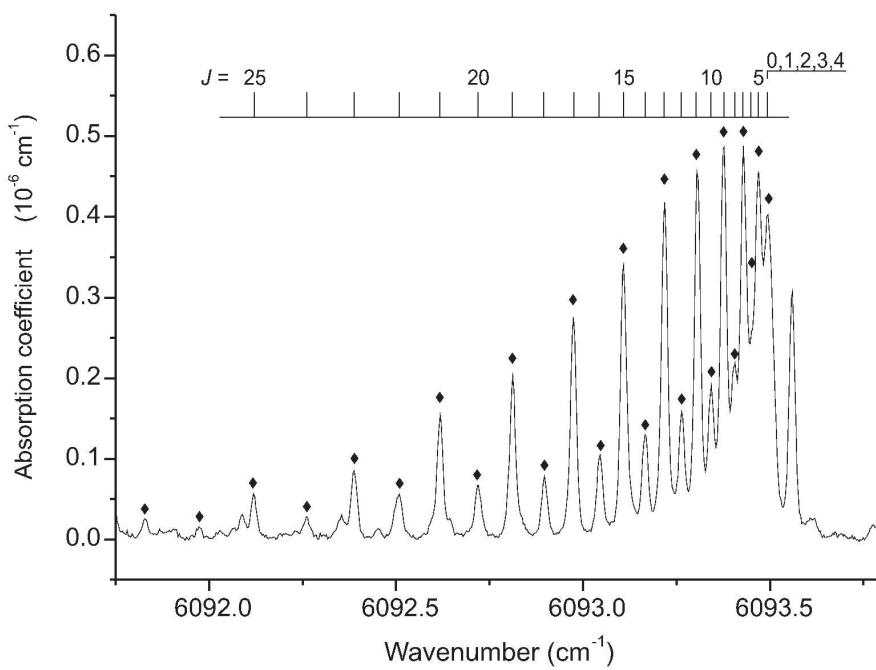


Fig. 2

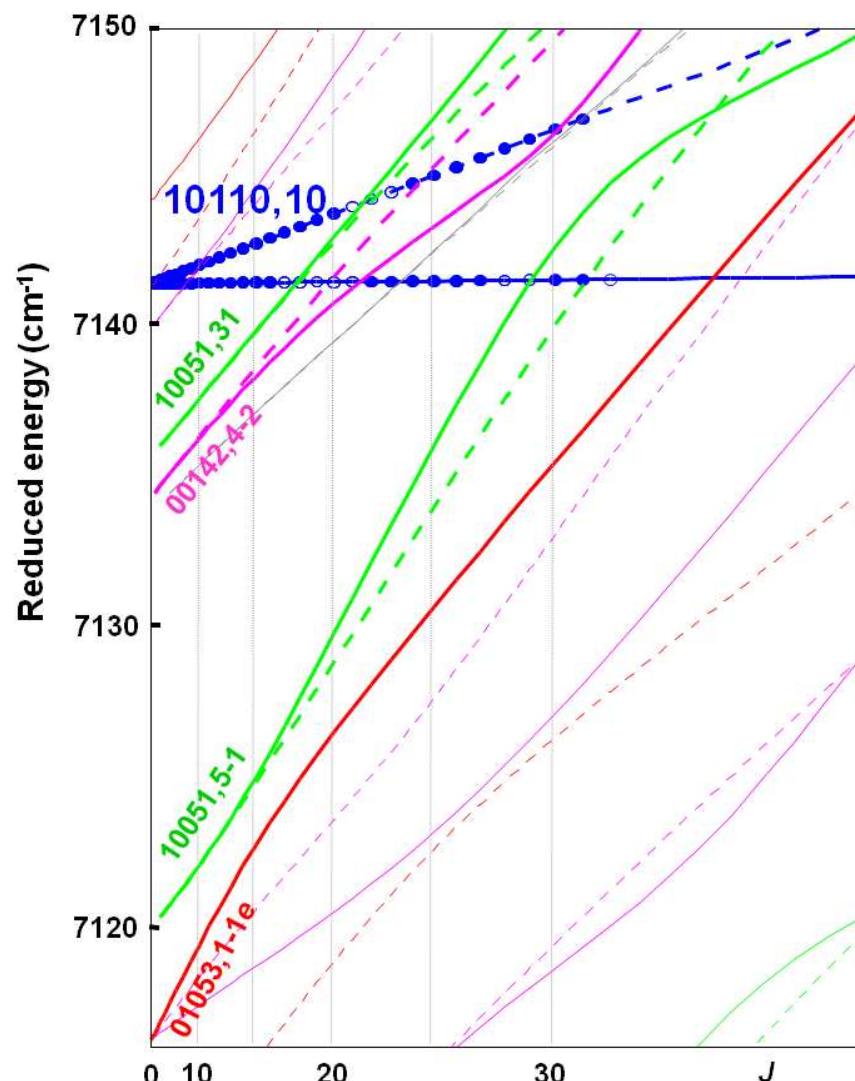
297x209mm (300 x 300 DPI)



297x209mm (300 x 300 DPI)



297x209mm (300 x 300 DPI)



190x254mm (96 x 96 DPI)

Molecular Physics: Supplementary Materials (29 pp) for the paper

Acetylene, $^{12}\text{C}_2\text{H}_2$: New CRDS data and global vibration-rotation analysis up to 8600 cm^{-1}

by

S. Robert, M. Herman, A. Fayt, A. Campargue, S. Kassi, A. Liu, L. Wang, G. Di Lonardo, and L. Fusina

Table of the bands newly reported from CRDS spectra (rob08), or including updated information with respect to the literature (kep96).

Assignment, experimental line wavenumbers (cm^{-1}), uncertainties (in unit of 10^{-3} cm^{-1}), observed-calculated values from the global fit procedure (in unit of 10^{-3} cm^{-1}) are provided.

(kep96): K. A. Keppler, G. C. Mellau, S. Klee, B. P. Winnewisser, M. Winnewisser, J. Plíva, and K. N. Rao, *J. Mol. Spectrosc.* **175**, 411 (1996).

(rob08): This work

(v_{sup})	$-$	(v_{inf})			
$v_1 v_2 v_3 v_4 v_5, l_4 l_5 e/f$	$-$	$v_1 v_2 v_3 v_4 v_5, l_4 l_5 e/f$			
J_{sup}	J_{inf}	$\tilde{\nu}_{\text{exp}}$	unc.	obs-calc	ref

1 1 0 0 1,	0 1e -	0 0 0 0 0,	0 0e		
3 2 6058.97591	0.90	-1.51	rob08		
4 3 6061.22752	0.0	2.38	rob08		
5 4 6063.44578	0.90	-0.59	rob08		
6 5 6065.64183	0.90	0.77	rob08		
7 6 6067.80822	0.90	-0.97	rob08		
8 7 6069.94999	0.90	-0.71	rob08		
9 8 6072.06539	0.90	-0.17	rob08		
10 9 6074.15383	0.90	0.10	rob08		
11 10 6076.21437	0.90	-0.79	rob08		
12 11 6078.25094	0.90	1.12	rob08		
13 12 6080.25679	0.90	-0.88	rob08		
14 13 6082.23784	0.90	-0.82	rob08		
15 14 6084.19240	0.90	-0.35	rob08		
16 15 6086.11963	0.90	-0.27	rob08		
17 16 6088.01995	0.90	-0.12	rob08		
18 17 6089.89309	0.90	-0.13	rob08		
19 18 6091.73890	0.90	-0.40	rob08		
20 19 6093.55914	0.90	0.86	rob08		
21 20 6095.35221	0.0	2.09	rob08		
22 21 6097.11498	0.90	0.20	rob08		
23 22 6098.85154	0.90	-0.66	rob08		
24 23 6100.56348	0.90	1.11	rob08		
25 24 6102.24472	0.90	-0.50	rob08		
26 25 6103.90071	0.90	-0.02	rob08		
27 26 6105.52791	0.90	-0.94	rob08		
28 27 6107.12924	0.90	-0.30	rob08		
29 28 6108.70111	0.90	-1.65	rob08		
30 29 6110.24687	0.90	-1.61	rob08		

1 1 0 0 1,	0 1f -	0 0 0 0 0,	0 0e		
1 1 6052.05776	0.70	-1.39	rob08		
2 2 6052.02657	0.70	0.56	rob08		
3 3 6051.97660	0.70	0.30	rob08		
4 4 6051.90904	0.70	-0.97	rob08		
5 5 6051.82618	0.70	-0.96	rob08		
6 6 6051.72780	0.70	0.14	rob08		
7 7 6051.61096	0.70	-0.62	rob08		
8 8 6051.47822	0.70	-0.66	rob08		
9 9 6051.32920	0.70	-0.34	rob08		
10 10 6051.16482	0.70	1.28	rob08		
11 11 6050.98053	0.70	-0.33	rob08		
12 12 6050.78204	0.70	0.54	rob08		
13 13 6050.56611	0.70	0.70	rob08		
14 14 6050.33260	0.70	0.01	rob08		
15 15 6050.08327	0.70	0.27	rob08		
16 16 6049.81547	0.70	-1.15	rob08		
17 17 6049.53397	0.70	0.55	rob08		
18 18 6049.23385	0.70	0.47	rob08		
19 19 6048.91304	0.0	-3.42	rob08		
20 20 6048.58199	0.70	-0.64	rob08		
21 21 6048.23229	0.70	0.43	rob08		
23 23 6047.47962	0.70	0.25	rob08		

1 0 0 1 3, 1 -1e - 0 0 0 0 0, 0 0e

1
 2
 3 0 1 6077.33968 2.00 1.00 rob08
 4 1 0 6082.05301 2.00 2.77 rob08
 5 1 2 6074.99282 2.00 2.40 rob08
 6 2 1 6084.41406 2.00 0.79 rob08
 7 2 3 6072.64910 2.00 2.06 rob08
 8 3 2 6086.79881 0.0 18.15 rob08
 9 3 4 6070.30978 2.00 1.57 rob08
 10 4 3 6089.15383 2.00 2.00 rob08
 11 4 5 6067.97486 2.00 1.43 rob08
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 13 5 6 6065.64261 2.00 0.60 rob08
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58 12 11 6388.39799 0.40 -0.01 kep96
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60 13 12 6390.41961 0.40 0.10 kep96
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20	21	6307.46499	0.0	7.97	kep96
21	20	6405.64762	0.0	32.54	kep96
21	22	6304.60367	0.0	32.64	kep96
22	21	6407.37057	0.0	-18.67	kep96
22	23	6301.64553	0.0	-12.84	kep96
23	22	6409.13093	0.0	-3.88	kep96
23	24	6298.71487	0.0	-4.03	kep96
24	23	6410.85101	0.40	-0.59	kep96
24	25	6295.75177	0.0	-0.71	kep96
25	24	6412.54033	0.40	0.95	kep96
25	26	6292.76002	0.40	1.06	kep96
26	27	6289.73813	2.00	-0.06	rob08
27	26	6415.83291	0.0	5.87	kep96
27	28	6286.69682	0.0	6.76	kep96
28	29	6283.63319	0.0	18.79	rob08
29	30	6280.50469	0.0	-6.37	rob08
30	31	6277.38056	2.00	0.64	rob08
31	32	6274.22436	2.00	3.56	rob08
32	33	6271.04127	0.0	7.71	rob08
33	34	6267.77779	0.0	-40.24	rob08
34	35	6264.58543	0.0	11.38	rob08
35	36	6261.31552	0.0	14.07	rob08

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6	5	6375.88423	0.40	-0.07	kep96
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7	6	6378.10638	0.40	0.03	kep96
7	8	6342.67759	0.40	-0.29	kep96
8	7	6380.30745	0.40	-0.14	kep96
8	9	6340.15698	0.40	-0.15	kep96
9	10	6337.61591	0.40	-0.06	kep96
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10	11	6335.05415	0.40	-0.01	kep96
11	10	6386.78325	0.40	-0.21	kep96
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12	13	6329.86783	0.40	0.19	kep96
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13	14	6327.24233	0.40	-0.07	kep96
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18	17	6401.10490	0.40	0.52	kep96
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19	18	6403.05474	0.40	0.17	kep96
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20	19	6404.98109	0.0	1.39	kep96
20	21	6308.24297	0.0	1.45	kep96
21	20	6406.87781	0.0	-1.58	kep96
21	22	6305.43277	0.0	-1.57	kep96
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22	23	6302.60244	0.40	-0.62	kep96
23	22	6410.59881	0.0	-2.16	kep96
23	24	6299.74705	0.40	-0.35	kep96
24	23	6412.42173	0.40	-0.41	kep96
24	25	6296.86668	0.40	-0.41	kep96

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 4 25 26 6293.96146 0.40 -0.39 kep96
 5 26 25 6415.98538 0.0 1.92 kep96
 6 26 27 6291.03064 0.0 -0.78 kep96
 7 27 26 6417.72360 0.40 0.67 kep96
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 9 28 27 6419.43606 0.0 1.57 kep96
 10 28 29 6285.09406 0.40 0.14 kep96
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 28 6 5 6630.39432 0.0 2.99 kep96
 29 6 7 6599.83786 0.0 1.26 kep96
 30 7 6 6632.64070 0.0 -7.84 rob08
 31 7 8 6597.39519 0.40 0.73 kep96
 32 8 7 6634.89483 0.40 0.22 kep96
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 34 9 8 6637.12958 0.40 -0.06 kep96
 35 10 9 6639.35296 0.40 -0.44 kep96
 36 10 11 6589.99654 0.0 -8.58 rob08
 37 11 10 6641.56502 0.40 -0.46 kep96
 38 11 12 6587.52020 0.40 -0.49 kep96
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 7 18 17 6712.88346 1.60 -0.97 rob08
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 9 20 19 6716.71621 1.60 -1.98 rob08
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 12 23 22 6722.33785 0.0 -5.87 rob08
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 16 27 26 6858.67633 2.00 -0.91 rob08
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 42 12 12 6803.53008 1.20 0.54 rob08
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 44 14 14 6803.11983 1.20 -1.96 rob08
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 46 16 16 6802.65390 1.20 0.45 rob08

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3 18 18 6798.67853 1.00 -0.17 rob08

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9 3 2 6861.78386 1.00 0.66 rob08
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19 8 7 6873.28470 1.00 0.71 rob08
20 8 9 6833.15231 1.00 -1.20 rob08
21 9 8 6875.55194 1.00 0.43 rob08
22 9 10 6830.70206 1.00 -0.03 rob08
23 10 9 6877.81008 1.00 2.57 rob08
24 10 11 6828.23981 1.00 -0.11 rob08
25 11 10 6880.05218 1.00 0.55 rob08
26 11 12 6825.76698 1.00 0.27 rob08
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57 27 26 6913.87510 1.00 -0.18 rob08
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59 28 29 6781.54430 1.00 0.25 rob08

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53 2 3 6847.64940 1.60 -0.33 rob08
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59 5 6 6840.36648 1.60 -0.40 rob08
60 6 5 6868.45537 1.60 0.09 rob08

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 3 6 7 6837.90036 1.60 -0.19 rob08
 4 7 6 6870.66842 1.60 -0.37 rob08
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 7 8 9 6832.90930 1.60 0.08 rob08
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 9 9 10 6830.38540 1.60 1.44 rob08
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 19 14 15 6817.45287 1.60 -1.72 rob08
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 28 19 18 6895.57611 1.60 -1.82 rob08
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 30 20 19 6897.50792 1.60 0.98 rob08
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 32 21 20 6899.40994 1.60 -1.95 rob08
 33 21 22 6798.46378 1.60 -0.85 rob08
 34 22 21 6901.29051 1.60 -1.93 rob08
 35 22 23 6795.66193 1.60 -1.02 rob08
 36 23 22 6903.14627 1.60 -2.04 rob08
 37 23 24 6792.83659 1.60 -1.74 rob08
 38 24 23 6904.97740 1.60 -1.78 rob08
 39 24 25 6789.98926 1.60 -1.31 rob08
 40 25 24 6906.78411 1.60 -0.65 rob08
 41 25 26 6787.11771 1.60 -1.73 rob08
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 44 27 26 6910.31435 0.0 -4.62 rob08

45 1 1 0 0 3, 0 1e - 0 0 0 1 0, 1 0e
 46 1 1 6854.76329 2.00 3.34 rob08

47 1 1 0 0 3, 0 1e - 0 0 0 1 0, 1 0f
 48 1 1 6854.73341 1.40 3.80 rob08
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 51 4 4 6854.46091 1.40 -0.71 rob08
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 56 9 9 6853.41338 1.40 -0.06 rob08
 57 10 10 6853.11175 1.40 -0.50 rob08

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 59 3 4 6333.09009 2.00 -1.03 rob08
 60 4 5 6330.62667 2.00 -1.86 rob08
 61 5 4 6354.08678 0.40 0.48 kep96
 62 5 6 6328.13225 0.0 2.40 kep96
 63 6 5 6356.26651 0.40 -0.93 kep96
 64 6 7 6325.59206 0.40 0.47 kep96
 65 7 6 6358.40889 0.0 1.50 kep96
 66 7 8 6323.01269 0.40 0.56 kep96
 67 8 7 6360.50606 0.40 0.12 kep96

8	9	6320.39811	0.0	6.86	kep96
9	8	6362.56630	0.0	2.73	kep96
9	10	6317.73254	0.0	3.11	kep96
10	9	6364.59119	0.0	10.40	kep96
10	11	6315.03446	0.0	7.28	kep96
11	10	6366.53495	0.0	-23.03	kep96
11	12	6312.26170	0.0	-23.18	kep96
12	11	6368.48882	0.0	-6.46	kep96
12	13	6309.49572	0.0	-6.94	kep96
13	12	6370.38589	0.0	-6.71	kep96
13	14	6306.67547	0.0	-5.00	kep96
14	15	6303.81282	2.00	-5.23	rob08
15	16	6300.90919	2.00	-5.86	rob08

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2	3	6335.52367	0.40	-0.58	kep96
3	4	6333.09761	2.00	-2.59	rob08
4	3	6351.89030	0.40	-0.22	kep96
4	5	6330.65459	0.40	-0.08	kep96
5	4	6354.14128	0.40	-0.54	kep96
5	6	6328.18845	0.40	0.84	kep96
6	5	6356.37215	0.40	1.05	kep96
6	7	6325.69812	0.40	-0.86	kep96
8	9	6320.65657	0.40	-0.07	kep96
9	8	6362.92570	0.40	0.49	kep96
9	10	6318.10271	0.40	-0.03	kep96
10	9	6365.06513	0.40	0.43	kep96
10	11	6315.52693	0.40	0.08	kep96
11	10	6367.18053	0.40	-0.71	kep96
11	12	6312.92949	0.40	0.66	kep96
12	11	6369.27499	0.40	0.40	kep96
13	14	6307.66664	0.40	0.83	kep96
14	13	6373.39132	0.40	0.55	kep96
14	15	6305.00102	0.40	0.55	kep96
15	14	6375.41219	0.40	-0.92	kep96
15	16	6302.31300	0.40	0.63	kep96
16	15	6377.41084	0.40	-0.41	kep96
16	17	6299.60209	0.40	0.80	kep96
17	16	6379.38477	0.40	-0.19	kep96
17	18	6296.86668	0.40	-0.40	kep96
18	19	6294.11014	0.40	0.61	kep96
19	18	6383.25806	0.40	0.13	kep96
19	20	6291.32803	0.40	-0.42	kep96
20	19	6385.15714	0.40	0.45	kep96
20	21	6288.52436	0.40	0.71	kep96
21	22	6285.69470	0.40	-0.26	kep96
22	23	6282.84227	0.40	0.12	kep96
23	24	6279.96461	0.40	-0.45	kep96
24	25	6277.06192	0.0	-1.59	kep96
25	26	6274.13485	2.00	-2.44	rob08
26	27	6271.18353	2.00	-2.71	rob08
27	28	6268.21123	2.00	1.05	rob08
28	29	6265.19587	0.0	-13.06	rob08

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1	1	6956.90016	2.00	-0.17	rob08
2	2	6956.85428	2.00	0.24	rob08
3	3	6956.78798	2.00	-0.78	rob08
4	4	6956.70822	2.00	-0.64	rob08
5	5	6956.61836	2.00	-0.40	rob08
6	6	6956.52169	2.00	0.15	rob08
7	7	6956.41879	2.00	0.40	rob08
8	8	6956.31342	2.00	4.45	rob08
9	9	6956.19402	2.00	1.81	rob08
10	10	6956.06849	2.00	1.58	rob08
11	11	6955.93338	2.00	1.41	rob08
12	12	6955.78445	2.00	-2.01	rob08
13	13	6955.63176	2.00	2.16	rob08
14	14	6955.46147	2.00	0.74	rob08

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2						
3	15	15	6955.28085	2.00	1.57	rob08
4	16	16	6955.08740	2.00	2.65	rob08
5	17	17	6954.87794	2.00	1.28	rob08
6	18	18	6954.65611	2.00	1.53	rob08
7	19	19	6954.42587	0.0	7.76	rob08
8	20	20	6954.17045	2.00	3.60	rob08
9	21	21	6953.90045	2.00	0.01	rob08
10	22	22	6953.61181	0.0	-6.70	rob08
11	23	23	6953.31904	2.00	-1.69	rob08
12	24	24	6953.00606	2.00	-0.69	rob08
13	25	25	6952.67448	2.00	-1.78	rob08
14	26	26	6952.32610	0.0	-2.83	rob08
15	27	27	6951.96261	2.00	-1.84	rob08
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17	0	0	2	2	0,	0e - 0 0 0 0 1, 0 1e
18	0	1	6954.57196	1.40	0.52	rob08
19	1	2	6952.20428	1.40	0.27	rob08
20	2	1	6961.58856	1.40	0.62	rob08
21	2	3	6949.82298	1.40	-0.78	rob08
22	3	2	6963.90302	1.40	-0.58	rob08
23	3	4	6947.43350	1.40	-0.52	rob08
24	4	3	6966.21321	1.40	-0.71	rob08
25	4	5	6945.03867	1.40	-0.55	rob08
26	5	4	6968.52314	1.40	-0.13	rob08
27	5	6	6942.64347	1.40	-0.32	rob08
28	6	5	6970.83380	1.40	-0.89	rob08
29	6	7	6940.25023	1.40	-0.64	rob08
30	7	6	6973.14888	1.40	-0.44	rob08
31	7	8	6937.86194	1.40	0.27	rob08
32	8	7	6975.46773	1.40	0.96	rob08
33	8	9	6935.47717	1.40	1.30	rob08
34	9	8	6977.78816	1.40	2.23	rob08
35	9	10	6933.09313	1.40	0.67	rob08
36	10	9	6980.10694	1.40	1.38	rob08
37	10	11	6930.71285	1.40	2.60	rob08
38	11	10	6982.42615	1.40	1.65	rob08
39	11	12	6928.32979	1.40	1.61	rob08
40	12	11	6984.73702	0.0	-4.76	rob08
41	12	13	6925.94652	1.40	1.18	rob08
42	13	12	6987.05974	1.40	3.18	rob08
43	13	14	6923.56356	1.40	2.57	rob08
44	14	13	6989.37066	1.40	2.52	rob08
45	14	15	6921.17524	1.40	0.75	rob08
46	15	14	6991.67462	1.40	-1.28	rob08
47	15	16	6918.78628	1.40	0.98	rob08
48	<hr/>					
49	0	0	2	2	0,	2 0e - 0 0 0 0 1, 0 1e
50	2	1	6960.97393	1.80	-1.59	rob08
51	2	3	6949.21128	1.80	-0.06	rob08
52	3	2	6963.27674	1.80	-0.55	rob08
53	3	4	6946.79913	0.0	-8.58	rob08
54	4	3	6965.55272	1.80	-1.89	rob08
55	4	5	6944.37850	1.80	-1.41	rob08
56	5	4	6967.80029	1.80	-2.61	rob08
57	5	6	6941.92391	1.80	0.49	rob08
58	6	5	6970.01912	1.80	0.30	rob08
59	6	7	6939.43420	1.80	-0.80	rob08
60	7	6	6972.20143	1.80	0.47	rob08

13	12	6984.60656	1.80	-4.66	rob08
13	14	6921.11088	1.80	-4.77	rob08
14	13	6986.56813	1.80	-3.25	rob08
14	15	6918.37293	1.80	-4.80	rob08
15	14	6988.49827	1.80	-3.12	rob08
15	16	6915.60712	1.80	-3.68	rob08
16	15	6990.39742	1.80	-3.89	rob08
16	17	6912.81185	1.80	-3.14	rob08
17	16	6992.26816	1.80	-2.98	rob08
17	18	6909.98797	1.80	-2.41	rob08
18	17	6994.10353	0.0	-7.31	rob08
18	19	6907.13494	1.80	-2.07	rob08

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2	1	6960.96809	1.20	0.25	rob08
2	3	6949.15659	1.20	-0.09	rob08
3	2	6963.25791	1.20	0.34	rob08
3	4	6946.72041	1.20	-1.81	rob08
4	3	6965.52429	1.20	1.35	rob08
4	5	6944.26289	1.20	-0.81	rob08
5	4	6967.76384	1.20	0.00	rob08
5	6	6941.78035	1.20	-0.70	rob08
6	5	6969.98007	1.20	-0.06	rob08
6	7	6939.27484	1.20	0.60	rob08
7	6	6972.16863	1.20	-3.03	rob08
7	8	6936.74051	1.20	-2.68	rob08
8	7	6974.33697	1.20	-1.28	rob08
8	9	6934.18681	1.20	-0.99	rob08
9	8	6976.48009	1.20	0.38	rob08
9	10	6931.60382	0.0	-4.14	rob08
10	9	6978.59451	1.20	-1.34	rob08
10	11	6929.00415	1.20	0.58	rob08
11	10	6980.68811	1.20	1.65	rob08
11	12	6926.37340	1.20	-1.08	rob08
12	11	6982.75112	1.20	-0.19	rob08
12	13	6923.72019	1.20	-0.37	rob08
13	12	6984.78853	1.20	-1.64	rob08
13	14	6921.04197	1.20	0.32	rob08
14	13	6986.80298	1.20	0.18	rob08
14	15	6918.33738	1.20	-0.20	rob08
15	14	6988.78790	1.20	-1.05	rob08
15	16	6915.60712	1.20	-1.08	rob08
16	15	6990.74823	1.20	-0.14	rob08
16	17	6912.85316	1.20	-0.17	rob08
17	16	6992.67759	1.20	-3.21	rob08
17	18	6910.07230	1.20	-0.50	rob08
18	17	6994.58504	1.20	-0.94	rob08
18	19	6907.26514	1.20	-1.28	rob08
19	18	6996.46211	1.20	-1.55	rob08
19	20	6904.43423	1.20	0.22	rob08
20	19	6998.31059	1.20	-2.98	rob08
20	21	6901.57377	1.20	-1.64	rob08

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2	2	6956.27761	0.0	6.09	rob08
3	3	6956.22810	1.60	0.81	rob08
4	4	6956.16799	1.60	-0.22	rob08
5	5	6956.09358	1.60	-0.62	rob08
6	6	6956.00461	1.60	-0.56	rob08
7	7	6955.90099	1.60	0.00	rob08
8	8	6955.78442	1.60	2.90	rob08
9	9	6955.64305	1.60	-3.57	rob08
10	10	6955.49566	1.60	-0.45	rob08
11	11	6955.32874	1.60	-1.07	rob08
12	12	6955.14610	1.60	-1.43	rob08
13	13	6954.94928	1.60	0.22	rob08
14	14	6954.73458	1.60	0.38	rob08
15	15	6954.50099	1.60	-1.72	rob08

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0	1	6353.52974	1.00	-1.16	rob08
1	2	6351.15515	0.0	8.68	rob08
2	3	6348.73959	0.40	-0.47	kep96
3	4	6346.31002	0.0	-1.75	kep96
4	3	6365.11897	0.40	-1.02	kep96
4	5	6343.86159	0.40	-0.10	kep96
5	4	6367.37005	0.40	-0.42	kep96
5	6	6341.39024	0.40	0.33	kep96
6	5	6369.59804	0.40	-0.21	kep96
6	7	6338.89592	0.40	-0.61	kep96
7	6	6371.79767	0.0	-5.56	kep96
7	8	6336.38238	0.40	0.75	kep96
8	7	6373.98524	0.40	-0.07	kep96
8	9	6333.84567	0.40	0.36	kep96
9	8	6376.14648	0.0	2.08	kep96
9	10	6331.28955	0.0	1.88	kep96
10	9	6378.27658	0.0	-3.85	kep96
10	11	6328.70501	0.0	-3.83	kep96
11	12	6326.11068	0.0	1.74	kep96
12	13	6323.48957	0.0	1.43	kep96
13	12	6384.54722	0.0	-2.76	kep96
13	14	6320.84747	0.40	0.79	kep96
14	13	6386.59449	0.40	0.62	kep96
14	15	6318.18525	0.40	0.40	kep96
15	16	6315.50362	1.00	0.58	rob08
16	17	6312.80084	1.00	-0.93	rob08
17	18	6310.07941	0.0	-2.36	rob08
18	19	6307.34139	0.0	-2.56	rob08

0	1	6761.64265	2.00	-2.75	rob08
1	0	6766.34214	2.00	3.49	rob08
1	2	6759.26516	2.00	3.01	rob08
2	1	6768.65105	2.00	2.12	rob08
2	3	6756.85594	2.00	2.39	rob08
3	2	6770.93638	2.00	1.96	rob08
3	4	6754.42106	2.00	2.73	rob08
4	3	6773.19586	2.00	1.72	rob08
4	5	6751.95630	2.00	1.43	rob08
5	4	6775.42827	2.00	1.62	rob08
5	6	6749.46201	2.00	0.82	rob08
6	5	6777.63170	2.00	1.54	rob08
6	7	6746.93762	2.00	2.46	rob08
7	6	6779.80337	2.00	0.84	rob08
7	8	6744.37589	2.00	1.27	rob08
8	7	6781.94223	2.00	0.77	rob08
8	9	6741.77882	2.00	1.24	rob08
9	8	6784.04456	2.00	-0.05	rob08
9	10	6739.14251	2.00	0.13	rob08
10	9	6786.10879	2.00	-1.05	rob08
10	11	6736.46676	2.00	-1.00	rob08
11	10	6788.13326	2.00	-2.05	rob08
11	12	6733.75014	2.00	-2.71	rob08
12	11	6790.11677	2.00	-2.83	rob08
12	13	6730.99357	2.00	-3.55	rob08
13	12	6792.05611	2.00	-5.58	rob08
13	14	6728.19536	2.00	-4.90	rob08
14	13	6793.95229	0.0	-8.59	rob08
14	15	6725.35705	2.00	-5.01	rob08
15	14	6795.80355	0.0	-13.16	rob08
15	16	6722.46891	0.0	-13.49	rob08
16	15	6797.71038	0.0	81.53	rob08
16	17	6719.54054	0.0	-20.57	rob08
17	16	6799.53238	0.0	135.36	rob08
18	17	6801.36335	0.0	242.43	rob08
19	18	6803.33221	0.0	531.94	rob08
20	19	6805.41651	0.0	981.81	rob08
21	20	6807.80831	0.0	1784.48	rob08
22	21	6810.67582	0.0	3108.57	rob08

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2	3	6772.28729	0.80	0.76	rob08
3	2	6786.36067	0.80	0.11	rob08
3	4	6769.85461	0.80	0.93	rob08
4	3	6788.62092	0.80	2.25	rob08
4	5	6767.39653	0.80	0.50	rob08
5	4	6790.85267	0.80	1.00	rob08
5	6	6764.91443	0.80	0.79	rob08
6	5	6793.05885	0.80	-0.67	rob08
6	7	6762.40641	0.80	-0.12	rob08
7	6	6795.24227	0.80	0.08	rob08
7	8	6759.87477	0.80	0.00	rob08
8	7	6797.40013	0.80	0.50	rob08
8	9	6757.31893	0.80	0.53	rob08
9	8	6799.53243	0.80	0.60	rob08
9	10	6754.73811	0.80	0.64	rob08
10	9	6801.63988	0.80	1.13	rob08
10	11	6752.13181	0.80	-0.21	rob08
11	10	6803.71984	0.80	-0.51	rob08
11	12	6749.50222	0.80	0.11	rob08
12	11	6805.77668	0.80	0.07	rob08
12	13	6746.84777	0.80	-0.03	rob08
13	12	6807.80796	0.80	0.45	rob08
13	14	6744.17001	0.80	0.88	rob08
14	13	6809.81309	0.80	0.08	rob08
14	15	6741.46567	0.80	-0.49	rob08
15	14	6811.79353	0.80	0.44	rob08
15	16	6738.74122	0.80	2.28	rob08
16	15	6813.74705	0.80	-0.68	rob08
16	17	6735.98791	0.80	0.37	rob08
17	16	6815.67675	0.80	-0.16	rob08
17	18	6733.21191	0.80	-0.10	rob08
18	17	6817.58005	0.80	-0.54	rob08
18	19	6730.41223	0.80	-0.18	rob08
19	18	6819.45794	0.80	-0.83	rob08
19	20	6727.58868	0.80	-0.11	rob08
20	19	6821.31106	0.80	-0.36	rob08
20	21	6724.74182	0.80	0.59	rob08
21	20	6823.13804	0.80	-0.49	rob08
21	22	6721.86046	0.0	-9.32	rob08
22	21	6824.93681	0.0	-3.27	rob08
22	23	6718.97483	0.80	0.31	rob08
23	22	6826.71524	0.80	-0.81	rob08
23	24	6716.05668	0.80	1.19	rob08
24	23	6828.46656	0.80	0.13	rob08
24	25	6713.11435	0.80	1.57	rob08
25	24	6830.19131	0.80	0.10	rob08
25	26	6710.14543	0.80	-1.02	rob08
26	25	6831.88932	0.80	-1.05	rob08
26	27	6707.15995	0.0	3.39	rob08
27	26	6833.56348	0.80	-0.44	rob08
27	28	6704.14223	0.80	-0.97	rob08
28	27	6835.20973	0.80	-2.10	rob08
29	28	6836.83262	0.80	-1.49	rob08
30	29	6838.42781	0.0	-2.93	rob08

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2	3	6772.28827	0.70	-0.35	rob08
3	2	6786.36188	0.70	0.69	rob08
3	4	6769.86128	0.70	1.27	rob08
4	3	6788.62128	0.70	-0.10	rob08
4	5	6767.41025	0.70	-0.60	rob08
5	4	6790.85927	0.70	-0.05	rob08
5	6	6764.94287	0.70	-0.32	rob08
6	5	6793.07645	0.70	-0.32	rob08
6	7	6762.45907	0.70	-0.20	rob08
7	6	6795.27614	0.70	0.38	rob08
7	8	6759.96146	0.70	0.13	rob08

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 2
 3 8 7 6797.45866 0.70 0.11 rob08
 4 8 9 6757.45152 0.70 0.07 rob08
 5 9 8 6799.62781 0.70 0.42 rob08
 6 9 10 6754.93205 0.70 0.66 rob08
 7 10 9 6801.78480 0.70 0.42 rob08
 8 10 11 6752.40210 0.70 -0.42 rob08
 9 11 10 6803.93116 0.70 -0.11 rob08
 10 11 12 6749.86581 0.70 0.02 rob08
 11 12 11 6806.06860 0.70 -0.83 rob08
 12 12 13 6747.32246 0.70 0.62 rob08
 13 13 12 6808.19847 0.70 -1.36 rob08
 14 13 14 6744.77101 0.70 -0.08 rob08
 15 14 13 6810.32182 0.70 -1.29 rob08
 16 14 15 6742.21387 0.70 0.04 rob08
 17 15 14 6812.43874 0.70 -0.92 rob08
 18 15 16 6739.65039 0.70 0.06 rob08
 19 16 15 6814.54909 0.70 -0.69 rob08
 20 16 17 6737.08134 0.70 0.51 rob08
 21 17 16 6816.65224 0.70 -1.45 rob08
 22 17 18 6734.50121 0.0 -4.44 rob08
 23 18 17 6818.75001 0.70 -1.61 rob08
 24 18 19 6731.92134 0.0 -3.81 rob08
 25 19 18 6820.84344 0.70 -0.40 rob08
 26 19 20 6729.33989 0.70 0.16 rob08
 27 20 19 6822.92921 0.70 -1.45 rob08
 28 20 21 6726.74843 0.70 -1.45 rob08

24 2 0 0 1 1, 1 1f - 0 0 0 2 0, 2 0e
 25
 26 2 2 6779.36149 0.80 0.09 rob08
 27 3 3 6779.28760 0.80 -0.54 rob08
 28 4 4 6779.19316 0.80 0.80 rob08
 29 5 5 6779.07640 0.80 0.79 rob08
 30 6 6 6778.93886 0.80 -0.86 rob08
 31 7 7 6778.78756 0.80 0.89 rob08
 32 8 8 6778.61953 0.80 1.14 rob08
 33 9 9 6778.43697 0.80 0.35 rob08
 34 10 10 6778.24227 0.80 -0.46 rob08
 35 11 11 6778.03669 0.80 -0.96 rob08
 36 12 12 6777.82161 0.80 -0.23 rob08
 37 13 13 6777.59572 0.80 0.28 rob08

36 2 0 0 1 1, 1 1e - 0 0 0 2 0, 2 0f
 37
 38 2 2 6779.36149 0.70 0.46 rob08
 39 3 3 6779.28760 0.70 1.28 rob08
 40 4 4 6779.18838 0.70 1.47 rob08
 41 5 5 6779.06362 0.70 0.62 rob08
 42 6 6 6778.91516 0.70 0.37 rob08
 43 7 7 6778.74234 0.70 -0.23 rob08
 44 8 8 6778.54698 0.70 0.32 rob08
 45 9 9 6778.32728 0.70 -0.12 rob08
 46 10 10 6778.08607 0.70 0.85 rob08
 47 11 11 6777.81994 0.70 -0.62 rob08
 48 12 12 6777.53284 0.70 -1.06 rob08

47 2 0 0 0 2, 0 0e - 0 0 0 1 1, 1 -1e
 48 0 1 6783.92912 1.80 0.15 rob08
 49 1 0 6788.62164 1.80 -4.07 rob08
 50 1 2 6781.54237 1.80 -0.60 rob08
 51 2 1 6790.93597 1.80 -0.31 rob08
 52 2 3 6779.13141 1.80 -0.57 rob08
 53 3 2 6793.22184 1.80 0.36 rob08
 54 3 4 6776.69697 1.80 0.93 rob08
 55 4 3 6795.48199 1.80 0.82 rob08
 56 4 5 6774.23523 1.80 0.07 rob08
 57 5 4 6797.71034 1.80 -4.86 rob08
 58 5 6 6771.74826 1.80 -1.10 rob08
 59 6 5 6799.92595 1.80 2.58 rob08
 60 6 7 6769.24062 1.80 2.01 rob08

3	7	6	6802.10625	1.80	0.77	rob08
4	7	8	6766.70233	1.80	-0.53	rob08
5	8	7	6804.26274	1.80	1.44	rob08
6	8	9	6764.14395	1.80	1.88	rob08
7	9	8	6806.39114	1.80	0.53	rob08
8	9	10	6761.55575	1.80	-0.41	rob08
9	10	9	6808.49367	1.80	0.54	rob08
10	10	11	6758.94404	1.80	-0.98	rob08
11	11	10	6810.56828	1.80	-0.33	rob08
12	11	12	6756.30865	1.80	0.09	rob08
13	12	13	6812.61749	1.80	0.74	rob08
14	13	12	6753.64987	1.80	3.23	rob08
15	13	14	6814.63674	1.80	-0.54	rob08
16	14	13	6750.96027	1.80	1.13	rob08
17	14	15	6816.62981	1.80	-0.09	rob08
18	14	15	6748.24596	1.80	0.04	rob08
19	15	14	6818.59452	1.80	0.17	rob08
20	15	16	6745.50767	1.80	0.83	rob08
21	16	15	6820.51654	0.0	-13.80	rob08
22	16	17	6742.74261	1.80	0.82	rob08
23	17	16	6822.43796	1.80	0.31	rob08
24	17	18	6739.95070	1.80	0.06	rob08
25	18	17	6824.31654	1.80	0.49	rob08
26	18	19	6737.13584	1.80	2.54	rob08
27	19	18	6826.16584	1.80	0.46	rob08
28	19	20	6734.28906	1.80	-0.64	rob08
29	20	19	6827.98574	1.80	0.23	rob08
30	20	21	6731.42237	1.80	2.54	rob08
31	21	20	6829.77672	1.80	0.36	rob08
32	21	22	6728.52455	1.80	0.87	rob08
33	22	21	6831.53753	1.80	-0.39	rob08
34	22	23	6725.60330	1.80	1.98	rob08
35	23	22	6833.27077	1.80	0.52	rob08
36	23	24	6722.65284	1.80	-0.01	rob08
37	24	23	6835.06198	0.0	88.52	rob08
38	24	25	6719.68262	1.80	4.20	rob08
39	25	24	6836.64780	1.80	0.08	rob08
40	25	26	6716.68093	1.80	2.69	rob08
41	26	25	6838.29335	1.80	0.08	rob08
42	27	26	6839.90967	1.80	-0.71	rob08
43	28	27	6841.49610	1.80	-3.28	rob08
44	29	28	6843.05929	1.80	-1.33	rob08
45	30	29	6844.60784	0.0	13.37	rob08
46	31	30	6846.10210	1.80	0.77	rob08
47	32	31	6847.58016	1.80	-1.41	rob08
48	33	32	6849.03501	1.80	-0.55	rob08
49	34	33	6850.47097	0.0	7.31	rob08
50	35	34	6851.88390	0.0	17.69	rob08

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43	2	3	6773.80564	1.80	-0.39	rob08
44	3	2	6787.88933	1.80	0.18	rob08
45	3	4	6771.37157	1.80	-0.44	rob08
46	4	3	6790.15470	0.0	5.57	rob08
47	4	5	6768.91313	1.80	-0.15	rob08
48	5	4	6792.38519	1.80	1.11	rob08
49	5	6	6766.42952	1.80	-0.35	rob08
50	6	5	6794.59586	1.80	1.89	rob08
51	6	7	6763.92199	1.80	0.15	rob08
52	7	6	6796.78161	1.80	2.87	rob08
53	7	8	6761.40302	0.0	13.80	rob08
54	8	7	6798.93846	1.80	0.09	rob08
55	8	9	6758.83128	1.80	-0.75	rob08
56	9	8	6801.07538	1.80	2.57	rob08
57	9	10	6756.25026	1.80	-0.07	rob08
58	10	9	6803.18217	1.80	0.16	rob08
59	10	11	6753.64956	0.0	5.41	rob08
60	11	10	6805.26579	1.80	-0.15	rob08
57	11	12	6751.01633	1.80	2.81	rob08
58	12	11	6807.32345	1.80	-1.09	rob08

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 2
 3 12 13 6748.35878 1.80 0.29 rob08
 4 13 12 6809.35329 1.80 -4.50 rob08
 5 13 14 6745.68878 0.0 9.71 rob08
 6 14 13 6811.36430 1.80 -1.32 rob08
 7 14 15 6742.97403 1.80 -1.29 rob08
 8 15 14 6813.34692 1.80 -1.09 rob08
 9 15 16 6740.24689 1.80 -0.38 rob08
 10 16 15 6815.30464 1.80 -0.27 rob08
 11 16 17 6737.49525 1.80 0.30 rob08
 12 17 16 6817.23524 1.80 -1.03 rob08
 13 17 18 6734.71931 1.80 0.92 rob08
 14 18 17 6819.14090 1.80 -1.14 rob08
 15 18 19 6731.92111 1.80 3.48 rob08
 16 19 18 6821.02198 1.80 -0.21 rob08
 17 19 20 6729.09616 1.80 3.45 rob08
 18 20 19 6822.87609 1.80 -0.59 rob08
 19 20 21 6726.24728 1.80 3.63 rob08
 20 21 20 6824.70468 1.80 -0.76 rob08
 21 21 22 6723.37051 1.80 0.02 rob08
 22 22 23 6720.47305 1.80 -0.22 rob08
 23 22 21 6826.50779 1.80 -0.65 rob08
 24 23 22 6828.28444 1.80 -1.20 rob08
 25 24 23 6830.03588 1.80 -1.11 rob08
 26 25 24 6831.76050 1.80 -1.94 rob08
 27 26 25 6833.46005 1.80 -1.90 rob08
 28 27 26 6835.13347 1.80 -1.99 rob08
 29 28 27 6836.78171 1.80 -1.23 rob08
 30 29 28 6838.39810 0.0 -6.24 rob08
 31 30 29 6839.99808 1.80 -1.53 rob08

26
 27 2 0 0 0 2, 0 2e - 0 0 0 1 1, 1 1e

28 2 3 6773.80564 1.80 -0.25 rob08
 29 3 2 6787.88933 1.80 -0.09 rob08
 30 3 4 6771.37157 1.80 -0.14 rob08
 31 4 3 6790.15470 1.80 4.84 rob08
 32 4 5 6768.91313 1.80 0.35 rob08
 33 5 4 6792.38519 1.80 -0.45 rob08
 34 5 6 6766.42952 1.80 0.33 rob08
 35 6 5 6794.59586 1.80 -1.03 rob08
 36 6 7 6763.92010 1.80 -0.94 rob08
 37 7 6 6796.78241 1.80 -1.30 rob08
 38 7 8 6761.40302 0.0 14.57 rob08
 39 8 7 6798.94592 1.80 -0.35 rob08
 40 8 9 6758.83128 1.80 -0.30 rob08
 41 9 8 6801.08397 1.80 -0.74 rob08
 42 9 10 6756.25026 1.80 -0.32 rob08
 43 10 9 6803.19949 1.80 0.25 rob08
 44 10 11 6753.64956 1.80 3.93 rob08
 45 11 10 6805.28929 1.80 -0.74 rob08
 46 11 12 6751.01633 1.80 -0.60 rob08
 47 12 11 6807.35638 1.80 -0.92 rob08
 48 12 13 6748.35916 0.0 -5.53 rob08
 49 13 12 6809.40064 1.80 -0.62 rob08
 50 13 14 6745.68878 1.80 -0.34 rob08
 51 14 13 6811.42159 1.80 -0.54 rob08
 52 14 15 6742.98972 1.80 -0.75 rob08
 53 15 14 6813.42039 1.80 0.29 rob08
 54 15 16 6740.26932 1.80 0.38 rob08
 55 16 15 6815.39427 1.80 -1.12 rob08
 56 16 17 6737.52529 1.80 0.53 rob08
 57 17 16 6817.34819 1.80 0.03 rob08
 58 17 18 6734.75775 1.80 -0.40 rob08
 59 18 17 6819.27930 1.80 0.74 rob08
 60 18 19 6731.96972 1.80 0.44 rob08
 59 19 18 6821.18675 1.80 0.05 rob08
 60 19 20 6729.15845 1.80 0.14 rob08
 59 20 19 6823.07168 1.80 -0.97 rob08
 60 20 21 6726.32457 1.80 -0.81 rob08
 59 21 22 6723.48708 0.0 16.50 rob08
 60 21 20 6824.93540 1.80 -1.00 rob08

1
 2
 3 22 23 6720.58368 0.0 -10.26 rob08
 4 22 21 6826.78880 0.0 10.88 rob08
 5 23 24 6717.68974 0.0 -5.73 rob08
 6 23 22 6828.59475 1.80 -2.34 rob08
 7 24 23 6830.36549 0.0 -28.26 rob08
 8 25 24 6832.16737 1.80 -0.30 rob08
 9 26 25 6833.95034 0.0 31.77 rob08
 10 27 26 6835.64594 1.80 -0.17 rob08
 11 28 27 6837.32929 0.0 -20.63 rob08
 12 29 28 6838.98393 0.0 -45.68 rob08
 30 29 6840.60469 0.0 -80.07 rob08
 31 30 6842.20659 0.0 -108.35 rob08

13 2 0 0 0 2, 0 2e - 0 0 0 1 1, 1 1 1f

14
 15 2 2 6780.88370 1.00 -1.25 rob08
 16 3 3 6780.81060 1.00 -0.01 rob08
 17 4 4 6780.70978 1.00 -1.99 rob08
 18 5 5 6780.58761 1.00 -1.08 rob08
 19 6 6 6780.43546 0.0 -6.21 rob08
 20 7 7 6780.27182 1.00 0.73 rob08
 21 9 9 6779.86101 1.00 0.00 rob08
 10 10 6779.62860 0.0 6.04 rob08

22 2 0 0 0 2, 0 2f - 0 0 0 1 1, 1 1 1e

23
 24 2 2 6780.88370 1.60 -1.15 rob08
 25 3 3 6780.81060 1.60 0.51 rob08
 26 4 4 6780.70978 1.60 -0.45 rob08
 27 5 5 6780.58761 1.60 2.52 rob08
 28 6 6 6780.43546 1.60 1.00 rob08
 29 7 7 6780.25983 1.60 1.72 rob08
 9 9 6779.86101 0.0 33.99 rob08
 10 10 6779.57215 1.60 0.57 rob08

30 0 1 1 0 3, 0 1e - 0 0 0 0 1, 0 0 1e

31
 32 1 2 6667.50737 1.40 -0.77 rob08
 33 2 1 6676.88398 1.40 0.39 rob08
 34 3 2 6679.18234 1.40 -0.06 rob08
 35 4 3 6681.46358 1.40 0.42 rob08
 36 5 4 6683.72915 1.40 3.24 rob08
 37 6 5 6685.97249 1.40 1.81 rob08
 38 7 6 6688.19881 1.40 1.21 rob08
 39 8 7 6690.40782 1.40 1.02 rob08
 40 9 8 6692.60007 1.40 1.54 rob08
 41 10 9 6694.77427 1.40 1.12 rob08
 42 11 10 6696.93085 1.40 -0.29 rob08
 43 12 11 6699.07261 1.40 -0.55 rob08
 44 13 12 6701.19976 1.40 -0.35 rob08
 45 14 13 6703.31219 1.40 -1.01 rob08
 46 15 14 6705.41275 1.40 -1.24 rob08
 47 16 15 6707.50379 1.40 -0.68 rob08
 48 17 16 6709.58713 1.40 -0.06 rob08
 49 18 17 6711.66496 1.40 -0.30 rob08
 50 19 18 6713.74391 0.0 1.56 rob08
 51 20 19 6715.82638 0.0 3.79 rob08
 52 21 20 6717.91519 0.0 4.95 rob08

53 0 1 1 0 3, 0 1f - 0 0 0 0 1, 0 0 1f

54
 55 1 2 6667.49660 1.80 0.18 rob08
 56 2 1 6676.92300 1.80 -0.55 rob08
 57 3 2 6679.25356 1.80 0.69 rob08
 58 4 3 6681.57382 1.80 2.73 rob08
 59 5 4 6683.87890 1.80 0.77 rob08
 60 6 5 6686.17581 1.80 1.91 rob08
 7 6 6688.45899 1.80 0.72 rob08
 8 7 6690.73297 1.80 1.88 rob08
 9 8 6692.99245 1.80 0.25 rob08
 10 9 6695.24274 1.80 1.40 rob08

11	10	6697.47888	1.80	0.62	rob08
12	11	6699.70240	1.80	-0.20	rob08
13	12	6701.91533	1.80	1.37	rob08
14	13	6704.11214	1.80	0.31	rob08
15	14	6706.29489	1.80	-0.74	rob08
16	15	6708.46364	1.80	-1.03	rob08
17	16	6710.61678	1.80	-1.38	rob08
18	17	6712.75410	1.80	-1.06	rob08
19	18	6714.87184	1.80	-2.81	rob08
20	19	6716.97344	1.80	-2.02	rob08
21	20	6719.05353	1.80	-2.80	rob08
22	21	6721.11287	1.80	-3.02	rob08
23	22	6723.14936	1.80	-3.33	rob08
24	23	6725.16151	1.80	-3.74	rob08
25	24	6727.12337	0.0	-28.71	rob08
26	25	6729.09609	0.0	-15.64	rob08
27	26	6731.03277	0.0	-10.06	rob08
28	27	6732.90375	0.0	-40.38	rob08

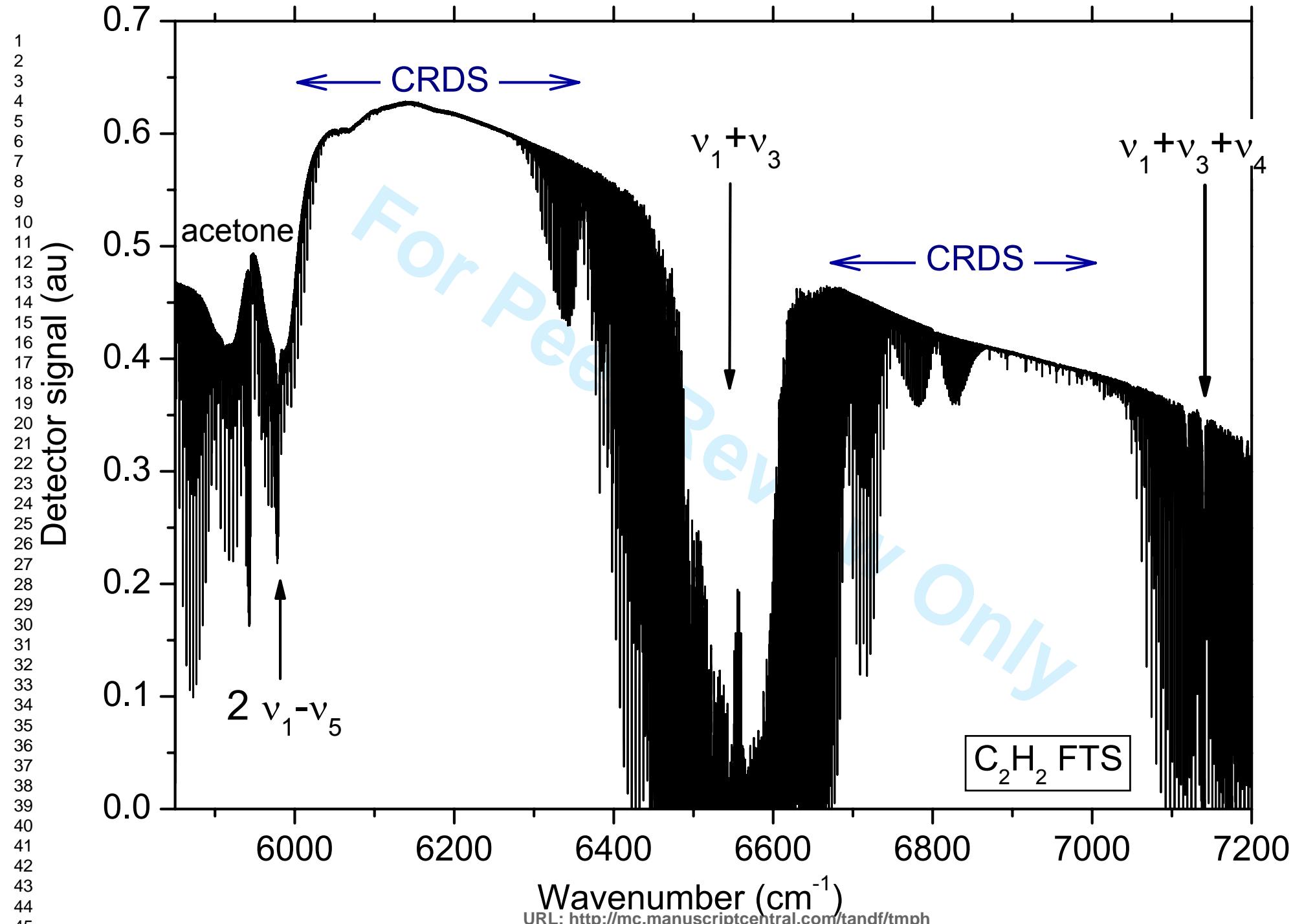


Fig. 1

Absorption coefficient (10^{-6} cm^{-1})