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A complete set of line parameters for CH_3Br in the 10-μm spectral region

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Abstract

Using FT spectra (Bruker IFS 120, unapodized FWHM resolution ≈ 0.001 cm^{-1}) of methyl bromide CH_3Br, absolute line positions and intensities, as well as self- and N_2-broadening coefficients have been measured for about 1200 lines, between 880 and 1050 cm^{-1}, in the ν_6 band of both $^{12}CH_3{}^{79}Br$ and $^{12}CH_3{}^{81}Br$ isotopologues. An absolute wavenumber calibration has been performed using the frequencies of the ν_2 band of NH_3. A multispectrum fitting procedure has been used to retrieve simultaneously the line parameters from 6 experimental spectra recorded at different pressures of CH_3Br and N_2. Average absolute accuracies of the measurements have been estimated to be equal to ± 0.0002 cm^{-1} for line positions, to ± 5% for line intensities, and to ± 5-10% for broadening coefficients. A theoretical treatment of measured line positions permitted a prediction of positions and assignments for the whole 10-μm spectral region. Measured line intensities have been analyzed in order to predict the intensities for the whole ν_6 band. The *J* and *K* dependences of the self- and N_2-broadening coefficients have been observed and modeled. These measurements improve the precision of wavenumbers and line intensities previously obtained and lead us, for the first time, to a complete set of self- and N_2-broadening coefficients for which clear *J*- and *K*-dependences have been observed and modeled. A complete line list containing line positions, intensities, self- and N_2-broadening coefficients has then been generated for atmospheric purposes from 820 to 1120 cm^{-1}.

Key words: Methyl bromide; Fourier transform spectroscopy; Infrared; Vibration-rotation; Line intensities; Broadening coefficients; Line list.

1. Introduction

Methyl bromide (CH_3Br) is a trace gas with a tropospheric concentration of about 10 parts per trillion per volume [1] and a total atmospheric life time of 0.6 to 0.9 years [2]. CH_3Br has the highest tropospheric concentration among all long-lived organobromides, making it the primary source of bromine to the stratosphere. Bromine radical in the stratosphere has been shown to contribute significantly to stratospheric ozone loss through coupled reactions with ClO, HO_2 and NO_2 radicals. Although the role of methyl bromide in the stratospheric ozone loss has been well documented, no spectroscopic data is available at the present time for methyl bromide in the atmospheric databases such as HITRAN [3] and GEISA [4]. Complete lists of spectroscopic line parameters are necessary to detect methyl bromide in atmospheric spectra and retrieve its concentrations in the atmosphere. Much work has been devoted to CH_3Br, almost concerning line positions. An extensive review on this molecule was given by Graner [5] for works prior to 1981. References on more recent works can be found in Ref. [6].

The present paper follows a series of recent works devoted to the measurements of line positions and line intensities for the ν_6 band around 10-μm [6], and for the interacting ν_2 and ν_5 bands around 7-μm [7,8]. This work is dedicated to an extensive study of the line parameters of the ν_6 band of CH_3Br. A multispectrum fitting procedure [10] has been used to adjust simultaneously six experimental spectra recorded at different pressures of CH_3Br and N_2. Line positions, intensities, as well as self- and N_2-broadening coefficients have been measured for about 1200 transitions between 880 and 1050 cm^{-1} in the ν_6 bands of $^{12}CH_3{}^{79}Br$ and $^{12}CH_3{}^{81}Br$. The average accuracy of the line parameters obtained in this work has been estimated to be ± 0.0002 cm^{-1} for line positions, ± 5% for line intensities, and ± 5-10% for broadening coefficients.

Measured line positions have been analyzed using the set of codes written by G. Tarrago [9] for C_{3v} symmetric-top molecules. Line intensities have been fitted using two different ways. The first one, in which all interactions have been neglected, led to the vibrational transition dipole moment for the ν_6 band as well as Herman-Wallis factors that describe the J and K dependences of the transition dipole moment. In the second one, the eigenvectors (determined previously from the calculation of line positions) have been used to model the dipole moment matrix with the set of codes written by G. Tarrago [9]. Both line intensity calculations are similar since the ν_6 band is isolated, and the ν_6 level presents weak *l*-type interactions. The extensive measurements for self- and N_2-broadening coefficients has been obtained for large sets of values of *J* and *K*, for which clear *J* and *K* dependences have been observed. Empirical polynomial expansions have been used to model the rotational dependence of the experimental widths. Such a study has, to our knowledge, never been done for CH_3Br.

The experimental procedure and the methodology of the analysis will be first presented respectively in Sections 2 and 3. Then, measurements and calculations of positions, intensities, and broadening coefficients will be presented in Section 4 together with comparisons of line positions and intensities obtained in Ref. [6]. The generation of a complete line list for the whole 10-μm spectral region will be described in Appendix.

2. Experimental procedure

The rapid scan Bruker IFS 120 HR interferometer of the Laboratoire de Dynamique Interactions, et Réactivités (LADIR in Paris) was used to record six spectra (see Figs. 1 and 2). The unapodized spectral resolution used for each spectrum was about 1.1×10^{-3} cm^{-1} (FWHM), corresponding to a maximal optical path difference of 450 cm. The interferometer was equipped with a Ge/KBr beamsplitter, a MCT photovoltaic detector, a Globar source, and an optical filter covering the 800 - 1100 cm^{-1} spectral region. Because of the spectral density of the ν_6 bands of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ (see Figs. 1 and 2) and of the strong values of the self-broadening coefficients, a line by line study could not have been possible with too high pressures of CH_3Br. The choice of the pressure for each spectrum has been done in order to have sufficient information on all the line parameters when analyzing a transition with the multispectrum fitting procedure. The experimental conditions of the six recorded spectra are summarized in Table 1. For all spectra the whole optical path was under vacuum. For five of them a multipass cell of one meter base length was used for a total absorption path of 415 ± 1 cm. One spectrum was recorded using a 30 cm cell. These cells were equipped with KCl windows. The commercial gas sample, furnished by Fluka, with a stated purity of 99.50 % in natural abundances, was used without further purification. Additional spectrum at low pressure of NH_3 has also been recorded with the multipass cell in order to measure line positions belonging to the ν_2 band of NH_3 and to be able to calibrate the wavenumber scale of the CH_3Br spectra.

The temperature of the gas in the cell was recorded with four platinum probes at different places in the cell. The uncertainty on the temperature measurements has been estimated to be ± 1 K. The pressure of the gas was measured with a capacitance MKS Baratron manometer with an accuracy estimated to be ± 1%. Every scan among the 200 recorded for each spectrum has then been individually transformed to spectrum using the Fourier transform procedure included in the Bruker software OPUS package [11], selecting a Mertz phase error correction [12,13]. The spectra were not numerically apodized. They were slightly over sampled (over sampling ratio equal to 2) by post-zero filling the interferograms. Averaging the 200 scans, the signal to noise ratio is nearly equal to 100. Symmetric line profiles were observed on the average spectrum, validating that the phase error was quite well corrected. A discussion on the apparatus function is presented in Section 3.1.1.

3. Description of the spectra analysis

First is described the apparatus function and the numerical treatment of the spectra that have been used in this study. Then the wavenumber calibration, using NH_3 transitions as references, is presented. Finally, conditions in which the multispectrum procedure has been used to retrieve line parameters are given.

3.1. Preliminaries

3.1.1. Apparatus function and numerical treatment of the spectra

For each spectrum, the apparatus function was calculated performing numerically the Fourier transform of the optical weighting function of the interferogram, due to the throughput, truncated at the maximum optical path difference [14].

In the definition of the apparatus function, the aperture and the focal length of the collimator are sensitive parameters: nominal value the focal length (418 mm) was used. In trying to use the nominal value of the aperture (0.65 mm), noticeable discrepancies were systematically observed on fit-residuals of spectra 1 and 2 (see Table 1 for the indexing of the spectra), when analyzing simultaneously the six spectra. These discrepancies are shown on the lower residuals panel of Fig. 3. Spectra 1 and 2 are the two lowest pressure spectra, in which the effect of the apparatus function is the most sensitive since the collisional widths are weak. Using effective value of 0.80 ± 0.05 mm, obtained in spectra 1 and 2 fitting isolated transitions, led to improvement in the residuals, as it can be seen on the upper residuals panel of Fig. 3. Difference between the use of nominal or effective value can lead to deviations of around 2 % on line intensities and broadening coefficients. Note that no signature appears in the residuals of the fit when the spectra are individually adjusted: the line parameters (especially the line intensity and the broadening parameters) compensate the effect of an "erroneous" apparatus function.

A multiplicative channel spectrum, due to the cell windows has been observed in all experimental spectra. Its period is around 0.60 cm^{-1} with maximum peak to peak amplitude of about 5 %. Because the adjusted spectral domains used are always less than the half-period of the channel, the channel can be reproduced by the polynomial expansion that adjusts the continuous background (see Ref. [10]).

3.1.2. Wavenumbers calibration

In the multispectrum fitting procedure, the absolute zero pressure line positions are the parameters that are looked for (considering the line pressure-shifts negligible). This is possible only if the wavenumber scale of the spectra can be calibrated with respect to standard wavenumbers. The HITRAN wavenumber values for the ν_2 transitions of NH_3 [3] were taken as etalon. The quantity $\varepsilon = (\nu_{HITRAN2004} - \nu_{this\ work}) / \nu_{HITRAN2004}$ has been calculated for around 50 transitions between 892 and 1034 cm^{-1}. These lines were adjusted only on spectra 1 and 2, where the most accurate measurements of line positions can be done, and an average of the ε values has been deduced. The mean value $< \varepsilon > = 1.79 \times 10^{-6}$ has been found with a scattering (1SD) smaller than 0.04×10^{-6}, which corresponds to a wavenumber deviation of 1.79×10^{-3} cm^{-1} at 1000 cm^{-1} with a scattering (1SD) of 0.04×10^{-3} cm^{-1}. Considering the scattering of the wavenumber calibration, and the accuracy of the line positions of NH_3 given by HITRAN [3] (better than 0.1×10^{-3} cm^{-1}), the accuracy of the wavenumber calibration has been estimated to be better than 0.1×10^{-3} cm^{-1}. We checked that the ε quantity did not significantly change from spectrum 1 to spectrum 2. As it has been observed previously in Ref. [15], this can be generalized to all spectra recorded with a rapid scan interferometer using the same optical arrangement. The average value of 1.79×10^{-6} has been used for ε in the absolute wavenumber calibration of the six experimental spectra.

3.2. The multispectrum fitting procedure

In the recent previous works on CH_3Br, line parameters have been retrieved with a nonlinear least-squares method that adjusts a calculated spectrum to the experimental spectrum [6,7,8]. We call multispectrum fitting procedure [10] a non linear least-squares method in which several laboratory spectra are analyzed simultaneously, and where the adjusted line parameters are the same for all the spectra.

Since methyl bromide has a significant dipole moment, the self-broadened half-widths of CH_3Br lines are significantly larger than the N_2-broadened half-widths. Indeed dipole–dipole interaction is dominant in self-broadening, whereas for collisions between methyl bromide and the homopolar molecules as nitrogen, this is the dipole–quadrupole interaction which is dominant. It results also that the rotational dependence of the self- and N_2-broadening coefficients are not the same (meaning that the ratio between the self- and N_2-broadening coefficients is not constant). Thus, in laboratory measurements in which appreciable amounts of methyl bromide are used, self-broadening must be considered while determining foreign-gas-broadened linewidths. Line positions (in cm^{-1}), intensities (in $cm.molecule^{-1}$ for natural CH_3Br at 296 K), and broadening coefficients (in $cm^{-1}.atm^{-1}$ at 296 K) were obtained in one simultaneous fit of the six spectra recorded with various experimental conditions. The total partition function calculated in Ref. [6] has been used to convert the line intensity at 296 K. For the broadening coefficients, we supposed that the effects of the collision for $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ are similar, so that the broadening coefficients can be written:

$$\gamma_{CH_3{}^{79}Br/CH_3{}^{79}Br} = \gamma_{CH_3{}^{81}Br/CH_3{}^{81}Br} = \gamma_{CH_3{}^{79}Br/CH_3{}^{81}Br} = \gamma_{CH_3{}^{81}Br/CH_3{}^{79}Br} = \gamma_{self}\ , \qquad (1)$$

$$\gamma_{CH_3{}^{79}Br/N_2} = \gamma_{CH_3{}^{81}Br/N_2} = \gamma_{N_2}\ . \qquad (2)$$

No temperature conversion has been done for the broadening coefficients, since temperatures of all spectra are very closed.

For all spectra, the profile of the line was calculated using a Voigt function. No characteristic signature due to the presence of collisional narrowing or line mixing has been observed in any residual. A study of these collisional phenomena is planed using higher pressures of CH_3Br and N_2.

4. Results

Analyses of the measured line parameters are presented in sub-section 4.1 for the line positions, in sub-section 4.2 for the line intensities, and in sub-section 4.3 for the self- and N_2-

broadening coefficients. Special care has been taken to measure a maximum of transitions with a large scale of *J* and *K* values in all type of branches. This effort was necessary to observe and reproduce the strong rotational dependences for the transition dipole moment squared as well as for the half-widths. The whole set of measured line positions, intensities, as well as self- and N_2-broadening coefficients for the ν_6 band of CH_3Br is given in Table 2, in which the observed transition dipole moments squared are also reported, as well as the differences between the observed and calculated line positions, intensities, self- and N_2-broadening coefficients. It can be noticed that the *A*+ and *A*– components for *K* = 3, 6, 9,… are not resolved. For these transitions, we supposed that the two components *A*+ and *A*– are sufficiently closed to be considerate as a single line noted *A*. In this case, line parameters have been obtained for the sum of the *A*+ and *A*– components, noted *A* in Table 2.

4.1. Line positions analysis

The wavenumber calibration, done from NH_3 line positions measurements (see section 3.2.2), allowed the determination of absolute line positions with a mean accuracy estimated better than ± 0.0002 cm^{-1}. These experimental positions have been compared to those obtained in Ref. [6]. The average discrepancy between line positions of this work and those of Ref. [6] is equal to 0.00024 ± 0.00020 cm^{-1} for 290 lines in common.

As mentioned above, the analysis of the measured line positions has been done using the set of codes written by G. Tarrago [9] for C_{3v} symmetric-top molecules, which takes into account the *l*-type interactions and allows the determination of the eigenvectors. For the ground state, the energy levels are calculated using equation and parameters of Ref. [16]. For the $v_6 = 1$ degenerate upper state, the diagonal matrix elements of the vibration-rotation Hamiltonian as also the *l*-type off-diagonal matrix elements given in Ref. [6,17] have been fitted. The molecular parameters used to fit the measured line positions are given in Table 3, together with those of Ref. [6]. In comparison with Ref. [6], two additional parameters were fitted, q_{2J}, the $J(J+1)$ dependence of the *l*-type parameter q_2 and one sixth order centrifugal distortion parameter H_J. Experimental line positions and the differences between the experimental and calculated line positions are given in Table 2. The average discrepancy of column labeled Dif in Table 2 (for 1166 transitions) is equal to $(0.002 \pm 0.118)\times10^{-3}$ cm^{-1}. The theoretical treatment developed in Ref. [9] appeared to reproduce very well the whole set of measurements.

4.2. Line intensities analysis

Theory on line intensities analysis of C_{3v} molecules as methyl bromide can be found in Refs. [18-20,21]. In order to check the consistency of the measured values, the transition dipole moment squared $\left|\langle A|\mu_Z^t|B\rangle\right|^2$ (in Debye^2) was deduced from the measured line intensities S_{obs} (obtained for natural CH_3Br at 296K in cm.molecule^{-1}, for a transition between two vibrational–rotational states $A \to B$) using the following equation:

$$S_{obs}(T_0) = \frac{1}{4\pi\varepsilon_0}\frac{8\pi^3}{3hc}\frac{\nu_0}{Z_{tot}(T_0)}\exp\left(-\frac{hcE''}{k_B T_0}\right)\left[1-\exp\left(-\frac{hc\nu_0}{k_B T_0}\right)\right]\left|\langle A|\mu_Z^t|B\rangle\right|^2 g_s \,, \qquad (3)$$

where $1/4\pi\varepsilon_0 = 10^{-36}$ erg·cm^3·D^{-2}; h is the Planck's constant equal to $6.6260755 \times 10^{-27}$ erg·s (1 erg = 10^{-7} J); c is the vacuum velocity of light equal to $2.99792458 \times 10^{10}$ cm·s^{-1}; g_s is the statistical weight due to nuclear spin of the lower level ($g_s = 4$ for the A+, A– and E rotational levels of the CH_3Br ground state, for A components if A+ and A- lines are degenerate $g_s = 8$); ν_0 is the transition wavenumber in cm^{-1}; $Z_{tot}(T_0)$ is the total partition function at temperature T_0 (calculated in Ref. [6]); E'', in cm^{-1}, is the energy of the lower level; k_B is the Boltzmann's constant equal to 1.380658×10^{-16} erg·K^{-1}.

Two models have then been used to reduce the data. All measurements and calculations are given in Table 2. For the first model (noted model 1), we decided to neglect all interactions that could perturb the lower and upper states of the transitions. The eigenvectors are approximated to be the $|\mathrm{v}, l, J, K\rangle$ vectors (zero order approximation). In these conditions, the transition dipole moment squared can be written as:

$$\left|\langle A|\mu_Z^t|B\rangle\right|^2 = |R_0|^2 F(m,K) L(J,K,\ell); \qquad (4)$$

$|R_0|^2$ is the vibrational transition dipole moment squared, $F(m,K)$ is the Herman-Wallis factor, and $L(J,K,\ell)$ is the Hönl-London factor. The $F(m,K)$ factor used in this work comes from the work of Watson [21]. The Herman-Wallis factor has been expressed, as it has been done by Pine and Dang-Nhu [22], using the coefficients A_J and A_K in the following expression of $F(m,K)$:

$$F(m,K) = \left(1 + A_J m + \frac{A_K}{2}\left(K'^2 - K^2\right)\right)^2, \qquad (5)$$

where *K'* is the rotational quantum number for the upper state, and *m* is equal to $-J$ for $\Delta J = -1$, 0 for $\Delta J = 0$, and J+1 for $\Delta J = +1$ [21,22]. Because no isotopologue's dependence has been observed, the values obtained for both $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ have been fitted together using Eqs. (10,11). Since the *J* dependence of the transition dipole moments squared is not significant, we chose to fix the coefficient A_J to zero. $|R_0|^2 = 2.688(6)10^{-3}$ Debye^2 and $A_K = 5.4(2)10^{-3}$ have then been obtained. The differences between observed and calculated values, as well as $\left|R_0\right|^2 F(m,K)$ values are listed in Table 2. The ΔK dependence can be easily observed when the values of $\left|R_0\right|^2 F(m,K)$ are plotted versus *J* for each value of *K* (see Fig. 4). The average discrepancy (100 × (obs – calc) / obs) between the experimental and calculated transition dipole moments squared (or line intensities) is equal to –0.01% ± 3.84%.

The second model (model 2) as developed in the set of codes written by G. Tarrago [9] for C_{3v} symmetric-top molecules that takes into account the *l*-type interactions and Coriolis interactions. With this method, the eigenvectors obtained from the treatment of the Hamiltonian, can be described as a linear combination of the zero-order basis wavefunctions $\left|\mathrm{v}, l, J, K\right\rangle$. The matrix elements of the M-reduced transition moment [6,19,23] for perpendicular bands are given by:

$$\left\langle v_6 = 0, l = 0; J, K \left\| \mu_Z^t \right\| v_6 = 1, l = \pm 1; J, K \pm 1 \right\rangle = \pm \frac{1}{2}\left[d_6 \pm d_6^{(2)}(2K \pm 1)\right] F_{01}^{\pm}(J,K), \qquad (6)$$

$$\left\langle v_6 = 0, l = 0; J, K \left\| \mu_Z^t \right\| v_6 = 1, l = \pm 1; J', K \pm 1 \right\rangle = \pm \frac{1}{2}\left[d_6 \pm d_6^{(2)}(2K \pm 1)\right] F_{11}^{\pm}(m,K). \qquad (7)$$

$\mathrm{d}_6 = \dfrac{\partial \mu}{\partial q_6}$ is the leading term of the dipole moment transition and $\mathrm{d}_6^{(2)}$ represents a correction factor in *K* [19]. The *F* function for perpendicular bands, as defined in Ref. [19], depends on *m* and *K*:

$$F_{01}^{\pm}(J,K) = -\frac{[2J+1]^{1/2}}{[J(J+1)]^{1/2}}\left[(J \mp K)(J \pm K + 1)\right]^{1/2}, \qquad (8)$$

$$F_{11}^{\pm}(m,K) = \pm \frac{m}{|m|}\left[\frac{(m \pm K)(m \pm K + 1)}{|m|}\right]^{1/2}. \qquad (9)$$

The *F* function is also called Höln-London factor, but is different from a factor 4 to the expression of $L(J,K,\ell)$ in order to have consistency with Eqs. (4) and (5). The following expression of $L(J,K,\ell)$ [23] has been used:

$$L(J,K) = (J + K\Delta K + 2)(J + K\Delta K + 1)/4(J+1) \;\; (\Delta J = +1), \tag{10}$$

$$L(J,K) = (2J+1)[J(J+1) - K(K+\Delta K)]/4J(J+1) \;\; (\Delta J = 0), \tag{11}$$

$$L(J,K) = (J - K\Delta K - 1)/4J \;\; (\Delta J = -1). \tag{12}$$

For $K = 0$, the Hönl-London factors from Ref. [22] used for model 1 in Eqs. (10-12) and those from Refs. [6,9,18-20] used for model 2 and reported in Eqs. (8,9) have to be multiplied by a factor 2. This is due to the statistical weight g_{KJ} which is included in the Hönl-London factors. Indeed, in these expressions, the value of g_{KJ} has been chosen equal to 2J+1, which is true for $K \neq 0$, but not for $K = 0$ where the statistical weight g_{KJ} is equal to 2×(2J+1). Note that in the work of Hertzberg [24], the g_{KJ} statistical weight has deliberately not been included in the expression of the Hönl-London factors.

Supposing that the l-type interactions of the levels are weak (the eigenvectors are close to $\left|\mathrm{v}, l, J, K\right\rangle$ vectors), it is possible to compare the intensity parameters deduced from both methods: d_6 should be close to $|R_0|$. However, due to the fact that the parameter d_6 in Eqs. (6,7) is inside the brackets whereas in Eq. (4) $|R_0|^2$ is outside the parentheses, no direct comparison can be done between the correction factor $d_6^{(2)}$, and the Herman-Wallis coefficient A_K given in Refs. [22,23]. We checked that the two polynomial expressions $\left|R_0\right|^2 F(m,K)$ for model 1, and $\left[d_6 \pm d_6^{(2)}(2K \pm 1)\right]^2$ for model 2 give very close results for same J and K. If differences are observed between the two calculations, it should come from the effects of l-type interactions neglected in model 1.

Values equal to 0.05188(4) and 0.05176(4) Debye have been obtained for d_6 in the case of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$, respectively. The correction factor $d_6^{(2)}$ have been found equal to $1.41(4)\times10^{-4}$ Debye for both $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ isotopologues. The average discrepancy between observed and calculated intensities using model 2 is equal to 0.2% ± 3.7% (100 × (obs – calc) / obs). The values of $|R_0|$ and d_6 obtained respectively using model 1 and 2 are very close, as well as the standard deviation on the discrepancy between observed and calculated intensities (3.8% with model 1, and 3.7% with model 2). However, it can be seen that a discrepancy (2-8%) between both calculations appears for K = 1 and 2 sub-branches and increases with high J values (between 30-60). The difference between the results of the two models is due to effects of l-type interactions for close levels having K = 1 and 2, and high J values. For the other transitions, it seems that l-type interactions could be neglected for the line intensities analysis.

Comparisons with experimental results of Ref. [6] led to an average discrepancy between the observed line intensities of this work and those of Ref. [6] equal to –2.3% ± 5.4% (100 × (this work – Ref. [6]) / Ref. [6]) for 290 lines in common. If we use the calculated line intensities of Ref. [6] and our measured line intensities (around 1200 transitions), an average discrepancy of –5.6 ± 7.0 % (100 × (this work – Ref. [6]) / Ref. [6]) is found. These discrepancies are too large to be only due to the experimental accuracy of both studies. Indeed, due to a lack of measured line intensities in Ref. [6], especially for values of *K* greater than 5, the *K* dependence of the M-reduced transition moment has not been taking account in Ref. [6]. The effect can be seen in Table 4 and 5 of Ref. [6], where systematic negative discrepancies between the calculated and observed line intensities are observed for transitions with $\Delta K = +1$ and high value of *K*, whereas systematic positive discrepancies are observed for transitions with $\Delta K = -1$ and high value of *K*. The values of d_6 = 0.05369(9) and 0.05352(9) Debye, obtained for $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ respectively [6], are 3.5% different to the value we obtained using model 2, resulting in a 7% mean difference on the line intensities.

4.3. Self- and N_2-broadening coefficients analysis

Extensive measurements of broadening coefficients, obtained for various values of *K* and for a large scale of *J* values, can allow the study of the rotational dependence (in *J* and *K*) of broadening coefficients. Such a work requires a great amount of accurate measurements. For C_{3v} molecules, the study of Nemtchinov et al. [25] on NH_3, and the study on CH_3D of Predoi-Cross et al. [26,27] can be cited as recent works dealing with the rotational dependence of broadening coefficients for large sets of *J* and *K* values. For methyl bromide, such a study has, to our knowledge, never been done. The experimental self- and N_2-broadening coefficients, obtained for *J* and *K* values ranging from 0 to 55 and 0 to 9 respectively, are listed in Table 2. In order to correctly model the line widths, we chose to fit the broadening coefficients for each value of *J* as a function of *K*. As it has been observed in numerous works concerning C_{3v} molecules [25-31], for a set of broadening coefficients with same value of *J*, the widths decrease with *K*. Each set of same value of *J* was fitted by a polynomial expansion of order two in *K* (fixing the first-order term to zero):

$$\gamma_J(K) = a_J^0 + a_J^2 K^2 . \qquad (13)$$

Example of these fits is given in Fig. 5 for *J* = 7, 10, 20, 35. The two coefficients a_J^0 and a_J^2 obtained for each set of same value of *J* have then been plotted versus *J* in Figs. 6 and

7 for the self-broadening coefficients respectively, and in Figs. 8 and 9 for the N_2-broadening coefficients. As it can be observed in these figures, the zero and second order coefficients are monotonously *J* dependent, and can be fitted by effective polynomial expansion in *J*.

The polynomial expansions chosen to fit the a_J^0 and a_J^2 coefficients obtained for the self-broadening coefficients are equal to:

$$a^0_{J,self} = a^{0,0}_{self} + a^{0,1}_{self} J + a^{0,2}_{self} J^2 + a^{0,3}_{self} J^3 + a^{0,4}_{self} J^4 + a^{0,5}_{self} J^5 . \quad (14)$$

$$a^2_{J,self} = a^{2,0}_{self} + a^{2,1}_{self} J + a^{2,2}_{self} J^2 + a^{2,3}_{self} J^3 + a^{2,4}_{self} J^4 + a^{2,5}_{self} J^5 + a^{2,6}_{self} J^6 , \; J \leq 39. \quad (15)$$

$$a^2_{J,self} = a^{2,0}_{self} + a^{2,1}_{self} J \text{ , for } J \geq 40. \quad (16)$$

For the N_2-broadening coefficients, we used:

$$a^0_{J,N_2} = a^{0,0}_{N_2} + a^{0,1}_{N_2} J + a^{0,2}_{N_2} J^2 + a^{0,3}_{N_2} J^3 . \quad (17)$$

$$a^2_{J,N_2} = a^{2,0}_{N_2} + a^{2,1}_{N_2} J + a^{2,2}_{N_2} J^2 + a^{2,3}_{N_2} J^3 + a^{2,4}_{N_2} J^4 + a^{2,5}_{N_2} J^5 \text{ , for } J \leq 16. \quad (18)$$

$$a^2_{J,N_2} = a^{2,0}_{N_2} + a^{2,1}_{N_2} J \text{ , for } J \geq 17. \quad (19)$$

The coefficients resulting from the fits in *J* of the a_J^0 and a_J^2 parameters are summarized in Table 4 for both self- and N_2-broadening coefficients. All these parameters allowed us to calculate the self- or N_2-broadening coefficients for any value of *J* and *K*. Because of the lack of measurements for low and high values of *J* and to avoid any extrapolation, we decided to constrain the self-broadening coefficient a_J^0 to the value of 0.380 for $J < 4$, and to the value of 0.150 for $J > 52$. In the same way, we chose to constrain the N_2-broadening coefficient a_J^0 to the value of 0.090 when $J > 55$. This empirical treatment has been used to calculate the self- and N_2-broadening widths for the line list presented in Appendix, where a discussion on the limit of the extrapolation of this model is also discussed. Experimental and calculated self- and N_2-broadening coefficients are plotted for each value of *K* and versus *J* in Figs. 10 and 11. The discrepancies between experimental and calculated broadening coefficients are presented in column named %self and %N_2 of Table 2. The average discrepancy %self is equal to 0.8% ± 6.4 %, and the average discrepancy %N_2 is equal to –0.3% ± 3.3 %. The *J* and *K* dependences of the measurement is reproduced with accuracy better than 10 % for the self-broadening coefficients, and around 5 % for the N_2-broadening coefficients.

5. Conclusion

Absolute line positions, intensities, self- and N_2-broadening coefficients have been measured for around 1200 transitions belonging to the ν_6 band of CH_3Br near 10 μm. Constants for the energy of the $v_6 = 1$ level, as well as intensity parameters for ν_6 band have been deduced and can be considered as an improvement of line positions and intensities previously obtained in Ref. [6]. Measurements of numerous self- and N_2-broadening coefficients for different values of J and K led to a fitting of self- and N_2-broadening coefficients. All the parameters obtained in this work allowed to generate a complete line list for atmospheric observation of CH_3Br transitions around 10 μm (see Appendix).

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Appendix

The line list is available upon requests to the authors, and will be proposed to the HITRAN [3] and GEISA [4] databases. An extract of this list is presented in Table 5.

In order to produce a complete line list of transitions for the ν_6 band of CH_3Br, interpolation and extrapolation of our measurements have been done. All allowed transitions that have line intensities greater than 10^{-26} cm.molecule^{-1} (for a natural CH_3Br at 296K) have been generated. 14909 lines corresponding to rotational quanta numbers J and K, respectively included between 0 and 59, and 0 and 22, have been calculated. Line positions have been calculated using the spectroscopic constants of this work for the rovibrational levels of the ν_6 state, and those of Ref. [16] for the rovibrational levels of the ground-state. For line intensities, we chose the calculation using G. Tarrago's set of codes [9] which include the *l*-type interactions. Using the values of $\left|R_0\right|^2$ and A_K (model 1), and the values of d_6 and $\mathrm{d}_6^{(2)}$ (model 2), the calculated line intensities obtained using both models have been compared. The average ratio between the results of the two models is equal to 0.994±0.012 (average on 14909 transitions). For the self- and N_2-broadening coefficients, the model developed in Section 4.3 has been used to calculate both widths.

We used for transitions with J less than 55 and K less than 9, an error code [3] of 4 (10^{-4} to 10^{-3} cm^{-1}) for positions, 6 (2-5%) for intensities, 5 (5-10%) for self-broadening coefficients, and 6 (2-5%) for air-broadening coefficients. Because the reliability of the extrapolation (for positions, intensities, and widths) is not known, the uncertainty codes of extrapolated calculations have been degraded. For J greater than 55, and for K greater than 9, we chose the error codes 3 (10^{-3} to 10^{-2} cm^{-1}) for line positions, 5 (5-10%) for intensities, 4 (10-20%) for self-broadening coefficients, and 5 (5-10%) for air-broadening coefficients. The error codes for the temperature-dependence exponent and for the air-shifting coefficients have been fixed to 1 (default value). All these codes are those of the HITRAN database and can be found in Ref. [3].

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Captions of tables

Table 1. Experimental conditions and characteristics of the recorded spectra

Table 2. Line parameters obtained in this study for the ν_6 bands of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$

Table 3. Molecular parameters of the ν_6 band of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ (cm^{-1})[a]

Table 4. Empirical coefficients of Eqs. (18-23) modeling the rotational dependence of self- and N_2-broadening widths

Table 5. Extract of the line list of the ν_6 band of CH_3Br around 10 μm

Captions of figures

Fig. 1. Overview of the 6 spectra recorded in this work with the Bruker IFS 120 HR interferometer of the LADIR. We assigned a number from 1 to 6 to these experimental spectra (see Table 1 for details).

Fig. 2. Spectral region of the ^{P}Q branch of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ for $K = 4$ in the six spectra recorded in this work. (see Table 1 for the spectra numbers)

Fig. 3. Multispectrum fitting of an isolated transition centered at 1035.932 cm^{-1}. The lower residuals panel corresponds to the residual obtained from the multispectrum fitting procedure using nominal value of the aperture, whereas the upper residuals panel is obtained using effective value of the aperture (see section 3.1.1). Signatures observed for the two lowest pressure spectra (#1 and #2: see Table 1 for the numbering of spectra) disappear when using effective values of the aperture.

Fig. 4. Experimental and calculated transition dipole moments squared of the ν_6 band of CH_3Br. Open symbols represents $\Delta K = +1$ transitions, whereas black symbols are used for $\Delta K = -1$ transitions. Squared symbols have been used for $\Delta J = 0$ transitions, and up- and down-triangles have been employed respectively for $\Delta J = -1$ and $\Delta J = +1$ transitions. Black lines represent calculation done using model 1 (see text).

Fig. 5. Example of the polynomial fit in K (see Eq. 13) of the self- and N_2-broadening widths for sets of measurements corresponding to $J = 7$, $J = 10$, $J = 20$, and $J = 35$. The open squares and triangles symbols represent respectively the measured self- and N_2-broadening widths, whereas the black squares and triangles have been used to reproduce respectively the calculated self- and N_2-broadening widths.

Fig. 6. Parameters a_J^0 deduced from the fit of the measured self-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eq. (14). The error bars are 1SD.

Fig. 7. Parameters a_J^2 deduced from the fit of the measured self-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eqs. (15,16). The error bars are 1SD.

Fig. 8. Parameters a_J^0 deduced from the fit of the measured N_2-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eqs. (17). The error bars are 1SD.

Fig. 9. Parameters a_J^2 deduced from the fit of the measured N_2-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eq. (18,19). The error bars are 1SD.

Fig. 10. J and K dependence observed and calculated for all the self-broadening coefficients measured in this work. The squared symbols symbolize the measured widths, and the continuous line has been used to represent the calculated widths using the algorithm described in section 4.3.

Fig. 11. J and K dependence observed and calculated for all the N_2-broadening coefficients measured in this work. The squared symbols symbolize the measured widths, and the continuous line has been used to represent the calculated widths using the algorithm described in section 4.3.

Table 1. Experimental conditions and characteristics of the recorded spectra

Unapodized apparatus function	
Maximum optical path difference	450 cm
FWHM	$\approx 1.1 \times 10^{-3}$ cm^{-1}
Nominal aperture radius	0.65 mm
Effective aperture radius	0.80 mm
Collimator focal length	418 mm
Absorbing sample	
Natural CH_3Br	50.54 % of $CH_3{}^{79}Br$
	49.46 % of $CH_3{}^{81}Br$
Stated purity	99.50 %
Experimental conditions	
S/N ratio	≈ 100

#	CH_3Br pressure (mbar)	N_2 pressure (mbar)	Temperature (K)	Absorption path (cm)
1	0.471_2	0	298.1_5	415
2	0.874_5	0	297.1_5	415
3	4.73_8	0	298.1_5	415
4	7.20_0	0	298.1_5	30
5	2.03_0	25.3_0	297.5_5	415
6	3.37_6	32.9_0	296.4_5	415

Table 2. Line parameters obtained in this study for the ν_6 bands of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$

Assignment	Position	Dif	S_{obs}	$\lvert R\rvert^2_{obs}$	%1	%2	γ_{self}	%self	γ_{N_2}	%N_2
81 RP(5,A+, 0)	954.17981	-0.05	1.96E-22	2.74E-03	1.3	1.9	0.3934	-2.1	0.1265	2.0
79 RP(5,A+, 0)	954.22797	-0.03	1.98E-22	2.72E-03	0.4	0.0	0.3857	-0.1	0.1269	1.7
79 RR(5,A+, 0)	961.22084	0.00	3.46E-22	2.69E-03	-0.5	-0.8	0.3820	0.9	0.1242	3.9
79 RR(6,A+, 0)	961.84102	-0.01	3.84E-22	2.66E-03	-1.6	-2.0	0.3909	0.2	0.1212	4.8
79 RR(7,A+, 0)	962.45857	-0.01	4.31E-22	2.71E-03	0.2	-0.2	0.4015	-0.4	0.1202	4.0
79 RR(8,A+, 0)	963.07344	-0.07	4.67E-22	2.71E-03	0.1	-0.2	0.3962	3.2	0.1205	2.2
81 RR(9,A+, 0)	963.60176	-0.01	4.78E-22	2.64E-03	-2.1	-2.0	0.4090	2.3	0.1176	3.2
81 RP(10,A+, 0)	950.91204	-0.01	4.05E-22	2.86E-03	6.0	6.6	0.4572	-6.3	0.1173	1.9
79 RP(10,A+, 0)	950.94763	-0.05	3.94E-22	2.73E-03	0.9	0.6	0.4247	0.8	0.1167	2.5
81 RP(12,A+, 0)	949.58752	-0.01	4.36E-22	2.71E-03	0.3	1.0	0.4388	1.9	0.1172	-0.8
81 RP(14,A+, 0)	948.25317	0.02	4.78E-22	2.73E-03	1.2	2.1	0.4357	6.2	0.1124	0.7
79 RP(14,A+, 0)	948.27856	-0.02	4.80E-22	2.69E-03	-0.4	-0.9	0.4671	-1.0	0.1121	1.0
81 RP(15,A+, 0)	947.58227	0.00	4.89E-22	2.72E-03	0.8	1.0	0.4645	0.9	0.1111	0.6
79 RP(15,A+, 0)	947.60509	-0.05	4.90E-22	2.68E-03	-1.0	-1.3	0.4685	0.0	0.1107	1.0
81 RP(19,A+, 0)	944.87449	0.01	4.84E-22	2.61E-03	-3.3	-2.4	0.4692	1.9	0.1054	1.2
79 RP(19,A+, 0)	944.88694	0.01	4.81E-22	2.54E-03	-5.9	-6.2	0.4401	8.7	0.1054	1.2
81 RP(20,A+, 0)	944.19144	-0.05	5.04E-22	2.74E-03	1.5	2.4	0.4935	-3.4	0.1090	-3.1
79 RP(20,A+, 0)	944.20133	0.01	5.13E-22	2.74E-03	1.3	0.9	0.4912	-2.9	0.1053	0.3
81 RR(20,A+, 0)	970.13577	0.02	5.90E-22	2.70E-03	-0.1	0.3	0.4750	0.4	0.1049	0.7
81 RP(21,A+, 0)	943.50608	-0.01	4.86E-22	2.68E-03	-0.7	-0.4	0.4865	-2.6	0.1016	2.9
79 RP(21,A+, 0)	943.51328	0.00	5.08E-22	2.76E-03	1.9	1.6	0.5001	-5.2	0.1012	3.3
81 RQ(22,A+, 0)	956.88770	-0.04	1.01E-21	2.61E-03	-3.5	-2.8	0.4397	6.8	0.0989	4.6
81 RQ(23,A+, 0)	956.84247	-0.03	1.00E-21	2.67E-03	-1.4	-0.6	0.4406	5.2	0.1068	-4.0
79 RQ(23,A+, 0)	956.90076	-0.02	1.02E-21	2.68E-03	-0.9	-1.1	0.4417	4.9	0.0982	4.4
81 RR(23,A+, 0)	971.86099	0.03	5.22E-22	2.57E-03	-4.9	-4.1	0.4558	1.7	0.1020	0.5
81 RQ(24,A+, 0)	956.79529	-0.01	9.49E-22	2.61E-03	-3.4	-2.7	0.4221	8.1	0.1010	0.6
79 RQ(24,A+, 0)	956.85340	0.01	9.74E-22	2.63E-03	-2.7	-3.0	0.4348	4.9	0.0979	3.8
81 RQ(25,A+, 0)	956.74610	-0.02	9.22E-22	2.63E-03	-2.7	-2.4	0.4290	4.4	0.0980	2.8
79 RQ(25,A+, 0)	956.80402	0.00	9.37E-22	2.63E-03	-2.8	-3.2	0.4230	5.8	0.0987	2.1
81 RR(25,A+, 0)	972.99741	0.04	5.30E-22	2.81E-03	3.9	4.4	0.4953	-9.6	0.0973	3.5
81 RQ(26,A+, 0)	956.69495	0.00	8.75E-22	2.60E-03	-3.7	-3.1	0.4129	6.1	0.0911	9.7
79 RQ(26,A+, 0)	956.75269	0.03	9.18E-22	2.69E-03	-0.7	-1.0	0.4234	3.5	0.1026	-2.6
81 RR(26,A+, 0)	973.56143	0.00	4.91E-22	2.71E-03	0.4	0.6	0.4412	-0.7	0.0987	1.2
79 RP(27,A+, 0)	939.33487	0.01	4.30E-22	2.84E-03	5.0	4.4	0.4603	-7.1	0.1003	-1.2
81 RP(27,A+, 0)	939.34366	-0.01	4.07E-22	2.73E-03	1.2	1.7	0.4246	0.7	0.1009	-1.7
79 RQ(27,A+, 0)	956.69935	0.03	8.56E-22	2.62E-03	-3.0	-3.1	0.3960	7.9	0.0944	5.0
79 RR(27,A+, 0)	974.24631	0.01	4.72E-22	2.69E-03	-0.6	-0.9	0.4707	-9.2	0.1011	-1.9
79 RP(28,A+, 0)	938.63015	0.01	4.17E-22	2.90E-03	7.1	6.8	0.4758	-12.6	0.1013	-2.8
81 RP(28,A+, 0)	938.64169	0.02	3.84E-22	2.71E-03	0.4	1.0	0.4089	1.7	0.0996	-1.2
81 RP(29,A+, 0)	937.93734	0.02	3.62E-22	2.70E-03	-0.2	0.3	0.4039	0.0	0.0996	-1.9
79 RP(30,A+, 0)	937.21365	-0.02	3.86E-22	3.00E-03	11.1	10.8	0.4593	-14.9	0.0984	-1.3
79 RP(31,A+, 0)	936.50192	0.00	3.36E-22	2.78E-03	3.0	2.7	0.4085	-7.5	0.0978	-1.3
81 RP(31,A+, 0)	936.52163	0.00	3.21E-22	2.70E-03	-0.1	0.4	0.4004	-5.6	0.0984	-1.9
79 RP(32,A+, 0)	935.78786	0.01	3.08E-22	2.73E-03	0.9	0.5	0.3790	-3.8	0.0968	-0.9
81 RP(32,A+, 0)	935.81026	-0.03	3.09E-22	2.78E-03	2.9	3.5	0.4089	-10.9	0.0963	-0.4
81 RQ(32,A+, 0)	956.34638	0.01	6.39E-22	2.67E-03	-1.0	-0.4	0.3635	0.3	0.0951	0.9
79 RR(32,A+, 0)	977.02103	-0.01	3.44E-22	2.65E-03	-1.9	-2.2	0.3576	1.9	0.0959	0.0
81 RQ(33,A+, 0)	956.28132	-0.01	5.81E-22	2.61E-03	-3.3	-2.7	0.3372	4.1	0.0930	2.6
79 RQ(33,A+, 0)	956.33753	0.07	6.04E-22	2.68E-03	-1.0	-1.5	0.3325	5.5	0.0963	-0.9
79 RR(33,A+, 0)	977.56748	-0.02	3.33E-22	2.76E-03	2.0	1.6	0.3589	-2.2	0.0941	1.4
79 RQ(34,A+, 0)	956.27015	-0.01	5.84E-22	2.79E-03	3.3	2.6	0.3525	-4.3	0.0948	0.1
79 RR(34,A+, 0)	978.11112	0.02	3.01E-22	2.70E-03	-0.2	-0.5	0.3229	4.5	0.0946	0.3
81 RQ(36,A+, 0)	956.07428	0.04	4.69E-22	2.68E-03	-1.0	-0.7	0.3139	-0.9	0.0936	0.5
79 RP(37,A+, 0)	932.18276	0.01	2.21E-22	2.90E-03	7.3	7.0	0.3360	-11.2	0.0941	-0.5
81 RQ(37,A+, 0)	956.00123	0.01	4.38E-22	2.73E-03	1.1	1.6	0.3042	-1.9	0.0938	-0.2
79 RQ(37,A+, 0)	956.05634	0.05	4.34E-22	2.67E-03	-1.3	-1.3	0.2859	4.4	0.0947	-1.1
81 RR(37,A+, 0)	979.58091	-0.05	2.38E-22	2.78E-03	3.0	3.5	0.3107	-3.9	0.0937	-0.1
81 RQ(38,A+, 0)	955.92621	0.00	3.90E-22	2.66E-03	-1.6	-1.1	0.2718	5.4	0.0930	0.3
79 RQ(38,A+, 0)	955.98096	-0.04	4.09E-22	2.76E-03	2.0	1.7	0.2878	-0.5	0.0934	-0.1
81 RQ(39,A+, 0)	955.84919	-0.01	3.58E-22	2.69E-03	-0.6	-0.1	0.2777	-1.0	0.0926	0.4
79 RQ(39,A+, 0)	955.90375	0.05	3.55E-22	2.63E-03	-2.6	-3.0	0.2613	5.2	0.0912	1.9
79 RQ(40,A+, 0)	955.82441	0.02	3.25E-22	2.66E-03	-1.5	-1.8	0.2575	2.5	0.0910	1.8
79 RP(41,A+, 0)	929.25746	0.01	1.57E-22	3.03E-03	12.1	11.8	0.2622	-3.3	0.0926	-0.2
79 RP(42,A+, 0)	928.52040	-0.06	1.24E-22	2.67E-03	-1.1	-1.3	0.2405	1.4	0.0945	-2.5
81 RP(42,A+, 0)	928.57075	-0.11	1.21E-22	2.62E-03	-2.9	-2.3	0.2362	3.3	0.0903	2.1
81 RQ(42,A+, 0)	955.60614	-0.02	2.58E-22	2.63E-03	-2.7	-2.1	0.2421	0.7	0.0875	5.3
79 RQ(42,A+, 0)	955.65973	0.00	2.72E-22	2.74E-03	1.3	0.9	0.2454	-0.6	0.0924	-0.3
79 RQ(43,A+, 0)	955.57441	0.03	2.44E-22	2.74E-03	1.3	1.0	0.2477	-5.2	0.0910	1.0
79 RR(43,A+, 0)	982.87395	0.02	1.21E-22	2.55E-03	-5.5	-6.0	0.2023	16.1	0.0911	0.9
79 RP(45,A+, 0)	926.29597	-0.03	9.36E-23	2.83E-03	4.7	4.5	0.2176	0.3	0.0954	-4.0
79 RQ(45,A+, 0)	955.39765	0.02	1.85E-22	2.62E-03	-3.1	-3.4	0.2101	3.8	0.0891	2.8

79	RP(46,A+, 0)	925.54999	-0.04	7.95E-23	2.71E-03	0.3	0.0	0.2038	3.2	0.0922	-0.9
81	RP(46,A+, 0)	925.61182	-0.07	7.93E-23	2.73E-03	1.1	1.5	0.1998	5.3	0.0913	0.1
81	RQ(46,A+, 0)	955.25397	-0.02	1.60E-22	2.58E-03	-4.3	-3.9	0.1900	10.7	0.0906	0.9
79	RQ(46,A+, 0)	955.30622	0.00	1.67E-22	2.67E-03	-1.1	-1.4	0.1991	5.6	0.0908	0.7
81	RQ(47,A+, 0)	955.16083	-0.08	1.60E-22	2.92E-03	8.0	8.5	0.2251	-10.0	0.0903	1.1
79	RQ(47,A+, 0)	955.21277	-0.02	1.51E-22	2.72E-03	0.6	0.3	0.1849	9.6	0.0937	-2.6
79	RR(47,A+, 0)	984.91472	0.02	7.94E-23	2.70E-03	-0.2	-0.5	0.1998	1.4	0.0921	-0.9
81	RQ(48,A+, 0)	955.06586	0.05	1.26E-22	2.61E-03	-3.4	-2.8	0.2047	-4.8	0.0904	0.8
81	RR(48,A+, 0)	985.25292	-0.19	6.77E-23	2.63E-03	-2.6	-2.3	0.1845	5.6	0.0923	-1.3
79	RR(48,A+, 0)	985.41753	0.05	6.87E-23	2.64E-03	-2.2	-2.3	0.1824	6.8	0.0926	-1.6
81	RQ(49,A+, 0)	954.96869	0.00	1.14E-22	2.67E-03	-1.2	-0.7	0.1947	-4.1	0.0913	-0.3
79	RQ(49,A+, 0)	955.01984	0.00	1.23E-22	2.88E-03	6.5	6.3	0.2006	-6.9	0.0914	-0.4
79	RR(49,A+, 0)	985.91729	0.02	6.37E-23	2.80E-03	3.6	3.3	0.2214	-15.7	0.0893	1.9
79	RP(50,A+, 0)	922.54395	-0.06	4.73E-23	2.70E-03	-0.1	-0.8	0.1661	7.1	0.0903	0.7
79	RP(51,A+, 0)	921.78699	0.01	4.24E-23	2.78E-03	2.9	2.9	0.1769	-5.0	0.0916	-0.8
81	RQ(51,A+, 0)	954.76837	-0.02	8.64E-23	2.67E-03	-1.3	-0.9	0.1734	-3.1	0.0920	-1.3
79	RQ(53,A+, 0)	954.60956	0.05	6.58E-23	2.69E-03	-0.5	-0.6	0.1497	0.2	0.0910	-0.3
81	RQ(54,A+, 0)	954.45270	0.02	5.49E-23	2.61E-03	-3.3	-2.9	0.1388	8.1	0.0915	-0.9
81	RQ(56,A+, 0)	954.23200	-0.03	4.53E-23	2.92E-03	8.0	8.7	0.1601	-6.3	0.0935	-3.7
79	RQ(57,A+, 0)	954.16651	0.07	3.68E-23	2.77E-03	2.5	2.1	0.1493	0.5	0.0938	-4.1
79	PP(4,E , 1)	947.43987	0.05	1.14E-22	2.54E-03	-4.9	-5.4	0.3739	-0.2	0.1315	-1.8
79	PP(5,E , 1)	946.79253	0.02	1.42E-22	2.67E-03	-0.1	-0.6	0.3818	-0.7	0.1283	-0.5
79	RR(6,E , 1)	969.34884	-0.04	2.58E-22	2.82E-03	3.2	2.9	0.4134	-6.4	0.1216	3.7
81	PR(7,E , 1)	954.94770	0.09	1.68E-22	2.87E-03	7.5	8.0	0.4225	-6.3	0.1239	0.4
79	PR(7,E , 1)	955.03070	0.02	1.67E-22	2.79E-03	4.2	3.8	0.3912	1.2	0.1243	0.1
79	RR(7,E , 1)	969.96884	0.01	2.67E-22	2.73E-03	-0.2	-0.5	0.3849	2.9	0.1212	2.7
79	PR(8,E , 1)	955.64826	-0.01	1.84E-22	2.75E-03	2.6	2.0	0.3872	4.8	0.1229	-0.2
79	RR(8,E , 1)	970.58639	-0.07	2.93E-22	2.82E-03	3.2	3.0	0.4400	-7.7	0.1203	2.0
79	PP(9,E , 1)	944.18101	0.00	2.18E-22	2.71E-03	1.3	0.9	0.3831	8.7	0.1205	0.4
79	PR(9,E , 1)	956.26349	-0.02	1.96E-22	2.68E-03	0.1	-0.4	0.3984	4.5	0.1149	5.3
81	PP(10,E , 1)	943.48331	0.04	2.24E-22	2.68E-03	0.1	0.5	0.4084	4.4	0.1194	-0.1
79	PP(10,E , 1)	943.52262	0.01	2.42E-22	2.83E-03	5.8	5.3	0.4186	1.9	0.1167	2.2
81	PR(10,E , 1)	956.78632	-0.01	1.89E-22	2.44E-03	-8.6	-8.4	0.3628	17.6	0.1220	-2.3
79	PR(10,E , 1)	956.87641	0.02	2.04E-22	2.58E-03	-3.5	-4.2	0.3734	14.2	0.1215	-1.9
81	PP(12,E , 1)	942.16495	0.01	2.40E-22	2.61E-03	-2.5	-2.1	0.4115	8.3	0.1147	1.2
79	RR(12,E , 1)	973.03348	-0.01	3.25E-22	2.69E-03	-1.6	-1.6	0.4434	0.5	0.1120	3.6
79	PP(13,E , 1)	941.53427	0.00	2.64E-22	2.72E-03	1.5	0.9	0.4410	3.0	0.1178	-2.7
81	RR(13,E , 1)	973.54959	-0.02	3.32E-22	2.75E-03	0.6	1.5	0.4746	-4.3	0.1118	2.5
81	PP(14,E , 1)	940.83792	-0.01	2.73E-22	2.80E-03	4.7	5.0	0.4777	-3.4	0.1137	-0.5
79	RP(14,E , 1)	955.80555	-0.01	2.03E-22	2.70E-03	-1.3	-1.2	0.4412	4.6	0.1147	-1.4
81	PP(15,E , 1)	940.17117	0.00	2.65E-22	2.67E-03	0.0	0.2	0.4671	0.1	0.1129	-1.0
79	PP(15,E , 1)	940.19784	0.00	2.80E-22	2.76E-03	3.2	2.5	0.4696	-0.4	0.1147	-2.6
79	RP(15,E , 1)	955.13630	-0.04	2.16E-22	2.76E-03	1.1	1.3	0.4758	-1.7	0.1163	-3.9
81	RP(16,E , 1)	954.44806	-0.03	2.12E-22	2.69E-03	-1.4	-0.4	0.4613	2.4	0.1142	-3.3
79	RP(16,E , 1)	954.46497	-0.01	2.13E-22	2.65E-03	-3.0	-2.8	0.4517	4.6	0.1137	-2.9
81	PQ(17,E , 1)	949.59637	-0.01	5.25E-22	2.65E-03	-0.8	0.2	0.4606	3.3	0.1072	1.8
81	PQ(18,E , 1)	949.55566	0.04	5.04E-22	2.54E-03	-4.9	-3.8	0.4604	3.7	0.1079	0.0
79	RR(18,E , 1)	976.63279	-0.01	3.27E-22	2.63E-03	-3.6	-3.2	0.4431	7.8	0.1066	1.2
79	PP(19,E , 1)	937.49917	0.06	2.84E-22	2.80E-03	4.6	3.7	0.4780	-0.1	0.1098	-2.8
81	PQ(19,E , 1)	949.51263	0.06	5.16E-22	2.62E-03	-2.0	-0.8	0.4457	7.2	0.1069	-0.2
79	PQ(19,E , 1)	949.57482	0.03	5.34E-22	2.66E-03	-0.6	-0.5	0.4635	3.1	0.1042	2.4
79	PR(19,E , 1)	962.28499	-0.01	2.73E-22	2.75E-03	2.8	1.5	0.4803	-0.5	0.1067	0.0
81	RR(19,E , 1)	977.12095	-0.06	3.23E-22	2.68E-03	-1.8	-0.5	0.4809	-0.7	0.1061	0.6
79	RR(19,E , 1)	977.22422	-0.04	3.45E-22	2.81E-03	3.0	3.4	0.4810	-0.7	0.1046	2.0
79	PQ(20,E , 1)	949.52935	0.05	5.27E-22	2.66E-03	-0.7	-0.3	0.4788	-0.5	0.1052	0.4
81	PP(21,E , 1)	936.12576	0.00	2.69E-22	2.79E-03	4.5	4.2	0.5112	-7.4	0.1077	-3.0
79	PP(21,E , 1)	936.13699	0.05	2.74E-22	2.79E-03	4.2	3.0	0.4811	-1.6	0.1063	-1.7
81	PQ(21,E , 1)	949.41973	0.05	4.80E-22	2.51E-03	-6.3	-4.9	0.4352	8.8	0.1046	-0.1
81	RP(21,E , 1)	951.07226	0.02	2.28E-22	2.83E-03	3.6	5.0	0.5083	-6.9	0.1029	1.6
79	RP(21,E , 1)	951.07623	0.03	2.24E-22	2.73E-03	0.0	0.7	0.4824	-1.9	0.1124	-7.0
81	RR(21,E , 1)	978.29222	-0.03	3.07E-22	2.67E-03	-2.3	-0.9	0.4814	-1.7	0.1031	1.4
79	PQ(22,E , 1)	949.43151	0.07	4.93E-22	2.59E-03	-3.2	-2.2	0.4574	2.5	0.1030	0.5
81	PR(22,E , 1)	963.92720	0.06	2.58E-22	2.77E-03	3.7	3.1	0.4750	-1.3	0.1051	-1.5
81	PQ(24,E , 1)	949.26330	0.06	4.66E-22	2.64E-03	-1.2	0.3	0.4730	-3.6	0.1000	1.6
79	RP(25,E , 1)	948.32732	-0.01	2.01E-22	2.69E-03	-1.6	-0.6	0.4545	-1.6	0.1039	-3.1
81	RP(25,E , 1)	948.33385	0.00	2.02E-22	2.75E-03	0.7	2.7	0.4224	5.9	0.1054	-4.4
79	PQ(25,E , 1)	949.26757	0.08	4.57E-22	2.64E-03	-1.2	0.2	0.4303	3.9	0.0957	5.3
81	RR(25,E , 1)	980.60545	-0.05	2.80E-22	2.79E-03	2.3	4.2	0.4909	-8.9	0.1025	-1.7
81	RQ(26,E , 1)	964.09542	-0.02	4.49E-22	2.72E-03	-0.4	-1.5	0.4203	4.1	0.0986	1.3
81	PQ(27,E , 1)	949.08636	0.10	3.96E-22	2.55E-03	-4.6	-2.7	0.3933	8.6	0.1029	-3.7
79	RQ(27,E , 1)	964.08773	-0.01	4.44E-22	2.77E-03	1.3	-0.9	0.4149	2.9	0.0991	0.0
81	RR(27,E , 1)	981.74736	-0.02	2.45E-22	2.69E-03	-1.5	0.5	0.4239	0.7	0.1007	-1.6
79	PQ(28,E , 1)	949.08300	0.09	4.13E-22	2.75E-03	2.7	4.1	0.4340	-4.2	0.0966	1.9
79	RR(28,E , 1)	982.43743	-0.03	2.31E-22	2.64E-03	-3.3	-2.0	0.3907	6.4	0.0987	-0.3
81	RQ(29,E , 1)	963.90578	-0.03	3.85E-22	2.72E-03	-0.6	-1.7	0.3798	6.2	0.0968	1.0
79	RQ(29,E , 1)	963.95851	-0.03	3.94E-22	2.73E-03	0.0	-2.0	0.3890	3.7	0.1022	-4.4
81	RR(29,E , 1)	982.87932	-0.04	2.02E-22	2.48E-03	-9.2	-7.1	0.3582	12.6	0.0987	-1.0
81	RP(30,E , 1)	944.86454	-0.01	1.43E-22	2.47E-03	-9.7	-7.5	0.3592	8.8	0.1003	-3.2

81	PQ(30,E , 1)	948.88879	0.08	3.44E-22	2.61E-03	-2.3	0.1	0.3875	0.8	0.0986	-1.5
79	RQ(30,E , 1)	963.89052	-0.02	3.79E-22	2.79E-03	2.2	0.0	0.3781	3.3	0.0991	-2.0
81	RR(30,E , 1)	983.44158	-0.03	2.02E-22	2.64E-03	-3.2	-0.8	0.3817	2.4	0.0963	0.8
79	RR(30,E , 1)	983.56865	-0.04	1.94E-22	2.50E-03	-8.5	-7.1	0.3553	10.0	0.0965	0.6
81	RP(31,E , 1)	944.16453	-0.07	1.46E-22	2.66E-03	-2.7	-0.3	0.3546	6.5	0.0989	-2.4
79	PQ(31,E , 1)	948.87774	0.10	3.25E-22	2.59E-03	-3.2	-1.6	0.3553	6.3	0.0970	-0.5
79	PP(32,E , 1)	928.49488	0.04	1.56E-22	2.67E-03	-0.1	-2.3	0.3483	4.5	0.0988	-2.9
81	PP(32,E , 1)	928.51295	0.16	1.68E-22	2.94E-03	9.9	8.6	0.3784	-3.8	0.0981	-2.2
79	RP(32,E , 1)	943.43741	-0.07	1.48E-22	2.85E-03	4.1	6.1	0.3902	-6.7	0.0962	-0.3
81	RP(32,E , 1)	943.46262	0.00	1.31E-22	2.54E-03	-6.9	-4.4	0.3395	7.3	0.0969	-1.0
79	RR(32,E , 1)	984.68987	0.00	1.80E-22	2.66E-03	-2.7	-0.9	0.3535	3.0	0.0954	0.5
81	RQ(33,E , 1)	963.62135	-0.03	2.97E-22	2.73E-03	-0.2	-1.9	0.3287	6.7	0.0960	-0.6
81	PR(33,E , 1)	970.16195	0.06	1.38E-22	2.53E-03	-5.2	-7.1	0.3146	11.5	0.0991	-3.7
79	RR(33,E , 1)	985.24663	-0.05	1.67E-22	2.66E-03	-2.7	-1.0	0.3429	2.3	0.0968	-1.5
79	RP(34,E , 1)	942.02201	-0.13	1.25E-22	2.77E-03	1.5	3.7	0.3245	3.9	0.1026	-7.5
81	PQ(34,E , 1)	948.59325	0.06	2.67E-22	2.68E-03	0.2	3.3	0.3327	1.3	0.0956	-0.7
79	RQ(34,E , 1)	963.59584	-0.04	2.96E-22	2.89E-03	5.6	2.8	0.3781	-10.8	0.0922	2.9
79	PP(35,E , 1)	926.36732	0.10	1.33E-22	2.88E-03	7.7	5.1	0.3529	-8.2	0.0973	-2.9
81	PP(35,E , 1)	926.39332	0.03	1.25E-22	2.73E-03	2.2	0.7	0.3246	-0.2	0.0986	-4.2
79	RP(35,E , 1)	941.31143	-0.05	1.11E-22	2.66E-03	-2.7	-0.4	0.3055	6.0	0.0975	-3.1
81	PQ(35,E , 1)	948.51360	0.04	2.40E-22	2.61E-03	-2.5	0.7	0.3101	4.4	0.0945	0.0
79	PQ(35,E , 1)	948.57177	0.10	2.45E-22	2.62E-03	-1.9	0.3	0.3172	2.1	0.0940	0.5
79	PP(36,E , 1)	925.65394	0.00	1.27E-22	2.98E-03	11.5	8.7	0.3273	-5.0	0.0926	1.6
79	RP(36,E , 1)	940.59879	-0.03	1.02E-22	2.63E-03	-3.6	-1.2	0.2955	5.2	0.0973	-3.4
81	RP(36,E , 1)	940.63474	-0.05	1.00E-22	2.64E-03	-3.4	-0.4	0.3038	2.3	0.0983	-4.3
81	PQ(36,E , 1)	948.43169	0.06	2.19E-22	2.59E-03	-3.2	0.0	0.3023	2.8	0.0939	0.1
79	PQ(36,E , 1)	948.48949	0.10	2.22E-22	2.58E-03	-3.7	-1.3	0.2919	6.5	0.0950	-1.0
81	RQ(36,E , 1)	963.38429	-0.07	2.36E-22	2.75E-03	0.5	-1.5	0.3061	1.5	0.0940	0.0
79	PP(37,E , 1)	924.93873	0.10	1.11E-22	2.85E-03	6.7	3.8	0.3050	-2.2	0.0947	-1.1
81	PP(37,E , 1)	924.97016	0.02	1.03E-22	2.69E-03	0.7	-1.2	0.2869	3.9	0.0918	2.0
79	RP(37,E , 1)	939.88412	-0.06	1.05E-22	2.95E-03	7.9	10.7	0.3455	-13.7	0.0978	-4.2
81	RP(37,E , 1)	939.92276	-0.11	9.90E-23	2.83E-03	3.5	7.0	0.3200	-6.8	0.0955	-1.9
81	PQ(37,E , 1)	948.34747	0.08	1.95E-22	2.51E-03	-6.1	-2.8	0.2867	4.0	0.0922	1.6
79	PQ(37,E , 1)	948.40490	0.10	2.00E-22	2.54E-03	-5.0	-2.6	0.2906	2.6	0.0944	-0.8
79	RQ(37,E , 1)	963.35103	-0.05	2.21E-22	2.76E-03	1.0	-2.0	0.2709	10.1	0.0936	0.1
81	PP(38,E , 1)	924.25562	0.08	9.26E-23	2.64E-03	-1.3	-3.4	0.2648	8.0	0.0948	-1.6
79	RP(38,E , 1)	939.16751	-0.07	8.90E-23	2.75E-03	0.7	3.3	0.2964	-3.5	0.0969	-3.7
81	RP(38,E , 1)	939.20889	-0.10	8.49E-23	2.66E-03	-2.6	1.0	0.2837	0.8	0.0971	-3.9
81	PQ(38,E , 1)	948.26092	0.09	2.00E-22	2.81E-03	5.2	9.0	0.2965	-3.5	0.0931	0.2
79	PQ(38,E , 1)	948.31799	0.10	1.80E-22	2.50E-03	-6.4	-3.9	0.2640	8.4	0.0948	-1.6
79	PQ(39,E , 1)	948.22875	0.09	1.69E-22	2.58E-03	-3.6	-0.7	0.2672	2.8	0.0935	-0.6
81	RQ(39,E , 1)	963.12697	-0.05	1.86E-22	2.83E-03	3.6	1.1	0.2819	-2.6	0.0942	-1.3
79	PR(39,E , 1)	973.58530	0.12	8.96E-23	2.70E-03	0.9	-2.6	0.2522	8.9	0.0941	-1.2
79	PP(40,E , 1)	922.78064	0.06	8.22E-23	2.82E-03	5.6	2.0	0.2499	5.5	0.0903	2.6
81	PP(40,E , 1)	922.82038	0.07	7.73E-23	2.69E-03	0.6	-1.5	0.2467	6.9	0.0874	6.0
81	PQ(40,E , 1)	948.08092	0.13	1.64E-22	2.80E-03	4.9	9.1	0.2761	-4.5	0.0938	-1.2
81	RQ(40,E , 1)	963.03663	-0.09	1.67E-22	2.82E-03	3.1	0.5	0.2586	1.9	0.0928	-0.1
79	RQ(40,E , 1)	963.08583	-0.05	1.71E-22	2.85E-03	4.1	0.5	0.2629	0.3	0.0915	1.3
81	PP(41,E , 1)	922.09967	-0.03	7.36E-23	2.84E-03	6.3	3.4	0.2684	-5.6	0.0946	-2.3
81	PQ(41,E , 1)	947.98736	0.07	1.35E-22	2.55E-03	-4.7	-0.6	0.2475	2.4	0.0934	-1.1
81	PP(42,E , 1)	921.37707	-0.01	6.52E-23	2.80E-03	4.7	1.9	0.2330	4.6	0.0891	3.4
81	PQ(42,E , 1)	947.89153	0.06	1.23E-22	2.59E-03	-3.2	1.0	0.2316	5.2	0.0932	-1.1
79	PQ(42,E , 1)	947.94707	0.07	1.22E-22	2.54E-03	-4.9	-1.6	0.2317	5.2	0.0918	0.4
79	RR(42,E , 1)	990.14276	-0.05	6.95E-23	2.55E-03	-6.8	-3.9	0.2306	5.7	0.0936	-1.5
81	RP(43,E , 1)	935.61025	-0.12	5.10E-23	2.65E-03	-3.1	0.8	0.2401	-2.3	0.0968	-5.0
81	PQ(43,E , 1)	947.79339	0.05	1.06E-22	2.50E-03	-6.6	-2.2	0.2113	11.0	0.0936	-1.8
79	PQ(43,E , 1)	947.84856	0.11	1.13E-22	2.62E-03	-2.0	1.4	0.2422	-3.1	0.0933	-1.5
81	RQ(43,E , 1)	962.75220	-0.09	1.13E-22	2.62E-03	-4.1	-7.0	0.2114	11.0	0.0909	1.1
81	RR(43,E , 1)	990.52026	-0.13	6.45E-23	2.67E-03	-2.1	1.9	0.2170	8.1	0.0831	10.6
79	RR(43,E , 1)	990.67383	-0.06	6.04E-23	2.48E-03	-9.2	-6.3	0.1983	18.3	0.0958	-4.0
79	PQ(44,E , 1)	947.74767	0.10	9.67E-23	2.52E-03	-5.9	-2.4	0.2090	8.2	0.0923	-0.6
81	PQ(45,E , 1)	947.59014	0.07	8.99E-23	2.65E-03	-0.8	4.2	0.2247	-3.0	0.0866	5.7
79	PQ(46,E , 1)	947.53893	0.16	8.03E-23	2.65E-03	-1.0	3.1	0.2083	0.9	0.0958	-4.6
81	RQ(46,E , 1)	962.44740	-0.12	8.39E-23	2.75E-03	0.6	-2.8	0.1896	10.8	0.0901	1.4
81	PR(46,E , 1)	977.12821	0.10	4.22E-23	2.76E-03	3.1	-0.9	0.2096	0.3	0.0899	1.7
79	PR(46,E , 1)	977.29466	0.15	4.01E-23	2.58E-03	-3.6	-8.3	0.1803	16.6	0.0943	-3.1
79	PQ(47,E , 1)	947.43096	0.12	6.94E-23	2.59E-03	-3.2	1.2	0.2041	-0.8	0.0943	-3.2
79	RR(47,E , 1)	992.77173	-0.18	3.97E-23	2.64E-03	-3.3	0.9	0.2019	0.3	0.0963	-5.2
81	RP(48,E , 1)	931.96364	-0.13	3.13E-23	2.94E-03	7.8	13.5	0.1933	0.7	0.0913	-0.2
81	PQ(48,E , 1)	947.26775	0.09	5.84E-23	2.50E-03	-6.5	-1.4	0.1786	9.0	0.0919	-0.8
79	PQ(48,E , 1)	947.32073	0.16	6.27E-23	2.65E-03	-0.9	4.0	0.1889	3.1	0.0949	-4.0
81	RQ(48,E , 1)	962.23292	-0.13	6.44E-23	2.71E-03	-0.6	-4.2	0.1747	11.4	0.0907	0.5
79	RQ(48,E , 1)	962.27876	-0.12	6.98E-23	2.91E-03	6.6	1.8	0.1820	7.0	0.0892	2.2
79	PR(48,E , 1)	978.33012	0.16	3.22E-23	2.67E-03	0.0	-5.2	0.1663	17.1	0.0886	2.9
81	PQ(49,E , 1)	947.15551	-0.01	5.26E-23	2.55E-03	-4.5	0.8	0.1827	2.1	0.0938	-2.9
79	RR(49,E , 1)	993.80500	-0.04	2.84E-23	2.42E-03	-11.3	-7.2	0.1641	13.7	0.0903	0.8
81	PQ(52,E , 1)	946.80498	0.00	3.55E-23	2.61E-03	-2.4	3.8	0.1767	-11.4	0.0916	-0.9
79	RQ(52,E , 1)	961.82075	-0.14	4.08E-23	2.93E-03	7.3	1.5	0.1741	-10.1	0.0988	-8.1

79	PQ(53,E , 1)	946.73400	0.20	2.82E-23	2.39E-03	-10.8	-5.7	0.1460	2.6	0.0933	-2.8
81	PR(7,E , 2)	947.56756	0.01	1.14E-22	2.81E-03	6.1	6.8	0.4123	-6.6	0.1241	-1.3
79	PP(8,E , 2)	937.46127	0.06	2.43E-22	2.83E-03	6.9	6.5	0.3824	3.9	0.1184	2.4
79	PR(8,E , 2)	948.27184	0.03	1.24E-22	2.59E-03	-2.3	-2.8	0.3824	3.9	0.1163	4.2
81	RR(8,E , 2)	978.07072	-0.03	3.07E-22	2.68E-03	-2.8	-2.3	0.3487	14.0	0.1249	-3.0
79	RR(8,E , 2)	978.14530	-0.08	3.16E-22	2.70E-03	-2.1	-2.4	0.3844	3.4	0.1202	0.8
81	PQ(9,E , 2)	942.46097	0.01	3.46E-22	2.55E-03	-3.6	-2.9	0.3785	8.2	0.1230	-2.6
81	RR(9,E , 2)	978.68364	-0.05	3.32E-22	2.80E-03	1.4	2.0	0.4256	-3.7	0.1179	1.6
79	RR(9,E , 2)	978.76060	-0.05	3.51E-22	2.90E-03	4.8	4.6	0.4586	-10.7	0.1207	-0.8
81	PP(10,E , 2)	936.10360	-0.06	2.43E-22	2.61E-03	-1.2	-0.7	0.3883	8.5	0.1210	-2.3
79	PP(10,E , 2)	936.14663	-0.01	2.52E-22	2.66E-03	0.5	0.2	0.3975	6.0	0.1189	-0.5
81	PQ(10,E , 2)	942.43833	0.01	3.76E-22	2.57E-03	-2.7	-2.0	0.4085	3.1	0.1209	-2.2
81	PR(10,E , 2)	949.40624	0.09	1.47E-22	2.51E-03	-5.0	-4.7	0.4066	3.6	0.1279	-7.5
79	PP(11,E , 2)	935.48605	0.00	2.66E-22	2.70E-03	2.0	1.5	0.4255	1.6	0.1185	-1.4
81	PQ(11,E , 2)	942.41342	0.00	3.78E-22	2.44E-03	-7.8	-7.1	0.3733	15.8	0.1185	-1.4
79	PQ(12,E , 2)	942.45316	0.00	4.27E-22	2.57E-03	-2.9	-2.8	0.4213	5.0	0.1187	-2.8
79	RR(12,E , 2)	980.59227	-0.09	3.55E-22	2.74E-03	-0.7	-1.0	0.4528	-2.3	0.1152	0.2
79	PQ(13,E , 2)	942.42362	0.02	4.33E-22	2.51E-03	-5.2	-5.0	0.4109	9.8	0.1166	-2.1
79	PR(13,E , 2)	951.32415	-0.01	2.02E-22	2.78E-03	5.1	4.6	0.4451	1.4	0.1165	-2.0
81	PQ(14,E , 2)	942.32511	0.01	4.51E-22	2.59E-03	-2.1	-1.0	0.4134	11.0	0.1088	3.7
79	RP(14,E , 2)	963.36507	-0.06	1.59E-22	2.66E-03	-3.7	-3.9	0.4279	7.3	0.1144	-1.4
81	RR(14,E , 2)	981.71318	-0.03	3.48E-22	2.69E-03	-2.6	-1.9	0.4549	0.9	0.1109	1.8
79	RR(15,E , 2)	982.40276	0.02	3.62E-22	2.74E-03	-0.6	-0.8	0.4583	1.5	0.1099	1.5
79	PP(16,E , 2)	932.15047	0.02	2.81E-22	2.65E-03	0.0	-0.4	0.4673	0.6	0.1123	-1.8
79	PQ(16,E , 2)	942.32126	0.01	5.09E-22	2.76E-03	4.5	4.4	0.5147	-8.6	0.1078	2.3
81	PQ(17,E , 2)	942.21640	0.04	4.54E-22	2.50E-03	-5.6	-4.6	0.4433	6.8	0.1064	2.5
81	RP(17,E , 2)	961.34035	-0.04	1.79E-22	2.72E-03	-1.5	-0.7	0.4650	1.9	0.1124	-2.9
79	RP(17,E , 2)	961.35115	0.00	1.80E-22	2.68E-03	-3.0	-3.0	0.4526	4.6	0.1108	-1.5
81	RR(17,E , 2)	983.50243	-0.05	3.55E-22	2.78E-03	0.7	1.4	0.4868	-2.7	0.1083	0.7
81	PQ(18,E , 2)	942.17563	0.05	4.74E-22	2.60E-03	-1.5	-0.3	0.4533	4.9	0.1082	-0.3
81	PR(18,E , 2)	954.20496	0.05	2.20E-22	2.72E-03	2.9	3.0	0.4965	-4.2	0.1091	-1.1
81	RR(18,E , 2)	984.09404	-0.08	3.39E-22	2.69E-03	-2.6	-1.9	0.4462	6.6	0.1057	2.0
81	PR(19,E , 2)	954.79401	0.06	2.09E-22	2.58E-03	-2.6	-2.5	0.4636	2.6	0.1059	0.7
81	RR(19,E , 2)	984.68328	-0.06	3.36E-22	2.71E-03	-1.7	-1.0	0.4796	-0.8	0.1056	1.0
81	PR(20,E , 2)	955.38062	0.06	2.22E-22	2.75E-03	4.1	4.2	0.5062	-6.3	0.1081	-2.4
81	RR(20,E , 2)	985.27007	-0.08	3.37E-22	2.79E-03	1.0	2.0	0.5019	-5.5	0.1055	0.0
81	PP(21,E , 2)	928.74629	0.07	2.73E-22	2.80E-03	5.9	6.1	0.5182	-9.0	0.1065	-1.9
79	PP(21,E , 2)	928.76106	0.00	2.79E-22	2.81E-03	6.2	5.5	0.5020	-6.1	0.1066	-2.0
81	PQ(21,E , 2)	942.03964	0.05	4.39E-22	2.49E-03	-5.7	-4.5	0.4444	6.1	0.1013	3.1
81	PR(21,E , 2)	955.96485	0.12	1.96E-22	2.46E-03	-6.8	-6.9	0.4311	9.4	0.1080	-3.3
79	PR(21,E , 2)	956.08338	0.10	2.10E-22	2.59E-03	-2.2	-3.2	0.4654	1.3	0.1035	0.9
81	RR(21,E , 2)	985.85448	-0.06	3.26E-22	2.77E-03	0.4	1.3	0.4873	-3.2	0.1048	-0.3
79	RR(21,E , 2)	985.95861	-0.04	3.30E-22	2.75E-03	-0.4	-0.4	0.4730	-0.3	0.1035	0.9
81	PQ(22,E , 2)	941.98978	0.06	4.64E-22	2.70E-03	2.0	2.9	0.4716	-0.9	0.1073	-3.6
79	PR(22,E , 2)	956.66730	0.11	2.30E-22	2.87E-03	8.6	7.6	0.5097	-8.3	0.0964	7.3
79	RR(22,E , 2)	986.54278	-0.02	3.12E-22	2.68E-03	-2.8	-2.6	0.4386	6.5	0.1042	-0.7
79	PQ(23,E , 2)	942.00272	0.09	4.43E-22	2.59E-03	-2.0	-2.1	0.4219	9.4	0.1025	0.0
79	PP(24,E , 2)	926.70203	0.07	2.52E-22	2.80E-03	5.8	5.0	0.4965	-8.5	0.1030	-1.4
81	PQ(24,E , 2)	941.88315	0.02	4.30E-22	2.65E-03	0.3	1.6	0.4571	-0.6	0.0989	2.7
81	PQ(25,E , 2)	941.82651	0.09	4.00E-22	2.56E-03	-3.4	-1.9	0.4060	9.8	0.0965	4.4
79	PQ(25,E , 2)	941.89108	0.05	4.38E-22	2.76E-03	4.1	4.5	0.4532	-1.6	0.1005	0.2
79	RP(25,E , 2)	955.88721	-0.04	1.84E-22	2.86E-03	3.5	3.9	0.4711	-5.3	0.1059	-4.9
81	RP(25,E , 2)	955.89728	-0.05	1.75E-22	2.76E-03	0.0	1.2	0.4443	0.4	0.0997	1.0
81	PR(25,E , 2)	958.27693	0.11	1.91E-22	2.64E-03	-0.2	-0.4	0.4212	5.9	0.1026	-1.8
79	PQ(26,E , 2)	941.83188	0.08	4.02E-22	2.64E-03	-0.3	0.1	0.4326	0.9	0.0963	3.7
79	RP(26,E , 2)	955.19483	-0.03	1.71E-22	2.76E-03	-0.2	0.2	0.4298	1.5	0.1013	-1.4
81	RP(26,E , 2)	955.20752	-0.07	1.69E-22	2.77E-03	0.3	1.4	0.4364	0.0	0.1045	-4.4
79	PR(26,E , 2)	958.97822	0.14	1.91E-22	2.69E-03	1.8	0.6	0.4280	2.0	0.1005	-0.6
81	RQ(27,E , 2)	971.59726	-0.05	4.06E-22	2.76E-03	-0.2	-0.4	0.4156	2.5	0.0991	0.0
79	RR(27,E , 2)	989.42651	-0.08	2.55E-22	2.75E-03	-0.6	-0.3	0.4341	-1.9	0.0953	4.0
81	RQ(28,E , 2)	971.53403	-0.06	3.79E-22	2.70E-03	-2.0	-2.3	0.4062	2.1	0.0975	0.9
79	RQ(28,E , 2)	971.58346	-0.04	3.92E-22	2.75E-03	-0.4	-1.5	0.3971	4.4	0.0978	0.6
79	RQ(29,E , 2)	971.51767	-0.07	3.77E-22	2.80E-03	1.5	0.3	0.3930	2.4	0.0963	1.5
81	RR(29,E , 2)	990.44128	-0.06	2.23E-22	2.74E-03	-0.6	0.7	0.4009	0.4	0.0979	-0.2
79	PP(30,E , 2)	922.52741	0.06	1.82E-22	2.78E-03	5.0	3.9	0.4199	-7.2	0.0983	-1.3
81	PP(30,E , 2)	922.53638	0.11	1.88E-22	2.90E-03	9.8	9.7	0.4085	-4.6	0.0990	-1.9
81	PQ(30,E , 2)	941.50876	0.11	3.04E-22	2.50E-03	-5.5	-4.0	0.3898	0.0	0.0910	6.7
81	RR(30,E , 2)	991.00342	-0.11	2.11E-22	2.77E-03	0.4	1.7	0.4134	-5.7	0.0987	-1.7
79	PP(31,E , 2)	921.82440	0.06	1.74E-22	2.83E-03	6.8	5.7	0.4093	-8.0	0.1020	-5.4
81	PP(31,E , 2)	921.83600	0.06	1.71E-22	2.82E-03	6.7	6.5	0.4265	-11.7	0.1012	-4.7
79	PR(31,E , 2)	961.81038	0.14	1.40E-22	2.56E-03	-3.4	-4.9	0.3395	10.9	0.1005	-4.0
81	PR(32,E , 2)	962.22707	0.14	1.36E-22	2.70E-03	2.0	1.2	0.3585	1.3	0.0983	-2.4
81	RR(33,E , 2)	992.67487	-0.14	1.67E-22	2.71E-03	-1.8	-0.2	0.3462	1.0	0.0966	-1.3
79	RR(33,E , 2)	992.80475	-0.01	1.65E-22	2.65E-03	-4.2	-3.5	0.3303	5.9	0.0963	-0.9
79	PQ(34,E , 2)	941.27548	0.10	2.43E-22	2.60E-03	-1.7	-0.8	0.3233	4.0	0.0966	-1.8
81	PR(34,E , 2)	963.33290	0.19	1.15E-22	2.62E-03	-1.0	-1.7	0.3097	8.6	0.0961	-1.2
81	RR(34,E , 2)	993.22699	-0.13	1.47E-22	2.60E-03	-5.8	-4.4	0.3039	10.7	0.0942	0.7
79	RR(34,E , 2)	993.35883	-0.11	1.61E-22	2.79E-03	1.2	2.0	0.3426	-1.8	0.0945	0.4

81	PQ(35,E , 2)	941.13382	0.12	2.13E-22	2.51E-03	-5.1	-3.3	0.3105	4.0	0.0914	3.3
79	RP(35,E , 2)	948.87133	-0.01	1.05E-22	2.83E-03	2.6	3.6	0.3263	-1.0	0.0970	-2.6
81	PR(35,E , 2)	963.88191	0.16	1.13E-22	2.78E-03	5.0	4.1	0.3258	-0.9	0.0972	-2.8
81	RR(35,E , 2)	993.77662	-0.07	1.51E-22	2.89E-03	4.5	6.2	0.3467	-6.8	0.0961	-1.7
79	RR(35,E , 2)	993.91047	-0.09	1.38E-22	2.60E-03	-5.8	-5.0	0.2977	8.5	0.0940	0.5
79	RQ(37,E , 2)	970.90970	-0.10	2.07E-22	2.76E-03	0.1	-1.7	0.2913	2.1	0.0942	-0.6
81	PQ(38,E , 2)	940.88138	0.19	1.68E-22	2.57E-03	-2.9	-1.0	0.2663	7.1	0.0946	-1.4
79	RP(38,E , 2)	946.72722	-0.05	7.91E-23	2.75E-03	-0.6	0.5	0.2805	1.7	0.0944	-1.2
81	RP(38,E , 2)	946.77221	-0.07	7.58E-23	2.67E-03	-3.4	-1.6	0.2796	2.0	0.0950	-1.8
79	RR(38,E , 2)	995.54993	-0.07	1.04E-22	2.58E-03	-6.7	-5.8	0.2638	8.1	0.0923	1.1
81	PQ(39,E , 2)	940.79257	0.14	1.48E-22	2.48E-03	-6.3	-4.2	0.2586	5.8	0.0928	0.2
79	PQ(39,E , 2)	940.85294	0.14	1.55E-22	2.57E-03	-2.7	-1.5	0.2611	4.8	0.0954	-2.5
81	RQ(40,E , 2)	970.59854	-0.17	1.53E-22	2.74E-03	-0.8	-1.8	0.2487	5.7	0.0916	1.2
81	PQ(41,E , 2)	940.60812	0.15	1.24E-22	2.53E-03	-4.3	-1.9	0.2375	6.5	0.0932	-0.8
79	RQ(41,E , 2)	970.55105	-0.14	1.45E-22	2.86E-03	3.4	1.4	0.2565	-1.4	0.0915	1.0
81	RR(41,E , 2)	997.02009	-0.11	7.37E-23	2.50E-03	-9.3	-7.6	0.2286	10.6	0.1047	-11.7
79	PQ(42,E , 2)	940.57162	0.11	1.17E-22	2.64E-03	-0.4	1.0	0.2474	-1.7	0.0942	-2.2
81	PP(43,E , 2)	913.27452	0.13	5.05E-23	2.49E-03	-5.7	-6.7	0.2049	14.3	0.0924	-0.5
81	PQ(43,E , 2)	940.41446	0.17	1.04E-22	2.63E-03	-0.4	2.0	0.2265	3.4	0.0946	-2.8
79	RP(43,E , 2)	943.11429	-0.12	5.17E-23	2.95E-03	6.8	8.5	0.2304	1.6	0.0926	-0.7
79	RR(44,E , 2)	998.75862	-0.12	5.79E-23	2.73E-03	-1.3	0.0	0.2183	3.3	0.0955	-3.9
81	PQ(45,E , 2)	940.21146	0.11	8.07E-23	2.58E-03	-2.5	0.0	0.2082	4.4	0.0912	0.4
81	RQ(45,E , 2)	970.11239	-0.17	9.03E-23	2.80E-03	1.4	0.0	0.2110	3.1	0.0906	1.1
79	RQ(45,E , 2)	970.15591	-0.17	9.10E-23	2.80E-03	1.3	-0.9	0.2082	4.4	0.0966	-5.2
81	PQ(46,E , 2)	940.10660	0.19	7.06E-23	2.54E-03	-3.9	-1.1	0.1935	8.3	0.0932	-1.9
79	PQ(46,E , 2)	940.16409	0.14	6.87E-23	2.45E-03	-7.4	-5.6	0.1790	17.1	0.0884	3.4
79	RP(47,E , 2)	940.18899	-0.15	2.79E-23	2.54E-03	-8.2	-6.4	0.1737	16.3	0.0994	-8.2
79	RQ(47,E , 2)	969.94461	-0.21	7.56E-23	2.96E-03	7.1	4.5	0.2076	-2.7	0.0919	-0.7
79	RP(48,E , 2)	939.45285	-0.17	2.74E-23	2.83E-03	2.6	4.8	0.1929	0.7	0.0892	2.2
81	PQ(48,E , 2)	939.88974	0.19	5.47E-23	2.54E-03	-4.0	-0.7	0.1852	4.8	0.0883	3.2
79	PQ(48,E , 2)	939.94650	0.30	5.66E-23	2.59E-03	-2.0	0.0	0.1827	6.3	0.0923	-1.2
79	RQ(48,E , 2)	969.83560	-0.16	6.51E-23	2.89E-03	4.7	1.9	0.1962	-1.0	0.0926	-1.5
81	PQ(49,E , 2)	939.77780	0.15	4.84E-23	2.55E-03	-3.5	-0.8	0.1740	6.9	0.0943	-3.4
81	PQ(52,E , 2)	939.42819	0.26	3.31E-23	2.63E-03	-0.5	3.0	0.1742	-10.4	0.0908	0.0
81	RQ(52,E , 2)	969.33596	-0.41	3.47E-23	2.67E-03	-3.1	-5.2	0.1397	11.7	0.0938	-3.2
79	RQ(52,E , 2)	969.37643	-0.17	3.61E-23	2.75E-03	-0.3	-3.2	0.1533	1.8	0.0931	-2.4
81	PP(54,E , 2)	905.17673	0.11	1.33E-23	2.81E-03	6.4	4.4	0.1567	-4.7	0.0803	13.0
81	PQ(54,E , 2)	939.18332	0.21	2.17E-23	2.32E-03	-12.3	-9.1	0.1182	26.3	0.0891	1.8
79	PP(55,E , 2)	904.35135	0.68	1.18E-23	2.87E-03	8.5	5.5	0.1195	25.0	0.0745	21.7
81	RR(6,A , 3)	984.45830	-0.04	6.63E-22	2.88E-03	3.2	3.7	0.3525	-1.1	0.1185	0.4
81	PR(9,A , 3)	941.47885	-0.05	1.93E-22	2.66E-03	1.6	2.4	0.4355	-8.4	0.1204	-2.2
81	RP(9,A , 3)	974.26859	-0.01	1.23E-22	2.74E-03	-1.6	-1.0	0.3954	0.8	0.1189	-1.0
79	RP(9,A , 3)	974.29642	0.28	1.23E-22	2.68E-03	-4.0	-4.4	0.4223	-5.6	0.1166	1.0
81	RR(9,A , 3)	986.30401	-0.03	6.87E-22	2.77E-03	-0.7	-0.2	0.3920	1.7	0.1167	0.9
81	PP(10,A , 3)	928.78779	-0.01	5.26E-22	2.72E-03	3.9	4.5	0.4338	-4.9	0.1183	-1.4
79	PP(10,A , 3)	928.83442	-0.04	5.34E-22	2.70E-03	3.2	2.9	0.4326	-4.6	0.1188	-1.9
79	PR(10,A , 3)	942.18674	0.01	2.19E-22	2.60E-03	-0.5	-0.9	0.4300	-4.0	0.1205	-3.2
81	PP(11,A , 3)	928.12977	0.01	5.13E-22	2.59E-03	-1.0	-0.4	0.4193	1.5	0.1160	-0.5
79	PP(11,A , 3)	928.17384	-0.06	5.35E-22	2.64E-03	1.0	0.6	0.4235	0.4	0.1165	-0.9
79	RP(11,A , 3)	972.97745	0.03	1.80E-22	2.75E-03	-1.7	-2.0	0.4264	-0.2	0.1222	-5.5
81	PR(12,A , 3)	943.30320	-0.01	2.57E-22	2.58E-03	-1.3	-0.9	0.4426	-1.4	0.1170	-2.2
79	PP(13,A , 3)	926.84620	-0.02	5.59E-22	2.68E-03	2.4	2.1	0.4609	-3.2	0.1175	-3.5
81	PP(14,A , 3)	926.14258	0.01	5.44E-22	2.64E-03	1.0	1.5	0.4478	1.5	0.1147	-2.0
79	PP(14,A , 3)	926.17908	-0.03	5.55E-22	2.64E-03	1.0	0.6	0.4561	-0.3	0.1140	-1.4
79	RR(14,A , 3)	989.41833	-0.03	7.32E-22	2.77E-03	-0.7	-1.0	0.4674	-2.7	0.1097	2.4
81	PP(15,A , 3)	925.47584	0.00	5.41E-22	2.62E-03	0.3	0.9	0.4546	1.5	0.1137	-2.1
79	PP(15,A , 3)	925.50983	-0.01	5.62E-22	2.67E-03	2.1	1.8	0.4747	-2.8	0.1111	0.2
81	RR(15,A , 3)	989.93219	-0.03	6.93E-22	2.69E-03	-3.5	-3.0	0.4493	2.7	0.1094	1.7
81	RR(16,A , 3)	990.52856	-0.06	7.07E-22	2.77E-03	-0.6	0.0	0.4743	-1.7	0.1085	1.4
79	RR(16,A , 3)	990.61804	-0.03	7.48E-22	2.88E-03	3.1	2.9	0.4758	-2.0	0.1105	-0.4
79	PR(18,A , 3)	947.00316	0.03	3.35E-22	2.60E-03	-0.8	-1.5	0.4830	-2.3	0.1071	0.6
81	PP(19,A , 3)	922.78754	0.04	5.08E-22	2.57E-03	-1.7	-1.2	0.4666	1.2	0.1076	-0.9
79	PP(19,A , 3)	922.81122	0.03	5.58E-22	2.78E-03	6.1	5.6	0.5274	-10.4	0.1072	-0.6
79	PR(19,A , 3)	947.59435	0.04	3.43E-22	2.63E-03	0.5	-0.1	0.4731	-0.2	0.1041	2.4
81	RR(19,A , 3)	992.30341	-0.05	6.86E-22	2.84E-03	1.8	2.5	0.4951	-4.6	0.1048	1.7
81	PP(20,A , 3)	922.11011	0.03	4.94E-22	2.56E-03	-2.0	-1.6	0.4763	-1.1	0.1047	0.7
79	PP(20,A , 3)	922.13117	-0.03	5.09E-22	2.59E-03	-1.1	-1.6	0.4779	-1.4	0.1057	-0.2
81	PR(20,A , 3)	948.06310	0.04	3.48E-22	2.73E-03	4.2	4.3	0.5099	-7.6	0.1065	-1.0
81	RR(20,A , 3)	992.89020	-0.04	6.58E-22	2.79E-03	0.2	0.8	0.4790	-1.6	0.1053	0.2
79	RR(20,A , 3)	992.98859	-0.02	7.00E-22	2.92E-03	4.6	4.5	0.5052	-6.7	0.1066	-1.0
81	PP(21,A , 3)	921.43060	0.05	4.95E-22	2.64E-03	0.9	1.3	0.4704	-0.4	0.1065	-2.0
79	PP(21,A , 3)	921.44910	0.04	5.22E-22	2.73E-03	4.3	3.7	0.4953	-5.4	0.1089	-4.1
81	PQ(21,A , 3)	934.72298	-0.01	7.95E-22	2.58E-03	-1.2	-0.2	0.4574	2.4	0.1041	0.3
81	PQ(22,A , 3)	934.67312	0.04	8.13E-22	2.70E-03	3.2	4.2	0.4763	-2.5	0.1069	-3.3
81	PQ(23,A , 3)	934.62093	0.04	7.44E-22	2.54E-03	-3.0	-2.1	0.4270	7.4	0.1037	-1.2
79	PQ(23,A , 3)	934.68966	0.04	7.81E-22	2.62E-03	-0.1	0.0	0.4633	-1.0	0.1028	-0.3
79	RR(23,A , 3)	994.74091	-0.06	5.93E-22	2.75E-03	-1.6	-1.5	0.4664	-1.6	0.1001	2.3
81	PQ(24,A , 3)	934.56649	0.07	7.50E-22	2.64E-03	1.0	2.0	0.4283	5.5	0.1021	-0.6

79	PQ(24,A , 3)	934.63497	0.03	7.43E-22	2.57E-03	-1.9	-1.9	0.4310	4.8	0.1032	-1.6
81	PP(25,A , 3)	918.69146	0.07	4.31E-22	2.68E-03	2.3	2.6	0.4436	0.0	0.1005	0.2
79	PP(25,A , 3)	918.69946	0.03	4.41E-22	2.69E-03	2.9	2.2	0.4622	-4.0	0.1007	0.0
79	PQ(25,A , 3)	934.57802	0.07	7.24E-22	2.60E-03	-0.8	-0.7	0.4195	5.8	0.0992	1.5
81	PR(25,A , 3)	950.95898	0.06	2.99E-22	2.55E-03	-2.4	-2.4	0.4297	3.2	0.0991	1.6
79	PR(25,A , 3)	951.08996	0.10	3.11E-22	2.61E-03	-0.3	-1.3	0.4509	-1.6	0.1006	0.1
81	RR(25,A , 3)	995.78761	-0.04	5.34E-22	2.76E-03	-1.2	-0.4	0.4338	2.3	0.1007	0.0
79	RR(25,A , 3)	995.89692	-0.01	5.43E-22	2.75E-03	-1.4	-1.3	0.4488	-1.2	0.0992	1.5
81	PQ(26,A , 3)	934.45070	0.06	6.64E-22	2.52E-03	-3.5	-2.4	0.4174	4.1	0.0928	7.6
81	RR(26,A , 3)	996.35969	-0.08	5.16E-22	2.80E-03	0.3	1.1	0.4313	0.7	0.0997	0.2
79	PQ(27,A , 3)	934.45717	0.04	6.68E-22	2.62E-03	-0.1	0.1	0.4325	-2.0	0.0978	1.3
81	RR(27,A , 3)	996.92933	-0.08	4.81E-22	2.76E-03	-1.2	-0.3	0.4366	-2.9	0.0981	1.0
81	RQ(28,A , 3)	979.15513	-0.08	6.95E-22	2.79E-03	0.0	-0.1	0.4006	3.0	0.1006	-2.2
79	RQ(29,A , 3)	979.13530	-0.05	6.63E-22	2.76E-03	-1.0	-1.9	0.3817	5.0	0.0940	3.9
79	RR(29,A , 3)	998.17897	-0.09	4.32E-22	2.75E-03	-1.6	-1.4	0.3904	2.7	0.0973	0.4
79	RR(30,A , 3)	998.74324	-0.08	4.06E-22	2.76E-03	-1.1	-0.9	0.3836	1.2	0.0959	1.2
79	PP(31,A , 3)	914.51250	0.08	3.05E-22	2.66E-03	1.5	0.7	0.3804	-1.4	0.0960	0.5
81	RR(31,A , 3)	999.18294	-0.11	3.69E-22	2.73E-03	-2.1	-1.0	0.3818	-1.7	0.0940	2.6
79	PP(32,A , 3)	913.80748	0.12	2.87E-22	2.69E-03	2.8	1.9	0.3733	-3.1	0.0976	-1.7
81	PP(32,A , 3)	913.81804	0.08	2.85E-22	2.71E-03	3.5	3.7	0.3804	-4.9	0.0979	-2.0
79	PR(32,A , 3)	955.05445	0.17	2.14E-22	2.52E-03	-3.5	-4.8	0.3390	6.7	0.0929	3.2
79	RQ(32,A , 3)	978.92435	-0.13	5.49E-22	2.77E-03	-0.9	-1.9	0.3599	0.5	0.0941	1.9
79	PR(33,A , 3)	955.61060	0.15	2.04E-22	2.58E-03	-1.5	-2.9	0.3323	4.8	0.0874	9.1
81	RQ(33,A , 3)	978.80510	-0.11	4.99E-22	2.74E-03	-1.8	-2.1	0.3289	5.9	0.0927	2.9
79	RR(33,A , 3)	1000.42091	-0.08	3.28E-22	2.78E-03	-0.4	-0.1	0.3674	-5.2	0.0936	1.9
81	PR(34,A , 3)	956.01423	0.11	1.88E-22	2.58E-03	-1.4	-1.7	0.3106	7.8	0.0969	-2.1
81	RQ(34,A , 3)	978.72831	-0.10	4.60E-22	2.72E-03	-2.3	-2.6	0.3328	0.6	0.0907	4.6
79	RQ(34,A , 3)	978.77244	-0.08	4.96E-22	2.89E-03	3.6	2.4	0.3647	-8.2	0.0938	1.2
79	RR(34,A , 3)	1000.97505	-0.08	3.03E-22	2.79E-03	-0.1	0.3	0.3305	1.3	0.0962	-1.4
81	PQ(35,A , 3)	933.81673	0.14	3.85E-22	2.57E-03	-1.7	-0.1	0.3140	2.4	0.0939	0.6
79	PR(35,A , 3)	956.71522	0.14	1.97E-22	2.88E-03	9.9	8.7	0.3275	-1.8	0.0969	-2.5
79	RQ(35,A , 3)	978.69303	-0.10	4.39E-22	2.77E-03	-0.6	-1.7	0.3272	-1.7	0.0911	3.7
79	PQ(36,A , 3)	933.79995	0.13	3.72E-22	2.67E-03	1.8	2.3	0.3200	-3.6	0.0951	-1.1
81	RP(36,A , 3)	955.82087	-0.09	1.68E-22	2.95E-03	5.7	7.2	0.3407	-9.5	0.0906	3.8
81	RQ(36,A , 3)	978.56791	-0.10	3.98E-22	2.77E-03	-0.7	-1.0	0.2988	3.2	0.0934	0.7
79	RQ(36,A , 3)	978.61137	-0.08	4.07E-22	2.80E-03	0.1	-1.0	0.3106	-0.7	0.0924	1.8
79	RP(37,A , 3)	955.06317	-0.05	1.54E-22	2.90E-03	3.9	4.4	0.3083	-4.1	0.0920	1.8
81	RP(37,A , 3)	955.10889	-0.14	1.47E-22	2.80E-03	0.4	1.7	0.3040	-2.7	0.0923	1.5
81	RQ(37,A , 3)	978.48429	-0.11	3.63E-22	2.75E-03	-1.3	-1.7	0.2889	2.4	0.0917	2.1
81	RR(37,A , 3)	1002.48763	-0.16	2.15E-22	2.61E-03	-6.3	-5.0	0.2859	3.5	0.0942	-0.6
81	PR(38,A , 3)	958.19465	0.19	1.34E-22	2.53E-03	-3.2	-3.8	0.2595	9.3	0.0947	-1.5
79	PR(38,A , 3)	958.35273	0.18	1.41E-22	2.64E-03	0.8	-0.9	0.2887	-1.7	0.0950	-1.8
79	RQ(38,A , 3)	978.44114	-0.13	3.39E-22	2.78E-03	-0.3	-1.4	0.2891	-1.9	0.0914	2.1
79	PR(39,A , 3)	958.89338	0.24	1.35E-22	2.78E-03	6.3	4.3	0.2806	-3.0	0.0955	-2.6
81	RQ(39,A , 3)	978.31022	-0.16	3.08E-22	2.81E-03	0.7	0.3	0.2782	-2.2	0.0921	1.0
79	RQ(40,A , 3)	978.26182	-0.14	2.95E-22	2.93E-03	5.0	3.5	0.2848	-8.2	0.0888	4.4
81	PQ(41,A , 3)	933.29085	0.15	2.23E-22	2.60E-03	-0.6	1.3	0.2639	-4.5	0.0923	0.1
81	RQ(41,A , 3)	978.12712	-0.15	2.45E-22	2.73E-03	-2.3	-2.7	0.2450	2.8	0.0912	1.4
79	RR(41,A , 3)	1004.78182	-0.20	1.55E-22	2.77E-03	-0.6	0.0	0.2642	-4.6	0.0926	-0.2
81	PQ(42,A , 3)	933.19521	0.21	2.01E-22	2.61E-03	-0.4	1.4	0.2539	-4.6	0.0923	-0.1
79	RR(42,A , 3)	1005.31533	-0.13	1.40E-22	2.80E-03	0.2	0.9	0.2495	-2.9	0.0935	-1.4
81	RP(43,A , 3)	950.79602	-0.22	8.72E-23	2.95E-03	5.7	8.0	0.2494	-6.5	0.0940	-2.1
79	RQ(43,A , 3)	977.97581	-0.06	1.97E-22	2.69E-03	-3.7	-5.1	0.2389	-2.4	0.0846	8.7
79	PP(44,A , 3)	905.18936	0.20	9.03E-23	2.70E-03	3.0	1.8	0.2274	-1.2	0.0944	-2.8
81	PP(44,A , 3)	905.23276	0.22	8.66E-23	2.61E-03	-0.1	-0.5	0.2249	-0.1	0.0922	-0.4
81	PR(44,A , 3)	961.38667	0.17	7.46E-23	2.58E-03	-1.2	-2.1	0.2193	2.5	0.0952	-3.6
79	RQ(44,A , 3)	977.87577	-0.15	1.80E-22	2.75E-03	-1.7	-3.3	0.2136	5.2	0.0897	2.3
79	RP(45,A , 3)	949.27502	-0.16	6.20E-23	2.60E-03	-6.8	-5.8	0.1903	13.8	0.0831	10.3
79	RQ(45,A , 3)	977.77348	-0.22	1.60E-22	2.75E-03	-1.7	-3.4	0.1826	18.6	0.0905	1.2
81	RR(45,A , 3)	1006.74961	-0.22	9.98E-23	2.85E-03	2.0	3.8	0.2267	-4.5	0.0926	-1.1
79	RR(45,A , 3)	1006.89969	-0.27	9.74E-23	2.75E-03	-1.4	-0.4	0.2098	3.2	0.0915	0.1
79	RP(46,A , 3)	948.54278	-0.15	5.36E-23	2.53E-03	-9.5	-8.4	0.1711	22.0	0.0919	-0.5
81	RP(46,A , 3)	948.61333	-0.29	5.78E-23	2.74E-03	-1.8	0.1	0.2001	4.3	0.0939	-2.6
81	PR(46,A , 3)	962.42952	0.25	6.02E-23	2.62E-03	0.2	-0.9	0.2227	-6.3	0.0961	-4.8
81	PP(47,A , 3)	903.04184	0.21	6.30E-23	2.74E-03	4.7	4.1	0.2261	-11.1	0.0952	-4.1
79	RP(47,A , 3)	947.80852	-0.22	5.70E-23	3.02E-03	8.3	9.6	0.2223	-9.5	0.0938	-2.6
81	RP(47,A , 3)	947.88201	-0.22	4.99E-23	2.68E-03	-3.9	-2.1	0.1916	5.0	0.0916	-0.3
79	RQ(47,A , 3)	977.56223	-0.15	1.27E-22	2.80E-03	0.1	-1.9	0.1958	2.7	0.0891	2.5
81	RP(48,A , 3)	947.14867	-0.27	4.62E-23	2.81E-03	0.9	3.0	0.1939	-0.3	0.0930	-1.9
79	PQ(49,A , 3)	932.52053	0.33	8.45E-23	2.52E-03	-3.7	-2.8	0.1890	-2.0	0.0901	1.1
81	RQ(49,A , 3)	977.30351	-0.26	9.53E-23	2.72E-03	-2.5	-3.3	0.1695	9.2	0.0896	1.7
81	RR(49,A , 3)	1008.81754	-0.15	6.18E-23	2.94E-03	5.3	7.3	0.2037	-9.1	0.0918	-0.7
81	PQ(50,A , 3)	932.34639	0.29	7.67E-23	2.62E-03	0.3	2.7	0.2054	-14.1	0.0903	0.8
81	RQ(50,A , 3)	977.19022	-0.35	8.29E-23	2.70E-03	-3.2	-4.2	0.1662	6.1	0.0921	-1.2
79	RQ(50,A , 3)	977.22800	-0.20	8.95E-23	2.91E-03	4.1	1.8	0.2056	-14.2	0.0874	4.2
81	RQ(51,A , 3)	977.07468	-0.40	7.57E-23	2.84E-03	1.8	0.6	0.1734	-4.0	0.0917	-0.8
79	RQ(51,A , 3)	977.11204	-0.17	7.68E-23	2.86E-03	2.3	0.2	0.1708	-2.5	0.0910	0.0
79	RR(55,A , 3)	1012.00737	-0.09	2.31E-23	2.59E-03	-7.1	-5.6	0.1447	2.6	0.0882	2.9

81	PP(4,E , 4)	925.43873	0.03	2.13E-22	2.53E-03	-2.3	-1.7	0.3042	-16.9	0.0997	-2.3
79	PP(4,E , 4)	925.50391	-0.06	2.25E-22	2.62E-03	1.0	0.7	0.3413	-25.9	0.0991	-1.8
79	RR(7,E , 4)	992.81787	-0.04	3.48E-22	2.85E-03	1.1	0.7	0.3760	-9.3	0.1116	3.0
81	PP(8,E , 4)	922.84638	0.01	2.42E-22	2.65E-03	2.6	3.3	0.3665	-0.8	0.1193	-3.3
79	PP(8,E , 4)	922.90161	-0.11	2.32E-22	2.49E-03	-3.8	-4.0	0.3455	5.2	0.1182	-2.4
81	RR(8,E , 4)	993.36786	0.02	3.43E-22	2.84E-03	0.7	1.2	0.3788	-4.0	0.1134	1.7
79	RR(8,E , 4)	993.43543	-0.01	3.44E-22	2.78E-03	-1.3	-1.6	0.3736	-2.7	0.1127	2.4
81	PP(9,E , 4)	922.19275	0.00	2.49E-22	2.66E-03	3.0	3.5	0.4021	-4.7	0.1180	-2.6
81	PP(10,E , 4)	921.53693	-0.01	2.44E-22	2.57E-03	-0.6	0.0	0.3809	5.2	0.1179	-3.1
79	PP(10,E , 4)	921.58722	-0.06	2.55E-22	2.64E-03	1.8	1.4	0.3996	0.3	0.1163	-1.8
81	RR(10,E , 4)	994.59119	-0.05	3.53E-22	2.86E-03	1.6	2.1	0.4251	-5.7	0.1108	3.1
81	PP(11,E , 4)	920.87890	-0.03	2.49E-22	2.59E-03	0.1	0.7	0.4084	1.8	0.1158	-2.0
79	PP(11,E , 4)	920.92670	-0.06	2.53E-22	2.58E-03	-0.4	-0.8	0.4079	1.9	0.1162	-2.3
81	PP(12,E , 4)	920.21875	0.01	2.46E-22	2.54E-03	-1.9	-1.3	0.4005	7.0	0.1181	-4.4
81	PR(12,E , 4)	936.05093	0.06	8.76E-23	2.56E-03	-1.0	-0.5	0.4310	-0.6	0.1109	1.8
79	PR(12,E , 4)	936.15652	-0.01	8.31E-23	2.38E-03	-8.0	-8.4	0.4063	5.5	0.1135	-0.5
81	RR(12,E , 4)	995.80525	-0.02	3.54E-22	2.85E-03	1.2	1.7	0.4585	-6.5	0.1120	0.8
79	RR(12,E , 4)	995.88209	-0.03	3.52E-22	2.78E-03	-1.3	-1.6	0.4489	-4.5	0.1126	0.3
81	RR(13,E , 4)	996.40876	0.00	3.49E-22	2.82E-03	0.0	0.5	0.4557	-3.6	0.1094	2.7
81	RR(14,E , 4)	997.00984	-0.04	3.34E-22	2.71E-03	-3.7	-3.3	0.4377	2.5	0.1119	-0.2
81	RP(15,E , 4)	977.97977	0.02	9.41E-23	2.82E-03	0.2	0.9	0.4644	-1.9	0.1056	5.0
81	RP(16,E , 4)	977.31114	0.02	1.04E-22	2.92E-03	3.6	4.5	0.4726	-2.4	0.1178	-6.8
79	RP(16,E , 4)	977.31742	-0.02	1.05E-22	2.89E-03	2.4	2.4	0.4690	-1.7	0.1161	-5.4
81	RR(16,E , 4)	998.20497	-0.02	3.24E-22	2.71E-03	-4.0	-3.5	0.4575	0.8	0.1090	0.7
79	PR(17,E , 4)	939.16031	-0.06	1.30E-22	2.78E-03	7.3	6.6	0.4842	-4.0	0.1098	-0.8
81	RP(17,E , 4)	976.64036	-0.01	1.07E-22	2.85E-03	0.9	1.5	0.4518	2.9	0.1050	3.7
79	RP(17,E , 4)	976.64414	0.04	1.09E-22	2.84E-03	0.8	0.7	0.4609	0.9	0.1105	-1.4
79	PR(18,E , 4)	939.75387	-0.04	1.23E-22	2.58E-03	-0.4	-1.0	0.4574	2.1	0.1094	-1.6
79	RR(18,E , 4)	999.48097	0.01	3.26E-22	2.78E-03	-1.5	-1.7	0.4714	-0.9	0.1059	1.7
81	PP(19,E , 4)	915.53685	-0.03	2.29E-22	2.52E-03	-2.6	-2.1	0.4429	5.6	0.1080	-1.4
81	PR(19,E , 4)	940.22354	0.02	1.24E-22	2.60E-03	0.6	1.0	0.4681	-0.1	0.1073	-0.7
81	PP(20,E , 4)	914.85955	0.06	2.31E-22	2.61E-03	1.0	1.6	0.4819	-3.1	0.1078	-2.2
79	PP(20,E , 4)	914.88427	-0.04	2.40E-22	2.66E-03	2.7	2.2	0.4835	-3.5	0.1103	-4.4
81	PR(20,E , 4)	940.81003	0.08	1.15E-22	2.38E-03	-8.0	-7.8	0.4210	10.9	0.1036	1.7
81	RR(20,E , 4)	1000.56648	0.02	3.00E-22	2.75E-03	-2.3	-1.7	0.4836	-3.5	0.1030	2.3
81	PP(21,E , 4)	914.17998	-0.01	2.22E-22	2.59E-03	0.0	0.4	0.4505	3.1	0.1043	0.0
79	PR(21,E , 4)	941.51987	0.04	1.21E-22	2.48E-03	-4.3	-5.0	0.4229	9.8	0.1053	-0.9
79	RP(22,E , 4)	973.24569	0.04	1.11E-22	2.61E-03	-7.6	-7.7	0.4430	3.9	0.1061	-2.6
81	RP(22,E , 4)	973.25479	-0.08	1.20E-22	2.89E-03	2.3	3.1	0.4338	6.1	0.1067	-3.2
81	RQ(22,E , 4)	987.17803	0.01	3.55E-22	2.70E-03	-4.2	-3.9	0.4234	8.7	0.1008	2.5
79	RR(22,E , 4)	1001.83199	0.04	2.85E-22	2.76E-03	-2.3	-2.5	0.4598	0.1	0.1020	1.3
81	PP(23,E , 4)	912.81462	-0.01	2.07E-22	2.60E-03	0.4	1.0	0.4627	-1.7	0.1063	-3.7
79	RP(23,E , 4)	972.55966	0.02	1.28E-22	3.03E-03	7.4	7.5	0.4651	-2.2	0.1014	1.0
79	RQ(23,E , 4)	987.16973	-0.02	3.64E-22	2.79E-03	-1.1	-1.6	0.4441	2.5	0.1003	2.1
81	PP(24,E , 4)	912.12883	0.02	1.96E-22	2.57E-03	-0.6	-0.2	0.4372	2.5	0.1041	-2.5
79	PP(24,E , 4)	912.14323	0.06	2.04E-22	2.63E-03	1.4	0.8	0.4592	-2.4	0.1062	-4.5
81	PQ(24,E , 4)	927.31446	0.04	2.90E-22	2.45E-03	-5.2	-4.3	0.4085	9.8	0.0999	1.6
81	PR(24,E , 4)	943.13126	0.10	1.14E-22	2.46E-03	-4.8	-4.7	0.4132	8.5	0.1014	0.1
81	RP(24,E , 4)	971.88607	0.05	1.14E-22	2.79E-03	-1.1	-0.4	0.5032	-10.9	0.1259	-19.4
81	PP(25,E , 4)	911.44090	0.02	1.91E-22	2.63E-03	1.6	2.2	0.4409	-0.1	0.1045	-3.7
79	PP(25,E , 4)	911.45262	0.00	1.98E-22	2.68E-03	3.4	2.9	0.4633	-4.9	0.1056	-4.7
81	PQ(25,E , 4)	927.25764	0.02	2.96E-22	2.59E-03	0.3	1.2	0.4393	0.3	0.1014	-0.8
81	PP(26,E , 4)	910.75096	0.08	1.73E-22	2.51E-03	-3.0	-2.5	0.4012	7.5	0.1020	-2.2
79	PP(26,E , 4)	910.75999	0.00	1.89E-22	2.69E-03	3.8	3.3	0.4450	-3.1	0.1026	-2.7
81	PQ(26,E , 4)	927.19862	0.08	2.84E-22	2.59E-03	0.3	1.3	0.4212	2.4	0.1024	-2.5
79	PQ(26,E , 4)	927.27033	0.04	2.91E-22	2.61E-03	0.8	0.8	0.4230	2.0	0.0966	3.3
79	RP(26,E , 4)	970.48910	-0.04	1.24E-22	3.12E-03	10.4	10.4	0.4751	-9.2	0.1053	-5.2
81	PP(27,E , 4)	910.05888	0.08	1.74E-22	2.65E-03	2.5	2.9	0.4341	-2.9	0.1012	-2.1
79	PP(27,E , 4)	910.06529	0.03	1.81E-22	2.72E-03	5.2	4.7	0.4278	-1.5	0.0998	-0.8
79	PQ(27,E , 4)	927.20875	0.07	2.80E-22	2.62E-03	1.4	1.5	0.4256	-1.0	0.0987	0.3
81	RP(27,E , 4)	969.81723	0.01	1.16E-22	3.04E-03	8.0	9.1	0.4459	-5.5	0.1036	-4.4
81	PP(28,E , 4)	909.36473	0.07	1.62E-22	2.62E-03	1.4	1.8	0.4072	0.8	0.0988	-0.5
79	PP(28,E , 4)	909.36851	0.05	1.71E-22	2.74E-03	5.7	5.2	0.4175	-1.7	0.1002	-1.9
79	RR(28,E , 4)	1005.28469	-0.01	2.18E-22	2.87E-03	1.6	1.5	0.4161	-1.4	0.0993	-1.0
79	PQ(30,E , 4)	927.01026	0.16	2.17E-22	2.40E-03	-7.2	-7.1	0.3164	22.0	0.1023	-5.2
81	RR(30,E , 4)	1006.29929	0.00	1.74E-22	2.66E-03	-5.7	-4.8	0.3640	6.0	0.0970	0.0
79	PP(31,E , 4)	907.26578	0.11	1.34E-22	2.61E-03	0.6	0.0	0.3898	-4.3	0.0937	2.9
81	PP(31,E , 4)	907.27000	0.14	1.36E-22	2.69E-03	4.1	4.3	0.4259	-12.4	0.1088	-11.4
81	PQ(31,E , 4)	926.86903	0.13	2.13E-22	2.55E-03	-1.5	-0.4	0.3702	0.8	0.0961	0.3
79	RP(31,E , 4)	966.99709	-0.01	9.10E-23	2.82E-03	0.0	0.0	0.3595	3.8	0.0997	-3.3
81	RQ(31,E , 4)	986.62969	-0.05	2.41E-22	2.72E-03	-3.6	-3.6	0.3449	8.2	0.0949	1.6
81	RR(31,E , 4)	1006.85886	-0.05	1.54E-22	2.53E-03	-10.2	-9.5	0.3270	14.1	0.0936	3.0
79	PQ(32,E , 4)	926.86628	0.06	2.15E-22	2.71E-03	4.5	4.7	0.3661	-1.7	0.1000	-4.1
79	PR(32,E , 4)	947.80376	0.23	9.65E-23	2.89E-03	11.6	10.6	0.3490	3.1	0.0974	-1.6
79	RP(32,E , 4)	966.29250	-0.08	8.73E-23	2.86E-03	1.2	1.4	0.3511	2.5	0.1019	-5.9
81	RP(32,E , 4)	966.32832	-0.02	8.71E-23	2.90E-03	2.8	3.8	0.3684	-2.3	0.0990	-3.1
81	RQ(32,E , 4)	986.55749	-0.02	2.36E-22	2.85E-03	0.9	0.9	0.3532	1.9	0.0962	-0.3
81	RR(32,E , 4)	1007.41599	-0.03	1.71E-22	3.02E-03	7.1	8.2	0.3609	-0.3	0.0946	1.4

81	PQ(33,E , 4)	926.72114	0.11	1.93E-22	2.65E-03	2.4	3.7	0.3436	0.8	0.0950	0.4
79	RQ(33,E , 4)	986.52386	-0.06	2.26E-22	2.88E-03	1.9	1.1	0.3521	-1.7	0.0945	0.9
81	RR(33,E , 4)	1007.97056	-0.03	1.59E-22	3.04E-03	7.7	8.5	0.3356	3.2	0.0980	-2.7
79	RR(33,E , 4)	1008.09318	-0.08	1.62E-22	3.05E-03	8.2	8.4	0.3671	-5.7	0.0977	-2.4
79	PQ(34,E , 4)	926.71326	0.11	1.79E-22	2.60E-03	0.6	0.9	0.3266	1.9	0.0949	0.0
81	RR(34,E , 4)	1008.52256	-0.08	1.36E-22	2.81E-03	-0.3	0.6	0.3270	1.8	0.0969	-2.1
79	RR(34,E , 4)	1008.64732	-0.04	1.34E-22	2.75E-03	-2.7	-2.6	0.3225	3.2	0.0936	1.4
81	RQ(35,E , 4)	986.32708	-0.12	1.93E-22	2.91E-03	3.3	3.2	0.3264	-2.1	0.0954	-1.0
79	RQ(36,E , 4)	986.28570	-0.11	1.70E-22	2.75E-03	-2.5	-3.4	0.2948	3.9	0.0934	0.7
81	RR(36,E , 4)	1009.61906	-0.02	1.11E-22	2.75E-03	-2.5	-1.4	0.2996	2.2	0.0957	-1.7
79	RR(36,E , 4)	1009.74778	-0.11	1.22E-22	2.98E-03	5.5	5.6	0.3376	-9.3	0.0969	-2.9
79	PP(37,E , 4)	903.00497	0.11	8.69E-23	2.80E-03	8.0	7.0	0.3241	-9.4	0.1007	-7.0
81	PP(37,E , 4)	903.02542	0.15	8.12E-23	2.65E-03	2.3	2.6	0.3112	-5.6	0.1013	-7.5
81	PQ(37,E , 4)	926.39790	0.11	1.33E-22	2.51E-03	-2.8	-1.5	0.2787	5.4	0.0914	2.5
79	RR(37,E , 4)	1010.29423	-0.07	1.02E-22	2.74E-03	-2.9	-2.7	0.2849	3.1	0.0952	-1.6
81	PQ(38,E , 4)	926.31141	0.18	1.23E-22	2.56E-03	-1.1	0.3	0.2760	2.0	0.0965	-3.3
79	PQ(38,E , 4)	926.37952	0.16	1.36E-22	2.78E-03	7.2	7.7	0.3003	-6.2	0.0949	-1.7
79	PR(38,E , 4)	951.10119	0.10	5.51E-23	2.60E-03	0.5	-0.7	0.2863	-1.6	0.0984	-5.2
81	PQ(39,E , 4)	926.22254	0.17	1.17E-22	2.66E-03	3.0	4.7	0.2931	-7.8	0.0933	-0.3
79	PQ(39,E , 4)	926.29023	0.08	1.23E-22	2.76E-03	6.6	7.0	0.2660	1.6	0.0935	-0.5
81	RP(39,E , 4)	961.35951	-0.01	5.05E-23	2.84E-03	0.7	1.6	0.2757	-2.0	0.0978	-4.9
81	RQ(39,E , 4)	985.98821	-0.13	1.23E-22	2.64E-03	-6.4	-6.7	0.2419	11.7	0.0934	-0.4
79	RQ(39,E , 4)	986.02709	-0.09	1.33E-22	2.82E-03	0.0	-0.9	0.2559	5.6	0.0883	5.3
79	RR(39,E , 4)	1011.37925	-0.11	8.22E-23	2.68E-03	-5.1	-4.7	0.2497	8.2	0.0933	-0.3
79	PP(40,E , 4)	900.84744	0.23	5.97E-23	2.60E-03	0.2	-0.7	0.2588	0.3	0.0905	2.5
81	PP(40,E , 4)	900.87600	0.19	5.63E-23	2.48E-03	-4.0	-4.1	0.2433	6.6	0.0921	0.7
81	PQ(40,E , 4)	926.13135	0.13	1.02E-22	2.55E-03	-1.3	0.4	0.2462	5.4	0.0954	-2.8
79	PQ(40,E , 4)	926.19880	0.17	1.11E-22	2.75E-03	6.0	6.6	0.2922	-11.2	0.0933	-0.6
79	RQ(40,E , 4)	985.93633	-0.09	1.23E-22	2.89E-03	2.3	1.3	0.2663	-2.6	0.0939	-1.2
81	RR(40,E , 4)	1011.78105	-0.11	7.22E-23	2.63E-03	-6.5	-5.3	0.2467	5.2	0.0909	2.0
79	RR(40,E , 4)	1011.91789	-0.11	7.61E-23	2.75E-03	-2.5	-2.1	0.2395	8.3	0.0860	7.8
79	PP(41,E , 4)	900.12411	0.12	5.58E-23	2.69E-03	4.0	3.0	0.2570	-2.4	0.0975	-5.2
81	PP(41,E , 4)	900.15560	0.25	5.32E-23	2.60E-03	0.6	0.8	0.2396	4.6	0.0924	0.1
79	PQ(41,E , 4)	926.10499	0.21	9.39E-23	2.59E-03	-0.1	0.4	0.2513	-0.2	0.0945	-2.2
79	RQ(41,E , 4)	985.84325	-0.11	1.18E-22	3.06E-03	8.5	7.3	0.2531	-0.9	0.0932	-0.8
81	RR(44,E , 4)	1013.90148	-0.18	4.82E-23	2.74E-03	-3.0	-1.7	0.2146	4.1	0.0902	1.8
79	RR(44,E , 4)	1014.04607	-0.23	5.06E-23	2.85E-03	0.9	1.6	0.2200	1.6	0.0952	-3.5
79	PP(45,E , 4)	897.21145	0.14	3.69E-23	2.85E-03	10.1	8.7	0.2432	-11.4	0.0945	-3.0
81	PQ(45,E , 4)	925.64112	0.27	5.98E-23	2.59E-03	-0.1	1.4	0.2233	-3.6	0.0967	-5.2
81	RQ(45,E , 4)	985.41161	-0.25	7.38E-23	3.01E-03	6.6	5.8	0.2177	-1.1	0.0927	-1.1
79	RQ(45,E , 4)	985.44805	-0.21	7.23E-23	2.91E-03	3.3	1.7	0.2114	1.9	0.0948	-3.3
81	PQ(46,E , 4)	925.53602	0.19	5.16E-23	2.52E-03	-2.6	-0.8	0.2098	-1.1	0.0933	-1.9
79	PQ(46,E , 4)	925.60102	0.22	5.46E-23	2.64E-03	1.8	2.3	0.1927	7.7	0.0907	0.9
79	RQ(46,E , 4)	985.34362	-0.14	6.10E-23	2.77E-03	-1.7	-3.2	0.1850	12.2	0.0913	0.2
81	PP(47,E , 4)	895.79128	0.11	2.57E-23	2.57E-03	-0.7	-0.9	0.1747	14.4	0.0949	-3.7
79	PQ(47,E , 4)	925.49329	0.26	4.49E-23	2.45E-03	-5.3	-4.3	0.1692	18.1	0.0841	8.7
79	RQ(47,E , 4)	985.23675	-0.22	5.48E-23	2.83E-03	0.1	-1.4	0.1857	7.6	0.0947	-3.5
81	PQ(50,E , 4)	925.09296	0.34	3.12E-23	2.53E-03	-2.1	-0.1	0.1674	4.6	0.0879	3.6
79	RQ(50,E , 4)	984.90264	-0.17	3.77E-23	2.86E-03	1.3	-0.2	0.1682	4.1	0.0903	0.9
81	PP(51,E , 4)	892.84303	0.28	1.49E-23	2.55E-03	-1.3	-1.9	0.1166	41.8	0.0907	0.4
81	PQ(51,E , 4)	924.97645	0.43	2.49E-23	2.34E-03	-9.5	-7.7	0.1209	36.7	0.0812	12.1
79	RQ(52,E , 4)	984.66851	-0.04	2.59E-23	2.60E-03	-7.9	-9.3	0.1277	20.6	0.0967	-5.9
79	RR(52,E , 4)	1018.17492	-0.23	1.78E-23	2.88E-03	2.2	3.0	--	--	0.0955	-4.7
81	PP(6,E , 5)	916.96185	-0.11	2.16E-22	2.53E-03	-1.2	-0.6	0.2722	0.0	0.1086	-3.7
79	PP(6,E , 5)	917.02581	-0.19	2.30E-22	2.63E-03	2.8	2.5	0.3243	-16.1	0.1062	-1.5
81	PP(7,E , 5)	916.31280	-0.02	2.24E-22	2.61E-03	1.9	2.6	0.3034	1.5	0.1128	-3.2
79	RR(7,E , 5)	1000.54591	0.00	3.33E-22	2.88E-03	0.9	0.6	0.3324	-7.4	0.1078	1.3
81	PP(9,E , 5)	915.00780	-0.11	2.13E-22	2.44E-03	-4.6	-4.0	0.3402	6.9	0.1146	-2.8
79	PP(9,E , 5)	915.06438	-0.10	2.32E-22	2.60E-03	1.7	1.4	0.3797	-4.2	0.1163	-4.2
81	RR(11,E , 5)	1002.93068	0.03	3.04E-22	2.68E-03	-5.9	-5.5	0.3927	2.7	0.1167	-4.8
81	RR(14,E , 5)	1004.74093	0.02	3.07E-22	2.78E-03	-2.5	-2.2	0.4431	-0.6	0.1072	3.4
81	RR(15,E , 5)	1005.33968	0.08	3.29E-22	3.01E-03	5.8	6.3	0.4819	-6.9	0.1097	0.6
81	RR(16,E , 5)	1005.93594	0.03	3.02E-22	2.82E-03	-0.9	-0.5	0.4575	-0.7	0.1071	2.1
81	PP(17,E , 5)	909.70079	-0.05	2.20E-22	2.64E-03	3.1	3.8	0.4386	4.5	0.1096	-0.7
79	RR(17,E , 5)	1006.61454	0.00	3.07E-22	2.87E-03	0.7	0.4	0.4689	-2.2	0.1066	2.1
81	PQ(19,E , 5)	920.37829	-0.04	2.52E-22	2.46E-03	-4.1	-3.3	0.4409	4.7	0.1055	0.9
81	RQ(19,E , 5)	995.05237	0.01	2.95E-22	2.73E-03	-4.2	-3.9	0.4295	7.5	0.1016	4.7
81	RR(19,E , 5)	1007.71055	0.08	2.70E-22	2.72E-03	-4.4	-4.0	0.4934	-6.4	0.0951	11.9
81	PQ(20,E , 5)	920.33282	-0.05	2.58E-22	2.53E-03	-1.1	-0.3	0.4672	-1.3	0.1064	-1.0
79	RQ(20,E , 5)	995.04804	0.01	3.16E-22	2.88E-03	1.1	0.5	0.4597	0.3	0.1036	1.6
79	RR(20,E , 5)	1008.38859	0.05	2.88E-22	2.94E-03	3.2	3.0	0.4815	-4.3	0.1052	0.1
81	PP(21,E , 5)	906.99558	-0.07	1.94E-22	2.60E-03	1.5	2.1	0.4645	-1.2	0.1083	-3.7
79	PP(21,E , 5)	907.02152	-0.07	1.95E-22	2.58E-03	0.7	0.2	0.4647	-1.3	0.1056	-1.3
81	PQ(21,E , 5)	920.28509	-0.05	2.62E-22	2.60E-03	1.7	2.5	0.4615	-0.6	0.1068	-2.4
79	PQ(21,E , 5)	920.36169	-0.02	2.61E-22	2.55E-03	-0.5	-0.6	0.4390	4.5	0.1047	-0.4
81	RQ(21,E , 5)	994.95997	0.02	2.98E-22	2.80E-03	-1.9	-1.6	0.4500	2.0	0.1033	0.9
81	PQ(22,E , 5)	920.23510	-0.04	2.53E-22	2.57E-03	0.3	1.1	0.4579	-0.6	0.1042	-0.9
79	PQ(22,E , 5)	920.31146	-0.04	2.58E-22	2.56E-03	0.1	0.0	0.4322	5.3	0.1015	1.7

81	RQ(22,E , 5)	994.91041	0.05	2.98E-22	2.84E-03	-0.2	0.0	0.4480	1.6	0.1028	0.4
79	RQ(22,E , 5)	994.95075	0.04	3.03E-22	2.83E-03	-0.6	-1.2	0.4426	2.8	0.1029	0.3
81	PQ(23,E , 5)	920.18286	0.00	2.55E-22	2.65E-03	3.5	4.5	0.4479	0.5	0.1036	-1.3
79	PQ(23,E , 5)	920.25897	-0.03	2.63E-22	2.68E-03	4.5	4.5	0.4541	-0.9	0.0983	4.1
79	PR(23,E , 5)	935.50057	0.01	8.91E-23	2.56E-03	-0.2	-0.9	0.4570	-1.5	0.1106	-7.5
79	RQ(23,E , 5)	994.89869	0.05	2.98E-22	2.85E-03	0.1	-0.4	0.4423	1.8	0.1017	0.6
79	RR(23,E , 5)	1010.14067	0.02	2.45E-22	2.83E-03	-0.6	-0.8	0.4473	0.6	0.0945	8.2
81	PP(24,E , 5)	904.94455	-0.01	1.67E-22	2.54E-03	-0.6	0.0	0.4301	3.2	0.1018	-0.4
81	PQ(24,E , 5)	920.12823	-0.05	2.44E-22	2.61E-03	1.9	2.9	0.4489	-1.1	0.1015	-0.1
79	PQ(24,E , 5)	920.20422	0.01	2.52E-22	2.64E-03	3.2	3.1	0.4588	-3.3	0.1015	-0.1
79	PR(24,E , 5)	936.07919	-0.02	9.07E-23	2.64E-03	3.1	2.3	0.4496	-1.3	0.1027	-1.3
79	RP(24,E , 5)	979.60221	-0.08	8.81E-23	2.88E-03	0.9	0.9	0.3856	15.1	0.1182	-14.2
81	RP(24,E , 5)	979.62021	0.00	8.32E-23	2.76E-03	-3.0	-2.4	0.4473	-0.8	0.1143	-11.3
81	PP(25,E , 5)	904.25669	0.03	1.65E-22	2.64E-03	3.2	3.8	0.4465	-2.3	0.1033	-2.7
79	PP(25,E , 5)	904.27207	-0.06	1.66E-22	2.61E-03	1.8	1.5	0.4402	-0.9	0.1040	-3.3
79	PQ(25,E , 5)	920.14709	-0.04	2.35E-22	2.55E-03	-0.3	-0.3	0.4264	2.3	0.1017	-1.1
81	PR(25,E , 5)	936.51705	0.00	8.68E-23	2.62E-03	2.4	2.9	0.4661	-6.4	0.1117	-10.0
81	RP(25,E , 5)	978.93284	0.06	8.92E-23	3.01E-03	5.5	6.3	0.3968	10.0	0.1012	-0.6
81	RQ(25,E , 5)	994.74805	0.02	2.70E-22	2.80E-03	-1.7	-1.6	0.4234	3.1	0.0995	1.0
81	RR(25,E , 5)	1011.19420	0.04	2.11E-22	2.74E-03	-3.8	-3.3	0.4189	4.2	0.1002	0.3
81	PP(26,E , 5)	903.56668	0.00	1.62E-22	2.74E-03	7.3	7.8	0.3931	8.8	0.0996	0.1
79	PP(26,E , 5)	903.57950	-0.02	1.60E-22	2.65E-03	3.6	3.1	0.4312	-0.8	0.1019	-2.1
81	RP(26,E , 5)	978.24332	0.04	8.81E-23	3.03E-03	6.2	6.9	0.4505	-5.1	0.1056	-5.5
79	RQ(26,E , 5)	994.72883	0.00	2.66E-22	2.81E-03	-1.3	-1.9	0.4181	2.3	0.0984	1.4
81	RR(26,E , 5)	1011.76622	0.03	1.97E-22	2.71E-03	-5.0	-4.5	0.3917	9.2	0.0973	2.5
81	PP(27,E , 5)	902.87466	0.03	1.37E-22	2.45E-03	-4.4	-4.0	0.3891	7.4	0.0998	-0.8
79	PP(27,E , 5)	902.88480	-0.01	1.47E-22	2.58E-03	0.8	0.3	0.4272	-2.2	0.1021	-3.0
81	RP(27,E , 5)	977.55173	-0.01	7.78E-23	2.75E-03	-3.5	-2.5	0.4018	4.0	0.1052	-5.9
79	PP(28,E , 5)	902.18802	-0.01	1.29E-22	2.42E-03	-5.4	-5.9	0.3661	11.2	0.0997	-1.4
79	RQ(28,E , 5)	994.60425	-0.02	2.38E-22	2.76E-03	-3.3	-3.9	0.3799	7.2	0.0989	-0.6
81	RR(28,E , 5)	1012.90288	0.04	1.87E-22	2.89E-03	1.5	2.2	0.4122	-1.2	0.0992	-0.9
81	RQ(29,E , 5)	994.50001	0.05	2.29E-22	2.85E-03	-0.1	0.0	0.3867	2.3	0.0979	-0.3
81	PQ(30,E , 5)	919.75293	0.01	1.81E-22	2.56E-03	-0.1	0.9	0.3581	7.0	0.0968	0.2
81	PR(30,E , 5)	939.34952	-0.01	6.87E-23	2.50E-03	-2.5	-2.3	0.3501	9.5	0.0949	2.2
79	RP(30,E , 5)	975.43088	-0.08	7.58E-23	2.96E-03	3.8	3.9	0.3417	12.1	0.1029	-5.7
81	RQ(30,E , 5)	994.43232	0.03	2.09E-22	2.75E-03	-3.5	-3.5	0.3551	7.9	0.0953	1.8
81	RR(30,E , 5)	1014.02953	0.01	1.59E-22	2.81E-03	-1.2	-0.5	0.3772	1.6	0.0956	1.5
79	RR(30,E , 5)	1014.14244	0.01	1.62E-22	2.82E-03	-1.1	-1.2	0.3719	3.0	0.0976	-0.6
79	PQ(31,E , 5)	919.75653	0.07	1.70E-22	2.51E-03	-2.1	-2.1	0.3467	6.8	0.0981	-1.7
81	PR(31,E , 5)	939.90848	0.03	6.40E-23	2.46E-03	-3.9	-3.6	0.3408	8.7	0.0969	-0.5
81	RQ(31,E , 5)	994.36237	0.03	2.01E-22	2.81E-03	-1.4	-1.2	0.3554	4.2	0.0953	1.2
79	RR(31,E , 5)	1014.70409	-0.01	1.46E-22	2.73E-03	-4.2	-4.2	0.3368	10.0	0.0945	2.0
79	PR(32,E , 5)	940.61813	0.12	6.03E-23	2.41E-03	-6.1	-6.9	0.3179	12.3	0.0984	-2.6
81	RQ(32,E , 5)	994.29017	0.03	1.86E-22	2.78E-03	-2.3	-2.3	0.3406	4.9	0.0970	-1.2
81	PQ(33,E , 5)	919.53442	0.08	1.53E-22	2.64E-03	3.1	4.4	0.3527	-2.6	0.0991	-3.8
81	RQ(33,E , 5)	994.21570	0.03	1.76E-22	2.82E-03	-1.1	-1.1	0.3206	7.2	0.0962	-0.9
79	PQ(34,E , 5)	919.53015	0.05	1.42E-22	2.60E-03	1.4	1.7	0.3263	1.2	0.0956	-0.7
81	PP(35,E , 5)	897.26418	0.06	8.21E-23	2.66E-03	3.8	4.1	0.3169	-0.1	0.1006	-6.1
79	RQ(35,E , 5)	994.09669	-0.01	1.64E-22	3.01E-03	5.6	4.9	0.2974	6.5	0.0954	-1.0
81	RR(35,E , 5)	1016.80218	0.03	1.11E-22	2.92E-03	2.4	3.0	0.3236	-2.1	0.1008	-6.3
79	RR(35,E , 5)	1016.92535	-0.06	1.07E-22	2.79E-03	-2.1	-1.8	0.3128	1.3	0.0953	-0.9
79	PP(36,E , 5)	896.53975	0.04	7.24E-23	2.53E-03	-1.2	-1.6	0.2925	3.8	0.0955	-1.5
81	PP(36,E , 5)	896.55373	0.07	6.60E-23	2.34E-03	-8.7	-8.4	0.2602	16.7	0.0931	1.0
81	RR(36,E , 5)	1017.34899	-0.07	9.66E-23	2.80E-03	-1.9	-1.2	0.2913	4.2	0.0883	6.5
79	PP(37,E , 5)	895.82460	0.09	6.74E-23	2.58E-03	0.7	0.0	0.2943	-1.1	0.0966	-3.0
81	PP(37,E , 5)	895.84127	0.09	6.67E-23	2.58E-03	0.8	1.2	0.2889	0.7	0.1002	-6.5
81	RQ(37,E , 5)	993.89503	-0.08	1.31E-22	2.88E-03	1.1	0.9	0.2955	-1.5	0.0956	-2.0
81	RR(37,E , 5)	1017.89343	0.03	8.03E-23	2.54E-03	-10.7	-10.0	0.2552	14.0	0.0908	3.2
79	PP(38,E , 5)	895.10738	0.09	6.16E-23	2.60E-03	1.7	0.7	0.2854	-2.3	0.0950	-1.7
81	PP(38,E , 5)	895.12679	0.10	5.89E-23	2.52E-03	-1.7	-1.4	0.2715	2.7	0.0950	-1.7
81	PQ(38,E , 5)	919.12426	0.09	9.29E-23	2.41E-03	-5.8	-4.6	0.2462	13.3	0.0917	1.8
81	RP(38,E , 5)	969.81094	-0.07	4.34E-23	2.93E-03	2.7	3.8	0.3071	-9.2	0.0968	-3.6
81	RQ(38,E , 5)	993.80927	-0.03	1.17E-22	2.83E-03	-0.6	-0.7	0.2767	0.8	0.0951	-1.8
79	RQ(38,E , 5)	993.84498	-0.03	1.19E-22	2.83E-03	-0.6	-1.3	0.2712	2.8	0.0929	0.5
79	PQ(39,E , 5)	919.10681	0.09	8.63E-23	2.44E-03	-4.9	-4.5	0.2552	4.8	0.0917	1.5
81	RQ(39,E , 5)	993.72113	-0.08	1.12E-22	2.98E-03	4.6	4.5	0.2817	-5.0	0.0941	-1.1
79	RQ(40,E , 5)	993.66578	-0.03	1.05E-22	3.01E-03	5.7	4.9	0.2676	-4.0	0.0941	-1.4
79	RR(40,E , 5)	1019.64422	-0.05	6.57E-23	2.79E-03	-2.3	-2.4	0.2537	1.3	0.0880	5.4
79	PP(41,E , 5)	892.94362	-0.02	4.30E-23	2.49E-03	-2.7	-3.6	0.2515	-0.9	0.0974	-5.0
81	RR(41,E , 5)	1020.04492	-0.05	5.95E-23	2.85E-03	0.0	0.0	0.2510	-0.7	0.0903	2.4
81	RQ(42,E , 5)	993.44318	-0.13	7.85E-23	2.82E-03	-1.0	-1.0	0.2255	6.2	0.0941	-1.9
81	PQ(43,E , 5)	918.65661	0.15	5.82E-23	2.51E-03	-2.1	-0.7	0.2196	4.9	0.0944	-2.5
79	PQ(43,E , 5)	918.72662	0.21	5.88E-23	2.52E-03	-1.8	-1.4	0.2102	9.6	0.0968	-4.9
81	RQ(43,E , 5)	993.34601	-0.12	7.06E-23	2.82E-03	-1.0	-1.1	0.2208	4.3	0.0993	-7.3
79	RQ(43,E , 5)	993.37989	0.00	7.26E-23	2.87E-03	0.8	0.0	0.2252	2.3	0.0937	-1.7
79	RR(43,E , 5)	1021.24420	-0.13	4.81E-23	2.84E-03	-0.4	0.0	0.2354	-2.1	0.0890	3.5
79	PP(44,E , 5)	890.76228	0.20	2.92E-23	2.36E-03	-7.7	-8.5	0.1715	29.4	0.0888	3.5
81	RQ(44,E , 5)	993.24659	-0.08	6.84E-23	3.07E-03	7.6	7.6	--	--	0.0920	-0.1

79	PP(45,E , 5)	890.03108	0.14	2.86E-23	2.63E-03	2.8	1.9	0.2065	3.5	0.0919	-0.2
81	PR(47,E , 5)	948.49932	0.45	1.59E-23	2.51E-03	-2.0	-2.5	0.1812	9.4	0.0961	-4.8
79	RQ(47,E , 5)	992.96656	-0.03	4.36E-23	2.76E-03	-3.1	-4.4	--	--	0.0910	0.5
81	PP(6,A , 6)	909.84385	-0.14	3.84E-22	2.45E-03	-3.1	-2.4	0.2270	-3.3	0.0922	2.7
79	RR(6,A , 6)	1007.70737	0.11	6.18E-22	2.94E-03	1.9	1.6	0.2353	-6.7	0.0927	2.1
81	PP(7,A , 6)	909.19480	-0.14	3.81E-22	2.45E-03	-3.0	-2.4	0.2800	-4.5	0.1019	0.3
79	PP(7,A , 6)	909.26005	-0.18	4.11E-22	2.59E-03	2.4	2.2	0.3098	-13.7	0.1039	-1.6
79	RR(8,A , 6)	1008.94444	0.09	5.91E-22	2.86E-03	-0.6	-0.9	0.3212	-4.4	0.1040	1.6
81	PP(10,A , 6)	907.23435	-0.13	3.88E-22	2.53E-03	0.0	0.7	0.3707	-1.2	0.1141	-5.7
81	RR(10,A , 6)	1010.10685	0.09	5.62E-22	2.82E-03	-1.9	-1.6	0.3574	2.5	0.1071	0.5
81	RQ(12,A , 6)	1003.09011	0.10	3.44E-22	2.85E-03	-1.0	-0.7	0.4347	-6.7	0.1042	4.3
81	RR(12,A , 6)	1011.32060	0.08	5.79E-22	2.97E-03	3.2	3.7	0.4336	-6.5	0.1099	-1.1
79	RR(12,A , 6)	1011.39055	0.10	5.80E-22	2.91E-03	1.1	0.8	0.4290	-5.5	0.1093	-0.6
81	PP(13,A , 6)	905.25418	-0.10	3.79E-22	2.52E-03	-0.4	0.3	0.4227	-0.7	0.1110	-1.5
79	PP(13,A , 6)	905.30436	-0.14	4.01E-22	2.62E-03	3.4	3.0	0.4521	-7.2	0.1132	-3.4
81	PR(13,A , 6)	922.34723	-0.10	7.53E-23	2.52E-03	-0.5	0.1	0.4535	-7.4	0.1128	-3.1
81	RQ(13,A , 6)	1003.06081	0.07	3.87E-22	2.93E-03	1.8	2.0	0.4804	-12.6	0.1086	0.7
81	RR(13,A , 6)	1011.92399	0.12	5.59E-22	2.90E-03	0.8	1.2	0.4286	-2.1	0.1073	1.9
79	RR(13,A , 6)	1011.99614	0.05	5.75E-22	2.93E-03	1.5	1.1	0.4335	-3.2	0.1088	0.5
81	PP(14,A , 6)	904.58975	-0.09	3.78E-22	2.55E-03	0.7	1.4	0.4466	-3.5	0.1087	1.0
79	RQ(14,A , 6)	1003.06759	0.06	4.14E-22	2.88E-03	-0.2	-0.7	0.4693	-8.2	0.1054	4.2
81	RR(14,A , 6)	1012.52495	0.10	5.62E-22	2.97E-03	3.1	3.5	0.4769	-9.6	0.1087	1.0
79	RR(14,A , 6)	1012.59941	0.06	5.77E-22	2.99E-03	3.7	3.4	0.4732	-8.9	0.1079	1.7
81	PP(15,A , 6)	903.92313	-0.12	3.70E-22	2.54E-03	0.2	0.9	0.4533	-3.0	0.1100	-0.3
79	PP(15,A , 6)	903.96823	-0.16	3.90E-22	2.62E-03	3.6	3.2	0.4558	-3.5	0.1110	-1.2
79	RR(15,A , 6)	1013.20030	0.08	5.42E-22	2.86E-03	-0.6	-1.0	0.4428	-0.7	0.1068	2.7
81	PP(16,A , 6)	903.25436	-0.14	3.66E-22	2.56E-03	1.0	1.7	0.4876	-8.5	0.1081	0.8
79	PR(16,A , 6)	924.26416	-0.12	1.03E-22	2.55E-03	0.6	0.0	0.4518	-1.3	0.1116	-2.4
81	RR(16,A , 6)	1013.71977	0.06	5.24E-22	2.88E-03	0.2	0.7	0.4535	-1.6	0.1062	2.6
79	RR(16,A , 6)	1013.79881	0.09	5.55E-22	2.99E-03	4.0	3.5	0.4636	-3.8	0.1028	6.0
81	RR(17,A , 6)	1014.31365	0.10	5.01E-22	2.83E-03	-1.6	-1.2	0.4538	-0.7	0.1040	4.5
79	RR(17,A , 6)	1014.39488	0.08	5.22E-22	2.89E-03	0.3	0.1	0.4669	-3.5	0.1055	3.0
81	PP(18,A , 6)	901.91043	-0.12	3.51E-22	2.58E-03	1.9	2.5	0.4611	-1.7	0.1086	-1.1
79	PP(18,A , 6)	901.94784	-0.15	3.54E-22	2.55E-03	0.6	0.1	0.4780	-5.2	0.1097	-2.1
81	PQ(18,A , 6)	913.30248	-0.10	3.97E-22	2.61E-03	3.3	4.1	0.5026	-9.8	0.1075	-0.1
79	PR(18,A , 6)	925.45319	-0.05	1.16E-22	2.61E-03	2.9	2.1	0.4775	-5.1	0.1119	-4.0
79	RQ(18,A , 6)	1002.91835	0.09	4.88E-22	2.97E-03	3.1	2.6	0.4472	1.4	0.1011	6.3
81	RR(18,A , 6)	1014.90508	0.08	4.99E-22	2.90E-03	0.8	1.2	0.4690	-3.3	0.1028	4.5
81	PP(19,A , 6)	901.23526	-0.10	3.43E-22	2.60E-03	2.6	3.3	0.4888	-7.0	0.1102	-3.6
79	PP(19,A , 6)	901.27005	-0.17	3.34E-22	2.48E-03	-2.1	-2.4	0.4585	-0.9	0.1067	-0.4
81	PQ(19,A , 6)	913.25926	-0.10	4.00E-22	2.63E-03	3.8	4.7	0.4775	-4.8	0.1069	-0.6
81	RQ(19,A , 6)	1002.83785	0.07	4.57E-22	2.82E-03	-2.2	-1.9	0.4618	-1.6	0.1009	5.3
79	RR(19,A , 6)	1015.57982	0.07	4.86E-22	2.86E-03	-0.6	-0.8	0.4617	-1.6	0.1035	2.7
81	PP(20,A , 6)	900.55795	-0.09	3.24E-22	2.53E-03	0.1	0.9	0.4745	-4.3	0.1084	-3.0
79	PP(20,A , 6)	900.59024	-0.08	3.46E-22	2.65E-03	4.8	4.5	0.4741	-4.2	0.1087	-3.2
81	PQ(20,A , 6)	913.21379	-0.07	3.79E-22	2.49E-03	-1.5	-0.7	0.4500	0.9	0.1060	-0.8
79	PQ(20,A , 6)	913.29424	-0.11	4.07E-22	2.63E-03	3.9	3.7	0.4747	-4.4	0.1066	-1.3
81	RP(20,A , 6)	990.13653	0.07	1.16E-22	2.94E-03	2.1	2.9	0.4745	-4.3	0.1039	1.2
81	RQ(20,A , 6)	1002.79281	0.09	4.56E-22	2.81E-03	-2.5	-2.2	0.4524	0.4	0.0997	5.5
79	RQ(20,A , 6)	1002.83010	0.06	4.63E-22	2.80E-03	-2.9	-3.2	0.4507	0.7	0.0997	5.5
81	RR(20,A , 6)	1016.08074	0.07	4.65E-22	2.90E-03	0.6	1.0	0.5015	-9.5	0.1004	4.8
79	RR(20,A , 6)	1016.16869	0.09	4.63E-22	2.83E-03	-1.8	-2.0	0.4615	-1.6	0.1008	4.3
81	PP(21,A , 6)	899.87850	-0.11	3.25E-22	2.64E-03	4.3	4.9	--	--	0.1109	-6.1
79	PP(21,A , 6)	899.90817	-0.11	3.28E-22	2.62E-03	3.2	2.9	0.4779	-5.4	0.1077	-3.3
81	PQ(21,A , 6)	913.16594	-0.14	4.02E-22	2.67E-03	5.5	6.4	0.4933	-8.3	0.1034	0.7
79	PQ(21,A , 6)	913.24626	-0.11	3.86E-22	2.52E-03	-0.5	-0.7	0.4620	-2.1	0.1025	1.6
79	PR(21,A , 6)	927.21827	-0.09	1.19E-22	2.49E-03	-1.8	-2.3	0.4540	-0.4	0.1026	1.5
79	RP(21,A , 6)	989.44409	0.12	1.20E-22	2.89E-03	0.4	0.3	0.4711	-4.0	0.1079	-3.5
81	RP(21,A , 6)	989.45739	-0.08	1.12E-22	2.75E-03	-4.6	-3.8	--	--	0.1047	-0.5
79	RQ(21,A , 6)	1002.78255	0.02	4.73E-22	2.88E-03	-0.1	-0.5	0.4588	-1.4	0.1016	2.5
79	PQ(22,A , 6)	913.19603	-0.08	3.73E-22	2.47E-03	-2.3	-2.5	0.4442	1.1	0.1024	0.7
81	RR(22,A , 6)	1017.24676	0.10	4.25E-22	2.87E-03	-0.3	0.3	0.4773	-5.9	0.0998	3.3
79	RR(22,A , 6)	1017.33904	0.06	4.33E-22	2.87E-03	-0.3	-0.5	0.4705	-4.6	0.0982	5.0
81	PR(23,A , 6)	928.24501	-0.10	1.23E-22	2.62E-03	3.3	4.1	0.4846	-8.3	0.1045	-2.2
79	PR(23,A , 6)	928.38270	-0.10	1.28E-22	2.65E-03	4.7	3.9	0.4662	-4.7	0.1053	-3.0
79	RR(23,A , 6)	1017.92053	0.03	4.15E-22	2.89E-03	0.3	0.0	0.4674	-4.9	0.1004	1.8
81	PP(24,A , 6)	897.82760	-0.03	2.77E-22	2.57E-03	1.7	2.2	0.4504	-2.7	0.1056	-4.1
79	PP(24,A , 6)	897.84939	-0.08	2.76E-22	2.52E-03	-0.4	-0.7	0.4429	-1.0	0.1034	-2.0
81	PR(24,A , 6)	928.82136	-0.07	1.11E-22	2.36E-03	-6.6	-6.2	--	--	0.0999	1.4
81	RQ(24,A , 6)	1002.59005	0.10	4.22E-22	2.78E-03	-3.5	-3.3	0.4369	0.4	0.0979	3.5
81	PP(25,A , 6)	897.13967	-0.10	2.64E-22	2.59E-03	2.2	2.7	0.4488	-3.9	0.1042	-3.6
79	PP(25,A , 6)	897.15896	-0.02	2.76E-22	2.66E-03	4.9	4.4	0.4229	2.0	0.1026	-2.1
81	PQ(25,A , 6)	912.95207	-0.07	3.33E-22	2.45E-03	-3.3	-2.4	0.4172	3.4	0.1004	0.1
79	RQ(25,A , 6)	1002.56990	0.07	4.24E-22	2.83E-03	-1.8	-2.4	0.4225	2.1	0.0979	2.6
81	PP(26,A , 6)	896.44973	-0.09	2.47E-22	2.56E-03	1.1	1.8	0.4268	-0.9	0.1040	-4.2
79	PP(26,A , 6)	896.46633	-0.06	2.57E-22	2.61E-03	3.0	2.6	0.4564	-7.3	0.1012	-1.5
81	PQ(26,A , 6)	912.89287	-0.07	3.24E-22	2.47E-03	-2.3	-1.4	0.4012	5.4	0.1001	-0.4
79	PQ(26,A , 6)	912.97203	-0.09	3.44E-22	2.59E-03	2.1	1.9	0.4446	-4.9	0.1010	-1.3

79	RP(26,A , 6)	986.00475	0.10	1.22E-22	2.92E-03	1.3	1.0	0.4374	-3.3	0.1026	-2.9
81	RP(26,A , 6)	986.03136	0.07	1.24E-22	3.02E-03	4.8	5.5	0.4423	-4.4	0.0989	0.8
81	RQ(26,A , 6)	1002.47512	0.11	4.02E-22	2.83E-03	-1.5	-1.3	0.4111	2.9	0.0976	2.1
81	RR(26,A , 6)	1019.54943	0.13	3.45E-22	2.86E-03	-0.5	0.0	0.4435	-4.6	0.0972	2.5
79	RR(26,A , 6)	1019.65033	0.07	3.51E-22	2.87E-03	-0.4	-0.6	0.4461	-5.2	0.0963	3.5
81	PP(27,A , 6)	895.75771	-0.08	2.39E-22	2.62E-03	3.6	4.2	0.4518	-8.5	0.1029	-3.9
79	PP(27,A , 6)	895.77163	-0.09	2.37E-22	2.56E-03	1.1	0.7	0.4234	-2.3	0.0992	-0.3
79	PQ(27,A , 6)	912.91032	-0.07	3.21E-22	2.51E-03	-0.8	-0.9	0.4175	-0.9	0.0964	2.6
79	RP(27,A , 6)	985.31066	0.09	1.18E-22	2.89E-03	0.5	0.7	0.4356	-5.1	0.0971	1.9
81	RP(27,A , 6)	985.33996	0.10	1.19E-22	2.98E-03	3.6	4.2	0.4215	-1.9	0.1036	-4.5
81	RR(27,A , 6)	1020.11889	0.08	3.15E-22	2.77E-03	-3.6	0.0	0.4102	0.8	0.0955	3.6
79	RR(27,A , 6)	1020.22198	0.08	3.38E-22	2.94E-03	1.9	1.8	0.4315	-4.1	0.0967	2.3
81	PP(28,A , 6)	895.06362	-0.06	2.22E-22	2.59E-03	2.5	3.0	0.4268	-5.5	0.1022	-3.9
79	PP(28,A , 6)	895.07485	-0.11	2.23E-22	2.57E-03	1.3	0.9	0.4083	-1.3	0.1012	-2.9
81	PQ(28,A , 6)	912.76762	-0.07	2.95E-22	2.47E-03	-2.3	-1.2	0.3908	3.2	0.0978	0.4
79	PQ(28,A , 6)	912.84630	-0.06	3.00E-22	2.47E-03	-2.5	-2.6	0.3865	4.3	0.0978	0.4
81	RP(28,A , 6)	984.64647	0.10	1.07E-22	2.76E-03	-4.2	-3.6	0.3873	4.1	0.0992	-1.0
81	RQ(28,A , 6)	1002.35109	0.06	3.50E-22	2.70E-03	-6.4	-6.3	0.3868	4.2	0.0942	4.3
81	RR(28,A , 6)	1020.68597	0.15	2.98E-22	2.80E-03	-2.8	0.0	0.4072	-1.0	0.0933	5.3
79	RR(28,A , 6)	1020.79114	0.10	3.11E-22	2.88E-03	0.0	-0.3	0.4171	-3.3	0.0967	1.6
81	PQ(29,A , 6)	912.70158	-0.05	2.81E-22	2.48E-03	-2.1	-1.0	0.3783	3.6	0.0977	-0.1
79	PQ(29,A , 6)	912.77995	-0.08	2.92E-22	2.53E-03	-0.2	-0.1	0.3831	2.3	0.1005	-2.9
81	RR(29,A , 6)	1021.25043	0.08	2.83E-22	2.85E-03	-1.1	0.0	0.3976	-1.4	0.0957	1.9
79	RR(29,A , 6)	1021.35779	0.11	2.87E-22	2.84E-03	-1.5	-1.8	0.3863	1.4	0.0965	1.1
81	PQ(30,A , 6)	912.63323	-0.05	2.70E-22	2.52E-03	-0.5	0.5	0.3740	1.5	0.0992	-2.3
79	PQ(30,A , 6)	912.71135	-0.05	2.75E-22	2.53E-03	-0.1	-0.1	0.3737	1.6	0.0951	1.9
79	RQ(30,A , 6)	1002.25295	0.07	3.28E-22	2.77E-03	-3.9	-4.6	0.3635	4.5	0.0934	3.8
81	RR(30,A , 6)	1021.81250	0.12	2.60E-22	2.81E-03	-2.5	0.0	0.3813	-0.4	0.0941	3.0
79	RR(30,A , 6)	1021.92181	0.00	2.75E-22	2.93E-03	1.6	1.3	0.3701	2.6	0.0952	1.8
79	PQ(31,A , 6)	912.64043	-0.05	2.68E-22	2.62E-03	3.6	3.7	0.3917	-6.3	0.0992	-2.9
79	RQ(31,A , 6)	1002.18276	0.08	3.10E-22	2.78E-03	-3.6	-4.2	0.3487	5.3	0.0942	2.3
81	RR(31,A , 6)	1022.37195	0.05	2.46E-22	2.85E-03	-0.8	0.0	0.3794	-3.2	0.0962	0.2
79	RR(31,A , 6)	1022.48352	0.10	2.47E-22	2.82E-03	-1.9	-1.9	0.3568	2.9	0.0951	1.3
79	RQ(32,A , 6)	1002.11025	0.04	2.87E-22	2.75E-03	-4.6	-5.3	0.3264	8.4	0.0932	2.8
79	PP(34,A , 6)	890.85102	-0.08	1.38E-22	2.50E-03	-1.3	-1.7	0.3279	-0.3	0.0958	-1.0
81	PP(34,A , 6)	890.85578	-0.11	1.37E-22	2.52E-03	-0.4	0.0	0.3362	-2.8	0.0950	-0.1
81	PR(34,A , 6)	934.44668	0.04	8.43E-23	2.72E-03	7.5	7.6	0.3246	0.7	--	--
81	RR(34,A , 6)	1024.03540	0.08	1.94E-22	2.88E-03	0.1	0.0	0.3505	-6.7	0.0935	1.5
79	RR(34,A , 6)	1024.15308	0.03	1.91E-22	2.79E-03	-3.1	-3.3	0.3359	-2.7	0.0893	6.2
79	PP(35,A , 6)	890.13996	0.00	1.27E-22	2.51E-03	-0.7	-1.6	0.3041	3.1	0.0979	-3.5
81	PP(35,A , 6)	890.14735	-0.10	1.33E-22	2.67E-03	5.5	5.8	0.3526	-11.1	0.0961	-1.7
81	PQ(35,A , 6)	912.25706	-0.07	1.92E-22	2.54E-03	0.3	1.3	0.3127	0.2	0.0939	0.6
81	RQ(35,A , 6)	1001.84590	0.09	2.42E-22	2.92E-03	1.6	1.5	0.3237	-3.2	0.0928	1.8
79	RR(35,A , 6)	1024.70447	-0.02	1.78E-22	2.84E-03	-1.3	-1.3	0.3167	-1.0	0.0938	0.7
79	PP(36,A , 6)	889.42677	-0.02	1.28E-22	2.78E-03	9.8	8.9	0.3527	-14.9	0.1005	-6.4
81	PP(36,A , 6)	889.43696	-0.03	1.14E-22	2.50E-03	-1.2	-0.7	0.3034	-1.0	0.0941	0.0
81	PQ(36,A , 6)	912.17497	-0.05	1.72E-22	2.46E-03	-2.6	-1.4	0.2876	4.4	0.0944	-0.4
79	PQ(36,A , 6)	912.25127	-0.02	1.81E-22	2.56E-03	1.2	1.6	0.3038	-1.2	0.0939	0.2
79	PR(36,A , 6)	935.70620	-0.02	7.41E-23	2.72E-03	7.5	6.5	0.3047	-1.4	0.0950	-1.0
79	PP(37,A , 6)	888.71149	-0.11	1.05E-22	2.51E-03	-0.9	-1.1	0.2804	2.6	0.0986	-5.0
81	PP(37,A , 6)	888.72456	0.04	1.12E-22	2.70E-03	6.7	7.4	0.3238	-11.2	0.0968	-3.2
81	PQ(37,A , 6)	912.09056	-0.04	1.58E-22	2.48E-03	-2.1	-0.8	0.2891	-0.5	0.0938	-0.1
79	PQ(37,A , 6)	912.16655	0.02	1.62E-22	2.50E-03	-1.5	-1.2	0.2777	3.6	0.0942	-0.5
81	PR(37,A , 6)	936.08437	-0.07	6.57E-23	2.64E-03	4.4	4.5	0.2931	-1.9	0.0958	-2.2
81	RP(37,A , 6)	978.31413	0.05	6.92E-23	2.93E-03	1.6	2.6	0.2947	-2.4	0.0892	5.0
79	PP(38,A , 6)	887.99427	-0.13	1.02E-22	2.68E-03	5.6	5.0	0.2873	-4.1	0.0937	-0.4
81	PP(38,A , 6)	888.01008	0.04	9.66E-23	2.58E-03	1.9	2.6	0.2921	-5.7	0.0966	-3.3
79	PQ(38,A , 6)	912.07945	-0.02	1.49E-22	2.51E-03	-0.8	-0.3	0.2710	1.7	0.0937	-0.4
79	RP(38,A , 6)	977.54154	-0.01	6.81E-23	3.09E-03	7.4	7.6	0.3019	-8.7	0.0988	-5.5
81	RQ(38,A , 6)	1001.59535	0.06	1.82E-22	2.85E-03	-1.0	-0.9	0.2944	-6.4	0.0902	3.5
79	RQ(38,A , 6)	1001.62758	0.03	1.83E-22	2.83E-03	-1.9	-2.6	0.2734	0.8	0.0908	2.8
79	PP(39,A , 6)	887.27521	0.02	8.90E-23	2.60E-03	2.6	2.3	0.2851	-7.3	0.0912	2.1
81	PP(39,A , 6)	887.29352	-0.04	8.98E-23	2.65E-03	4.8	5.2	0.2716	-2.7	0.0904	3.0
79	RP(39,A , 6)	976.82334	0.07	5.93E-23	2.93E-03	1.7	1.9	0.2786	-5.1	0.0960	-3.1
81	RQ(39,A , 6)	1001.50728	0.03	1.64E-22	2.82E-03	-1.9	-1.9	0.2726	-3.0	0.0914	1.8
79	RR(39,A , 6)	1026.88465	0.12	1.18E-22	2.77E-03	-3.9	-3.9	0.2524	4.7	0.0924	0.7
79	RQ(40,A , 6)	1001.44844	0.02	1.54E-22	2.89E-03	0.2	-0.8	0.2588	-1.9	0.0925	0.3
81	RR(40,A , 6)	1027.29322	-0.03	1.04E-22	2.75E-03	-4.5	0.0	0.2438	4.2	0.0910	2.0
79	PP(41,A , 6)	885.83081	0.05	6.88E-23	2.49E-03	-1.7	-2.4	0.2397	3.1	0.0888	4.2
81	PP(41,A , 6)	885.85449	-0.12	6.92E-23	2.53E-03	0.1	0.4	0.2332	6.0	0.0924	0.2
79	RR(41,A , 6)	1027.95899	0.01	1.02E-22	2.97E-03	3.1	2.8	0.2603	-5.0	0.0908	1.9
81	PQ(42,A , 6)	911.63396	0.01	9.94E-23	2.52E-03	-0.3	0.8	0.2320	2.4	0.0924	-0.1
81	RR(42,A , 6)	1028.35853	-0.01	8.31E-23	2.73E-03	-5.1	0.0	0.2250	5.6	0.0926	-0.3
79	RR(42,A , 6)	1028.49244	0.17	8.55E-23	2.78E-03	-3.4	-3.6	0.2402	-1.1	0.0919	0.5
81	PQ(43,A , 6)	911.53569	-0.01	8.59E-23	2.43E-03	-3.8	-2.3	0.2138	6.9	0.0913	0.9
79	PQ(43,A , 6)	911.60954	0.15	9.06E-23	2.55E-03	0.5	1.4	0.2197	4.0	0.0938	-1.8
81	RR(43,A , 6)	1028.88734	0.08	8.21E-23	3.02E-03	4.9	0.0	0.2555	-10.6	0.0944	-2.4
79	RR(43,A , 6)	1029.02296	0.03	7.84E-23	2.86E-03	-0.8	-0.6	0.2314	-1.3	0.0935	-1.5

81	PP(44,A , 6)	883.68126	-0.07	5.15E-23	2.66E-03	5.2	5.4	0.2202	-0.1	0.0973	-5.5
81	PQ(44,A , 6)	911.43523	0.09	8.18E-23	2.60E-03	2.5	4.0	0.2134	3.1	0.0933	-1.4
79	PQ(44,A , 6)	911.50847	0.05	7.79E-23	2.44E-03	-3.5	-3.1	0.2064	6.6	0.0915	0.5
81	RR(44,A , 6)	1029.41346	0.09	6.57E-23	2.73E-03	-5.2	0.0	0.2125	3.5	0.0908	1.3
81	PQ(45,A , 6)	911.33232	0.06	7.02E-23	2.50E-03	-1.3	0.1	0.2086	1.6	0.0921	-0.3
79	PQ(45,A , 6)	911.40520	0.08	7.09E-23	2.50E-03	-1.2	-0.7	0.2010	5.4	0.0925	-0.7
79	RQ(45,A , 6)	1000.96065	0.05	9.44E-23	3.04E-03	5.4	4.5	0.2255	-6.1	0.0928	-1.1
81	RR(45,A , 6)	1029.93678	-0.05	6.01E-23	2.82E-03	-2.1	0.0	0.2206	-4.0	0.0892	2.9
79	PQ(46,A , 6)	911.29967	0.18	6.65E-23	2.65E-03	4.5	5.0	0.2063	-1.1	0.0923	-0.7
81	RR(47,A , 6)	1030.97584	0.03	4.58E-23	2.78E-03	-3.6	0.0	0.1883	4.3	0.0921	-0.6
79	RR(48,A , 6)	1031.63661	0.13	4.22E-23	2.89E-03	0.4	0.8	0.1926	-2.1	0.0910	0.5
79	RQ(49,A , 6)	1000.52913	0.02	5.46E-23	2.89E-03	0.2	-0.9	0.1763	2.4	0.0938	-2.6
79	PP(7,E , 7)	902.21396	-0.14	1.61E-22	2.38E-03	-4.8	-5.0	0.2012	9.2	0.0887	5.9
79	RR(7,E , 7)	1016.15941	0.08	2.51E-22	2.85E-03	-2.1	-2.5	0.2140	2.7	0.0848	10.8
81	RR(8,E , 7)	1016.71947	0.13	2.38E-22	2.80E-03	-3.7	-3.3	0.2744	-1.5	0.0957	3.8
81	PP(9,E , 7)	900.84042	-0.06	1.60E-22	2.48E-03	-0.9	-0.3	0.3100	0.3	0.1079	-5.6
79	PP(9,E , 7)	900.90445	-0.09	1.84E-22	2.80E-03	12.0	11.8	0.3903	-20.3	0.1124	-9.4
81	RR(9,E , 7)	1017.33202	0.07	2.40E-22	2.87E-03	-1.3	-0.8	0.3312	-6.1	0.0994	2.5
79	RR(9,E , 7)	1017.39166	0.10	2.48E-22	2.90E-03	-0.3	-0.6	0.3291	-5.5	0.1013	0.6
81	PP(10,E , 7)	900.18478	-0.11	1.59E-22	2.50E-03	0.0	0.8	0.3470	-0.9	0.1096	-5.7
79	PP(10,E , 7)	900.24630	-0.13	1.61E-22	2.49E-03	-0.6	-1.0	0.3372	2.0	0.1101	-6.2
79	RR(11,E , 7)	1018.61450	0.08	2.38E-22	2.87E-03	-1.3	-1.7	0.3719	-0.5	0.1062	-1.5
81	PP(12,E , 7)	898.86703	-0.05	1.51E-22	2.44E-03	-2.6	-1.8	0.3627	7.7	0.1129	-6.2
79	PP(12,E , 7)	898.92349	-0.10	1.61E-22	2.54E-03	1.5	1.3	0.3972	-1.6	0.1118	-5.2
81	PQ(12,E , 7)	906.46317	-0.08	9.67E-23	2.42E-03	-3.3	-2.4	0.3796	2.9	0.1145	-7.5
81	PP(13,E , 7)	898.20480	-0.11	1.50E-22	2.46E-03	-1.8	-1.1	0.4030	1.0	0.1105	-2.8
79	PP(13,E , 7)	898.25881	-0.08	1.59E-22	2.56E-03	2.4	2.1	0.3928	3.6	0.1109	-3.2
81	PQ(13,E , 7)	906.43357	-0.10	1.17E-22	2.68E-03	7.0	7.8	0.4412	-7.8	0.1156	-7.1
81	RQ(13,E , 7)	1010.89775	0.28	1.37E-22	3.10E-03	6.7	6.9	0.4130	-1.5	0.1122	-4.3
81	PP(14,E , 7)	897.54043	-0.13	1.45E-22	2.41E-03	-3.5	-2.7	0.4019	4.4	0.1109	-2.1
81	PQ(14,E , 7)	906.40177	-0.03	1.13E-22	2.42E-03	-3.5	-2.8	0.3992	5.1	0.1143	-5.0
79	RQ(14,E , 7)	1010.90104	0.19	1.40E-22	2.86E-03	-1.8	-2.3	0.3991	5.1	0.1110	-2.2
81	RR(14,E , 7)	1020.36010	0.14	2.31E-22	3.01E-03	3.3	0.0	0.4296	-2.3	0.1044	4.0
81	PP(15,E , 7)	896.87398	-0.05	1.43E-22	2.44E-03	-2.3	-1.7	0.4040	6.2	0.1100	-0.9
79	PP(15,E , 7)	896.92281	-0.12	1.51E-22	2.52E-03	0.5	0.3	0.4318	-0.6	0.1119	-2.6
81	PQ(15,E , 7)	906.36753	-0.12	1.19E-22	2.43E-03	-3.0	-2.3	0.4182	2.6	0.1118	-2.5
79	PQ(15,E , 7)	906.45255	-0.17	1.31E-22	2.62E-03	4.6	4.5	0.4629	-7.3	0.1135	-4.0
81	PP(16,E , 7)	896.20534	-0.01	1.55E-22	2.71E-03	8.2	9.1	0.4585	-4.8	0.1103	-1.7
79	PP(17,E , 7)	895.57814	-0.15	1.30E-22	2.29E-03	-8.7	-9.0	0.4029	9.5	0.1063	2.0
79	PQ(17,E , 7)	906.37717	-0.11	1.35E-22	2.52E-03	0.6	0.3	0.4455	-1.0	0.1082	0.2
81	RQ(17,E , 7)	1010.75798	0.07	1.66E-22	2.99E-03	2.9	3.2	0.4313	2.3	0.1108	-2.1
79	PP(18,E , 7)	894.90261	-0.12	1.42E-22	2.58E-03	2.9	2.6	0.4276	3.9	0.1052	2.0
79	RQ(18,E , 7)	1010.75175	0.10	1.70E-22	2.93E-03	0.7	0.2	0.4451	-0.2	0.1212	-11.5
81	PP(19,E , 7)	894.18623	-0.17	1.27E-22	2.43E-03	-2.9	-2.2	0.4295	3.8	0.1066	-0.5
81	PQ(19,E , 7)	906.20817	-0.09	1.34E-22	2.50E-03	-0.1	0.6	0.4206	6.0	0.1053	0.8
79	RR(19,E , 7)	1023.41107	0.11	2.02E-22	2.99E-03	2.7	2.4	0.4733	-5.8	0.1036	2.4
81	PQ(20,E , 7)	906.16257	-0.14	1.27E-22	2.36E-03	-5.5	-4.8	0.4238	5.2	0.1043	0.7
79	PQ(20,E , 7)	906.24674	-0.20	1.40E-22	2.56E-03	2.0	1.8	0.4409	1.1	0.0984	6.7
81	PP(21,E , 7)	892.82973	-0.04	1.22E-22	2.52E-03	0.6	1.3	0.4582	-3.0	0.1054	-1.3
79	PP(21,E , 7)	892.86305	-0.16	1.29E-22	2.61E-03	4.2	3.9	0.4720	-5.9	0.1043	-0.3
81	PQ(21,E , 7)	906.11472	-0.15	1.27E-22	2.38E-03	-4.9	-4.0	0.4193	6.0	0.1041	-0.1
79	PQ(21,E , 7)	906.19883	-0.08	1.35E-22	2.48E-03	-1.1	-1.2	0.4317	2.9	0.1031	0.9
81	RR(21,E , 7)	1024.49952	0.16	1.72E-22	2.80E-03	-3.7	0.0	0.4314	3.0	0.1040	0.0
81	PQ(22,E , 7)	906.06455	-0.21	1.26E-22	2.40E-03	-4.2	-3.4	0.3998	10.4	0.1004	2.6
81	RQ(22,E , 7)	1010.53288	0.12	1.71E-22	2.99E-03	2.8	2.9	0.4436	-0.5	0.1015	1.5
81	RR(22,E , 7)	1025.08118	0.13	1.65E-22	2.81E-03	-3.5	0.0	0.4244	4.0	0.1023	0.7
79	RR(22,E , 7)	1025.17005	0.13	1.74E-22	2.91E-03	0.0	-0.2	0.4521	-2.3	0.1030	0.0
81	PQ(23,E , 7)	906.01218	-0.17	1.35E-22	2.61E-03	4.3	5.4	0.4662	-6.2	0.1048	-2.6
79	PQ(23,E , 7)	906.09586	-0.10	1.27E-22	2.41E-03	-3.7	-4.0	0.4182	4.6	0.1026	-0.5
79	RQ(23,E , 7)	1010.51426	0.05	1.64E-22	2.86E-03	-1.7	-2.2	0.4106	6.5	0.1060	-3.7
79	PP(24,E , 7)	890.80433	-0.21	1.09E-22	2.55E-03	1.7	1.5	0.4396	-1.7	0.1066	-5.1
79	PQ(24,E , 7)	906.04093	-0.12	1.21E-22	2.36E-03	-5.6	-5.7	0.3829	12.8	0.0998	1.4
81	RQ(24,E , 7)	1010.42698	0.08	1.61E-22	2.93E-03	0.7	1.0	0.4054	6.6	0.1000	1.2
79	RQ(24,E , 7)	1010.46006	0.13	1.64E-22	2.94E-03	0.9	0.5	0.4312	0.2	0.1021	-0.9
81	PP(25,E , 7)	890.09101	-0.12	9.98E-23	2.50E-03	0.1	0.8	0.4313	-1.4	0.1044	-3.9
79	PP(25,E , 7)	890.11402	-0.07	1.05E-22	2.60E-03	3.9	3.6	0.4445	-4.3	0.1029	-2.5
79	RQ(25,E , 7)	1010.40348	0.11	1.56E-22	2.87E-03	-1.4	-2.0	0.4021	5.8	0.1010	-0.6
79	RR(25,E , 7)	1026.90699	0.15	1.58E-22	3.10E-03	6.6	6.2	0.4128	3.0	0.0978	2.6
81	PP(26,E , 7)	889.40113	-0.09	9.40E-23	2.50E-03	0.0	0.9	0.4212	-0.9	0.1038	-4.1
81	RQ(26,E , 7)	1010.31218	0.17	1.47E-22	2.87E-03	-1.5	-1.3	0.3990	4.7	0.0991	0.5
81	RR(26,E , 7)	1027.38355	0.20	1.46E-22	3.08E-03	6.0	0.0	0.4152	0.6	0.0991	0.5
81	PP(27,E , 7)	888.70918	-0.06	9.22E-23	2.62E-03	4.5	5.0	0.4069	0.4	0.1036	-4.6
79	PP(27,E , 7)	888.72694	0.01	8.92E-23	2.48E-03	-0.9	-1.3	0.4646	-12.1	0.0932	6.0
81	RQ(27,E , 7)	1010.25132	0.14	1.41E-22	2.84E-03	-2.5	-2.2	0.3908	4.6	0.1010	-2.1
79	RQ(27,E , 7)	1010.28355	0.08	1.41E-22	2.79E-03	-4.2	-4.7	0.3744	9.1	0.0997	-0.9
81	RR(27,E , 7)	1027.95301	0.23	1.42E-22	3.20E-03	9.9	0.0	0.4525	-9.7	0.0994	-0.6
79	RR(27,E , 7)	1028.05250	0.07	1.41E-22	3.10E-03	6.5	6.4	0.4508	-9.4	0.0987	0.1
81	PP(28,E , 7)	888.01490	-0.27	8.02E-23	2.42E-03	-3.1	-2.5	0.3899	2.2	0.0981	0.0

79	PP(28,E , 7)	888.03004	-0.17	8.57E-23	2.55E-03	1.9	1.4	0.4126	-3.4	0.1034	-5.1
79	RQ(28,E , 7)	1010.22026	0.15	1.37E-22	2.84E-03	-2.3	-2.9	0.3838	3.8	0.1015	-3.3
79	RR(28,E , 7)	1028.62171	0.22	1.31E-22	3.08E-03	5.9	5.5	0.4087	-2.5	0.0988	-0.7
81	PP(29,E , 7)	887.31885	-0.18	7.55E-23	2.44E-03	-2.5	-2.1	0.3829	1.2	0.0999	-2.4
79	PP(29,E , 7)	887.33136	-0.06	8.17E-23	2.59E-03	3.5	3.1	0.4110	-5.7	0.1041	-6.3
81	RQ(29,E , 7)	1010.12291	0.18	1.26E-22	2.79E-03	-4.1	-4.0	0.3565	8.7	0.1016	-4.0
81	RR(29,E , 7)	1029.08436	0.20	1.13E-22	2.91E-03	0.1	0.0	0.3900	-0.6	0.0965	1.0
81	PQ(30,E , 7)	905.58127	-0.18	9.04E-23	2.34E-03	-6.5	-5.5	0.3340	12.5	0.0982	-1.3
81	RR(30,E , 7)	1029.64625	0.14	9.67E-23	2.67E-03	-8.1	0.0	0.3348	12.2	0.0940	3.1
81	PP(31,E , 7)	885.92047	-0.11	6.24E-23	2.34E-03	-6.4	-6.1	0.3359	8.1	0.0984	-2.1
79	PP(31,E , 7)	885.92749	-0.14	7.09E-23	2.62E-03	4.5	4.1	0.3816	-4.8	0.1030	-6.5
81	PQ(31,E , 7)	905.51059	-0.13	8.75E-23	2.41E-03	-3.8	-2.7	0.3324	9.3	0.0952	1.2
79	PQ(31,E , 7)	905.59220	-0.11	9.16E-23	2.48E-03	-1.0	-0.9	0.3430	5.9	0.0973	-1.0
79	RQ(31,E , 7)	1010.01652	0.12	1.12E-22	2.75E-03	-5.5	-6.1	0.3266	11.2	0.1039	-7.3
81	RR(31,E , 7)	1030.20570	0.15	9.79E-23	2.92E-03	0.3	0.0	0.3601	0.9	0.0979	-1.6
79	RR(31,E , 7)	1030.31373	0.11	9.65E-23	2.83E-03	-2.9	-3.2	0.3665	-0.9	0.0942	2.3
81	PQ(32,E , 7)	905.43766	-0.05	9.60E-23	2.82E-03	12.6	13.9	0.4153	-15.7	0.1001	-4.3
79	PQ(32,E , 7)	905.51889	-0.11	8.48E-23	2.45E-03	-2.2	-2.3	0.3376	3.7	0.0978	-2.0
81	RR(32,E , 7)	1030.76259	0.11	8.54E-23	2.75E-03	-5.3	0.0	0.3305	5.9	0.0949	0.9
79	RR(32,E , 7)	1030.87270	0.07	9.08E-23	2.88E-03	-1.1	-1.3	0.3528	-0.8	0.0963	-0.5
81	PQ(33,E , 7)	905.36234	-0.05	8.04E-23	2.52E-03	0.9	2.1	0.3671	-8.3	0.0974	-2.1
79	PQ(33,E , 7)	905.44321	-0.17	7.76E-23	2.40E-03	-4.2	-4.0	0.3141	7.2	0.0944	1.0
81	RR(33,E , 7)	1031.31691	0.03	7.66E-23	2.68E-03	-7.9	0.0	0.3060	10.0	0.0930	2.5
79	PQ(34,E , 7)	905.36551	0.05	7.41E-23	2.48E-03	-1.1	-1.1	0.3188	1.4	0.0942	0.7
81	RQ(34,E , 7)	1009.76213	0.10	9.51E-23	2.91E-03	0.0	0.0	0.3228	0.1	0.0945	0.4
79	RQ(34,E , 7)	1009.79234	0.09	9.86E-23	2.97E-03	1.9	1.2	0.3304	-2.2	0.0947	0.2
79	PR(35,E , 7)	928.10566	0.03	2.73E-23	2.74E-03	9.3	8.3	0.3331	-7.1	0.0958	-1.4
81	RR(35,E , 7)	1032.41823	0.15	6.49E-23	2.70E-03	-7.1	0.0	0.2926	5.8	0.0948	-0.4
79	RR(35,E , 7)	1032.53456	0.18	6.97E-23	2.86E-03	-1.6	-1.7	0.3077	0.6	0.0915	3.2
79	PP(36,E , 7)	882.38213	-0.14	4.66E-23	2.63E-03	4.9	4.5	0.3272	-9.4	0.0982	-4.2
81	PP(36,E , 7)	882.38848	-0.21	4.12E-23	2.36E-03	-5.6	-4.7	0.2759	7.4	0.1002	-6.1
79	PQ(36,E , 7)	905.20255	-0.13	6.92E-23	2.72E-03	8.4	8.9	0.2864	3.5	0.0994	-5.4
81	PR(36,E , 7)	928.48487	0.30	2.10E-23	2.28E-03	-9.0	-8.8	0.2736	8.3	0.0909	3.5
81	RQ(36,E , 7)	1009.60197	0.07	7.92E-23	2.83E-03	-2.8	-3.0	0.2821	5.1	0.0932	0.9
79	RQ(36,E , 7)	1009.63151	0.08	9.24E-23	3.26E-03	12.0	11.2	0.3256	-9.0	0.0970	-3.0
79	PP(37,E , 7)	881.66692	-0.17	3.84E-23	2.39E-03	-4.6	-5.0	0.2678	5.9	0.1031	-9.1
81	PP(37,E , 7)	881.67595	-0.29	3.80E-23	2.40E-03	-4.3	-3.8	0.2705	4.9	0.1060	-11.6
81	PQ(37,E , 7)	905.03800	-0.15	5.63E-23	2.44E-03	-2.5	-1.4	0.2854	-0.6	0.0988	-5.1
81	PQ(38,E , 7)	904.95114	-0.19	5.22E-23	2.48E-03	-1.0	0.0	0.2640	2.9	0.0872	7.1
79	PQ(38,E , 7)	905.03055	-0.11	5.20E-23	2.43E-03	-3.1	-3.0	0.2576	5.5	0.0945	-1.2
81	RP(38,E , 7)	985.44225	0.20	2.11E-23	2.77E-03	-4.8	-3.9	0.2765	-1.8	0.0959	-2.6
81	PQ(39,E , 7)	904.86209	-0.12	4.70E-23	2.45E-03	-2.3	-0.8	0.2624	-0.7	0.0916	1.6
79	PQ(39,E , 7)	904.94113	-0.05	5.20E-23	2.66E-03	6.4	6.6	0.2728	-4.5	0.1013	-8.1
81	PQ(40,E , 7)	904.77054	-0.24	5.01E-23	2.86E-03	14.1	15.9	0.2458	1.8	0.0931	-0.3
79	PQ(40,E , 7)	904.84928	-0.10	4.30E-23	2.44E-03	-2.7	-2.7	0.2267	10.4	0.0935	-0.7
79	PQ(41,E , 7)	904.75528	0.02	4.06E-23	2.54E-03	1.6	1.8	0.2369	3.4	0.0940	-1.5
79	RR(41,E , 7)	1035.78860	0.18	3.90E-23	2.95E-03	1.2	1.3	0.2501	-2.1	0.0941	-1.6
81	PQ(42,E , 7)	904.58090	-0.09	3.57E-23	2.52E-03	0.6	1.9	0.2398	-1.9	0.0857	7.8
79	PQ(43,E , 7)	904.55997	-0.10	3.06E-23	2.37E-03	-5.4	-5.1	0.1861	21.5	0.0911	1.2
79	RR(43,E , 7)	1036.85244	0.20	3.07E-23	2.90E-03	-0.3	-0.3	0.2363	-4.3	0.0973	-5.2
79	RR(44,E , 7)	1037.38027	0.09	2.93E-23	3.14E-03	7.9	8.0	0.2341	-7.0	0.0966	-4.7
81	PQ(45,E , 7)	904.27884	-0.12	2.61E-23	2.57E-03	2.7	4.2	0.2088	0.4	0.0908	1.2
79	PQ(45,E , 7)	904.35544	-0.13	2.62E-23	2.55E-03	1.7	2.0	0.1840	13.9	0.0932	-1.4
81	RQ(45,E , 7)	1008.76896	0.10	3.47E-23	3.05E-03	5.0	4.9	0.2158	-2.9	0.0907	1.3
79	RQ(45,E , 7)	1008.79502	0.21	3.42E-23	2.99E-03	2.8	1.9	0.2092	0.2	0.0916	0.3
81	PQ(46,E , 7)	904.17337	-0.27	2.25E-23	2.49E-03	-0.3	1.1	0.1846	9.3	0.0991	-7.4
79	PQ(46,E , 7)	904.24997	0.14	2.26E-23	2.47E-03	-1.3	-0.9	0.1947	3.6	0.0911	0.8
81	RQ(46,E , 7)	1008.66514	0.22	3.29E-23	3.28E-03	12.7	12.5	0.2063	-2.2	0.0947	-3.1
81	PP(8,E , 8)	894.51296	-0.02	1.19E-22	2.31E-03	-6.8	-6.0	0.1896	20.2	0.0843	9.2
79	PP(8,E , 8)	894.58333	0.03	1.37E-22	2.59E-03	4.7	4.3	0.2474	-7.9	0.0888	3.7
81	PP(9,E , 8)	893.85970	0.01	1.20E-22	2.36E-03	-4.8	-4.2	0.2537	9.6	0.0967	-0.8
79	PP(9,E , 8)	893.92751	0.00	1.23E-22	2.38E-03	-3.7	-4.1	0.2517	10.5	0.0955	0.4
81	RR(9,E , 8)	1025.21705	0.06	1.89E-22	2.85E-03	-3.0	0.0	0.2662	4.5	0.0966	-0.7
81	PP(10,E , 8)	893.20424	0.05	1.26E-22	2.53E-03	2.3	3.0	0.3029	5.0	0.1038	-5.3
79	PP(10,E , 8)	893.26948	-0.02	1.29E-22	2.54E-03	2.7	2.2	0.3052	4.2	0.1066	-7.8
79	RR(10,E , 8)	1025.88563	-0.04	1.94E-22	2.92E-03	-0.6	-1.0	0.3212	-1.0	0.1001	-1.8
81	PP(11,E , 8)	892.54646	-0.02	1.17E-22	2.40E-03	-3.2	-2.4	0.3338	4.6	0.1040	-3.4
81	RR(11,E , 8)	1026.43507	0.07	1.87E-22	2.94E-03	0.0	0.0	0.3489	0.1	0.1018	-1.3
81	RR(12,E , 8)	1027.04053	0.03	1.87E-22	2.99E-03	1.9	0.0	0.3843	-2.8	0.1047	-1.8
79	RR(12,E , 8)	1027.10365	0.05	1.88E-22	2.96E-03	0.6	0.2	0.3620	3.2	0.1019	0.9
81	RR(13,E , 8)	1027.64369	0.05	1.81E-22	2.97E-03	1.1	0.0	0.3970	-1.2	0.1070	-1.7
79	RR(13,E , 8)	1027.70912	0.10	1.88E-22	3.03E-03	3.2	2.9	0.4053	-3.2	0.1061	-0.9
81	RR(14,E , 8)	1028.24452	0.10	1.67E-22	2.81E-03	-4.3	0.0	0.3961	2.6	0.1024	4.6
79	RR(14,E , 8)	1028.31214	0.06	1.90E-22	3.14E-03	6.6	6.3	0.4350	-6.6	0.1059	1.1
81	RR(15,E , 8)	1028.84291	0.08	1.80E-22	3.11E-03	5.9	0.0	0.4327	-3.6	0.1037	4.2
81	RR(16,E , 8)	1029.43885	-0.02	1.64E-22	2.92E-03	-0.7	0.0	0.4299	-1.1	0.1046	3.0
81	RQ(17,E , 8)	1018.64434	0.02	1.20E-22	3.25E-03	10.5	0.0	0.4595	-6.3	0.1068	1.4
81	RR(17,E , 8)	1030.03261	0.10	1.63E-22	2.99E-03	1.8	0.0	0.4524	-4.8	0.1052	2.9

79	RR(17,E , 8)	1030.10695	0.03	1.58E-22	2.85E-03	-3.2	-3.5	0.4265	0.9	0.1043	3.8
79	PP(18,E , 8)	887.92646	-0.05	1.03E-22	2.48E-03	-0.1	-0.4	0.4320	0.5	0.1103	-2.9
81	RQ(18,E , 8)	1018.60388	0.07	1.09E-22	2.86E-03	-2.7	0.0	0.4164	4.2	0.1089	-1.7
79	RQ(18,E , 8)	1018.63476	0.08	1.08E-22	2.79E-03	-5.3	-5.6	0.3942	10.1	0.1032	3.7
79	RR(18,E , 8)	1030.70045	0.05	1.55E-22	2.91E-03	-1.1	-1.3	0.4279	1.4	0.1046	2.4
81	PP(19,E , 8)	887.20643	-0.05	9.17E-23	2.33E-03	-5.9	-5.0	0.4195	3.9	0.1027	3.1
79	PP(19,E , 8)	887.24884	-0.04	9.31E-23	2.33E-03	-6.1	-6.5	0.4243	2.7	0.1110	-4.6
79	RQ(19,E , 8)	1018.59173	0.00	1.15E-22	2.90E-03	-1.3	-1.7	0.4218	3.3	0.1077	-1.6
81	RR(19,E , 8)	1031.21266	0.05	1.50E-22	2.97E-03	1.0	0.0	0.4375	-0.4	0.1033	2.5
79	RR(19,E , 8)	1031.29152	0.06	1.49E-22	2.90E-03	-1.5	-1.9	0.4368	-0.2	0.1018	4.1
81	PQ(20,E , 8)	899.18020	-0.06	8.78E-23	2.44E-03	-1.4	-0.5	0.4382	-0.4	0.1050	-0.1
81	PP(21,E , 8)	885.85004	0.05	9.26E-23	2.56E-03	3.6	4.5	0.3984	9.2	0.1033	0.5
79	PP(21,E , 8)	885.88715	-0.05	9.00E-23	2.44E-03	-1.5	-1.8	0.4353	0.0	0.1080	-3.9
81	PQ(21,E , 8)	899.13229	-0.07	8.51E-23	2.37E-03	-4.3	-3.2	0.4206	3.5	0.1074	-3.3
81	PQ(22,E , 8)	899.08206	-0.13	8.22E-23	2.31E-03	-6.5	-5.6	0.4120	5.1	0.0997	3.2
79	PQ(22,E , 8)	899.16970	-0.07	9.23E-23	2.55E-03	3.0	2.7	0.4417	-2.0	0.1066	-3.5
81	PQ(23,E , 8)	899.02969	-0.01	8.65E-23	2.48E-03	0.3	1.4	0.4249	1.1	0.1038	-1.8
79	PQ(23,E , 8)	899.11697	-0.12	8.68E-23	2.44E-03	-1.6	-1.8	0.4228	1.6	0.1033	-1.3
81	RQ(23,E , 8)	1018.36755	0.07	1.17E-22	3.04E-03	3.3	3.6	0.4523	-5.1	0.0940	8.4
81	PQ(24,E , 8)	898.97482	-0.13	8.59E-23	2.52E-03	1.7	2.9	0.4198	1.1	0.0994	1.7
79	PQ(24,E , 8)	899.06197	-0.13	8.20E-23	2.36E-03	-4.8	-5.1	0.4069	4.3	0.1012	-0.1
81	RQ(24,E , 8)	1018.31353	0.07	1.07E-22	2.83E-03	-3.6	-3.3	0.3907	8.7	0.0991	2.0
79	RQ(24,E , 8)	1018.34326	0.19	1.22E-22	3.16E-03	7.5	7.1	0.4162	2.0	0.1054	-4.1
81	PQ(25,E , 8)	898.91781	-0.09	7.83E-23	2.36E-03	-4.6	-3.5	0.3950	6.0	0.1024	-2.1
79	PQ(25,E , 8)	899.00478	-0.04	8.57E-23	2.54E-03	2.4	2.4	0.4308	-2.8	0.1028	-2.5
81	RQ(25,E , 8)	1018.25720	0.03	1.11E-22	3.01E-03	2.4	2.6	0.3831	9.2	0.1009	-0.7
79	RQ(25,E , 8)	1018.28668	0.13	1.07E-22	2.87E-03	-2.4	-2.9	0.4072	2.8	0.0979	2.4
81	PP(26,E , 8)	882.42162	-0.13	6.90E-23	2.48E-03	0.3	1.2	0.4180	-1.6	0.1041	-4.4
79	PP(26,E , 8)	882.44567	-0.19	6.82E-23	2.41E-03	-2.6	-2.9	0.3939	4.4	0.0988	0.7
81	PQ(26,E , 8)	898.85854	-0.02	8.03E-23	2.51E-03	1.3	2.1	0.4268	-3.6	0.1042	-4.5
79	PQ(26,E , 8)	898.94521	-0.03	8.79E-23	2.70E-03	9.0	9.0	0.4103	0.2	0.1022	-2.7
81	RQ(26,E , 8)	1018.19872	0.10	1.04E-22	2.92E-03	-0.8	-0.8	0.4035	1.9	0.0978	1.7
81	PP(27,E , 8)	881.72978	-0.03	6.56E-23	2.52E-03	1.9	2.5	0.4297	-6.3	0.1003	-1.6
81	PQ(27,E , 8)	898.79678	-0.14	7.87E-23	2.56E-03	3.3	4.3	0.4079	-1.2	0.1024	-3.6
79	PQ(27,E , 8)	898.88332	-0.03	7.45E-23	2.39E-03	-3.7	-3.6	0.3934	2.4	0.0999	-1.2
81	RQ(27,E , 8)	1018.13787	0.05	1.08E-22	3.16E-03	7.5	7.6	0.4394	-8.3	0.0967	2.1
79	RQ(27,E , 8)	1018.16680	0.11	1.04E-22	2.99E-03	1.7	1.2	0.3992	0.9	0.0985	0.2
81	RR(27,E , 8)	1035.83596	0.08	9.97E-23	2.99E-03	1.8	0.0	0.4038	-0.2	0.1030	-4.1
79	RR(27,E , 8)	1035.93215	0.06	1.00E-22	2.96E-03	0.8	0.4	0.4049	-0.5	0.1007	-1.9
79	PQ(28,E , 8)	898.81899	-0.19	7.26E-23	2.43E-03	-1.9	-2.2	0.3965	-0.8	0.0971	1.0
81	RQ(28,E , 8)	1018.07494	0.19	8.72E-23	2.66E-03	-9.5	-9.2	0.3254	20.9	0.0962	1.9
79	RQ(30,E , 8)	1017.96990	0.01	8.91E-23	2.96E-03	0.8	0.5	0.3716	-0.1	0.1027	-5.7
81	RR(30,E , 8)	1037.52908	0.15	7.90E-23	2.93E-03	-0.3	0.0	0.3774	-1.7	0.0949	2.0
79	RR(30,E , 8)	1037.63174	0.27	8.74E-23	3.19E-03	8.5	8.5	0.3668	1.2	0.0971	-0.3
81	PQ(31,E , 8)	898.52731	-0.14	5.64E-23	2.26E-03	-8.5	-7.3	0.3217	11.5	0.0990	-2.7
81	RQ(31,E , 8)	1017.87200	0.00	7.08E-23	2.54E-03	-13.5	-13.3	0.2974	20.6	0.0948	1.6
79	RQ(31,E , 8)	1017.89990	0.16	7.60E-23	2.67E-03	-9.1	-9.6	0.3087	16.2	0.0949	1.5
79	RR(31,E , 8)	1038.19302	0.12	7.59E-23	2.99E-03	1.6	1.6	0.3426	4.7	0.0965	-0.2
81	PQ(32,E , 8)	898.45425	-0.10	5.53E-23	2.36E-03	-4.6	-3.5	0.3272	5.7	0.0957	0.1
81	RR(32,E , 8)	1038.64529	0.18	6.60E-23	2.87E-03	-2.5	0.0	0.3615	-4.4	0.0963	-0.6
79	RR(32,E , 8)	1038.75174	-0.07	7.01E-23	3.00E-03	1.9	1.8	0.3519	-1.8	0.0963	-0.6
81	PQ(33,E , 8)	898.37868	-0.26	6.05E-23	2.77E-03	11.8	12.8	0.3110	6.9	0.0996	-4.3
79	PQ(33,E , 8)	898.46359	-0.10	5.21E-23	2.35E-03	-5.3	-5.1	0.3116	6.6	0.0968	-1.6
81	RQ(33,E , 8)	1017.72564	0.12	6.92E-23	2.83E-03	-3.7	-3.9	0.3101	7.2	0.0917	3.9
79	RQ(33,E , 8)	1017.75286	0.22	7.40E-23	2.98E-03	1.4	0.5	0.3373	-1.5	0.0984	-3.2
81	PQ(34,E , 8)	898.30111	-0.12	5.35E-23	2.64E-03	6.6	8.1	0.3439	-7.3	0.1004	-5.5
79	PQ(34,E , 8)	898.38546	-0.20	4.87E-23	2.37E-03	-4.5	-4.7	0.2876	10.8	0.0936	1.3
81	RR(34,E , 8)	1039.75125	0.06	5.63E-23	2.90E-03	-1.3	0.0	0.3156	1.0	0.0946	0.3
79	PQ(35,E , 8)	898.30514	-0.20	4.96E-23	2.60E-03	4.9	5.1	0.3292	-7.3	0.0946	-0.2
81	PR(35,E , 8)	920.95044	-0.08	1.49E-23	2.32E-03	-6.2	-5.9	0.2973	2.6	0.0954	-1.0
81	RR(35,E , 8)	1040.30057	0.14	5.28E-23	2.97E-03	1.1	0.0	0.3228	-5.5	0.0947	-0.3
81	RQ(37,E , 8)	1017.40557	0.19	5.43E-23	3.03E-03	3.1	3.1	0.3010	-7.3	0.0994	-5.7
81	RQ(38,E , 8)	1017.31988	0.20	4.95E-23	3.02E-03	2.6	2.5	0.2862	-6.7	0.0961	-2.8
79	RQ(38,E , 8)	1017.34521	0.16	5.28E-23	3.17E-03	7.8	7.4	0.2811	-5.0	0.0793	17.8
81	PQ(39,E , 8)	897.87783	-0.31	3.12E-23	2.33E-03	-5.7	-4.6	0.2358	8.6	0.0975	-4.5
81	RQ(39,E , 8)	1017.23180	0.09	4.24E-23	2.82E-03	-4.0	-3.7	0.2627	-2.5	0.0905	2.9
79	RQ(39,E , 8)	1017.25683	0.13	4.47E-23	2.95E-03	0.2	0.0	0.2459	4.1	0.0910	2.4
79	PQ(40,E , 8)	897.86867	-0.28	2.85E-23	2.34E-03	-5.5	-5.3	0.2232	10.3	0.0907	2.4
81	PP(9,A , 9)	886.94892	0.39	1.80E-22	2.37E-03	-3.0	-2.2	0.1963	22.7	0.0855	4.3
79	PP(9,A , 9)	887.02051	0.38	1.82E-22	2.35E-03	-4.0	-4.4	0.1977	21.8	0.0842	5.9
79	RR(9,A , 9)	1033.20217	-0.24	2.98E-22	2.94E-03	-1.0	-1.3	0.2037	18.3	0.0827	7.8
81	PP(10,A , 9)	886.29352	0.38	1.78E-22	2.41E-03	-1.3	-0.5	0.2789	3.5	0.0952	-2.6
79	PP(10,A , 9)	886.36261	0.37	1.82E-22	2.42E-03	-1.3	-1.7	0.2571	12.3	0.0968	-4.2
81	RR(12,A , 9)	1034.97255	-0.19	2.69E-22	2.92E-03	-1.6	0.0	0.3511	0.8	0.1000	-0.8
81	PQ(13,A , 9)	892.53926	0.32	7.62E-23	2.40E-03	-1.9	-1.2	0.3931	-4.5	0.1035	-0.9
81	RR(13,A , 9)	1035.57558	-0.17	2.64E-22	2.94E-03	-0.9	0.0	0.3801	-1.2	0.0998	2.8
79	RR(13,A , 9)	1035.63759	-0.13	2.72E-22	2.98E-03	0.2	-0.1	0.3840	-2.2	0.1015	1.1
79	PP(14,A , 9)	883.70897	0.34	1.63E-22	2.39E-03	-2.4	-2.7	0.3791	3.3	0.1073	-1.7

81	PQ(14,A , 9)	892.50752	0.54	8.74E-23	2.46E-03	0.7	1.4	0.3987	-1.8	0.1066	-1.1
81	RQ(14,A , 9)	1026.68629	-0.14	1.09E-22	3.05E-03	2.6	0.0	0.4089	-4.3	0.1055	0.0
79	RR(14,A , 9)	1036.24050	-0.14	2.67E-22	3.00E-03	0.9	0.5	0.4094	-4.4	0.1019	3.5
79	PP(15,A , 9)	883.04003	0.28	1.56E-22	2.37E-03	-3.3	-3.5	0.4019	0.4	0.1071	0.0
81	PQ(15,A , 9)	892.47316	0.41	9.02E-23	2.34E-03	-4.4	-3.4	0.3605	11.9	0.1109	-3.4
79	PQ(15,A , 9)	892.56593	0.57	9.97E-23	2.53E-03	3.2	2.9	0.3636	11.0	0.1105	-3.1
81	RQ(15,A , 9)	1026.65260	-0.11	1.21E-22	3.02E-03	1.8	0.0	0.4097	-1.5	0.1066	0.5
79	RQ(15,A , 9)	1026.68043	-0.23	1.25E-22	3.07E-03	3.3	2.6	0.4228	-4.6	0.1026	4.4
81	RR(15,A , 9)	1036.77456	-0.13	2.46E-22	2.91E-03	-2.0	0.0	0.3998	0.9	0.1036	3.4
79	RR(15,A , 9)	1036.84109	-0.10	2.56E-22	2.97E-03	-0.1	-0.5	0.4092	-1.4	0.1043	2.7
81	PP(16,A , 9)	882.31505	0.27	1.53E-22	2.43E-03	-0.7	0.0	0.4156	-0.8	0.1091	-1.9
79	PP(16,A , 9)	882.36894	0.25	1.62E-22	2.53E-03	3.2	2.8	0.4149	-0.7	0.1096	-2.3
81	PQ(16,A , 9)	892.43660	0.38	9.59E-23	2.34E-03	-4.6	-4.0	0.4062	1.5	0.1028	4.1
79	PQ(16,A , 9)	892.52894	0.26	1.01E-22	2.41E-03	-1.8	-2.3	0.4011	2.8	0.1081	-1.0
81	RQ(16,A , 9)	1026.61658	-0.14	1.33E-22	3.06E-03	3.2	0.0	0.4227	-2.5	0.1096	-2.3
79	RQ(16,A , 9)	1026.64442	-0.10	1.30E-22	2.96E-03	-0.4	-0.6	0.4165	-1.0	0.1019	5.1
81	RR(16,A , 9)	1037.37039	-0.20	2.41E-22	2.94E-03	-0.9	0.0	0.4161	-1.0	0.1035	3.4
79	RR(16,A , 9)	1037.43911	-0.23	2.49E-22	2.99E-03	0.5	0.0	0.4208	-2.1	0.1042	2.7
79	PP(17,A , 9)	881.69573	0.26	1.47E-22	2.38E-03	-2.8	-2.9	0.4106	1.9	0.1056	2.3
79	PQ(17,A , 9)	892.48970	-0.02	1.10E-22	2.50E-03	2.1	2.3	0.4601	-9.1	0.1083	-0.3
81	RQ(17,A , 9)	1026.57838	-0.11	1.35E-22	2.93E-03	-1.3	0.0	0.4107	1.8	0.1054	2.5
79	RQ(17,A , 9)	1026.60596	-0.17	1.39E-22	2.97E-03	-0.1	-0.3	0.4200	-0.4	0.1035	4.4
81	RR(17,A , 9)	1037.96389	-0.22	2.30E-22	2.91E-03	-1.9	0.0	0.4203	-0.5	0.1019	6.0
79	RR(17,A , 9)	1038.03494	-0.16	2.39E-22	2.97E-03	-0.1	-0.5	0.4349	-3.8	0.1029	5.0
79	PQ(18,A , 9)	892.44844	-0.01	1.04E-22	2.30E-03	-6.2	-6.5	0.4117	2.6	0.1019	4.9
81	RQ(18,A , 9)	1026.53785	-0.16	1.50E-22	3.12E-03	5.0	0.0	0.4571	-7.6	0.1045	2.2
79	RQ(18,A , 9)	1026.56532	-0.14	1.46E-22	2.99E-03	0.7	0.3	0.4218	0.1	0.1034	3.3
81	RR(18,A , 9)	1038.55508	-0.16	2.27E-22	2.98E-03	0.5	0.0	0.4458	-5.3	0.1001	6.7
79	RR(18,A , 9)	1038.62832	-0.13	2.29E-22	2.95E-03	-0.7	-1.0	0.4398	-4.0	0.1031	3.6
81	PP(19,A , 9)	880.29649	0.14	1.38E-22	2.45E-03	-0.1	0.9	0.4141	2.5	0.1057	0.0
79	RQ(19,A , 9)	1026.52247	-0.07	1.56E-22	3.09E-03	4.1	3.8	0.4432	-4.2	0.0994	6.4
81	RR(19,A , 9)	1039.14383	-0.13	2.16E-22	2.95E-03	-0.6	0.0	0.4277	-0.7	0.1028	2.8
79	RR(19,A , 9)	1039.21927	-0.13	2.17E-22	2.92E-03	-1.8	-2.0	0.4387	-3.2	0.1021	3.5
81	RQ(20,A , 9)	1026.45020	-0.08	1.50E-22	2.98E-03	0.5	0.0	0.4163	2.2	0.1066	-1.8
81	RR(20,A , 9)	1039.73013	-0.15	2.08E-22	2.97E-03	0.1	0.0	0.4386	-3.0	0.1039	0.7
79	RQ(21,A , 9)	1026.42982	-0.09	1.57E-22	3.04E-03	2.4	1.8	0.4505	-5.7	0.1007	2.9
81	RR(21,A , 9)	1040.31399	-0.19	1.95E-22	2.91E-03	-1.9	0.0	0.4230	0.5	0.0994	4.3
81	RQ(23,A , 9)	1026.30164	-0.15	1.43E-22	2.85E-03	-3.9	0.0	0.4069	3.3	0.0994	2.4
79	RQ(24,A , 9)	1026.27393	-0.06	1.49E-22	2.98E-03	0.2	0.0	0.4114	1.2	0.1017	-0.8
81	RQ(25,A , 9)	1026.19141	-0.10	1.53E-22	3.17E-03	6.8	0.0	0.4482	-8.3	0.1031	-2.9
81	RQ(26,A , 9)	1026.13282	-0.18	1.45E-22	3.11E-03	4.8	0.0	0.4178	-3.3	0.0980	1.4
79	RQ(26,A , 9)	1026.15870	-0.01	1.49E-22	3.13E-03	5.2	4.5	0.4332	-6.7	0.0996	-0.3
81	RR(26,A , 9)	1043.19693	-0.15	1.50E-22	2.96E-03	-0.3	0.0	0.4073	-0.8	0.1006	-1.2
79	RR(26,A , 9)	1043.28763	-0.09	1.56E-22	3.03E-03	1.9	1.8	0.4230	-4.5	0.0995	-0.1
81	RQ(27,A , 9)	1026.07215	-0.06	1.37E-22	3.04E-03	2.3	0.0	0.4069	-2.6	0.0986	0.0
79	RQ(27,A , 9)	1026.09754	-0.13	1.37E-22	3.00E-03	0.8	0.6	0.3879	2.2	0.0986	0.0
81	PQ(28,A , 9)	891.81947	0.07	9.51E-23	2.49E-03	1.7	2.6	0.4155	-6.8	0.1029	-4.8
81	RQ(28,A , 9)	1026.00916	-0.02	1.29E-22	3.00E-03	1.0	0.0	0.3917	-1.1	0.0988	-0.8
79	RQ(28,A , 9)	1026.03431	-0.06	1.31E-22	2.98E-03	0.2	-0.6	0.3799	1.9	0.0970	1.0
81	PQ(29,A , 9)	891.75313	0.04	8.63E-23	2.37E-03	-3.2	-1.8	0.3533	6.7	0.0995	-2.2
79	PQ(29,A , 9)	891.84285	0.07	9.08E-23	2.45E-03	0.1	-0.4	0.3723	1.3	0.1023	-4.8
81	RQ(29,A , 9)	1025.94373	-0.15	1.26E-22	3.06E-03	3.2	0.0	0.3860	-2.3	0.0982	-0.9
79	RQ(29,A , 9)	1025.96876	-0.03	1.27E-22	3.02E-03	1.7	1.3	0.3699	1.9	0.0989	-1.6
81	RR(29,A , 9)	1044.89713	-0.11	1.21E-22	2.93E-03	-1.3	0.0	0.3742	0.8	0.0955	1.9
81	PQ(30,A , 9)	891.68446	-0.03	8.06E-23	2.34E-03	-4.5	-3.8	0.3528	3.7	0.0984	-1.7
79	PQ(30,A , 9)	891.77388	-0.01	8.13E-23	2.32E-03	-5.2	-5.6	0.3414	7.1	0.0985	-1.8
79	PR(30,A , 9)	911.42992	-0.02	2.69E-23	2.60E-03	6.0	5.3	0.3779	-3.2	0.0989	-2.2
81	RQ(30,A , 9)	1025.87635	0.02	1.17E-22	2.98E-03	0.3	0.0	0.4021	-9.0	0.0915	5.8
81	RR(30,A , 9)	1045.45902	0.03	1.13E-22	2.95E-03	-0.7	0.0	0.3703	-1.2	0.0956	1.2
79	RR(30,A , 9)	1045.55802	-0.05	1.17E-22	2.99E-03	0.7	0.3	0.3818	-4.2	0.0942	2.7
79	PQ(31,A , 9)	891.70271	0.01	7.70E-23	2.33E-03	-5.0	-5.4	0.3231	9.4	0.0957	0.5
81	RR(31,A , 9)	1046.01823	0.00	1.09E-22	3.07E-03	3.5	0.0	0.3615	-2.2	0.0956	0.7
79	PQ(32,A , 9)	891.62922	0.02	7.90E-23	2.54E-03	3.9	3.8	0.3635	-6.3	0.0984	-2.7
81	RR(33,A , 9)	1047.12919	0.05	8.72E-23	2.90E-03	-2.3	0.0	0.3486	-6.1	0.0938	1.6
81	PQ(34,A , 9)	891.38691	-0.15	6.34E-23	2.38E-03	-2.9	-1.8	0.3015	4.1	0.0985	-3.7
79	PQ(35,A , 9)	891.39473	-0.09	6.03E-23	2.40E-03	-2.0	-2.0	0.2928	2.5	0.0962	-1.8
81	RQ(36,A , 9)	1025.42396	0.47	7.68E-23	2.94E-03	-0.8	0.0	0.3051	-6.0	0.0914	2.9
79	RQ(36,A , 9)	1025.44617	0.00	8.09E-23	3.06E-03	2.9	2.4	0.3066	-6.5	0.0916	2.7
81	RP(39,A , 9)	1000.55891	-0.03	1.67E-23	2.82E-03	-4.8	-4.2	0.2718	-7.6	0.0973	-4.2
81	RQ(39,A , 9)	1025.16651	0.02	6.43E-23	3.20E-03	7.8	0.0	0.2953	-15.0	0.0960	-2.9
79	RQ(39,A , 9)	1025.18811	0.06	6.19E-23	3.04E-03	2.4	1.7	0.2636	-4.7	0.0926	0.6
81	RQ(40,A , 9)	1025.07630	0.01	5.54E-23	3.03E-03	2.2	0.0	0.2423	-0.3	0.0979	-5.0
79	RQ(40,A , 9)	1025.09742	-0.03	5.49E-23	2.98E-03	0.2	-0.4	0.2537	-4.8	0.0949	-2.0
79	PQ(41,A , 9)	890.86311	-0.40	3.44E-23	2.35E-03	-3.9	-3.8	0.2403	-0.5	0.0950	-2.4
79	PQ(42,A , 9)	890.76667	-0.16	3.13E-23	2.37E-03	-3.4	-3.3	0.2069	10.9	0.0988	-6.3
79	RQ(44,A , 9)	1024.71241	0.19	3.67E-23	3.04E-03	2.1	1.3	0.2221	-4.5	0.0922	0.1
79	RQ(46,A , 9)	1024.50623	0.35	3.00E-23	3.12E-03	4.9	4.2	0.2052	-4.4	0.0909	1.3
81	PQ(47,A , 9)	890.16474	-0.43	1.85E-23	2.53E-03	3.5	5.0	0.1888	-0.1	--	--

81	PQ(48,A , 9)	890.05488	-0.06	1.70E-23	2.62E-03	7.2	8.8	0.2256	-19.8	--	--
79	PQ(49,A , 9)	890.02455	-0.20	1.39E-23	2.40E-03	-2.1	-1.7	0.1623	6.5	--	--
81	RQ(50,A , 9)	1024.04944	0.38	1.62E-23	2.82E-03	-5.0	0.0	0.1410	16.3	--	--

Note: The assignment column gives the type of isotopologues (79 for $CH_3{}^{79}Br$ and 81 for $CH_3{}^{81}Br$) for which the transition is observed, the type of branch for *K* and *J*, the rotational quantum number *J* of the lower state, its symmetry, and the rotational quantum number *K* of the lower state. Position column corresponds to line positions at zero pressure measured in this work. The Dif column is the difference between the experimental and calculated positions in 10^{-3} cm^{-1}. S_{obs} are the line intensities for natural CH_3Br at 296K in $cm.molecule^{-1}$. $|R|^2_{obs}$ are the observed transition dipole moment squared deduced from the measured line intensities. %1 and %2 represent the difference in % ((obs-calc)/calc×100) between the experimental and calculated intensity obtained using respectively the empirical analysis based on the Herman-Wallis factor or the set of codes of Ref. [9]. γ_{self} and γ_{N_2} are the measured self- and N_2-broadening coefficients in $cm^{-1}.atm^{-1}$. %self and $\%N_2$ are the differences in % between the experimental and calculated widths.

Table 3. Molecular parameters of the ν_6 band of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ (cm^{-1})[a]

ν_6 state	$CH_3{}^{79}Br$		$CH_3{}^{81}Br$	
	From Ref. [6]	Present Work	From Ref. [6]	Present Work
ν_0	954.86785(1)	954.86800(2)	954.80509(1)	954.80519(2)
A	5.210153(2)	5.2101669(6)	5.210133(1)	5.2101408(7)
B	0.31802118(3)	0.31802097(5)	0.31681287(2)	0.31681280(6)
$A\zeta$	1.157528(3)	1.157529(1)	1.156915(2)	1.156908(1)
$D_J \times 10^7$	3.3081(1)	3.3060(4)	3.28205(9)	3.2829(5)
$D_{JK} \times 10^6$	4.3156(9)	4.3243(3)	4.2920(6)	4.2961(3)
$D_K \times 10^5$	8.810(3)	8.7832(7)	8.778(2)	8.7916(8)
$\eta_J \times 10^6$	9.443(5)	9.504(1)	9.417(3)	9.456(2)
$\eta_K \times 10^4$	1.231(3)	1.1948(5)	1.206(2)	1.1936(5)
$H_J \times 10^{13}$	[-1.9][b]	-2.4(1)	[-1.9][b]	-2.1(1)
$H_{JK} \times 10^{12}$	[3.2][b]	[3.2][b]	[4.7][b]	[4.7][b]
$H_{KJ} \times 10^{10}$	[1.97][b]	[1.97][b]	[1.95][b]	[1.95][b]
$H_K \times 10^9$	[4.1][b]	[4.1][b]	[4.6][b]	[4.6][b]
$q_2 \times 10^5$	-7.434(1)	-7.466(2)	-7.398(1)	-7.4235(2)
$q_{2J} \times 10^{10}$	0.[c]	2.86(9)	0.[c]	3.0(1)

[a]Error in parentheses is one standard deviation in units of the last digit.
[b]Fixed to the ground state value of Ref. [16].
[c]Fixed in Ref. [6].

Table 4. Empirical coefficients of Eqs. (18-23) modeling the rotational dependence of self- and N_2-broadening widths

$a_{self}^{0,0} = 0.401 \pm 0.085$	$a_{N_2}^{0,0} = 0.1405 \pm 0.0014$
$a_{self}^{0,1} = -0.015 \pm 0.020$	$a_{N_2}^{0,1} = -0.00248 \pm 0.00022$
$a_{self}^{0,2} = 0.0031 \pm 0.0018$	$a_{N_2}^{0,2} = (4.15 \pm 0.91)\times10^{-5}$
$a_{self}^{0,3} = (-1.64 \pm 0.70)\times10^{-4}$	$a_{N_2}^{0,3} = (-2.3 \pm 1.1)\times10^{-7}$
$a_{self}^{0,4} = (3.2 \pm 1.3)\times10^{-6}$	
$a_{self}^{0,5} = (-2.17 \pm 0.990)\times10^{-8}$	

for $J \leq 39$	for $J \geq 40$	for $J \leq 17$	for $J \geq 16$
$a_{self}^{2,0} = -0.0208 \pm 0.0052$	$a_{self}^{2,0} = (-2.06 \pm 0.59)\times10^{-4}$	$a_{N_2}^{2,0} = (-1.14 \pm 0.25)\times10^{-2}$	$a_{N_2}^{2,0} = (-2.7 \pm 2.9)\times10^{-5}$
$a_{self}^{2,1} = 0.0046 \pm 0.0015$	$a_{self}^{2,1} = (7.0 \pm 5.1)\times10^{-7}$	$a_{N_2}^{2,1} = (4.3 \pm 1.3)\times10^{-3}$	$a_{N_2}^{2,1} = (7.6 \pm 7.6)\times10^{-7}$
$a_{self}^{2,2} = (-4.4 \pm 1.7)\times10^{-4}$		$a_{N_2}^{2,2} = (-6.8 \pm 2.7)\times10^{-4}$	
$a_{self}^{2,3} = (2.15 \pm 0.92)\times10^{-5}$		$a_{N_2}^{2,3} = (5.4 \pm 2.5)\times10^{-5}$	
$a_{self}^{2,4} = (-5.7 \pm 2.7)\times10^{-7}$		$a_{N_2}^{2,4} = (-2.1 \pm 1.1)\times10^{-6}$	
$a_{self}^{2,5} = (7.8 \pm 4.0)\times10^{-9}$		$a_{N_2}^{2,5} = (3.1 \pm 1.8)\times10^{-8}$	
$a_{self}^{2,6} = (-4.3 \pm 2.3)\times10^{-11}$			

Note: The given error bars are one standard deviation (1SD) of the fit and are given for indication.

Table 5. Extract of the line list of the ν_6 band of CH_3Br around 10 μm

Iso	ν_0	S_0	R^2	γ_{air}	γ_{self}	E_{inf}	n_{air}	δ_{air}	Vibrational and Rotational attribution								error codes
81	927.00762	0.242E-21	0.260E-02	0.0937	0.3985	354.08860	0.75	0.000000	NU6	GROUND	29	3	1E	29	4	0E	466511
79	927.01010	0.234E-21	0.260E-02	0.0931	0.3860	374.23240	0.75	0.000000	NU6	GROUND	30	3	1E	30	4	0E	466511
79	927.03972	0.101E-21	0.269E-02	0.0881	0.2263	630.64530	0.75	0.000000	NU6	GROUND	43	1	1A+	44	0	0A+	466511
81	927.04048	0.334E-22	0.257E-02	0.1070	0.3636	150.11680	0.75	0.000000	NU6	GROUND	10	4	1E	9	5	0E	466511
81	927.07354	0.255E-21	0.260E-02	0.0944	0.4103	335.68350	0.75	0.000000	NU6	GROUND	28	3	1E	28	4	0E	466511
79	927.07847	0.137E-21	0.269E-02	0.0911	0.3372	384.19070	0.75	0.000000	NU6	GROUND	33	0	1E	34	1	0E	466511
79	927.07859	0.248E-21	0.260E-02	0.0937	0.3985	355.12250	0.75	0.000000	NU6	GROUND	29	3	1E	29	4	0E	466511
81	927.08505	0.593E-22	0.255E-02	0.1000	0.4522	321.69760	0.75	0.000000	NU6	GROUND	22	5	1A-	21	6	0A-	466511
81	927.08505	0.593E-22	0.255E-02	0.1000	0.4522	321.69760	0.75	0.000000	NU6	GROUND	22	5	1A+	21	6	0A+	466511
81	927.09583	0.988E-22	0.269E-02	0.0881	0.2263	628.25310	0.75	0.000000	NU6	GROUND	43	1	1A+	44	0	0A+	466511
81	927.10182	0.134E-21	0.269E-02	0.0911	0.3372	382.75190	0.75	0.000000	NU6	GROUND	33	0	1E	34	1	0E	466511
81	927.13719	0.268E-21	0.260E-02	0.0951	0.4213	317.91100	0.75	0.000000	NU6	GROUND	27	3	1E	27	4	0E	466511
79	927.14292	0.344E-22	0.257E-02	0.1070	0.3636	150.19610	0.75	0.000000	NU6	GROUND	10	4	1E	9	5	0E	466511
79	927.14478	0.262E-21	0.260E-02	0.0944	0.4103	336.64730	0.75	0.000000	NU6	GROUND	28	3	1E	28	4	0E	466511
81	927.19854	0.281E-21	0.260E-02	0.0958	0.4314	300.77120	0.75	0.000000	NU6	GROUND	26	3	1E	26	4	0E	466511
79	927.20868	0.275E-21	0.260E-02	0.0951	0.4213	318.80710	0.75	0.000000	NU6	GROUND	27	3	1E	27	4	0E	466511
79	927.21836	0.609E-22	0.255E-02	0.1000	0.4522	322.21400	0.75	0.000000	NU6	GROUND	22	5	1A+	21	6	0A+	466511
79	927.21836	0.609E-22	0.255E-02	0.1000	0.4522	322.21400	0.75	0.000000	NU6	GROUND	22	5	1A-	21	6	0A-	466511
81	927.25762	0.292E-21	0.260E-02	0.0966	0.4404	284.26450	0.75	0.000000	NU6	GROUND	25	3	1E	25	4	0E	466511
79	927.27029	0.288E-21	0.260E-02	0.0958	0.4314	301.60210	0.75	0.000000	NU6	GROUND	26	3	1E	26	4	0E	466511
81	927.31442	0.303E-21	0.260E-02	0.0974	0.4483	268.39090	0.75	0.000000	NU6	GROUND	24	3	1E	24	4	0E	466511
81	927.32295	0.524E-23	0.249E-02	0.0882	0.1915	1025.87590	0.75	0.000000	NU6	GROUND	48	7	1E	47	8	0E	466511
79	927.32960	0.300E-21	0.260E-02	0.0966	0.4404	285.03250	0.75	0.000000	NU6	GROUND	25	3	1E	25	4	0E	466511
81	927.36894	0.313E-21	0.260E-02	0.0983	0.4550	253.15080	0.75	0.000000	NU6	GROUND	23	3	1E	23	4	0E	466511
81	927.38083	0.242E-21	0.266E-02	0.0984	0.4614	194.84730	0.75	0.000000	NU6	GROUND	22	1	1E	23	2	0E	466511
79	927.38663	0.312E-21	0.260E-02	0.0974	0.4483	269.09850	0.75	0.000000	NU6	GROUND	24	3	1E	24	4	0E	466511
79	927.39044	0.249E-21	0.266E-02	0.0984	0.4614	195.51130	0.75	0.000000	NU6	GROUND	22	1	1E	23	2	0E	466511
81	927.39052	0.264E-22	0.252E-02	0.0911	0.3231	615.71430	0.75	0.000000	NU6	GROUND	35	6	1E	34	7	0E	466511
81	927.42117	0.321E-21	0.260E-02	0.0992	0.4603	238.54430	0.75	0.000000	NU6	GROUND	22	3	1E	22	4	0E	466511
79	927.43977	0.121E-22	0.272E-02	0.0871	0.1498	949.84560	0.75	0.000000	NU6	GROUND	53	2	1E	54	1	0E	466511
79	927.44137	0.321E-21	0.260E-02	0.0983	0.4550	253.80030	0.75	0.000000	NU6	GROUND	23	3	1E	23	4	0E	466511

Note: Iso is the isotopologue's identifier (79 for $CH_3{}^{79}Br$ and 81 for $CH_3{}^{81}Br$), ν_0 is the wavenumber of the transition in cm^{-1}, S_0 is the calculated line intensity for natural abundances of CH_3Br at 296 K in cm.molecule^{-1}, R^2 is the calculated transition dipole moment squared for pure $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ in debye^2, γ_{air} and γ_{self} are respectively the air- and self-broadening coefficients in $cm^{-1}.atm^{-1}$ at 296 K, E_{inf} is the energy of the lower level in cm^{-1}, n_{air} is the temperature dependence of the air-broadening coefficient at 296 K, δ_{air} is the air-shifting coefficient in $cm^{-1}.atm^{-1}$. Vibrational attribution is self explanatory, and the rotational attribution is given first for the upper state, then for the lower, it corresponds to the rotational quantum numbers J, and K, and the symmetry of the rovibrational state $A+$, $A–$, or E [19,21]. Finally the error codes related to the wavenumber, the intensity, the air- and self-broadening coefficients, the temperature dependence, and the air-shifting coefficient are given (see Appendix for details)

Fig. 1. Overview of the 6 spectra recorded in this work with the Bruker IFS 120 HR interferometer of the LADIR. We assigned a number from 1 to 6 to these experimental spectra (see Table 1 for details).

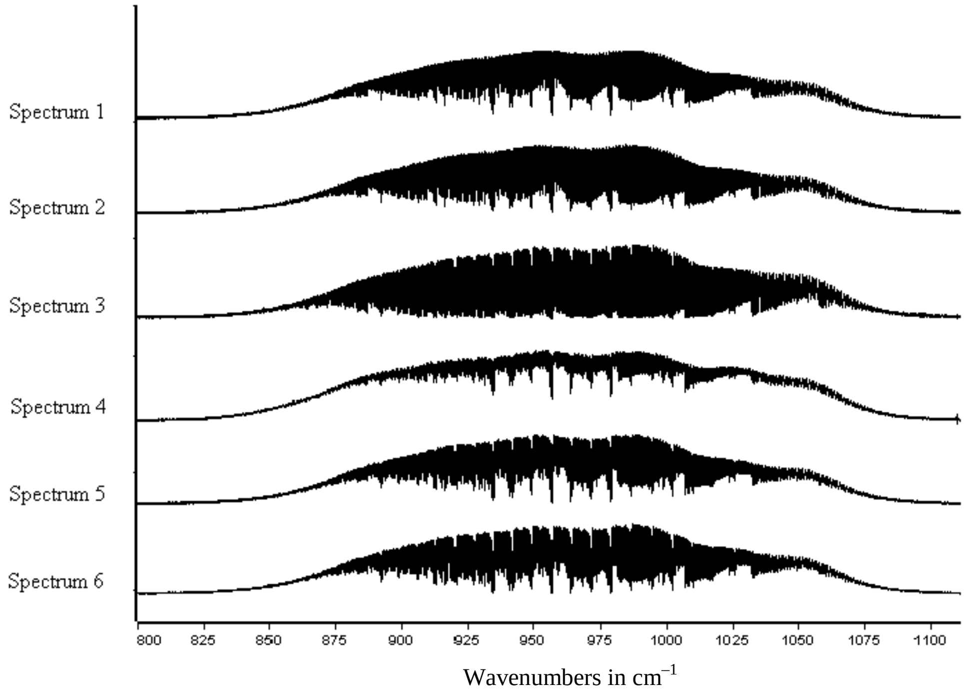

Fig. 2. Spectral region of the ^{P}Q branch of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ for $K = 4$ in the six spectra recorded in this work. (see Table 1 for the spectra numbers)

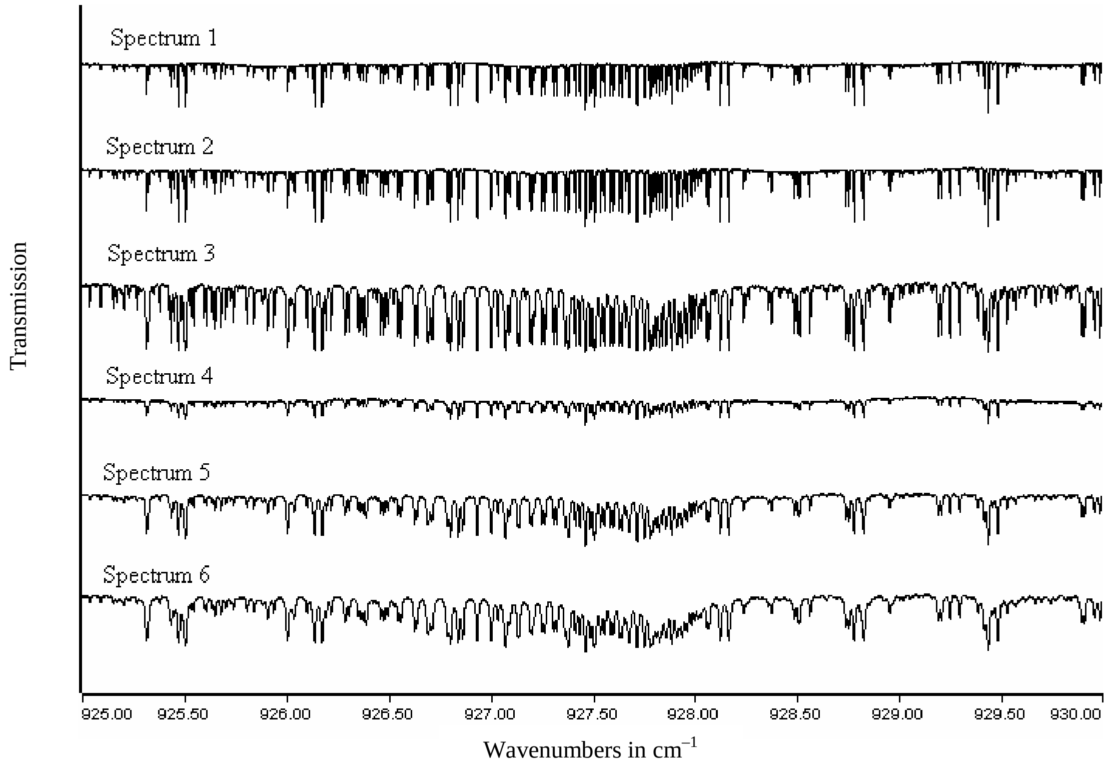

Fig. 3. Multispectrum fitting of an isolated transition centered at 1035.932 cm^{-1}. The lower residuals panel corresponds to the residual obtained from the multispectrum fitting procedure using nominal value of the aperture, whereas the upper residuals panel is obtained using effective value of the aperture (see section 3.1.1). Signatures observed for the two lowest pressure spectra (#1 and #2: see Table 1 for the numbering of spectra) disappear when using effective values of the aperture.

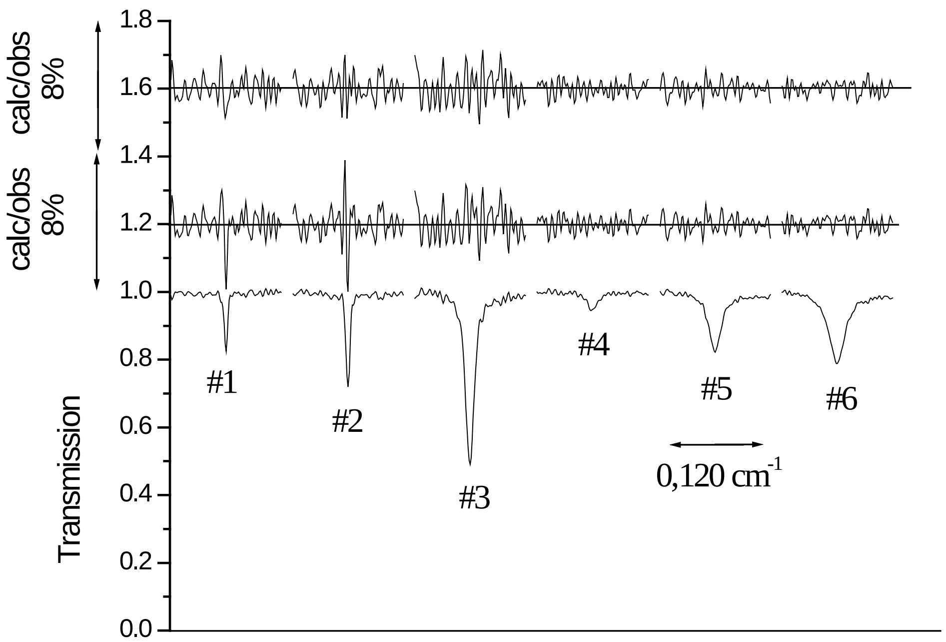

Fig. 4. Experimental and calculated transition dipole moments squared of the ν_6 band of CH_3Br. Open symbols represents $\Delta K = +1$ transitions, whereas black symbols are used for $\Delta K = -1$ transitions. Squared symbols have been used for $\Delta J = 0$ transitions, and up- and down-triangles have been employed respectively for $\Delta J = -1$ and $\Delta J = +1$ transitions. Black lines represent calculation done using model 1 (see text).

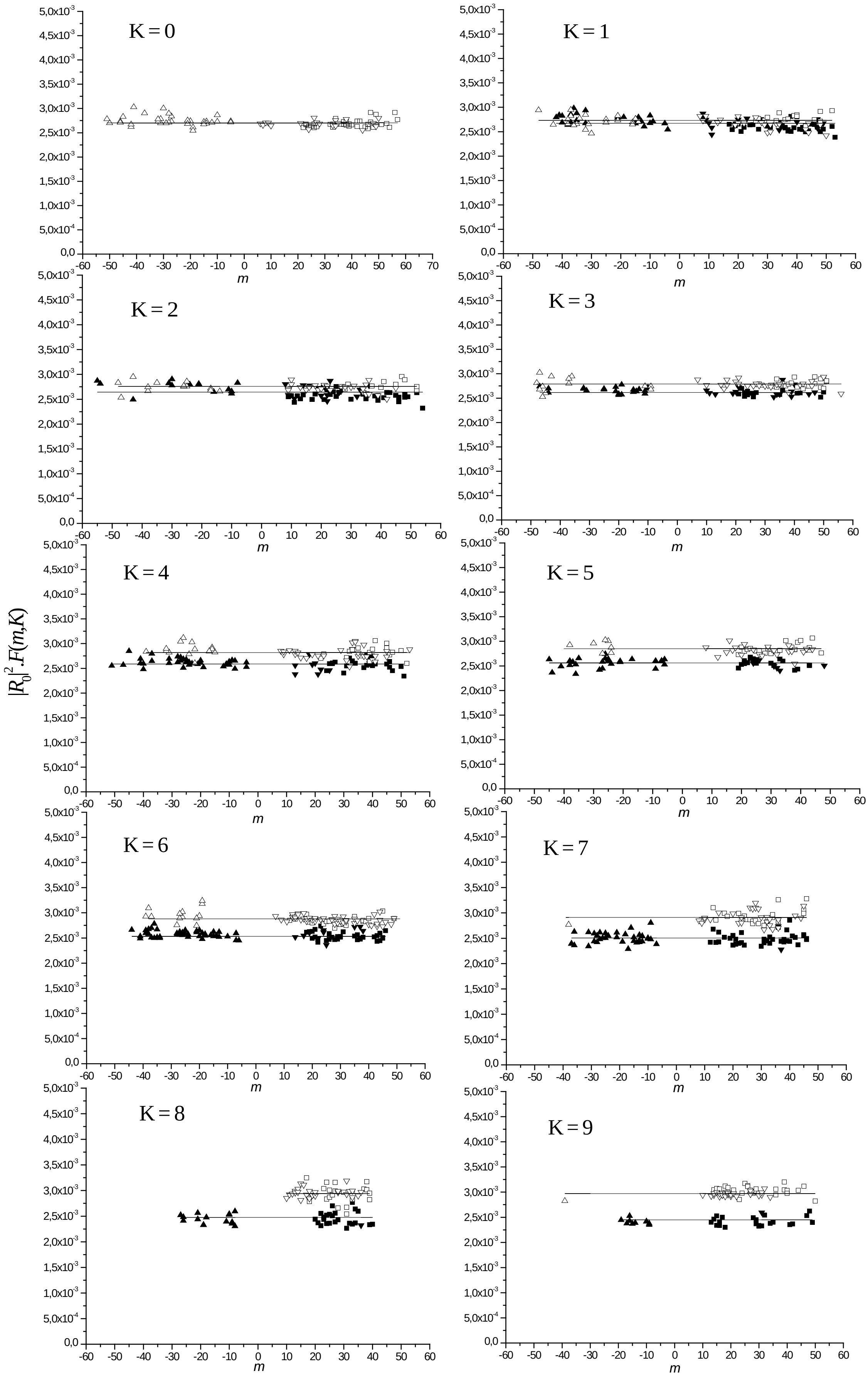

Fig.5. Example of the polynomial fit in K (see Eq. 13) of the self- and N_2-broadening widths for sets of measurements corresponding to $J = 7$, $J = 10$, $J = 20$, and $J = 35$. The open squares and triangles symbols represent respectively the measured self- and N_2-broadening widths, whereas the black squares and triangles have been used to reproduce respectively the calculated self- and N_2-broadening widths.

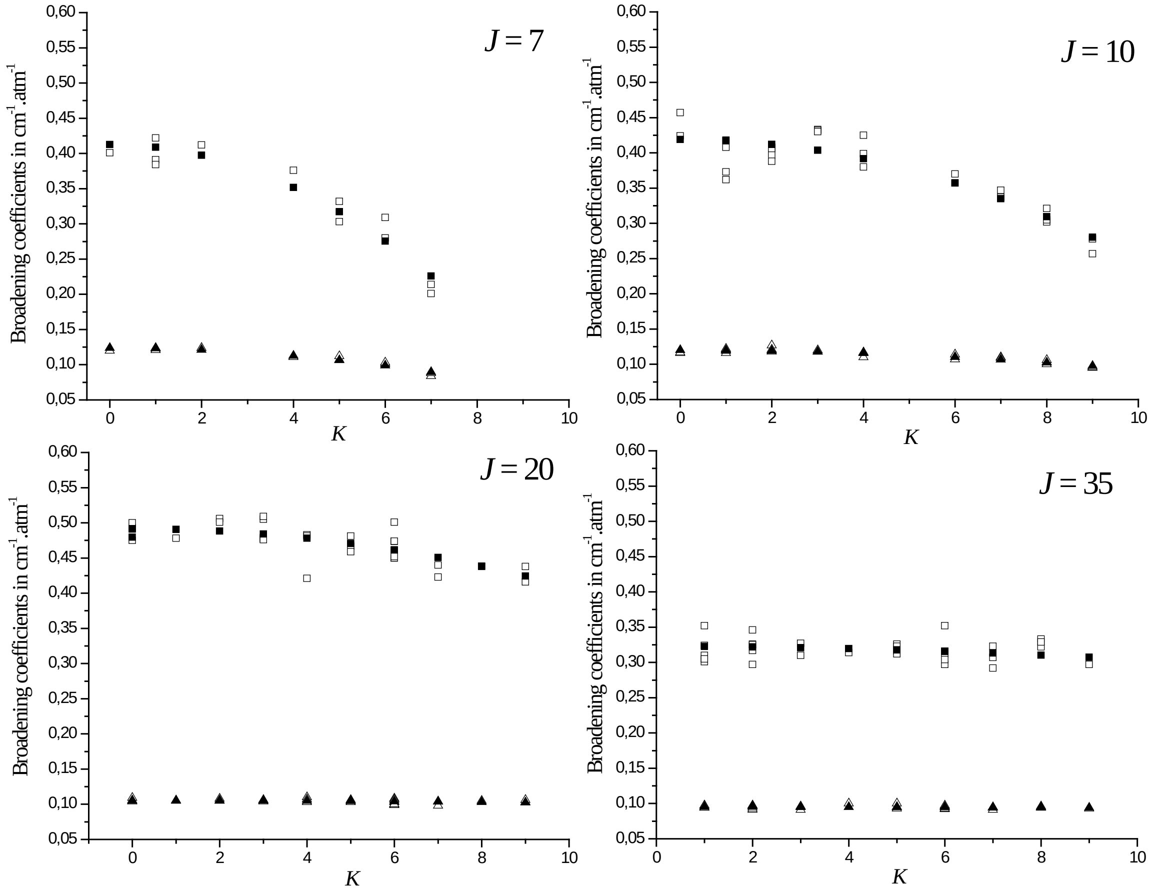

Fig. 6. Parameters a_J^0 deduced from the fit of the measured self-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eq. (14). The error bars are 1SD.

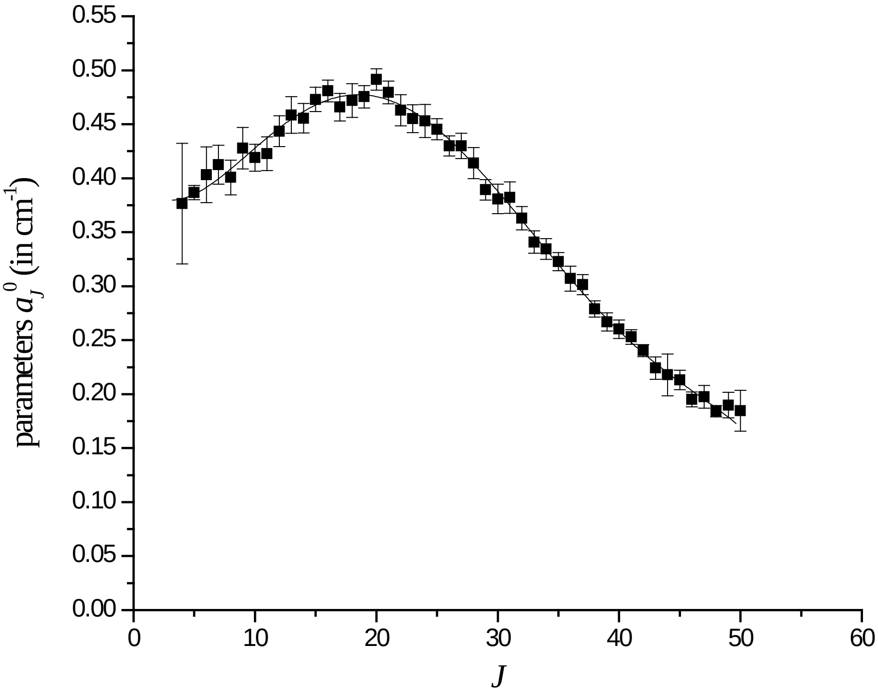

Fig. 7. Parameters a_J^2 deduced from the fit of the measured self-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eqs. (15,16). The error bars are 1SD.

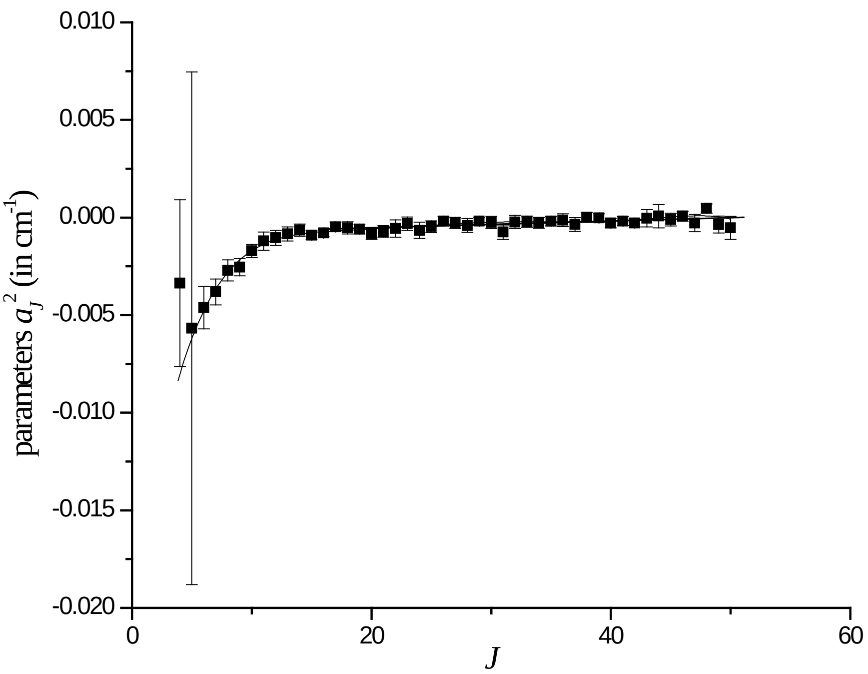

Fig. 8. Parameters a_J^0 deduced from the fit of the measured N_2-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eq. (17). The error bars are 1SD.

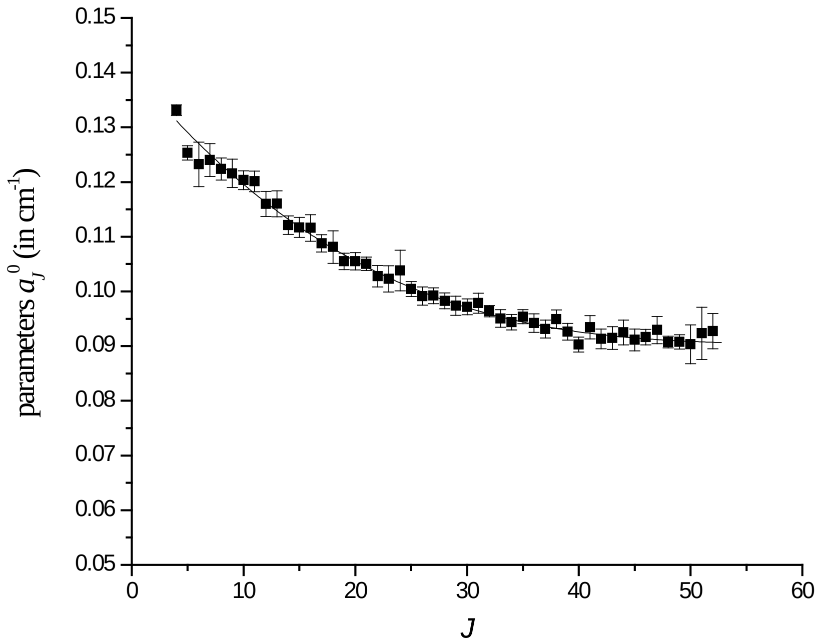

Fig. 9. Parameters a_J^2 deduced from the fit of the measured N_2-broadening coefficients using Eq. (13). The continuous line symbolizes the fit of these coefficients using Eqs. (18,19). The error bars are 1SD.

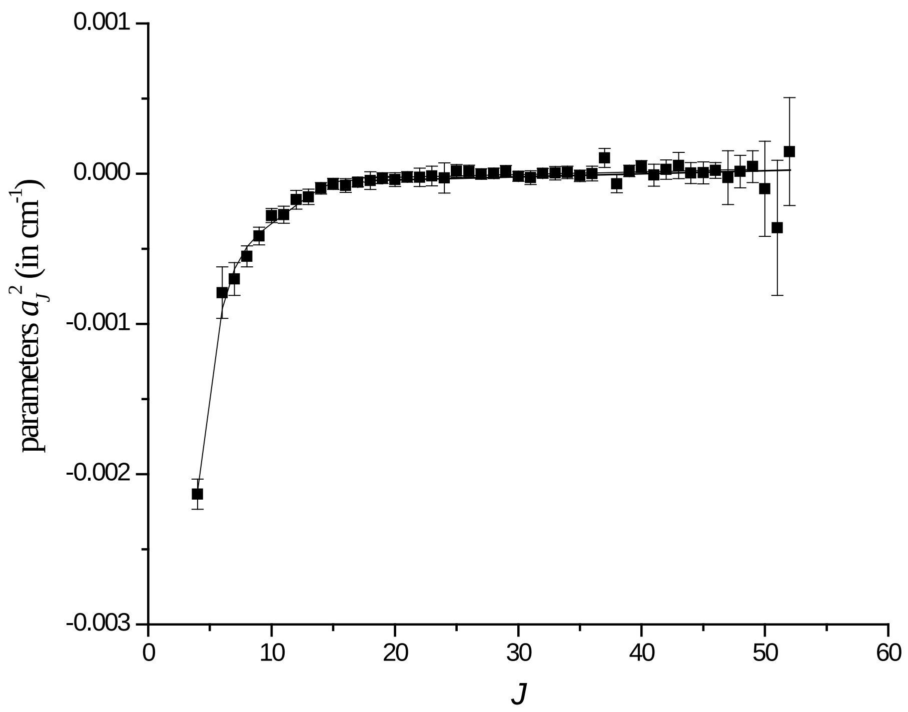

Fig. 10. *J* and *K* dependence observed and calculated for all the self-broadening coefficients measured in this work. The squared symbols symbolize the measured widths, and the continuous line has been used to represent the calculated widths using the algorithm described in section 4.3.

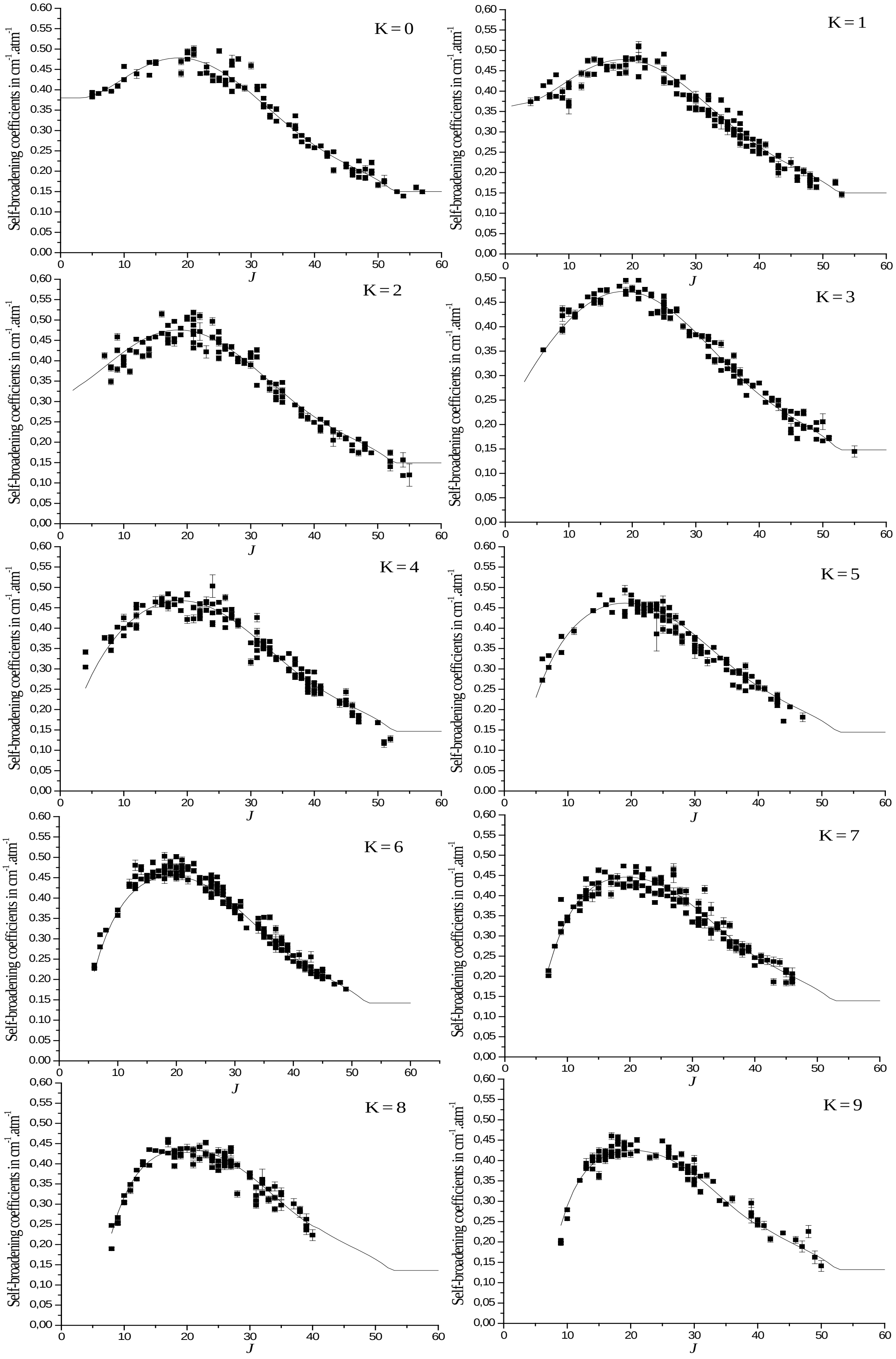

Fig. 11. *J* and *K* dependence observed and calculated for all the N_2-broadening coefficients measured in this work. The squared symbols symbolize the measured widths, and the continuous line has been used to represent the calculated widths using the algorithm described in section 4.3.