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Acetylene, 12C2H2: new CRDS data and global vibration-rotation analysis up to 8600 cm⁻¹

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Revised manuscript

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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Abstract

The absorption spectrum of $^{12}\text{C}_2\text{H}_2$ has been recorded using cavity ringdown spectroscopy and analyzed in the ranges 6000–6356 cm^{-1} and 6667–7015 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 i 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. Introduction

The high resolution spectrum of acetylene, $^{12}\text{C}_2\text{H}_2$, has been already investigated in the 1.5 μm spectral range using Fourier transform infrared spectroscopy (FTIR) ¹⁻⁴. The strong $\nu_1+\nu_3$ band, of metrological relevance, is observed in this range, together with various combination and hot bands. Nowadays, cavity ~~ringdown~~ spectroscopy (CRDS) (*e.g.* ^{5,6}) allows the experimental sensitivity to be significantly increased with respect to FTIR measurements. We have ~~used CW-CRDS~~ ^{7,8} to record the acetylene spectrum around 1.5 μm in Grenoble. Experimental details are provided in section 2 and the results of the band-by-band analyses performed in Bologna, between 6000–6356 cm^{-1} and 6667–7015 cm^{-1} , are listed in section 3.

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The new spectra revealed very weak bands compared to the existing literature data. Their analysis was facilitated by unpublished global constants obtained in Brussels from the simultaneous fit of many sets of already known vibration-rotation lines. Such a procedure, which was already achieved for $^{13}\text{CH}^{12}\text{CH}$ up to 6750 cm^{-1} using a set of programs developed in Louvain ⁹, exploits the very regular vibrational energy pattern in acetylene, as recently reviewed in ¹⁰. The present investigation stimulated an update of the still unpublished results of our $^{12}\text{C}_2\text{H}_2$ global fit, to include the new CRDS data reported here. The data base gathering the published vibration-rotation lines in $^{12}\text{C}_2\text{H}_2$ involving vibrational states up to 8600 cm^{-1} , is summarized in

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3 section 4. This range was selected to include all states observed through cold
4 and hot bands in the present CRDS spectra. The global model is presented in
5 section 5. The results, also updating a previously published global analysis by
6 Perevalov *et al.*¹¹, are detailed in section 6 and discussed in section 7, before
7 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
20 = $l_4 + l_5$.
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33 2. Experimental details

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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
38 ¹² and ¹²CO₂¹³⁻¹⁵ or O₃¹⁶. The fibered CW-CRDS spectrometer and the
39 procedure adopted for an accurate calibration of the wavenumber scale of the
40 recorded spectra were described in Refs.^{12 14 17}. Fig. 1 shows an overview of
41 the acetylene absorption spectrum recorded by FTS at ULB, highlighting the
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2 two spectral sections presently investigated. The 6000–6356 cm^{-1} and
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4 6667–7015 cm^{-1} regions were selected for the present CRDS recordings as
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6 they correspond to transparency windows located between strong absorption
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8 bands. These two regions were covered by using a set of 18 and 12
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10 Distributed Feed-Back (DFB) diode lasers, respectively. Only the range
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12 6122–6130 cm^{-1} could not be recorded due to the lack of diode.
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18 [Insert figure 1 about here]
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24 The tuning range of each DFB laser is about 7 nm ($\sim 30 \text{ cm}^{-1}$) by temperature
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26 variation from -10 to 65°C . The typical sensitivity (noise equivalent
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28 absorption $\alpha_{\text{min}} \sim 2\text{--}5 \times 10^{-10} \text{ cm}^{-1}$), wide spectral coverage and the four to five
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30 decades linear dynamic range, make it an ideal tool for high sensitivity
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32 absorption spectroscopy in the important atmospheric window of
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34 transparency around $1.5 \mu\text{m}$. The CRDS cell fitted by the super mirrors is
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36 1.40 m long. The typical ringdown times were of the order of $60 \mu\text{s}$. A few
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38 hundred ringdown events were averaged for each spectral data point, taking
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40 some 220 ms per averaged point, and the duration of a temperature scan was
41
42 about 70 minutes for each DFB laser. The pressure, measured by a
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44 capacitance gauge, as well as the ringdown cell temperature, were monitored
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46 during the spectrum recording. Different series of recordings were performed
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2 for pressure values of 667, 1333 and 2666 Pa depending on the spectral
3 region. The DFB line width is much smaller than the Doppler width and the
4 observed resolution is mostly Doppler limited in the adopted pressure
5 conditions. In cases of overlapped lines, whenever it was possible, a
6 deconvolution by means of Voigt profile was performed, keeping the full
7 width at half maximum at a value observed for close $^{12}\text{C}_2\text{H}_2$ isolated lines.
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18 The wavenumber calibration of the spectrum is based on the
19 wavelength values measured by a wavemeter (Burleigh WA1640) during the
20 DFB frequency scan. When necessary, it was further refined by simply
21 stretching the frequency scale (with an origin at 0) in agreement with highly
22 accurate positions of reference lines due to impurities. H_2^{16}O line positions as
23 provided by the HITRAN database ¹⁸ were used as reference lines. The
24 obtained absolute wavenumber calibration is estimated accurate within
25 better than $\pm 2 \times 10^{-3} \text{ cm}^{-1}$.
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36 The achieved sensitivity and dynamics are illustrated in Fig. 2 on a
37 small section of the spectrum near 6235 cm^{-1} . It is significantly improved
38 compared to the previous investigation by Keppler *et al.* ³, based on FTIR and
39 up to 352.5 m long absorption path. The improvement is best demonstrated
40 by the analysis of 14 additional, new bands in the present spectra.
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[Insert figure 2 about here]

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 database¹⁸, were observed in the region of the strong 2ν₃ band near 6000 cm⁻¹, while C₂H₄ lines belonging to the ν₅+ν₉ band at 6151 cm⁻¹ were identified between 6095 and 6210 cm⁻¹¹⁹. 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 $\bullet_{min} \sim 3 \times 10^{-9}$ 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 $\nu_{4^+} \nu_5 \leq 2$. 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 $2\nu_1(\Sigma_g^+) \leftarrow \nu_5(\Pi_u)$ hot band extending from 6000 to 6050 cm^{-1} (see Fig.1). At 6011 cm^{-1} the red degraded Q branch of the $\nu_1+\nu_2+\nu_4+\nu_5(\Sigma_u^+) \leftarrow \nu_4(\Pi_g)$ 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 $\nu_1+\nu_2+2\nu_5(\Sigma_g^+) \leftarrow \nu_5(\Pi_u)$, $\nu_1+\nu_2+\nu_5(\Pi_u) \leftarrow \text{G.S.}$ and $2\nu_2+3\nu_5(\Pi_u) \leftarrow \text{G.S.}$ 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 $\nu_1+\nu_2+2\nu_5(\Sigma_g^+) \leftarrow \nu_5(\Pi_u)$ band superimposed with the R branch of the $2\nu_1(\Sigma_g^+) \leftarrow \nu_5(\Pi_u)$ band, while the very weak Q branch of the $2\nu_2+3\nu_5(\Pi_u) \leftarrow \text{G.S.}$ band is presented in Fig. 4. A parallel band centred at 6079.7 cm^{-1}

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has been assigned to $\nu_1+\nu_4+3\nu_5(\Sigma_u^+) \leftarrow \text{G.S.}$. Between 6095 and 6210 cm^{-1} the spectrum is dominated by the strong lines of the C_2H_4 impurity, which overlap the weaker C_2H_2 transitions, making the assignment very difficult. In fact, only a few transitions have been added to previously observed bands³.

[Insert figures 3 and 4 about here]

At both ends of the region between 6667 and 7015 cm^{-1} the wings of the strong $\nu_1+\nu_3$ and $\nu_1+\nu_3+\nu_4$ band systems, centred at 6556 and 7141 cm^{-1} , respectively, are visible. In the FTIR spectrum only the $2\nu_1+\nu_5(\Pi_u) \leftarrow \nu_4(\Pi_g)$ and $\nu_2+\nu_3+2\nu_5(\Sigma_u^+) \leftarrow \text{G.S.}$ assigned in Keppler *et al.*³ at 6804.7 and 6690 cm^{-1} , respectively, have been identified. Most of the bands observed in the CRDS 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 $\Pi_{g/u} \leftarrow \Pi_{u/g}$ bands also the very weak *Q* branches have been observed and assigned. In the higher wavenumber side two perpendicular bands, $\Delta_g \leftarrow \Pi_u$ and $\Sigma_g^+ \leftarrow \Pi_u$, have been identified, both centered at about 6956 cm^{-1} and leading to states of the same manifold.

The spectral analysis was made difficult by the superposition of the different bands of $^{12}\text{C}_2\text{H}_2$ with lines due to impurities (in particular H_2O and C_2H_4) or to the $^{13}\text{CH}^{12}\text{CH}$ isotopologue. In fact, lines without intensity

alternation due to transitions already reported ⁶ in twelve bands for this molecule have been observed mainly in the 6667–7015 cm⁻¹ range.

The rotational analysis of the bands listed in Table 1 was performed using standard procedures. The energy of the rovibrational levels of the Σ^+ , Π , and Δ states was calculated according to the expression:

$$T(v, J) = G_c + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3 \pm \frac{1}{2} \{ q_v [J(J+1)] + q_v^J [J(J+1)]^2 + q_v^{JJ} [J(J+1)]^3 \} \quad (1)$$

with $q_v, q_v^J, q_v^{JJ} = 0$ for $l=0$, Σ states, and the centre term value defined as

$$G_c = G_v - B_v k^2 - D_v k^4 \quad (2)$$

and G_v the vibrational term value. In Eq. (1) upper signs refer to e -symmetry states, lower signs to f -symmetry states.

The constants resulting from the band-by-band analysis are listed in Table 1. The term values of the lower states of the transitions were calculated from literature data ²⁰. The number of lines assigned in the branches and the number of fitted lines are also indicated for each band.

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[Insert Table 1 about here]

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 $\nu_1+\nu_2+\nu_4+\nu_5$ (Σ_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.

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

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3 corresponding P (or R) counterpart is outside the investigated spectral region.
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5 With the help of the predicted line positions by means of the parameters of
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7 the global fit three R branches of this kind have been assigned to the $\Pi \leftarrow \Pi$
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9 bands centred at 6662, 6672 and 6674 cm^{-1} (see Table 1). Unassigned series
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11 could also correspond to hot bands from states with vibrational excitation
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13 higher than those considered in the predictions, limited to $v_4^+ v_5^- \bullet 2$. Another
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15 possibility, which has not been exploited, is represented by zero-order
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17 forbidden transitions with $|\Delta k| = 2$. These additional structures will be
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19 considered at a later stage of the global analysis.
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24 All line wavenumbers from the rotational analyses reported in Table 1,
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26 together with their assignments, are attached as Supplementary Material.
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28 Observed–calculated values obtained from the global procedure described in
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30 section 6, rather than from the band-by-band parameters listed in Table 1,
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32 are also provided.
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The data base consists of the assigned line wavenumbers from the literature, within the upper vibrational state energy limit of 8600 cm^{-1} . This limit was selected to include all new states from the present CRDS data.

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The bands involved in the data base are identified in Table 2. All data, except for the Raman ones by Bermejo *et al.*^{21,22}, come from various absorption techniques. It is interesting to notice that, besides the bending range investigated using FTIR^{20,23,24}, some low energy bands were only reported in the early literature, investigated using high resolution spectrographs, by Rao and coworkers²⁵⁻²⁸. The quality of these data, although optimal at the time of their publication, may possibly be improved nowadays. Some more recent data recorded using FTIR have actually since been published but the related list of assigned lines could unfortunately not be made available by the authors²⁹.

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The data base includes the vibration-rotation wavenumbers from the systematic investigation by Jacquemart and co-workers, using FTIR^{23,30-37}. Additional conventional FTIR results around 1.5^{2,3} and 1.17 μm ³⁸, as well as lines around 2.5 μm reported from very sensitive FTIR experiments using a femto laser as absorption source³⁹, are included. Finally, 14 new bands presently observed by CW-CRDS are also part of the data base, together with additional lines in 10 previously reported ones.

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[Insert Table 2 about here]

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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
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6 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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35 The data base amounts to 12137 vibration-rotation lines accessing
36 states up to 8600 cm^{-1} . They arise from bands linking 186 different l -
37 substates (counting e and f components separately). All states involved in the
38 data base are gathered in Table 3, together with their centre term value G_v ,
39 calculated from the global constants resulting from the procedure detailed in
40 the next sections. It is interesting to notice that, because of the u/g selection
41 rule, this data set is significantly reduced compared to $^{13}\text{CH}^{12}\text{CH}$, for which
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2 about the same number of lines was gathered from the literature, up to the
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4 limit of 6750 cm^{-1} as compared to 8600 cm^{-1} in the present case.
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13 It must be emphasized that, as the same states are observed from
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15 spectra recorded in different wavelength ranges and using various
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17 experimental conditions, spectral calibration is a critical issue when
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19 performing global fitting. We satisfactorily checked that the line
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21 measurement accuracy, described in the references just mentioned, was
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23 comparable to the quality of the standard deviation of the final fit.
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30 **5. Vibration-rotation Hamiltonian**

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32 For several isotopologues of acetylene, the vibrational state
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34 energies could be gathered into so-called polyads or vibrational clusters up to
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36 high excitation, block-diagonalizing the global vibrational Hamiltonian⁴¹⁻⁴⁶.
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38 Each of these blocks within the Hamiltonian matrix image of the molecule
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40 (MIME) shows a similar structure, accounting for the same set of anharmonic
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42 resonances, all characterized by well-defined interaction matrix elements. As
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44 a consequence of this regularity, new constants of the motion, N_r and N_s , can
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46 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} :
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$$N_r = 5v_1 + 3v_2 + 5v_3 + v_4 + v_5 \quad (3)$$

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

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 proceedings 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 coworkers 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 *ijkl* (*ii/jj*) refers to anharmonic resonance interaction terms of the type

$\Delta v_i = \pm 1, \Delta v_j = \mp 1, \Delta v_k = \mp 2$ ($\Delta v_i = \pm 2, \Delta v_j = \mp 2$) characterized by the interaction constant $K_{i/jkk}$ ($K_{i/ij}$). The related main coupling terms fulfill the $\Delta k = 0$ selection rule in various possible ways, thus with either $\Delta l_4 = \Delta l_5 = 0$, or $\Delta l_4 = -\Delta l_5 \neq 0$. Higher order terms, labeled $O_{ij/mn}$, apply for $\Delta k = \pm 2$ coupling schemes. For completeness, vibrational and rotational interaction terms in the global Hamiltonian are defined in Table 4. Only some of the anharmonic resonance terms are explicitly provided in this Table, namely those relevant to the 3/245 and 44/55 anharmonic couplings in eqs. (13-16) and (17-19), respectively. The selection of higher order terms was adapted to the results of the global fit presented in the next section.

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[Insert Table 4 about here]

As detailed in ⁹, vibration-rotation polyads include states with different values of $k = l_4 + l_5$, either even or odd. The e and f partition defined in ⁵⁶ is also included, with the symmetrized basis as defined in ⁵⁷ for pentatomic molecules. Also, g and u symmetry is used to classify the total wavefunction and to further block-diagonalize the Hamiltonian. Finally, the resulting vibration-rotation matrices are diagonal in J . Each block is characterized by the pseudo-quantum numbers N_r and N_s defined in Eqs (3) and (4), the total angular momentum quantum number J , and the symmetry properties e/f and u/g . Each block is therefore labeled using the $\{N_r, N_s, J, e/f, u/g\}$ notation.

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 states ⁴⁰ 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:

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

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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3 A statistical survey of the quality of the vibration-rotation data of $^{12}\text{C}_2\text{H}_2$
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5 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
11 satisfactory, meaning all those with observed-calculated value larger than
12
13 three times the uncertainty ε_i . Since we do not have access to all spectra, we
14
15 could not systematically check the quality of these rejected lines. About 80%
16
17 of these correspond to very low or high J -values. They are thus most likely
18
19 weaker or overlapped lines in different bands, less precisely measured. We
20
21 could clearly assess this in $^{13}\text{CH}^{12}\text{CH}$ ⁹, as further discussed below. Their
22
23 rejection, only occurs because they are characterized by the same
24
25 uncertainties as for the other more accurately measured lines in the same
26
27 bands and does therefore not affect the global picture.
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33 We identified specific high order Coriolis type vibration-rotation
34
35 interaction schemes, 14/22 in particular, likely to explain the rejection of the
36
37 remaining 20%. This coupling sometimes affects many rotational levels
38
39 within the same vibrational sub-state. It is *e.g.* the case for $(v_1 v_2 v_3 v_4 v_5, l_4 l_5) =$
40
41 $(10012, 10) \Pi^f$ sub-state at 5381.56 cm^{-1} , perturbed by the $(02002, 02) \Delta^f$ one.
42
43 Significant changes in the programs would be required to account for these
44
45 additional $\Delta k = 1$ couplings, affecting only a very small fraction, about 2%, of
46
47 the information available in the present data base. Depending on the various
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3 high order Coriolis type vibration-rotation interaction schemes to be
4 accounted for in acetylene, the block diagonal structure of the Hamiltonian
5
6 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
16 because a larger fraction of them results from a single series of high quality
17
18 FTIR spectra, probably also contributes to this comparison. One should
19
20 furthermore account for the energy ranges considered in both cases, up to
21
22 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
23
24 interaction schemes due to a denser pattern of states at the higher energies
25
26 considered are thus to be unraveled in the symmetric isotopologue. In
27
28 addition, since the number of data is almost identical in both data bases, the
29
30 information content is significantly higher in the asymmetric isotopologue,
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32 imposing more efficient constraints on the fitting procedure.
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41 [Insert Table 6 about here]
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48 7. Global constants

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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 $^{12}\text{C}_2\text{H}_2$ are different from those determined in the similar fit of $^{13}\text{CH}^{12}\text{CH}$ ⁹. It is interesting to notice that the number of parameters is higher in $^{12}\text{C}_2\text{H}_2$ (266), compared to $^{13}\text{CH}^{12}\text{CH}$ (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 $^{12}\text{C}_2\text{H}_2$, 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
4 adopting the same selection of diagonal and off diagonal interaction terms or
5
6 the same procedure and constraints. We thus only mention that all leading
7
8 and higher order rotational terms compare well, but not the vibrational ones.
9
10 Actually their constants (absolute values in cm^{-1}) x_{11} (18.96), x_{33} (30.02), x_{13}
11
12 (105.29), and $K_{11/33}$ (14.06)⁵⁴ do not fit the so-called x - K relations, *i.e.*
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14

$$x_{11} = x_{33} = \frac{1}{4}x_{13} = \frac{1}{4}K_{11/33} \quad (6)$$

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21 predicted to apply in all symmetric isotopologues of acetylene⁵⁹. These
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23 relations are reasonably well fulfilled by the present values, listed in the first
24
25 column of Table 8.
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31 [Insert Table 8 about here]
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35 It is interesting to notice that the values of the vibrational parameters
36
37 for $^{12}\text{C}_2\text{H}_2$ derived from a fit of the vibrational energies only⁴³ are very similar
38
39 to those presently obtained considering vibration-rotation data. This previous
40
41 set, listed in the second column of Table 8, was derived from vibrational data
42
43 covering a much broader spectral range, up to the visible region. This
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45 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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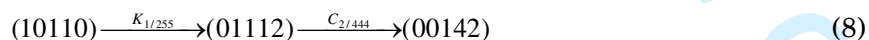
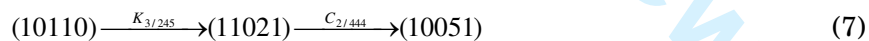
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3 Table 8, from ^{9,46}. Values for the same parameters in ¹³C₂H₂ ⁴⁴ and ¹²C₂D₂ ⁴²,
4
5 resulting from a vibrational fit, are also listed for completeness.
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9 Another test of the reliability of the present set of parameters comes
10 from their predictive efficiency. As already mentioned, the global approach
11 significantly facilitated the assignment of the new weaker bands on the CW-
12 CRDS spectrum discussed in section 3. Also, as demonstrated in a
13 preliminary report ⁶⁰, the global parameters are presently being used with
14 success to assign new emission spectra from very hot acetylene.
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25 [Insert figure 5 about here]
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29 As another example, Fig. 5 details the vibration-rotation states around
30 7135 cm⁻¹ from data reported in ^{3,38}, with their reduced energy plotted as
31 function of $J(J+1)$. Only *u*-symmetry vibrational states existing in the range
32 appear on Fig. 5, with those relevant assigned. We have selected the zero-
33 order state with the largest weight in the eigenvector at the lowest *J*-value to
34 label these eigenstates, as everywhere else in the text. The state of interest,
35 (10110,10) $\Pi^{e,f}$, appears to be perturbed for *J*-values from 21 to 23 for the *f*-
36 symmetry, and from 18 to 21 and 28-29 for the *e*-symmetry. As shown in Fig.
37 5, level crossings can be identified from the predictions. Predicted crossings
38 agree within no more than a fraction of a wavenumber from the observed
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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:



16 The composition of the eigenvectors of interest is very complicated and not
 17 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 6000–6356 cm^{-1} and 6667–7015 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 $\{N_v, N_s, J, e/f, u/g\}$ 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 saga ⁷, will consist in additional spectral assignments in the range presently considered and resulting updates

1
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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10 11 12 13 **Acknowledgments**

14
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16
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18
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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 $5 \times 10^{-10} \text{ cm}^{-1}$.

Figure 3: CW-CRDS spectrum of acetylene near 6028 cm^{-1} showing the very weak *Q* branch of the $\nu_1 + \nu_2 + 2\nu_5 (\Sigma_g^+) \leftarrow \nu_5 (\Pi_u)$ band centred at 6030.084 cm^{-1} , superimposed with the *R* branch of the $2\nu_1 (\Sigma_g^+) \leftarrow \nu_5 (\Pi_u)$ band. The sample pressure was 2666 Pa.

Figure 4: *Q* branch of the $2\nu_2 + 3\nu_5 (\Pi_u) \leftarrow \text{G.S}$ band newly observed by CW-CRDS near 6093 cm^{-1} . The sample pressure was 2666 Pa.

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3 Figure 5: Reduced energy graph (in cm^{-1}) defined as
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5 $E(v,r) - 1.162540 J(J+1) + 1.6265 \cdot 10^{-6} J^2(J+1)^2$, presenting vibration-rotation
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7 states of u -symmetry in $^{12}\text{C}_2\text{H}_2$, in a selected energy range. Only those
8
9 relevant to the perturbation affecting the $(v_1v_2v_3v_4v_5, l_4l_5) = (10110, 10)$ sub-
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11 state are assigned, using the dominant zero order state in the eigenvector
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13 composition at low J -values. Full and empty dots indicate unperturbed and
14
15 perturbed observed levels, respectively. Full and dashed lines indicate e - and
16
17 f - parity states, respectively. The color code is adapted to the sub-state
18
19 symmetry: in red, Σ ; in blue, Π ; in pink, Δ ; in green Γ .

Table legends

Table 1: Band centres ($\bar{\nu}_c$), 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_v , 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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5 Table 8: Check of x - K relations in acetylene isotopologues (all parameters in
6 cm^{-1}).
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4 Table 1

$v_1 v_2 v_3 v_4 v_5, l_4 l_5$	Transition	$\tilde{\nu}_c$	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 $\sigma_{\text{lines}} \times 10^3$
0 0 0 0, 0 0 ^b	$\Sigma_g^+ \leftarrow \Pi_u (v_5)$	5979.867032(61)	6709.0212	1.16309389(29)	1.60165(24)			P _e {1,34} ; R _e {2,36} Q _r {1,33}	93/99 0.32
1 0 1 1, 1 -1 ^b	$\Sigma_u^+ \leftarrow \Pi_g (v_4)$	6011.44215(27)	6623.1360	1.1679733(39)	3.995(14)	0.361(13)		P _e {1,23} ; R _e {1,26} Q _r {1,22}	59/66 0.78
1 0 0 2, 0 0	$\Sigma_g^+ \leftarrow \Pi_u (v_5)$	6030.08441(25)	6759.2386	1.1684360(34)	4.647(11)	0.7418(87)		P _e {2,10} ; R _e {1,28} Q _r {1,25}	49/61 0.77
1 0 0 1, 0 1	$\Pi_u \leftarrow \text{G.S.}$	6052.07472(14)	6053.2406	1.1659268(12)	1.6755(20)		-4.8871(15) 0.0779(33)	R _e {2,29} ; Q _e {1,23}	39/50 0.40
0 1 1 3, 1 -1	$\Sigma_u^+ \leftarrow \text{G.S.}$	6079.69351(40)	6079.6935	1.179181(12)	9.803(81)	2.67(15)		P _e {1,20} ; R _e {0,17}	35/38 1.02
1 0 0 3, 0 1	$\Pi_u \leftarrow \text{G.S.}$	6093.51086(27)	6094.6814	1.1705347(53)	2.454(27)		-9.4249 (79) 0.657(50)	P _e {2,15} ; R _e {0,12} Q _e {3,29}	46/53 0.80
2 2 2 0, 2 0 ^b	$\Delta_g \leftarrow \Delta_u (v_4+v_5)$	6342.66832(39)	7690.1434	1.168212(14)	17.22(16)	30.39(45)	-1.703(25) -29.64(31) 60.61(89)	P _e {4,16} ; R _e {4,12} P _r {3,29} ; R _r {3,19}	42/60 0.87

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5	0 0 2 1 1, 1 -1 ^b	$\Sigma_u^+ \leftarrow \Sigma_g^+ (2\nu_5)$	6355.89158(33)	7805.0040	1.170123(24)	4.48(10)	1.31(16)		$P_e\{1,19\}; R_e\{3,13\}$	21/28
6										0.61
7										
8	0 0 2 1 0, 1 0 ^b	$\Pi_g \leftarrow \Pi_u (\nu_5)$	6362.12705(20)	7092.4489	1.1676643(19)	2.6110(42)	0.1899(23)	-7.2812(22)	$P_e\{2,36\}; R_e\{1,26\}$	86/115
9								0.6875(61)	$P_f\{3,37\}; R_f\{1,28\}$	0.76
10								-0.1307(37)		
11										
12	0 0 2 0 1, 0 1 ^b	$\Pi_u \leftarrow \Pi_g (\nu_4)$	6606.50704(20)	7219.3685	1.1676694(16)	2.3259(30)	0.1270(15)	-2.3916(19)	$P_e\{3,29\}; R_e\{1,39\}$	79/93
13								-0.5588(43)	$P_f\{4,18\}; R_f\{4,37\}$	0.75
14								0.1431(24)		
15										
16										
17	0 2 1, 2 -1 ^b	$\Pi_u \leftarrow \Pi_g (\nu_4)$	6616.57126(86)	7229.4356	1.170534(18)	2.111(10)	-0.46(15)	-4.062(13)	$P_e\{4,17\}; R_e\{1,27\}$	43/85
18								7.38(10)	$P_f\{3,25\}; R_f\{1,27\}$	1.13
19								-8.94(18)		
20										
21	1 0 1 1, 1 -1 ^b	$\Sigma_u^+ \leftarrow G.S.$	6623.13568(23)	6623.1357	1.1679887(17)	4.0647(29)	0.4330(13)		$P_e\{1,32\}; R_e\{0,43\}$	64/72
22										0.86
23										
24	0 2 0 1 3, 1 -1 ^b	$\Sigma_u^+ \leftarrow G.S.$	6654.25168(29)	6654.2517	1.1718021(44)	8.233(15)	2.121(13)		$P_e\{2,20\}; R_e\{1,31\}$	37/44
25										0.81
26										
27										
28	1 1 1 2, 1 0	$\Pi_u \leftarrow \Pi_g (\nu_4)$	6662.07839(26)	7274.9429	1.1706463(32)	2.6856(98)	0.0323(80)	-10.3624(37)	$R_e\{2,29\}; R_f\{2,27\}$	41/54
29								0.111(15)		0.59
30								0.456(13)		
31										
32										
33	0 1 1 0 3, 0 1	$\Pi_g \leftarrow \Pi_u (\nu_5)$	6672.23153(17)	7402.5573	1.1716056(35)	2.088(19)	2.223(31)	-8.1878(50)	$P_e\{2\}; R_e\{1,20\}$	39/49
34								0.095(35)	$P_f\{2\}; R_f\{1,27\}$	0.46
35										
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4							6.683(59)			
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7	1 1 1 2, -1 2	${}^1\Pi_u \leftarrow \Pi_g(v_4)$	6674.42955(40)	7287.2938	1.170452(13)	4.48(10)	0.994(24)	3.708(23)	$P_e\{2,3\}; R_e\{1,10\}$	25/41
8								-6.35(19)	$P_f\{2,3\}; R_f\{1,27\}$	1.01
9										
10	0 0 1 1, 1 -1	$\Sigma_u^+ \leftarrow \Sigma_g^+(2v_4)$	6764.00626(27)	7994.3967	1.167236(11)	3.25(11)	-1.50(28)		$P_e\{1,17\}; R_e\{0,21\}$	29/39
11										0.60
12										
13	2 0 0 1 1, 1 1	$\Delta_u \leftarrow \Delta_g(2v_4)$	6779.43633(10)	8012.9029	1.1666208(12)	0.7283(28)		-0.0074(16)	$P_e\{3,21\}; R_e\{2,19\}$	93/114
14								1.8309(51)	$P_f\{3,28\}; R_f\{2,29\}$	0.49
15									$Q_e\{2,13\}; Q_f\{2,12\}$	
16										
17	2 0 0 0 2, 0 2	$\Delta_g \leftarrow \Delta_u(v_4+v_5)$	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
18								3.0252(89)	$P_f\{3,23\}; R_f\{2,29\}$	0.53
19								-0.9367(70)	$Q_e\{2,10\}; Q_f\{2,10\}$	
20										
21										
22	2 0 0 0 2, 0 0	$\Sigma_g^+ \leftarrow \Sigma_u^+(v_4+v_5)$	6786.28975(25)	8114.3630	1.1679559(26)	4.5797(62)	0.7045(38)		$P_e\{1,26\}; R_e\{0,34\}$	48/61
23										0.83
24										
25	2 0 0 0 1, 0 1 ^b	$\Pi_u \leftarrow \Pi_g(v_4)$	6804.706648(65)	7417.5658	1.16534366(30)	1.63375(23)		-4.87823(38)	$P_e\{2,32\}; R_e\{1,37\}$	142/172
26								0.05701(36)	$P_f\{2,35\}; R_f\{1,37\}$	0.42
27									$Q_e\{1,16\}; Q_f\{1,18\}$	
28										
29										
30	0 0 3, 0 1	$\Pi_u \leftarrow \Pi_g(v_4)$	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
31								0.189(13)	$P_f\{2,29\}; R_f\{1,26\}$	0.68
32								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)	$P_e\{3,19\} ; R_e\{1,17\}$	36/86
5								-33.49(33)	$P_f\{3,21\} ; R_f\{1,19\}$	0.72
6								75.3(11)	$Q_e\{2,15\}$	
7										
8										
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)		$P_e\{1,16\} ; R_e\{1,14\}$	25/57
10									$Q_f\{1,27\}$	1.21
11										

^a The vibrational assignments correspond to those of the dominant zero order state in the eigenvector composition at low J -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.

The last column gives the number of lines included in the fit and the corresponding standard deviation. The band centre is

$$\tilde{\nu}_c = G'_v - B'_v k'^2 - D'_v k'^4 - G''_v + B''_v k''2 + D''_v k''4.$$

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

Table 2

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

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

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2 1 2 0 1 1, 1-1e 0 0 0 0 0, 0 0e 34 2 22 vda02 0.449 8556.59101
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5 The vibrational states, v' and v'' , are identified using the labels $v_1v_2v_3v_4v_5, l_1l_2l_3l_4l_5, e/f$. 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_c value, in cm^{-1} , is $G'_c - G''_c$.
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.*²³; jac07: Jacquemart *et al.*³⁴; kep96: Keppler *et al.*³; kou94: Kou *et al.*²; lyu06: Lyulin
11 *et al.*³⁵; 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.*²⁵; rin82: Rinsland *et al.*²⁶; 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
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Table 3

$v_1 v_2 v_3 v_4 L_1 L_2 e/f$	G_c	$v_1 v_2 v_3 v_4 L_1 L_2 e/f$	G_c	$v_1 v_2 v_3 v_4 L_1 L_2 e/f$	G_c
0 0 0 0 0, 0 0e	0.00000	1 0 0 0 0, 0 0e	3372.84725	1 1 0 0 1, 0 1f	6052.07572
0 0 0 1 0, 1 0e	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 0f	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 0e	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 0f	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 0e	3933.89754	0 1 1 2 0, 2 0f	6447.81394
0 0 0 2 0, 0 0e	1230.38251	1 0 0 1 0, 1 0e	3968.88384	0 1 1 2 0, 0 0e	6449.09176
0 0 0 1 1, 1-1e	1328.07331	1 0 0 1 0, 1 0f	3968.88384	0 0 2 0 0, 0 0e	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 0e	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 0e	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 0e	6709.02113
0 0 0 3 0, 3 0e	1851.35850	0 1 0 0 3, 0 1f	4138.87768	1 1 0 0 2, 0 0e	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 0f	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 0e	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 0e	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 0e	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 0e	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 0f	2573.53545	1 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 0e	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 0e	7732.76330
0 1 0 0 1, 0 1e	2701.90945	0 1 1 0 0, 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, 1-1f	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 3e	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 0e	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 1 0 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 0e	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

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

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

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

$$D_v = D_0 + \sum_i \beta_i^0 v_i + \sum_{i \leq i'} \beta_{l_i l_{i'}}^0 l_i l_{i'} \quad (4)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

^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.

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	q4Jv1	-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	0.10182	0.01411	E-08	k4455v5	0.09946	0.00130	
z241414	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.

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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
xl4l4	0.82	0.76	K4455	-8.58	-8.61
xl4l5	6.55	6.54	O4455 (E-05)	3.92	16.35
xl5l5	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.

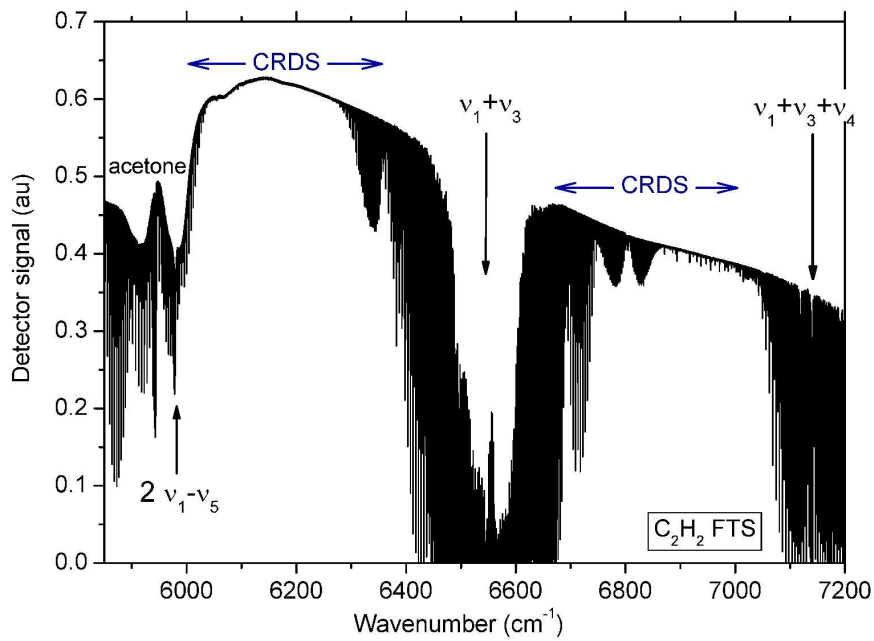


Fig. 1

297x209mm (300 x 300 DPI)

View Only

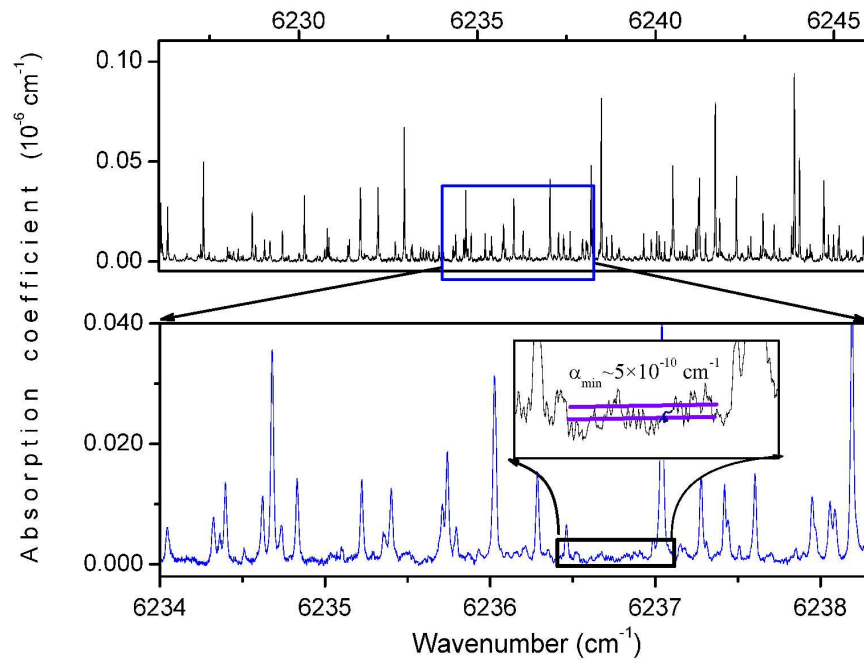
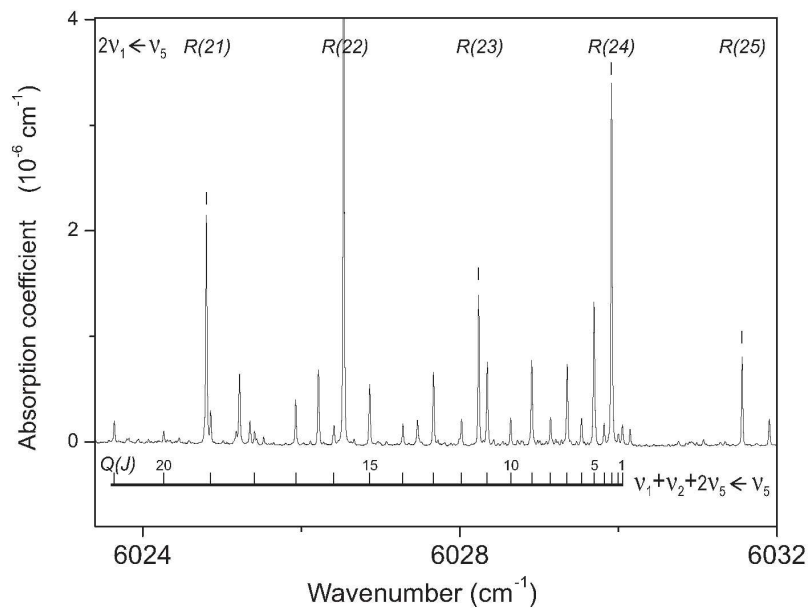


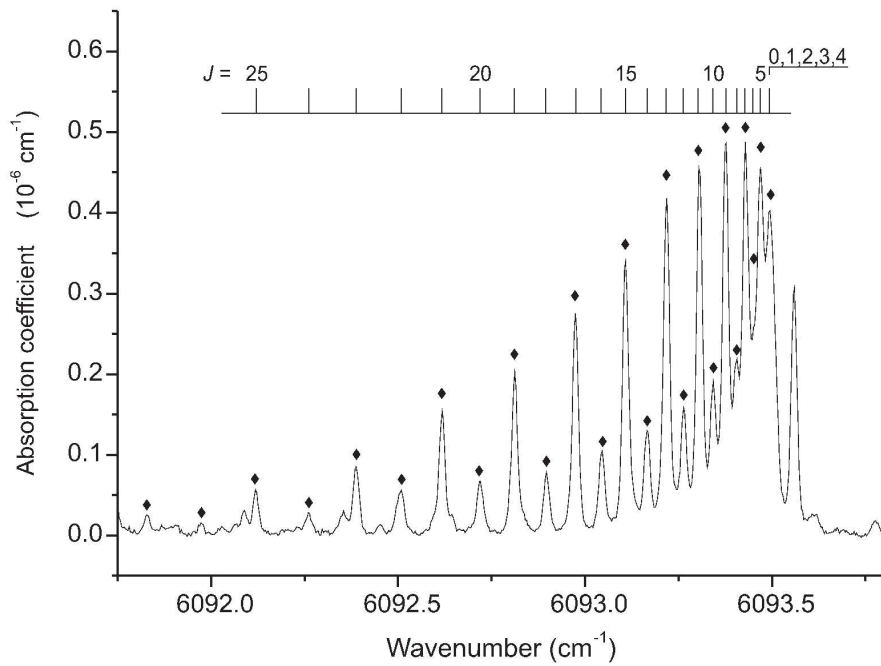
Fig. 2

297x209mm (300 x 300 DPI)

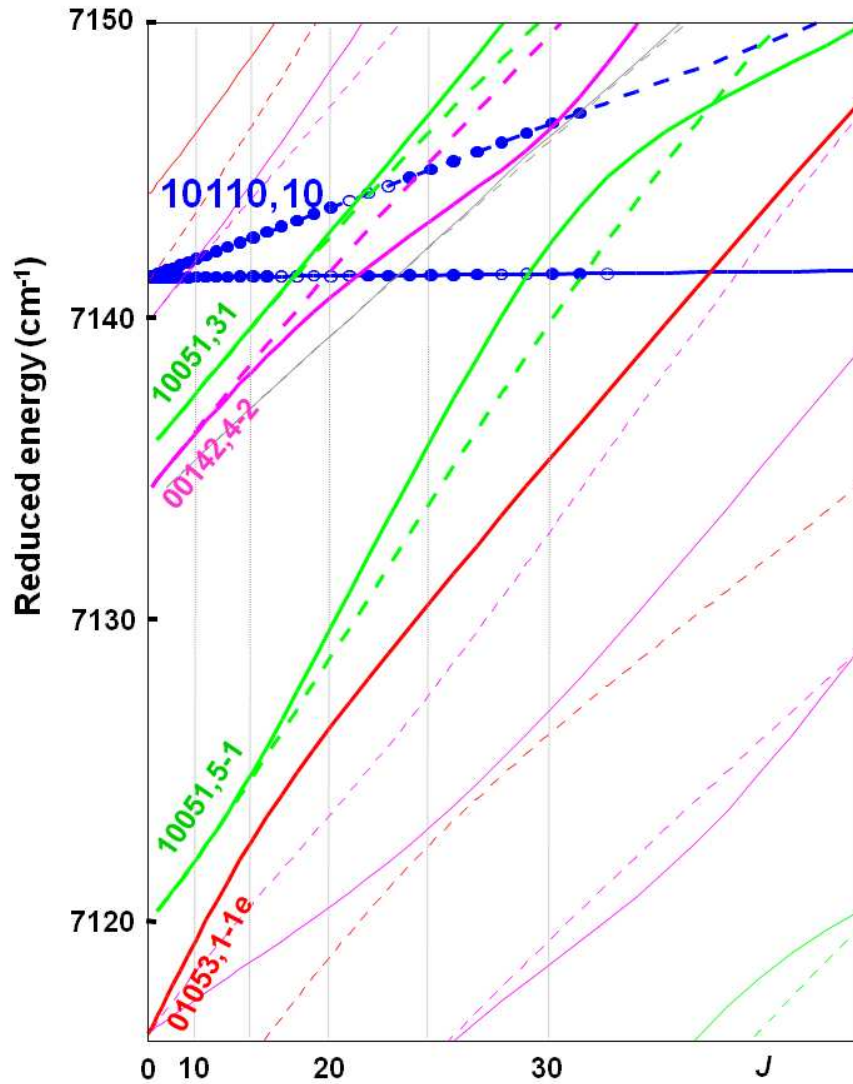


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Molecular Physics: Supplementary Materials (29 pp) for the paper

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{V}_{exp}	unc.	obs-calc	ref

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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

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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

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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
12	5	4	6091.52758	2.00	1.57	rob08
13	5	6	6065.64261	2.00	0.60	rob08
14	6	5	6093.90448	2.00	2.23	rob08
15	6	7	6063.31340	2.00	0.31	rob08
16	7	6	6096.28131	2.00	1.87	rob08
17	7	8	6060.98727	2.00	1.65	rob08
18	8	7	6098.65897	2.00	2.69	rob08
19	8	9	6058.65937	2.00	0.99	rob08
20	9	8	6101.03206	2.00	0.75	rob08
21	9	10	6056.33095	2.00	0.94	rob08
22	10	9	6103.40256	2.00	-0.40	rob08
23	10	11	6053.99971	2.00	0.73	rob08
24	11	10	6105.76986	2.00	0.37	rob08
25	11	12	6051.66509	2.00	1.43	rob08
26	12	11	6108.12965	2.00	0.57	rob08
27	12	13	6049.32029	2.00	-2.01	rob08
28	13	12	6110.47846	2.00	-1.39	rob08
29	13	14	6046.95895	0.0	-14.15	rob08
30	14	13	6112.81825	2.00	-1.64	rob08
31	14	15	6044.61115	2.00	-3.07	rob08
32	15	14	6115.14664	2.00	-0.65	rob08
33	15	16	6042.24021	2.00	-3.62	rob08
34	16	15	6117.45928	2.00	-0.93	rob08
35	16	17	6039.85678	2.00	-3.38	rob08
36	17	16	6119.75534	2.00	-1.57	rob08
37	17	18	6037.45674	0.0	-4.82	rob08
38	18	17	6122.03345	2.00	-2.31	rob08
39	18	19	6035.04278	2.00	-3.70	rob08
40	19	20	6032.60795	0.0	-5.62	rob08

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35	3	3	6093.49350	1.60	-1.64	rob08
36	5	5	6093.46954	1.60	0.93	rob08
37	6	6	6093.45062	1.60	0.07	rob08
38	7	7	6093.42847	1.60	-0.64	rob08
39	8	8	6093.40511	1.60	1.02	rob08
40	9	9	6093.37657	1.60	1.27	rob08
41	10	10	6093.34279	1.60	0.31	rob08
42	11	11	6093.30576	1.60	0.39	rob08
43	12	12	6093.26353	1.60	-0.12	rob08
44	13	13	6093.21849	1.60	1.53	rob08
45	14	14	6093.16577	1.60	0.85	rob08
46	15	15	6093.10828	1.60	1.18	rob08
47	16	16	6093.04575	1.60	2.74	rob08
48	17	17	6092.97447	1.60	2.36	rob08
49	18	18	6092.89664	1.60	2.82	rob08
50	19	19	6092.81223	1.60	4.72	rob08
51	20	20	6092.71895	0.0	6.49	rob08
52	21	21	6092.61777	0.0	9.86	rob08
53	22	22	6092.50668	0.0	13.63	rob08
54	23	23	6092.38570	0.0	18.74	rob08
55	24	24	6092.25582	0.0	27.12	rob08
56	25	25	6092.11723	0.0	39.98	rob08
57	26	26	6091.97126	0.0	59.75	rob08
58	27	27	6091.82845	0.0	98.11	rob08
59	28	28	6091.66122	0.0	128.67	rob08
60	29	29	6091.50089	0.0	183.98	rob08

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57	1	0	6095.83671	0.0	-7.45	rob08
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1						
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3	1	2	6088.78111	1.80	-3.23	rob08
4	2	1	6098.15102	1.80	-3.17	rob08
5	2	3	6086.38597	1.80	-1.99	rob08
6	3	2	6100.44160	1.80	-0.88	rob08
7	3	4	6083.96765	1.80	-2.37	rob08
8	4	3	6102.70850	1.80	-0.42	rob08
9	4	5	6081.52730	1.80	-3.22	rob08
10	5	4	6104.95297	1.80	-0.41	rob08
11	5	6	6079.06668	1.80	-2.70	rob08
12	6	5	6107.17289	1.80	-2.82	rob08
13	6	7	6076.58434	1.80	-2.20	rob08
14	7	6	6109.37384	1.80	-1.89	rob08
15	7	8	6074.08069	1.80	-1.22	rob08
16	8	7	6111.55223	1.80	-1.03	rob08
17	8	9	6071.55422	1.80	-1.14	rob08
18	9	8	6113.70827	1.80	0.19	rob08
19	9	10	6069.00523	1.80	-1.54	rob08
20	10	9	6115.84083	1.80	0.86	rob08
21	10	11	6066.43653	1.80	0.54	rob08
22	11	10	6117.95122	1.80	2.55	rob08
23	11	12	6063.84417	1.80	1.32	rob08
24	12	11	6120.03910	0.0	5.16	rob08
25	12	13	6061.23145	0.0	4.28	rob08
26	13	12	6122.10305	0.0	7.55	rob08
27	13	14	6058.59592	0.0	7.17	rob08
28	14	15	6055.96216	0.0	34.77	rob08

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29	0	1	6620.78612	0.0	2.92	kep96
30	1	0	6625.47265	0.40	0.27	kep96
31	1	2	6618.41276	0.40	0.19	kep96
32	2	1	6627.79094	0.40	0.14	kep96
33	2	3	6616.02469	0.40	0.13	kep96
34	3	2	6630.09174	0.40	0.17	kep96
35	3	4	6613.61931	0.40	0.19	kep96
36	4	3	6632.37464	0.40	0.12	kep96
37	4	5	6611.19616	0.40	0.03	kep96
38	5	4	6634.63961	0.40	0.21	kep96
39	5	6	6608.75549	0.40	0.09	kep96
40	6	5	6636.88587	0.40	-0.01	kep96
41	6	7	6606.29683	0.40	0.12	kep96
42	7	6	6639.11379	0.40	0.19	kep96
43	7	8	6603.81994	0.40	0.16	kep96
44	8	7	6641.32215	0.40	-0.02	kep96
45	8	9	6601.32424	0.40	-0.03	kep96
46	9	8	6643.51131	0.40	0.21	kep96
47	9	10	6598.80998	0.40	0.18	kep96
48	10	9	6645.67998	0.40	0.07	kep96
49	10	11	6596.27572	0.40	-0.21	kep96
50	11	10	6647.82821	0.40	0.20	kep96
51	11	12	6593.72235	0.40	0.17	kep96
52	12	11	6649.95483	0.40	0.05	kep96
53	12	13	6591.14814	0.40	0.13	kep96
54	13	12	6652.05985	0.40	0.25	kep96
55	13	14	6588.55317	0.40	0.32	kep96
56	14	13	6654.14185	0.40	0.10	kep96
57	14	15	6585.93618	0.40	0.10	kep96
58	15	14	6656.20074	0.40	0.23	kep96
59	15	16	6583.29731	0.40	0.27	kep96
60	16	15	6658.23527	0.40	0.16	kep96
61	17	16	6660.24499	0.40	0.21	kep96
62	17	18	6577.94958	0.40	0.16	kep96
63	18	17	6662.22888	0.40	0.20	kep96
64	18	19	6575.23953	0.40	0.12	kep96
65	19	18	6664.18627	0.40	0.24	kep96
66	19	20	6572.50450	0.40	0.23	kep96
67	20	19	6666.11618	0.40	0.19	kep96
68	20	21	6569.74349	0.40	0.24	kep96
69	21	20	6668.01798	0.40	0.22	kep96
70	21	22	6566.95581	0.40	0.16	kep96

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2							
3	22	21	6669.89074	0.40	0.22	kep96	
4	22	23	6564.14092	0.40	0.20	kep96	
5	23	22	6671.73367	0.40	0.16	kep96	
6	23	24	6561.29791	0.40	0.13	kep96	
7	24	23	6673.54605	0.40	0.05	kep96	
8	24	25	6558.42659	0.40	0.45	kep96	
9	25	24	6675.32742	0.40	0.15	kep96	
10	25	26	6555.52559	0.40	0.37	kep96	
11	26	25	6677.07676	0.40	0.08	kep96	
12	26	27	6552.59372	0.40	-0.70	kep96	
13	27	26	6678.79368	0.40	0.05	kep96	
14	28	27	6680.47797	0.40	0.40	kep96	
15	28	29	6546.64155	0.40	0.40	kep96	
16	29	28	6682.12777	0.40	-0.27	kep96	
17	30	29	6683.74429	0.40	-0.31	kep96	
18	31	30	6685.32728	0.40	0.36	kep96	
19	31	32	6537.47461	0.0	-1.47	kep96	
20	32	31	6686.87453	0.40	-0.16	kep96	
21	33	32	6688.38772	0.40	0.04	kep96	
22	34	33	6689.86548	0.40	-0.24	kep96	
23	35	34	6691.30841	0.40	-0.26	kep96	
24	36	35	6692.71575	0.40	-0.70	kep96	
25	37	36	6694.08917	0.40	0.15	kep96	
26	38	37	6695.42938	2.00	3.01	rob08	
27	39	38	6696.72987	2.00	1.35	rob08	
28	40	39	6697.99818	2.00	2.66	rob08	
29	41	40	6699.22990	2.00	2.48	rob08	
30	42	41	6700.42696	2.00	2.65	rob08	
31	43	42	6701.58742	2.00	1.14	rob08	
32	44	43	6702.71495	2.00	1.53	rob08	
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34	1	1	0	1	1,	1 -1e - 0 0 0 1 0,	1 0e
35	0	1	6016.10304	0.0	7010.98	kep96	
36	1	2	6006.72362	0.0	-3.10	kep96	
37	2	1	6016.10076	1.00	1.10	rob08	
38	2	3	6004.33904	0.0	-7.62	rob08	
39	3	2	6018.40521	0.40	-0.53	kep96	
40	4	3	6020.69743	0.40	0.81	kep96	
41	5	4	6022.97640	0.0	4.32	kep96	
42	5	6	5997.11636	0.40	-0.85	kep96	
43	6	5	6025.23100	0.40	-0.79	kep96	
44	6	7	5994.67859	0.0	1.52	kep96	
45	7	6	6027.47457	0.40	-0.84	kep96	
46	7	8	5992.22111	0.40	-0.22	kep96	
47	8	7	6029.70155	0.40	-0.97	kep96	
48	8	9	5989.74831	0.0	-1.38	kep96	
49	9	8	6031.91245	0.40	-0.21	kep96	
50	9	10	5987.26064	0.40	-1.09	kep96	
51	10	9	6034.10508	0.40	-0.24	kep96	
52	10	11	5984.75745	0.40	0.41	kep96	
53	11	10	6036.28031	0.40	0.37	kep96	
54	11	12	5982.23562	0.40	0.48	kep96	
55	12	11	6038.43460	0.0	-1.30	kep96	
56	13	12	6040.57190	0.40	-0.66	kep96	
57	14	13	6042.68903	0.40	-0.20	kep96	
58	14	15	5974.56079	0.40	0.16	kep96	
59	15	14	6044.78576	0.40	0.57	kep96	
60	15	16	5971.96409	0.40	-0.06	kep96	
61	16	15	6046.85959	0.40	-0.07	kep96	
62	16	17	5969.34694	0.40	-0.48	kep96	
63	17	16	6048.91276	0.40	0.88	kep96	
64	17	18	5966.70836	0.0	-1.37	kep96	
65	18	17	6050.94098	0.40	-0.07	kep96	
66	19	18	6052.94661	0.40	0.28	kep96	
67	19	20	5961.36734	0.0	-1.23	kep96	
68	20	19	6054.92695	0.40	0.01	kep96	
69	20	21	5958.66259	0.40	-1.04	kep96	
70	21	20	6056.87851	0.0	-3.55	kep96	
71	21	22	5955.93489	0.40	0.09	kep96	
72	22	21	6058.80939	0.0	-1.50	kep96	

22	23	5953.18371	0.0	2.32	kep96
23	22	6060.71107	0.0	-1.60	kep96
24	23	6062.58446	0.0	-2.21	kep96
25	24	6064.43089	1.00	-1.30	rob08
26	25	6066.24748	1.00	-1.11	rob08
27	26	6068.03331	1.00	-1.97	rob08
28	27	6069.79239	1.00	0.66	rob08

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1	1	6011.41354	0.0	-3.96	kep96
2	2	6011.36793	0.40	0.90	kep96
3	3	6011.29104	0.40	-0.18	kep96
4	4	6011.18986	0.40	-0.01	kep96
5	5	6011.06343	0.40	0.64	kep96
6	6	6010.90917	0.40	-0.56	kep96
7	7	6010.73761	0.0	7.25	kep96
8	8	6010.52421	0.40	-0.12	kep96
9	9	6010.29060	0.40	-0.61	kep96
10	10	6010.02996	0.40	-0.58	kep96
11	11	6009.74144	0.40	-0.37	kep96
12	12	6009.42408	0.40	-0.39	kep96
13	13	6009.08303	0.0	5.12	kep96
14	14	6008.70131	0.40	-0.20	kep96
15	15	6008.29482	0.40	0.26	kep96
16	16	6007.85610	0.40	-0.28	kep96
17	17	6007.38561	0.40	-0.63	kep96
18	18	6006.88307	0.40	-0.31	kep96
19	19	6006.34662	0.40	-0.46	kep96
20	20	6005.77626	0.40	-0.28	kep96
21	21	6005.17354	1.00	2.51	rob08
22	22	6004.52652	0.0	-3.30	rob08

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1	2	6649.53387	0.0	-2.45	kep96
2	1	6658.92994	0.40	0.36	kep96
2	3	6647.16313	0.40	-0.22	kep96
3	2	6661.25277	0.40	0.08	kep96
3	4	6644.78207	0.0	1.84	kep96
4	3	6663.56640	0.0	1.42	kep96
4	5	6642.38663	0.40	0.05	kep96
5	4	6665.86613	0.40	0.27	kep96
5	6	6639.98224	0.40	0.38	kep96
6	5	6668.15470	0.40	0.15	kep96
6	7	6637.56539	0.40	0.00	kep96
7	6	6670.43031	0.40	0.13	kep96
8	7	6672.69184	0.40	0.14	kep96
9	8	6674.93811	0.40	0.16	kep96
9	10	6630.23661	0.40	-0.03	kep96
10	9	6677.16784	0.40	0.20	kep96
11	10	6679.37950	0.40	0.13	kep96
11	12	6625.27359	0.40	0.04	kep96
12	11	6681.57154	0.40	-0.14	kep96
13	12	6683.72929	0.0	-13.68	rob08
14	15	6617.68632	0.40	0.33	kep96
14	13	6685.89151	0.40	-0.16	kep96
15	14	6688.01622	0.40	0.06	kep96
15	16	6615.11172	0.40	-0.97	kep96
16	15	6690.11479	0.40	-0.03	kep96
16	17	6612.51476	0.40	-0.01	kep96
17	16	6692.18850	0.0	2.36	kep96
18	17	6694.22847	0.40	-0.16	kep96
18	19	6607.23803	0.0	-1.32	kep96
19	18	6696.24089	0.40	-0.06	kep96
19	20	6604.56057	0.0	1.38	kep96
20	19	6698.22154	0.40	-0.35	kep96
21	20	6700.17043	0.40	0.05	kep96
22	21	6702.08537	0.40	-0.14	kep96
23	22	6703.96806	2.00	1.51	rob08
24	23	6705.81438	2.00	1.47	rob08

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3	25	24	6707.62513	2.00	0.97	rob08
4	26	25	6709.40088	2.00	0.92	rob08
5	27	26	6711.14099	2.00	0.85	rob08
6	28	27	6712.84552	2.00	0.95	rob08
7	29	28	6714.51362	2.00	0.40	rob08
8	30	29	6716.14627	2.00	0.16	rob08
9	31	30	6717.74298	2.00	-0.32	rob08
10	32	31	6719.30521	2.00	0.32	rob08
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12	0	1	5977.51427	0.40	0.18	kep96
13	1	2	5975.13466	0.40	0.10	kep96
14	2	3	5972.72841	0.40	0.00	kep96
15	3	2	5986.76541	0.40	0.14	kep96
16	3	4	5970.29571	0.40	0.02	kep96
17	4	3	5989.01155	0.40	0.41	kep96
18	4	5	5967.83638	0.40	-0.05	kep96
19	5	4	5991.23008	0.40	-0.08	kep96
20	5	6	5965.35077	0.40	0.09	kep96
21	6	5	5993.42232	0.40	0.02	kep96
22	6	7	5962.83851	0.40	0.03	kep96
23	7	6	5995.58737	0.40	-0.15	kep96
24	7	8	5960.29986	0.40	-0.01	kep96
25	8	7	5997.72582	0.40	0.03	kep96
26	8	9	5957.73491	0.40	0.01	kep96
27	9	8	5999.83703	0.40	-0.05	kep96
28	9	10	5955.14358	0.40	-0.03	kep96
29	10	9	6001.92151	0.40	0.16	kep96
30	10	11	5952.52645	0.40	0.41	kep96
31	11	10	6003.97849	0.40	-0.07	kep96
32	11	12	5949.88214	0.40	-0.11	kep96
33	12	11	6006.00900	0.40	0.30	kep96
34	12	13	5947.21227	0.40	0.01	kep96
35	13	12	6008.01175	0.40	0.03	kep96
36	13	14	5944.51607	0.40	-0.08	kep96
37	14	13	6009.98738	0.40	-0.21	kep96
38	14	15	5941.79401	0.40	0.07	kep96
39	15	14	6011.93618	0.40	-0.11	kep96
40	16	15	6013.85711	0.40	-0.68	kep96
41	16	17	5936.27139	0.40	-0.07	kep96
42	17	16	6015.75196	0.40	-0.09	kep96
43	17	18	5933.47126	0.40	-0.03	kep96
44	18	17	6017.61938	0.40	0.33	kep96
45	18	19	5930.64532	0.40	0.10	kep96
46	19	18	6019.45878	0.40	0.01	kep96
47	19	20	5927.79332	0.40	0.01	kep96
48	20	19	6021.27104	1.00	-0.13	rob08
49	20	21	5924.91493	0.40	-0.69	kep96
50	21	20	6023.05605	0.40	-0.19	kep96
51	21	22	5922.01229	0.40	0.10	kep96
52	22	21	6024.81396	1.00	0.02	rob08
53	22	23	5919.08384	0.40	0.76	kep96
54	23	22	6026.54427	0.40	0.00	kep96
55	23	24	5916.12824	0.40	-0.12	kep96
56	24	23	6028.24675	1.00	-0.43	rob08
57	25	24	6029.92339	0.40	0.73	kep96
58	25	26	5910.14020	0.0	-2.03	kep96
59	25	26	5910.14223	1.00	0.00	rob08
60	26	25	6031.56959	1.00	-1.11	rob08
	27	26	6033.18991	1.00	-1.35	rob08
	27	28	5904.05307	1.00	-1.21	rob08
	28	27	6034.78447	1.00	0.13	rob08
	28	29	5900.97069	1.00	-1.58	rob08
	29	28	6036.35005	1.00	0.13	rob08
	29	30	5897.86472	1.00	-0.26	rob08
	30	29	6037.88729	1.00	-0.68	rob08
	30	31	5894.73186	1.00	-0.61	rob08
	31	30	6039.39751	1.00	-0.97	rob08
	31	32	5891.57465	1.00	-0.15	rob08
	32	31	6040.88041	1.00	-1.03	rob08

32	33	5888.38947	0.0	-2.56	rob08
33	32	6042.33565	1.00	-1.18	rob08
33	34	5885.18526	0.0	1.02	rob08
34	33	6043.76360	1.00	-1.04	rob08
35	34	6045.16427	1.00	-0.59	rob08
36	35	6046.53586	1.00	-1.61	rob08
37	36	6047.88156	1.00	-0.91	rob08

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1	1	5979.83104	0.40	0.16	kep96
2	2	5979.75879	0.40	0.09	kep96
3	3	5979.65048	0.40	0.06	kep96
4	4	5979.50599	0.40	-0.08	kep96
5	5	5979.32567	0.40	0.02	kep96
6	6	5979.10920	0.40	0.05	kep96
7	7	5978.85662	0.40	0.02	kep96
8	8	5978.56795	0.40	-0.04	kep96
9	9	5978.24338	0.40	0.03	kep96
10	10	5977.88276	0.40	0.06	kep96
11	11	5977.48605	0.40	0.02	kep96
12	12	5977.05342	0.40	0.04	kep96
13	13	5976.58463	0.40	-0.12	kep96
14	14	5976.08015	0.40	-0.03	kep96
15	15	5975.53974	0.40	0.06	kep96
16	16	5974.96330	0.40	0.03	kep96
17	17	5974.35099	0.40	-0.01	kep96
18	18	5973.70265	0.40	-0.22	kep96
19	19	5973.01885	0.40	-0.06	kep96
20	20	5972.29919	0.40	0.01	kep96
21	21	5971.54378	0.40	0.11	kep96
22	22	5970.75243	0.40	-0.02	kep96
23	23	5969.92548	0.40	-0.05	kep96
25	25	5968.16492	0.40	0.12	kep96
26	26	5967.23193	0.40	0.87	kep96
27	27	5966.26190	0.40	0.11	kep96
28	28	5965.26233	0.0	5.29	rob08
29	29	5964.21460	0.0	-2.26	kep96
30	30	5963.13898	1.00	-2.31	rob08
31	31	5962.03075	1.00	0.37	rob08
32	32	5960.88468	1.00	0.48	rob08
33	33	5959.70204	1.00	-0.74	rob08

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1	2	6025.36402	1.60	0.57	rob08
2	1	6034.74322	1.60	0.64	rob08
2	3	6022.97521	1.60	-3.19	rob08
3	2	6037.04731	1.60	0.57	rob08
3	4	6020.57831	1.60	1.15	rob08
4	3	6039.33423	1.60	-0.05	rob08
4	5	6018.16161	1.60	2.04	rob08
5	4	6041.60482	1.60	-0.08	rob08
6	5	6043.85769	1.60	-0.54	rob08
6	7	6013.27332	1.60	-1.09	rob08
7	6	6046.09495	1.60	1.09	rob08
7	8	6010.80698	1.60	0.77	rob08
8	7	6048.31212	1.60	0.83	rob08
8	9	6008.31921	1.60	-1.18	rob08
9	8	6050.51224	1.60	2.28	rob08
9	10	6005.81499	1.60	-1.50	rob08
10	9	6052.69018	1.60	0.91	rob08
11	10	6054.84970	1.60	1.15	rob08
12	11	6056.98862	1.60	1.54	rob08
13	12	6059.10540	1.60	1.31	rob08
14	13	6061.19908	1.60	0.30	rob08
15	14	6063.27034	1.60	0.03	rob08
16	15	6065.31774	1.60	-0.09	rob08
17	16	6067.34085	1.60	0.37	rob08
18	17	6069.33758	1.60	0.20	rob08
19	18	6071.30780	1.60	0.09	rob08

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2						
3	20	19	6073.25168	1.60	1.03	rob08
4	21	20	6075.16510	1.60	-0.33	rob08
5	22	21	6077.03420	0.0	-17.13	rob08
6	23	22	6078.90730	1.60	-0.42	rob08
7	24	23	6080.73036	1.60	-3.64	rob08
8	25	24	6082.52869	1.60	-0.98	rob08
9	26	25	6084.29182	1.60	-2.50	rob08
10	27	26	6086.02624	1.60	-1.36	rob08
11	28	27	6087.72967	1.60	0.44	rob08
12	29	28	6089.39896	1.60	-0.08	rob08

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13	1	1	6030.05968	1.00	-0.09	rob08
14	2	2	6030.00839	1.00	-0.29	rob08
15	3	3	6029.92262	0.0	-9.27	rob08
16	4	4	6029.82927	1.00	0.06	rob08
17	5	5	6029.70219	1.00	1.81	rob08
18	6	6	6029.54522	1.00	0.14	rob08
19	7	7	6029.36335	1.00	0.42	rob08
20	8	8	6029.15408	1.00	0.59	rob08
21	9	9	6028.91663	1.00	0.39	rob08
22	10	10	6028.65123	1.00	0.61	rob08
23	11	11	6028.35620	1.00	0.18	rob08
24	12	12	6028.03180	1.00	0.04	rob08
25	13	13	6027.67728	1.00	0.15	rob08
26	14	14	6027.29204	1.00	0.67	rob08
27	15	15	6026.87340	1.00	-0.30	rob08
28	16	16	6026.42368	1.00	0.36	rob08
29	17	17	6025.93981	1.00	0.39	rob08
30	18	18	6025.42158	1.00	0.38	rob08
31	19	19	6024.86791	1.00	0.05	rob08
32	20	20	6024.27767	1.00	-0.98	rob08
33	21	21	6023.65301	1.00	0.15	rob08
34	22	22	6022.97540	0.0	-14.44	rob08
35	23	23	6022.28833	1.00	-0.66	rob08
36	24	24	6021.54899	1.00	-0.80	rob08
37	25	25	6020.77048	1.00	-1.33	rob08

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38	1	2	6357.39495	0.0	-1.53	kep96
39	2	1	6366.76102	0.0	2.78	kep96
40	3	2	6369.03607	0.40	-0.38	kep96
41	4	3	6371.29029	0.40	0.68	kep96
42	5	4	6373.51629	0.0	-1.34	kep96
43	5	6	6347.63817	0.40	0.02	kep96
44	6	5	6375.71997	0.40	-0.41	kep96
45	6	7	6345.13633	0.40	-0.24	kep96
46	7	6	6377.89738	0.40	-0.35	kep96
47	7	8	6342.60927	0.40	-0.81	kep96
48	8	7	6380.05079	0.0	1.25	kep96
49	8	9	6340.05821	0.40	-0.44	kep96
50	9	8	6382.17526	0.40	-0.39	kep96
51	9	10	6337.48183	0.40	-0.34	kep96
52	10	9	6384.27543	0.40	-0.44	kep96
53	10	11	6334.87943	0.40	-1.13	kep96
54	11	10	6386.34978	0.40	-0.27	kep96
55	11	12	6332.25361	0.40	-0.12	kep96
56	12	11	6388.39799	0.40	-0.01	kep96
57	12	13	6329.60165	0.40	0.09	kep96
58	13	12	6390.41961	0.40	0.10	kep96
59	13	14	6326.92397	0.40	0.04	kep96
60	14	13	6392.41372	0.40	-0.66	kep96
61	14	15	6324.22112	0.40	0.38	kep96
62	15	14	6394.38307	0.40	0.65	kep96
63	15	16	6321.49249	0.40	0.66	kep96
64	16	15	6396.32431	0.40	0.90	kep96
65	16	17	6318.73822	0.40	1.13	kep96
66	17	16	6398.23843	0.0	1.29	kep96
67	17	18	6315.95799	0.0	1.61	kep96

18	17	6400.12510	0.0	1.71	kep96
18	19	6313.15250	0.0	2.95	kep96
19	20	6310.31963	0.0	3.15	kep96
20	19	6403.82042	0.0	7.85	kep96
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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2	1	6366.79165	0.40	-0.89	kep96
2	3	6354.98266	0.0	1.27	kep96
3	2	6369.09544	0.40	-0.18	kep96
4	3	6371.37848	0.40	-0.24	kep96
5	4	6373.64173	0.40	0.06	kep96
6	5	6375.88423	0.40	-0.07	kep96
6	7	6345.17784	0.40	-0.57	kep96
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
10	9	6384.64623	0.40	-0.22	kep96
10	11	6335.05415	0.40	-0.01	kep96
11	10	6386.78325	0.40	-0.21	kep96
11	12	6332.47147	0.40	0.00	kep96
12	11	6388.89850	0.40	0.10	kep96
12	13	6329.86783	0.40	0.19	kep96
13	12	6390.99106	0.40	0.14	kep96
13	14	6327.24233	0.40	-0.07	kep96
14	13	6393.06113	0.40	0.46	kep96
14	15	6324.59568	0.40	0.22	kep96
15	14	6395.10762	0.40	0.34	kep96
15	16	6321.92684	0.40	0.31	kep96
16	15	6397.13147	0.40	1.11	kep96
16	17	6319.23564	0.40	0.32	kep96
17	16	6399.12947	0.40	-0.04	kep96
17	18	6316.52186	0.40	0.34	kep96
18	17	6401.10490	0.40	0.52	kep96
18	19	6313.78526	0.40	0.44	kep96
19	18	6403.05474	0.40	0.17	kep96
19	20	6311.02532	0.40	0.40	kep96
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
22	21	6408.75241	0.40	-0.85	kep96
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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3	25	24	6414.21270	0.0	-3.72	kep96
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
8	27	28	6288.07536	0.40	-0.17	kep96
9	28	27	6419.43606	0.0	1.57	kep96
10	28	29	6285.09406	0.40	0.14	kep96
11	29	28	6421.11999	0.0	2.20	kep96
12	29	30	6282.08593	0.0	-0.41	kep96
13	30	31	6279.05515	0.0	2.62	kep96
14	31	32	6275.99562	2.00	3.36	rob08
15	32	33	6272.94931	0.0	44.07	rob08
16	33	34	6269.77634	0.0	-14.87	rob08
17	34	35	6266.63883	0.0	-11.06	rob08
18	35	36	6263.47113	0.0	-9.87	rob08
19	36	37	6260.27984	0.0	-4.37	rob08

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20	2	1	6621.25078	0.0	10.35	rob08
21	3	2	6623.56704	0.0	19.17	rob08
22	3	4	6607.10343	0.0	9.49	rob08
23	4	3	6625.84788	0.0	6.18	rob08
24	4	5	6604.68728	0.40	0.16	kep96
25	5	4	6628.13092	0.0	8.31	kep96
26	5	6	6602.26756	2.00	-0.18	rob08
27	6	5	6630.39432	0.0	2.99	kep96
28	6	7	6599.83786	0.0	1.26	kep96
29	7	6	6632.64070	0.0	-7.84	rob08
30	7	8	6597.39519	0.40	0.73	kep96
31	8	7	6634.89483	0.40	0.22	kep96
32	8	9	6594.94241	0.40	0.64	kep96
33	9	8	6637.12958	0.40	-0.06	kep96
34	10	9	6639.35296	0.40	-0.44	kep96
35	10	11	6589.99654	0.0	-8.58	rob08
36	11	10	6641.56502	0.40	-0.46	kep96
37	11	12	6587.52020	0.40	-0.49	kep96
38	12	11	6643.76483	0.40	-0.56	kep96
39	12	13	6585.02279	2.00	-2.19	rob08
40	13	12	6645.95480	0.0	2.21	kep96
41	13	14	6582.51701	0.40	-0.54	kep96
42	14	13	6648.12626	0.40	-0.27	kep96
43	14	15	6579.99803	0.40	0.10	kep96
44	15	14	6650.28701	0.40	0.34	kep96
45	15	16	6577.46639	0.40	0.75	kep96
46	16	15	6652.43353	0.40	1.07	kep96
47	16	17	6574.92091	0.40	0.68	kep96
48	17	16	6654.56507	0.0	1.71	kep96
49	18	17	6656.68151	0.0	2.68	kep96
50	19	18	6658.78305	0.0	4.67	kep96
51	20	19	6660.86868	0.0	7.14	kep96
52	21	20	6662.93761	0.0	9.62	kep96
53	22	21	6664.98005	2.00	2.59	rob08
54	23	22	6667.01836	0.0	8.42	kep96
55	24	23	6669.03489	0.0	9.33	kep96
56	25	24	6671.04860	0.0	23.83	rob08
57	26	25	6673.02694	0.0	18.73	rob08
58	27	26	6674.94180	0.0	-34.96	rob08
59	28	27	6676.88280	0.0	-48.65	rob08

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52	2	1	6621.25078	2.00	-4.14	rob08
53	2	3	6609.45130	0.0	1.68	kep96
54	3	2	6623.56704	2.00	1.09	rob08
55	3	4	6607.04032	0.0	1.50	kep96
56	4	3	6625.84940	0.0	-10.83	rob08
57	4	5	6604.61508	0.0	3.54	kep96
58	5	4	6628.13207	2.00	-5.45	rob08
59	5	6	6602.16280	0.0	-4.84	kep96

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3	6	5	6630.39207	2.00	-5.36	rob08
4	6	7	6599.70671	0.40	-0.09	kep96
5	7	6	6632.64092	0.0	1.47	kep96
6	7	8	6597.22787	0.40	-0.73	kep96
7	8	7	6634.86306	0.40	0.04	kep96
8	8	9	6594.73261	0.40	0.07	kep96
9	9	10	6592.21804	0.40	-0.04	kep96
10	10	9	6639.25235	0.40	0.04	kep96
11	11	10	6641.41681	0.40	-0.09	kep96
12	12	11	6643.56086	0.40	0.05	kep96
13	12	13	6584.55985	0.40	0.36	kep96
14	14	13	6647.78540	0.40	0.22	kep96
15	14	15	6579.35416	0.40	0.00	kep96
16	15	14	6649.86523	0.40	-0.08	kep96
17	15	16	6576.72114	0.40	-0.01	kep96
18	16	15	6651.92418	0.40	0.09	kep96
19	16	17	6574.06765	0.40	-0.39	kep96
20	17	16	6653.96185	0.40	0.12	kep96
21	17	18	6571.39559	0.40	0.47	kep96
22	18	17	6655.97830	0.40	-0.31	kep96
23	18	19	6568.70295	0.40	0.12	kep96
24	19	18	6657.97436	2.00	-0.86	rob08
25	19	20	6565.99207	0.40	0.28	kep96
26	20	19	6659.95262	0.40	0.40	kep96
27	20	21	6563.26488	0.0	2.19	kep96
28	21	20	6661.91067	0.40	0.31	kep96
29	21	22	6560.51733	0.40	0.96	kep96
30	22	21	6663.85038	2.00	-0.08	rob08
31	22	23	6557.75214	0.0	-1.62	kep96
32	23	22	6665.77469	0.0	1.26	kep96
33	23	24	6554.97873	0.0	2.90	kep96
34	24	23	6667.69576	0.0	15.53	kep96
35	24	25	6552.20259	0.0	18.99	kep96
36	25	24	6669.60784	0.0	36.01	rob08
37	26	25	6671.44819	2.00	-1.05	rob08
38	27	26	6673.31455	2.00	1.12	rob08
39	28	27	6675.16437	2.00	-1.02	rob08

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40	2	1	6611.15540	0.0	1.36	kep96
41	2	3	6599.40144	0.40	0.40	kep96
42	3	2	6613.44986	0.0	-1.57	kep96
43	3	4	6597.00022	0.0	2.70	kep96
44	4	3	6615.73020	0.40	-0.70	kep96
45	4	5	6594.57630	0.40	-0.03	kep96
46	5	6	6592.13773	0.40	0.31	kep96
47	6	5	6620.23566	0.40	0.21	kep96
48	6	7	6589.68183	0.40	1.11	kep96
49	7	6	6622.46191	0.0	1.71	kep96
50	8	7	6624.66646	0.40	0.11	kep96
51	9	8	6626.85377	0.40	0.11	kep96
52	9	10	6582.20285	0.40	0.13	kep96
53	10	9	6629.02212	0.40	0.21	kep96
54	10	11	6579.67387	0.40	0.24	kep96
55	11	10	6631.17111	0.40	0.28	kep96
56	11	12	6577.12618	0.40	0.14	kep96
57	12	11	6633.30032	0.40	0.14	kep96
58	12	13	6574.55954	0.40	-0.23	kep96
59	13	12	6635.40982	0.40	0.16	kep96
60	13	14	6571.97501	0.40	0.39	kep96
61	14	13	6637.49918	0.40	0.20	kep96
62	14	15	6569.37064	0.40	0.27	kep96
63	15	14	6639.56826	0.40	0.42	kep96
64	15	16	6566.74723	0.40	0.42	kep96
65	16	15	6641.61727	0.0	1.34	kep96
66	16	17	6564.10508	0.0	1.39	kep96
67	17	16	6643.64145	0.0	-1.50	kep96
68	17	18	6561.43908	0.0	-1.72	kep96
69	18	17	6645.64858	0.40	0.00	kep96
70	19	18	6647.63631	0.0	3.80	kep96

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20	19	6649.59405	0.40	-0.38	kep96
20	21	6553.33027	0.40	-0.84	kep96
21	20	6651.53381	0.40	-0.22	kep96
22	21	6653.45076	0.40	-0.25	kep96
23	22	6655.34487	0.40	-0.24	kep96
24	23	6657.21588	0.40	-0.15	kep96
24	25	6542.22714	0.40	-0.29	kep96
25	24	6659.06364	0.40	0.11	kep96
26	25	6660.88707	0.40	-0.30	kep96
26	27	6536.54483	0.0	-2.51	kep96
27	26	6662.68668	0.40	-0.63	kep96
28	27	6664.46347	0.40	0.32	kep96
28	29	6530.77873	0.0	-1.30	kep96
29	28	6666.21451	0.40	-0.20	kep96
30	29	6667.94261	0.40	0.78	kep96
31	30	6669.64430	0.40	-0.07	kep96
32	31	6671.34163	0.0	19.43	rob08
33	32	6672.97986	2.00	4.63	rob08
34	33	6674.60629	2.00	2.92	rob08
35	34	6676.20635	2.00	-0.22	rob08
36	35	6677.78919	2.00	4.41	rob08
37	36	6679.34306	2.00	5.08	rob08
38	37	6680.87042	2.00	4.27	rob08
39	38	6682.37526	0.0	5.97	rob08
40	39	6683.85251	2.00	5.10	rob08

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3	4	6596.92189	0.40	0.18	kep96
4	5	6594.46570	0.0	-1.81	kep96
5	4	6617.96094	0.40	0.98	kep96
5	6	6591.99039	0.40	0.32	kep96
6	5	6620.18050	0.40	0.49	kep96
6	7	6589.48976	0.40	0.38	kep96
7	8	6586.96543	0.40	0.02	kep96
8	9	6584.41832	0.40	0.19	kep96
9	8	6626.69694	0.40	-0.01	kep96
10	9	6628.82147	0.40	0.32	kep96
10	11	6579.25259	0.40	-0.97	kep96
11	10	6630.92096	0.40	-0.12	kep96
11	12	6576.63605	0.40	-0.11	kep96
12	11	6632.99702	0.40	0.41	kep96
12	13	6573.99527	0.40	-0.02	kep96
13	12	6635.04749	0.40	-0.11	kep96
13	14	6571.33063	0.40	-0.26	kep96
14	13	6637.06901	0.0	-4.90	kep96
14	15	6568.64018	0.0	-2.71	kep96
15	14	6639.07518	0.40	-0.21	kep96
15	16	6565.93120	0.40	-0.03	kep96
16	15	6641.05185	0.40	-0.04	kep96
16	17	6563.19551	0.40	-0.33	kep96
17	16	6643.00377	0.40	0.51	kep96
17	18	6560.43867	0.0	2.03	kep96
18	17	6644.92820	0.0	-1.13	kep96
19	18	6646.82999	0.40	0.03	kep96
20	19	6648.70500	0.40	0.04	kep96
21	20	6650.55436	0.40	0.15	kep96
31	30	6667.59530	2.00	-0.37	rob08
32	31	6669.15117	2.00	-0.35	rob08
33	32	6670.68019	2.00	0.32	rob08
34	33	6672.18147	2.00	0.92	rob08
35	34	6673.65418	2.00	0.78	rob08
36	35	6675.09993	2.00	1.69	rob08
37	36	6676.51758	2.00	2.71	rob08
38	37	6677.90485	2.00	1.83	rob08

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3	2	6669.01159	2.00	-1.25	rob08
4	3	6671.28227	2.00	-1.82	rob08
5	4	6673.51333	0.0	-21.89	rob08

6	5	6675.76584	2.00	-0.23	rob08
7	6	6677.97604	2.00	-0.44	rob08
8	7	6680.16601	2.00	-0.24	rob08
9	8	6682.33478	2.00	-0.38	rob08
10	9	6684.48344	2.00	0.44	rob08
11	10	6686.60891	2.00	-0.61	rob08
12	11	6688.77171	0.0	57.25	rob08
13	12	6690.79365	2.00	-3.91	rob08
14	13	6692.85757	2.00	-0.96	rob08
15	14	6694.89889	2.00	1.79	rob08
16	15	6696.91191	2.00	-1.07	rob08
17	16	6698.90484	2.00	-1.03	rob08
18	17	6700.87365	2.00	-1.84	rob08
19	18	6702.82017	2.00	-1.40	rob08
20	19	6704.74208	2.00	-1.73	rob08
21	20	6706.63494	0.0	-7.01	rob08
22	21	6708.51334	2.00	-2.40	rob08
23	22	6710.36399	2.00	-0.96	rob08
24	23	6712.18820	2.00	-1.17	rob08
25	24	6713.98758	2.00	-1.22	rob08
26	25	6715.76286	2.00	-0.23	rob08
27	26	6717.50148	0.0	-10.65	rob08
28	27	6719.23101	0.0	-4.84	rob08
29	28	6720.93012	0.0	-4.12	rob08
30	29	6722.60616	2.00	-1.20	rob08

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3	2	6669.10428	1.80	-1.12	rob08
4	3	6671.42780	1.80	-0.10	rob08
5	4	6673.73962	1.80	-0.85	rob08
6	5	6676.04165	1.80	-1.32	rob08
7	6	6678.33436	1.80	-0.86	rob08
8	7	6680.61892	1.80	1.91	rob08
9	8	6682.88923	1.80	1.14	rob08
10	9	6685.14990	1.80	1.69	rob08
11	10	6687.39810	1.80	1.04	rob08
12	11	6689.63513	1.80	0.83	rob08
13	12	6691.86114	1.80	1.59	rob08
14	13	6694.07379	1.80	1.39	rob08
15	14	6696.27483	1.80	2.46	rob08
16	15	6698.46012	1.80	1.17	rob08
17	16	6700.63207	1.80	0.51	rob08
18	17	6702.78981	1.80	0.23	rob08
19	18	6704.93306	1.80	0.76	rob08
20	19	6707.06005	1.80	1.09	rob08
21	20	6709.16989	1.80	1.15	rob08
22	21	6711.26183	1.80	1.12	rob08
23	22	6713.33000	0.0	-3.90	rob08
24	23	6715.38693	1.80	-0.30	rob08
25	24	6717.42321	1.80	3.63	rob08
26	25	6719.43791	0.0	8.19	rob08
27	26	6721.42942	0.0	13.05	rob08
28	27	6723.39842	0.0	20.24	rob08

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1	2	6669.68323	1.60	-0.28	rob08
2	1	6679.08083	1.60	0.07	rob08
2	3	6667.27477	1.60	-0.69	rob08
3	2	6681.37038	1.60	-0.59	rob08
4	3	6683.63333	1.60	-3.88	rob08
5	4	6685.86340	0.0	-15.92	rob08
6	5	6688.09640	1.60	-0.80	rob08
7	6	6690.28922	1.60	-1.62	rob08
8	7	6692.45954	1.60	-0.76	rob08
9	8	6694.60643	1.60	0.72	rob08
10	9	6696.72864	1.60	1.37	rob08
11	10	6698.82480	1.60	-0.43	rob08
12	11	6700.90032	1.60	0.40	rob08
13	12	6702.95221	1.60	0.53	rob08

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3	14	13	6704.98096	1.60	-0.01	rob08
4	15	14	6706.98873	1.60	0.45	rob08
5	16	15	6708.97402	1.60	-0.15	rob08
6	17	16	6710.93861	1.60	-0.70	rob08
7	18	17	6712.88346	1.60	-0.97	rob08
8	19	18	6714.80774	1.60	-2.67	rob08
9	20	19	6716.71621	1.60	-1.98	rob08
10	21	20	6718.60485	1.60	-4.00	rob08
11	22	21	6720.47675	0.0	-6.84	rob08
12	23	22	6722.33785	0.0	-5.87	rob08
13	24	23	6724.18428	0.0	-6.36	rob08
14	25	24	6726.01162	0.0	-14.21	rob08
15	26	25	6727.83735	0.0	-13.45	rob08
16	27	26	6729.64940	0.0	-17.68	rob08
17	28	27	6731.44646	0.0	-29.61	rob08

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17	1	2	6669.72132	2.00	-0.23	rob08
18	2	1	6679.11139	2.00	0.19	rob08
19	2	3	6667.35600	2.00	-2.20	rob08
20	3	2	6681.44407	2.00	1.83	rob08
21	4	3	6683.74000	0.0	-26.19	rob08
22	5	4	6686.08706	2.00	4.51	rob08
23	6	5	6688.39338	2.00	2.69	rob08
24	7	6	6690.69376	2.00	3.95	rob08
25	8	7	6692.98328	2.00	4.23	rob08
26	9	8	6695.26351	2.00	5.88	rob08
27	10	9	6697.52659	2.00	1.60	rob08
28	11	10	6699.77714	0.0	-3.72	rob08

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29	1	2	6799.98045	0.40	-0.09	kep96
30	2	1	6809.33460	0.0	1.25	kep96
31	2	3	6797.58057	0.40	0.22	kep96
32	3	2	6811.60556	0.0	-3.80	kep96
33	3	4	6795.15500	0.40	-0.44	kep96
34	4	3	6813.86008	0.40	-0.34	kep96
35	4	5	6792.70552	0.40	-0.33	kep96
36	5	4	6816.08630	0.40	-0.20	kep96
37	5	6	6790.23109	0.40	-0.53	kep96
38	6	5	6818.28751	0.40	-0.03	kep96
39	6	7	6787.73279	0.40	-0.02	kep96
40	7	6	6820.46326	0.40	-0.28	kep96
41	7	8	6785.20950	0.40	0.05	kep96
42	8	7	6822.61438	0.40	-0.05	kep96
43	8	9	6782.66158	0.40	-0.01	kep96
44	9	8	6824.74062	0.40	0.42	kep96
45	9	10	6780.08907	0.40	-0.20	kep96
46	10	9	6826.84077	0.40	-0.05	kep96
47	10	11	6777.49240	0.40	-0.14	kep96
48	11	10	6828.91581	0.40	-0.43	kep96
49	11	12	6774.87174	0.40	0.30	kep96
50	12	11	6830.96632	0.40	-0.13	kep96
51	12	13	6772.22630	0.40	0.27	kep96
52	13	12	6832.99211	0.40	0.72	kep96
53	13	14	6769.55612	0.40	-0.24	kep96
54	14	13	6834.99139	0.40	0.33	kep96
55	14	15	6766.86255	0.40	0.10	kep96
56	15	14	6836.96529	0.40	-0.13	kep96
57	15	16	6764.14413	0.40	-0.26	kep96
58	16	15	6838.91413	0.40	-0.31	kep96
59	16	17	6761.40187	0.40	-0.33	kep96
60	17	16	6840.83763	0.40	-0.47	kep96
	17	18	6758.63592	0.40	-0.02	kep96
	18	17	6842.73683	0.40	0.47	kep96
	18	19	6755.84551	0.40	-0.17	kep96
	19	18	6844.60947	0.40	0.27	kep96
	19	20	6753.03175	0.40	0.32	kep96
	20	19	6846.45598	0.40	-0.64	kep96

20	21	6750.19360	0.40	0.30	kep96
21	20	6848.28055	0.0	2.00	kep96
21	22	6747.32640	0.0	-4.91	kep96
22	21	6850.07514	0.40	0.12	kep96
22	23	6744.44538	0.40	-0.13	kep96
23	22	6851.84563	0.40	-0.33	kep96
23	24	6741.53626	2.00	0.28	rob08
24	23	6853.59133	0.40	-0.04	kep96
24	25	6738.60346	0.40	0.69	kep96
25	24	6855.31130	0.40	0.05	kep96
25	26	6735.64679	2.00	0.86	rob08
26	25	6857.00557	0.40	0.03	kep96
26	27	6732.66587	2.00	0.35	rob08
27	26	6858.67592	0.0	1.65	kep96
27	28	6729.65896	0.0	-2.65	rob08
28	27	6860.31990	0.0	2.52	kep96
28	29	6726.63446	2.00	0.20	rob08
29	28	6861.93139	0.0	-3.48	kep96
29	30	6723.58415	2.00	0.63	rob08
30	29	6863.52697	2.00	0.24	rob08
30	31	6720.51053	2.00	1.06	rob08
31	30	6865.09311	2.00	0.16	rob08
31	32	6717.42327	0.0	11.11	rob08
32	31	6866.63299	2.00	-0.51	rob08
33	32	6868.14813	2.00	-0.25	rob08
34	33	6869.63782	2.00	0.24	rob08
35	34	6871.10118	2.00	0.10	rob08
36	35	6872.53815	2.00	-0.74	rob08
37	36	6873.95053	2.00	-0.45	rob08
38	37	6875.33752	2.00	0.16	rob08

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1	2	6799.95886	0.40	-0.06	kep96
2	1	6809.34974	0.0	-2.41	kep96
2	3	6797.54668	0.40	-0.17	kep96
3	2	6811.63631	0.40	-0.20	kep96
3	4	6795.10922	0.40	-0.15	kep96
4	3	6813.89385	0.0	-1.35	kep96
4	5	6792.64720	0.40	0.70	kep96
5	4	6816.12807	0.40	-0.11	kep96
5	6	6790.15814	0.40	-0.16	kep96
6	5	6818.33553	0.40	0.11	kep96
6	7	6787.64512	0.40	0.33	kep96
7	6	6820.51686	0.40	-0.04	kep96
7	8	6785.10576	0.40	-0.27	kep96
8	7	6822.67280	0.40	0.25	kep96
8	9	6782.54223	0.40	0.17	kep96
9	8	6824.80250	0.40	0.16	kep96
9	10	6779.95292	0.40	0.01	kep96
10	9	6826.90628	0.40	0.04	kep96
10	11	6777.33908	0.40	0.44	kep96
11	10	6828.98431	0.40	0.09	kep96
11	12	6774.69935	0.40	0.06	kep96
12	11	6831.03488	0.0	-1.34	kep96
12	13	6772.03590	0.40	1.00	kep96
13	12	6833.06238	0.40	0.16	kep96
13	14	6769.34562	0.40	0.12	kep96
14	13	6835.06225	0.40	0.07	kep96
14	15	6766.63196	0.40	0.80	kep96
15	14	6837.03660	0.40	0.53	kep96
15	16	6763.89249	0.40	0.58	kep96
16	15	6838.98336	0.40	-0.49	kep96
16	17	6761.12818	0.40	0.37	kep96
17	16	6840.90589	0.40	0.39	kep96
17	18	6758.33954	0.40	0.67	kep96
18	17	6842.80109	0.40	0.13	kep96
18	19	6755.52501	0.40	-0.18	kep96
19	18	6844.67026	0.40	0.05	kep96
19	20	6752.68660	0.40	-0.18	kep96
20	19	6846.51125	0.0	-1.99	kep96

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20	21	6749.82327	0.40	-0.44	kep96
21	20	6848.33058	0.40	0.59	kep96
21	22	6746.94013	0.0	4.12	kep96
22	21	6850.12027	0.40	-0.17	kep96
22	23	6744.02446	2.00	0.72	rob08
23	22	6851.88564	0.40	1.07	kep96
23	24	6741.08731	0.40	0.35	kep96
24	23	6853.62182	2.00	-0.51	rob08
24	25	6738.12614	2.00	0.43	rob08
25	24	6855.33455	0.40	0.83	kep96
25	26	6735.14081	0.40	0.76	kep96
26	25	6857.00794	0.0	-10.76	rob08
26	27	6732.12975	2.00	-0.28	rob08
27	26	6858.67633	2.00	-0.91	rob08
27	28	6729.09584	2.00	0.14	rob08
28	27	6860.30870	2.00	-0.63	rob08
28	29	6726.03647	2.00	-0.66	rob08
29	28	6861.91479	0.40	-0.15	kep96
29	30	6722.94607	0.0	-8.30	rob08
30	29	6863.49378	2.00	-0.27	rob08
30	31	6719.84739	2.00	-0.09	rob08
31	30	6865.04519	2.00	-1.44	rob08
31	32	6716.71621	2.00	-0.30	rob08
32	31	6866.56613	0.0	-6.55	rob08
32	33	6713.56475	2.00	3.21	rob08
33	32	6868.07015	2.00	-2.01	rob08
33	34	6710.38371	2.00	1.10	rob08
34	33	6869.54193	2.00	-3.15	rob08
34	35	6707.17958	2.00	-0.22	rob08
35	34	6870.98836	2.00	-3.04	rob08
36	35	6872.40660	2.00	-4.51	rob08
37	36	6873.80007	2.00	-4.14	rob08
38	37	6875.16580	2.00	-4.88	rob08

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1	1	6804.69205	1.20	0.51	rob08
2	2	6804.66484	1.20	3.46	rob08
3	3	6804.61422	1.20	-1.91	rob08
4	4	6804.55614	1.20	0.35	rob08
5	5	6804.48103	1.20	0.67	rob08
6	6	6804.38901	1.20	-0.84	rob08
7	7	6804.28394	1.20	-0.29	rob08
8	8	6804.16534	1.20	1.82	rob08
9	9	6804.02720	1.20	-0.50	rob08
10	10	6803.87673	1.20	-0.03	rob08
11	11	6803.72021	0.0	9.50	rob08
12	12	6803.53008	1.20	0.54	rob08
13	13	6803.33264	1.20	-0.59	rob08
14	14	6803.11983	1.20	-1.96	rob08
15	15	6802.89557	1.20	0.38	rob08
16	16	6802.65390	1.20	0.45	rob08

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1	1	6804.67141	1.00	0.08	rob08
2	2	6804.60156	1.00	0.83	rob08
3	3	6804.49370	1.00	-1.14	rob08
4	4	6804.35397	1.00	0.30	rob08
5	5	6804.17509	1.00	-2.12	rob08
6	6	6803.96481	1.00	-0.67	rob08
7	7	6803.72078	1.00	2.30	rob08
8	8	6803.43633	1.00	0.10	rob08
9	9	6803.11959	1.00	0.84	rob08
10	10	6802.76531	1.00	-0.73	rob08
11	11	6802.37915	1.00	1.02	rob08
12	12	6801.95485	1.00	-0.17	rob08
13	13	6801.49674	1.00	-0.01	rob08
14	14	6801.00216	1.00	-1.17	rob08
15	15	6800.47443	1.00	-0.36	rob08
17	17	6799.31211	1.00	-0.34	rob08

18 18 6798.67853 1.00 -0.17 rob08

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1	2	6850.02959	1.00	2.27	rob08
2	1	6859.45260	1.00	0.70	rob08
2	3	6847.64939	1.00	2.79	rob08
3	2	6861.78386	1.00	0.66	rob08
3	4	6845.25661	1.00	0.55	rob08
4	3	6864.10477	1.00	0.42	rob08
4	5	6842.85573	1.00	0.08	rob08
5	4	6866.41496	1.00	-0.24	rob08
5	6	6840.44563	1.00	0.32	rob08
6	5	6868.71577	1.00	0.20	rob08
6	7	6838.02415	1.00	-0.79	rob08
7	6	6871.00601	1.00	0.76	rob08
7	8	6835.59401	1.00	-0.38	rob08
8	7	6873.28470	1.00	0.71	rob08
8	9	6833.15231	1.00	-1.20	rob08
9	8	6875.55194	1.00	0.43	rob08
9	10	6830.70206	1.00	-0.03	rob08
10	9	6877.81008	1.00	2.57	rob08
10	11	6828.23981	1.00	-0.11	rob08
11	10	6880.05218	1.00	0.55	rob08
11	12	6825.76698	1.00	0.27	rob08
12	11	6882.28372	1.00	0.24	rob08
12	13	6823.28206	1.00	-0.10	rob08
13	12	6884.50287	1.00	0.24	rob08
13	14	6820.78571	1.00	-0.20	rob08
14	13	6886.70960	1.00	0.99	rob08
14	15	6818.28711	0.0	9.52	rob08
15	14	6888.90137	1.00	0.47	rob08
15	16	6815.75597	1.00	-0.77	rob08
16	15	6891.07879	1.00	-0.14	rob08
16	17	6813.22269	1.00	-0.19	rob08
17	16	6893.24203	1.00	-0.05	rob08
17	18	6810.67635	1.00	0.88	rob08
18	17	6895.38896	1.00	-0.71	rob08
18	19	6808.11362	1.00	-0.28	rob08
19	18	6897.52166	1.00	0.69	rob08
19	20	6805.53742	1.00	-0.11	rob08
20	19	6899.63487	1.00	-0.29	rob08
20	21	6802.94401	1.00	-1.62	rob08
21	20	6901.73105	1.00	-0.36	rob08
21	22	6800.33892	1.00	1.49	rob08
22	21	6903.80950	1.00	0.73	rob08
22	23	6797.71040	1.00	-1.67	rob08
23	22	6905.86623	1.00	-0.03	rob08
23	24	6795.06930	1.00	0.65	rob08
24	23	6907.90367	1.00	0.86	rob08
24	25	6792.38533	0.0	-20.85	rob08
25	24	6909.91810	1.00	0.80	rob08
25	26	6789.72423	1.00	0.61	rob08
26	25	6911.90918	1.00	0.65	rob08
26	27	6787.02132	1.00	1.46	rob08
27	26	6913.87510	1.00	-0.18	rob08
27	28	6784.29390	1.00	0.16	rob08
28	29	6781.54430	1.00	0.25	rob08

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1	2	6850.03431	1.60	-4.52	rob08
2	1	6859.40296	1.60	0.23	rob08
2	3	6847.64940	1.60	-0.33	rob08
3	2	6861.69639	1.60	1.07	rob08
3	4	6845.24409	1.60	2.69	rob08
4	3	6863.96892	1.60	0.54	rob08
4	5	6842.81379	1.60	-0.01	rob08
5	4	6866.22036	1.60	-1.39	rob08
5	6	6840.36648	1.60	-0.40	rob08
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
5	7	8	6835.41545	1.60	0.75	rob08
6	8	7	6872.86189	1.60	-0.18	rob08
7	8	9	6832.90930	1.60	0.08	rob08
8	9	8	6875.03529	1.60	0.40	rob08
9	9	10	6830.38540	1.60	1.44	rob08
10	10	9	6877.18688	1.60	-0.15	rob08
11	10	11	6827.83825	1.60	-0.50	rob08
12	11	10	6879.31741	1.60	-0.80	rob08
13	11	12	6825.27188	1.60	-1.53	rob08
14	12	11	6881.42781	1.60	-0.35	rob08
15	12	13	6822.68706	1.60	-0.69	rob08
16	13	12	6883.51595	1.60	-0.64	rob08
17	13	14	6820.08055	1.60	-1.00	rob08
18	14	13	6885.58235	1.60	-0.85	rob08
19	14	15	6817.45287	1.60	-1.72	rob08
20	15	14	6887.62760	1.60	-0.08	rob08
21	15	16	6814.80526	1.60	-1.39	rob08
22	16	15	6889.64794	1.60	-1.78	rob08
23	16	17	6812.13593	1.60	-1.55	rob08
24	17	16	6891.64858	1.60	-0.42	rob08
25	17	18	6809.44555	1.60	-1.29	rob08
26	18	17	6893.62338	1.60	-1.79	rob08
27	18	19	6806.73288	1.60	-1.61	rob08
28	19	18	6895.57611	1.60	-1.82	rob08
29	19	20	6803.99732	1.60	-2.84	rob08
30	20	19	6897.50792	1.60	0.98	rob08
31	20	21	6801.24086	1.60	-2.77	rob08
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
42	26	25	6908.55885	0.0	-5.93	rob08
43	26	27	6784.22474	1.60	-0.02	rob08
44	27	26	6910.31435	0.0	-4.62	rob08

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1	1	6854.76329	2.00	3.34	rob08
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1	1	6854.73341	1.40	3.80	rob08
2	2	6854.67152	1.40	1.41	rob08
3	3	6854.58106	1.40	0.26	rob08
4	4	6854.46091	1.40	-0.71	rob08
5	5	6854.31276	1.40	0.30	rob08
6	6	6854.13259	1.40	-0.62	rob08
7	7	6853.92365	1.40	-0.08	rob08
8	8	6853.68288	1.40	-0.99	rob08
9	9	6853.41338	1.40	-0.06	rob08
10	10	6853.11175	1.40	-0.50	rob08

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3	4	6333.09009	2.00	-1.03	rob08
4	5	6330.62667	2.00	-1.86	rob08
5	4	6354.08678	0.40	0.48	kep96
5	6	6328.13225	0.0	2.40	kep96
6	5	6356.26651	0.40	-0.93	kep96
6	7	6325.59206	0.40	0.47	kep96
7	6	6358.40889	0.0	1.50	kep96
7	8	6323.01269	0.40	0.56	kep96
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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15	15	6955.28085	2.00	1.57	rob08
16	16	6955.08740	2.00	2.65	rob08
17	17	6954.87794	2.00	1.28	rob08
18	18	6954.65611	2.00	1.53	rob08
19	19	6954.42587	0.0	7.76	rob08
20	20	6954.17045	2.00	3.60	rob08
21	21	6953.90045	2.00	0.01	rob08
22	22	6953.61181	0.0	-6.70	rob08
23	23	6953.31904	2.00	-1.69	rob08
24	24	6953.00606	2.00	-0.69	rob08
25	25	6952.67448	2.00	-1.78	rob08
26	26	6952.32610	0.0	-2.83	rob08
27	27	6951.96261	2.00	-1.84	rob08

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0	1	6954.57196	1.40	0.52	rob08
1	2	6952.20428	1.40	0.27	rob08
2	1	6961.58856	1.40	0.62	rob08
2	3	6949.82298	1.40	-0.78	rob08
3	2	6963.90302	1.40	-0.58	rob08
3	4	6947.43350	1.40	-0.52	rob08
4	3	6966.21321	1.40	-0.71	rob08
4	5	6945.03867	1.40	-0.55	rob08
5	4	6968.52314	1.40	-0.13	rob08
5	6	6942.64347	1.40	-0.32	rob08
6	5	6970.83380	1.40	-0.89	rob08
6	7	6940.25023	1.40	-0.64	rob08
7	6	6973.14888	1.40	-0.44	rob08
7	8	6937.86194	1.40	0.27	rob08
8	7	6975.46773	1.40	0.96	rob08
8	9	6935.47717	1.40	1.30	rob08
9	8	6977.78816	1.40	2.23	rob08
9	10	6933.09313	1.40	0.67	rob08
10	9	6980.10694	1.40	1.38	rob08
10	11	6930.71285	1.40	2.60	rob08
11	10	6982.42615	1.40	1.65	rob08
11	12	6928.32979	1.40	1.61	rob08
12	11	6984.73702	0.0	-4.76	rob08
12	13	6925.94652	1.40	1.18	rob08
13	12	6987.05974	1.40	3.18	rob08
13	14	6923.56356	1.40	2.57	rob08
14	13	6989.37066	1.40	2.52	rob08
14	15	6921.17524	1.40	0.75	rob08
15	14	6991.67462	1.40	-1.28	rob08
15	16	6918.78628	1.40	0.98	rob08

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2	1	6960.97393	1.80	-1.59	rob08
2	3	6949.21128	1.80	-0.06	rob08
3	2	6963.27674	1.80	-0.55	rob08
3	4	6946.79913	0.0	-8.58	rob08
4	3	6965.55272	1.80	-1.89	rob08
4	5	6944.37850	1.80	-1.41	rob08
5	4	6967.80029	1.80	-2.61	rob08
5	6	6941.92391	1.80	0.49	rob08
6	5	6970.01912	1.80	0.30	rob08
6	7	6939.43420	1.80	-0.80	rob08
7	6	6972.20143	1.80	0.47	rob08
7	8	6936.91336	1.80	0.05	rob08
8	7	6974.35045	1.80	1.10	rob08
8	9	6934.35876	1.80	0.30	rob08
9	8	6976.46741	1.80	2.67	rob08
9	10	6931.77346	1.80	2.19	rob08
10	9	6978.55425	0.0	6.26	rob08
10	11	6929.15946	0.0	6.78	rob08
11	10	6980.57462	0.0	-25.20	rob08
11	12	6926.48031	0.0	-23.19	rob08
12	11	6982.61132	0.0	-9.46	rob08
12	13	6923.81620	0.0	-8.14	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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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

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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

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

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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

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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	11	6812.61749	1.80	0.74	rob08
14	12	13	6753.64987	1.80	3.23	rob08
15	13	12	6814.63674	1.80	-0.54	rob08
16	13	14	6750.96027	1.80	1.13	rob08
17	14	13	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
	11	12	6751.01633	1.80	2.81	rob08
	12	11	6807.32345	1.80	-1.09	rob08

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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
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33	2	0	0	0	2,	0
34			2e	-		0
35				0	0	0
36				1	1,	1
37						1e
38	2	3	6773.80564	1.80	-0.25	rob08
39	3	2	6787.88933	1.80	-0.09	rob08
40	3	4	6771.37157	1.80	-0.14	rob08
41	4	3	6790.15470	1.80	4.84	rob08
42	4	5	6768.91313	1.80	0.35	rob08
43	5	4	6792.38519	1.80	-0.45	rob08
44	5	6	6766.42952	1.80	0.33	rob08
45	6	5	6794.59586	1.80	-1.03	rob08
46	6	7	6763.92010	1.80	-0.94	rob08
47	7	6	6796.78241	1.80	-1.30	rob08
48	7	8	6761.40302	0.0	14.57	rob08
49	8	7	6798.94592	1.80	-0.35	rob08
50	8	9	6758.83128	1.80	-0.30	rob08
51	9	8	6801.08397	1.80	-0.74	rob08
52	9	10	6756.25026	1.80	-0.32	rob08
53	10	9	6803.19949	1.80	0.25	rob08
54	10	11	6753.64956	1.80	3.93	rob08
55	11	10	6805.28929	1.80	-0.74	rob08
56	11	12	6751.01633	1.80	-0.60	rob08
57	12	11	6807.35638	1.80	-0.92	rob08
58	12	13	6748.35916	0.0	-5.53	rob08
59	13	12	6809.40064	1.80	-0.62	rob08
60	13	14	6745.68878	1.80	-0.34	rob08
61	14	13	6811.42159	1.80	-0.54	rob08
62	14	15	6742.98972	1.80	-0.75	rob08
63	15	14	6813.42039	1.80	0.29	rob08
64	15	16	6740.26932	1.80	0.38	rob08
65	16	15	6815.39427	1.80	-1.12	rob08
66	16	17	6737.52529	1.80	0.53	rob08
67	17	16	6817.34819	1.80	0.03	rob08
68	17	18	6734.75775	1.80	-0.40	rob08
69	18	17	6819.27930	1.80	0.74	rob08
70	18	19	6731.96972	1.80	0.44	rob08
71	19	18	6821.18675	1.80	0.05	rob08
72	19	20	6729.15845	1.80	0.14	rob08
73	20	19	6823.07168	1.80	-0.97	rob08
74	20	21	6726.32457	1.80	-0.81	rob08
75	21	22	6723.48708	0.0	16.50	rob08
76	21	20	6824.93540	1.80	-1.00	rob08

22	23	6720.58368	0.0	-10.26	rob08
22	21	6826.78880	0.0	10.88	rob08
23	24	6717.68974	0.0	-5.73	rob08
23	22	6828.59475	1.80	-2.34	rob08
24	23	6830.36549	0.0	-28.26	rob08
25	24	6832.16737	1.80	-0.30	rob08
26	25	6833.95034	0.0	31.77	rob08
27	26	6835.64594	1.80	-0.17	rob08
28	27	6837.32929	0.0	-20.63	rob08
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

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2	2	6780.88370	1.00	-1.25	rob08
3	3	6780.81060	1.00	-0.01	rob08
4	4	6780.70978	1.00	-1.99	rob08
5	5	6780.58761	1.00	-1.08	rob08
6	6	6780.43546	0.0	-6.21	rob08
7	7	6780.27182	1.00	0.73	rob08
9	9	6779.86101	1.00	0.00	rob08
10	10	6779.62860	0.0	6.04	rob08

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2	2	6780.88370	1.60	-1.15	rob08
3	3	6780.81060	1.60	0.51	rob08
4	4	6780.70978	1.60	-0.45	rob08
5	5	6780.58761	1.60	2.52	rob08
6	6	6780.43546	1.60	1.00	rob08
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

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1	2	6667.50737	1.40	-0.77	rob08
2	1	6676.88398	1.40	0.39	rob08
3	2	6679.18234	1.40	-0.06	rob08
4	3	6681.46358	1.40	0.42	rob08
5	4	6683.72915	1.40	3.24	rob08
6	5	6685.97249	1.40	1.81	rob08
7	6	6688.19881	1.40	1.21	rob08
8	7	6690.40782	1.40	1.02	rob08
9	8	6692.60007	1.40	1.54	rob08
10	9	6694.77427	1.40	1.12	rob08
11	10	6696.93085	1.40	-0.29	rob08
12	11	6699.07261	1.40	-0.55	rob08
13	12	6701.19976	1.40	-0.35	rob08
14	13	6703.31219	1.40	-1.01	rob08
15	14	6705.41275	1.40	-1.24	rob08
16	15	6707.50379	1.40	-0.68	rob08
17	16	6709.58713	1.40	-0.06	rob08
18	17	6711.66496	1.40	-0.30	rob08
19	18	6713.74391	0.0	1.56	rob08
20	19	6715.82638	0.0	3.79	rob08
21	20	6717.91519	0.0	4.95	rob08

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1	2	6667.49660	1.80	0.18	rob08
2	1	6676.92300	1.80	-0.55	rob08
3	2	6679.25356	1.80	0.69	rob08
4	3	6681.57382	1.80	2.73	rob08
5	4	6683.87890	1.80	0.77	rob08
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

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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

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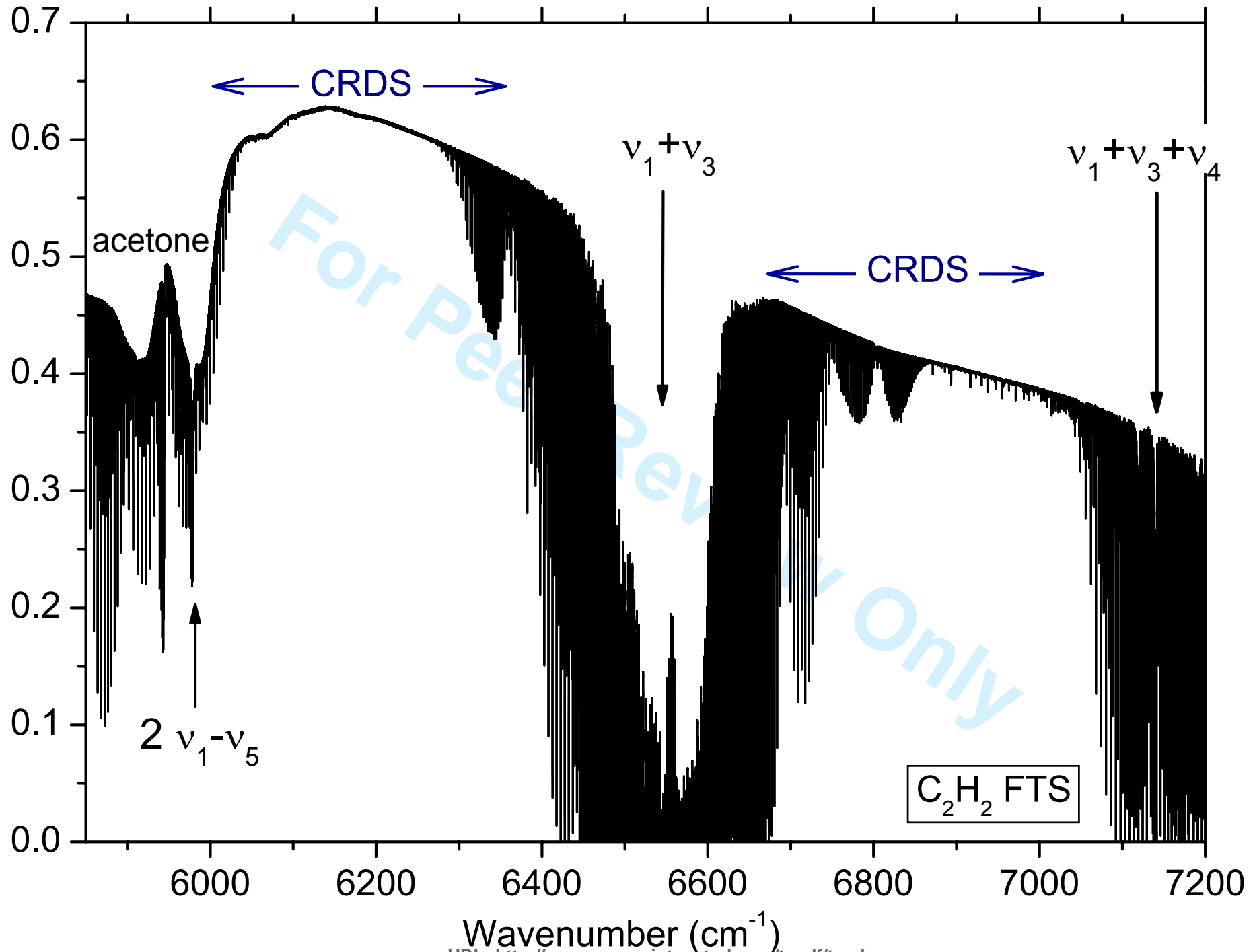
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47URL: <http://mc.manuscriptcentral.com/tandf/tmph>

Fig. 1

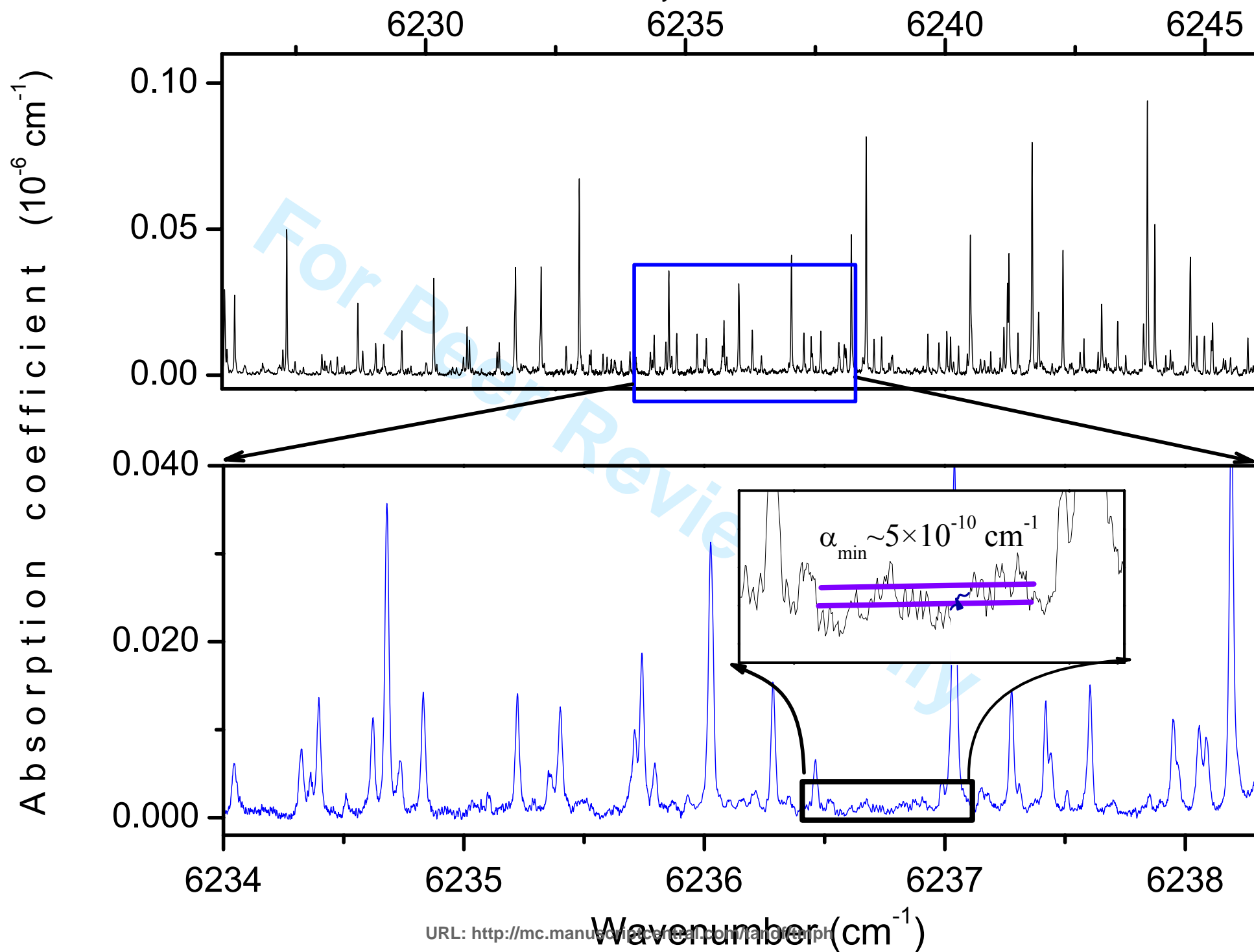


Fig. 2

