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Keywords:	Formaldehyde, InfraRed Spectroscopy, Vibrational analysis, Perturbations



# Rotational analysis of the $2\nu_5$ Band of Formaldehyde

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## Abstract

The spectrum of the  $2\nu_5$  C–H stretching band of formaldehyde has been measured by Barry *et al* [*Phys. Chem. Chem. Phys.*, 4, 445 (2002).] with FTIR spectroscopy. We have rotationally analysed this spectrum with the help of PGOPHER, a general purpose program for simulating and fitting rotational spectra. The spectrum shows several perturbations and there is sufficient information available on the vibrational structure from a dispersed fluorescence spectra study by Bowens *et al* [*J. Chem. Phys.* 104, 460 (1996)] and theoretical calculations by Burleigh *et al* [*J. Chem. Phys.* 104, 480 (1996)] to allow us to identify the perturbing states and deperturb the energy levels. The resulting perturbation parameters and rotational constants enabled us to reproduce the experimental line positions with an average error of  $0.013\text{ cm}^{-1}$ . We also present a list of line positions and relative intensities in the region around  $1.76\text{ }\mu\text{m}$ .

*Keywords:* Formaldehyde; InfraRed Spectroscopy; Vibrational analysis; Perturbations

## A. Introduction

Formaldehyde is one of the most widely studied polyatomic molecules, and has played a very important role in understanding the spectroscopy of polyatomic molecules. Recent interest in formaldehyde is due to its atmospheric importance as it is known to play an important part in tropospheric chemistry [1,2]. The molecule has been identified as a significant atmospheric pollutant [3], and long term exposure to it can cause considerable health problems [4,5]. Hence, there is a requirement to monitor atmospheric formaldehyde below the parts per million (ppmv) level, which would be convenient, portable, and instantaneous. There are a number of methods currently being used [6,7], and the most widely used method for atmospheric formaldehyde detection is with the help of a wet chemical formaldehyde analyser [8], but this cannot detect the fluctuations in formaldehyde concentration, as it is a time averaged method. Spectroscopic methods, using ultra violet (UV/VIS) [9,10] and infrared frequencies are more suitable due to better time resolution [6,7,11,12]. For infrared spectroscopy, both the C-H stretching ( $\nu_1$  and  $\nu_5$ ) region at  $3.6 \mu\text{m}$  [13,14,15,16,17,18,19], and the  $5\text{-}10 \mu\text{m}$  wavelength range corresponding to the  $\nu_4 / \nu_6$ ,  $\nu_3$  and  $\nu_2$  fundamental bands [20,21,22,23] of formaldehyde are being used. The  $3.6 \mu\text{m}$  bands, with strong  $\nu_1$  and  $\nu_5$  bands at  $2782 \text{ cm}^{-1}$  and  $2843 \text{ cm}^{-1}$  are most widely used for detection of formaldehyde in the atmosphere. Recently, Barry *et al* [24] studied the absorption of gaseous formaldehyde near  $1.76 \mu\text{m}$ , which is the region of the first overtone of the C-H asymmetric stretch, and evaluated the potential of using this band for detection of

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3 formaldehyde in the atmosphere. Given the commercial availability of stable, narrow  
4 band room temperature diode lasers in this region this is a very promising method, even  
5 though the absorption cross section for this overtone band is considerably lower than the  
6 fundamental band. Barry *et al* recorded the FTIR spectrum of formaldehyde in the range  
7 5600-5700  $\text{cm}^{-1}$ , and identified the band with origin near 5651  $\text{cm}^{-1}$  to be the transition  
8 from the ground state to the state with two quanta in the asymmetric stretch mode,  $2\nu_5$   
9 [25,26]. They performed a preliminary analysis of the recorded spectrum which  
10 resembles a parallel band of a prolate symmetric top, and identified the asymmetry  
11 doubled  $^{\text{Q}}\text{R}_1$  and  $^{\text{Q}}\text{P}_1$  lines for lower  $J'$  values. This preliminary analysis indicated that  
12 the spectrum had many perturbations. A more detailed analysis of the whole spectrum  
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25 We report here a detailed analysis of this  $2\nu_5$  band of formaldehyde recorded by  
26 Barry *et al*, with the help of PGOPHER [28], a general purpose program for simulating  
27 and fitting rotational spectra. We have been able to assign levels up to  $J' = 20$  and  
28  $K_a' = 5$  and have identified several perturbations. As information with moderate  
29 accuracy ( $\sim 1 \text{ cm}^{-1}$ ) on all the states in the region is available from previous work,  
30 including an experimental study by Bowens *et al* [29] and theoretical study by Burleigh  
31 *et al* [30], we were able to assign a source to all the perturbations. The model we  
32 developed for the perturbations enabled us to fit the spectrum with an average error of  
33 0.013  $\text{cm}^{-1}$ , compared to a line width of the experimental spectrum of 0.022  $\text{cm}^{-1}$ .  
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## B. Analysis of the $2\nu_5$ band of formaldehyde

The spectrum used for the analysis is described in [24]; it was of a 0.02 Torr sample of HCHO and covered the range  $5600 - 5730 \text{ cm}^{-1}$ . [The overall form of the band is typical of an A type band of a near prolate asymmetric top with distinct P, Q and R branch regions.](#) Sample portions of the spectra are shown in the upper traces of figures 1 (part of the P branch region) and 2 (covering the  $K'_a = 3, 4$  and  $5$  Q branches). The PGOPHER program [28] was used to assign and fit the spectra. The asymmetric top Hamiltonian used included Watson's standard A reduced form [31] for the centrifugal distortion. As in previous work on HCHO, we used the Ir representation, giving the  $K_a$  quantization along the  $a$  inertial axis (corresponding to the  $C_2$  axis of the molecule). Ground state rotational constants have been accurately determined in previous studies [32,33,34] and we used the most recent set of constants, reported by Muller *et al* [34] for this work. For calculating vibrationally excited states where perturbations are included (as described below), the Hamiltonian matrices are set up and diagonalised including all states of the required total angular momentum and symmetry. The basis was restricted to  $K'_a \leq 7$ ; this had little effect on the simulation and avoided problems with unphysical locations for the high  $K'_a$  states during the fitting process.

The spectrum is clearly dominated by a single band and, given the reliable ground state constants, assignment of most of the transitions with the aid of common differences was reasonably straightforward. [The assignments extended up to  \$J' \leq 20\$ ,  \$K'\_a = 5\$ . As can be seen from figure 2 the  \$K'\_a = 5\$  Q branch lines are strong and clear and thus the  \$K'\_a = 6\$  and  \$7\$  Q branches, while weaker because of Boltzmann factors \(and statistical weights for  \$K'\_a = 6\$ \), should be visible. No other Q branches can be found; the  \$K'\_a = 7\$  transitions may be shifted into the region at low frequency where there are](#)

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3 absorptions from other bands and the  $K'_a = 6$  is sufficiently weak to be easily obscured  
4 by much stronger  $P$  branch transitions. No  $P$  or  $R$  branch transitions could be assigned  
5 to  $K'_a > 5$  either. As extrapolations of positions from lower  $K'_a$  levels is likely to be poor  
6 as the constants derived below will only be appropriate for  $K'_a \leq 5$ .  
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11 The assignment clearly indicated several perturbations, with line shifts up to  
12  $2.5 \text{ cm}^{-1}$ . Fortunately, there is significant information on the other vibrational states at  
13 similar energies to allow us to identify the states responsible for the perturbations. The  
14 bulk of this information comes from dispersed fluorescence spectroscopy work via the  
15  $0_{00}$  rotational level of the zero point level,  $\nu_4$ ,  $\nu_5$ , and  $\nu_3+\nu_4$  vibrational states of the  $S_1$   
16 state of formaldehyde, with the measured states and band origins given in ref [29].  
17 Table 1 shows the available information on the states in the region of  $2\nu_5$  in the energy  
18 range of  $5540 \text{ cm}^{-1}$  to  $6100 \text{ cm}^{-1}$ . The table also includes estimates of the rotational  
19 constants for these states, generated from the standard expression for the vibrational  
20 dependence of rotational constants:  
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$$A = A_{eq} - \sum_i \alpha_i^A (\nu_i + 1/2) \quad (1)$$

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33 and analogous expressions for  $B$  and  $C$  rotational constants. The ground state rotational  
34 constants for our calculations have been taken from ref. [34], and their corresponding  
35 equilibrium values have been calculated using equation (1). The rovibrational  
36 interaction constants  $\alpha_i^A$ ,  $\alpha_i^B$  and  $\alpha_i^C$  have been taken from table III of ref [35],  
37 (previous experimentally determined values from a number of sources). The discussion  
38 in ref [35] indicates that the values for  $B$  and  $C$  calculated in this way are likely to be  
39 reliable, but also indicates a potential problem with values for  $A$ . There is a significant  $A$   
40 axis Coriolis interaction involving  $\nu_4$  and  $\nu_6$ , mixing clusters of states such as  $\nu_4+\nu_6$ ,  $2\nu_6$   
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3 and  $2\nu_4$  giving rise to anomalous effective values of  $A$  for such states. The matrix  
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5 elements are expected to be of the form (See equation 27 of ref [35]):  
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$$\langle v_4, v_6, J, K | H | v_4 + 1, v_6 - 1, J, K \rangle = \Xi K \sqrt{v_6(v_4 + 1)} \quad (2)$$

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9 and ref [26] suggests an average value for  $\Xi$  of  $8.354 \text{ cm}^{-1}$ .  
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12 Given these estimates for the rotational constants, origins and mutual  
13 interactions of the potential perturbing states, we used the PGOPHER program to calculate  
14 and plot energy level diagrams for each rovibronic symmetry to locate possible  
15 crossings. To take account of the  $A$  axis Coriolis interaction we explicitly included the  
16 perturbations between the appropriate states (according to equation (2) with the values  
17 tabulated in table 2), rather than use effective values for  $A$  for these states.  
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24 We show and discuss selected individual perturbations below, but the overall  
25 conclusion from these plots is that each observed perturbation in  $2\nu_5$  can be matched  
26 with a specific crossing with one of the other vibrational states. The crossings are  
27 predicted to within a few  $\text{cm}^{-1}$  which is consistent with the accuracy of the constants  
28 used for the predictions. It is also clear that almost all crossings lead to an observable  
29 perturbation, though with a significant variation in size. The published information thus  
30 provides a good starting point for a deperturbation, and we added perturbations between  
31 states as suggested by the symmetry of the states involved. (We did not attempt to  
32 determine the possible perturbations from considerations of the force field.) The  
33 perturbation operators are given in table 3.  
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### 47 ***B.1. The $K_a' = 1$ levels***

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3 As an example of the analysis process, consider the  $K_a' = 1$  levels. Because of  
4 the statistical weights, transitions to these odd  $K_a'$ -levels will be about 3-times stronger  
5 than transitions to even  $K_a'$ -levels and these give the strongest peaks in the spectrum.  
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7 The  $P$  and  $R$  branches show as a regular series of strong pairs of peaks and could be  
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9 unambiguously assigned up to  $J'=20$  though the  $Q$ -branches are weak due to large  $A/B$   
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11 ratio of formaldehyde [36].  
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15 The  $K_a' = 1$  levels are asymmetry doubled into two, which correspond to the  $O+$   
16 and  $O-$  Wang combinations. [These will also have different values of  \$K\_c\$ , such that](#)  
17  
18  [\$K\_a+K\_c = J\$  and  \$K\_a+K\_c = J+1\$  respectively.](#) For the purposes of this discussion it is  
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20 convenient to use  $O+$  and  $O-$  as symmetry labels as, for example, the  $O+$  matrix will  
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22 have a consistent form with  $J'$  though the overall rovibrational symmetry will alternate  
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24 between  $B_1$  and  $B_2$  for even and odd  $J'$ . Perturbing states must, of course, have the same  
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26 overall rovibronic symmetry which means that different Wang combinations must be  
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28 taken where the vibrational symmetry is different. Table 4 gives the correlation for our  
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30 choice of representation and symmetry axes.  
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34 Figure 3(b) shows the levels with the symmetry corresponding to  $O+$  for  $2\nu_5$ .  
35 The symbols (squares) indicate the observed energy levels, plotted by adding the  
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37 measured line positions to the ground state energy levels calculated using the constants  
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39 in ref [34]. The solid lines indicate levels calculated using our final constants. There is  
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41 one obvious perturbation, though careful examination indicates a second, much weaker  
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43 perturbation giving line shifts of only  $0.025 \text{ cm}^{-1}$ . The source of the perturbations is  
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45 easy to identify here; while the diagram indicates fitted positions our initial estimates  
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47 put the levels within  $2 \text{ cm}^{-1}$  of those plotted on the diagram. This shows that the strong  
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49 perturbation is caused by the crossing with the  $K_a' = 0$  level of the  $\nu_1+\nu_2+\nu_4$  state. Given  
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3 that the mixing corresponds to a change in  $K_a'$  of 1, and the mixing level has  $B_1$   
4 vibrational symmetry, this suggests the mixing operator should be  $J_b$ , and this is  
5 therefore included in our model (see Table 3), with a final fitted value of  $-0.2448 \text{ cm}^{-1}$ .  
6  
7 Similarly, the weak perturbation is due to the crossing with the  $K_a' = 0$  level of the  
8  
9  $3\nu_3 + \nu_4$  state at lower  $J'$ . As this has the same  $K_a'$  vibrational symmetry as  $\nu_1 + \nu_2 + \nu_4$  the  
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11 same operator ( $J_b$ ) is appropriate, though with a much smaller value ( $0.0108 \text{ cm}^{-1}$ ).  
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15 In O- symmetry, plotted in figure 3(c), there is only one significant perturbation,  
16 a large crossing with a component of the  $K_a' = 1$  level of the  $\nu_2 + \nu_3 + \nu_4 + \nu_6$  state. In this  
17 case the crossing happens at the limit of our assigned range of  $J'$ , but common  
18 differences and modelling of intensities indicate that we have the correct assignment. In  
19 this case the appropriate operator for mixing is  $i(J_b J_c + J_c J_b)$ . Note that the  $\nu_2 + \nu_3 + \nu_4 + \nu_6$   
20 state interacts strongly with the  $\nu_2 + \nu_3 + 2\nu_4$  and  $\nu_2 + \nu_3 + 2\nu_6$  states via the A axis Coriolis  
21 mixing discussed above, and hence to get this crossing right, we had to take into  
22 consideration the big interactions between these states, as shown in table 2. Figure 3(c)  
23 also indicates a crossing with  $\nu_1 + \nu_5$ , though in this case no perturbation is seen. There  
24 are two other nearby states ( $3\nu_3 + \nu_6$  and  $\nu_3 + \nu_5 + \nu_6$ ), and some interactions with these  
25 might well be expected though, as there is no crossing with these states in our range of  
26  $J'$ , there is no direct information available on such interactions.  
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## 43 **B.2. The $K_a' = 2$ levels**

44 While the statistical weights mean that these levels give weaker transitions, we  
45 were able to assign a similar range of  $J'$ . The E+ ( $K_a + K_c = J$ ) component has two major  
46 crossings – with the  $K_a' = 0$  level of the  $\nu_2 + \nu_3 + 2\nu_6$  state between  $J' = 12$  and 13, and  
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3 with the  $K_a' = 1$  level of the  $\nu_1+\nu_2+\nu_4$  state between  $J' = 19$  and 20, shown in figure 3(d).

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5 The E- ( $K_a+K_c = J+1$ ) component is not straightforward – as shown in figure 3(e) there  
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7 are crossings with two different perturbing states at nearly the same  $J'$ . The two  
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9 crossing levels are the  $K_a' = 1$  level of the  $\nu_1+\nu_2+\nu_4$  state and the  $K_a' = 1$  level of the  
10  
11  $3\nu_3+\nu_6$  state. This makes the levels difficult to assign around the crossing. Note that, as  
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13 mentioned above, a different component of the  $\nu_1+\nu_2+\nu_4$  level crosses the  $K_a' = 1$  O+  
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15 component, so 2 perturbation parameters were required to model the interaction to allow  
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17 for a different magnitude of the interaction at the two crossing points. The operator,  $J^2J_b$   
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19 essentially allows for a centrifugal distortion of the mixing.  
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### B.3. Overall fit

The same logic was applied to all our assigned transitions, adding perturbation parameters as necessary, and initially fitting each  $K_a'$  and symmetry independently to confirm the assignments. After completing the individual fits, we performed fits to all the available data simultaneously. Determining the constants for the perturbing states required a special procedure. For states with no direct crossings with  $2\nu_5$ , the constants were left at the values calculated as described above. Where there is a crossing it is clear that adjustments are necessary, given that the crossing points need shifts of  $1-2\text{ cm}^{-1}$ , and for best fit both the origin of the perturbing state and the rotational constants of the perturbing state need adjustment. Initially we allowed many parameters to float simultaneously, but constrained the parameters of the perturbing states by including the initial constants of these states as observations in the fit. In some cases, because of numerical instabilities in the fit the constraint value needed manual adjustment for best fit. When this process had converged we performed a slightly different procedure to give the final constants and uncertainties. We performed an individual fit for each state in turn, including all the experimental data but with the constants of the particular perturbing state and its perturbation parameters floated, but all other parameters held fixed. This resulted in only minor adjustments to the constants, and the results of these individual fits are given in tables 1 and 3. The final constants for  $2\nu_5$ , given in table 5 were determined similarly, from a fit to all data but with just the  $2\nu_5$  constants floated. The number of figures quoted in the uncertainties in these tables is determined by calculating the parameter sensitivity as described by Watson [37]. This takes account of possible correlations between the parameters, so that the values truncated to the figures

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3 quoted in the tables reproduce the final fit to well within the experimental error. A  
4 detailed line list is included as supplementary data, including observed – calculated  
5 values. Simulations of small sections of the observed spectrum are given in figures 1  
6 and 2 (lower traces). The (observed – calculated) values from this fit for all the  
7 observations are plotted in figure 4. The horizontal axis for this plot is simply  
8 observation number, but the observations have been grouped by symmetry and then  
9 sorted by  $J'$ . This serves to show that, even though the overall fit is good, with an  
10 average error of only  $0.013 \text{ cm}^{-1}$ , there are still some systematic trends to the remaining  
11 residuals. The origin of these can be seen by considering the plot of the  $K_a' = 0$  levels in  
12 figure 3(a). This shows that there are no observed crossings with this component, and  
13 indeed none are predicted. However there are some nearby states, and the perturbation  
14 parameters we have added to model crossings elsewhere are large enough to shift the  
15  $K_a' = 0$  levels. The size of these shifts is indicated by the dotted line on the figure which  
16 indicates the calculated position if all the perturbations (tables 2 and 3) are set to zero.  
17 (The interaction with the  $K_a' = 2$  level of the  $\nu_2+\nu_3+\nu_4+\nu_6$  state is giving half this shift;  
18 there is no direct interaction with  $\nu_2+\nu_3+2\nu_4$ , so the remaining shift is from a  
19 combination of other states.) In practice these shifts will not be modelled exactly, as we  
20 only have approximate values for the constants of the perturbing levels. The effect of  
21 these shifts will thus be partly absorbed into the many centrifugal distortion constants  
22 we have allowed to float for  $2\nu_5$ , but this will not give exactly the right functional  
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#### B.4. Intensities

Comparison of the intensities from the final simulation with experiment indicates that our model gives a reasonable qualitative description of the intensities (see for example figures 1 and 2), but by no means quantitative. This is as expected for a model using only a single dipole moment for the band; more detailed modelling of the intensity of lower energy transitions in HCHO [23] required  $J$  dependent operators in the transition moment, and contributions from several bands for a satisfactory intensity model. Our intensity model included only a constant  $a$  component of the transition dipole component to the  $2\nu_5$  state and assumed zero intensity to all the other states in the model.

Within the limitations of this model, we can reassess the value for the overall strength of the band. In the paper describing the experimental spectrum [24] the integrated intensity of one specific line,  $^oR_{1,10}(10)$  at  $5676.21 \text{ cm}^{-1}$  was accurately determined to be  $5.7 \pm 0.6 \times 10^{-22} \text{ cm}^2\text{cm}^{-1}$ . The present analysis confirms that this transition is relatively unperturbed; the perturbation shifts the transition down by only  $0.15 \text{ cm}^{-1}$  and decreases the intensity by 1.5%. The integrated intensity of the band can be estimated from this single measurement, given the partition function and the line strength factors, and both are available from our model. (The vibrational contribution can be ignored at the current level of accuracy.) This gives a total intensity of  $9.6 \times 10^{-20} \text{ cm}^2\text{cm}^{-1}$  ( $0.58 \text{ km mole}^{-1}$ ), corresponding to a transition moment of  $0.00640 \text{ Debye}$  for the vibrational transition. This is consistent with the values of  $0.53$  or  $0.84 \text{ km mole}^{-1}$  estimated in the previous work. The line list includes intensities calculated with these values.

## C. Conclusion

We have succeeded in assigning and modelling all the strong transitions associated with the  $2\nu_5$  band of formaldehyde up to  $J' \sim 20$ ,  $K_a' = 5$ . All the states in the region of this  $2\nu_5$  state have been included in our model, and the constants from previous work, though rather less precise than our experimental accuracy, allowed us to identify the perturbing states unambiguously, and gave a good starting point for the deperturbation. The results show that almost all the states that cross the  $2\nu_5$  state show a perturbation at our level of accuracy, so it is clear that an approach considering all the levels in the region is essential. Improving our model could only be done with more precise information about these other states.

## Acknowledgement

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**Table 1:** States perturbing the  $2\nu_5$  state, with their symmetry, initial and fitted origin and rotational constants.

State	Symmetry	Origin/cm <sup>-1</sup> Ref [28]	Origin/cm <sup>-1</sup> (Fitted)	A /cm <sup>-1</sup> (Calc.)	A /cm <sup>-1</sup> (Fitted)	B /cm <sup>-1</sup> (Calc.)	B /cm <sup>-1</sup> (Fitted)	C /cm <sup>-1</sup> (Calc.)	C /cm <sup>-1</sup> (Fitted)
$\nu_3+\nu_4+\nu_5^*$	A <sub>2</sub>	5489.0		9.2894		1.2901		1.1295	
$\nu_2+3\nu_6^*$	B <sub>2</sub>	5492.2		9.4000		1.2961		1.1053	
$\nu_1+\nu_5^*$	B <sub>2</sub>	5530.5		9.0721		1.2950		1.1282	
$\nu_2+\nu_3+2\nu_4$	A <sub>1</sub>	5546.5		9.4616		1.2712		1.1261	
$\nu_3+\nu_5+\nu_6^*$	A <sub>1</sub>	5551.3		9.2894		1.3061		1.1213	
$\nu_2+\nu_3+\nu_4+\nu_6$	A <sub>2</sub>	5625.5	5623.02(12)	9.4616	9.217(17)	1.2872	1.29064(47)	1.1179	1.12678(71)
$3\nu_3+\nu_4$	B <sub>1</sub>	5659.4	5660.759(48)	9.5903		1.3115		1.1288	
$3\nu_3+\nu_6$	B <sub>2</sub>	5666.6	5665.640(39)	9.5903	9.790(57)	1.3275	1.33674(82)	1.1206	1.1295(11)
$\nu_1+\nu_2+\nu_4$	B <sub>1</sub>	5680.0	5680.963(27)	9.2443	9.239(13)	1.2761	1.27485(24)	1.1248	1.12433(15)
$\nu_2+\nu_3+2\nu_6$	A <sub>1</sub>	5687.9	5685.636(94)	9.4616	9.462(13)	1.3032	1.3029(13)	1.1097	1.13767(54)
$\nu_2+\nu_4+\nu_5$	A <sub>2</sub>	5717.7	5718.77(12)	9.2223	9.39(12)	1.2729	1.26936(60)	1.1230	1.10211(82)
$\nu_1+2\nu_3$	A <sub>1</sub>	5729.2	5735.35(35)	9.3730	9.374(14)	1.3164	1.3082(15)	1.1275	1.0997(12)
$\nu_1+\nu_2+\nu_6$	B <sub>2</sub>	5765.2	5766.47(30)	9.2443	9.244(14)	1.2921	1.2851(33)	1.1166	1.1107(29)
$2\nu_2+2\nu_4^*$	A <sub>1</sub>	5768.8		9.3945		1.2540		1.1196	
$5\nu_4^*$	B <sub>1</sub>	5771.0		9.4055		1.2289		1.1417	
$\nu_2+\nu_5+\nu_6^*$	A <sub>1</sub>	5809.5		9.2223		1.2889		1.1148	
$2\nu_3+\nu_5^*$	B <sub>2</sub>	5822.0		9.3510		1.3132		1.1257	

$v_2+2v_3+v_4^*$	B <sub>1</sub>	5887.2		9.5232		1.2943		1.1222	
$2v_2+v_4+v_6^*$	A <sub>2</sub>	5887.5		9.3945		1.2700		1.1114	
$4v_4+v_6^*$	B <sub>2</sub>	5891.8		9.4055		1.2449		1.1335	
$v_2+2v_3+v_6^*$	B <sub>2</sub>	5936.1		9.5232		1.3103		1.1141	
$2v_2+2v_6^*$	A <sub>1</sub>	5986.2		9.3945		1.2860		1.1032	
$4v_3^*$	A <sub>1</sub>	5988.6		9.6519		1.3346		1.1250	
$v_1+v_2+v_3^*$	A <sub>1</sub>	5996.0		9.3059		1.2992		1.1210	
$3v_4+2v_6^*$	B <sub>1</sub>	6000.5		9.4055		1.2609		1.1253	
$v_2+v_3+v_5^*$	B <sub>2</sub>	6051.7		9.2839		1.2960		1.1192	
$2v_4+3v_6^*$	B <sub>2</sub>	6098.0		9.4055		1.2769		1.1171	

\* The final model has no direct or indirect coupling between these states and  $2v_5$

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**Table 2:** Perturbation constants for the states having significant interaction among themselves. The operator multiplying each of these is  $J_a$

Perturbing state	Perturbing state	$\Xi\sqrt{v_6(v_4+1)} / \text{cm}^{-1}$
$v_2+v_3+v_4+v_6$	$v_2+v_3+2v_4$	11.814
$v_2+v_3+2v_6$	$v_2+v_3+v_4+v_6$	11.814
$v_3+v_5+v_6$	$v_3+v_4+v_5$	8.354
$3v_3+v_6$	$3v_3+v_4$	8.354
$v_1+v_2+v_6$	$v_1+v_2+v_4$	8.354
$v_2+v_5+v_6$	$v_2+v_4+v_5$	8.354
$2v_2+v_4+v_6$	$2v_2+2v_4$	11.814
$2v_2+2v_6$	$2v_2+v_4+v_6$	11.814
$4v_4+v_6$	$5v_4$	18.680
$3v_4+2v_6$	$4v_4+v_6$	23.629
$2v_4+3v_6$	$3v_4+2v_6$	25.062
$v_2+2v_3+v_6$	$v_2+2v_3+v_4$	8.354

**Table 3:** Perturbation constants for the states interacting with the  $2\nu_5$  state

Perturbing state	Operator <sup>a</sup>	Perturbation constant / $\text{cm}^{-1}$
$\nu_2+\nu_3+\nu_4+\nu_6$	$i(J_b J_c + J_c J_b)$	0.014930(47)
$3\nu_3+\nu_4$	$J_b$	-0.02150(95)
$3\nu_3+\nu_6$	$iJ_c$	-0.13336(80)
$\nu_1+\nu_2+\nu_4$	$J_b$	-0.2448(11)
$\nu_1+\nu_2+\nu_4$	$J^2 J_b$	$1.232(46)\times 10^{-4}$
$\nu_2+\nu_3+2\nu_6$	$J_+^2 + J_-^2$	$3.009(20)\times 10^{-3}$
$\nu_2+\nu_4+\nu_5$	$i(J_b J_c + J_c J_b)$	0.012057(71)
$\nu_1+\nu_2+\nu_6$	$[J_a, J_+^3 + J_-^3]_+$	$3.33(15)\times 10^{-5}$
$\nu_1+2\nu_3$	$J_+^2 + J_-^2$	$5.557(36)\times 10^{-3}$

<sup>a</sup>  $J_{\pm} = J_b \pm iJ_c$ ; the phases of the wavefunctions are chosen such that the matrix elements of  $J_a$  and  $J_{\pm}$  are real and positive.

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**Table 4:** Correlation between Wang basis and rovibrational symmetry for each vibrational symmetry. The columns correspond to different vibrational symmetries, and the rows to different rovibrational symmetries.

Rovibrational Symmetry		Vibrational Symmetry			
Even $J$	Odd $J$	$A_1$	$A_2$	$B_1$	$B_2$
$A_1$	$A_2$	$E+ \quad Ka+Kc = J$	$E- \quad Ka+Kc = J+1$	$O+ \quad Ka+Kc = J$	$O- \quad Ka+Kc = J+1$
$A_2$	$A_1$	$E- \quad Ka+Kc = J+1$	$E+ \quad Ka+Kc = J$	$O- \quad Ka+Kc = J+1$	$O+ \quad Ka+Kc = J$
$B_1$	$B_2$	$O+ \quad Ka+Kc = J$	$O- \quad Ka+Kc = J+1$	$E+ \quad Ka+Kc = J$	$E- \quad Ka+Kc = J+1$
$B_2$	$B_1$	$O- \quad Ka+Kc = J+1$	$O+ \quad Ka+Kc = J$	$E- \quad Ka+Kc = J+1$	$E+ \quad Ka+Kc = J$

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**Table 5:** Fitted constants for the  $2\nu_5$  state

Constants	Values / $\text{cm}^{-1}$
Origin	5651.1904(29)
$A$	9.48110(205)
$B$	1.295856(74)
$C$	1.128606(65)
$\Delta_K$	0.0310516(3954)
$\Delta_{JK}$	$7.7822(857)\times 10^{-4}$
$\Delta_J$	$5.70(11)\times 10^{-6}$
$\delta_K$	$5.33(12)\times 10^{-4}$
$\delta_J$	$1.063(96)\times 10^{-6}$
$\Phi_K$	$1.46223(2644)\times 10^{-3}$
$\Phi_{KJ}$	$6.1465(958)\times 10^{-5}$
$L_K$	$-2.6465(553)\times 10^{-5}$
$L_{KKJ}$	$-1.6308(253)\times 10^{-6}$
$L_{JK}$	$4.69(64)\times 10^{-9}$

## Captions

**Figure 1.** Portion of the  $P$ -branch region of the observed spectrum, shown along with the simulation as the lower trace.

**Figure 2.** Portion of the  $Q$ -branch region of the observed spectra, covering the  $K_a' = 2, 3, 4$  and  $5$  levels of the  $2\nu_5$  band. The branches are indicated on the spectrum, though note that some other transitions also occur in this region.

**Figure 3.** Energy level diagrams for selected regions of the  $2\nu_5$  state. For clarity,  $1.2J(J+1)$  has been subtracted from all the energy levels, and each plot includes one rovibronic symmetry only. Calculated energy levels are shown as solid lines and observed energy levels (calculated from the observed line positions by adding the lower state energy) are shown as symbols. The regions covered are (a)  $K_a'=0$  (E+), (b)  $K_a'=1$  (O+,  $K_a+K_c=J$ ), (c)  $K_a'=1$  (O-,  $K_a+K_c=J+1$ ), (d)  $K_a'=2$  (E+,  $K_a+K_c=J$ ) and (e)  $K_a'=2$  (E-,  $K_a+K_c=J+1$ ). This dashed line in (a) is the calculated  $2\nu_5$   $K_a'=0$  component in the absence of perturbations.

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**Figure 4.** The (Observed-Calculated) positions for the points we have successfully assigned have been plotted against the observation number. The observations have been grouped by  $K_a'$  and symmetry and plotted in order of increasing  $J'$  values within each group.

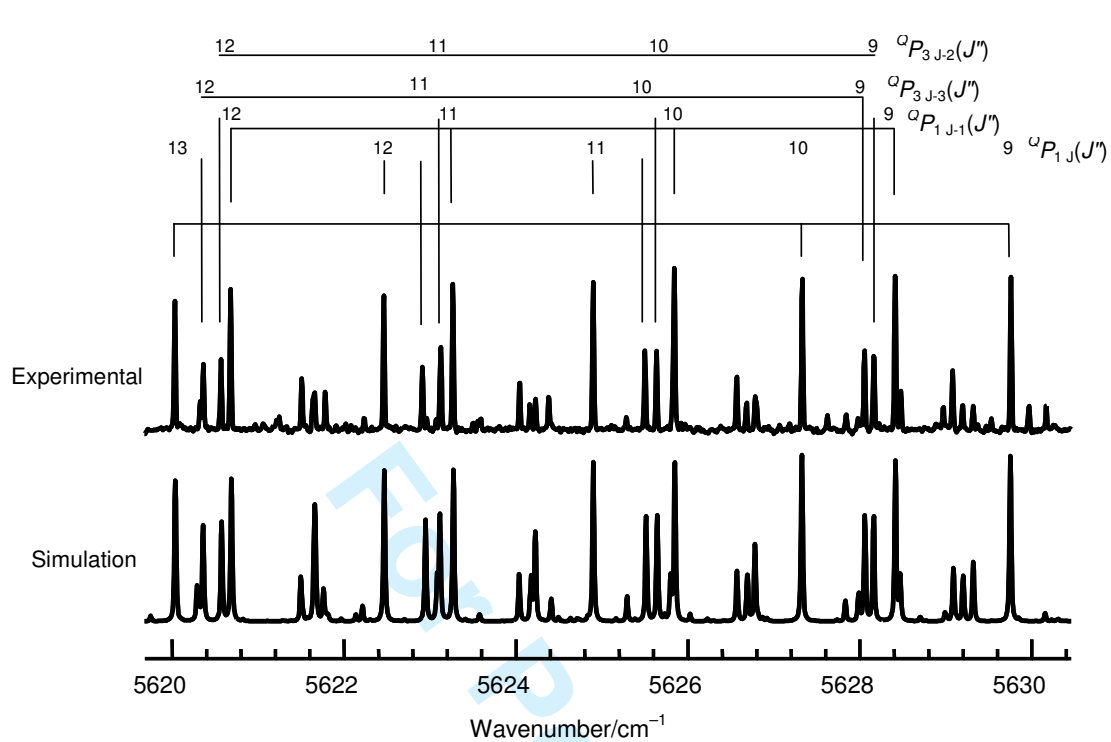


Figure 1.

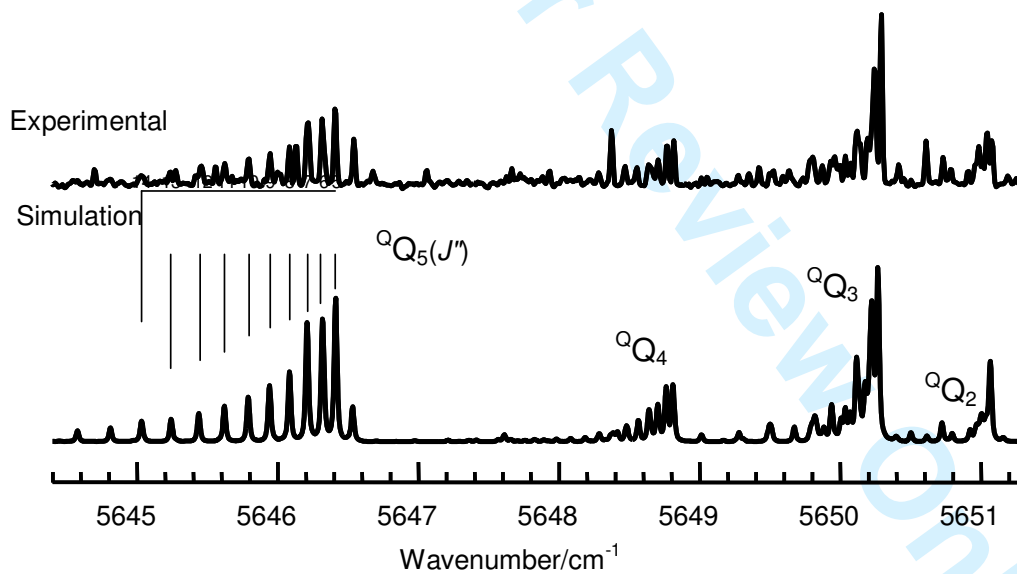


Figure 2.



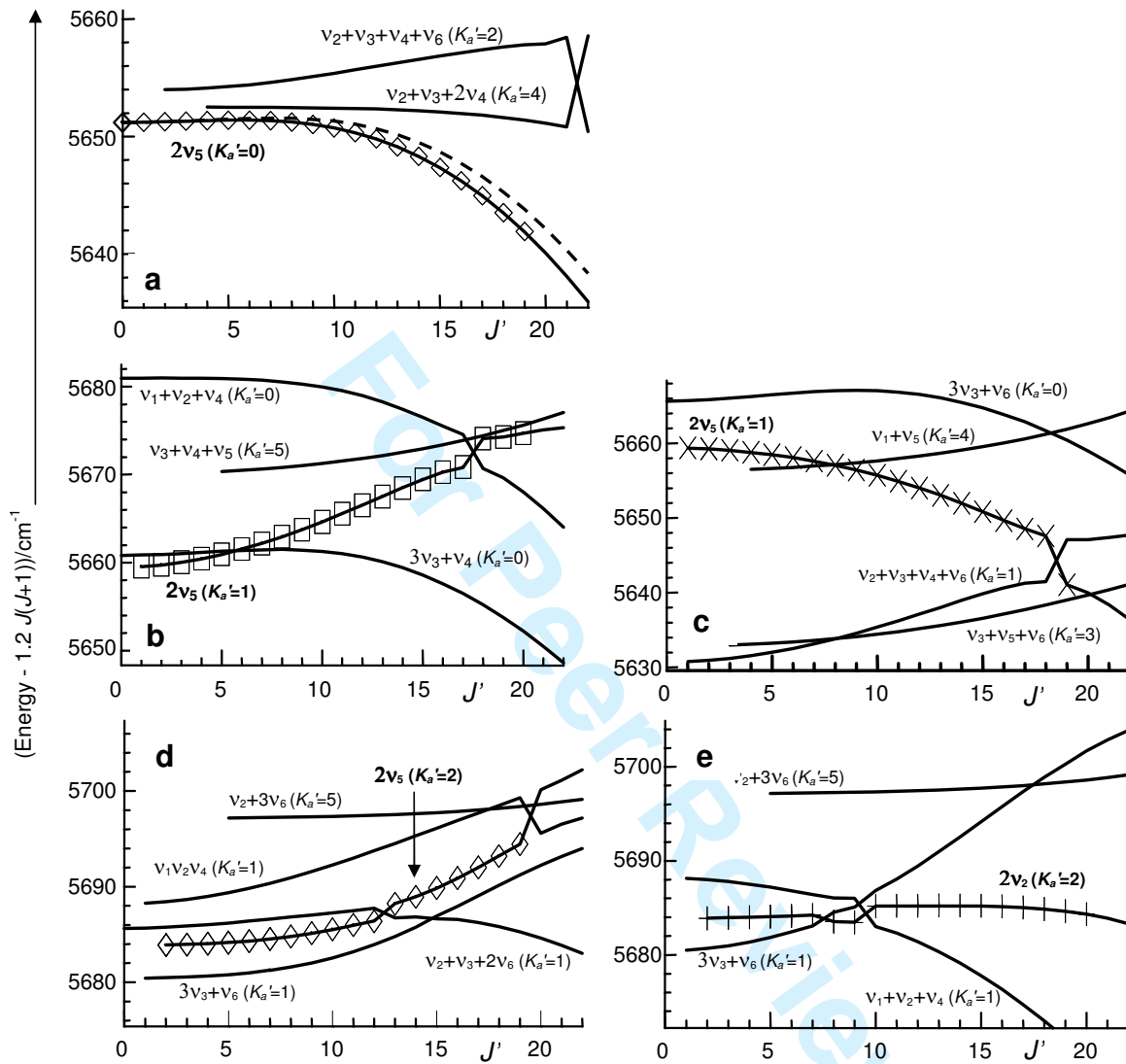


Figure 3

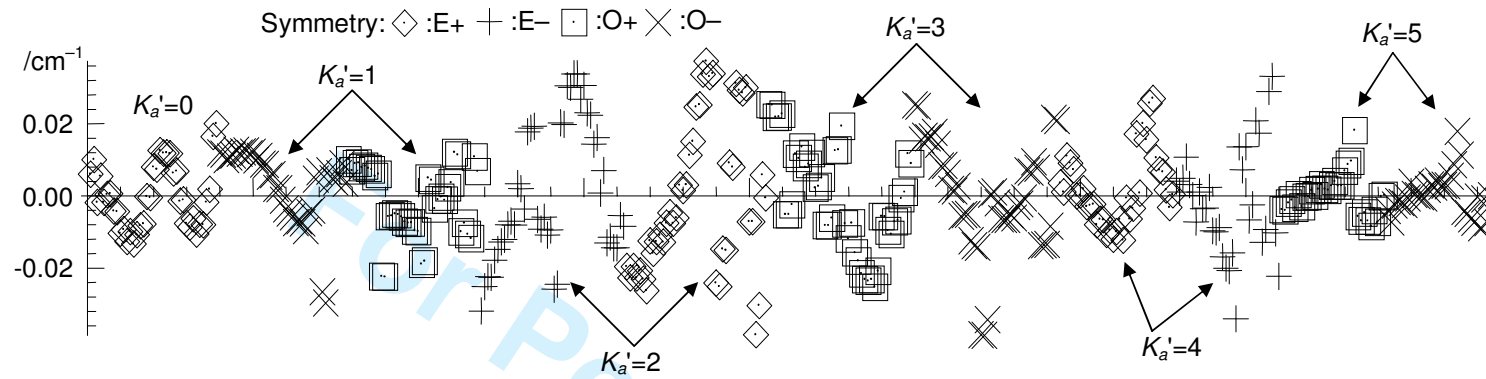


Figure 4.

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	J' S' #'	J" S" #"	Observed	Calculated	Obs-Calc	Weight	Intensity	Ka"Kc" J"	J' Ka'Kc'	J" Ka"Kc"
1										
2										
3	0 E+ 3	1 E+ 1	5648.7668	5648.7608	0.0060	1.0000	3.4025E-23	: qP 0 1( 1) : U v5=2	0 0 0 - X v=0	1 0 1
4	1 E+ 5	0 E+ 1	5653.6222	5653.6121	0.0101	1.0000	3.4457E-23	: qR 0 0( 0) : U v5=2	1 0 1 - X v=0	0 0 0
5	1 E+ 5	2 E+ 1	5646.3239	5646.3257	-0.0018	1.0000	6.6410E-23	: qP 0 2( 2) : U v5=2	1 0 1 - X v=0	2 0 2
6	2 E+ 8	1 E+ 1	5656.0278	5656.0224	0.0054	1.0000	6.8082E-23	: qR 0 1( 1) : U v5=2	2 0 2 - X v=0	1 0 1
7	2 E+ 8	3 E+ 1	5643.8847	5643.8865	-0.0018	1.0000	9.6016E-23	: qP 0 3( 3) : U v5=2	2 0 2 - X v=0	3 0 3
8	3 E+ 10	4 E+ 1	5641.4435	5641.4431	0.0004	1.0000	1.2179E-22	: qP 0 4( 4) : U v5=2	3 0 3 - X v=0	4 0 4
9	3 E+ 10	2 E+ 1	5658.4170	5658.4164	0.0006	1.0000	9.9566E-23	: qR 0 2( 2) : U v5=2	3 0 3 - X v=0	2 0 2
10	4 E+ 11	5 E+ 1	5638.9903	5638.9946	-0.0043	1.0000	1.4277E-22	: qP 0 5( 5) : U v5=2	4 0 4 - X v=0	5 0 5
11	4 E+ 11	3 E+ 1	5660.7839	5660.7883	-0.0044	1.0000	1.2759E-22	: qR 0 3( 3) : U v5=2	4 0 4 - X v=0	3 0 3
12	5 E+ 11	6 E+ 1	5636.5280	5636.5384	-0.0104	1.0000	1.5813E-22	: qP 0 6( 6) : U v5=2	5 0 5 - X v=0	6 0 6
13	5 E+ 11	4 E+ 1	5663.1217	5663.1311	-0.0094	1.0000	1.5083E-22	: qR 0 4( 4) : U v5=2	5 0 5 - X v=0	4 0 4
14	6 E+ 11	7 E+ 1	5634.0583	5634.0711	-0.0128	1.0000	1.6712E-22	: qP 0 7( 7) : U v5=2	6 0 6 - X v=0	7 0 7
15	6 E+ 11	5 E+ 1	5665.4270	5665.4370	-0.0100	1.0000	1.6797E-22	: qR 0 5( 5) : U v5=2	6 0 6 - X v=0	5 0 5
16	7 E+ 11	8 E+ 1	5631.5748	5631.5882	-0.0134	1.0000	1.6932E-22	: qP 0 8( 8) : U v5=2	7 0 7 - X v=0	8 0 8
17	7 E+ 11	6 E+ 1	5667.6871	5667.6980	-0.0109	1.0000	1.7795E-22	: qR 0 6( 6) : U v5=2	7 0 7 - X v=0	6 0 6
18	8 E+ 11	9 E+ 1	5629.0786	5629.0870	-0.0084	1.0000	1.6528E-22	: qP 0 9( 9) : U v5=2	8 0 8 - X v=0	9 0 9
19	8 E+ 11	7 E+ 1	5669.9003	5669.9082	-0.0079	1.0000	1.8071E-22	: qR 0 7( 7) : U v5=2	8 0 8 - X v=0	7 0 7
20	9 E+ 11	10 E+ 1	5626.5677	5626.5680	-0.0003	1.0000	1.5692E-22	: qP 0 10(10) : U v5=2	9 0 9 - X v=0	10 0 10
21	9 E+ 11	8 E+ 1	5672.0662	5672.0668	-0.0006	1.0000	1.7788E-22	: qR 0 8( 8) : U v5=2	9 0 9 - X v=0	8 0 8
22	10 E+ 11	9 E+ 1	5674.1860	5674.1781	0.0079	1.0000	1.7182E-22	: qR 0 9( 9) : U v5=2	10 0 10 - X v=0	9 0 9
23	10 E+ 11	11 E+ 1	5624.0433	5624.0361	0.0072	1.0000	1.4659E-22	: qP 0 11(11) : U v5=2	10 0 10 - X v=0	11 0 11
24	11 E+ 11	10 E+ 1	5676.2619	5676.2495	0.0124	1.0000	1.6424E-22	: qR 0 10(10) : U v5=2	11 0 11 - X v=0	10 0 10
25	11 E+ 11	12 E+ 1	5621.5088	5621.4971	0.0117	1.0000	1.3577E-22	: qP 0 12(12) : U v5=2	11 0 11 - X v=0	12 0 12
26	12 E+ 11	11 E+ 1	5678.2996	5678.2879	0.0117	1.0000	1.5577E-22	: qR 0 11(11) : U v5=2	12 0 12 - X v=0	11 0 11
27	12 E+ 11	13 E+ 1	5618.9672	5618.9557	0.0115	1.0000	1.2494E-22	: qP 0 13(13) : U v5=2	12 0 12 - X v=0	13 0 13
28	13 E+ 11	12 E+ 1	5680.3051	5680.2989	0.0062	1.0000	1.4647E-22	: qR 0 12(12) : U v5=2	13 0 13 - X v=0	12 0 12
29	13 E+ 11	14 E+ 1	5616.4201	5616.4134	0.0067	1.0000	1.1412E-22	: qP 0 14(14) : U v5=2	13 0 13 - X v=0	14 0 14
30	14 E+ 11	13 E+ 1	5682.2850	5682.2867	-0.0017	1.0000	1.3628E-22	: qR 0 13(13) : U v5=2	14 0 14 - X v=0	13 0 13
31	14 E+ 11	15 E+ 1	5613.8684	5613.8697	-0.0013	1.0000	1.0324E-22	: qP 0 15(15) : U v5=2	14 0 14 - X v=0	15 0 15
32	15 E+ 11	14 E+ 1	5684.2456	5684.2534	-0.0078	1.0000	1.2524E-22	: qR 0 14(14) : U v5=2	15 0 15 - X v=0	14 0 14
33	15 E+ 11	16 E+ 1	5611.3133	5611.3221	-0.0088	1.0000	9.2319E-23	: qP 0 16(16) : U v5=2	15 0 15 - X v=0	16 0 16
34	16 E+ 11	17 E+ 1	5608.7608	5608.7673	-0.0065	1.0000	8.1470E-23	: qP 0 17(17) : U v5=2	16 0 16 - X v=0	17 0 17
35	16 E+ 11	15 E+ 1	5686.1899	5686.2006	-0.0107	1.0000	1.1353E-22	: qR 0 15(15) : U v5=2	16 0 16 - X v=0	15 0 15
36	17 E+ 11	18 E+ 1	5606.1937	5606.2018	-0.0081	1.0000	7.0895E-23	: qP 0 18(18) : U v5=2	17 0 17 - X v=0	18 0 18
37	17 E+ 11	16 E+ 1	5688.1206	5688.1288	-0.0082	1.0000	1.0143E-22	: qR 0 16(16) : U v5=2	17 0 17 - X v=0	16 0 16
38	18 E+ 11	19 E+ 1	5603.6202	5603.6221	-0.0019	1.0000	6.0805E-23	: qP 0 19(19) : U v5=2	18 0 18 - X v=0	19 0 19
39	18 E+ 11	17 E+ 1	5690.0395	5690.0378	0.0017	1.0000	8.9281E-23	: qR 0 17(17) : U v5=2	18 0 18 - X v=0	17 0 17
40	19 E+ 11	20 E+ 1	5601.0419	5601.0256	0.0163	1.0000	5.1397E-23	: qP 0 20(20) : U v5=2	19 0 19 - X v=0	20 0 20
41	19 E+ 11	18 E+ 1	5691.9472	5691.9274	0.0198	1.0000	7.7424E-23	: qR 0 18(18) : U v5=2	19 0 19 - X v=0	18 0 18
42	2 0- 9	3 0- 1	5644.1707	5644.1587	0.0120	1.0000	2.4647E-22	: qP 1 3( 3) : U v5=2	2 1 2 - X v=0	3 1 3
43	2 0- 9	1 0- 1	5655.9135	5655.9019	0.0116	1.0000	1.4715E-22	: qR 1 1( 1) : U v5=2	2 1 2 - X v=0	1 1 1
44	2 0- 9	2 0+ 1	5650.7308	5650.7207	0.0101	1.0000	7.9630E-23	: qQ 1 1( 2) : U v5=2	2 1 2 - X v=0	2 1 1
45	1 0- 7	2 0- 1	5646.5411	5646.5304	0.0107	1.0000	1.4369E-22	: qP 1 2( 2) : U v5=2	1 1 1 - X v=0	2 1 2
46	1 0- 7	1 0+ 1	5651.0785	5651.0672	0.0113	1.0000	1.4703E-22	: qQ 1 0( 1) : U v5=2	1 1 1 - X v=0	1 1 0
47	3 0- 12	4 0- 1	5641.7899	5641.7773	0.0126	1.0000	3.3051E-22	: qP 1 4( 4) : U v5=2	3 1 3 - X v=0	4 1 4
	3 0- 12	2 0- 1	5658.2251	5658.2133	0.0118	1.0000	2.5546E-22	: qR 1 2( 2) : U v5=2	3 1 3 - X v=0	2 1 2
	4 0- 14	5 0- 1	5639.3991	5639.3869	0.0122	1.0000	3.9875E-22	: qP 1 5( 5) : U v5=2	4 1 4 - X v=0	5 1 5
	4 0- 14	3 0- 1	5660.5238	5660.5113	0.0125	1.0000	3.4676E-22	: qR 1 3( 3) : U v5=2	4 1 4 - X v=0	3 1 3
	5 0- 14	6 0- 1	5637.0000	5636.9883	0.0117	1.0000	4.5151E-22	: qP 1 6( 6) : U v5=2	5 1 5 - X v=0	6 1 6
	5 0- 14	4 0- 1	5662.8079	5662.7958	0.0121	1.0000	4.2349E-22	: qR 1 4( 4) : U v5=2	5 1 5 - X v=0	4 1 4
	6 0- 14	7 0- 1	5634.5923	5634.5824	0.0099	1.0000	4.8887E-22	: qP 1 7( 7) : U v5=2	6 1 6 - X v=0	7 1 7







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18 E- 15	17 E- 1	5692.4860	5692.4978	-0.0118	1.0000	8.0845E-23	: qR 2 16(17)	: U v5=2	18	2 17 - X v=0	17	2 16
19 E- 15	20 E- 1	5600.8678	5600.8826	-0.0148	1.0000	4.4871E-23	: qP 2 19(20)	: U v5=2	19	2 18 - X v=0	20	2 19
19 E- 15	18 E- 1	5694.5458	5694.5606	-0.0148	1.0000	6.8513E-23	: qR 2 17(18)	: U v5=2	19	2 18 - X v=0	18	2 17
20 E- 15	19 E- 1	5696.5698	5696.5756	-0.0058	1.0000	5.6638E-23	: qR 2 18(19)	: U v5=2	20	2 19 - X v=0	19	2 18
20 E- 15	21 E- 1	5598.1982	5598.2070	-0.0088	1.0000	3.6125E-23	: qP 2 20(21)	: U v5=2	20	2 19 - X v=0	21	2 20
2 E+ 12	3 E+ 2	5643.7493	5643.7689	-0.0196	1.0000	4.5284E-23	: qQ 2 1( 3)	: U v5=2	2	2 0 - X v=0	3	2 1
2 E+ 12	2 E- 1	5651.0456	5651.0683	-0.0227	1.0000	9.3979E-23	: qQ 2 1( 2)	: U v5=2	2	2 0 - X v=0	2	2 1
2 E+ 12	3 E+ 2	5643.7493	5643.7689	-0.0196	1.0000	4.5284E-23	: qP 2 1( 3)	: U v5=2	2	2 0 - X v=0	3	2 1
2 E+ 12	2 E- 1	5651.0456	5651.0683	-0.0227	1.0000	9.3979E-23	: qQ 2 1( 2)	: U v5=2	2	2 0 - X v=0	2	2 1
3 E+ 14	3 E- 1	5651.0127	5651.0334	-0.0207	1.0000	6.3070E-23	: qQ 2 2( 3)	: U v5=2	3	2 1 - X v=0	3	2 2
3 E+ 14	4 E+ 2	5641.2602	5641.2832	-0.0230	1.0000	7.7196E-23	: qP 2 2( 4)	: U v5=2	3	2 1 - X v=0	4	2 2
3 E+ 14	2 E+ 2	5658.2924	5658.3186	-0.0262	1.0000	4.6761E-23	: qR 2 0( 2)	: U v5=2	3	2 1 - X v=0	2	2 0
4 E+ 16	4 E- 1	5650.9854	5650.9978	-0.0124	1.0000	4.6000E-23	: qQ 2 3( 4)	: U v5=2	4	2 2 - X v=0	4	2 3
4 E+ 16	5 E+ 2	5638.7592	5638.7750	-0.0158	1.0000	1.0095E-22	: qP 2 3( 5)	: U v5=2	4	2 2 - X v=0	5	2 3
4 E+ 16	3 E+ 2	5660.6880	5660.7006	-0.0126	1.0000	8.0607E-23	: qR 2 1( 3)	: U v5=2	4	2 2 - X v=0	3	2 1
5 E+ 16	6 E+ 2	5636.2312	5636.2419	-0.0107	1.0000	1.1812E-22	: qP 2 4( 6)	: U v5=2	5	2 3 - X v=0	6	2 4
5 E+ 16	4 E+ 2	5663.0619	5663.0745	-0.0126	1.0000	1.0661E-22	: qR 2 2( 4)	: U v5=2	5	2 3 - X v=0	4	2 2
5 E+ 16	5 E- 1	5650.9628	5650.9701	-0.0073	1.0000	3.4941E-23	: qQ 2 4( 5)	: U v5=2	5	2 3 - X v=0	5	2 4
6 E+ 16	7 E+ 2	5633.6770	5633.6813	-0.0043	1.0000	1.2938E-22	: qP 2 5( 7)	: U v5=2	6	2 4 - X v=0	7	2 5
6 E+ 16	5 E+ 2	5665.4338	5665.4411	-0.0073	1.0000	1.2616E-22	: qR 2 3( 5)	: U v5=2	6	2 4 - X v=0	5	2 3
6 E+ 16	6 E- 1	5650.9552	5650.9610	-0.0058	1.0000	2.7102E-23	: qQ 2 5( 6)	: U v5=2	6	2 4 - X v=0	6	2 5
7 E+ 16	8 E+ 2	5631.0936	5631.0902	0.0034	1.0000	1.3518E-22	: qP 2 6( 8)	: U v5=2	7	2 5 - X v=0	8	2 6
7 E+ 16	6 E+ 2	5667.8019	5667.7999	0.0020	1.0000	1.3967E-22	: qR 2 4( 6)	: U v5=2	7	2 5 - X v=0	6	2 4
7 E+ 16	7 E- 1	5650.9854	5650.9819	0.0035	1.0000	2.1220E-23	: qQ 2 6( 7)	: U v5=2	7	2 5 - X v=0	7	2 6
8 E+ 16	9 E+ 2	5628.4765	5628.4647	0.0118	1.0000	1.3588E-22	: qP 2 7( 9)	: U v5=2	8	2 6 - X v=0	9	2 7
8 E+ 16	7 E+ 2	5670.1646	5670.1489	0.0157	1.0000	1.4728E-22	: qR 2 5( 7)	: U v5=2	8	2 6 - X v=0	7	2 5
9 E+ 16	8 E+ 2	5672.5083	5672.4829	0.0254	1.0000	1.4882E-22	: qR 2 6( 8)	: U v5=2	9	2 7 - X v=0	8	2 6
9 E+ 16	10 E+ 2	5625.8249	5625.7989	0.0260	1.0000	1.3165E-22	: qP 2 8(10)	: U v5=2	9	2 7 - X v=0	10	2 8
10 E+ 16	9 E+ 2	5674.8251	5674.7904	0.0347	1.0000	1.4343E-22	: qR 2 7( 9)	: U v5=2	10	2 8 - X v=0	9	2 7
10 E+ 16	11 E+ 2	5623.1205	5623.0822	0.0383	1.0000	1.2212E-22	: qP 2 9(11)	: U v5=2	10	2 8 - X v=0	11	2 9
11 E+ 16	12 E+ 2	5620.3236	5620.2895	0.0341	1.0000	1.0540E-22	: qP 2 10(12)	: U v5=2	11	2 9 - X v=0	12	2 10
11 E+ 16	10 E+ 2	5677.0790	5677.0440	0.0350	1.0000	1.2830E-22	: qR 2 8(10)	: U v5=2	11	2 9 - X v=0	10	2 8
12 E+ 16	11 E+ 2	5679.1526	5679.1756	-0.0230	1.0000	9.7502E-23	: qR 2 9(11)	: U v5=2	12	2 10 - X v=0	11	2 9
12 E+ 16	13 E+ 2	5617.3324	5617.3565	-0.0241	1.0000	7.7432E-23	: qP 2 11(13)	: U v5=2	12	2 10 - X v=0	13	2 11
13 E+ 17	14 E+ 2	5615.6477	5615.6618	-0.0141	1.0000	5.9181E-23	: qP 2 12(14)	: U v5=2	13	2 11 - X v=0	14	2 12
13 E+ 17	12 E+ 2	5682.5444	5682.5589	-0.0145	1.0000	7.7030E-23	: qR 2 10(12)	: U v5=2	13	2 11 - X v=0	12	2 10
14 E+ 17	13 E+ 2	5684.6926	5684.6826	0.0100	1.0000	9.4340E-23	: qR 2 11(13)	: U v5=2	14	2 12 - X v=0	13	2 11
14 E+ 17	15 E+ 2	5612.7090	5612.7001	0.0089	1.0000	7.0232E-23	: qP 2 13(15)	: U v5=2	14	2 12 - X v=0	15	2 13
15 E+ 17	16 E+ 2	5609.8285	5609.7962	0.0323	1.0000	6.7881E-23	: qP 2 14(16)	: U v5=2	15	2 13 - X v=0	16	2 14
15 E+ 17	14 E+ 2	5686.8956	5686.8652	0.0304	1.0000	9.4030E-23	: qR 2 12(14)	: U v5=2	15	2 13 - X v=0	14	2 12
16 E+ 17	17 E+ 2	5606.9273	5606.8976	0.0297	1.0000	5.9813E-23	: qP 2 15(17)	: U v5=2	16	2 14 - X v=0	17	2 15
16 E+ 17	15 E+ 2	5689.0794	5689.0483	0.0311	1.0000	8.5387E-23	: qR 2 13(15)	: U v5=2	16	2 14 - X v=0	15	2 13
17 E+ 17	16 E+ 2	5691.1856	5691.1917	-0.0061	1.0000	7.3237E-23	: qR 2 14(16)	: U v5=2	17	2 15 - X v=0	16	2 14
17 E+ 17	18 E+ 2	5603.9639	5603.9700	-0.0061	1.0000	4.9807E-23	: qP 2 16(18)	: U v5=2	17	2 15 - X v=0	18	2 16
18 E+ 17	19 E+ 2	5600.9431	5600.9807	-0.0376	1.0000	3.9298E-23	: qP 2 17(19)	: U v5=2	18	2 16 - X v=0	19	2 17
18 E+ 17	17 E+ 2	5693.2285	5693.2580	-0.0295	1.0000	5.9494E-23	: qR 2 15(17)	: U v5=2	18	2 16 - X v=0	17	2 15
19 E+ 17	20 E+ 2	5597.8903	5597.8838	0.0065	1.0000	2.8898E-23	: qP 2 18(20)	: U v5=2	19	2 17 - X v=0	20	2 18
19 E+ 17	18 E+ 2	5695.1970	5695.1969	0.0001	1.0000	4.5028E-23	: qR 2 16(18)	: U v5=2	19	2 17 - X v=0	18	2 16
3 O+ 18	3 O- 2	5650.2901	5650.2648	0.0253	1.0000	3.5162E-22	: qQ 3 1( 3)	: U v5=2	3	3 0 - X v=0	3	3 1
3 O+ 18	4 O+ 2	5640.5704	5640.5452	0.0252	1.0000	1.1158E-22	: qP 3 1( 4)	: U v5=2	3	3 0 - X v=0	4	3 1
4 O+ 20	4 O- 2	5650.2432	5650.2214	0.0218	1.0000	2.5597E-22	: qQ 3 2( 4)	: U v5=2	4	3 1 - X v=0	4	3 2
4 O+ 20	5 O+ 2	5638.0918	5638.0699	0.0219	1.0000	1.9019E-22	: qP 3 2( 5)	: U v5=2	4	3 1 - X v=0	5	3 2
4 O+ 20	3 O+ 2	5659.9635	5659.9408	0.0227	1.0000	1.1621E-22	: qR 3 0( 3)	: U v5=2	4	3 1 - X v=0	3	3 0



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8 O- 23	9 O- 2	5628.0530	5628.0585	-0.0055	1.0000	3.2782E-22	: qP 3 7( 9) : U v5=2	8 3 6 - X v=0	9 3 7
8 O- 23	7 O- 2	5669.3924	5669.3974	-0.0050	1.0000	3.4745E-22	: qR 3 5( 7) : U v5=2	8 3 6 - X v=0	7 3 5
8 O- 23	8 O+ 2	5649.9308	5649.9358	-0.0050	1.0000	9.7105E-23	: qQ 3 5( 8) : U v5=2	8 3 6 - X v=0	8 3 5
9 O- 23	8 O- 2	5671.7119	5671.7241	-0.0122	1.0000	3.6403E-22	: qR 3 6( 8) : U v5=2	9 3 7 - X v=0	8 3 6
9 O- 23	10 O- 2	5625.4993	5625.5129	-0.0136	1.0000	3.2754E-22	: qP 3 8(10) : U v5=2	9 3 7 - X v=0	10 3 8
9 O- 23	9 O+ 2	5649.8027	5649.8168	-0.0141	1.0000	7.7124E-23	: qQ 3 6( 9) : U v5=2	9 3 7 - X v=0	9 3 6
10 O- 23	11 O- 2	5622.9096	5622.9478	-0.0382	1.0000	3.1726E-22	: qP 3 9(11) : U v5=2	10 3 8 - X v=0	11 3 9
10 O- 23	10 O+ 2	5649.6335	5649.6719	-0.0384	1.0000	6.1029E-23	: qQ 3 7(10) : U v5=2	10 3 8 - X v=0	10 3 7
10 O- 23	9 O- 2	5673.9989	5674.0329	-0.0340	1.0000	3.6746E-22	: qR 3 7( 9) : U v5=2	10 3 8 - X v=0	9 3 7
11 O- 23	12 O- 2	5620.3620	5620.3611	0.0009	1.0000	2.9879E-22	: qP 3 10(12) : U v5=2	11 3 9 - X v=0	12 3 10
11 O- 23	10 O- 2	5676.3228	5676.3214	0.0014	1.0000	3.5924E-22	: qR 3 8(10) : U v5=2	11 3 9 - X v=0	10 3 8
11 O- 23	11 O+ 2	5649.4938	5649.4953	-0.0015	1.0000	4.7963E-23	: qQ 3 8(11) : U v5=2	11 3 9 - X v=0	11 3 8
12 O- 23	11 O- 2	5678.5802	5678.5860	-0.0058	1.0000	3.4082E-22	: qR 3 9(11) : U v5=2	12 3 10 - X v=0	11 3 9
12 O- 23	13 O- 2	5617.7441	5617.7501	-0.0060	1.0000	2.7380E-22	: qP 3 11(13) : U v5=2	12 3 10 - X v=0	13 3 11
12 O- 23	12 O+ 2	5649.2734	5649.2794	-0.0060	1.0000	3.7300E-23	: qQ 3 9(12) : U v5=2	12 3 10 - X v=0	12 3 9
13 O- 23	12 O- 2	5680.8179	5680.8224	-0.0045	1.0000	3.1322E-22	: qR 3 10(12) : U v5=2	13 3 11 - X v=0	12 3 10
13 O- 23	14 O- 2	5615.1056	5615.1110	-0.0054	1.0000	2.4350E-22	: qP 3 12(14) : U v5=2	13 3 11 - X v=0	14 3 12
13 O- 23	13 O+ 2	5649.0119	5649.0142	-0.0023	1.0000	2.8538E-23	: qQ 3 10(13) : U v5=2	13 3 11 - X v=0	13 3 10
14 O- 23	15 O- 2	5612.4370	5612.4381	-0.0011	1.0000	2.0776E-22	: qP 3 13(15) : U v5=2	14 3 12 - X v=0	15 3 13
14 O- 23	13 O- 2	5683.0245	5683.0239	0.0006	1.0000	2.7579E-22	: qR 3 11(13) : U v5=2	14 3 12 - X v=0	13 3 11
15 O- 23	14 O- 2	5685.1882	5685.1792	0.0090	1.0000	2.2075E-22	: qR 3 12(14) : U v5=2	15 3 13 - X v=0	14 3 12
15 O- 23	16 O- 2	5609.7297	5609.7211	0.0086	1.0000	1.6133E-22	: qP 3 14(16) : U v5=2	15 3 13 - X v=0	16 3 14
16 O- 23	17 O- 2	5606.9544	5606.9402	0.0142	1.0000	7.2594E-23	: qP 3 15(17) : U v5=2	16 3 14 - X v=0	17 3 15
16 O- 23	15 O- 2	5687.2798	5687.2673	0.0125	1.0000	1.0227E-22	: qR 3 13(15) : U v5=2	16 3 14 - X v=0	15 3 13
17 O- 24	16 O- 2	5690.9258	5690.9343	-0.0085	1.0000	7.6986E-23	: qR 3 14(16) : U v5=2	17 3 15 - X v=0	16 3 14
17 O- 24	18 O- 2	5605.7342	5605.7425	-0.0083	1.0000	5.2953E-23	: qP 3 16(18) : U v5=2	17 3 15 - X v=0	18 3 16
18 O- 23	17 O- 2	5691.4076	5691.4212	-0.0136	1.0000	1.1847E-22	: qR 3 15(17) : U v5=2	18 3 16 - X v=0	17 3 15
18 O- 23	19 O- 2	5601.3619	5601.3704	-0.0085	1.0000	7.9269E-23	: qP 3 17(19) : U v5=2	18 3 16 - X v=0	19 3 17
19 O- 23	18 O- 2	5693.3454	5693.3244	0.0210	1.0000	1.1384E-22	: qR 3 16(18) : U v5=2	19 3 17 - X v=0	18 3 16
19 O- 23	20 O- 2	5598.4421	5598.4217	0.0204	1.0000	7.4070E-23	: qP 3 18(20) : U v5=2	19 3 17 - X v=0	20 3 18
4 E+ 31	4 E- 2	5648.8142	5648.8106	0.0036	1.0000	1.1598E-22	: qQ 4 1( 4) : U v5=2	4 4 0 - X v=0	4 4 1
4 E+ 31	5 E+ 3	5636.6665	5636.6654	0.0011	1.0000	2.7265E-23	: qP 4 1( 5) : U v5=2	4 4 0 - X v=0	5 4 1
5 E+ 33	6 E+ 3	5634.1973	5634.1863	0.0110	1.0000	4.6974E-23	: qP 4 2( 6) : U v5=2	5 4 1 - X v=0	6 4 2
5 E+ 33	5 E- 2	5648.7707	5648.7616	0.0091	1.0000	8.9009E-23	: qQ 4 2( 5) : U v5=2	5 4 1 - X v=0	5 4 2
5 E+ 33	4 E+ 3	5660.9140	5660.9068	0.0072	1.0000	2.9047E-23	: qR 4 0( 4) : U v5=2	5 4 1 - X v=0	4 4 0
6 E+ 34	7 E+ 3	5631.6972	5631.6972	0.0000	1.0000	6.1063E-23	: qP 4 3( 7) : U v5=2	6 4 2 - X v=0	7 4 3
6 E+ 34	6 E- 2	5648.7035	5648.7033	0.0002	1.0000	6.9913E-23	: qQ 4 3( 6) : U v5=2	6 4 2 - X v=0	6 4 3
6 E+ 34	5 E+ 3	5663.2806	5663.2786	0.0020	1.0000	5.0676E-23	: qR 4 1( 5) : U v5=2	6 4 2 - X v=0	5 4 1
7 E+ 34	7 E- 2	5648.6331	5648.6360	-0.0029	1.0000	5.5608E-23	: qQ 4 4( 7) : U v5=2	7 4 3 - X v=0	7 4 4
7 E+ 34	8 E+ 3	5629.1958	5629.1984	-0.0026	1.0000	7.0564E-23	: qP 4 4( 8) : U v5=2	7 4 3 - X v=0	8 4 4
7 E+ 34	6 E+ 3	5665.6398	5665.6421	-0.0023	1.0000	6.6700E-23	: qR 4 2( 6) : U v5=2	7 4 3 - X v=0	6 4 2
8 E+ 34	8 E- 2	5648.5522	5648.5602	-0.0080	1.0000	4.4497E-23	: qQ 4 5( 8) : U v5=2	8 4 4 - X v=0	8 4 5
8 E+ 34	9 E+ 3	5626.6837	5626.6902	-0.0065	1.0000	7.6174E-23	: qP 4 5( 9) : U v5=2	8 4 4 - X v=0	9 4 5
8 E+ 34	7 E+ 3	5667.9911	5667.9977	-0.0066	1.0000	7.8036E-23	: qR 4 3( 7) : U v5=2	8 4 4 - X v=0	7 4 3
9 E+ 34	10 E+ 3	5624.1623	5624.1729	-0.0106	1.0000	7.8468E-23	: qP 4 6(10) : U v5=2	9 4 5 - X v=0	10 4 6
9 E+ 34	9 E- 2	5648.4668	5648.4763	-0.0095	1.0000	3.5664E-23	: qQ 4 6( 9) : U v5=2	9 4 5 - X v=0	9 4 6
9 E+ 34	8 E+ 3	5670.3340	5670.3460	-0.0120	1.0000	8.5276E-23	: qR 4 4( 8) : U v5=2	9 4 5 - X v=0	8 4 4
10 E+ 34	9 E+ 3	5672.6779	5672.6877	-0.0098	1.0000	8.8906E-23	: qR 4 5( 9) : U v5=2	10 4 6 - X v=0	9 4 5
10 E+ 34	11 E+ 3	5621.6406	5621.6470	-0.0064	1.0000	7.7976E-23	: qP 4 7(11) : U v5=2	10 4 6 - X v=0	11 4 7
10 E+ 34	10 E- 2	5648.3728	5648.3850	-0.0122	1.0000	2.8542E-23	: qQ 4 7(10) : U v5=2	10 4 6 - X v=0	10 4 7
11 E+ 34	12 E+ 3	5619.1129	5619.1134	-0.0005	1.0000	7.5212E-23	: qP 4 8(12) : U v5=2	11 4 7 - X v=0	12 4 8
11 E+ 34	11 E- 2	5648.2813	5648.2875	-0.0062	1.0000	2.2753E-23	: qQ 4 8(11) : U v5=2	11 4 7 - X v=0	11 4 8
11 E+ 34	10 E+ 3	5675.0207	5675.0240	-0.0033	1.0000	8.9391E-23	: qR 4 6(10) : U v5=2	11 4 7 - X v=0	10 4 6





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2 15 O- 44 14 O- 3 5681.2418 5681.2489 -0.0071 1.0000 1.4502E-22 : qR 5 10(14) : U v5=2 15 5 11 - X v=0 14 5 10  
3 15 O- 44 15 O+ 3 5644.8083 5644.8079 0.0004 1.0000 2.9130E-23 : qQ 5 10(15) : U v5=2 15 5 11 - X v=0 15 5 10

4 424 Observations  
5 Average Error: 0.0133968803218114  
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