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The far-infrared spectrum of 12C2HD

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The far-infrared spectrum of $^{12}\text{C}_2\text{HD}$

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Abstract

The infrared spectrum of $^{12}\text{C}_2\text{HD}$ has been studied using synchrotron radiation at the far-infrared beamline, Canadian Light Source, Saskatoon, Canada. The spectra were recorded at a resolution of 0.00096 cm^{-1} in the 60 to 360 cm^{-1} range using a Bruker IFS125 Fourier transform spectrometer. Altogether, 821 vibration rotation lines were observed and assigned to $P(J)$, $Q(J)$ and $R(J)$ transitions of the $\nu_5 \leftarrow \nu_4$ difference band and associated hot bands with J'' up to 35 and $(\nu_4 + \nu_5)$ up to 3. These new transitions were analyzed together with 4518 transitions involving bending states with $(\nu_4 + \nu_5)$ up to 3 available in the literature. The spectroscopic parameters obtained from the fit reproduce 4909 transitions with a standard deviation standard deviation of 0.00028 cm^{-1} . The $\nu_5 \leftarrow \nu_4$ bands of the $^{13}\text{CH}^{12}\text{CD}$ and $^{12}\text{CH}^{13}\text{CD}$ molecules were also detected and analyzed.

1. Introduction

Before its detection in the Titan atmosphere by the Composite Infrared Spectrometer (CIRS) instrument mounted on CASSINI spacecraft [1] monodeuterated acetylene ($^{12}\text{C}_2\text{HD}$) has never been considered a molecule of astrophysical interest. Prior to this finding, deuterated species of methane and hydrogen have been identified in the atmospheric spectra of Titan, where methane is considered to be the main reservoir of deuterium. The discovery of monodeuterated acetylene in Titan's atmosphere and inconsistencies in the H/D ratio retrieved from analysis of different vibrational bands of methane, have prompted a thorough investigation of the infrared intensities of $^{12}\text{C}_2\text{HD}$ in the range $400 - 2000 \text{ cm}^{-1}$ [2], with particular emphasis on the bending fundamentals, whose strong features could be useful for the evaluation of the H/D ratio in Titan's atmosphere.

Although the spectroscopy of this molecule in the infrared (IR) is very well known [3-9] the only observations reported so far in the far-IR refer to the pure rotational spectrum in the ground and in a few low lying vibrational states [10-12]. Monodeuterated acetylene has two doubly degenerate bending vibrations at 518.38 cm^{-1} (ν_4) and 677.86 cm^{-1} (ν_5). The spectral signatures of both these vibrations were observed in Titan's atmospheric spectra. From a spectroscopic point of view, it is expected that the difference band $\nu_5 \leftarrow \nu_4$ will appear near 159.48 cm^{-1} , as observed in normal acetylene at 116.28 cm^{-1} [13-16]. In addition, a large number of hot bands accompanying the difference band should appear in the same region. Synchrotron light offers a significant advantage compared to a thermal source over most of the far-infrared region and was adopted as source in our experiment in order to improve the S/N in the recorded spectra.

2. Experimental details

Two spectra were acquired during separate experiments involving a Bruker IFS 125 Fourier transform (FT) spectrometer located at the far-infrared beamline, Canadian Light Source, Saskatoon, Canada. The spectra were recorded in the $60 - 360 \text{ cm}^{-1}$ range at an unapodized

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3 resolution of 0.00096 cm^{-1} . Optimum instrumental performance was achieved using a synchrotron
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5 source, a 2 mm Mylar beam splitter, and a Si bolometer detector. The spectrometer aperture was set
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7 to 2 mm. A scanner velocity of 80 kHz was used with analog electronic filters set for a low band
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9 pass of 5 kHz. No optical filters were used. A boxcar apodization was used in the Fourier transform
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11 which leads to an instrumental linewidth of $0.61/\text{optical path difference}$, full width at half
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13 maximum. A zerofilling factor of two, a Mertz phase correction, and a phase resolution of 1.0 were
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15 also used in the Fourier transforms.
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20 A multipass coolable cell with a base of 2 m with wedged polypropylene windows adjusted
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22 for a 72 m pathlength contained the C_2HD sample. The sample was supplied by the Cambridge
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24 Isotope Laboratories and used without further purification. Isotopic purity was reported to be of
25
26 98%, but it turned out that C_2H_2 was more abundant than expected. In particular, transitions of the
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28 symmetric species interfere with the P branch of the $\nu_5 \leftarrow \nu_4$ band of C_2HD molecule. Nevertheless,
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30 due to the very high resolution, the number of overlapped lines is negligible. All far-infrared data of
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32 the C_2H_2 isotopologue, recorded under similar experimental conditions, are furthermore well known
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34 [16] and were easily identified in the spectra.
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39 The two spectra were recorded at total gas pressures and temperatures of 750 mTorr and
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41 298.35 K (I), and 3.026 Torr and 297.75 K (II). The gas pressure was measured using a 0-1 Torr
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43 and a 0-10 Torr Baratron gauge for spectrum (I) and (II), respectively. Rotational water lines [17,
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45 18] were used to calibrate the wavenumber scale. Lines of the intense $\nu_5 \leftarrow \nu_4$ band were measured
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47 on spectrum (I), while lines of all the other hot bands and of the $^{13}\text{CH}^{12}\text{CD}$ and $^{12}\text{CH}^{13}\text{CD}$
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49 molecules rely on spectrum (II).
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52

53 54 55 56 **3. Analysis**

57
58 The position of the lines expected in the investigated spectral range was calculated by means
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60 of the parameters derived from the analysis of the bending states up to $\nu_4 + \nu_5 = 3$ [4]. First, the
intense $\nu_5 \leftarrow \nu_4$ band was investigated. The P and R branches could be assigned up to high J values,

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3 while the weak Q branch lines were observed up to $J = 13$. Figure 1 illustrates the $f \leftarrow e$ and $e \leftarrow f$
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5 components of the Q branch. Subsequently, a systematic search of the lines belonging to all weak
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7 hot bands involving states up to $\nu_{\text{tot}} = \nu_4 + \nu_5 = 3$ present in the recorded region was undertaken.
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9 All bands involving states with $\nu_{\text{tot}} = 2$ were identified, but, within the investigated range, only P
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11 and Q branches of $2\nu_4 \leftarrow \nu_5$ ($\Sigma^+ \leftarrow \Pi$) band are present, while the expected P lines of the $\Delta \leftarrow \Pi$
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13 component are too weak to be observed. These latter branches are at the upper wavenumber limit of
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15 the spectrum which is characterized by a poor S/N. Of the transitions involving three quanta of the
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17 bending modes only the $\nu_4 + 2\nu_5 \leftarrow 2\nu_4 + \nu_5$ ($\Phi \leftarrow \Phi$) and $2\nu_4 + \nu_5 \leftarrow 3\nu_4$ (${}^1\Pi \leftarrow \Pi$) bands have
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19 been identified. After completing the assignment procedure a careful search of $\Delta(l_4 + l_5) = 2$
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21 transitions was undertaken by means of a list of computed wavenumbers. Three such bands with
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23 intensity slightly above the noise level of the spectrum were found with origins at 146.48, 161.78,
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25 and 161.81 cm^{-1} . The assignment of the transitions was straightforward due to the accuracy of their
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27 predicted positions. The analysed bands are listed in Table 1 together with the symmetry of the
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29 vibrational states, the band centre, the J values of the P , Q , and R branches, the RMS value of the
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31 residuals obtained from a simultaneous fit, and the number of lines assigned and retained in the
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33 final cycle of the least-squares procedure.
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42 After having completed the assignments, a simultaneous fit of all the transitions involving
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44 only excited states of the bending modes was performed. The data set includes: i) the presently
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46 observed far-IR transitions, ii) the IR bands listed in Table 1 of Ref. [4] involving all the states with
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48 $\nu_{\text{tot}} = 3$, with the exception of the $\nu_4 = 3$ Φ state which was not observed, iii) the $2\nu_4 + \nu_5 \leftarrow 2\nu_4$ (${}^1\Pi$
49
50 $\leftarrow \Delta$) band reported in Ref. [2] and iv) the rotational lines in the ground and first excited bending
51
52 states $\nu_4 = 1$ and $\nu_5 = 1$ [11-12]. The model Hamiltonian adopted for the analysis has already been
53
54 described (see Ref [4], Eqs. 2 to 6). It contains the usual vibration and rotation terms for a linear
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56 molecule with two bending modes, including the l -type interaction terms, both vibrational and
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58 rotational, connecting levels of the same vibrational manifold.
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60

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3 The weight of the experimental data were chosen proportional to the inverse of their squared
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5 estimated uncertainties. An uncertainty of $5 \times 10^{-5} \text{ cm}^{-1}$ (1.66 MHz) was given to wavenumbers of
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7 the main band $\nu_5 \leftarrow \nu_4$, $1 \times 10^{-4} \text{ cm}^{-1}$ to those of the weak bands involving $\nu_{\text{tot}} = 2$, but $2\nu_4 \leftarrow \nu_5$
8
9 ($\Sigma^+ \leftarrow \Pi$) which is at the edge of the response curve of the bolometer. An uncertainty of 2×10^{-4}
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11 cm^{-1} was given to this band and to the remaining far-IR transitions with $\nu_{\text{tot}} = 3$. The uncertainty of
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13 the IR lines was estimated to be $2 \times 10^{-4} \text{ cm}^{-1}$, while that of the pure rotational lines was set to $1 \times$
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15 10^{-6} cm^{-1} (30 kHz). Finally, all the transition wavenumbers that differed from their corresponding
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17 calculated values by more than 5 times their uncertainties were excluded from the data set in the
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19 final cycle of the analysis.
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25 A total of 5339 transitions were fitted to 62 parameters listed in Table 2. Based on the
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27 criterion adopted for rejection, 4909 observed wavenumbers were reproduced with a standard
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29 deviation of the fit of $2.8 \times 10^{-4} \text{ cm}^{-1}$. The RMS error for each band presently analysed is reported
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31 in column 5 of Table 1. For the bands previously observed, the RMS errors are practically identical
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33 to the values obtained in the fit without the far-IR transitions [4].
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37 The spectroscopic parameters in Table 2 can be compared to those listed in Table 2 of Ref.
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39 [4]. The same constants have been refined but δ_{45} (see Eq. 3 in [4]) resulted undetermined and was
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41 constrained to zero. The values of all the parameters are very similar, most of them being
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43 determined within one statistical error. Those presently obtained have smaller uncertainties, on the
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45 average about 20%, due to the high precision of the far-IR data and to the extension of pure
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47 rotational transitions measured with higher accuracy up to $J = 10$ [12].
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51 Finally, transitions of the $\nu_5 \leftarrow \nu_4$ bands of the $^{13}\text{CH}^{12}\text{CD}$ and $^{12}\text{CH}^{13}\text{CD}$ molecules were
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53 identified and analysed in single band fits. The band characteristics are listed in Table 1. A table
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55 with the list of transition wavenumbers, assignments, and residuals from the simultaneous fit
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57 associated with all the analysed bands can be made available from the Bologna authors.
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59
60

4. Conclusions

The very high resolution far-IR spectrum of the monodeuterated acetylene molecule, $^{12}\text{C}_2\text{HD}$, has been recorded in the $60 - 360 \text{ cm}^{-1}$ region by FT spectroscopy and synchrotron radiation source. The analysis of the observed bands complements and improves previous investigation on the bending states of the molecule. A simultaneous fit of 5339 transitions, including all previously measured lines and those presently assigned, provided a set of 62 accurate spectroscopic parameters which reproduces 4909 transitions with a standard deviation of the fit equal to $2.8 \times 10^{-4} \text{ cm}^{-1}$.

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References

- [1] A. Coustenis, D. J. Jennings, A. Jolly, Y. Benilan, C. A. Nixon, S. Vinatier, et al. *Icarus*, **197**, 539–48 (2008).
- [2] A. Jolly, Y. Benilan, E. Canè, L. Fusina, F. Tamassia, A. Fayt, S. Robert, M. Herman, *J. Quant. Spectrosc. Rad. Transf.*, **109**, 2846 (2008).
- [3] A. Baldacci, S. Gheretti, S. C. Hurlock, K. Narahari Rao, *J. Mol. Spectrosc.*, **59**, 116 (1976).
- [4] L. Fusina, E. Canè, F. Tamassia, G. Di Lonardo, *Mol. Phys.*, **103**, 3263 (2005).
- [5] L. Fusina, F. Tamassia, G. Di Lonardo, *Mol. Phys.*, **103**, 2613 (2005).
- [6] J. Liévin, M. Abbouti Temsamani, P. Gaspard, M. Herman, *Chem. Phys.*, **190**, 419 (1995).

- 1
2
3 [7] M. Abbouti Tamsamani, M. Herman, Chem. Phys. Lett., **260**, 253 (1996).
4
5
6 [8] M. Abbouti Tamsamani, M. Herman, Chem. Phys. Lett., **264**, 556 (1997).
7
8 [9] M. Herman, C. Depiesse, G. Di Lonardo, A. Fayt, L. Fusina, D. Hurtmans, S. Kassi, M.
9
10 Mollabashi, J. Vander Awera, J. Mol. Spectrosc., **228**, 499 (2004).
11
12 [10] K. Matsumura, T. Tanaka, Y. Endo, S. Saito, E. Hirota, J. Phys. Chem., **84**, 1793 (1980).
13
14 [11] G. Wlodarczak, J. Demaison, J. Burie, M. C. Lasne, Mol. Phys., **66**, 669 (1989).
15
16 [12] G. Cazzoli, C. Puzzarini, L. Fusina, F. Tamassia, J. Mol. Spectrosc., **247**, 115 (2008).
17
18 [13] Y. Kabbadj, M. Herman, G. Di Lonardo, L. Fusina, J.W.C. Johns, J. Mol. Spectrosc.,
19
20
21 **150**, 535 (1991)
22
23
24 [14] D. Jacquemart, L. Gomez, N. Lacombe, J.-Y. Mandin, O. Pirali, P. Roy, J. Quant. Spectrosc.
25
26 Radiat. Transf. **110**, 2102 (2009).
27
28 [15] S. Yu, B. J. Drouin, J.C. Pearson, Astrophys. J. **705**, 786 (2009).
29
30 [16] B. Amyay, M. Herman, A. Fayt, L. Fusina, A. Predoi-Cross, Chem. Phys. Letters, **491**, 17
31
32 (2010).
33
34 [17] J.W.C. Johns, J. Opt. Soc. Am. B **2**, 1340 (1985).
35
36 [18] F. Matsushima, H. Odashima, T. Iwasaki, S. Tsunekawa, K. Takagi, J. Mol. Structure,
37
38
39 **352/353**, 371 (1995).
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Table Captions

Table 1. Bands of $^{12}\text{C}_2\text{HD}$, $^{12}\text{CH}^{13}\text{CD}$, and $^{13}\text{CH}^{12}\text{CD}$ analyzed in the far-IR spectrum.

Table 2. Spectroscopic parameters (in cm^{-1}) for $^{12}\text{C}_2\text{HD}$ resulting from the simultaneous fit of all transitions involving bending levels up to $\nu_4 + \nu_5 = 3$

Figure Legend

Figure 1. A section of the FIR spectrum illustrating the Q branch of the $\nu_5 \leftarrow \nu_4$ band of $^{12}\text{C}_2\text{HD}$.

Experimental conditions: pressure, 3.026 Torr; path length, 72 m. **a:** $R(15)$ transition of $2\nu_5 \Sigma_g^+ \leftarrow$

$(\nu_4 + \nu_5) \Sigma_u^+$ in $^{12}\text{C}_2\text{H}_2$. **b:** rotational transition in H_2O . **c:** $R(18)$ transition of $(\nu_4 + \nu_5) \Delta_u(e) \leftarrow 2\nu_4$

$\Delta_g(e)$ in $^{12}\text{C}_2\text{H}_2$. **d:** $10_{4,6} \leftarrow 9_{4,5}$ rotational transition in HOD . **e:** $R(8)$ transition of $2\nu_5 \Sigma^+ \leftarrow (\nu_4 + \nu_5)$

Σ^+ in $^{12}\text{C}_2\text{HD}$.

Table 1. Bands of $^{12}\text{C}_2\text{HD}$, $^{12}\text{CH}^{13}\text{CD}$, and $^{13}\text{CH}^{12}\text{CD}$ analysed in the far-IR spectrum.

Vibrational transition	Symmetry	ν_C^a	$P, R, Q \{J_{\min}, J_{\max}\}$	$\sigma (\times 10^5)^b$	n. fitted/ assign. lines
$^{12}\text{C}_2\text{HD}$					
$\nu_5 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	159.4263	$P_{e-e} (2-33); R_{e-e} (1-35); Q_{f-e} (1-13)$ $P_{f-f} (2-34); R_{f-f} (1-35); Q_{f-e} (1-12)$	5	152/159
$2\nu_4 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	356.1275	$P_{e-e} (3-23); Q_{e-f} (2-23)$	26	42/43
$\nu_4 + \nu_5 \leftarrow 2\nu_4$	$\Sigma^+ \leftarrow \Sigma^+$	166.5628	$P_{e-e} (1-24); R_{e-e} (0-28)$	11	53/53
	$(\Sigma^+ \leftarrow \Delta)^c$	161.7773	$P_{e-e} (9-28); R_{e-e} (8-34)$	20	42/47
	$\Delta \leftarrow \Delta$	157.0286	$P_{e-e} (3-24); R_{e-e} (2-30); Q_{e-f} (2-11)$ $P_{f-f} (3-29); R_{f-f} (2-33); Q_{f-e} (2-14)$	13	129/133
	$(\Delta \leftarrow \Sigma^+)^c$	161.8141	$P_{e-e} (9-27); R_{e-e} (8-32)$	22	42/44
$2\nu_5 \leftarrow \nu_4 + \nu_5$	$\Sigma^+ \leftarrow \Sigma^+$	141.7283	$P_{e-e} (1-20); R_{e-e} (1-29)$	10	49/49
	$\Delta \leftarrow \Delta$	163.2996	$P_{e-e} (3-26); R_{e-e} (2-29); Q_{e-f} (2-11)$ $P_{f-f} (3-24); R_{f-f} (2-30); Q_{f-e} (2-12)$	13	119/124
	$(\Sigma^+ \leftarrow \Delta)^c$	146.4771	$P_{e-e} (12-19); R_{e-e} (15-29)$	14	20/23
$\nu_4 + 2\nu_5 \leftarrow 2\nu_4 + \nu_5$	$\Phi \leftarrow \Phi$	160.9732	$P_{e-e} (4-16); R_{e-e} (3-22); Q_{e-f} (3-8)$ $P_{f-f} (5-18); R_{f-f} (5-24); Q_{f-e} (3-10)$	25	71/77
$2\nu_4 + \nu_5 \leftarrow 3\nu_4$	${}^1\Pi \leftarrow \Pi$	171.3139	$P_{e-e} (3-20); R_{e-e} (1-19);$ $P_{f-f} (3-17); R_{f-f} (1-17); Q_{f-e} (1)$	22	63/69
$^{12}\text{CH}^{13}\text{CD}$					
$\nu_5 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	166.3566	$P_{e-e} (2-18); R_{e-e} (2-23)$ $P_{f-f} (3-21); R_{f-f} (1-25)$	22	72/81
$^{13}\text{CH}^{12}\text{CD}$					
$\nu_5 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	157.6795	$P_{e-e} (2-19); R_{e-e} (1-24)$ $P_{f-f} (3-18); R_{f-f} (1-24)$	22	76/82

$$^a \nu_C = G_v^0 - B_v k^2 - D_v k^4 - (G_v^0 - B_v k^2 - D_v k^4).$$

$^b \sigma$ (in cm^{-1}) corresponds to the RMS value of the residuals for the various assigned lines resulting from the simultaneous fit (see text).

c Perturbation allowed transition.

Table 2. Spectroscopic parameters (in cm^{-1}) for the bending states of $^{12}\text{C}_2\text{HD}$ resulting from the simultaneous fit of all transitions involving levels up to $\nu_4 + \nu_5 = 3$.^a

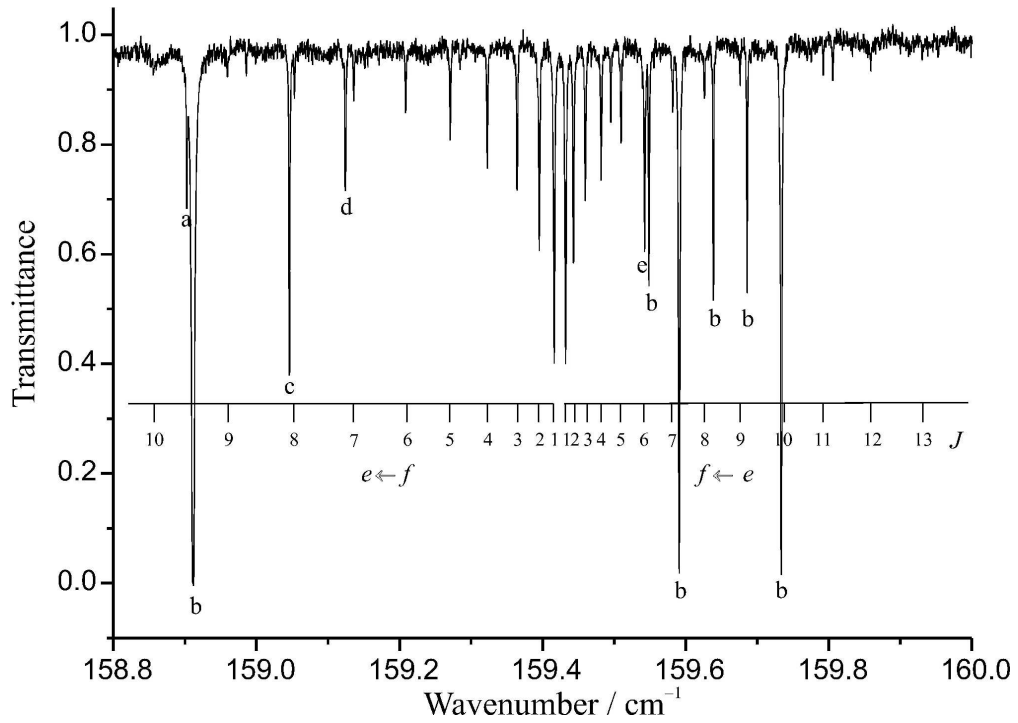
Parameter			Parameter		
ω_4^0	517.400373	(268)	g_{55}^0	5.1618252	(245)
ω_5^0	676.1870743	(371)	y_4^{44}	0.037851	(105)
x_{44}^0	-0.143558	(197)	y_4^{45}	-0.1020412	(223)
x_{45}^0	0.7075504	(548)	y_4^{55}	0.0218842	(201)
x_{55}^0	-2.5974508	(266)	y_5^{44}	0.0398552	(309)
y_{444}^0	-0.0364024	(323)	y_5^{45}	-0.0497324	(186)
y_{555}^0	0.03026340	(611)	y_5^{55}	0.01895520	(936)
y_{455}^0	0.0426422	(187)	r_{45}^0	1.557113	(195)
y_{445}^0	0.0427599	(215)	r_{445}	0.2380359	(560)
g_{44}^0	2.117292	(210)	r_{455}	0.067199	(103)
g_{45}^0	0.8521726	(394)	$r_{45}^J \times 10^3$	-0.0246653	(746)
B_0	0.9915272623	(434)	$\gamma_{445} \times 10^6$	2.0464	(460)
$\alpha_4^0 \times 10^3$	-2.643371	(138)	$\gamma_{455} \times 10^6$	0.2716	(367)
$\alpha_5^0 \times 10^3$	-1.481912	(103)	$\gamma_4^{44} \times 10^6$	-1.1851	(675)
$\gamma_{44} \times 10^3$	0.0313649	(561)	$\gamma_4^{45} \times 10^6$	2.2258	(709)
$\gamma_{45} \times 10^3$	-0.025949	(109)	$\gamma_4^{55} \times 10^6$	-0.3491	(279)
$\gamma_{55} \times 10^3$	0.0236638	(383)	$\gamma_5^{44} \times 10^6$	-2.1443	(526)
$\gamma^{44} \times 10^3$	-0.079675	(145)	$\gamma_5^{45} \times 10^6$	2.9576	(513)
$\gamma^{45} \times 10^3$	-0.003360	(151)	$\gamma_5^{55} \times 10^6$	-2.3959	(331)
$\gamma^{55} \times 10^3$	-0.1187171	(855)			
$D_0 \times 10^6$	1.133919	(183)	$\delta_{55} \times 10^9$	0.2737	(194)
$\beta_4 \times 10^6$	0.0345719	(927)	$\delta^{44} \times 10^9$	2.1478	(575)
$\beta_5 \times 10^6$	0.0167646	(773)	$\delta^{55} \times 10^9$	-2.0065	(302)
$\delta_{44} \times 10^9$	-0.9328	(301)			
$H_0 \times 10^{12}$	0.5733	(943)	$h_5 \times 10^{12}$	0.1947	(237)
$h_4 \times 10^{12}$	0.2021	(330)			

$q_4^0 \times 10^3$	4.3977317	(637)	$q_{55} \times 10^3$	0.0478092	(274)
$q_5^0 \times 10^3$	3.4783596	(639)	$q_4^J \times 10^6$	-0.0383910	(394)
$q_{44} \times 10^3$	0.0406380	(394)	$q_5^J \times 10^6$	-0.0221680	(437)
$q_{45} \times 10^3$	-0.0054381	(415)	$q_5^k \times 10^6$	-5.0948	(789)
$q_{54} \times 10^3$	0.0178707	(718)			
$\rho_4^0 \times 10^6$	-0.011018	(114)	$\rho_{55} \times 10^9$	5.490	(208)
$\rho_5^0 \times 10^6$	-0.012120	(447)	$\rho_{45}^0 \times 10^9$	-0.868	(258)

Number of fitted / assigned data = 4909 / 5339

St. dev. of the fit $\times 10^4 = 2.8$

^a Estimated uncertainties (1σ) are given in parentheses in units of the last figure quoted.



255x181mm (600 x 600 DPI)

view Only

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Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm^{-1}) for the bands involving the bending states up to $\nu_{\text{tot}} = 3$ of $^{12}\text{C}_2\text{HD}$ ^a (86 pp)

$\nu_4(\text{II}) \leftarrow G.S. (\Sigma^+)$

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$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 0 0 1	0 0 0 0 2	514.41615	0.00004	520.36524	5.94912
1 1 0 0 2	0 0 0 0 3	512.43467	0.00002	524.33282	11.89816
1 1 0 0 3	0 0 0 0 4	510.45392	-0.00011	530.28412	19.83009
1 1 0 0 4	0 0 0 0 5	508.47420	-0.00006	538.21906	29.74480
1 1 0 0 5	0 0 0 0 6	506.49535	-0.00003	548.13753	41.64214
1 1 0 0 6	0 0 0 0 7	504.51737	-0.00004	560.03938	55.52197
1 1 0 0 7	0 0 0 0 8	502.54048	0.00010	573.92447	71.38408
1 1 0 0 8	0 0 0 0 9	500.56423	-0.00008	589.79258	89.22827
1 1 0 0 9	0 0 0 0 10	498.58920	-0.00002	607.64350	109.05428
1 1 0 0 10	0 0 0 0 11	496.61513	-0.00001	627.47699	130.86184
1 1 0 0 11	0 0 0 0 12	494.64209	0.00000	649.29275	154.65066
1 1 0 0 12	0 0 0 0 13	492.67012	0.00002	673.09051	180.42041
1 1 0 0 13	0 0 0 0 14	490.69922	0.00004	698.86991	208.17072
1 1 0 0 14	0 0 0 0 15	488.72938	0.00001	726.63060	237.90124
1 1 0 0 15	0 0 0 0 16	486.76069	0.00002	756.37220	269.61154
1 1 0 0 16	0 0 0 0 17	484.79270	-0.00041	788.09430	303.30118
1 1 0 0 17	0 0 0 0 18	482.82675	0.00003	821.79644	338.96972
1 1 0 0 18	0 0 0 0 19	480.86156	0.00005	857.47816	376.61665
1 1 0 0 19	0 0 0 0 20	478.89752	0.00002	895.13897	416.24147
1 1 0 0 20	0 0 0 0 21	476.93475	0.00003	934.77834	457.84362
1 1 0 0 21	0 0 0 0 22	474.97318	0.00000	976.39572	501.42254
1 1 0 0 22	0 0 0 0 23	473.01294	0.00004	1019.99053	546.97764
1 1 0 0 23	0 0 0 0 24	471.05389	-0.00001	1065.56217	594.50827
1 1 0 0 24	0 0 0 0 25	469.09614	-0.00005	1113.10999	644.01380
1 1 0 0 25	0 0 0 0 26	467.13988	0.00007	1162.63334	695.49354
1 1 0 0 26	0 0 0 0 27	465.18470	-0.00006	1214.13154	748.94678
1 1 0 0 27	0 0 0 0 28	463.23119	0.00014	1267.60385	804.37280
1 1 0 0 28	0 0 0 0 29	461.27873	0.00001	1323.04955	861.77083
1 1 0 0 29	0 0 0 0 30	459.32778	0.00001	1380.46786	921.14009
1 1 0 0 30	0 0 0 0 31	457.37839	0.00017	1439.85797	982.47976
1 1 0 0 31	0 0 0 0 32	455.43011	0.00003	1501.21907	1045.78899
1 1 0 0 32	0 0 0 0 33	453.48309	-0.00029	1564.55030	1111.06693
1 1 0 0 33	0 0 0 0 34	451.53811	-0.00001	1629.85078	1178.31267
1 1 0 0 2	0 0 0 0 1	522.34972	-0.00005	524.33282	1.98305
1 1 0 0 3	0 0 0 0 2	524.33499	-0.00001	530.28412	5.94912
1 1 0 0 4	0 0 0 0 3	526.32074	-0.00015	538.21906	11.89816
1 1 0 0 5	0 0 0 0 4	528.30739	-0.00004	548.13753	19.83009
1 1 0 0 6	0 0 0 0 5	530.29452	-0.00007	560.03938	29.74480
1 1 0 0 7	0 0 0 0 6	532.28226	-0.00006	573.92447	41.64214
1 1 0 0 8	0 0 0 0 7	534.27056	-0.00005	589.79258	55.52197
1 1 0 0 9	0 0 0 0 8	536.25933	-0.00009	607.64350	71.38408
1 1 0 0 10	0 0 0 0 9	538.24864	-0.00008	627.47699	89.22827
1 1 0 0 11	0 0 0 0 10	540.23839	-0.00009	649.29275	109.05428
1 1 0 0 12	0 0 0 0 11	542.22859	-0.00007	673.09051	130.86184
1 1 0 0 13	0 0 0 0 12	544.21916	-0.00009	698.86991	154.65066
1 1 0 0 14	0 0 0 0 13	546.21000	-0.00020	726.63060	180.42041
1 1 0 0 15	0 0 0 0 14	548.20138	-0.00010	756.37220	208.17072
1 1 0 0 16	0 0 0 0 15	550.19297	-0.00009	788.09430	237.90124
1 1 0 0 17	0 0 0 0 16	552.18481	-0.00009	821.79644	269.61154
1 1 0 0 18	0 0 0 0 17	554.17689	-0.00009	857.47816	303.30118
1 1 0 0 19	0 0 0 0 18	556.16913	-0.00012	895.13897	338.96972
1 1 0 0 20	0 0 0 0 19	558.16155	-0.00014	934.77834	376.61665
1 1 0 0 21	0 0 0 0 20	560.15411	-0.00014	976.39572	416.24147
1 1 0 0 22	0 0 0 0 21	562.14677	-0.00014	1019.99053	457.84362
1 1 0 0 23	0 0 0 0 22	564.13948	-0.00014	1065.56217	501.42254
1 1 0 0 24	0 0 0 0 23	566.13220	-0.00016	1113.10999	546.97764

URL: <http://mc.manuscriptcentral.com/tandf/tmlp>

1	1	0	0	25	0	0	0	0	24	568.12491	-0.00016	1162.63334	594.50827
1	1	0	0	26	0	0	0	0	25	570.11757	-0.00017	1214.13154	644.01380
1	1	0	0	27	0	0	0	0	26	572.11013	-0.00019	1267.60385	695.49354
2	1	1	0	0	28	0	0	0	27	574.10258	-0.00019	1323.04955	748.94678
3	1	1	0	0	29	0	0	0	28	576.09482	-0.00023	1380.46786	804.37280
4	1	1	0	0	30	0	0	0	29	578.08688	-0.00026	1439.85797	861.77083
5	1	1	0	0	31	0	0	0	30	580.07867	-0.00031	1501.21907	921.14009
6	1	-1	0	0	2	0	0	0	2	518.41029	-0.00003	524.35945	5.94912
7	1	-1	0	0	3	0	0	0	3	518.43915	-0.00006	530.33737	11.89816
8	1	-1	0	0	4	0	0	0	4	518.47766	-0.00006	538.30781	19.83009
9	1	-1	0	0	5	0	0	0	5	518.52579	-0.00006	548.27064	29.74480
10	1	-1	0	0	6	0	0	0	6	518.58351	-0.00007	560.22573	41.64214
11	1	-1	0	0	7	0	0	0	7	518.65084	-0.00008	574.17289	55.52197
12	1	-1	0	0	8	0	0	0	8	518.72778	-0.00008	590.11194	71.38408
13	1	-1	0	0	9	0	0	0	9	518.81431	-0.00006	608.04264	89.22827
14	1	-1	0	0	10	0	0	0	10	518.91034	-0.00012	627.96474	109.05428
15	1	-1	0	0	11	0	0	0	11	519.01603	-0.00008	649.87795	130.86184
16	1	-1	0	0	12	0	0	0	12	519.13120	-0.00010	673.78196	154.65066
17	1	-1	0	0	13	0	0	0	13	519.25592	-0.00010	699.67642	180.42041
18	1	-1	0	0	14	0	0	0	14	519.39014	-0.00010	727.56097	208.17072
19	1	-1	0	0	15	0	0	0	15	519.53387	-0.00009	757.43520	237.90124
20	1	-1	0	0	16	0	0	0	16	519.68701	-0.00015	789.29869	269.61154
21	1	-1	0	0	17	0	0	0	17	519.84968	-0.00012	823.15099	303.30118
22	1	-1	0	0	18	0	0	0	18	520.02173	-0.00015	858.99160	338.96972
23	1	-1	0	0	19	0	0	0	19	520.20320	-0.00016	896.82001	376.61665
24	1	-1	0	0	20	0	0	0	20	520.39423	0.00001	936.63569	416.24147
25	1	-1	0	0	21	0	0	0	21	520.59426	-0.00017	978.43806	457.84362
26	1	-1	0	0	22	0	0	0	22	520.80381	-0.00016	1022.22652	501.42254
27	1	-1	0	0	23	0	0	0	23	521.02263	-0.00018	1068.00045	546.97764
28	1	-1	0	0	24	0	0	0	24	521.25070	-0.00022	1115.75919	594.50827
29	1	-1	0	0	25	0	0	0	25	521.48805	-0.00022	1165.50207	644.01380
30	1	-1	0	0	26	0	0	0	26	521.73461	-0.00021	1217.22835	695.49354
31	1	-1	0	0	27	0	0	0	27	521.99033	-0.00021	1270.93732	748.94678
32	1	-1	0	0	28	0	0	0	28	522.25513	-0.00026	1326.62819	804.37280
33	1	-1	0	0	29	0	0	0	29	522.52961*	0.00026	1384.30018	861.77083
34	1	-1	0	0	30	0	0	0	30	522.81237	0.00001	1443.95245	921.14009
35	1	-1	0	0	31	0	0	0	31	523.10413	-0.00027	1505.58415	982.47976
36	1	-1	0	0	32	0	0	0	32	523.40523	-0.00019	1569.19441	1045.78899
37	1	-1	0	0	33	0	0	0	33	523.71526	-0.00012	1634.78230	1111.06693
38	1	-1	0	0	34	0	0	0	34	524.03419	-0.00005	1702.34690	1178.31267
39	1	-1	0	0	35	0	0	0	35	524.36186	-0.00009	1771.88724	1247.52529
40	1	-1	0	0	36	0	0	0	36	524.69852	0.00005	1843.40231	1318.70384
41	1	-1	0	0	37	0	0	0	37	525.04382	0.00007	1916.89110	1391.84735
42	1	-1	0	0	38	0	0	0	38	525.39796	0.00021	1992.35257	1466.95482
43	1	-1	0	0	39	0	0	0	39	525.76002	-0.00039	2069.78561	1544.02520
44	1	-1	0	0	40	0	0	0	40	526.13208	0.00039	2149.18914	1623.05745
45	1	-1	0	0	41	0	0	0	41	526.51080	-0.00074	2230.56202	1704.05048

rms = 0.00016 cm⁻¹

^a Observed wavenumbers identified by an asterisk have not been included in the fit.
Transitions identified by a W have been discarded because they do not satisfy the rejection limit criterion (see text).

$\nu_5 (\Pi) \leftarrow G.S. (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	0 0 0 0 2	673.84111	0.00018	679.79005	5.94912
0 0 1 1 2	0 0 0 0 3	671.85671	0.00025	683.75462	11.89816
0 0 1 1 3	0 0 0 0 4	669.87155	0.00024	689.70140	19.83009
0 0 1 1 4	0 0 0 0 5	667.88580	0.00028	697.63032	29.74480
0 0 1 1 5	0 0 0 0 6	665.89937	0.00026	707.54126	41.64214
0 0 1 1 6	0 0 0 0 7	663.91232	0.00020	719.43409	55.52197
0 0 1 1 7	0 0 0 0 8	661.92480	0.00025	733.30864	71.38408
0 0 1 1 8	0 0 0 0 9	659.93670	0.00025	749.16472	89.22827

URL: <http://mc.manuscriptcentral.com/and/tmph>

1	0	0	1	1	9	0	0	0	0	10	657.94806	0.00022	767.00212	109.05428
2	0	0	1	1	10	0	0	0	0	11	655.95896	0.00021	786.82059	130.86184
3	0	0	1	1	11	0	0	0	0	12	653.96947	0.00028	808.61985	154.65066
4	0	0	1	1	12	0	0	0	0	13	651.97944	0.00023	832.39961	180.42041
5	0	0	1	1	13	0	0	0	0	14	649.98908	0.00027	858.15954	208.17072
6	0	0	1	1	14	0	0	0	0	15	647.99820	0.00016	885.89928	237.90124
7	0	0	1	1	15	0	0	0	0	16	646.00712	0.00021	915.61845	269.61154
8	0	0	1	1	16	0	0	0	0	17	644.01571	0.00025	947.31664	303.30118
9	0	0	1	1	17	0	0	0	0	18	642.02392	0.00022	980.99342	338.96972
10	0	0	1	1	18	0	0	0	0	19	640.03191	0.00025	1016.64832	376.61665
11	0	0	1	1	19	0	0	0	0	20	638.03958	0.00020	1054.28084	416.24147
12	0	0	1	1	20	0	0	0	0	21	636.04711	0.00025	1093.89049	457.84362
13	0	0	1	1	21	0	0	0	0	22	634.05434	0.00019	1135.47669	501.42254
14	0	0	1	1	22	0	0	0	0	23	632.06096	-0.00030	1179.03889	546.97764
15	0	0	1	1	23	0	0	0	0	24	630.06812	-0.00010	1224.57649	594.50827
16	0	0	1	1	24	0	0	0	0	25	628.07548	0.00043	1272.08885	644.01380
17	0	0	1	1	25	0	0	0	0	26	626.08161	-0.00018	1321.57533	695.49354
18	0	0	1	1	26	0	0	0	0	27	624.08834	-0.00011	1373.03523	748.94678
19	0	0	1	1	27	0	0	0	0	28	622.09499	-0.00007	1426.46786	804.37280
20	0	0	1	1	28	0	0	0	0	29	620.10156	-0.00009	1481.87248	861.77083
21	0	0	1	1	29	0	0	0	0	30	618.10818	-0.00005	1539.24832	921.14009
22	0	0	1	1	30	0	0	0	0	31	616.11474	-0.00011	1598.59460	982.47976
23	0	0	1	1	31	0	0	0	0	32	614.12136	-0.00015	1659.91050	1045.78899
24	0	0	1	1	32	0	0	0	0	33	612.12816	-0.00009	1723.19517	1111.06693
25	0	0	1	1	33	0	0	0	0	34	610.13498	-0.00010	1788.44775	1178.31267
26	0	0	1	1	34	0	0	0	0	35	608.14172	-0.00032	1855.66733	1247.52529
27	0	0	1	1	35	0	0	0	0	36	606.14904	-0.00011	1924.85299	1318.70384
28	0	0	1	1	36	0	0	0	0	37	604.15614	-0.00029	1996.00378	1391.84735
29	0	0	1	1	37	0	0	0	0	38	602.16369	-0.00022	2069.11873	1466.95482
30	0	0	1	1	38	0	0	0	0	39	600.17150	-0.00011	2144.19682	1544.02520
31	0	0	1	1	39	0	0	0	0	40	598.17914	-0.00042	2221.23702	1623.05745
32	0	0	1	1	40	0	0	0	0	41	596.18725	-0.00054	2300.23827	1704.05048
33	0	0	1	1	1	0	0	0	0	0	679.79030	0.00025	679.79005	0.00000
34	0	0	1	1	2	0	0	0	0	1	681.77184	0.00027	683.75462	1.98305
35	0	0	1	1	3	0	0	0	0	2	683.75250	0.00022	689.70140	5.94912
36	0	0	1	1	4	0	0	0	0	3	685.73249	0.00034	697.63032	11.89816
37	0	0	1	1	5	0	0	0	0	4	687.71144	0.00027	707.54126	19.83009
38	0	0	1	1	6	0	0	0	0	5	689.68954	0.00025	719.43409	29.74480
39	0	0	1	1	7	0	0	0	0	6	691.66676	0.00027	733.30864	41.64214
40	0	0	1	1	8	0	0	0	0	7	693.64303	0.00028	749.16472	55.52197
41	0	0	1	1	9	0	0	0	0	8	695.61830	0.00026	767.00212	71.38408
42	0	0	1	1	10	0	0	0	0	9	697.59251	0.00019	786.82059	89.22827
43	0	0	1	1	11	0	0	0	0	10	699.56583	0.00026	808.61985	109.05428
44	0	0	1	1	12	0	0	0	0	11	701.53804	0.00027	832.39961	130.86184
45	0	0	1	1	13	0	0	0	0	12	703.50909	0.00021	858.15954	154.65066
46	0	0	1	1	14	0	0	0	0	13	705.47913	0.00026	885.89928	180.42041
47	0	0	1	1	15	0	0	0	0	14	707.44796	0.00024	915.61845	208.17072
48	0	0	1	1	16	0	0	0	0	15	709.41565	0.00025	947.31664	237.90124
49	0	0	1	1	17	0	0	0	0	16	711.38212	0.00024	980.99342	269.61154
50	0	0	1	1	18	0	0	0	0	17	713.34741	0.00028	1016.64832	303.30118
51	0	0	1	1	19	0	0	0	0	18	715.31136	0.00023	1054.28084	338.96972
52	0	0	1	1	20	0	0	0	0	19	717.27415	0.00032	1093.89049	376.61665
53	0	0	1	1	21	0	0	0	0	20	719.23547	0.00025	1135.47669	416.24147
54	0	0	1	1	22	0	0	0	0	21	721.19557	0.00030	1179.03889	457.84362
55	0	0	1	1	23	0	0	0	0	22	723.15417	0.00023	1224.57649	501.42254
56	0	0	1	1	24	0	0	0	0	23	725.11146	0.00025	1272.08885	546.97764
57	0	0	1	1	25	0	0	0	0	24	727.06734	0.00028	1321.57533	594.50827
58	0	0	1	1	26	0	0	0	0	25	729.02172	0.00028	1373.03523	644.01380
59	0	0	1	1	27	0	0	0	0	26	730.97458	0.00025	1426.46786	695.49354
60	0	0	1	1	28	0	0	0	0	27	732.92596	0.00026	1481.87248	748.94678
	0	0	1	1	29	0	0	0	0	28	734.87592	0.00040	1539.24832	804.37280
	0	0	1	1	30	0	0	0	0	29	736.82395	0.00018	1598.59460	861.77083
	0	0	1	1	31	0	0	0	0	30	738.77077	0.00036	1659.91050	921.14009
	0	0	1	1	32	0	0	0	0	31	740.71567	0.00025	1723.19517	982.47976
	0	0	1	1	33	0	0	0	0	32	742.65859	-0.00017	1788.44775	1045.78899
	0	0	1	1	34	0	0	0	0	33	744.60030	-0.00010	1855.66733	1111.06693
	0	0	1	1	35	0	0	0	0	34	746.54021	-0.00012	1924.85299	1178.31267
	0	0	1	1	36	0	0	0	0	35	748.47835	-0.00015	1996.00378	1247.52529
	0	0	1	1	37	0	0	0	0	36	750.41467	-0.00022	2069.11873	1318.70384

1	0	0	1	1	38	0	0	0	0	37	752.34918	-0.00028	2144.19682	1391.84735
2	0	0	1	1	39	0	0	0	0	38	754.28190	-0.00030	2221.23702	1466.95482
3	0	0	1	1	40	0	0	0	0	39	756.21267	-0.00040	2300.23827	1544.02520
4	0	0	1	1	41	0	0	0	0	40	758.14173	-0.00031	2381.19949	1623.05745
5	0	0	1	1	42	0	0	0	0	41	760.06846	-0.00062	2464.11956	1704.05048
6	0	0	1	1	43	0	0	0	0	42	761.99359	-0.00057	2548.99734	1787.00318
7	0	0	1	-1	1	0	0	0	0	1	677.81436	0.00031	679.79710	1.98305
8	0	0	1	-1	2	0	0	0	0	2	677.82690	0.00025	683.77578	5.94912
9	0	0	1	-1	3	0	0	0	0	3	677.84578	0.00023	689.74371	11.89816
10	0	0	1	-1	4	0	0	0	0	4	677.87103	0.00029	697.70083	19.83009
11	0	0	1	-1	5	0	0	0	0	5	677.90247	0.00024	707.64702	29.74480
12	0	0	1	-1	6	0	0	0	0	6	677.94020	0.00020	719.58215	41.64214
13	0	0	1	-1	7	0	0	0	0	7	677.98431	0.00025	733.50603	55.52197
14	0	0	1	-1	8	0	0	0	0	8	678.03461	0.00020	749.41849	71.38408
15	0	0	1	-1	9	0	0	0	0	9	678.09119	0.00016	767.31930	89.22827
16	0	0	1	-1	10	0	0	0	0	10	678.15410	0.00018	787.20820	109.05428
17	0	0	1	-1	11	0	0	0	0	11	678.22324	0.00016	809.08492	130.86184
18	0	0	1	-1	12	0	0	0	0	12	678.29867	0.00017	832.94916	154.65066
19	0	0	1	-1	13	0	0	0	0	13	678.38036	0.00020	858.80057	180.42041
20	0	0	1	-1	14	0	0	0	0	14	678.46821	0.00014	886.63880	208.17072
21	0	0	1	-1	15	0	0	0	0	15	678.56235	0.00013	916.46345	237.90124
22	0	0	1	-1	16	0	0	0	0	16	678.66276	0.00018	948.27412	269.61154
23	0	0	1	-1	17	0	0	0	0	17	678.76928	0.00011	982.07035	303.30118
24	0	0	1	-1	18	0	0	0	0	18	678.88210	0.00015	1017.85167	338.96972
25	0	0	1	-1	19	0	0	0	0	19	679.00107	0.00014	1055.61759	376.61665
26	0	0	1	-1	20	0	0	0	0	20	679.12617	0.00007	1095.36757	416.24147
27	0	0	1	-1	21	0	0	0	0	21	679.25752	0.00009	1137.10105	457.84362
28	0	0	1	-1	22	0	0	0	0	22	679.39502	0.00011	1180.81746	501.42254
29	0	0	1	-1	23	0	0	0	0	23	679.53860	0.00006	1226.51618	546.97764
30	0	0	1	-1	24	0	0	0	0	24	679.68838	0.00008	1274.19657	594.50827
31	0	0	1	-1	25	0	0	0	0	25	679.84420	0.00003	1323.85797	644.01380
32	0	0	1	-1	26	0	0	0	0	26	680.00618	0.00004	1375.49968	695.49354
33	0	0	1	-1	27	0	0	0	0	27	680.17421	0.00002	1429.12098	748.94678
34	0	0	1	-1	28	0	0	0	0	28	680.34829	-0.00002	1484.72111	804.37280
35	0	0	1	-1	29	0	0	0	0	29	680.52854	0.00006	1542.29931	861.77083
36	0	0	1	-1	30	0	0	0	0	30	680.71486	0.00018	1601.85477	921.14009
37	0	0	1	-1	31	0	0	0	0	31	680.90680	-0.00009	1663.38664	982.47976
38	0	0	1	-1	32	0	0	0	0	32	681.10504	-0.00005	1726.89408	1045.78899
39	0	0	1	-1	33	0	0	0	0	33	681.30943	0.00015	1792.37620	1111.06693
40	0	0	1	-1	34	0	0	0	0	34	681.51943	0.00002	1859.83208	1178.31267
41	0	0	1	-1	35	0	0	0	0	35	681.73531	-0.00017	1929.26077	1247.52529
42	0	0	1	-1	36	0	0	0	0	36	681.95726	-0.00021	2000.66131	1318.70384
43	0	0	1	-1	37	0	0	0	0	37	682.18521	-0.00014	2074.03270	1391.84735
44	0	0	1	-1	38	0	0	0	0	38	682.41903	-0.00006	2149.37391	1466.95482
45	0	0	1	-1	39	0	0	0	0	39	682.65870	0.00001	2226.68389	1544.02520
46	0	0	1	-1	40	0	0	0	0	40	682.90410	-0.00001	2305.96156	1623.05745
47	0	0	1	-1	41	0	0	0	0	41	683.15891*	0.00358	2387.20581	1704.05048W
48	0	0	1	-1	42	0	0	0	0	42	683.41237	0.00004	2470.41551	1787.00318

rms = 0.00023 cm⁻¹

2v₄(Σ⁺) ← v₄(Π)

v ₄ ' l ₄ ' v ₅ ' l ₅ ' J'	v ₄ '' l ₄ '' v ₅ '' l ₅ '' J''	OBS	OBS - CALC	E'	E''
2 0 0 0 0	1 1 0 0 1	513.57016	0.00010	1033.93529	520.36524
2 0 0 0 1	1 1 0 0 2	511.59606	-0.00029	1035.92917	524.33282
2 0 0 0 2	1 1 0 0 3	509.63244	-0.00023	1039.91679	530.28412
2 0 0 0 3	1 1 0 0 4	507.67859	-0.00024	1045.89789	538.21906
2 0 0 0 4	1 1 0 0 5	505.73440	-0.00017	1053.87209	548.13753
2 0 0 0 5	1 1 0 0 6	503.79939	-0.00010	1063.83887	560.03938
2 0 0 0 6	1 1 0 0 7	501.87302	-0.00010	1075.79759	573.92447
2 0 0 0 7	1 1 0 0 8	499.95487	-0.00002	1089.74746	589.79258
2 0 0 0 8	1 1 0 0 9	498.04403	-0.00008	1105.68761	607.64350
2 0 0 0 9	1 1 0 0 10	496.13998	-0.00005	1123.61701	627.47699
2 0 0 0 10	1 1 0 0 11	494.24184	0.00003	1143.53456	649.29275
2 0 0 0 11	1 1 0 0 12	492.34970	0.00000	1165.43907	673.09051

URL: <http://mc.manuscriptcentral.com/andf/andf>

1	2	0	0	0	12	1	1	0	0	13	490.45938	0.00004	1189.32925	698.86991
2	2	0	0	0	13	1	1	0	0	14	488.57331	0.00012	1215.20380	726.63060
3	2	0	0	0	14	1	1	0	0	15	486.68930	0.00013	1243.06138	756.37220
4	2	0	0	0	15	1	1	0	0	16	484.80654	0.00019	1272.90065	788.09430
5	2	0	0	0	16	1	1	0	0	17	482.92403	0.00014	1304.72033	821.79644
6	2	0	0	0	17	1	1	0	0	18	481.04215*	0.00113	1338.51918	857.47816W
7	2	0	0	0	18	1	1	0	0	19	479.15700	-0.00007	1374.29604	895.13897
8	2	0	0	0	19	1	1	0	0	20	477.27158	0.00008	1412.04985	934.77834
9	2	0	0	0	20	1	1	0	0	21	475.38368	-0.00022	1451.77962	976.39572
10	2	0	0	0	21	1	1	0	0	22	473.49399	0.00003	1493.48450	1019.99053
11	2	0	0	0	22	1	1	0	0	23	471.60127	-0.00024	1537.16368	1065.56217
12	2	0	0	0	23	1	1	0	0	24	469.70656	0.00009	1582.81646	1113.10999
13	2	0	0	0	24	1	1	0	0	25	467.80886	0.00002	1630.44219	1162.63334
14	2	0	0	0	25	1	1	0	0	26	465.90856	-0.00015	1680.04024	1214.13154
15	2	0	0	0	26	1	1	0	0	27	464.00624	0.00004	1731.61005	1267.60385
16	2	0	0	0	27	1	1	0	0	28	462.10154	0.00005	1785.15104	1323.04955
17	2	0	0	0	28	1	1	0	0	29	460.19509	0.00031	1840.66263	1380.46786
18	2	0	0	0	2	1	1	0	0	1	519.55138	-0.00017	1039.91679	520.36524
19	2	0	0	0	3	1	1	0	0	2	521.56481	-0.00026	1045.89789	524.33282
20	2	0	0	0	4	1	1	0	0	3	523.58776	-0.00021	1053.87209	530.28412
21	2	0	0	0	5	1	1	0	0	4	525.62059*	0.00077	1063.83887	538.21906
22	2	0	0	0	6	1	1	0	0	5	527.66020	0.00014	1075.79759	548.13753
23	2	0	0	0	7	1	1	0	0	6	529.70794	-0.00014	1089.74746	560.03938
24	2	0	0	0	8	1	1	0	0	7	531.76300	-0.00014	1105.68761	573.92447
25	2	0	0	0	9	1	1	0	0	8	533.82436	-0.00007	1123.61701	589.79258
26	2	0	0	0	10	1	1	0	0	9	535.89097	-0.00009	1143.53456	607.64350
27	2	0	0	0	11	1	1	0	0	10	537.96178	-0.00030	1165.43907	627.47699
28	2	0	0	0	12	1	1	0	0	11	540.03642	-0.00008	1189.32925	649.29275
29	2	0	0	0	13	1	1	0	0	12	542.11327	-0.00002	1215.20380	673.09051
30	2	0	0	0	14	1	1	0	0	13	544.19143	-0.00004	1243.06138	698.86991
31	2	0	0	0	15	1	1	0	0	14	546.27009	0.00004	1272.90065	726.63060
32	2	0	0	0	16	1	1	0	0	15	548.34808	-0.00005	1304.72033	756.37220
33	2	0	0	0	17	1	1	0	0	16	550.42483	-0.00006	1338.51918	788.09430
34	2	0	0	0	18	1	1	0	0	17	552.49948	-0.00012	1374.29604	821.79644
35	2	0	0	0	19	1	1	0	0	18	554.57157	-0.00011	1412.04985	857.47816
36	2	0	0	0	20	1	1	0	0	19	556.64051	-0.00014	1451.77962	895.13897
37	2	0	0	0	21	1	1	0	0	20	558.70603	-0.00012	1493.48450	934.77834
38	2	0	0	0	22	1	1	0	0	21	560.76774	-0.00022	1537.16368	976.39572
39	2	0	0	0	23	1	1	0	0	22	562.82574	-0.00019	1582.81646	1019.99053
40	2	0	0	0	24	1	1	0	0	23	564.87987	-0.00015	1630.44219	1065.56217
41	2	0	0	0	25	1	1	0	0	24	566.93002	-0.00023	1680.04024	1113.10999
42	2	0	0	0	26	1	1	0	0	25	568.97644	-0.00027	1731.61005	1162.63334
43	2	0	0	0	27	1	1	0	0	26	571.01927	-0.00023	1785.15104	1214.13154
44	2	0	0	0	28	1	1	0	0	27	573.05848	-0.00030	1840.66263	1267.60385
45	2	0	0	0	29	1	1	0	0	28	575.09438	-0.00032	1898.14425	1323.04955
46	2	0	0	0	30	1	1	0	0	29	577.12699	-0.00043	1957.59528	1380.46786
47	2	0	0	0	31	1	1	0	0	30	579.15688	-0.00025	2019.01510	1439.85797
48	2	0	0	0	9	1	-1	0	0	9	515.57459	0.00022	1123.61701	608.04264
49	2	0	0	0	10	1	-1	0	0	10	515.56960	-0.00022	1143.53456	627.96474
50	2	0	0	0	11	1	-1	0	0	11	515.56096	-0.00016	1165.43907	649.87795
51	2	0	0	0	12	1	-1	0	0	12	515.54738	0.00009	1189.32925	673.78196
52	2	0	0	0	13	1	-1	0	0	13	515.52751	0.00013	1215.20380	699.67642
53	2	0	0	0	14	1	-1	0	0	14	515.50221*	0.00180	1243.06138	727.56097W
54	2	0	0	0	15	1	-1	0	0	15	515.46543	-0.00002	1272.90065	757.43520
55	2	0	0	0	16	1	-1	0	0	16	515.42171	0.00007	1304.72033	789.29869
56	2	0	0	0	17	1	-1	0	0	17	515.36829	0.00009	1338.51918	823.15099
57	2	0	0	0	18	1	-1	0	0	18	515.30499	0.00054	1374.29604	858.99160
58	2	0	0	0	19	1	-1	0	0	19	515.22996	0.00012	1412.04985	896.82001
59	2	0	0	0	20	1	-1	0	0	20	515.14403	0.00009	1451.77962	936.63569
60	2	0	0	0	21	1	-1	0	0	21	515.04638	-0.00006	1493.48450	978.43806
	2	0	0	0	22	1	-1	0	0	22	514.93728	0.00012	1537.16368	1022.22652
	2	0	0	0	23	1	-1	0	0	23	514.81637	0.00036	1582.81646	1068.00045
	2	0	0	0	24	1	-1	0	0	24	514.68452*	0.00153	1630.44219	1115.75919W
	2	0	0	0	25	1	-1	0	0	25	514.53836	0.00018	1680.04024	1165.50207
	2	0	0	0	26	1	-1	0	0	26	514.38214	0.00044	1731.61005	1217.22835
	2	0	0	0	27	1	-1	0	0	27	514.21309*	-0.00063	1785.15104	1270.93732
	2	0	0	0	28	1	-1	0	0	28	514.03654*	0.00210	1840.66263	1326.62819W
	2	0	0	0	29	1	-1	0	0	29	513.84560*	0.00153	1898.14425	1384.30018W

rms = 0.00019 cm⁻¹ $2\nu_4(\Delta) \leftarrow \nu_4(\Pi)$

ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
2	2	0	0	2	1	1	0	0	3	514.41615	-0.00032	1044.70059	530.28412
2	2	0	0	3	1	1	0	0	4	512.46105	-0.00048	1050.68059	538.21906
2	2	0	0	4	1	1	0	0	5	510.51694	0.00021	1058.65425	548.13753
2	2	0	0	5	1	1	0	0	6	508.58229	-0.00019	1068.62187	560.03938
2	2	0	0	6	1	1	0	0	7	506.65911	-0.00022	1080.58379	573.92447
2	2	0	0	7	1	1	0	0	8	504.74800	0.00012	1094.54045	589.79258
2	2	0	0	8	1	1	0	0	9	502.84866	-0.00018	1110.49234	607.64350
2	2	0	0	9	1	1	0	0	10	500.96297	-0.00003	1128.43999	627.47699
2	2	0	0	10	1	1	0	0	11	499.09116	-0.00008	1148.38399	649.29275
2	2	0	0	11	1	1	0	0	12	497.23441	-0.00006	1170.32497	673.09051
2	2	0	0	12	1	1	0	0	13	495.39365	-0.00001	1194.26357	698.86991
2	2	0	0	13	1	1	0	0	14	493.56976	-0.00003	1220.20039	726.63060
2	2	0	0	14	1	1	0	0	15	491.76390	0.00007	1248.13603	756.37220
2	2	0	0	15	1	1	0	0	16	489.97645	-0.00026	1278.07100	788.09430
2	2	0	0	16	1	1	0	0	17	488.20926	-0.00004	1310.00574	821.79644
2	2	0	0	17	1	1	0	0	18	486.46295*	0.00057	1343.94054	857.47816
2	2	0	0	18	1	1	0	0	19	484.73704	0.00042	1379.87559	895.13897
2	2	0	0	19	1	1	0	0	20	483.03248	-0.00010	1417.81092	934.77834
2	2	0	0	2	1	1	0	0	1	524.33499*	-0.00036	1044.70059	520.36524
2	2	0	0	3	1	1	0	0	2	526.34786	0.00009	1050.68059	524.33282
2	2	0	0	4	1	1	0	0	3	528.37005	-0.00008	1058.65425	530.28412
2	2	0	0	5	1	1	0	0	4	530.40278	-0.00003	1068.62187	538.21906
2	2	0	0	6	1	1	0	0	5	532.44618	-0.00009	1080.58379	548.13753
2	2	0	0	7	1	1	0	0	6	534.50103	-0.00004	1094.54045	560.03938
2	2	0	0	8	1	1	0	0	7	536.56775	-0.00012	1110.49234	573.92447
2	2	0	0	9	1	1	0	0	8	538.64732	-0.00009	1128.43999	589.79258
2	2	0	0	10	1	1	0	0	9	540.74038	-0.00011	1148.38399	607.64350
2	2	0	0	11	1	1	0	0	10	542.84786	-0.00013	1170.32497	627.47699
2	2	0	0	12	1	1	0	0	11	544.97065	-0.00016	1194.26357	649.29275
2	2	0	0	13	1	1	0	0	12	547.10979	-0.00009	1220.20039	673.09051
2	2	0	0	14	1	1	0	0	13	549.26598	-0.00014	1248.13603	698.86991
2	2	0	0	15	1	1	0	0	14	551.44033	-0.00007	1278.07100	726.63060
2	2	0	0	16	1	1	0	0	15	553.63079*	-0.00274	1310.00574	756.37220W
2	2	0	0	17	1	1	0	0	16	555.84616	-0.00009	1343.94054	788.09430
2	2	0	0	18	1	1	0	0	17	558.07905	-0.00010	1379.87559	821.79644
2	2	0	0	19	1	1	0	0	18	560.33285	0.00009	1417.81092	857.47816
2	2	0	0	20	1	1	0	0	19	562.60731	-0.00011	1457.74639	895.13897
2	2	0	0	21	1	1	0	0	20	564.90329	-0.00009	1499.68172	934.77834
2	2	0	0	22	1	1	0	0	21	567.22108	0.00031	1543.61649	976.39572
2	2	0	0	23	1	1	0	0	22	569.55980	0.00019	1589.55014	1019.99053
2	2	0	0	24	1	1	0	0	23	571.91974	-0.00008	1637.48199	1065.56217
2	2	0	0	25	1	1	0	0	24	574.30121	-0.00007	1687.41127	1113.10999
2	2	0	0	5	1	-1	0	0	5	520.35150	0.00027	1068.62187	548.27064
2	2	0	0	6	1	-1	0	0	6	520.35803	-0.00004	1080.58379	560.22573
2	2	0	0	7	1	-1	0	0	7	520.36614*	-0.00142	1094.54045	574.17289W
2	2	0	0	8	1	-1	0	0	8	520.38031	-0.00009	1110.49234	590.11194
2	2	0	0	9	1	-1	0	0	9	520.39423*	-0.00311	1128.43999	608.04264W
2	2	0	0	10	1	-1	0	0	10	520.41921	-0.00004	1148.38399	627.96474
2	2	0	0	11	1	-1	0	0	11	520.44706	0.00004	1170.32497	649.87795
2	2	0	0	12	1	-1	0	0	12	520.48128	-0.00033	1194.26357	673.78196
2	2	0	0	13	1	-1	0	0	13	520.52394	-0.00003	1220.20039	699.67642
2	2	0	0	14	1	-1	0	0	14	520.57508	0.00002	1248.13603	727.56097
2	2	0	0	15	1	-1	0	0	15	520.63575	-0.00005	1278.07100	757.43520
2	2	0	0	16	1	-1	0	0	16	520.70705	0.00001	1310.00574	789.29869
2	2	0	0	17	1	-1	0	0	17	520.78959	0.00003	1343.94054	823.15099
2	2	0	0	18	1	-1	0	0	18	520.88403	0.00003	1379.87559	858.99160
2	2	0	0	19	1	-1	0	0	19	520.99102	0.00011	1417.81092	896.82001
2	2	0	0	20	1	-1	0	0	20	521.11086	0.00016	1457.74639	936.63569
2	2	0	0	21	1	-1	0	0	21	521.24384	0.00017	1499.68172	978.43806
2	2	0	0	22	1	-1	0	0	22	521.38209	0.00017	1543.61649	1022.22652

1	2	2	0	0	23	1	-1	0	0	23	521.54998	0.00029	1589.55014	1068.00045
2	2	2	0	0	24	1	-1	0	0	24	521.72305	0.00025	1637.48199	1115.75919
3	2	2	0	0	25	1	-1	0	0	25	521.90941	0.00020	1687.41127	1165.50207
4	2	2	0	0	26	1	-1	0	0	26	522.10905	0.00029	1739.33712	1217.22835
5	2	2	0	0	27	1	-1	0	0	27	522.32149	0.00021	1793.25860	1270.93732
6	2	2	0	0	28	1	-1	0	0	28	522.54670	0.00016	1849.17473	1326.62819
7	2	2	0	0	29	1	-1	0	0	29	522.78567*	0.00137	1907.08448	1384.30018W
8	2	2	0	0	30	1	-1	0	0	30	523.03812*	0.00379	1966.98678	1443.95245W
9	2	2	0	0	31	1	-1	0	0	31	523.29666	0.00029	2028.88052	1505.58415
10	2	2	0	0	32	1	-1	0	0	32	523.56820*	-0.00198	2092.76459	1569.19441W
11	2	2	0	0	33	1	-1	0	0	33	523.85561	0.00008	2158.63783	1634.78230
12	2	2	0	0	34	1	-1	0	0	34	524.15173	-0.00045	2226.49908	1702.34690
13	2	-2	0	0	2	1	-1	0	0	3	514.36336	0.00024	1044.70049	530.33737
14	2	-2	0	0	3	1	-1	0	0	4	512.37218	-0.00009	1050.68009	538.30781
15	2	-2	0	0	4	1	-1	0	0	5	510.38520*	0.00310	1058.65275	548.27064W
16	2	-2	0	0	5	1	-1	0	0	6	508.39359*	0.00096	1068.61835	560.22573
17	2	-2	0	0	6	1	-1	0	0	7	506.40382	-0.00005	1080.57677	574.17289
18	2	-2	0	0	7	1	-1	0	0	8	504.41588	0.00001	1094.52781	590.11194
19	2	-2	0	0	8	1	-1	0	0	9	502.42868	0.00004	1110.47128	608.04264
20	2	-2	0	0	9	1	-1	0	0	10	500.44210	-0.00011	1128.40695	627.96474
21	2	-2	0	0	10	1	-1	0	0	11	498.45649	-0.00012	1148.33456	649.87795
22	2	-2	0	0	11	1	-1	0	0	12	496.47180	-0.00006	1170.25382	673.78196
23	2	-2	0	0	12	1	-1	0	0	13	494.48785	-0.00014	1194.16442	699.67642
24	2	-2	0	0	13	1	-1	0	0	14	492.50490	-0.00013	1220.06599	727.56097
25	2	-2	0	0	14	1	-1	0	0	15	490.52291	-0.00007	1247.95819	757.43520
26	2	-2	0	0	15	1	-1	0	0	16	488.54187	-0.00002	1277.84059	789.29869
27	2	-2	0	0	16	1	-1	0	0	17	486.56453*	0.00275	1309.71276	823.15099W
28	2	-2	0	0	17	1	-1	0	0	18	484.58274	0.00008	1343.57425	858.99160
29	2	-2	0	0	18	1	-1	0	0	19	482.60456	0.00000	1379.42457	896.82001
30	2	-2	0	0	19	1	-1	0	0	20	480.62721	-0.00029	1417.26319	936.63569
31	2	-2	0	0	20	1	-1	0	0	21	478.65149	-0.00002	1457.08957	978.43806
32	2	-2	0	0	21	1	-1	0	0	22	476.67660	-0.00001	1498.90313	1022.22652
33	2	-2	0	0	22	1	-1	0	0	23	474.70260	-0.00021	1542.70326	1068.00045
34	2	-2	0	0	23	1	-1	0	0	24	472.72996	-0.00019	1588.48935	1115.75919
35	2	-2	0	0	24	1	-1	0	0	25	470.75823	-0.00041	1636.26071	1165.50207
36	2	-2	0	0	25	1	-1	0	0	26	468.78810	-0.00021	1686.01666	1217.22835
37	2	-2	0	0	26	1	-1	0	0	27	466.81927	0.00011	1737.75648	1270.93732
38	2	-2	0	0	27	1	-1	0	0	28	464.85113	-0.00011	1791.47943	1326.62819
39	2	-2	0	0	28	1	-1	0	0	29	462.88434	-0.00020	1847.18472	1384.30018
40	2	-2	0	0	2	1	-1	0	0	1	524.32641	0.00003	1044.70049	520.37411
41	2	-2	0	0	3	1	-1	0	0	2	526.32074	0.00010	1050.68009	524.35945
42	2	-2	0	0	4	1	-1	0	0	3	528.31523	-0.00014	1058.65275	530.33737
43	2	-2	0	0	5	1	-1	0	0	4	530.31045	-0.00009	1068.61835	538.30781
44	2	-2	0	0	6	1	-1	0	0	5	532.30606	-0.00006	1080.57677	548.27064
45	2	-2	0	0	7	1	-1	0	0	6	534.30198	-0.00010	1094.52781	560.22573
46	2	-2	0	0	8	1	-1	0	0	7	536.29827	-0.00012	1110.47128	574.17289
47	2	-2	0	0	9	1	-1	0	0	8	538.29490	-0.00011	1128.40695	590.11194
48	2	-2	0	0	10	1	-1	0	0	9	540.29173	-0.00019	1148.33456	608.04264
49	2	-2	0	0	11	1	-1	0	0	10	542.28859	-0.00049	1170.25382	627.96474
50	2	-2	0	0	12	1	-1	0	0	11	544.28633	-0.00013	1194.16442	649.87795
51	2	-2	0	0	13	1	-1	0	0	12	546.28388	-0.00016	1220.06599	673.78196
52	2	-2	0	0	14	1	-1	0	0	13	548.28162	-0.00015	1247.95819	699.67642
53	2	-2	0	0	15	1	-1	0	0	14	550.27932	-0.00030	1277.84059	727.56097
54	2	-2	0	0	16	1	-1	0	0	15	552.27754	-0.00002	1309.71276	757.43520
55	2	-2	0	0	17	1	-1	0	0	16	554.27532	-0.00024	1343.57425	789.29869
56	2	-2	0	0	18	1	-1	0	0	17	556.27329	-0.00029	1379.42457	823.15099
57	2	-2	0	0	19	1	-1	0	0	18	558.27132	-0.00027	1417.26319	858.99160
58	2	-2	0	0	20	1	-1	0	0	19	560.26933	-0.00023	1457.08957	896.82001
59	2	-2	0	0	21	1	-1	0	0	20	562.26726	-0.00018	1498.90313	936.63569
60	2	-2	0	0	22	1	-1	0	0	21	564.26503	-0.00018	1542.70326	978.43806
	2	-2	0	0	23	1	-1	0	0	22	566.26247	-0.00036	1588.48935	1022.22652
	2	-2	0	0	24	1	-1	0	0	23	568.26005	-0.00021	1636.26071	1068.00045
	2	-2	0	0	25	1	-1	0	0	24	570.25672	-0.00075	1686.01666	1115.75919
	2	-2	0	0	26	1	-1	0	0	25	572.25426	-0.00016	1737.75648	1165.50207
	2	-2	0	0	27	1	-1	0	0	26	574.25095	-0.00013	1791.47943	1217.22835
	2	-2	0	0	28	1	-1	0	0	27	576.24705	-0.00035	1847.18472	1270.93732
	2	-2	0	0	29	1	-1	0	0	28	578.24298	-0.00038	1904.87155	1326.62819
	2	-2	0	0	30	1	-1	0	0	29	580.23856	-0.00035	1964.53909	1384.30018
	2	-2	0	0	3	1	-1	0	0	3	520.39423*	-0.00174	1050.68009	530.28412W

1	2	-2	0	0	4	1	1	0	0	4	520.43359	-0.00010	1058.65275	538.21906
2	2	-2	0	0	5	1	1	0	0	5	520.48128*	0.00045	1068.61835	548.13753
3	2	-2	0	0	6	1	1	0	0	6	520.53726	-0.00012	1080.57677	560.03938
4	2	-2	0	0	7	1	1	0	0	7	520.60322	-0.00012	1094.52781	573.92447
5	2	-2	0	0	8	1	1	0	0	8	520.67860	-0.00010	1110.47128	589.79258
6	2	-2	0	0	9	1	1	0	0	9	520.76335	-0.00010	1128.40695	607.64350
7	2	-2	0	0	10	1	1	0	0	10	520.85741	-0.00017	1148.33456	627.47699
8	2	-2	0	0	11	1	1	0	0	11	520.96092	-0.00015	1170.25382	649.29275
9	2	-2	0	0	12	1	1	0	0	12	521.07380	-0.00011	1194.16442	673.09051
10	2	-2	0	0	13	1	1	0	0	13	521.19586	-0.00023	1220.06599	698.86991
11	2	-2	0	0	14	1	1	0	0	14	521.32736	-0.00022	1247.95819	726.63060
12	2	-2	0	0	15	1	1	0	0	15	521.46814	-0.00024	1277.84059	756.37220
13	2	-2	0	0	16	1	1	0	0	16	521.61823	-0.00024	1309.71276	788.09430
14	2	-2	0	0	17	1	1	0	0	17	521.77752	-0.00029	1343.57425	821.79644
15	2	-2	0	0	18	1	1	0	0	18	521.94611	-0.00029	1379.42457	857.47816
16	2	-2	0	0	19	1	1	0	0	19	522.12397	-0.00024	1417.26319	895.13897
17	2	-2	0	0	20	1	1	0	0	20	522.31132	0.00010	1457.08957	934.77834
18	2	-2	0	0	21	1	1	0	0	21	522.50689	-0.00051	1498.90313	976.39572
19	2	-2	0	0	22	1	1	0	0	22	522.71249	-0.00024	1542.70326	1019.99053
20	2	-2	0	0	23	1	1	0	0	23	522.92665	-0.00053	1588.48935	1065.56217
21	2	-2	0	0	24	1	1	0	0	24	523.15036	-0.00036	1636.26071	1113.10999
22	2	-2	0	0	25	1	1	0	0	25	523.38309	-0.00023	1686.01666	1162.63334
23	2	-2	0	0	26	1	1	0	0	26	523.62473	-0.00022	1737.75648	1214.13154
24	2	-2	0	0	27	1	1	0	0	27	523.87561	0.00004	1791.47943	1267.60385
25	2	-2	0	0	28	1	1	0	0	28	524.13522	0.00005	1847.18472	1323.04955
26	2	-2	0	0	29	1	1	0	0	29	524.40347	-0.00023	1904.87155	1380.46786
27	2	-2	0	0	30	1	1	0	0	30	524.68072	-0.00040	1964.53909	1439.85797
28	2	-2	0	0	31	1	1	0	0	31	524.96735	-0.00005	2026.18647	1501.21907
29	2	-2	0	0	32	1	1	0	0	32	525.26337*	0.00087	2089.81280	1564.55030
30	2	-2	0	0	33	1	1	0	0	33	525.56635	-0.00003	2155.41717	1629.85078
31	2	-2	0	0	34	1	1	0	0	34	525.87939	0.00038	2222.99862	1697.11961
32	2	-2	0	0	35	1	1	0	0	35	526.20087	0.00054	2292.55617	1766.35584
33	2	-2	0	0	36	1	1	0	0	36	526.53095	0.00063	2364.08883	1837.55852

rms = 0.00022 cm⁻¹

$v_4 + v_5 (\Sigma^+) \leftarrow v_4 (\Pi)$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
1	1	1	-1	0	1	1	0	0	1	680.13284	-0.00002	1200.49810	520.36524
2	1	1	-1	1	1	1	0	0	2	678.15740*	0.00122	1202.48900	524.33282W
3	1	1	-1	2	1	1	0	0	3	676.18675	0.00001	1206.47085	530.28412
4	1	1	-1	3	1	1	0	0	4	674.22527	0.00056	1212.44377	538.21906
5	1	1	-1	4	1	1	0	0	5	672.27034	-0.00002	1220.40789	548.13753
6	1	1	-1	5	1	1	0	0	6	670.32404	-0.00001	1230.36343	560.03938
7	1	1	-1	6	1	1	0	0	7	668.38613	-0.00005	1242.31065	573.92447
8	1	1	-1	7	1	1	0	0	8	666.45724	-0.00002	1256.24984	589.79258
9	1	1	-1	8	1	1	0	0	9	664.53777	-0.00010	1272.18137	607.64350
10	1	1	-1	9	1	1	0	0	10	662.62945	0.00083	1290.10561	627.47699
11	1	1	-1	10	1	1	0	0	11	660.73006	-0.00017	1310.02298	649.29275
12	1	1	-1	11	1	1	0	0	12	658.84328	-0.00015	1331.93393	673.09051
13	1	1	-1	12	1	1	0	0	13	656.96884	-0.00016	1355.83891	698.86991
14	1	1	-1	13	1	1	0	0	14	655.10773	-0.00001	1381.73835	726.63060
15	1	1	-1	14	1	1	0	0	15	653.26030	-0.00017	1409.63267	756.37220
16	1	1	-1	15	1	1	0	0	16	651.42783	-0.00012	1439.52224	788.09430
17	1	1	-1	16	1	1	0	0	17	649.61076	-0.00018	1471.40738	821.79644
18	1	1	-1	17	1	1	0	0	18	647.80992	-0.00020	1505.28829	857.47816
19	1	1	-1	18	1	1	0	0	19	646.02583	-0.00030	1541.16510	895.13897
20	1	1	-1	19	1	1	0	0	20	644.25923	-0.00025	1579.03782	934.77834
21	1	1	-1	20	1	1	0	0	21	642.51045	-0.00018	1618.90635	976.39572
22	1	1	-1	21	1	1	0	0	22	640.77962	-0.00030	1660.77045	1019.99053
23	1	1	-1	22	1	1	0	0	23	639.06739	-0.00021	1704.62977	1065.56217
24	1	1	-1	23	1	1	0	0	24	637.37364	-0.00020	1750.48383	1113.10999
25	1	1	-1	24	1	1	0	0	25	635.69752	-0.00119	1798.33206	1162.63334W
26	1	1	-1	25	1	1	0	0	26	634.04240	0.00016	1848.17378	1214.13154
27	1	1	-1	26	1	1	0	0	27	632.40082	0.00082	1900.00824	1267.60385

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1	1	1	-1	2	1	1	0	0	1	686.10525	-0.00037	1206.47085	520.36524
2	1	1	1	-1	3	1	1	0	0	688.11096	0.00001	1212.44377	524.33282
3	1	1	1	-1	4	1	1	0	0	690.12374	-0.00003	1220.40789	530.28412
4	1	1	1	-1	5	1	1	0	0	692.14437	0.00000	1230.36343	538.21906
5	1	1	1	-1	6	1	1	0	0	694.17304	-0.00008	1242.31065	548.13753
6	1	1	1	-1	7	1	1	0	0	696.21040	-0.00006	1256.24984	560.03938
7	1	1	1	-1	8	1	1	0	0	698.25687	-0.00003	1272.18137	573.92447
8	1	1	1	-1	9	1	1	0	0	700.31294	-0.00009	1290.10561	589.79258
9	1	1	1	-1	10	1	1	0	0	702.37938	-0.00010	1310.02298	607.64350
10	1	1	1	-1	11	1	1	0	0	704.45689	-0.00006	1331.93393	627.47699
11	1	1	1	-1	12	1	1	0	0	706.54607	-0.00008	1355.83891	649.29275
12	1	1	1	-1	13	1	1	0	0	708.64771	-0.00013	1381.73835	673.09051
13	1	1	1	-1	14	1	1	0	0	710.76266	-0.00010	1409.63267	698.86991
14	1	1	1	-1	15	1	1	0	0	712.89403*	0.00239	1439.52224	726.63060W
15	1	1	1	-1	16	1	1	0	0	715.03507	-0.00010	1471.40738	756.37220
16	1	1	1	-1	17	1	1	0	0	717.19394	-0.00005	1505.28829	788.09430
17	1	1	1	-1	18	1	1	0	0	719.36852	-0.00014	1541.16510	821.79644
18	1	1	1	-1	19	1	1	0	0	721.55951	-0.00015	1579.03782	857.47816
19	1	1	1	-1	20	1	1	0	0	723.76720	-0.00018	1618.90635	895.13897
20	1	1	1	-1	21	1	1	0	0	725.99194	-0.00017	1660.77045	934.77834
21	1	1	1	-1	22	1	1	0	0	728.23398	-0.00006	1704.62977	976.39572
22	1	1	1	-1	23	1	1	0	0	730.49311	-0.00018	1750.48383	1019.99053
23	1	1	1	-1	24	1	1	0	0	732.77052	0.00063	1798.33206	1065.56217
24	1	1	1	-1	25	1	1	0	0	735.06331	-0.00048	1848.17378	1113.10999
25	1	1	1	-1	26	1	1	0	0	737.37451	-0.00039	1900.00824	1162.63334
26	1	1	1	-1	27	1	1	0	0	739.70363	0.00056	1953.83461	1214.13154
27	1	1	1	-1	28	1	1	0	0	742.04820	0.00007	2009.65198	1267.60385
28	1	1	1	-1	3	1	-1	0	0	682.10764*	0.00125	1212.44377	530.33737W
29	1	1	1	-1	4	1	-1	0	0	682.10764*	0.00756	1220.40789	538.30781W
30	1	1	1	-1	5	1	-1	0	0	682.09284	0.00005	1230.36343	548.27064
31	1	1	1	-1	6	1	-1	0	0	682.08585*	0.00093	1242.31065	560.22573
32	1	1	1	-1	7	1	-1	0	0	682.07647	-0.00048	1256.24984	574.17289
33	1	1	1	-1	8	1	-1	0	0	682.07055*	0.00112	1272.18137	590.11194W
34	1	1	1	-1	9	1	-1	0	0	682.06270*	-0.00026	1290.10561	608.04264
35	1	1	1	-1	10	1	-1	0	0	682.05702*	-0.00122	1310.02298	627.96474W
36	1	1	1	-1	11	1	-1	0	0	682.05702*	0.00104	1331.93393	649.87795W
37	1	1	1	-1	12	1	-1	0	0	682.05702*	0.00007	1355.83891	673.78196
38	1	1	1	-1	13	1	-1	0	0	682.06280	0.00087	1381.73835	699.67642
39	1	1	1	-1	14	1	-1	0	0	682.07055*	-0.00115	1409.63267	727.56097W
40	1	1	1	-1	15	1	-1	0	0	682.08655	-0.00049	1439.52224	757.43520
41	1	1	1	-1	16	1	-1	0	0	682.10835	-0.00033	1471.40738	789.29869
42	1	1	1	-1	17	1	-1	0	0	682.13774	0.00044	1505.28829	823.15099
43	1	1	1	-1	18	1	-1	0	0	682.17338	-0.00012	1541.16510	858.99160
44	1	1	1	-1	19	1	-1	0	0	682.21763	-0.00018	1579.03782	896.82001
45	1	1	1	-1	20	1	-1	0	0	682.27050	-0.00017	1618.90635	936.63569
46	1	1	1	-1	21	1	-1	0	0	682.33226	-0.00014	1660.77045	978.43806
47	1	1	1	-1	22	1	-1	0	0	682.40284	-0.00041	1704.62977	1022.22652
48	1	1	1	-1	23	1	-1	0	0	682.48332	-0.00006	1750.48383	1068.00045
49	1	1	1	-1	24	1	-1	0	0	682.57274	-0.00012	1798.33206	1115.75919
50	1	1	1	-1	25	1	-1	0	0	682.67162	-0.00010	1848.17378	1165.50207
51	1	1	1	-1	26	1	-1	0	0	682.77985	-0.00004	1900.00824	1217.22835
52	1	1	1	-1	27	1	-1	0	0	682.89730	0.00001	1953.83461	1270.93732
53	1	1	1	-1	28	1	-1	0	0	683.02381	0.00002	2009.65198	1326.62819
54	1	1	1	-1	29	1	-1	0	0	683.15891	-0.00033	2067.45942	1384.30018
55	1	1	1	-1	30	1	-1	0	0	683.30210	-0.00137	2127.25592	1443.95245W
56	1	1	1	-1	31	1	-1	0	0	683.45782	0.00151	2189.04046	1505.58415W
57	1	1	1	-1	32	1	-1	0	0	683.61804	0.00048	2252.81197	1569.19441
58	1	1	1	-1	33	1	-1	0	0	683.78820*	0.00114	2318.56937	1634.78230W
59	1	1	1	-1	34	1	-1	0	0	683.96525	0.00063	2386.31153	1702.34690
60	1	1	1	-1	35	1	-1	0	0	684.15010*	0.00003	2456.03731	1771.88724
	1	1	1	-1	36	1	-1	0	0	684.34314	-0.00010	2527.74555	1843.40231
	1	1	1	-1	37	1	-1	0	0	684.54458	0.00061	2601.43508	1916.89110

rms = 0.00029 cm⁻¹

$$v_4 + v_5 (\Sigma^-) \leftarrow v_4 (\Pi)$$

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	$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS – CALC	E'	E''
1	1 -1 1 1 0	1 -1 0 0 1	675.78894	0.00012	1196.16293	520.37411
2	1 -1 1 1 1	1 -1 0 0 2	673.79458	0.00009	1198.15393	524.35945
3	1 -1 1 1 2	1 -1 0 0 3	671.79870	0.00016	1202.13592	530.33737
4	1 -1 1 1 3	1 -1 0 0 4	669.80111	0.00007	1208.10885	538.30781
5	1 -1 1 1 4	1 -1 0 0 5	667.80214	0.00010	1216.07268	548.27064
6	1 -1 1 1 5	1 -1 0 0 6	665.80164	0.00003	1226.02734	560.22573
7	1 -1 1 1 6	1 -1 0 0 7	663.79988	0.00003	1237.97275	574.17289
8	1 -1 1 1 7	1 -1 0 0 8	661.79692	0.00006	1251.90880	590.11194
9	1 -1 1 1 8	1 -1 0 0 9	659.79277	0.00005	1267.83537	608.04264
10	1 -1 1 1 9	1 -1 0 0 10	657.78755	-0.00002	1285.75232	627.96474
11	1 -1 1 1 10	1 -1 0 0 11	655.78150	-0.00003	1305.65948	649.87795
12	1 -1 1 1 11	1 -1 0 0 12	653.77462	-0.00008	1327.55666	673.78196
13	1 -1 1 1 12	1 -1 0 0 13	651.76721	-0.00002	1351.44366	699.67642
14	1 -1 1 1 13	1 -1 0 0 14	649.75914	-0.00010	1377.32021	727.56097
15	1 -1 1 1 14	1 -1 0 0 15	647.75072	-0.00013	1405.18605	757.43520
16	1 -1 1 1 15	1 -1 0 0 16	645.74208	-0.00009	1435.04086	789.29869
17	1 -1 1 1 16	1 -1 0 0 17	643.73313	-0.00017	1466.88429	823.15099
18	1 -1 1 1 17	1 -1 0 0 18	641.72417	-0.00017	1500.71593	858.99160
19	1 -1 1 1 18	1 -1 0 0 19	639.71519	-0.00016	1536.53536	896.82001
20	1 -1 1 1 19	1 -1 0 0 20	637.70632	-0.00010	1574.34210	936.63569
21	1 -1 1 1 20	1 -1 0 0 21	635.69752	-0.00006	1614.13563	978.43806
22	1 -1 1 1 21	1 -1 0 0 22	633.68871	-0.00017	1655.91539	1022.22652
23	1 -1 1 1 22	1 -1 0 0 23	631.68020	-0.00014	1699.68079	1068.00045
24	1 -1 1 1 23	1 -1 0 0 24	629.67193	-0.00007	1745.43120	1115.75919
25	1 -1 1 1 24	1 -1 0 0 25	627.66377	-0.00010	1793.16594	1165.50207
26	1 -1 1 1 25	1 -1 0 0 26	625.65593	-0.00003	1842.88432	1217.22835
27	1 -1 1 1 26	1 -1 0 0 27	623.64839	0.00010	1894.58561	1270.93732
28	1 -1 1 1 27	1 -1 0 0 28	621.64086	0.00002	1948.26904	1326.62819
29	1 -1 1 1 28	1 -1 0 0 29	619.63365	0.00000	2003.93383	1384.30018
30	1 -1 1 1 29	1 -1 0 0 30	617.62776	0.00106	2061.57915	1443.95245W
31	1 -1 1 1 30	1 -1 0 0 31	615.62011	0.00010	2121.20417	1505.58415
32	1 -1 1 1 31	1 -1 0 0 32	613.61327	-0.00032	2182.80800	1569.19441
33	1 -1 1 1 32	1 -1 0 0 33	611.60770	0.00026	2246.38975	1634.78230
34	1 -1 1 1 2	1 -1 0 0 1	681.76230*	0.00050	1202.13592	520.37411
35	1 -1 1 1 3	1 -1 0 0 2	683.75093*	0.00153	1208.10885	524.35945W
36	1 -1 1 1 4	1 -1 0 0 3	685.73430*	-0.00100	1216.07268	530.33737W
37	1 -1 1 1 5	1 -1 0 0 4	687.71871	-0.00082	1226.02734	538.30781
38	1 -1 1 1 6	1 -1 0 0 5	689.70207	-0.00003	1237.97275	548.27064
39	1 -1 1 1 7	1 -1 0 0 6	691.68301	-0.00006	1251.90880	560.22573
40	1 -1 1 1 8	1 -1 0 0 7	693.66245	-0.00002	1267.83537	574.17289
41	1 -1 1 1 9	1 -1 0 0 8	695.64035	-0.00002	1285.75232	590.11194
42	1 -1 1 1 10	1 -1 0 0 9	697.61678	-0.00005	1305.65948	608.04264
43	1 -1 1 1 11	1 -1 0 0 10	699.59192	0.00000	1327.55666	627.96474
44	1 -1 1 1 12	1 -1 0 0 11	701.56559	-0.00011	1351.44366	649.87795
45	1 -1 1 1 13	1 -1 0 0 12	703.53818	-0.00007	1377.32021	673.78196
46	1 -1 1 1 14	1 -1 0 0 13	705.50949	-0.00014	1405.18605	699.67642
47	1 -1 1 1 15	1 -1 0 0 14	707.47978	-0.00011	1435.04086	727.56097
48	1 -1 1 1 16	1 -1 0 0 15	709.44896	-0.00012	1466.88429	757.43520
49	1 -1 1 1 17	1 -1 0 0 16	711.41711	-0.00013	1500.71593	789.29869
50	1 -1 1 1 18	1 -1 0 0 17	713.38418	-0.00020	1536.53536	823.15099
51	1 -1 1 1 19	1 -1 0 0 18	715.35035	-0.00016	1574.34210	858.99160
52	1 -1 1 1 20	1 -1 0 0 19	717.31552	-0.00010	1614.13563	896.82001
53	1 -1 1 1 21	1 -1 0 0 20	719.27965	-0.00006	1655.91539	936.63569
54	1 -1 1 1 22	1 -1 0 0 21	721.24259	-0.00015	1699.68079	978.43806
55	1 -1 1 1 23	1 -1 0 0 22	723.20460	-0.00008	1745.43120	1022.22652
56	1 -1 1 1 24	1 -1 0 0 23	725.16538	-0.00011	1793.16594	1068.00045
57	1 -1 1 1 25	1 -1 0 0 24	727.12510	-0.00003	1842.88432	1115.75919
58	1 -1 1 1 26	1 -1 0 0 25	729.08352	-0.00002	1894.58561	1165.50207
59	1 -1 1 1 27	1 -1 0 0 26	731.04042	-0.00026	1948.26904	1217.22835
60	1 -1 1 1 28	1 -1 0 0 27	732.99654	0.00003	2003.93383	1270.93732
	1 -1 1 1 29	1 -1 0 0 28	734.95102	0.00006	2061.57915	1326.62819
	1 -1 1 1 30	1 -1 0 0 29	736.90417	0.00018	2121.20417	1384.30018
	1 -1 1 1 31	1 -1 0 0 30	738.85577	0.00022	2182.80800	1443.95245
	1 -1 1 1 32	1 -1 0 0 31	740.80585	0.00026	2246.38975	1505.58415
	1 -1 1 1 33	1 -1 0 0 32	742.75432	0.00025	2311.94848	1569.19441
	1 -1 1 1 34	1 -1 0 0 33	744.70136	0.00043	2379.48324	1634.78230
	1 -1 1 1 35	1 -1 0 0 34	746.64660	0.00044	2448.99304	1702.34690

1	-1	1	1	36	1	-1	0	0	35	748.59023	0.00058	2520.47689	1771.88724
1	-1	1	1	37	1	-1	0	0	36	750.53210	0.00068	2593.93373	1843.40231
1	-1	1	1	1	1	1	0	0	1	677.78899	0.00029	1198.15393	520.36524
1	-1	1	1	2	1	1	0	0	2	677.80350	0.00040	1202.13592	524.33282
1	-1	1	1	4	1	1	0	0	4	677.85323	-0.00039	1216.07268	538.21906
1	-1	1	1	5	1	1	0	0	5	677.89006	0.00025	1226.02734	548.13753
1	-1	1	1	6	1	1	0	0	6	677.93270*	-0.00066	1237.97275	560.03938
1	-1	1	1	7	1	1	0	0	7	677.98370*	-0.00063	1251.90880	573.92447
1	-1	1	1	8	1	1	0	0	8	678.04298	0.00019	1267.83537	589.79258
1	-1	1	1	9	1	1	0	0	9	678.10872	-0.00009	1285.75232	607.64350
1	-1	1	1	10	1	1	0	0	10	678.18251	0.00002	1305.65948	627.47699
1	-1	1	1	11	1	1	0	0	11	678.26389	-0.00002	1327.55666	649.29275
1	-1	1	1	12	1	1	0	0	12	678.35317	0.00002	1351.44366	673.09051
1	-1	1	1	13	1	1	0	0	13	678.45031	0.00001	1377.32021	698.86991
1	-1	1	1	14	1	1	0	0	14	678.55675*	0.00130	1405.18605	726.63060W
1	-1	1	1	15	1	1	0	0	15	678.66770*	-0.00096	1435.04086	756.37220
1	-1	1	1	16	1	1	0	0	16	678.78989	-0.00010	1466.88429	788.09430
1	-1	1	1	17	1	1	0	0	17	678.91931	-0.00018	1500.71593	821.79644
1	-1	1	1	18	1	1	0	0	18	679.05700	-0.00020	1536.53536	857.47816
1	-1	1	1	19	1	1	0	0	19	679.20294	-0.00019	1574.34210	895.13897
1	-1	1	1	20	1	1	0	0	20	679.35710	-0.00019	1614.13563	934.77834
1	-1	1	1	21	1	1	0	0	21	679.51953	-0.00014	1655.91539	976.39572
1	-1	1	1	22	1	1	0	0	22	679.68780	-0.00246	1699.68079	1019.99053W
1	-1	1	1	23	1	1	0	0	23	679.86889	-0.00014	1745.43120	1065.56217
1	-1	1	1	24	1	1	0	0	24	680.05415	-0.00180	1793.16594	1113.10999W
1	-1	1	1	25	1	1	0	0	25	680.25092	-0.00005	1842.88432	1162.63334
1	-1	1	1	26	1	1	0	0	26	680.45397	-0.00010	1894.58561	1214.13154
1	-1	1	1	27	1	1	0	0	27	680.66502	-0.00016	1948.26904	1267.60385

rms = 0.00020 cm⁻¹ $v_4 + v_5 (\Delta) \leftarrow v_4 (\Pi)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 2	1 1 0 0 1	681.35686	-0.00009	1201.72219	520.36524
1 1 1 1 3	1 1 0 0 2	683.36169	-0.00018	1207.69469	524.33282
1 1 1 1 4	1 1 0 0 3	685.37322	-0.00017	1215.65751	530.28412
1 1 1 1 5	1 1 0 0 4	687.39099	-0.00017	1225.61022	538.21906
1 1 1 1 6	1 1 0 0 5	689.41459	-0.00016	1237.55228	548.13753
1 1 1 1 7	1 1 0 0 6	691.44356	-0.00010	1251.48305	560.03938
1 1 1 1 8	1 1 0 0 7	693.47719	-0.00011	1267.40177	573.92447
1 1 1 1 9	1 1 0 0 8	695.51489	-0.00014	1285.30761	589.79258
1 1 1 1 10	1 1 0 0 9	697.55603	-0.00010	1305.19963	607.64350
1 1 1 1 11	1 1 0 0 10	699.59969	-0.00015	1327.07683	627.47699
1 1 1 1 12	1 1 0 0 11	701.64523	-0.00014	1350.93813	649.29275
1 1 1 1 13	1 1 0 0 12	703.69180	-0.00010	1376.78240	673.09051
1 1 1 1 14	1 1 0 0 13	705.73852	-0.00007	1404.60850	698.86991
1 1 1 1 15	1 1 0 0 14	707.78459	-0.00007	1434.41526	726.63060
1 1 1 1 17	1 1 0 0 16	711.87182	-0.00002	1499.96614	788.09430
1 1 1 1 18	1 1 0 0 17	713.91159	-0.00001	1535.70804	821.79644
1 1 1 1 19	1 1 0 0 18	715.94800	-0.00003	1573.42620	857.47816
1 1 1 1 20	1 1 0 0 19	717.98064	-0.00001	1613.11962	895.13897
1 1 1 1 21	1 1 0 0 20	720.00899	-0.00010	1654.78743	934.77834
1 1 1 1 22	1 1 0 0 21	722.03304	-0.00001	1698.42877	976.39572
1 1 1 1 23	1 1 0 0 22	724.05231	-0.00002	1744.04287	1019.99053
1 1 1 1 24	1 1 0 0 23	726.06684	0.00001	1791.62900	1065.56217
1 1 1 1 25	1 1 0 0 24	728.07647	-0.00001	1841.18647	1113.10999
1 1 1 1 26	1 1 0 0 25	730.08133	0.00005	1892.71462	1162.63334
1 1 1 1 27	1 1 0 0 26	732.08125	-0.00003	1946.21281	1214.13154
1 1 1 1 28	1 1 0 0 27	734.07656	0.00000	2001.68041	1267.60385
1 1 1 1 29	1 1 0 0 28	736.06719	-0.00004	2059.11678	1323.04955
1 1 1 1 30	1 1 0 0 29	738.05332	-0.00008	2118.52125	1380.46786
1 1 1 1 31	1 1 0 0 30	740.03515	-0.00006	2179.89318	1439.85797
1 1 1 1 32	1 1 0 0 31	742.01276	-0.00002	2243.23185	1501.21907
1 1 1 1 33	1 1 0 0 32	743.98624	-0.00002	2308.53656	1564.55030
1 1 1 1 34	1 1 0 0 33	745.95570	-0.00002	2375.80655	1629.85078

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1	1	1	1	35	1	1	0	0	34	747.92134	-0.00010	2445.04104	1697.11961
1	1	1	1	36	1	1	0	0	35	749.88310	-0.00027	2516.23921	1766.35584
1	1	1	1	37	1	1	0	0	36	751.84140	-0.00029	2589.40020	1837.55852
2	1	1	1	2	1	1	0	0	3	671.43798	-0.00009	1201.72219	530.28412
3	1	1	1	3	1	1	0	0	4	669.47543	-0.00020	1207.69469	538.21906
4	1	1	1	4	1	1	0	0	5	667.51982	-0.00016	1215.65751	548.13753
5	1	1	1	5	1	1	0	0	6	665.57073	-0.00010	1225.61022	560.03938
6	1	1	1	6	1	1	0	0	7	663.62766	-0.00015	1237.55228	573.92447
7	1	1	1	7	1	1	0	0	8	661.69138	0.00091	1251.48305	589.79258
8	1	1	1	8	1	1	0	0	9	659.75813	-0.00014	1267.40177	607.64350
9	1	1	1	9	1	1	0	0	10	657.83053	-0.00009	1285.30761	627.47699
10	1	1	1	10	1	1	0	0	11	655.90678	-0.00010	1305.19963	649.29275
11	1	1	1	11	1	1	0	0	12	653.98620	-0.00012	1327.07683	673.09051
12	1	1	1	12	1	1	0	0	13	652.06858	0.00036	1350.93813	698.86991
13	1	1	1	13	1	1	0	0	14	650.15164	-0.00016	1376.78240	726.63060
14	1	1	1	14	1	1	0	0	15	648.23613	-0.00017	1404.60850	756.37220
15	1	1	1	15	1	1	0	0	16	646.32091	-0.00005	1434.41526	788.09430
16	1	1	1	16	1	1	0	0	17	644.40502	-0.00006	1466.20152	821.79644
17	1	1	1	17	1	1	0	0	18	642.48791	-0.00007	1499.96614	857.47816
18	1	1	1	18	1	1	0	0	19	640.56902	-0.00005	1535.70804	895.13897
19	1	1	1	19	1	1	0	0	20	638.64775	-0.00010	1573.42620	934.77834
20	1	1	1	20	1	1	0	0	21	636.72385	-0.00005	1613.11962	976.39572
21	1	1	1	21	1	1	0	0	22	634.79693	0.00003	1654.78743	1019.99053
22	1	1	1	22	1	1	0	0	23	632.86660	0.00000	1698.42877	1065.56217
23	1	1	1	23	1	1	0	0	24	630.93286	-0.00002	1744.04287	1113.10999
24	1	1	1	24	1	1	0	0	25	628.99564	-0.00001	1791.62900	1162.63334
25	1	1	1	25	1	1	0	0	26	627.05493	0.00000	1841.18647	1214.13154
26	1	1	1	26	1	1	0	0	27	625.11078	0.00001	1892.71462	1267.60385
27	1	1	1	27	1	1	0	0	28	623.16322	-0.00004	1946.21281	1323.04955
28	1	1	1	28	1	1	0	0	29	621.21256	0.00000	2001.68041	1380.46786
29	1	1	1	29	1	1	0	0	30	619.25875	-0.00005	2059.11678	1439.85797
30	1	1	1	30	1	1	0	0	31	617.30207	-0.00011	2118.52125	1501.21907
31	1	1	1	31	1	1	0	0	32	615.34289	0.00001	2179.89318	1564.55030
32	1	1	1	32	1	1	0	0	33	613.38075	-0.00032	2243.23185	1629.85078
33	1	1	1	33	1	1	0	0	34	611.41690	-0.00006	2308.53656	1697.11961
34	1	1	1	34	1	1	0	0	35	609.45004	-0.00067	2375.80655	1766.35584
35	1	1	1	2	1	-1	0	0	2	677.36257	-0.00017	1201.72219	524.35945
36	1	1	1	3	1	-1	0	0	3	677.35683	-0.00048	1207.69469	530.33737
37	1	1	1	4	1	-1	0	0	4	677.34963	-0.00007	1215.65751	538.30781
38	1	1	1	5	1	-1	0	0	5	677.33943	-0.00015	1225.61022	548.27064
39	1	1	1	6	1	-1	0	0	6	677.32642	-0.00013	1237.55228	560.22573
40	1	1	1	7	1	-1	0	0	7	677.30994	-0.00021	1251.48305	574.17289
41	1	1	1	8	1	-1	0	0	8	677.28983	0.00000	1267.40177	590.11194
42	1	1	1	9	1	-1	0	0	9	677.26485	-0.00011	1285.30761	608.04264
43	1	1	1	10	1	-1	0	0	10	677.23482	-0.00007	1305.19963	627.96474
44	1	1	1	11	1	-1	0	0	11	677.19890	0.00002	1327.07683	649.87795
45	1	1	1	12	1	-1	0	0	12	677.15609	-0.00008	1350.93813	673.78196
46	1	1	1	13	1	-1	0	0	13	677.10575	-0.00023	1376.78240	699.67642
47	1	1	1	14	1	-1	0	0	14	677.04754	0.00001	1404.60850	727.56097
48	1	1	1	15	1	-1	0	0	15	676.97959	-0.00047	1434.41526	757.43520
49	1	1	1	16	1	-1	0	0	16	676.90293	0.00011	1466.20152	789.29869
50	1	1	1	17	1	-1	0	0	17	676.81519	0.00004	1499.96614	823.15099
51	1	1	1	18	1	-1	0	0	18	676.71654	0.00009	1535.70804	858.99160
52	1	1	1	19	1	-1	0	0	19	676.60619	0.00000	1573.42620	896.82001
53	1	1	1	20	1	-1	0	0	20	676.48411	0.00017	1613.11962	936.63569
54	1	1	1	21	1	-1	0	0	21	676.34952	0.00015	1654.78743	978.43806
55	1	1	1	22	1	-1	0	0	22	676.20274	0.00049	1698.42877	1022.22652
56	1	1	1	23	1	-1	0	0	23	676.04260	0.00018	1744.04287	1068.00045
57	1	1	1	24	1	-1	0	0	24	675.86992	0.00012	1791.62900	1115.75919
58	1	1	1	25	1	-1	0	0	25	675.68453	0.00013	1841.18647	1165.50207
59	1	1	1	26	1	-1	0	0	26	675.48641	0.00014	1892.71462	1217.22835
60	1	1	1	27	1	-1	0	0	27	675.27339*	-0.00210	1946.21281	1270.93732W
	1	1	1	28	1	-1	0	0	28	675.05233	0.00011	2001.68041	1326.62819
	1	1	1	29	1	-1	0	0	29	674.81644	-0.00016	2059.11678	1384.30018
	1	1	1	30	1	-1	0	0	30	674.56900	0.00020	2118.52125	1443.95245
	1	-1	1	-1	2	1	-1	0	1	681.34796	-0.00019	1201.72226	520.37411
	1	-1	1	-1	3	1	-1	0	2	683.33551	-0.00007	1207.69503	524.35945
	1	-1	1	-1	4	1	-1	0	3	685.32106	-0.00010	1215.65854	530.33737
	1	-1	1	-1	5	1	-1	0	4	687.30464	-0.00017	1225.61262	538.30781

1	-1	1	-1	6	1	-1	0	0	5	689.28625	-0.00019	1237.55708	548.27064
2	-1	1	-1	7	1	-1	0	0	6	691.26584	-0.00012	1251.49169	560.22573
3	-1	1	-1	8	1	-1	0	0	7	693.24318	-0.00008	1267.41616	574.17289
4	-1	1	-1	9	1	-1	0	0	8	695.21846	0.00023	1285.33018	590.11194
5	-1	1	-1	10	1	-1	0	0	9	697.19063	-0.00013	1305.23340	608.04264
6	-1	1	-1	11	1	-1	0	0	10	699.16060	-0.00011	1327.12545	627.96474
7	-1	1	-1	12	1	-1	0	0	11	701.12797	0.00000	1351.00592	649.87795
8	-1	1	-1	13	1	-1	0	0	12	703.09238	-0.00003	1376.87436	673.78196
9	-1	1	-1	14	1	-1	0	0	13	705.05388	-0.00003	1404.73033	699.67642
10	-1	1	-1	15	1	-1	0	0	14	707.01236	-0.00001	1434.57334	727.56097
11	-1	1	-1	16	1	-1	0	0	15	708.96763	-0.00006	1466.40289	757.43520
12	-1	1	-1	17	1	-1	0	0	16	710.91986	0.00009	1500.21846	789.29869
13	-1	1	-1	18	1	-1	0	0	17	712.86852	-0.00003	1536.01954	823.15099
14	-1	1	-1	19	1	-1	0	0	18	714.81395	-0.00001	1573.80556	858.99160
15	-1	1	-1	20	1	-1	0	0	19	716.75581	-0.00015	1613.57597	896.82001
16	-1	1	-1	21	1	-1	0	0	20	718.69451	-0.00001	1655.33020	936.63569
17	-1	1	-1	22	1	-1	0	0	21	720.62953	-0.00006	1699.06765	978.43806
18	-1	1	-1	23	1	-1	0	0	22	722.56110	-0.00008	1744.78769	1022.22652
19	-1	1	-1	24	1	-1	0	0	23	724.48920	-0.00005	1792.48970	1068.00045
20	-1	1	-1	25	1	-1	0	0	24	726.41383	0.00001	1842.17301	1115.75919
21	-1	1	-1	26	1	-1	0	0	25	728.33473	-0.00014	1893.83694	1165.50207
22	-1	1	-1	27	1	-1	0	0	26	730.25217	-0.00023	1947.48076	1217.22835
23	-1	1	-1	28	1	-1	0	0	27	732.16640	-0.00002	2003.10374	1270.93732
24	-1	1	-1	2	1	-1	0	0	3	671.38949*	0.00460	1201.72226	530.33737W
25	-1	1	-1	3	1	-1	0	0	4	669.38704	-0.00018	1207.69503	538.30781
26	-1	1	-1	4	1	-1	0	0	5	667.38770	-0.00019	1215.65854	548.27064
27	-1	1	-1	5	1	-1	0	0	6	665.38613	-0.00076	1225.61262	560.22573
28	-1	1	-1	6	1	-1	0	0	7	663.38412	-0.00007	1237.55708	574.17289
29	-1	1	-1	7	1	-1	0	0	8	661.37959	-0.00016	1251.49169	590.11194
30	-1	1	-1	8	1	-1	0	0	9	659.38064	0.00713	1267.41616	608.04264W
31	-1	1	-1	9	1	-1	0	0	10	657.36530	-0.00013	1285.33018	627.96474
32	-1	1	-1	10	1	-1	0	0	11	655.35538	-0.00007	1305.23340	649.87795
33	-1	1	-1	11	1	-1	0	0	12	653.34339	-0.00010	1327.12545	673.78196
34	-1	1	-1	12	1	-1	0	0	13	651.32947	-0.00003	1351.00592	699.67642
35	-1	1	-1	13	1	-1	0	0	14	649.31334	-0.00006	1376.87436	727.56097
36	-1	1	-1	14	1	-1	0	0	15	647.29517	0.00004	1404.73033	757.43520
37	-1	1	-1	15	1	-1	0	0	16	645.27467	0.00002	1434.57334	789.29869
38	-1	1	-1	16	1	-1	0	0	17	643.25195	0.00005	1466.40289	823.15099
39	-1	1	-1	17	1	-1	0	0	18	641.22681	-0.00006	1500.21846	858.99160
40	-1	1	-1	18	1	-1	0	0	19	639.19807*	-0.00146	1536.01954	896.82001W
41	-1	1	-1	19	1	-1	0	0	20	637.16987	0.00000	1573.80556	936.63569
42	-1	1	-1	20	1	-1	0	0	21	635.13804	0.00012	1613.57597	978.43806
43	-1	1	-1	21	1	-1	0	0	22	633.10372	0.00004	1655.33020	1022.22652
44	-1	1	-1	22	1	-1	0	0	23	631.06687	-0.00033	1699.06765	1068.00045
45	-1	1	-1	23	1	-1	0	0	24	629.02889	0.00039	1744.78769	1115.75919
46	-1	1	-1	2	1	1	0	0	2	677.38932	-0.00012	1201.72226	524.33282
47	-1	1	-1	3	1	1	0	0	3	677.41080	-0.00011	1207.69503	530.28412
48	-1	1	-1	4	1	1	0	0	4	677.43937	-0.00011	1215.65854	538.21906
49	-1	1	-1	5	1	1	0	0	5	677.47490	-0.00020	1225.61262	548.13753
50	-1	1	-1	6	1	1	0	0	6	677.51751	-0.00019	1237.55708	560.03938
51	-1	1	-1	7	1	1	0	0	7	677.56695	-0.00027	1251.49169	573.92447
52	-1	1	-1	8	1	1	0	0	8	677.62345	-0.00013	1267.41616	589.79258
53	-1	1	-1	9	1	1	0	0	9	677.68651	-0.00016	1285.33018	607.64350
54	-1	1	-1	10	1	1	0	0	10	677.75629	-0.00013	1305.23340	627.47699
55	-1	1	-1	11	1	1	0	0	11	677.83315	0.00045	1327.12545	649.29275
56	-1	1	-1	12	1	1	0	0	12	677.91521	-0.00020	1351.00592	673.09051
57	-1	1	-1	13	1	1	0	0	13	678.00428	-0.00018	1376.87436	698.86991
58	-1	1	-1	14	1	1	0	0	14	678.09858	-0.00115	1404.73033	726.63060W
59	-1	1	-1	15	1	1	0	0	15	678.20159	0.00046	1434.57334	756.37220
60	-1	1	-1	16	1	1	0	0	16	678.30808	-0.00051	1466.40289	788.09430
61	-1	1	-1	17	1	1	0	0	17	678.42219	0.00017	1500.21846	821.79644
62	-1	1	-1	18	1	1	0	0	18	678.54133	-0.00004	1536.01954	857.47816
63	-1	1	-1	20	1	1	0	0	20	678.79759	-0.00004	1613.57597	934.77834
64	-1	1	-1	21	1	1	0	0	21	678.93429	-0.00019	1655.33020	976.39572
65	-1	1	-1	22	1	1	0	0	22	679.07687	-0.00024	1699.06765	1019.99053
66	-1	1	-1	23	1	1	0	0	23	679.22527	-0.00026	1744.78769	1065.56217
67	-1	1	-1	24	1	1	0	0	24	679.37952	-0.00019	1792.48970	1113.10999
68	-1	1	-1	25	1	1	0	0	25	679.53768*	-0.00019	1842.17301	1162.63334W
69	-1	1	-1	26	1	1	0	0	26	679.70615*	0.00075	1893.83694	1214.13154

1	-1	1	-1	27	1	1	0	0	27	679.87651	-0.00039	1947.48076	1267.60385	
1	-1	1	-1	28	1	1	0	0	28	680.05415	-0.00004	2003.10374	1323.04955	
1	-1	1	-1	29	1	1	0	0	29	680.23685	-0.00041	2060.70512	1380.46786	
2	1	-1	1	-1	30	1	1	0	0	30	680.42555	-0.00057	2120.28409	1439.85797
3	1	-1	1	-1	31	1	1	0	0	31	680.62012	-0.00064	2181.83983	1501.21907
4	1	-1	1	-1	32	1	1	0	0	32	680.82049	-0.00070	2245.37149	1564.55030
5	1	-1	1	-1	33	1	1	0	0	33	681.02584*	-0.00156	2310.87818	1629.85078W
6	1	-1	1	-1	34	1	1	0	0	34	681.23760*	-0.00179	2378.35899	1697.11961W
7	1	-1	1	-1	35	1	1	0	0	35	681.45344*	-0.00371	2447.81298	1766.35584W
8	1	-1	1	-1	36	1	1	0	0	36	681.67991	-0.00076	2519.23919	1837.55852
9	1	-1	1	-1	37	1	1	0	0	37	681.90919	-0.00076	2592.63660	1910.72665

rms = 0.00022 cm⁻¹ $v_4 + v_5 (\Sigma^+) \leftarrow v_5 (\Pi)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 2	0 0 1 1 3	516.76965	0.00020	1206.47085	689.70140
1 1 1 -1 3	0 0 1 1 4	514.81360	0.00015	1212.44377	697.63032
1 1 1 -1 4	0 0 1 1 5	512.86658	-0.00005	1220.40789	707.54126
1 1 1 -1 5	0 0 1 1 6	510.92951	0.00017	1230.36343	719.43409
1 1 1 -1 6	0 0 1 1 7	509.00180	-0.00021	1242.31065	733.30864
1 1 1 -1 7	0 0 1 1 8	507.08696*	0.00184	1256.24984	749.16472W
1 1 1 -1 8	0 0 1 1 9	505.17916	-0.00008	1272.18137	767.00212
1 1 1 -1 9	0 0 1 1 10	503.28510	0.00008	1290.10561	786.82059
1 1 1 -1 10	0 0 1 1 11	501.40256	-0.00057	1310.02298	808.61985
1 1 1 -1 11	0 0 1 1 12	499.53248*	-0.00184	1331.93393	832.39961W
1 1 1 -1 12	0 0 1 1 13	497.67889	-0.00048	1355.83891	858.15954
1 1 1 -1 13	0 0 1 1 14	495.83905	-0.00002	1381.73835	885.89928
1 1 1 -1 14	0 0 1 1 15	494.01374	-0.00048	1409.63267	915.61845
1 1 1 -1 15	0 0 1 1 16	492.20539	-0.00021	1439.52224	947.31664
1 1 1 -1 16	0 0 1 1 17	490.41312	-0.00084	1471.40738	980.99342
1 1 1 -1 17	0 0 1 1 18	488.63970	-0.00027	1505.28829	1016.64832
1 1 1 -1 3	0 0 1 1 2	528.68897	-0.00018	1212.44377	683.75462
1 1 1 -1 4	0 0 1 1 3	530.70588	-0.00061	1220.40789	689.70140
1 1 1 -1 5	0 0 1 1 4	532.73346	0.00035	1230.36343	697.63032
1 1 1 -1 6	0 0 1 1 5	534.76910	-0.00029	1242.31065	707.54126
1 1 1 -1 7	0 0 1 1 6	536.81586	0.00010	1256.24984	719.43409
1 1 1 -1 8	0 0 1 1 7	538.87246	-0.00027	1272.18137	733.30864
1 1 1 -1 9	0 0 1 1 8	540.94185*	0.00097	1290.10561	749.16472
1 1 1 -1 10	0 0 1 1 9	543.02063	-0.00023	1310.02298	767.00212
1 1 1 -1 11	0 0 1 1 10	545.11322	-0.00012	1331.93393	786.82059
1 1 1 -1 12	0 0 1 1 11	547.21875	-0.00030	1355.83891	808.61985
1 1 1 -1 13	0 0 1 1 12	549.33872	-0.00002	1381.73835	832.39961
1 1 1 -1 14	0 0 1 1 13	551.47296	-0.00017	1409.63267	858.15954
1 1 1 -1 15	0 0 1 1 14	553.62310*	0.00013	1439.52224	885.89928
1 1 1 -1 16	0 0 1 1 15	555.78894	0.00001	1471.40738	915.61845
1 1 1 -1 17	0 0 1 1 16	557.97120	-0.00045	1505.28829	947.31664
1 1 1 -1 18	0 0 1 1 17	560.17126	-0.00042	1541.16510	980.99342
1 1 1 -1 19	0 0 1 1 18	562.38940	-0.00011	1579.03782	1016.64832
1 1 1 -1 20	0 0 1 1 19	564.62585	0.00034	1618.90635	1054.28084
1 1 1 -1 21	0 0 1 1 20	566.87921	-0.00076	1660.77045	1093.89049
1 1 1 -1 1	0 0 1 -1 1	522.69125	-0.00065	1202.48900	679.79710
1 1 1 -1 2	0 0 1 -1 2	522.69464	-0.00044	1206.47085	683.77578
1 1 1 -1 3	0 0 1 -1 3	522.70050	0.00045	1212.44377	689.74371
1 1 1 -1 4	0 0 1 -1 4	522.70715	0.00009	1220.40789	697.70083
1 1 1 -1 5	0 0 1 -1 5	522.71680	0.00039	1230.36343	707.64702
1 1 1 -1 7	0 0 1 -1 7	522.74374	-0.00007	1256.24984	733.50603
1 1 1 -1 8	0 0 1 -1 8	522.76326	0.00039	1272.18137	749.41849
1 1 1 -1 9	0 0 1 -1 9	522.78567	-0.00064	1290.10561	767.31930
1 1 1 -1 10	0 0 1 -1 10	522.81220*	-0.00258	1310.02298	787.20820W
1 1 1 -1 11	0 0 1 -1 11	522.84934	0.00033	1331.93393	809.08492
1 1 1 -1 12	0 0 1 -1 12	522.88953	-0.00022	1355.83891	832.94916
1 1 1 -1 13	0 0 1 -1 13	522.93769	-0.00009	1381.73835	858.80057
1 1 1 -1 14	0 0 1 -1 14	522.99343	-0.00044	1409.63267	886.63880
1 1 1 -1 15	0 0 1 -1 15	523.05224	-0.00039	1439.52224	916.46345

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1	1	1	-1	16	0	0	1	-1	16	523.13311	-0.00015	1471.40738	948.27412
1	1	1	-1	17	0	0	1	-1	17	523.21788	-0.00006	1505.28829	982.07035
1	1	1	-1	18	0	0	1	-1	18	523.31388	0.00045	1541.16510	1017.85167
1	1	1	-1	19	0	0	1	-1	19	523.41996	-0.00028	1579.03782	1055.61759
1	1	1	-1	20	0	0	1	-1	20	523.53864	-0.00015	1618.90635	1095.36757
1	1	1	-1	21	0	0	1	-1	21	523.66934	-0.00006	1660.77045	1137.10105
1	1	1	-1	22	0	0	1	-1	22	523.81221	-0.00010	1704.62977	1180.81746
1	1	1	-1	23	0	0	1	-1	23	523.96738	-0.00027	1750.48383	1226.51618
1	1	1	-1	24	0	0	1	-1	24	524.13522	-0.00027	1798.33206	1274.19657
1	1	1	-1	25	0	0	1	-1	25	524.31573	-0.00008	1848.17378	1323.85797
1	1	1	-1	26	0	0	1	-1	26	524.50910	0.00054	1900.00824	1375.49968
1	1	1	-1	27	0	0	1	-1	27	524.71368	0.00005	1953.83461	1429.12098

rms = 0.00034 cm⁻¹

$v_4 + v_5 (\Sigma^-) \leftarrow v_5 (\Pi)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 1 1 5	0 0 1 -1 6	506.44549	0.00030	1226.02734	719.58215
1 -1 1 1 6	0 0 1 -1 7	504.46677	0.00006	1237.97275	733.50603
1 -1 1 1 7	0 0 1 -1 8	502.49026	-0.00004	1251.90880	749.41849
1 -1 1 1 8	0 0 1 -1 9	500.51585	-0.00022	1267.83537	767.31930
1 -1 1 1 9	0 0 1 -1 10	498.54474	0.00063	1285.75232	787.20820
1 -1 1 1 10	0 0 1 -1 11	496.57474	0.00019	1305.65948	809.08492
1 -1 1 1 11	0 0 1 -1 12	494.60740	-0.00011	1327.55666	832.94916
1 -1 1 1 12	0 0 1 -1 13	492.64301	-0.00008	1351.44366	858.80057
1 -1 1 1 14	0 0 1 -1 15	488.72250	-0.00010	1405.18605	916.46345
1 -1 1 1 15	0 0 1 -1 16	486.76698	0.00024	1435.04086	948.27412
1 -1 1 1 17	0 0 1 -1 18	482.86634*	0.00208	1500.71593	1017.85167W
1 -1 1 1 18	0 0 1 -1 19	480.91766	-0.00011	1536.53536	1055.61759
1 -1 1 1 19	0 0 1 -1 20	478.97504	0.00050	1574.34210	1095.36757
1 -1 1 1 20	0 0 1 -1 21	477.03448	-0.00010	1614.13563	1137.10105
1 -1 1 1 4	0 0 1 -1 3	526.32955	0.00058	1216.07268	689.74371
1 -1 1 1 5	0 0 1 -1 4	528.32672	0.00021	1226.02734	697.70083
1 -1 1 1 6	0 0 1 -1 5	530.32538	-0.00034	1237.97275	707.64702
1 -1 1 1 7	0 0 1 -1 6	532.32611	-0.00054	1251.90880	719.58215
1 -1 1 1 8	0 0 1 -1 7	534.32947	0.00014	1267.83537	733.50603
1 -1 1 1 9	0 0 1 -1 8	536.33398	0.00016	1285.75232	749.41849
1 -1 1 1 10	0 0 1 -1 9	538.34006	-0.00012	1305.65948	767.31930
1 -1 1 1 11	0 0 1 -1 10	540.34851	0.00005	1327.55666	787.20820
1 -1 1 1 12	0 0 1 -1 11	542.35825	-0.00048	1351.44366	809.08492
1 -1 1 1 13	0 0 1 -1 12	544.37122	0.00016	1377.32021	832.94916
1 -1 1 1 14	0 0 1 -1 13	546.38525	-0.00024	1405.18605	858.80057
1 -1 1 1 15	0 0 1 -1 14	548.40186	-0.00021	1435.04086	886.63880
1 -1 1 1 17	0 0 1 -1 16	552.44185	0.00004	1500.71593	948.27412
1 -1 1 1 19	0 0 1 -1 18	556.49036	-0.00007	1574.34210	1017.85167
1 -1 1 1 20	0 0 1 -1 19	558.51750	-0.00054	1614.13563	1055.61759
1 -1 1 1 21	0 0 1 -1 20	560.54908*	0.00125	1655.91539	1095.36757W
1 -1 1 1 1	0 0 1 1 1	518.36328	-0.00060	1198.15393	679.79005
1 -1 1 1 2	0 0 1 1 2	518.38121	-0.00009	1202.13592	683.75462
1 -1 1 1 5	0 0 1 1 5	518.48587	-0.00021	1226.02734	707.54126
1 -1 1 1 6	0 0 1 1 6	518.53860	-0.00006	1237.97275	719.43409
1 -1 1 1 7	0 0 1 1 7	518.60002	-0.00014	1251.90880	733.30864
1 -1 1 1 8	0 0 1 1 8	518.67057	-0.00007	1267.83537	749.16472
1 -1 1 1 9	0 0 1 1 9	518.75029	0.00010	1285.75232	767.00212
1 -1 1 1 10	0 0 1 1 10	518.83870	-0.00019	1305.65948	786.82059
1 -1 1 1 11	0 0 1 1 11	518.93677	-0.00004	1327.55666	808.61985
1 -1 1 1 12	0 0 1 1 12	519.04390	-0.00014	1351.44366	832.39961
1 -1 1 1 13	0 0 1 1 13	519.16055	-0.00012	1377.32021	858.15954
1 -1 1 1 14	0 0 1 1 14	519.28679	0.00002	1405.18605	885.89928
1 -1 1 1 15	0 0 1 1 15	519.42182	-0.00059	1435.04086	915.61845
1 -1 1 1 16	0 0 1 1 16	519.56755	-0.00010	1466.88429	947.31664
1 -1 1 1 17	0 0 1 1 17	519.72247	-0.00004	1500.71593	980.99342
1 -1 1 1 18	0 0 1 1 18	519.88675	-0.00030	1536.53536	1016.64832
1 -1 1 1 19	0 0 1 1 19	520.05873*	-0.00253	1574.34210	1054.28084W
1 -1 1 1 20	0 0 1 1 20	520.23709	0.00002	1614.13563	1093.89049

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1	-1	1	1	21	0	0	1	1	21	520.43840	-0.00030	1655.91539	1135.47669
1	-1	1	1	22	0	0	1	1	22	520.64148	-0.00042	1699.68079	1179.03889
1	-1	1	1	24	0	0	1	1	24	521.07764	0.00055	1793.16594	1272.08885

rms = 0.00029 cm⁻¹

$$v_4 + v_5 (\Delta) \leftarrow v_5 (\Pi)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 5	0 0 1 1 6	506.17606	-0.00007	1225.61022	719.43409
1 1 1 1 6	0 0 1 1 7	504.24359	-0.00005	1237.55228	733.30864
1 1 1 1 7	0 0 1 1 8	502.31816	-0.00016	1251.48305	749.16472
1 1 1 1 8	0 0 1 1 9	500.39950	-0.00015	1267.40177	767.00212
1 1 1 1 10	0 0 1 1 11	496.57977	-0.00001	1305.19963	808.61985
1 1 1 1 11	0 0 1 1 12	494.67699	-0.00023	1327.07683	832.39961
1 1 1 1 12	0 0 1 1 13	492.77880	0.00021	1350.93813	858.15954
1 1 1 1 13	0 0 1 1 14	490.88265	-0.00047	1376.78240	885.89928
1 1 1 1 14	0 0 1 1 15	488.99060	0.00055	1404.60850	915.61845
1 1 1 1 15	0 0 1 1 16	487.09850	-0.00012	1434.41526	947.31664
1 1 1 1 16	0 0 1 1 17	485.20832	0.00022	1466.20152	980.99342
1 1 1 1 17	0 0 1 1 18	483.31749	-0.00033	1499.96614	1016.64832
1 1 1 1 18	0 0 1 1 19	481.42714	-0.00006	1535.70804	1054.28084
1 1 1 1 19	0 0 1 1 20	479.53594	0.00023	1573.42620	1093.89049
1 1 1 1 20	0 0 1 1 21	477.64233*	-0.00060	1613.11962	1135.47669
1 1 1 1 21	0 0 1 1 22	475.74911	0.00057	1654.78743	1179.03889
1 1 1 1 22	0 0 1 1 23	473.85262	0.00034	1698.42877	1224.57649
1 1 1 1 23	0 0 1 1 24	471.95428	0.00026	1744.04287	1272.08885
1 1 1 1 24	0 0 1 1 25	470.05398	0.00031	1791.62900	1321.57533
1 1 1 1 2	0 0 1 1 1	521.93188	-0.00026	1201.72219	679.79005
1 1 1 1 3	0 0 1 1 2	523.93984	-0.00023	1207.69469	683.75462
1 1 1 1 5	0 0 1 1 4	527.97980	-0.00010	1225.61022	697.63032
1 1 1 1 6	0 0 1 1 5	530.01088	-0.00014	1237.55228	707.54126
1 1 1 1 7	0 0 1 1 6	532.04872	-0.00024	1251.48305	719.43409
1 1 1 1 8	0 0 1 1 7	534.09302	-0.00011	1267.40177	733.30864
1 1 1 1 9	0 0 1 1 8	536.14280	-0.00008	1285.30761	749.16472
1 1 1 1 10	0 0 1 1 9	538.19733	-0.00018	1305.19963	767.00212
1 1 1 1 11	0 0 1 1 10	540.25609	-0.00015	1327.07683	786.82059
1 1 1 1 12	0 0 1 1 11	542.31817	-0.00010	1350.93813	808.61985
1 1 1 1 13	0 0 1 1 12	544.38280	0.00001	1376.78240	832.39961
1 1 1 1 14	0 0 1 1 13	546.44899	0.00003	1404.60850	858.15954
1 1 1 1 15	0 0 1 1 14	548.51581	-0.00017	1434.41526	885.89928
1 1 1 1 16	0 0 1 1 15	550.58402*	0.00095	1466.20152	915.61845
1 1 1 1 17	0 0 1 1 16	552.64943	-0.00007	1499.96614	947.31664
1 1 1 1 18	0 0 1 1 17	554.71434	-0.00029	1535.70804	980.99342
1 1 1 1 19	0 0 1 1 18	556.77780	-0.00008	1573.42620	1016.64832
1 1 1 1 20	0 0 1 1 19	558.83895	0.00017	1613.11962	1054.28084
1 1 1 1 21	0 0 1 1 20	560.89679	-0.00015	1654.78743	1093.89049
1 1 1 1 22	0 0 1 1 21	562.95189	-0.00019	1698.42877	1135.47669
1 1 1 1 23	0 0 1 1 22	565.00379	-0.00018	1744.04287	1179.03889
1 1 1 1 24	0 0 1 1 23	567.05238	-0.00013	1791.62900	1224.57649
1 1 1 1 25	0 0 1 1 24	569.09741	-0.00021	1841.18647	1272.08885
1 1 1 1 26	0 0 1 1 25	571.13895	-0.00035	1892.71462	1321.57533
1 1 1 1 27	0 0 1 1 26	573.17737	-0.00021	1946.21281	1373.03523
1 1 1 1 28	0 0 1 1 27	575.21179	-0.00076	2001.68041	1426.46786
1 1 1 1 29	0 0 1 1 28	577.24390	-0.00040	2059.11678	1481.87248
1 1 1 1 30	0 0 1 1 29	579.27232	-0.00061	2118.52125	1539.24832
1 1 1 1 2	0 0 1 -1 2	517.94653	0.00011	1201.72219	683.77578
1 1 1 1 3	0 0 1 -1 3	517.95154*	0.00057	1207.69469	689.74371
1 1 1 1 4	0 0 1 -1 4	517.95671	0.00004	1215.65751	697.70083
1 1 1 1 5	0 0 1 -1 5	517.96295	-0.00024	1225.61022	707.64702
1 1 1 1 6	0 0 1 -1 6	517.96988	-0.00025	1237.55228	719.58215
1 1 1 1 7	0 0 1 -1 7	517.97662	-0.00039	1251.48305	733.50603
1 1 1 1 8	0 0 1 -1 8	517.98254	-0.00074	1267.40177	749.41849
1 1 1 1 9	0 0 1 -1 9	517.98900	0.00069	1285.30761	767.31930
1 1 1 1 10	0 0 1 -1 10	517.99137	-0.00006	1305.19963	787.20820
1 1 1 1 11	0 0 1 -1 11	517.99374	-0.00006	1327.07683	809.08492

1	1	1	1	12	0	0	1	-1	12	517.98900	0.00003	1350.93813	832.94916	
2	1	1	1	13	0	0	1	-1	13	517.98254	0.00070	1376.78240	858.80057	
3	1	1	1	14	0	0	1	-1	14	517.96988	0.00017	1404.60850	886.63880	
4	1	1	1	15	0	0	1	-1	15	517.95154	-0.00027	1434.41526	916.46345	
5	1	1	1	16	0	0	1	-1	16	517.92976*	0.00236	1466.20152	948.27412W	
6	1	1	1	17	0	0	1	-1	17	517.89472*	-0.00107	1499.96614	982.07035W	
7	1	1	1	20	0	0	1	-1	20	517.75232	0.00026	1613.11962	1095.36757	
8	1	-1	1	-1	3	0	0	1	-1	4	509.99356	-0.00064	1207.69503	697.70083
9	1	-1	1	-1	4	0	0	1	-1	5	508.01152	0.00001	1215.65854	707.64702
10	1	-1	1	-1	5	0	0	1	-1	6	506.03000	-0.00048	1225.61262	719.58215
11	1	-1	1	-1	6	0	0	1	-1	7	504.05111	0.00006	1237.55708	733.50603
12	1	-1	1	-1	8	0	0	1	-1	9	500.09674	-0.00012	1267.41616	767.31930
13	1	-1	1	-1	9	0	0	1	-1	10	498.12182	-0.00015	1285.33018	787.20820
14	1	-1	1	-1	10	0	0	1	-1	11	496.14835	-0.00013	1305.23340	809.08492
15	1	-1	1	-1	11	0	0	1	-1	12	494.17451*	-0.00179	1327.12545	832.94916W
16	1	-1	1	-1	12	0	0	1	-1	13	492.20539	0.00004	1351.00592	858.80057
17	1	-1	1	-1	13	0	0	1	-1	14	490.23538	-0.00019	1376.87436	886.63880
18	1	-1	1	-1	14	0	0	1	-1	15	488.26723	0.00035	1404.73033	916.46345
19	1	-1	1	-1	15	0	0	1	-1	16	486.29935	0.00013	1434.57334	948.27412
20	1	-1	1	-1	16	0	0	1	-1	17	484.33310	0.00056	1466.40289	982.07035
21	1	-1	1	-1	17	0	0	1	-1	18	482.36718	0.00039	1500.21846	1017.85167
22	1	-1	1	-1	18	0	0	1	-1	19	480.40191	-0.00004	1536.01954	1055.61759
23	1	-1	1	-1	19	0	0	1	-1	20	478.43808	0.00009	1573.80556	1095.36757
24	1	-1	1	-1	20	0	0	1	-1	21	476.47464	-0.00028	1613.57597	1137.10105
25	1	-1	1	-1	21	0	0	1	-1	22	474.51220	-0.00054	1655.33020	1180.81746
26	1	-1	1	-1	22	0	0	1	-1	23	472.55248	0.00101	1699.06765	1226.51618W
27	1	-1	1	-1	2	0	0	1	-1	1	521.92504	-0.00012	1201.72226	679.79710
28	1	-1	1	-1	3	0	0	1	-1	2	523.91880	-0.00045	1207.69503	683.77578
29	1	-1	1	-1	4	0	0	1	-1	3	525.91468	-0.00014	1215.65854	689.74371
30	1	-1	1	-1	5	0	0	1	-1	4	527.91045*	-0.00134	1225.61262	697.70083W
31	1	-1	1	-1	6	0	0	1	-1	5	529.91001	-0.00005	1237.55708	707.64702
32	1	-1	1	-1	7	0	0	1	-1	6	531.90955	0.00001	1251.49169	719.58215
33	1	-1	1	-1	8	0	0	1	-1	7	533.91007	-0.00005	1267.41616	733.50603
34	1	-1	1	-1	9	0	0	1	-1	8	535.91168	0.00000	1285.33018	749.41849
35	1	-1	1	-1	10	0	0	1	-1	9	537.91369	-0.00041	1305.23340	767.31930
36	1	-1	1	-1	11	0	0	1	-1	10	539.91719	-0.00006	1327.12545	787.20820
37	1	-1	1	-1	12	0	0	1	-1	11	541.92086	-0.00014	1351.00592	809.08492
38	1	-1	1	-1	13	0	0	1	-1	12	543.92518	-0.00003	1376.87436	832.94916
39	1	-1	1	-1	14	0	0	1	-1	13	545.92978	0.00002	1404.73033	858.80057
40	1	-1	1	-1	15	0	0	1	-1	14	547.93442	-0.00012	1434.57334	886.63880
41	1	-1	1	-1	16	0	0	1	-1	15	549.93941	-0.00003	1466.40289	916.46345
42	1	-1	1	-1	17	0	0	1	-1	16	551.94445	0.00011	1500.21846	948.27412
43	1	-1	1	-1	18	0	0	1	-1	17	553.94915	-0.00004	1536.01954	982.07035
44	1	-1	1	-1	19	0	0	1	-1	18	555.95381	-0.00008	1573.80556	1017.85167
45	1	-1	1	-1	20	0	0	1	-1	19	557.95846	0.00007	1613.57597	1055.61759
46	1	-1	1	-1	21	0	0	1	-1	20	559.96251	-0.00013	1655.33020	1095.36757
47	1	-1	1	-1	22	0	0	1	-1	21	561.96711	0.00051	1699.06765	1137.10105
48	1	-1	1	-1	23	0	0	1	-1	22	563.96995	-0.00029	1744.78769	1180.81746
49	1	-1	1	-1	24	0	0	1	-1	23	565.97343	-0.00009	1792.48970	1226.51618
50	1	-1	1	-1	25	0	0	1	-1	24	567.97620	-0.00024	1842.17301	1274.19657
51	1	-1	1	-1	26	0	0	1	-1	25	569.97821	-0.00076	1893.83694	1323.85797
52	1	-1	1	-1	27	0	0	1	-1	26	571.98059	-0.00049	1947.48076	1375.49968
53	1	-1	1	-1	28	0	0	1	-1	27	573.98235	-0.00042	2003.10374	1429.12098
54	1	-1	1	-1	29	0	0	1	-1	28	575.98386	-0.00015	2060.70512	1484.72111
55	1	-1	1	-1	30	0	0	1	-1	29	577.98474	-0.00004	2120.28409	1542.29931
56	1	-1	1	-1	4	0	0	1	1	4	518.02867	0.00045	1215.65854	697.63032
57	1	-1	1	-1	5	0	0	1	1	5	518.07129	-0.00007	1225.61262	707.54126
58	1	-1	1	-1	6	0	0	1	1	6	518.12285	-0.00015	1237.55708	719.43409
59	1	-1	1	-1	7	0	0	1	1	7	518.18282	-0.00023	1251.49169	733.30864
60	1	-1	1	-1	8	0	0	1	1	8	518.25139	-0.00004	1267.41616	749.16472
61	1	-1	1	-1	9	0	0	1	1	9	518.32794	-0.00011	1285.33018	767.00212
62	1	-1	1	-1	11	0	0	1	1	11	518.50540	-0.00020	1327.12545	808.61985
63	1	-1	1	-1	12	0	0	1	1	12	518.60644	0.00013	1351.00592	832.39961
64	1	-1	1	-1	13	0	0	1	1	13	518.71498	0.00015	1376.87436	858.15954
65	1	-1	1	-1	14	0	0	1	1	14	518.83108	0.00003	1404.73033	885.89928
66	1	-1	1	-1	15	0	0	1	1	15	518.95496	0.00007	1434.57334	915.61845
67	1	-1	1	-1	16	0	0	1	1	16	519.08854*	0.00229	1466.40289	947.31664W
68	1	-1	1	-1	17	0	0	1	1	17	519.22498	-0.00007	1500.21846	980.99342
69	1	-1	1	-1	18	0	0	1	1	18	519.37236*	0.00114	1536.01954	1016.64832W

1 -1 1 -1 19 0 0 1 1 19 519.52479 0.00007 1573.80556 1054.28084

rms = 0.00029 cm⁻¹

$2\nu_5(\Sigma^+) \leftarrow \nu_5(\Pi)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 2	0 0 1 1 1	668.40380	-0.00006	1348.19391	679.79005
0 0 2 0 3	0 0 1 1 2	670.40655	-0.00005	1354.16122	683.75462
0 0 2 0 4	0 0 1 1 3	672.41598	-0.00005	1362.11743	689.70140
0 0 2 0 5	0 0 1 1 4	674.43171	-0.00031	1372.06234	697.63032
0 0 2 0 6	0 0 1 1 5	676.45450	0.00004	1383.99572	707.54126
0 0 2 0 7	0 0 1 1 6	678.48351	0.00030	1397.91730	719.43409
0 0 2 0 8	0 0 1 1 7	680.51817	0.00006	1413.82675	733.30864
0 0 2 0 9	0 0 1 1 8	682.55876	-0.00022	1431.72370	749.16472
0 0 2 0 10	0 0 1 1 9	684.60558	-0.00004	1451.60774	767.00212
0 0 2 0 11	0 0 1 1 10	686.65777	-0.00004	1473.47840	786.82059
0 0 2 0 12	0 0 1 1 11	688.71522	-0.00010	1497.33518	808.61985
0 0 2 0 13	0 0 1 1 12	690.77780	-0.00010	1523.17752	832.39961
0 0 2 0 14	0 0 1 1 13	692.84518	-0.00010	1551.00481	858.15954
0 0 2 0 15	0 0 1 1 14	694.91709	-0.00006	1580.81643	885.89928
0 0 2 0 16	0 0 1 1 15	696.99311	-0.00011	1612.61167	915.61845
0 0 2 0 17	0 0 1 1 16	699.07310	-0.00007	1646.38981	947.31664
0 0 2 0 18	0 0 1 1 17	701.15648	-0.00017	1682.15007	980.99342
0 0 2 0 19	0 0 1 1 18	703.24324	-0.00007	1719.89163	1016.64832
0 0 2 0 20	0 0 1 1 19	705.33265	-0.00013	1759.61363	1054.28084
0 0 2 0 21	0 0 1 1 20	707.42463	-0.00005	1801.31517	1093.89049
0 0 2 0 22	0 0 1 1 21	709.51849	-0.00013	1844.99532	1135.47669
0 0 2 0 23	0 0 1 1 22	711.61403	-0.00017	1890.65309	1179.03889
0 0 2 0 24	0 0 1 1 23	713.71086	-0.00015	1938.28750	1224.57649
0 0 2 0 25	0 0 1 1 24	715.80847	-0.00016	1987.89749	1272.08885
0 0 2 0 26	0 0 1 1 25	717.90651	-0.00015	2039.48198	1321.57533
0 0 2 0 27	0 0 1 1 26	720.00490*	0.00024	2093.03990	1373.03523
0 0 2 0 28	0 0 1 1 27	722.10204	-0.00020	2148.57010	1426.46786
0 0 2 0 29	0 0 1 1 28	724.19888	-0.00008	2206.07144	1481.87248
0 0 2 0 30	0 0 1 1 29	726.29429	-0.00014	2265.54275	1539.24832
0 0 2 0 31	0 0 1 1 30	728.38805	-0.00020	2326.98286	1598.59460
0 0 2 0 32	0 0 1 1 31	730.47977	-0.00027	2390.39054	1659.91050
0 0 2 0 33	0 0 1 1 32	732.56936	-0.00007	2455.76460	1723.19517
0 0 2 0 34	0 0 1 1 33	734.65565	-0.00041	2523.10381	1788.44775
0 0 2 0 35	0 0 1 1 34	736.73970	0.00011	2592.40692	1855.66733
0 0 2 0 36	0 0 1 1 35	738.81990	0.00018	2663.67271	1924.85299
0 0 2 0 6	0 0 1 -1 6	664.41003*	-0.00354	1383.99572	719.58215W
0 0 2 0 7	0 0 1 -1 7	664.41003*	-0.00123	1397.91730	733.50603W
0 0 2 0 8	0 0 1 -1 8	664.41003*	0.00177	1413.82675	749.41849W
0 0 2 0 9	0 0 1 -1 9	664.40551	0.00111	1431.72370	767.31930W
0 0 2 0 10	0 0 1 -1 10	664.40014	0.00060	1451.60774	787.20820
0 0 2 0 11	0 0 1 -1 11	664.39371	0.00023	1473.47840	809.08492
0 0 2 0 12	0 0 1 -1 12	664.38613	0.00011	1497.33518	832.94916
0 0 2 0 13	0 0 1 -1 13	664.37696	0.00001	1523.17752	858.80057
0 0 2 0 14	0 0 1 -1 14	664.36603	0.00001	1551.00481	886.63880
0 0 2 0 15	0 0 1 -1 15	664.35298	0.00000	1580.81643	916.46345
0 0 2 0 16	0 0 1 -1 16	664.33759	0.00004	1612.61167	948.27412
0 0 2 0 17	0 0 1 -1 17	664.31947	0.00001	1646.38981	982.07035
0 0 2 0 18	0 0 1 -1 18	664.29842	0.00002	1682.15007	1017.85167
0 0 2 0 19	0 0 1 -1 19	664.27404	0.00000	1719.89163	1055.61759
0 0 2 0 20	0 0 1 -1 20	664.24604	-0.00002	1759.61363	1095.36757
0 0 2 0 21	0 0 1 -1 21	664.21408	-0.00004	1801.31517	1137.10105
0 0 2 0 22	0 0 1 -1 22	664.17786	0.00000	1844.99532	1180.81746
0 0 2 0 23	0 0 1 -1 23	664.13690	-0.00002	1890.65309	1226.51618
0 0 2 0 24	0 0 1 -1 24	664.09085	-0.00008	1938.28750	1274.19657
0 0 2 0 25	0 0 1 -1 25	664.03953	0.00001	1987.89749	1323.85797
0 0 2 0 26	0 0 1 -1 26	663.98229	-0.00002	2039.48198	1375.49968
0 0 2 0 28	0 0 1 -1 28	663.84910	0.00012	2148.57010	1484.72111
0 0 2 0 29	0 0 1 -1 29	663.77215	0.00002	2206.07144	1542.29931
0 0 2 0 30	0 0 1 -1 30	663.65427	0.00002	2265.54275	1601.85477

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1	0	0	2	0	31	0	0	1	-1	31	663.59612	-0.00009	2326.98286	1663.38664
2	0	0	2	0	32	0	0	1	-1	32	663.49650	0.00004	2390.39054	1726.89408
3	0	0	2	0	34	0	0	1	-1	34	663.27184	0.00011	2523.10381	1859.83208
4	0	0	2	0	36	0	0	1	-1	36	663.01261	0.00121	2663.67271	2000.66131W
5	0	0	2	0	0	0	0	1	1	1	662.43662	0.00022	1342.22645	679.79005
6	0	0	2	0	1	0	0	1	1	2	660.46103	0.00003	1344.21562	683.75462
7	0	0	2	0	2	0	0	1	1	3	658.49257	0.00006	1348.19391	689.70140
8	0	0	2	0	3	0	0	1	1	4	656.53093	0.00003	1354.16122	697.63032
9	0	0	2	0	4	0	0	1	1	5	654.57609	-0.00008	1362.11743	707.54126
10	0	0	2	0	5	0	0	1	1	6	652.62820	-0.00005	1372.06234	719.43409
11	0	0	2	0	6	0	0	1	1	7	650.68700	-0.00008	1383.99572	733.30864
12	0	0	2	0	7	0	0	1	1	8	648.75247	-0.00010	1397.91730	749.16472
13	0	0	2	0	8	0	0	1	1	9	646.82458	-0.00005	1413.82675	767.00212
14	0	0	2	0	9	0	0	1	1	10	644.90304	-0.00007	1431.72370	786.82059
15	0	0	2	0	10	0	0	1	1	11	642.98782	-0.00007	1451.60774	808.61985
16	0	0	2	0	11	0	0	1	1	12	641.07866	-0.00013	1473.47840	832.39961
17	0	0	2	0	12	0	0	1	1	13	639.17555	-0.00009	1497.33518	858.15954
18	0	0	2	0	13	0	0	1	1	14	637.27816	-0.00008	1523.17752	885.89928
19	0	0	2	0	14	0	0	1	1	15	635.38631	-0.00006	1551.00481	915.61845
20	0	0	2	0	15	0	0	1	1	16	633.49969	-0.00010	1580.81643	947.31664
21	0	0	2	0	16	0	0	1	1	17	631.61809	-0.00017	1612.61167	980.99342
22	0	0	2	0	17	0	0	1	1	18	629.74133	-0.00017	1646.38981	1016.64832
23	0	0	2	0	18	0	0	1	1	19	627.86901	-0.00021	1682.15007	1054.28084
24	0	0	2	0	19	0	0	1	1	20	626.00102	-0.00012	1719.89163	1093.89049
25	0	0	2	0	20	0	0	1	1	21	624.13675	-0.00018	1759.61363	1135.47669
26	0	0	2	0	21	0	0	1	1	22	622.27612	-0.00015	1801.31517	1179.03889
27	0	0	2	0	22	0	0	1	1	23	620.41867	-0.00016	1844.99532	1224.57649
28	0	0	2	0	23	0	0	1	1	24	618.56404	-0.00020	1890.65309	1272.08885
29	0	0	2	0	24	0	0	1	1	25	616.71208	-0.00009	1938.28750	1321.57533
30	0	0	2	0	25	0	0	1	1	26	614.86220	-0.00005	1987.89749	1373.03523
31	0	0	2	0	26	0	0	1	1	27	613.01406	-0.00006	2039.48198	1426.46786
32	0	0	2	0	27	0	0	1	1	28	611.16709	-0.00033	2093.03990	1481.87248
33	0	0	2	0	28	0	0	1	1	29	609.32164	-0.00013	2148.57010	1539.24832
34	0	0	2	0	29	0	0	1	1	30	607.47688	0.00004	2206.07144	1598.59460
35	0	0	2	0	30	0	0	1	1	31	605.63219	-0.00006	2265.54275	1659.91050
36	0	0	2	0	31	0	0	1	1	32	603.78770	0.00002	2326.98286	1723.19517
37	0	0	2	0	32	0	0	1	1	33	601.94271	-0.00009	2390.39054	1788.44775
38	0	0	2	0	33	0	0	1	1	34	600.09780	0.00053	2455.76460	1855.66733

rms = 0.00015 cm⁻¹

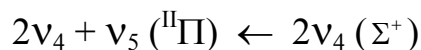
$2\nu_5(\Delta) \leftarrow \nu_5(\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 2 2	0 0 1 1 1	685.22346	-0.00008	1365.01359	679.79005
0 0 2 2 3	0 0 1 1 2	687.22343	-0.00010	1370.97815	683.75462
0 0 2 2 4	0 0 1 1 3	689.22933	-0.00011	1378.93084	689.70140
0 0 2 2 5	0 0 1 1 4	691.24119	-0.00012	1388.87163	697.63032
0 0 2 2 6	0 0 1 1 5	693.25915	-0.00007	1400.80048	707.54126
0 0 2 2 7	0 0 1 1 6	695.28312	-0.00011	1414.71732	719.43409
0 0 2 2 8	0 0 1 1 7	697.31330	-0.00014	1430.62208	733.30864
0 0 2 2 9	0 0 1 1 8	699.34989	-0.00008	1448.51470	749.16472
0 0 2 2 10	0 0 1 1 9	701.39287	-0.00008	1468.39508	767.00212
0 0 2 2 11	0 0 1 1 10	703.44237	-0.00016	1490.26312	786.82059
0 0 2 2 12	0 0 1 1 11	705.49873	-0.00014	1514.11873	808.61985
0 0 2 2 13	0 0 1 1 12	707.56206	-0.00010	1539.96178	832.39961
0 0 2 2 14	0 0 1 1 13	709.63245	-0.00015	1567.79214	858.15954
0 0 2 2 15	0 0 1 1 14	711.71031	-0.00010	1597.60969	885.89928
0 0 2 2 16	0 0 1 1 15	713.79574	-0.00007	1629.41426	915.61845
0 0 2 2 17	0 0 1 1 16	715.88901	-0.00006	1663.20571	947.31664
0 0 2 2 18	0 0 1 1 17	717.99034	-0.00009	1698.98385	980.99342
0 0 2 2 19	0 0 1 1 18	720.10010	-0.00008	1736.74850	1016.64832
0 0 2 2 20	0 0 1 1 19	722.21858	-0.00003	1776.49946	1054.28084
0 0 2 2 21	0 0 1 1 20	724.34595	-0.00007	1818.23651	1093.89049
0 0 2 2 22	0 0 1 1 21	726.48262	-0.00010	1861.95941	1135.47669
0 0 2 2 23	0 0 1 1 22	728.62929	-0.00009	1907.66792	1179.03889

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1	0	0	2	-2	8	0	0	1	-1	9	663.29887	-0.00010	1430.61827	767.31930
2	0	0	2	-2	9	0	0	1	-1	10	661.30043	-0.00007	1448.50870	787.20820
3	0	0	2	-2	10	0	0	1	-1	11	659.30111	-0.00005	1468.38608	809.08492
4	0	0	2	-2	11	0	0	1	-1	12	657.30093	-0.00005	1490.25013	832.94916
5	0	0	2	-2	12	0	0	1	-1	13	655.29987	-0.00010	1514.10054	858.80057
6	0	0	2	-2	13	0	0	1	-1	14	653.29810	-0.00008	1539.93697	886.63880
7	0	0	2	-2	15	0	0	1	-1	16	649.29229	-0.00004	1597.56645	948.27412
8	0	0	2	-2	16	0	0	1	-1	17	647.28807	-0.00026	1629.35868	982.07035
9	0	0	2	-2	18	0	0	1	-1	19	643.27831	-0.00001	1698.89591	1055.61759
10	0	0	2	-2	19	0	0	1	-1	20	641.27234	-0.00003	1736.63994	1095.36757
11	0	0	2	-2	20	0	0	1	-1	21	639.26582	-0.00001	1776.36688	1137.10105
12	0	0	2	-2	21	0	0	1	-1	22	637.25866	-0.00006	1818.07617	1180.81746
13	0	0	2	-2	22	0	0	1	-1	23	635.25107	0.00001	1861.76724	1226.51618
14	0	0	2	-2	23	0	0	1	-1	24	633.24290	0.00000	1907.43947	1274.19657
15	0	0	2	-2	24	0	0	1	-1	25	631.23432	0.00006	1955.09223	1323.85797
16	0	0	2	-2	25	0	0	1	-1	26	629.22529	0.00013	2004.72483	1375.49968
17	0	0	2	-2	26	0	0	1	-1	27	627.21571	0.00008	2056.33660	1429.12098
18	0	0	2	-2	27	0	0	1	-1	28	625.20588	0.00018	2109.92681	1484.72111
19	0	0	2	-2	28	0	0	1	-1	29	623.19524	-0.00016	2165.49472	1542.29931
20	0	0	2	-2	29	0	0	1	-1	30	621.18431	-0.00045	2223.03953	1601.85477
21	0	0	2	-2	30	0	0	1	-1	31	619.17380	-0.00001	2282.56045	1663.38664
22	0	0	2	-2	31	0	0	1	-1	32	617.16310	0.00053	2344.05666	1726.89408

rms = 0.00019 cm⁻¹



$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 1 1 1	2 0 0 0 2	674.24970	-0.00059	1714.16707	1039.91679
2 0 1 1 2	2 0 0 0 3	672.26431	0.00002	1718.16218	1045.89789
2 0 1 1 3	2 0 0 0 4	670.28258	0.00005	1724.15462	1053.87209
2 0 1 1 4	2 0 0 0 5	668.30523	-0.00003	1732.14413	1063.83887
2 0 1 1 5	2 0 0 0 6	666.33271	-0.00005	1742.13035	1075.79759
2 0 1 1 6	2 0 0 0 7	664.36603*	0.00067	1754.11283	1089.74746
2 0 1 1 7	2 0 0 0 8	662.40327	-0.00012	1768.09099	1105.68761
2 0 1 1 8	2 0 0 0 9	660.44688	-0.00029	1784.06418	1123.61701
2 0 1 1 9	2 0 0 0 10	658.49700*	-0.00003	1802.03159	1143.53456
2 0 1 1 10	2 0 0 0 11	656.55297	-0.00028	1821.99232	1165.43907
2 0 1 1 11	2 0 0 0 12	654.61576	-0.00030	1843.94531	1189.32925
2 0 1 1 12	2 0 0 0 13	652.68526	-0.00032	1867.88938	1215.20380
2 0 1 1 13	2 0 0 0 14	650.76129	-0.00055	1893.82321	1243.06138
2 0 1 1 14	2 0 0 0 15	648.84435	-0.00033	1921.74533	1272.90065
2 0 1 1 15	2 0 0 0 16	646.93340	-0.00041	1951.65414	1304.72033
2 0 1 1 16	2 0 0 0 17	645.02870	-0.00005	1983.54793	1338.51918
2 0 1 1 17	2 0 0 0 18	643.12624*	-0.00260	2017.42488	1374.29604W
2 0 1 1 18	2 0 0 0 19	641.23295	-0.00031	2053.28311	1412.04985
2 0 1 1 19	2 0 0 0 20	639.34089	-0.00019	2091.12070	1451.77962
2 0 1 1 20	2 0 0 0 21	637.45100	-0.00027	2130.93576	1493.48450
2 0 1 1 21	2 0 0 0 22	635.56269	-0.00006	2172.72643	1537.16368
2 0 1 1 22	2 0 0 0 23	633.67227*	-0.00223	2216.49097	1582.81646W
2 0 1 1 23	2 0 0 0 24	631.78555	0.00002	2262.22772	1630.44219
2 0 1 1 1	2 0 0 0 0	680.23260	0.00082	1714.16707	1033.93529
2 0 1 1 2	2 0 0 0 1	682.23302	0.00001	1718.16218	1035.92917
2 0 1 1 3	2 0 0 0 2	684.23766	-0.00017	1724.15462	1039.91679
2 0 1 1 4	2 0 0 0 3	686.24653	0.00029	1732.14413	1045.89789
2 0 1 1 5	2 0 0 0 4	688.25812	-0.00014	1742.13035	1053.87209
2 0 1 1 6	2 0 0 0 5	690.27387	-0.00008	1754.11283	1063.83887
2 0 1 1 7	2 0 0 0 6	692.29321	-0.00019	1768.09099	1075.79759
2 0 1 1 8	2 0 0 0 7	694.31657	-0.00014	1784.06418	1089.74746
2 0 1 1 9	2 0 0 0 8	696.34381	-0.00017	1802.03159	1105.68761
2 0 1 1 10	2 0 0 0 9	698.37513	-0.00018	1821.99232	1123.61701
2 0 1 1 11	2 0 0 0 10	700.41049	-0.00025	1843.94531	1143.53456
2 0 1 1 12	2 0 0 0 11	702.45008	-0.00023	1867.88938	1165.43907
2 0 1 1 13	2 0 0 0 12	704.49366	-0.00030	1893.82321	1189.32925
2 0 1 1 14	2 0 0 0 13	706.54607*	0.00454	1921.74533	1215.20380W
2 0 1 1 15	2 0 0 0 14	708.59848	-0.00041	1951.65414	1243.06138

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2	0	1	1	16	2	0	0	0	15	710.64697	-0.00031	1983.54793	1272.90065
2	0	1	1	17	2	0	0	0	16	712.70422	-0.00033	2017.42488	1304.72033
2	0	1	1	18	2	0	0	0	17	714.76407	0.00014	2053.28311	1338.51918
2	0	1	1	19	2	0	0	0	18	716.82541	0.00075	2091.12070	1374.29604
2	0	1	1	20	2	0	0	0	19	718.88501	-0.00091	2130.93576	1412.04985
2	0	1	1	21	2	0	0	0	20	720.94657	-0.00024	2172.72643	1451.77962
2	0	1	1	22	2	0	0	0	21	723.00623	-0.00024	2216.49097	1493.48450
2	0	1	1	23	2	0	0	0	22	725.06382	-0.00022	2262.22772	1537.16368
2	0	1	1	24	2	0	0	0	23	727.11868	-0.00006	2309.93520	1582.81646
2	0	1	-1	1	2	0	0	0	1	678.23780*	0.00201	1714.16495	1035.92917W
2	0	1	-1	2	2	0	0	0	2	678.23780*	-0.00123	1718.15582	1039.91679W
2	0	1	-1	3	2	0	0	0	3	678.24388	-0.00012	1724.14189	1045.89789
2	0	1	-1	4	2	0	0	0	4	678.25071	-0.00010	1732.12291	1053.87209
2	0	1	-1	5	2	0	0	0	5	678.25890*	-0.00076	1742.09853	1063.83887
2	0	1	-1	6	2	0	0	0	6	678.27102	0.00027	1754.06834	1075.79759
2	0	1	-1	7	2	0	0	0	7	678.28480	0.00043	1768.03183	1089.74746
2	0	1	-1	8	2	0	0	0	8	678.29970*	-0.00114	1783.98845	1105.68761W
2	0	1	-1	9	2	0	0	0	9	678.32040	-0.00017	1801.93758	1123.61701
2	0	1	-1	10	2	0	0	0	10	678.34423	0.00024	1821.87855	1143.53456
2	0	1	-1	11	2	0	0	0	11	678.37783*	0.00624	1843.81066	1165.43907W
2	0	1	-1	12	2	0	0	0	12	678.40378	-0.00012	1867.73315	1189.32925
2	0	1	-1	13	2	0	0	0	13	678.44144	-0.00005	1893.64529	1215.20380
2	0	1	-1	14	2	0	0	0	14	678.48351*	-0.00139	1921.54628	1243.06138W
2	0	1	-1	15	2	0	0	0	15	678.53465	-0.00005	1951.43535	1272.90065
2	0	1	-1	16	2	0	0	0	16	678.59125	-0.00015	1983.31173	1304.72033
2	0	1	-1	17	2	0	0	0	17	678.65560*	0.00014	2017.17464	1338.51918
2	0	1	-1	18	2	0	0	0	18	678.72721	-0.00008	2053.02334	1374.29604
2	0	1	-1	19	2	0	0	0	19	678.80725	0.00003	2090.85706	1412.04985
2	0	1	-1	20	2	0	0	0	20	678.89486	-0.00061	2130.67509	1451.77962
2	0	1	-1	21	2	0	0	0	21	678.99300*	0.00080	2172.47670	1493.48450
2	0	1	-1	22	2	0	0	0	22	679.09747	-0.00003	2216.26118	1537.16368
2	0	1	-1	23	2	0	0	0	23	679.21138	0.00002	2262.02782	1582.81646
2	0	1	-1	24	2	0	0	0	24	679.33370	-0.00004	2309.77593	1630.44219
2	0	1	-1	25	2	0	0	0	25	679.46427	-0.00028	2359.50479	1680.04024
2	0	1	-1	26	2	0	0	0	26	679.60349	-0.00016	2411.21370	1731.61005
2	0	1	-1	27	2	0	0	0	27	679.75068	-0.00022	2464.90194	1785.15104
2	0	1	-1	28	2	0	0	0	28	679.90596	-0.00017	2520.56876	1840.66263
2	0	1	-1	29	2	0	0	0	29	680.06910	-0.00007	2578.21342	1898.14425

rms = 0.00030 cm⁻¹

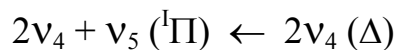
$$2\nu_4 + \nu_5 (\Phi) \leftarrow 2\nu_4 (\Delta)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 1 1 22	2 2 0 0 23	630.99388	-0.00041	2220.54443	1589.55014
2 2 1 1 21	2 2 0 0 22	633.01458	0.00024	2176.63083	1543.61649
2 2 1 1 20	2 2 0 0 21	635.03269	-0.00002	2134.71443	1499.68172
2 2 1 1 19	2 2 0 0 20	637.04860	-0.00027	2094.79526	1457.74639
2 2 1 1 18	2 2 0 0 19	639.06206	-0.00023	2056.87321	1417.81092
2 2 1 1 17	2 2 0 0 18	641.07232	-0.00020	2020.94812	1379.87559
2 2 1 1 16	2 2 0 0 17	643.07913	-0.00006	1987.01973	1343.94054
2 2 1 1 15	2 2 0 0 16	645.08191	-0.00015	1955.08779	1310.00574
2 2 1 1 14	2 2 0 0 15	647.08097	-0.00008	1925.15205	1278.07100
2 2 1 1 13	2 2 0 0 14	649.07619	-0.00006	1897.21228	1248.13603
2 2 1 1 12	2 2 0 0 13	651.06762	-0.00027	1871.26829	1220.20039
2 2 1 1 11	2 2 0 0 12	653.05543	-0.00094	1847.31994	1194.26357
2 2 1 1 10	2 2 0 0 11	655.04215	-0.00001	1825.36714	1170.32497
2 2 1 1 9	2 2 0 0 10	657.02588	0.00003	1805.40985	1148.38399
2 2 1 1 8	2 2 0 0 9	659.00797	-0.00010	1787.44806	1128.43999
2 2 1 1 6	2 2 0 0 7	662.97117	0.00052	1757.51111	1094.54045
2 2 1 1 5	2 2 0 0 6	664.95250	0.00024	1745.53606	1080.58379
2 2 1 1 4	2 2 0 0 5	666.93605	0.00121	1735.55671	1068.62187W
2 2 1 1 3	2 2 0 0 2	682.87259	0.00004	1727.57314	1044.70059
2 2 1 1 4	2 2 0 0 3	684.87644	0.00031	1735.55671	1050.68059
2 2 1 1 5	2 2 0 0 4	686.88251	0.00070	1745.53606	1058.65425
2 2 1 1 6	2 2 0 0 5	688.88858	0.00107	1757.51111	1068.62187W

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1	2	-2	1	-1	5	2	-2	0	0	4	686.88251	-0.00074	1745.53600	1058.65275
2	2	-2	1	-1	6	2	-2	0	0	5	688.89053	-0.00204	1757.51093	1068.61835W
3	2	-2	1	-1	7	2	-2	0	0	6	690.90470	0.00012	1771.48134	1080.57677
4	2	-2	1	-1	8	2	-2	0	0	7	692.91935	0.00010	1787.44706	1094.52781
5	2	-2	1	-1	9	2	-2	0	0	8	694.93532*	-0.00126	1805.40786	1110.47128W
6	2	-2	1	-1	10	2	-2	0	0	9	696.95632	-0.00019	1825.36346	1128.40695
7	2	-2	1	-1	11	2	-2	0	0	10	698.97907	0.00011	1847.31352	1148.33456
8	2	-2	1	-1	12	2	-2	0	0	11	701.00388	0.00005	1871.25765	1170.25382
9	2	-2	1	-1	13	2	-2	0	0	12	703.03112	0.00016	1897.19537	1194.16442
10	2	-2	1	-1	14	2	-2	0	0	13	705.06054	0.00038	1925.12616	1220.06599
11	2	-2	1	-1	15	2	-2	0	0	14	707.09127	0.00008	1955.04938	1247.95819
12	2	-2	1	-1	16	2	-2	0	0	15	709.12395	0.00018	1986.96435	1277.84059
13	2	-2	1	-1	17	2	-2	0	0	16	711.15761	0.00005	2020.87032	1309.71276
14	2	-2	1	-1	18	2	-2	0	0	17	713.19241	0.00020	2056.76646	1343.57425
15	2	-2	1	-1	19	2	-2	0	0	18	715.22740	0.00009	2094.65187	1379.42457
16	2	-2	1	-1	20	2	-2	0	0	19	717.26344*	0.00100	2134.52563	1417.26319
17	2	-2	1	-1	21	2	-2	0	0	20	719.29732	0.00014	2176.38674	1457.08957
18	2	-2	1	-1	22	2	-2	0	0	21	721.33128	0.00020	2220.23421	1498.90313
19	2	-2	1	-1	23	2	-2	0	0	22	723.36376	0.00004	2266.06698	1542.70326
20	2	-2	1	-1	24	2	-2	0	0	23	725.39484	0.00016	2313.88402	1588.48935
21	2	-2	1	-1	25	2	-2	0	0	24	727.42390	0.00033	2363.68428	1636.26071
22	2	-2	1	-1	26	2	-2	0	0	25	729.45016*	0.00012	2415.46670	1686.01666
23	2	-2	1	-1	27	2	-2	0	0	26	731.47436	0.00061	2469.23024	1737.75648
24	2	-2	1	-1	28	2	-2	0	0	27	733.49400	-0.00043	2524.97386	1791.47943
25	2	-2	1	-1	29	2	-2	0	0	28	735.51180	-0.00003	2582.69655	1847.18472
26	2	-2	1	-1	30	2	-2	0	0	29	737.52610	0.00036	2642.39729	1904.87155
27	2	2	1	1	3	2	-2	0	0	3	676.89195	-0.00111	1727.57314	1050.68009W
28	2	2	1	1	4	2	-2	0	0	4	676.90293*	-0.00104	1735.55671	1058.65275W
29	2	2	1	1	5	2	-2	0	0	5	676.91700*	-0.00070	1745.53606	1068.61835
30	2	2	1	1	6	2	-2	0	0	6	676.93430	-0.00004	1757.51111	1080.57677
31	2	2	1	1	7	2	-2	0	0	7	676.95460*	0.00062	1771.48179	1094.52781
32	2	2	1	1	8	2	-2	0	0	8	676.97959*	0.00282	1787.44806	1110.47128W
33	2	2	1	1	9	2	-2	0	0	9	677.00290	0.00001	1805.40985	1128.40695
34	2	2	1	1	10	2	-2	0	0	10	677.03269	0.00012	1825.36714	1148.33456
35	2	2	1	1	11	2	-2	0	0	11	677.06602	-0.00009	1847.31994	1170.25382
36	2	2	1	1	12	2	-2	0	0	12	677.10575*	0.00188	1871.26829	1194.16442W
37	2	2	1	1	13	2	-2	0	0	13	677.14626	-0.00002	1897.21228	1220.06599
38	2	2	1	1	14	2	-2	0	0	14	677.19420*	0.00034	1925.15205	1247.95819
39	2	2	1	1	15	2	-2	0	0	15	677.24754	0.00033	1955.08779	1277.84059
40	2	2	1	1	16	2	-2	0	0	16	677.30693	-0.00004	1987.01973	1309.71276
41	2	2	1	1	17	2	-2	0	0	17	677.37396	0.00010	2020.94812	1343.57425
42	2	2	1	1	18	2	-2	0	0	18	677.44928	0.00063	2056.87321	1379.42457
43	2	2	1	1	19	2	-2	0	0	19	677.53220	0.00013	2094.79526	1417.26319
44	2	2	1	1	20	2	-2	0	0	20	677.62345*	-0.00141	2134.71443	1457.08957W
45	2	2	1	1	21	2	-2	0	0	21	677.72819	0.00049	2176.63083	1498.90313
46	2	2	1	1	22	2	-2	0	0	22	677.84540*	0.00423	2220.54443	1542.70326W

rms = 0.00034 cm⁻¹



$\nu_4' l_4' \nu_5' l_5' J'$	$\nu_4'' l_4'' \nu_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 1 -1 1	2 2 0 0 2	679.76212	0.00014	1724.46257	1044.70059
2 2 1 -1 2	2 2 0 0 3	677.76478	0.00023	1728.44514	1050.68059
2 2 1 -1 3	2 2 0 0 4	675.76492	0.00013	1734.41904	1058.65425
2 2 1 -1 4	2 2 0 0 5	673.76265	0.00019	1742.38433	1068.62187
2 2 1 -1 5	2 2 0 0 6	671.75712	-0.00015	1752.34107	1080.58379
2 2 1 -1 6	2 2 0 0 7	669.74895	0.00007	1764.28934	1094.54045
2 2 1 -1 7	2 2 0 0 8	667.73661	-0.00031	1778.22926	1110.49234
2 2 1 -1 8	2 2 0 0 9	665.72083	-0.00012	1794.16094	1128.43999
2 2 1 -1 9	2 2 0 0 10	663.70024	-0.00029	1812.08452	1148.38399
2 2 1 -1 10	2 2 0 0 11	661.67508	-0.00011	1832.00016	1170.32497
2 2 1 -1 11	2 2 0 0 12	659.64442	-0.00004	1853.90802	1194.26357
2 2 1 -1 12	2 2 0 0 13	657.60782	-0.00007	1877.80829	1220.20039
2 2 1 -1 13	2 2 0 0 14	655.56507	-0.00003	1903.70113	1248.13603
2 2 1 -1 14	2 2 0 0 15	653.51632	0.00000	1931.58675	1278.07100

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2	-2	1	1	25	2	2	0	0	25	685.47074	-0.00053	2372.88254	1687.41127
2	-2	1	1	27	2	2	0	0	27	685.70587	-0.00165	2478.96612	1793.25860W

rms = 0.00032 cm⁻¹

$$v_4 + 2v_5 (^{\text{II}}\Pi) \leftarrow v_4 + v_5 (\Sigma^+)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 2 0 1	1 1 1 -1 1	661.36680	0.00037	1863.85543	1202.48900
1 -1 2 0 3	1 1 1 -1 3	661.39660	0.00008	1873.84028	1212.44377
1 -1 2 0 4	1 1 1 -1 4	661.42020	0.00020	1881.82789	1220.40789
1 -1 2 0 5	1 1 1 -1 5	661.44860	-0.00003	1891.81206	1230.36343
1 -1 2 0 6	1 1 1 -1 6	661.48180	-0.00011	1903.79255	1242.31065
1 -1 2 0 7	1 1 1 -1 7	661.51935	0.00009	1917.76910	1256.24984
1 -1 2 0 8	1 1 1 -1 8	661.55970	-0.00032	1933.74139	1272.18137
1 -1 2 0 9	1 1 1 -1 9	661.60305	-0.00039	1951.70905	1290.10561
1 -1 2 0 10	1 1 1 -1 10	661.64870	0.00001	1971.67167	1310.02298
1 -1 2 0 12	1 1 1 -1 12	661.74050	-0.00054	2017.57995	1355.83891
1 -1 2 0 13	1 1 1 -1 13	661.78590	-0.00033	2043.52458	1381.73835
1 -1 2 0 14	1 1 1 -1 14	661.82900	-0.00043	2071.46210	1409.63267
1 -1 2 0 15	1 1 1 -1 15	661.86930	-0.00036	2101.39190	1439.52224
1 -1 2 0 16	1 1 1 -1 16	661.90630	0.00036	2133.31332	1471.40738
1 -1 2 0 18	1 1 1 -1 18	661.96260	-0.00044	2203.12814	1541.16510
1 -1 2 0 19	1 1 1 -1 19	661.98150	-0.00072	2241.02004	1579.03782
1 -1 2 0 20	1 1 1 -1 20	661.99380	-0.00037	2280.90052	1618.90635
1 -1 2 0 21	1 1 1 -1 21	661.99760	-0.00069	2322.76874	1660.77045
1 -1 2 0 22	1 1 1 -1 22	661.99380	-0.00024	2366.62381	1704.62977

rms = 0.00038 cm⁻¹

$$v_4 + 2v_5 (^{\text{I}}\Pi) \leftarrow v_4 + v_5 (\Sigma^+)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 2 2 21	1 1 1 -1 22	637.90515	-0.00009	2342.53501	1704.62977
1 -1 2 2 20	1 1 1 -1 21	639.93638	0.00019	2300.70664	1660.77045
1 -1 2 2 19	1 1 1 -1 20	641.96329	-0.00029	2260.86993	1618.90635
1 -1 2 2 18	1 1 1 -1 19	643.98720	-0.00002	2223.02504	1579.03782
1 -1 2 2 17	1 1 1 -1 18	646.00624	-0.00075	2187.17209	1541.16510
1 -1 2 2 16	1 1 1 -1 17	648.02298	0.00011	2153.31116	1505.28829
1 -1 2 2 15	1 1 1 -1 16	650.03466	-0.00024	2121.44228	1471.40738
1 -1 2 2 14	1 1 1 -1 15	652.04313	-0.00010	2091.56547	1439.52224
1 -1 2 2 13	1 1 1 -1 14	654.04794	-0.00012	2063.68073	1409.63267
1 -1 2 2 12	1 1 1 -1 13	656.04965	-0.00003	2037.78803	1381.73835
1 -1 2 2 11	1 1 1 -1 12	658.04796	-0.00047	2013.88734	1355.83891
1 -1 2 2 10	1 1 1 -1 11	660.04454	-0.00014	1991.97861	1331.93393
1 -1 2 2 9	1 1 1 -1 10	662.03885	0.00004	1972.06179	1310.02298
1 -1 2 2 8	1 1 1 -1 9	664.03130	0.00008	1954.13683	1290.10561
1 -1 2 2 7	1 1 1 -1 8	666.02210	-0.00021	1938.20368	1272.18137
1 -1 2 2 6	1 1 1 -1 7	668.01274	0.00029	1924.26229	1256.24984
1 -1 2 2 5	1 1 1 -1 6	670.00188	-0.00009	1912.31262	1242.31065
1 -1 2 2 4	1 1 1 -1 5	671.99082	-0.00037	1902.35462	1230.36343
1 -1 2 2 3	1 1 1 -1 4	673.98038	0.00000	1894.38827	1220.40789
1 -1 2 2 2	1 1 1 -1 3	675.96960	-0.00016	1888.41352	1212.44377
1 -1 2 2 1	1 1 1 -1 2	677.95900	-0.00052	1884.43037	1206.47085
1 -1 2 2 1	1 1 1 -1 0	683.93240	0.00012	1884.43037	1200.49810
1 -1 2 2 2	1 1 1 -1 1	685.92452	0.00000	1888.41352	1202.48900
1 -1 2 2 3	1 1 1 -1 2	687.91711	-0.00030	1894.38827	1206.47085
1 -1 2 2 4	1 1 1 -1 3	689.91059	-0.00027	1902.35462	1212.44377
1 -1 2 2 5	1 1 1 -1 4	691.90459	-0.00014	1912.31262	1220.40789
1 -1 2 2 6	1 1 1 -1 5	693.89879	-0.00007	1924.26229	1230.36343
1 -1 2 2 7	1 1 1 -1 6	695.89280	-0.00023	1938.20368	1242.31065
1 -1 2 2 8	1 1 1 -1 7	697.88688	-0.00011	1954.13683	1256.24984

1	1	-1	2	2	9	1	1	1	-1	8	699.88022	-0.00020	1972.06179	1272.18137
2	1	-1	2	2	10	1	1	1	-1	9	701.87276	-0.00024	1991.97861	1290.10561
3	1	-1	2	2	11	1	1	1	-1	10	703.86415	-0.00021	2013.88734	1310.02298
4	1	-1	2	2	12	1	1	1	-1	11	705.85400	-0.00010	2037.78803	1331.93393
5	1	-1	2	2	13	1	1	1	-1	12	707.84174	-0.00008	2063.68073	1355.83891
6	1	-1	2	2	14	1	1	1	-1	13	709.82905*	0.00193	2091.56547	1381.73835W
7	1	-1	2	2	15	1	1	1	-1	14	711.80961	0.00000	2121.44228	1409.63267
8	1	-1	2	2	16	1	1	1	-1	15	713.78898	0.00007	2153.31116	1439.52224
9	1	-1	2	2	17	1	1	1	-1	16	715.77282*	0.00810	2187.17209	1471.40738W
10	1	-1	2	2	18	1	1	1	-1	17	717.73645	-0.00031	2223.02504	1505.28829
11	1	-1	2	2	19	1	1	1	-1	18	719.70469	-0.00014	2260.86993	1541.16510
12	1	-1	2	2	20	1	1	1	-1	19	721.66857	-0.00024	2300.70664	1579.03782
13	1	-1	2	2	21	1	1	1	-1	20	723.62853	-0.00012	2342.53501	1618.90635
14	1	-1	2	2	22	1	1	1	-1	21	725.58425	-0.00012	2386.35482	1660.77045
15	1	-1	2	2	23	1	1	1	-1	22	727.53630	0.00025	2432.16581	1704.62977
16	1	1	2	-2	3	1	1	1	-1	3	681.96444	-0.00007	1894.40827	1212.44377
17	1	1	2	-2	4	1	1	1	-1	4	681.97998	-0.00010	1902.38797	1220.40789
18	1	1	2	-2	5	1	1	1	-1	5	681.99913	-0.00009	1912.36265	1230.36343
19	1	1	2	-2	6	1	1	1	-1	6	682.02170	0.00000	1924.33235	1242.31065
20	1	1	2	-2	7	1	1	1	-1	7	682.04760	0.00033	1938.29711	1256.24984
21	1	1	2	-2	10	1	1	1	-1	10	682.14040*	0.00098	1992.16240	1310.02298
22	1	1	2	-2	11	1	1	1	-1	11	682.17345*	-0.00069	2014.10807	1331.93393
23	1	1	2	-2	12	1	1	1	-1	12	682.21036	0.00011	2038.04916	1355.83891
24	1	1	2	-2	13	1	1	1	-1	13	682.24740*	0.00000	2063.98575	1381.73835
25	1	1	2	-2	14	1	1	1	-1	14	682.28531	0.00003	2091.91795	1409.63267
26	1	1	2	-2	15	1	1	1	-1	15	682.32381	0.00022	2121.84584	1439.52224
27	1	1	2	-2	16	1	1	1	-1	16	682.35930*	-0.00283	2153.76950	1471.40738W
28	1	1	2	-2	17	1	1	1	-1	17	682.40290*	0.00215	2187.68903	1505.28829W
29	1	1	2	-2	18	1	1	1	-1	18	682.43945	0.00006	2223.60449	1541.16510
30	1	1	2	-2	19	1	1	1	-1	19	682.47660*	-0.00150	2261.51593	1579.03782W
31	1	1	2	-2	20	1	1	1	-1	20	682.51706	0.00004	2301.42338	1618.90635
32	1	1	2	-2	21	1	1	1	-1	21	682.55880*	0.00242	2343.32683	1660.77045W
33	1	1	2	-2	22	1	1	1	-1	22	682.59920*	0.00270	2387.22627	1704.62977W
34	1	1	2	-2	23	1	1	1	-1	23	682.63775	-0.00002	2433.12160	1750.48383
35	1	1	2	-2	24	1	1	1	-1	24	682.68028	-0.00037	2481.01271	1798.33206
36	1	1	2	-2	25	1	1	1	-1	25	682.72810*	0.00246	2530.89942	1848.17378W
37	1	1	2	-2	26	1	1	1	-1	26	682.77271	-0.00056	2582.78151	1900.00824
38	1	1	2	-2	27	1	1	1	-1	27	682.82386	-0.00023	2636.65870	1953.83461
39	1	1	2	-2	28	1	1	1	-1	28	682.87840	-0.00023	2692.53061	2009.65198

rms = 0.00023 cm⁻¹

$$v_4 + 2v_5 (^{\Pi}\Pi) \leftarrow v_4 + v_5 (\Sigma^-)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''	
46	1 -1 2 0 18	1 -1 1 1 19	628.78580	-0.00024	2203.12814	1574.34210
47	1 -1 2 0 17	1 -1 1 1 18	630.68986	-0.00042	2167.22564	1536.53536
48	1 -1 2 0 16	1 -1 1 1 17	632.59764	0.00025	2133.31332	1500.71593
49	1 -1 2 0 15	1 -1 1 1 16	634.50737	-0.00025	2101.39190	1466.88429
50	1 -1 2 0 14	1 -1 1 1 15	636.42075	-0.00049	2071.46210	1435.04086
51	1 -1 2 0 13	1 -1 1 1 14	638.33784	-0.00069	2043.52458	1405.18605
52	1 -1 2 0 12	1 -1 1 1 13	640.25940	-0.00034	2017.57995	1377.32021
53	1 -1 2 0 11	1 -1 1 1 12	642.18477	-0.00038	1993.62880	1351.44366
54	1 -1 2 0 10	1 -1 1 1 11	644.11461	-0.00040	1971.67167	1327.55666
55	1 -1 2 0 9	1 -1 1 1 10	646.04947	-0.00010	1951.70905	1305.65948
56	1 -1 2 0 8	1 -1 1 1 9	647.98960*	0.00052	1933.74139	1285.75232
57	1 -1 2 0 7	1 -1 1 1 8	649.93360	-0.00014	1917.76910	1267.83537
58	1 -1 2 0 6	1 -1 1 1 7	651.88332	-0.00044	1903.79255	1251.90880
59	1 -1 2 0 5	1 -1 1 1 6	653.83881	-0.00050	1891.81206	1237.97275
60	1 -1 2 0 4	1 -1 1 1 5	655.79995	-0.00060	1881.82789	1226.02734
	1 -1 2 0 3	1 -1 1 1 4	657.76738	-0.00023	1873.84028	1216.07268
	1 -1 2 0 2	1 -1 1 1 3	659.74100	0.00043	1867.84942	1208.10885
	1 -1 2 0 1	1 -1 1 1 2	661.72060	0.00109	1863.85543	1202.13592W
	1 -1 2 0 1	1 -1 1 1 0	667.69530	0.00280	1863.85543	1196.16293W
	1 -1 2 0 6	1 -1 1 1 5	677.76475	-0.00046	1903.79255	1226.02734
	1 -1 2 0 7	1 -1 1 1 6	677.76910	-0.00046	1903.79255	1226.02734

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1	-1	2	0	8	1	-1	1	1	7	681.83248	-0.00011	1933.74139	1251.90880
1	-1	2	0	9	1	-1	1	1	8	683.87262*	-0.00106	1951.70905	1267.83537W
1	-1	2	0	10	1	-1	1	1	9	685.91890	-0.00046	1971.67167	1285.75232
1	-1	2	0	11	1	-1	1	1	10	687.96904	-0.00029	1993.62880	1305.65948
1	-1	2	0	12	1	-1	1	1	11	690.02291	-0.00038	2017.57995	1327.55666
1	-1	2	0	13	1	-1	1	1	12	692.08053	-0.00039	2043.52458	1351.44366
1	-1	2	0	14	1	-1	1	1	13	694.14160	-0.00029	2071.46210	1377.32021
1	-1	2	0	15	1	-1	1	1	14	696.21040*	0.00455	2101.39190	1405.18605W
1	-1	2	0	16	1	-1	1	1	15	698.27200	-0.00046	2133.31332	1435.04086
1	-1	2	0	17	1	-1	1	1	16	700.34098	-0.00038	2167.22564	1466.88429
1	-1	2	0	18	1	-1	1	1	17	702.41190	-0.00031	2203.12814	1500.71593
1	-1	2	0	19	1	-1	1	1	18	704.48445	-0.00023	2241.02004	1536.53536
1	-1	2	0	20	1	-1	1	1	19	706.55813	-0.00029	2280.90052	1574.34210
1	-1	2	0	21	1	-1	1	1	20	708.63273	-0.00038	2322.76874	1614.13563
1	-1	2	0	22	1	-1	1	1	21	710.70813	-0.00029	2366.62381	1655.91539
1	-1	2	0	23	1	-1	1	1	22	712.78380	-0.00024	2412.46483	1699.68079
1	1	2	0	12	1	-1	1	1	12	665.70745	0.00096	2017.15015	1351.44366
1	1	2	0	13	1	-1	1	1	13	665.70410*	0.00112	2043.02319	1377.32021W
1	1	2	0	14	1	-1	1	1	14	665.69832	0.00077	2070.88360	1405.18605
1	1	2	0	15	1	-1	1	1	15	665.69066	0.00079	2100.73073	1435.04086
1	1	2	0	16	1	-1	1	1	16	665.68004	0.00043	2132.56390	1466.88429
1	1	2	0	17	1	-1	1	1	17	665.66711	0.00069	2166.38235	1500.71593
1	1	2	0	18	1	-1	1	1	18	665.65059	0.00066	2202.18530	1536.53536
1	1	2	0	19	1	-1	1	1	19	665.63010	0.00030	2239.97191	1574.34210
1	1	2	0	20	1	-1	1	1	20	665.60595	0.00030	2279.74129	1614.13563
1	1	2	0	21	1	-1	1	1	21	665.57760	0.00049	2321.49251	1655.91539
1	1	2	0	22	1	-1	1	1	22	665.54380*	0.00001	2365.22458	1699.68079
1	1	2	0	23	1	-1	1	1	23	665.50560	0.00032	2410.93648	1745.43120

rms = 0.00044 cm⁻¹

$$v_4 + 2v_5 (\text{I}\Pi) \leftarrow v_4 + v_5 (\Sigma^-)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 2 -2 18	1 -1 1 1 19	649.26300	0.00061	2223.60449	1574.34210
1 1 2 -2 17	1 -1 1 1 18	651.15408	0.00041	2187.68903	1536.53536
1 1 2 -2 16	1 -1 1 1 17	653.05543*	0.00186	2153.76950	1500.71593W
1 1 2 -2 15	1 -1 1 1 16	654.96817*	0.00662	2121.84584	1466.88429W
1 1 2 -2 14	1 -1 1 1 15	656.87710	0.00001	2091.91795	1435.04086
1 1 2 -2 13	1 -1 1 1 14	658.79958	-0.00012	2063.98575	1405.18605
1 1 2 -2 12	1 -1 1 1 13	660.73006	0.00111	2038.04916	1377.32021W
1 1 2 -2 11	1 -1 1 1 12	662.66451	0.00009	2014.10807	1351.44366
1 1 2 -2 10	1 -1 1 1 11	664.60555	-0.00019	1992.16240	1327.55666
1 1 2 -2 9	1 -1 1 1 10	666.55194	-0.00066	1972.21207	1305.65948
1 1 2 -2 8	1 -1 1 1 9	668.50450	-0.00018	1954.25700	1285.75232
1 1 2 -2 7	1 -1 1 1 8	670.46140	-0.00034	1938.29711	1267.83537
1 1 2 -2 6	1 -1 1 1 7	672.42352	-0.00003	1924.33235	1251.90880
1 1 2 -2 5	1 -1 1 1 6	674.38965	-0.00025	1912.36265	1237.97275
1 1 2 -2 4	1 -1 1 1 5	676.35957	-0.00106	1902.38797	1226.02734W
1 1 2 -2 3	1 -1 1 1 4	678.33560*	0.00001	1894.40827	1216.07268
1 1 2 -2 2	1 -1 1 1 3	680.31450	-0.00018	1888.42353	1208.10885
1 1 2 -2 1	1 -1 1 1 2	682.29810	0.00031	1884.43371	1202.13592
1 1 2 -2 1	1 -1 1 1 0	688.26980	-0.00098	1884.43371	1196.16293
1 1 2 -2 3	1 -1 1 1 2	692.27227	-0.00009	1894.40827	1202.13592
1 1 2 -2 4	1 -1 1 1 3	694.27875	-0.00037	1902.38797	1208.10885
1 1 2 -2 5	1 -1 1 1 4	696.28970	-0.00027	1912.36265	1216.07268
1 1 2 -2 6	1 -1 1 1 5	698.30480	-0.00021	1924.33235	1226.02734
1 1 2 -2 7	1 -1 1 1 6	700.32415	-0.00021	1938.29711	1237.97275
1 1 2 -2 8	1 -1 1 1 7	702.34799	-0.00021	1954.25700	1251.90880
1 1 2 -2 9	1 -1 1 1 8	704.37664	-0.00007	1972.21207	1267.83537
1 1 2 -2 10	1 -1 1 1 9	706.40985	-0.00024	1992.16240	1285.75232
1 1 2 -2 11	1 -1 1 1 10	708.44851	-0.00008	2014.10807	1305.65948
1 1 2 -2 12	1 -1 1 1 11	710.49246	-0.00004	2038.04916	1327.55666
1 1 2 -2 13	1 -1 1 1 12	712.54212	0.00002	2063.98575	1351.44366
1 1 2 -2 14	1 -1 1 1 13	714.59778	0.00004	2091.91795	1377.32021
1 1 2 -2 15	1 -1 1 1 14	716.65344	0.00001	2121.84584	1405.18605

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1	1	1	2	-2	16	1	-1	1	1	15	718.72864	0.00000	2153.76950	1435.04086
2	1	1	2	-2	17	1	-1	1	1	16	720.80510	0.00035	2187.68903	1466.88429
3	1	1	2	-2	18	1	-1	1	1	17	722.88855	-0.00001	2223.60449	1500.71593
4	1	-1	2	2	6	1	-1	1	1	6	686.28904	-0.00050	1924.26229	1237.97275
5	1	-1	2	2	7	1	-1	1	1	7	686.29502	0.00014	1938.20368	1251.90880
6	1	-1	2	2	8	1	-1	1	1	8	686.30148	0.00002	1954.13683	1267.83537
7	1	-1	2	2	9	1	-1	1	1	9	686.30933	-0.00014	1972.06179	1285.75232
8	1	-1	2	2	10	1	-1	1	1	10	686.31918	0.00005	1991.97861	1305.65948
9	1	-1	2	2	11	1	-1	1	1	11	686.33045	-0.00023	2013.88734	1327.55666
10	1	-1	2	2	12	1	-1	1	1	12	686.34402	-0.00036	2037.78803	1351.44366
11	1	-1	2	2	13	1	-1	1	1	13	686.36018	-0.00034	2063.68073	1377.32021
12	1	-1	2	2	14	1	-1	1	1	14	686.37923	-0.00019	2091.56547	1405.18605
13	1	-1	2	2	15	1	-1	1	1	15	686.40130	-0.00012	2121.44228	1435.04086
14	1	-1	2	2	16	1	-1	1	1	16	686.42677	-0.00010	2153.31116	1466.88429
15	1	-1	2	2	17	1	-1	1	1	17	686.45610	-0.00006	2187.17209	1500.71593
16	1	-1	2	2	18	1	-1	1	1	18	686.48969	0.00001	2223.02504	1536.53536
17	1	-1	2	2	19	1	-1	1	1	19	686.52788	0.00005	2260.86993	1574.34210
18	1	-1	2	2	20	1	-1	1	1	20	686.57126	0.00025	2300.70664	1614.13563
19	1	-1	2	2	21	1	-1	1	1	21	686.62003	0.00042	2342.53501	1655.91539
20	1	-1	2	2	22	1	-1	1	1	22	686.67412	0.00009	2386.35482	1699.68079
21	1	-1	2	2	23	1	-1	1	1	23	686.73538	0.00077	2432.16581	1745.43120
22	1	-1	2	2	24	1	-1	1	1	24	686.80250	0.00079	2479.96765	1793.16594
23	1	-1	2	2	25	1	-1	1	1	25	686.87549	-0.00012	2529.75993	1842.88432
24	1	-1	2	2	26	1	-1	1	1	26	686.95665	0.00005	2581.54220	1894.58561
25	1	-1	2	2	27	1	-1	1	1	27	687.04465	-0.00025	2635.31393	1948.26904

rms = 0.00031 cm⁻¹

$$v_4 + 2v_5 (\text{II}\Pi) \leftarrow v_4 + v_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 2 0 18	1 1 1 1 19	628.75960	0.00050	2202.18530	1573.42620
1 1 2 0 17	1 1 1 1 18	630.67500	0.00070	2166.38235	1535.70804
1 1 2 0 16	1 1 1 1 17	632.59764	-0.00012	2132.56390	1499.96614
1 1 2 0 15	1 1 1 1 16	634.52937	0.00015	2100.73073	1466.20152
1 1 2 0 14	1 1 1 1 15	636.46890	0.00056	2070.88360	1434.41526
1 1 2 0 13	1 1 1 1 14	638.41478	0.00009	2043.02319	1404.60850
1 1 2 0 12	1 1 1 1 13	640.36803	0.00029	2017.15015	1376.78240
1 1 2 0 11	1 1 1 1 12	642.32733	0.00039	1993.26507	1350.93813
1 1 2 0 10	1 1 1 1 11	644.29153	-0.00014	1971.36850	1327.07683
1 1 2 0 9	1 1 1 1 10	646.26123	-0.00009	1951.46095	1305.19963
1 1 2 0 8	1 1 1 1 9	648.23613*	0.00087	1933.54287	1285.30761
1 1 2 0 7	1 1 1 1 8	650.21296	0.00006	1917.61467	1267.40177
1 1 2 0 6	1 1 1 1 7	652.19413	0.00047	1903.67670	1251.48305
1 1 2 0 5	1 1 1 1 6	654.17710	0.00009	1891.72929	1237.55228
1 1 2 0 4	1 1 1 1 5	656.16209	-0.00040	1881.77271	1225.61022
1 1 2 0 3	1 1 1 1 4	658.14961	-0.00005	1873.80717	1215.65751
1 1 2 0 2	1 1 1 1 3	660.13820	0.00003	1867.83286	1207.69469
1 1 2 0 1	1 1 1 1 2	662.12761	-0.00011	1863.84991	1201.72219
1 1 2 0 4	1 1 1 1 3	674.07820	0.00018	1881.77271	1207.69469
1 1 2 0 5	1 1 1 1 4	676.07210	0.00032	1891.72929	1215.65751
1 1 2 0 6	1 1 1 1 5	678.06601	-0.00047	1903.67670	1225.61022
1 1 2 0 7	1 1 1 1 6	680.06250*	0.00011	1917.61467	1237.55228
1 1 2 0 8	1 1 1 1 7	682.06020*	0.00037	1933.54287	1251.48305
1 1 2 0 9	1 1 1 1 8	684.06040*	0.00122	1951.46095	1267.40177W
1 1 2 0 10	1 1 1 1 9	686.06103	0.00013	1971.36850	1285.30761
1 1 2 0 11	1 1 1 1 10	688.06570	0.00026	1993.26507	1305.19963
1 1 2 0 12	1 1 1 1 11	690.07361	0.00029	2017.15015	1327.07683
1 1 2 0 13	1 1 1 1 12	692.08570	0.00064	2043.02319	1350.93813
1 1 2 0 14	1 1 1 1 13	694.10152	0.00032	2070.88360	1376.78240
1 1 2 0 15	1 1 1 1 14	696.12250	0.00027	2100.73073	1404.60850
1 1 2 0 16	1 1 1 1 15	698.14882	0.00018	2132.56390	1434.41526
1 1 2 0 17	1 1 1 1 16	700.18130	0.00047	2166.38235	1466.20152
1 1 2 0 18	1 1 1 1 17	702.21939	0.00023	2202.18530	1499.96614
1 1 2 0 19	1 1 1 1 18	704.26410	0.00024	2239.97191	1535.70804
1 1 2 0 20	1 1 1 1 19	706.30881	0.00024	2279.74129	1573.42620

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1	1	2	0	21	1	1	1	1	20	708.37340	0.00052	2321.49251	1613.11962	
2	1	1	2	0	22	1	1	1	1	21	710.43780	0.00065	2365.22458	1654.78743
3	1	-1	2	0	5	1	1	1	1	5	666.20169	-0.00015	1891.81206	1225.61022
4	1	-1	2	0	6	1	1	1	1	6	666.24014	-0.00013	1903.79255	1237.55228
5	1	-1	2	0	7	1	1	1	1	7	666.28568	-0.00038	1917.76910	1251.48305
6	1	-1	2	0	8	1	1	1	1	8	666.33953	-0.00009	1933.74139	1267.40177
7	1	-1	2	0	9	1	1	1	1	9	666.40125	-0.00019	1951.70905	1285.30761
8	1	-1	2	0	10	1	1	1	1	10	666.47188	-0.00016	1971.67167	1305.19963
9	1	-1	2	0	11	1	1	1	1	11	666.55194	-0.00004	1993.62880	1327.07683
10	1	-1	2	0	12	1	1	1	1	12	666.64141	-0.00042	2017.57995	1350.93813
11	1	-1	2	0	13	1	1	1	1	13	666.74170	-0.00048	2043.52458	1376.78240
12	1	-1	2	0	14	1	1	1	1	14	666.85300	-0.00060	2071.46210	1404.60850
13	1	-1	2	0	15	1	1	1	1	15	666.97630	-0.00034	2101.39190	1434.41526
14	1	-1	2	0	18	1	-1	1	-1	19	629.32230	-0.00028	2203.12814	1573.80556
15	1	-1	2	0	17	1	-1	1	-1	18	631.20650	0.00039	2167.22564	1536.01954
16	1	-1	2	0	16	1	-1	1	-1	17	633.09550	0.00065	2133.31332	1500.21846
17	1	-1	2	0	15	1	-1	1	-1	16	634.98900	-0.00002	2101.39190	1466.40289
18	1	-1	2	0	14	1	-1	1	-1	15	636.88880	0.00004	2071.46210	1434.57334
19	1	-1	2	0	13	1	-1	1	-1	14	638.79390	-0.00035	2043.52458	1404.73033
20	1	-1	2	0	12	1	-1	1	-1	13	640.70500	-0.00059	2017.57995	1376.87436
21	1	-1	2	0	11	1	-1	1	-1	12	642.62233	-0.00056	1993.62880	1351.00592
22	1	-1	2	0	10	1	-1	1	-1	11	644.54590	-0.00032	1971.67167	1327.12545
23	1	-1	2	0	9	1	-1	1	-1	10	646.47550	-0.00015	1951.70905	1305.23340
24	1	-1	2	0	8	1	-1	1	-1	9	648.41097	-0.00025	1933.74139	1285.33018
25	1	-1	2	0	7	1	-1	1	-1	8	650.35270	-0.00025	1917.76910	1267.41616
26	1	-1	2	0	6	1	-1	1	-1	7	652.30024	-0.00063	1903.79255	1251.49169
27	1	-1	2	0	5	1	-1	1	-1	6	654.25490	-0.00007	1891.81206	1237.55708
28	1	-1	2	0	4	1	-1	1	-1	5	656.21500	-0.00027	1881.82789	1225.61262
29	1	-1	2	0	3	1	-1	1	-1	4	658.18160	-0.00015	1873.84028	1215.65854
30	1	-1	2	0	2	1	-1	1	-1	3	660.15430	-0.00009	1867.84942	1207.69503
31	1	-1	2	0	1	1	-1	1	-1	2	662.13300	-0.00017	1863.85543	1201.72226
32	1	-1	2	0	3	1	-1	1	-1	2	672.11760	-0.00042	1873.84028	1201.72226
33	1	-1	2	0	5	1	-1	1	-1	4	676.15340	-0.00012	1891.81206	1215.65854
34	1	-1	2	0	7	1	-1	1	-1	6	680.21140	-0.00062	1917.76910	1237.55708
35	1	-1	2	0	9	1	-1	1	-1	8	684.29220	-0.00069	1951.70905	1267.41616
36	1	-1	2	0	11	1	-1	1	-1	10	688.39500	-0.00040	1993.62880	1305.23340
37	1	-1	2	0	12	1	-1	1	-1	11	690.45430	-0.00020	2017.57995	1327.12545
38	1	-1	2	0	13	1	-1	1	-1	12	692.51810	-0.00056	2043.52458	1351.00592
39	1	-1	2	0	14	1	-1	1	-1	13	694.58750	-0.00024	2071.46210	1376.87436
40	1	-1	2	0	15	1	-1	1	-1	14	696.66170	0.00013	2101.39190	1404.73033
41	1	-1	2	0	16	1	-1	1	-1	15	698.73940	-0.00058	2133.31332	1434.57334
42	1	-1	2	0	18	1	-1	1	-1	17	702.90990	0.00022	2203.12814	1500.21846
43	1	1	2	0	4	1	-1	1	-1	4	666.11430	0.00013	1881.77271	1215.65854
44	1	1	2	0	5	1	-1	1	-1	5	666.11430*	-0.00237	1891.72929	1225.61262W
45	1	1	2	0	6	1	-1	1	-1	6	666.11890	-0.00072	1903.67670	1237.55708
46	1	1	2	0	7	1	-1	1	-1	7	666.12270	-0.00028	1917.61467	1251.49169
47	1	1	2	0	8	1	-1	1	-1	8	666.12710	0.00038	1933.54287	1267.41616
48	1	1	2	0	9	1	-1	1	-1	9	666.13210*	0.00132	1951.46095	1285.33018W
49	1	1	2	0	10	1	-1	1	-1	10	666.13600	0.00090	1971.36850	1305.23340
50	1	1	2	0	11	1	-1	1	-1	11	666.13980	0.00018	1993.26507	1327.12545
51	1	1	2	0	12	1	-1	1	-1	12	666.14490	0.00067	2017.15015	1351.00592
52	1	1	2	0	13	1	-1	1	-1	13	666.14920	0.00038	2043.02319	1376.87436
53	1	1	2	0	14	1	-1	1	-1	14	666.15440*	0.00113	2070.88360	1404.73033W
54	1	1	2	0	15	1	-1	1	-1	15	666.15440*	-0.00299	2100.73073	1434.57334W

rms = 0.00038 cm⁻¹

$$v_4 + 2v_5 (\Phi) \leftarrow v_4 + v_5 (\Delta)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 2 2 21	1 1 1 1 22	638.19950	-0.00084	2336.62911	1698.42877
1 1 2 2 20	1 1 1 1 21	640.04900	0.00000	2294.83643	1654.78743
1 1 2 2 19	1 1 1 1 20	641.90910	0.00008	2255.02864	1613.11962
1 1 2 2 18	1 1 1 1 19	643.77985	-0.00031	2217.20636	1573.42620
1 1 2 2 17	1 1 1 1 18	645.66220	0.00004	2181.37021	1535.70804
1 1 2 2 16	1 1 1 1 17	647.55470	0.00004	2147.52082	1499.96614

1	-1	2	-2	3	1	-1	1	-1	2	686.80845	0.00012	1888.53059	1201.72226
1	-1	2	-2	4	1	-1	1	-1	3	688.80839	-0.00002	1896.50344	1207.69503
1	-1	2	-2	5	1	-1	1	-1	4	690.81112	0.00052	1906.46914	1215.65854
1	-1	2	-2	6	1	-1	1	-1	5	692.81604	0.00122	1918.42744	1225.61262W
1	-1	2	-2	7	1	-1	1	-1	6	694.82118	0.00021	1932.37805	1237.55708
1	-1	2	-2	8	1	-1	1	-1	7	696.82904	0.00009	1948.32063	1251.49169
1	-1	2	-2	9	1	-1	1	-1	8	698.83869	0.00006	1966.25479	1267.41616
1	-1	2	-2	10	1	-1	1	-1	9	700.84995	0.00005	1986.18007	1285.33018
1	-1	2	-2	11	1	-1	1	-1	10	702.86259	-0.00001	2008.09600	1305.23340
1	-1	2	-2	12	1	-1	1	-1	11	704.87653	-0.00003	2032.00201	1327.12545
1	-1	2	-2	13	1	-1	1	-1	12	706.89118*	-0.00043	2057.89753	1351.00592
1	-1	2	-2	14	1	-1	1	-1	13	708.90757	0.00002	2085.78191	1376.87436
1	-1	2	-2	15	1	-1	1	-1	14	710.92743*	0.00329	2115.65447	1404.73033W
1	-1	2	-2	16	1	-1	1	-1	15	712.94109	-0.00006	2147.51449	1434.57334
1	-1	2	-2	17	1	-1	1	-1	16	714.95813	-0.00017	2181.36119	1466.40289
1	-1	2	-2	18	1	-1	1	-1	17	716.97542	0.00011	2217.19377	1500.21846
1	-1	2	-2	19	1	-1	1	-1	18	718.99202	0.00015	2255.01141	1536.01954
1	-1	2	-2	20	1	-1	1	-1	19	721.00745	-0.00022	2294.81323	1573.80556
1	-1	2	-2	21	1	-1	1	-1	20	723.02201	-0.00038	2336.59836	1613.57597
1	-1	2	-2	22	1	-1	1	-1	21	725.03738*	0.00170	2380.36588	1655.33020W
1	-1	2	-2	23	1	-1	1	-1	22	727.04738	0.00014	2426.11489	1699.06765
1	-1	2	-2	24	1	-1	1	-1	23	731.06500*	0.00108	2523.55362	1792.48970W
1	-1	2	-2	25	1	-1	1	-1	24	733.06760	-0.00087	2575.24148	1842.17301
1	-1	2	-2	26	1	-1	1	-1	25	735.07015	0.00001	2628.90708	1893.83694
1	-1	2	-2	27	1	-1	1	-1	26	737.06920	0.00048	2684.54948	1947.48076
1	-1	2	-2	28	1	-1	1	-1	27	739.06450	0.00049	2742.16775	2003.10374
1	1	2	2	3	1	-1	1	-1	3	680.83599	0.00043	1888.53059	1207.69503
1	1	2	2	4	1	-1	1	-1	4	680.84552	0.00062	1896.50344	1215.65854
1	1	2	2	5	1	-1	1	-1	5	680.85778	0.00126	1906.46914	1225.61262W
1	1	2	2	6	1	-1	1	-1	6	680.87071	0.00034	1918.42746	1237.55708
1	1	2	2	7	1	-1	1	-1	7	680.88624	-0.00017	1932.37810	1251.49169
1	1	2	2	8	1	-1	1	-1	8	680.90639*	0.00180	1948.32074	1267.41616W
1	1	2	2	9	1	-1	1	-1	9	680.92501	0.00018	1966.25501	1285.33018
1	1	2	2	10	1	-1	1	-1	10	680.94716	0.00008	1986.18048	1305.23340
1	1	2	2	11	1	-1	1	-1	11	680.97131	0.00006	2008.09670	1327.12545
1	1	2	2	12	1	-1	1	-1	12	680.99724	-0.00003	2032.00319	1351.00592
1	1	2	2	13	1	-1	1	-1	13	681.02584	0.00079	2057.89941	1376.87436
1	1	2	2	14	1	-1	1	-1	14	681.05457	0.00009	2085.78481	1404.73033
1	1	2	2	15	1	-1	1	-1	15	681.08554	0.00006	2115.65882	1434.57334
1	1	2	2	16	1	-1	1	-1	16	681.11640*	-0.00153	2147.52082	1466.40289W
1	1	2	2	22	1	-1	1	-1	22	681.33893	0.00050	2380.40608	1699.06765
1	1	2	2	23	1	-1	1	-1	23	681.37923	0.00018	2426.16675	1744.78769
1	1	2	2	24	1	-1	1	-1	24	681.42097	0.00012	2473.91055	1792.48970
1	1	2	2	25	1	-1	1	-1	25	681.46360	-0.00034	2523.63695	1842.17301
1	1	2	2	27	1	-1	1	-1	27	681.55470	-0.00004	2629.03550	1947.48076
1	1	2	2	28	1	-1	1	-1	28	681.60350	0.00056	2684.70668	2003.10374

rms = 0.00031 cm⁻¹

3v₅ (Π) ← 2v₅ (Σ⁺)

v ₄ ' l ₄ ' v ₅ ' l ₅ ' J'	v ₄ '' l ₄ '' v ₅ '' l ₅ '' J''	OBS	OBS - CALC	E'	E''
0 0 3 1 1	0 0 2 0 2	664.01500	0.00012	2012.20878	1348.19391
0 0 3 1 2	0 0 2 0 3	662.01720	-0.00009	2016.17851	1354.16122
0 0 3 1 3	0 0 2 0 4	660.01553	-0.00005	2022.13301	1362.11743
0 0 3 1 4	0 0 2 0 5	658.00937	-0.00048	2030.07218	1372.06234
0 0 3 1 5	0 0 2 0 6	655.99983	-0.00034	2039.99589	1383.99572
0 0 3 1 6	0 0 2 0 7	653.98620	-0.00045	2051.90395	1397.91730
0 0 3 1 7	0 0 2 0 8	651.97050	0.00108	2065.79617	1413.82675W
0 0 3 1 8	0 0 2 0 9	649.94859	0.00000	2081.67229	1431.72370
0 0 3 1 9	0 0 2 0 10	647.92414	-0.00016	2099.53204	1451.60774
0 0 3 1 10	0 0 2 0 11	645.89657	-0.00014	2119.37511	1473.47840
0 0 3 1 11	0 0 2 0 12	643.86585	-0.00013	2141.20116	1497.33518
0 0 3 1 12	0 0 2 0 13	641.83207	-0.00022	2165.00981	1523.17752
0 0 3 1 13	0 0 2 0 14	639.79560	-0.00022	2190.80064	1551.00481
0 0 3 1 14	0 0 2 0 15	637.75609	-0.00022	2218.57321	1580.81643

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1	0	0	3	1	15	0	0	2	0	16	635.71504	-0.00033	2248.32704	1612.61167
2	0	0	3	1	16	0	0	2	0	17	633.67227	0.00046	2280.06163	1646.38981
3	0	0	3	1	17	0	0	2	0	18	631.62612	-0.00023	2313.77642	1682.15007
4	0	0	3	1	18	0	0	2	0	19	629.57900	-0.00021	2349.47084	1719.89163
5	0	0	3	1	19	0	0	2	0	20	627.53050	-0.00016	2387.14429	1759.61363
6	0	0	3	1	1	0	0	2	0	0	669.98210	-0.00023	2012.20878	1342.22645
7	0	0	3	1	2	0	0	2	0	1	671.96260	-0.00029	2016.17851	1344.21562
8	0	0	3	1	3	0	0	2	0	2	673.93907	-0.00003	2022.13301	1348.19391
9	0	0	3	1	4	0	0	2	0	3	675.90970*	-0.00126	2030.07218	1354.16122W
10	0	0	3	1	7	0	0	2	0	6	681.80037	-0.00008	2065.79617	1383.99572
11	0	0	3	1	9	0	0	2	0	8	685.70587	0.00058	2099.53204	1413.82675
12	0	0	3	1	10	0	0	2	0	9	687.65132	-0.00009	2119.37511	1431.72370
13	0	0	3	1	11	0	0	2	0	10	689.59329	-0.00013	2141.20116	1451.60774
14	0	0	3	1	12	0	0	2	0	11	691.53357*	0.00216	2165.00981	1473.47840W
15	0	0	3	1	13	0	0	2	0	12	693.46545	-0.00001	2190.80064	1497.33518
16	0	0	3	1	14	0	0	2	0	13	695.39523	-0.00046	2218.57321	1523.17752
17	0	0	3	1	15	0	0	2	0	14	697.32193	-0.00030	2248.32704	1551.00481
18	0	0	3	1	16	0	0	2	0	15	699.24483	-0.00037	2280.06163	1580.81643
19	0	0	3	1	17	0	0	2	0	16	701.16448	-0.00026	2313.77642	1612.61167
20	0	0	3	1	18	0	0	2	0	17	703.08081	-0.00022	2349.47084	1646.38981
21	0	0	3	1	19	0	0	2	0	18	704.99419	-0.00003	2387.14429	1682.15007
22	0	0	3	1	20	0	0	2	0	19	706.90423	-0.00027	2426.79612	1719.89163
23	0	0	3	1	21	0	0	2	0	20	708.81195	-0.00010	2468.42567	1759.61363
24	0	0	3	1	22	0	0	2	0	21	710.71687	-0.00020	2512.03224	1801.31517
25	0	0	3	1	23	0	0	2	0	22	712.61974	-0.00004	2557.61509	1844.99532
26	0	0	3	1	25	0	0	2	0	24	716.41910	0.00001	2654.70659	1938.28750
27	0	0	3	-1	1	0	0	2	0	1	668.00794	0.00029	2012.22327	1344.21562
28	0	0	3	-1	2	0	0	2	0	2	668.02778	-0.00028	2016.22197	1348.19391
29	0	0	3	-1	3	0	0	2	0	3	668.05867	-0.00003	2022.21993	1354.16122
30	0	0	3	-1	4	0	0	2	0	4	668.09953	-0.00008	2030.21704	1362.11743
31	0	0	3	-1	5	0	0	2	0	5	668.15068	-0.00014	2040.21315	1372.06234
32	0	0	3	-1	6	0	0	2	0	6	668.21223	-0.00015	2052.20810	1383.99572
33	0	0	3	-1	7	0	0	2	0	7	668.28423	-0.00013	2066.20166	1397.91730
34	0	0	3	-1	8	0	0	2	0	8	668.36612	-0.00070	2082.19357	1413.82675
35	0	0	3	-1	9	0	0	2	0	9	668.45983	-0.00003	2100.18356	1431.72370
36	0	0	3	-1	10	0	0	2	0	10	668.56360	0.00005	2120.17129	1451.60774
37	0	0	3	-1	11	0	0	2	0	11	668.67797	-0.00003	2142.15640	1473.47840
38	0	0	3	-1	12	0	0	2	0	12	668.80328	-0.00004	2166.13850	1497.33518
39	0	0	3	-1	13	0	0	2	0	13	668.93956	-0.00006	2192.11714	1523.17752
40	0	0	3	-1	14	0	0	2	0	14	669.08705	0.00003	2220.09184	1551.00481
41	0	0	3	-1	15	0	0	2	0	15	669.24578	0.00011	2250.06210	1580.81643
42	0	0	3	-1	16	0	0	2	0	16	669.41574	0.00006	2282.02735	1612.61167
43	0	0	3	-1	17	0	0	2	0	17	669.59727	0.00006	2315.98702	1646.38981
44	0	0	3	-1	18	0	0	2	0	18	669.79057	0.00018	2351.94046	1682.15007
45	0	0	3	-1	19	0	0	2	0	19	669.99540	0.00002	2389.88701	1719.89163
46	0	0	3	-1	20	0	0	2	0	20	670.21248	0.00016	2429.82595	1759.61363
47	0	0	3	-1	21	0	0	2	0	21	670.44138	0.00002	2471.75653	1801.31517
48	0	0	3	-1	22	0	0	2	0	22	670.68260	-0.00004	2515.67796	1844.99532
49	0	0	3	-1	23	0	0	2	0	23	670.93650	0.00020	2561.58939	1890.65309
50	0	0	3	-1	24	0	0	2	0	24	671.20260	0.00015	2609.48995	1938.28750
51	0	0	3	-1	25	0	0	2	0	25	671.48140	0.00017	2659.37872	1987.89749

rms = 0.00023 cm⁻¹

$$3\nu_5(\Phi) \leftarrow 2\nu_5(\Delta)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 3 3 3	0 0 2 -2 3	684.97659	-0.00002	2055.95466	1370.97805
0 0 3 3 4	0 0 2 -2 4	684.98421	-0.00023	2063.91501	1378.93057
0 0 3 3 5	0 0 2 -2 5	684.99384	-0.00045	2073.86528	1388.87100
0 0 3 3 6	0 0 2 -2 6	685.00548	-0.00069	2085.80538	1400.79921
0 0 3 3 7	0 0 2 -2 7	685.01897	-0.00117	2099.73517	1414.71503W
0 0 3 3 8	0 0 2 -2 8	685.03270	-0.00354	2115.65451	1430.61827W
0 0 3 3 9	0 0 2 -2 9	685.05440	-0.00011	2133.56322	1448.50870
0 0 3 3 10	0 0 2 -2 10	685.07483	-0.00020	2153.46111	1468.38608
0 0 3 3 11	0 0 2 -2 11	685.09748	0.00017	2175.34797	1490.25013

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1	0	0	3	-3	7	0	0	2	-2	8	669.11650	-0.00041	2099.73518	1430.61827
2	0	0	3	-3	8	0	0	2	-2	9	667.14611	0.00029	2115.65453	1448.50870
3	0	0	3	-3	9	0	0	2	-2	10	665.17760	0.00042	2133.56326	1468.38608
4	0	0	3	-3	10	0	0	2	-2	11	663.21080	-0.00026	2153.46119	1490.25013
5	0	0	3	-3	11	0	0	2	-2	12	661.24800	0.00043	2175.34811	1514.10054
6	0	0	3	-3	12	0	0	2	-2	13	659.28711	0.00029	2199.22379	1539.93697
7	0	0	3	-3	13	0	0	2	-2	14	657.32855	-0.00038	2225.08800	1567.75907
8	0	0	3	-3	14	0	0	2	-2	15	655.37370	-0.00031	2252.94045	1597.56645
9	0	0	3	-3	15	0	0	2	-2	16	653.42220	0.00000	2282.78088	1629.35868
10	0	0	3	-3	16	0	0	2	-2	17	651.47305	-0.00060	2314.60898	1663.13533
11	0	0	3	-3	17	0	0	2	-2	18	649.52830	-0.00021	2348.42442	1698.89591
12	0	0	3	-3	18	0	0	2	-2	19	647.58680	-0.00014	2384.22688	1736.63994
13	0	0	3	-3	19	0	0	2	-2	20	645.64880	-0.00032	2422.01600	1776.36688
14	0	0	3	-3	20	0	0	2	-2	21	643.71710	0.00186	2461.79141	1818.07617W
15	0	0	3	-3	3	0	0	2	-2	2	690.94103*	-0.00006	2055.95466	1365.01357
16	0	0	3	-3	4	0	0	2	-2	3	692.93681*	-0.00014	2063.91501	1370.97805
17	0	0	3	-3	5	0	0	2	-2	4	694.93522*	0.00050	2073.86528	1378.93057
18	0	0	3	-3	6	0	0	2	-2	5	696.93399	-0.00040	2085.80538	1388.87100
19	0	0	3	-3	7	0	0	2	-2	6	698.93553	-0.00044	2099.73518	1400.79921
20	0	0	3	-3	8	0	0	2	-2	7	700.93816	-0.00134	2115.65453	1414.71503W
21	0	0	3	-3	9	0	0	2	-2	8	702.94840	0.00341	2133.56326	1430.61827W
22	0	0	3	-3	10	0	0	2	-2	9	704.95195*	-0.00054	2153.46119	1448.50870
23	0	0	3	-3	11	0	0	2	-2	10	706.96157	-0.00046	2175.34811	1468.38608
24	0	0	3	-3	12	0	0	2	-2	11	708.97403	0.00037	2199.22379	1490.25013
25	0	0	3	-3	13	0	0	2	-2	12	710.98753	0.00007	2225.08800	1514.10054
26	0	0	3	-3	14	0	0	2	-2	13	713.00340	-0.00008	2252.94045	1539.93697
27	0	0	3	-3	15	0	0	2	-2	14	715.02196	0.00015	2282.78088	1567.75907
28	0	0	3	-3	16	0	0	2	-2	15	717.04260	0.00007	2314.60898	1597.56645
29	0	0	3	-3	17	0	0	2	-2	16	719.06587	0.00013	2348.42442	1629.35868
30	0	0	3	-3	18	0	0	2	-2	17	721.09153	-0.00003	2384.22688	1663.13533
31	0	0	3	-3	19	0	0	2	-2	18	723.12004	-0.00005	2422.01600	1698.89591
32	0	0	3	-3	20	0	0	2	-2	19	725.15158	0.00011	2461.79141	1736.63994

rms = 0.00037 cm⁻¹

$2\nu_4(\Sigma^+) \leftarrow G.S.(\Sigma^+)$

ν_4'	ν_4''	ν_5'	ν_5''	J'	J''	OBS	OBS - CALC	E'	E''
2	0	0	0	0	1	1031.95232	0.00008	1033.93529	1.98305
2	0	0	0	1	2	1029.98007	0.00002	1035.92917	5.94912
2	0	0	0	2	3	1028.01865	0.00003	1039.91679	11.89816
2	0	0	0	3	4	1026.06784	0.00004	1045.89789	19.83009
2	0	0	0	4	5	1024.12740	0.00010	1053.87209	29.74480
2	0	0	0	5	6	1022.19676	0.00003	1063.83887	41.64214
2	0	0	0	6	7	1020.27562	0.00000	1075.79759	55.52197
2	0	0	0	7	8	1018.36336	-0.00002	1089.74746	71.38408
2	0	0	0	8	9	1016.45928	-0.00006	1105.68761	89.22827
2	0	0	0	9	10	1014.56300	0.00027	1123.61701	109.05428
2	0	0	0	10	11	1012.67264	-0.00008	1143.53456	130.86184
2	0	0	0	11	12	1010.78882	0.00041	1165.43907	154.65066
2	0	0	0	12	13	1008.90889	0.00004	1189.32925	180.42041
2	0	0	0	13	14	1007.03274	-0.00033	1215.20380	208.17072
2	0	0	0	14	15	1005.16006	-0.00008	1243.06138	237.90124
2	0	0	0	15	16	1003.28906	-0.00006	1272.90065	269.61154
2	0	0	0	16	17	1001.41927	0.00012	1304.72033	303.30118
2	0	0	0	17	18	999.54983	0.00037	1338.51918	338.96972
2	0	0	0	18	19	997.67965	0.00026	1374.29604	376.61665
2	0	0	0	19	20	995.80863	0.00025	1412.04985	416.24147
2	0	0	0	20	21	993.93637	0.00037	1451.77962	457.84362
2	0	0	0	21	22	992.06205	0.00010	1493.48450	501.42254
2	0	0	0	22	23	990.18639	0.00034	1537.16368	546.97764
2	0	0	0	23	24	988.30863	0.00044	1582.81646	594.50827
2	0	0	0	24	25	986.42873	0.00034	1630.44219	644.01380
2	0	0	0	25	26	984.54693	0.00022	1680.04024	695.49354
2	0	0	0	26	27	982.66306	-0.00021	1731.61005	748.94678
2	0	0	0	27	28	980.77920	0.00011	1785.15104	804.37280

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	$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS – CALC	E'	E''
1	2 2 0 0 41	0 0 0 0 42	970.08701	-0.00004	2757.09023	1787.00318
2	2 2 0 0 40	0 0 0 0 41	971.29577	-0.00087	2675.34712	1704.05048
3	2 2 0 0 39	0 0 0 0 40	972.52554	-0.00035	2595.58334	1623.05745
4	2 2 0 0 38	0 0 0 0 39	973.77464	-0.00035	2517.80019	1544.02520
5	2 2 0 0 37	0 0 0 0 38	975.04392	-0.00021	2441.99894	1466.95482
6	2 2 0 0 36	0 0 0 0 37	976.33353	0.00003	2368.18085	1391.84735
7	2 2 0 0 35	0 0 0 0 36	977.64303	-0.00029	2296.34716	1318.70384
8	2 2 0 0 34	0 0 0 0 35	978.97381	0.00001	2226.49908	1247.52529
9	2 2 0 0 33	0 0 0 0 34	980.32533	0.00016	2158.63783	1178.31267
10	2 2 0 0 32	0 0 0 0 33	981.69771	0.00004	2092.76459	1111.06693
11	2 2 0 0 31	0 0 0 0 32	983.09180	0.00027	2028.88052	1045.78899
12	2 2 0 0 30	0 0 0 0 31	984.50650	-0.00052	1966.98678	982.47976
13	2 2 0 0 29	0 0 0 0 30	985.94463	0.00024	1907.08448	921.14009
14	2 2 0 0 28	0 0 0 0 29	987.40396	0.00006	1849.17473	861.77083
15	2 2 0 0 27	0 0 0 0 28	988.88574	-0.00006	1793.25860	804.37280
16	2 2 0 0 26	0 0 0 0 27	990.39092	0.00059	1739.33712	748.94678
17	2 2 0 0 25	0 0 0 0 26	991.91716	-0.00057	1687.41127	695.49354
18	2 2 0 0 24	0 0 0 0 25	993.46851	0.00032	1637.48199	644.01380
19	2 2 0 0 23	0 0 0 0 24	995.04214	0.00027	1589.55014	594.50827
20	2 2 0 0 22	0 0 0 0 23	996.63934	0.00049	1543.61649	546.97764
21	2 2 0 0 21	0 0 0 0 22	998.25959	0.00041	1499.68172	501.42254
22	2 2 0 0 20	0 0 0 0 21	999.90292	0.00016	1457.74639	457.84362
23	2 2 0 0 19	0 0 0 0 20	1001.56977	0.00032	1417.81092	416.24147
24	2 2 0 0 18	0 0 0 0 19	1003.25939	0.00045	1379.87559	376.61665
25	2 2 0 0 17	0 0 0 0 18	1004.97088	0.00006	1343.94054	338.96972
26	2 2 0 0 16	0 0 0 0 17	1006.70505	0.00050	1310.00574	303.30118
27	2 2 0 0 15	0 0 0 0 16	1008.45969	0.00022	1278.07100	269.61154
28	2 2 0 0 14	0 0 0 0 15	1010.23523	0.00044	1248.13603	237.90124
29	2 2 0 0 13	0 0 0 0 14	1012.02998	0.00031	1220.20039	208.17072
30	2 2 0 0 12	0 0 0 0 13	1013.84333	0.00017	1194.26357	180.42041
31	2 2 0 0 11	0 0 0 0 12	1015.67454	0.00023	1170.32497	154.65066
32	2 2 0 0 10	0 0 0 0 11	1017.52243	0.00028	1148.38399	130.86184
33	2 2 0 0 9	0 0 0 0 10	1019.38624	0.00053	1128.43999	109.05428
34	2 2 0 0 8	0 0 0 0 9	1021.26446	0.00039	1110.49234	89.22827
35	2 2 0 0 7	0 0 0 0 8	1023.15649	0.00012	1094.54045	71.38408
36	2 2 0 0 6	0 0 0 0 7	1025.06227	0.00045	1080.58379	55.52197
37	2 2 0 0 5	0 0 0 0 6	1026.97990	0.00018	1068.62187	41.64214
38	2 2 0 0 5	0 0 0 0 4	1048.79270	0.00092	1068.62187	19.83009
39	2 2 0 0 6	0 0 0 0 5	1050.83957	0.00057	1080.58379	29.74480
40	2 2 0 0 7	0 0 0 0 6	1052.89812	-0.00019	1094.54045	41.64214
41	2 2 0 0 8	0 0 0 0 7	1054.97074	0.00037	1110.49234	55.52197
42	2 2 0 0 9	0 0 0 0 8	1057.05595	0.00005	1128.43999	71.38408
43	2 2 0 0 10	0 0 0 0 9	1059.15576	0.00004	1148.38399	89.22827
44	2 2 0 0 11	0 0 0 0 10	1061.27082	0.00012	1170.32497	109.05428
45	2 2 0 0 12	0 0 0 0 11	1063.40199	0.00027	1194.26357	130.86184
46	2 2 0 0 13	0 0 0 0 12	1065.55027	0.00054	1220.20039	154.65066
47	2 2 0 0 14	0 0 0 0 13	1067.71578	0.00016	1248.13603	180.42041
48	2 2 0 0 15	0 0 0 0 14	1069.90050	0.00022	1278.07100	208.17072
49	2 2 0 0 16	0 0 0 0 15	1072.10477	0.00027	1310.00574	237.90124
50	2 2 0 0 17	0 0 0 0 16	1074.32908	0.00007	1343.94054	269.61154
51	2 2 0 0 18	0 0 0 0 17	1076.57460	0.00019	1379.87559	303.30118
52	2 2 0 0 19	0 0 0 0 18	1078.84140	0.00020	1417.81092	338.96972
53	2 2 0 0 20	0 0 0 0 19	1081.12972	-0.00001	1457.74639	376.61665
54	2 2 0 0 21	0 0 0 0 20	1083.44043	0.00018	1499.68172	416.24147
55	2 2 0 0 22	0 0 0 0 21	1085.77319	0.00032	1543.61649	457.84362
56	2 2 0 0 23	0 0 0 0 22	1088.12771	0.00012	1589.55014	501.42254
57	2 2 0 0 24	0 0 0 0 23	1090.50457	0.00021	1637.48199	546.97764
58	2 2 0 0 25	0 0 0 0 24	1092.90327	0.00027	1687.41127	594.50827
59	2 2 0 0 26	0 0 0 0 25	1095.32340	0.00008	1739.33712	644.01380
60	2 2 0 0 27	0 0 0 0 26	1097.76528	0.00022	1793.25860	695.49354
	2 2 0 0 28	0 0 0 0 27	1100.22819	0.00024	1849.17473	748.94678
	2 2 0 0 29	0 0 0 0 28	1102.71194	0.00026	1907.08448	804.37280
	2 2 0 0 30	0 0 0 0 29	1105.21610	0.00015	1966.98678	861.77083
	2 2 0 0 31	0 0 0 0 30	1107.74054	0.00011	2028.88052	921.14009
	2 2 0 0 32	0 0 0 0 31	1110.28492	0.00008	2092.76459	982.47976
	2 2 0 0 33	0 0 0 0 32	1112.84898	0.00014	2158.63783	1045.78899
	2 2 0 0 34	0 0 0 0 33	1115.43315	0.00011	2226.49908	1111.06693

2	2	0	0	35	0	0	0	0	34	1118.03439	-0.00010	2296.34716	1178.31267
2	2	0	0	36	0	0	0	0	35	1120.65547	-0.00009	2368.18085	1247.52529
2	2	0	0	37	0	0	0	0	36	1123.29498	-0.00012	2441.99894	1318.70384
2	2	0	0	38	0	0	0	0	37	1125.95271	-0.00013	2517.80019	1391.84735
2	2	0	0	39	0	0	0	0	38	1128.62817	-0.00036	2595.58334	1466.95482
2	2	0	0	40	0	0	0	0	39	1131.32173	-0.00019	2675.34712	1544.02520
2	2	0	0	41	0	0	0	0	40	1134.03242	-0.00036	2757.09023	1623.05745
2	2	0	0	42	0	0	0	0	41	1136.76096	0.00008	2840.81136	1704.05048
2	2	0	0	43	0	0	0	0	42	1139.50590	-0.00009	2926.50917	1787.00318

rms = 0.00031 cm⁻¹

$v_4 + v_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	0 0 0 0 1	1198.51557	0.00052	1200.49810	1.98305
1 1 1 -1 1	0 0 0 0 2	1196.54002	0.00014	1202.48900	5.94912
1 1 1 -1 2	0 0 0 0 3	1194.57270	0.00001	1206.47085	11.89816
1 1 1 -1 3	0 0 0 0 4	1192.61363	-0.00004	1212.44377	19.83009
1 1 1 -1 4	0 0 0 0 5	1190.66321	0.00012	1220.40789	29.74480
1 1 1 -1 5	0 0 0 0 6	1188.72140	0.00011	1230.36343	41.64214
1 1 1 -1 6	0 0 0 0 7	1186.78878	0.00010	1242.31065	55.52197
1 1 1 -1 7	0 0 0 0 8	1184.86581	0.00005	1256.24984	71.38408
1 1 1 -1 8	0 0 0 0 9	1182.95292	-0.00018	1272.18137	89.22827
1 1 1 -1 9	0 0 0 0 10	1181.05155	0.00022	1290.10561	109.05428
1 1 1 -1 10	0 0 0 0 11	1179.16124	0.00010	1310.02298	130.86184
1 1 1 -1 11	0 0 0 0 12	1177.28288	-0.00039	1331.93393	154.65066
1 1 1 -1 12	0 0 0 0 13	1175.41817	-0.00033	1355.83891	180.42041
1 1 1 -1 13	0 0 0 0 14	1173.56761	-0.00001	1381.73835	208.17072
1 1 1 -1 14	0 0 0 0 15	1171.73147	0.00004	1409.63267	237.90124
1 1 1 -1 15	0 0 0 0 16	1169.91054	-0.00017	1439.52224	269.61154
1 1 1 -1 16	0 0 0 0 17	1168.10622	0.00003	1471.40738	303.30118
1 1 1 -1 17	0 0 0 0 18	1166.31870	0.00013	1505.28829	338.96972
1 1 1 -1 18	0 0 0 0 19	1164.54858	0.00013	1541.16510	376.61665
1 1 1 -1 19	0 0 0 0 20	1162.79659	0.00023	1579.03782	416.24147
1 1 1 -1 20	0 0 0 0 21	1161.06281	0.00008	1618.90635	457.84362
1 1 1 -1 21	0 0 0 0 22	1159.34761	-0.00030	1660.77045	501.42254
1 1 1 -1 22	0 0 0 0 23	1157.65208	-0.00005	1704.62977	546.97764
1 1 1 -1 23	0 0 0 0 24	1155.97523	-0.00033	1750.48383	594.50827
1 1 1 -1 24	0 0 0 0 25	1154.31881	0.00055	1798.33206	644.01380
1 1 1 -1 25	0 0 0 0 26	1152.68002	-0.00023	1848.17378	695.49354
1 1 1 -1 26	0 0 0 0 27	1151.06137	-0.00009	1900.00824	748.94678
1 1 1 -1 27	0 0 0 0 28	1149.46205	0.00024	1953.83461	804.37280
1 1 1 -1 28	0 0 0 0 29	1147.88120	0.00005	2009.65198	861.77083
1 1 1 -1 29	0 0 0 0 30	1146.31963	0.00030	2067.45942	921.14009
1 1 1 -1 30	0 0 0 0 31	1144.77594	-0.00023	2127.25592	982.47976
1 1 1 -1 31	0 0 0 0 32	1143.25198	0.00051	2189.04046	1045.78899
1 1 1 -1 32	0 0 0 0 33	1141.74540	0.00035	2252.81197	1111.06693
1 1 1 -1 33	0 0 0 0 34	1140.25730	0.00060	2318.56937	1178.31267
1 1 1 -1 34	0 0 0 0 35	1138.78690	0.00066	2386.31153	1247.52529
1 1 1 -1 35	0 0 0 0 36	1137.33410	0.00063	2456.03731	1318.70384
1 1 1 -1 36	0 0 0 0 37	1135.89862	0.00042	2527.74555	1391.84735
1 1 1 -1 37	0 0 0 0 38	1134.48082	0.00056	2601.43508	1466.95482
1 1 1 -1 38	0 0 0 0 39	1133.07993	0.00045	2677.10468	1544.02520
1 1 1 -1 39	0 0 0 0 40	1131.69644	0.00076	2754.75313	1623.05745
1 1 1 -1 40	0 0 0 0 41	1130.32938	0.00067	2834.37920	1704.05048
1 1 1 -1 41	0 0 0 0 42	1128.97966	0.00123	2915.98161	1787.00318W
1 1 1 -1 42	0 0 0 0 43	1127.64639	0.00172	2999.55909	1871.91441W
1 1 1 -1 1	0 0 0 0 0	1202.48927	0.00027	1202.48900	0.00000
1 1 1 -1 2	0 0 0 0 1	1204.48768	-0.00012	1206.47085	1.98305
1 1 1 -1 3	0 0 0 0 2	1206.49404	-0.00060	1212.44377	5.94912
1 1 1 -1 4	0 0 0 0 3	1208.51003	0.00030	1220.40789	11.89816
1 1 1 -1 5	0 0 0 0 4	1210.53320	-0.00014	1230.36343	19.83009
1 1 1 -1 6	0 0 0 0 5	1212.56578	-0.00007	1242.31065	29.74480
1 1 1 -1 7	0 0 0 0 6	1214.60747	-0.00023	1256.24984	41.64214
1 1 1 -1 8	0 0 0 0 7	1216.66777	0.00017	1272.18137	55.52197

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1	1	1	-1	9	0	0	0	0	8	1218.72149	-0.00003	1290.10561	71.38408
1	1	1	-1	10	0	0	0	0	9	1220.79484	0.00013	1310.02298	89.22827
1	1	1	-1	11	0	0	0	0	10	1222.87941	-0.00024	1331.93393	109.05428
2	1	1	1	-1	12	0	0	0	11	1224.97715	0.00008	1355.83891	130.86184
3	1	1	1	-1	13	0	0	0	12	1227.08785	0.00016	1381.73835	154.65066
4	1	1	1	-1	14	0	0	0	13	1229.21226	-0.00001	1409.63267	180.42041
5	1	1	1	-1	15	0	0	0	14	1231.35122	-0.00030	1439.52224	208.17072
6	1	1	1	-1	16	0	0	0	15	1233.50595	-0.00019	1471.40738	237.90124
7	1	1	1	-1	17	0	0	0	16	1235.67679	0.00004	1505.28829	269.61154
8	1	1	1	-1	18	0	0	0	17	1237.86371	-0.00021	1541.16510	303.30118
9	1	1	1	-1	19	0	0	0	18	1240.06800	-0.00011	1579.03782	338.96972
10	1	1	1	-1	20	0	0	0	19	1242.28958	-0.00012	1618.90635	376.61665
11	1	1	1	-1	21	0	0	0	20	1244.52883	-0.00015	1660.77045	416.24147
12	1	1	1	-1	22	0	0	0	21	1246.78654	0.00040	1704.62977	457.84362
13	1	1	1	-1	23	0	0	0	22	1249.06108	-0.00020	1750.48383	501.42254
14	1	1	1	-1	24	0	0	0	23	1251.35374	-0.00068	1798.33206	546.97764
15	1	1	1	-1	25	0	0	0	24	1253.66481	-0.00070	1848.17378	594.50827
16	1	1	1	-1	26	0	0	0	25	1255.99446	0.00001	1900.00824	644.01380
17	1	1	1	-1	27	0	0	0	26	1258.34107	0.00000	1953.83461	695.49354
18	1	1	1	-1	28	0	0	0	27	1260.70550	0.00030	2009.65198	748.94678
19	1	1	1	-1	29	0	0	0	28	1263.08653	-0.00009	2067.45942	804.37280
20	1	1	1	-1	30	0	0	0	29	1265.48515	0.00006	2127.25592	861.77083
21	1	1	1	-1	31	0	0	0	30	1267.90077	0.00040	2189.04046	921.14009
22	1	1	1	-1	32	0	0	0	31	1270.33245	0.00023	2252.81197	982.47976
23	1	1	1	-1	33	0	0	0	32	1272.78072	0.00034	2318.56937	1045.78899
24	1	1	1	-1	34	0	0	0	33	1275.24474	0.00014	2386.31153	1111.06693
25	1	1	1	-1	35	0	0	0	34	1277.72482	0.00018	2456.03731	1178.31267
26	1	1	1	-1	36	0	0	0	35	1280.22075	0.00048	2527.74555	1247.52529
27	1	1	1	-1	37	0	0	0	36	1282.73185	0.00062	2601.43508	1318.70384
28	1	1	1	-1	38	0	0	0	37	1285.25731	-0.00001	2677.10468	1391.84735
29	1	1	1	-1	39	0	0	0	38	1287.79919	0.00087	2754.75313	1466.95482
30	1	1	1	-1	40	0	0	0	39	1290.35422	0.00022	2834.37920	1544.02520
31	1	1	1	-1	41	0	0	0	40	1292.92593	0.00177	2915.98161	1623.05745W
32	1	1	1	-1	42	0	0	0	41	1295.50788	-0.00073	2999.55909	1704.05048
33	1	1	1	-1	43	0	0	0	42	1298.10927	0.00212	3085.11033	1787.00318W
34	1	1	1	-1	44	0	0	0	43	1300.71869	-0.00090	3172.63400	1871.91441

rms = 0.00035 cm⁻¹

$$v_4 + v_5 (\Delta) \leftarrow G.S. (\Sigma^+)$$

v_4'	l_4'	v_5'	l_5'	J'	v_4''	l_4''	v_5''	l_5''	J''	OBS	OBS - CALC	E'	E''
1	1	1	1	6	0	0	0	0	7	1182.03050	0.00019	1237.55228	55.52197
1	1	1	1	7	0	0	0	0	8	1180.09780	-0.00116	1251.48305	71.38408W
1	1	1	1	8	0	0	0	0	9	1178.17399	0.00049	1267.40177	89.22827
1	1	1	1	9	0	0	0	0	10	1176.25360	0.00027	1285.30761	109.05428
1	1	1	1	10	0	0	0	0	11	1174.33778	-0.00001	1305.19963	130.86184
1	1	1	1	11	0	0	0	0	12	1172.42620	0.00003	1327.07683	154.65066
1	1	1	1	13	0	0	0	0	14	1168.61180	0.00012	1376.78240	208.17072
1	1	1	1	14	0	0	0	0	15	1166.70744	0.00017	1404.60850	237.90124
1	1	1	1	15	0	0	0	0	16	1164.80361	-0.00011	1434.41526	269.61154
1	1	1	1	16	0	0	0	0	17	1162.90033	0.00000	1466.20152	303.30118
1	1	1	1	17	0	0	0	0	18	1160.99595	-0.00047	1499.96614	338.96972
1	1	1	1	18	0	0	0	0	19	1159.09166	0.00027	1535.70804	376.61665
1	1	1	1	20	0	0	0	0	21	1155.27657	0.00057	1613.11962	457.84362
1	1	1	1	21	0	0	0	0	22	1153.36543	0.00055	1654.78743	501.42254
1	1	1	1	22	0	0	0	0	23	1151.45145	0.00032	1698.42877	546.97764
1	1	1	1	23	0	0	0	0	24	1149.53443	-0.00017	1744.04287	594.50827
1	1	1	1	24	0	0	0	0	25	1147.61553	0.00033	1791.62900	644.01380
1	1	1	1	25	0	0	0	0	26	1145.69338	0.00045	1841.18647	695.49354
1	1	1	1	26	0	0	0	0	27	1143.76780	-0.00004	1892.71462	748.94678
1	1	1	1	27	0	0	0	0	28	1141.83980	-0.00021	1946.21281	804.37280
1	1	1	1	28	0	0	0	0	29	1139.90971	0.00013	2001.68041	861.77083
1	1	1	1	29	0	0	0	0	30	1137.97694*	0.00025	2059.11678	921.14009
1	1	1	1	30	0	0	0	0	31	1136.04160	0.00010	2118.52125	982.47976
1	1	1	1	31	0	0	0	0	32	1134.10627	0.00079	2179.89318	1045.78899

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1	1	1	1	32	0	0	0	0	33	1132.16488	-0.00005	2243.23185	1111.06693
1	1	1	1	33	0	0	0	0	34	1130.22399	0.00009	2308.53656	1178.31267
1	1	1	1	34	0	0	0	0	35	1128.28112	-0.00015	2375.80655	1247.52529
2	1	1	1	35	0	0	0	0	36	1126.33743	0.00023	2445.04104	1318.70384
3	1	1	1	36	0	0	0	0	37	1124.39114	-0.00072	2516.23921	1391.84735
4	1	1	1	37	0	0	0	0	38	1122.44525	-0.00014	2589.40020	1466.95482
5	1	1	1	38	0	0	0	0	39	1120.49751	-0.00042	2664.52313	1544.02520
6	1	1	1	39	0	0	0	0	40	1118.54960	-0.00002	2741.60707	1623.05745
7	1	1	1	5	0	0	0	0	4	1205.77960	-0.00053	1225.61022	19.83009
8	1	1	1	6	0	0	0	0	5	1207.80661	-0.00087	1237.55228	29.74480
9	1	1	1	7	0	0	0	0	6	1209.84157	0.00067	1251.48305	41.64214
10	1	1	1	8	0	0	0	0	7	1211.88018	0.00038	1267.40177	55.52197
11	1	1	1	9	0	0	0	0	8	1213.92367	0.00015	1285.30761	71.38408
12	1	1	1	10	0	0	0	0	9	1215.97159	0.00023	1305.19963	89.22827
13	1	1	1	11	0	0	0	0	10	1218.02260	0.00005	1327.07683	109.05428
14	1	1	1	12	0	0	0	0	11	1220.07627	-0.00001	1350.93813	130.86184
15	1	1	1	13	0	0	0	0	12	1222.13167	-0.00007	1376.78240	154.65066
16	1	1	1	14	0	0	0	0	13	1224.18824	0.00014	1404.60850	180.42041
17	1	1	1	15	0	0	0	0	14	1226.24459	0.00006	1434.41526	208.17072
18	1	1	1	16	0	0	0	0	15	1228.30047	0.00019	1466.20152	237.90124
19	1	1	1	17	0	0	0	0	16	1230.35460	-0.00001	1499.96614	269.61154
20	1	1	1	18	0	0	0	0	17	1232.40684	-0.00002	1535.70804	303.30118
21	1	1	1	19	0	0	0	0	18	1234.45659	0.00011	1573.42620	338.96972
22	1	1	1	20	0	0	0	0	19	1236.50291	-0.00006	1613.11962	376.61665
23	1	1	1	21	0	0	0	0	20	1238.54603	0.00007	1654.78743	416.24147
24	1	1	1	22	0	0	0	0	21	1240.58510	-0.00005	1698.42877	457.84362
25	1	1	1	23	0	0	0	0	22	1242.62043	0.00011	1744.04287	501.42254
26	1	1	1	24	0	0	0	0	23	1244.65129	-0.00007	1791.62900	546.97764
27	1	1	1	25	0	0	0	0	24	1246.67844	0.00024	1841.18647	594.50827
28	1	1	1	26	0	0	0	0	25	1248.70128	0.00046	1892.71462	644.01380
29	1	1	1	27	0	0	0	0	26	1250.71968	0.00040	1946.21281	695.49354
30	1	1	1	28	0	0	0	0	27	1252.73367	0.00004	2001.68041	748.94678
31	1	1	1	29	0	0	0	0	28	1254.74428	0.00031	2059.11678	804.37280
32	1	1	1	30	0	0	0	0	29	1256.75040	-0.00002	2118.52125	861.77083
33	1	1	1	31	0	0	0	0	30	1258.75325	0.00016	2179.89318	921.14009
34	1	1	1	32	0	0	0	0	31	1260.75209	-0.00001	2243.23185	982.47976
35	1	1	1	33	0	0	0	0	32	1262.74751	-0.00006	2308.53656	1045.78899
36	1	1	1	34	0	0	0	0	33	1264.73951	-0.00012	2375.80655	1111.06693
37	1	1	1	35	0	0	0	0	34	1266.72840	0.00002	2445.04104	1178.31267
38	1	1	1	36	0	0	0	0	35	1268.71377	-0.00015	2516.23921	1247.52529
39	1	1	1	37	0	0	0	0	36	1270.69603	-0.00033	2589.40020	1318.70384
40	1	1	1	38	0	0	0	0	37	1272.67546	-0.00032	2664.52313	1391.84735
41	1	1	1	39	0	0	0	0	38	1274.65131	-0.00094	2741.60707	1466.95482
42	1	1	1	40	0	0	0	0	39	1276.62495	-0.00090	2820.65105	1544.02520
43	1	1	1	41	0	0	0	0	40	1278.59590	-0.00073	2901.65408	1623.05745
44	1	1	1	42	0	0	0	0	41	1280.56340	-0.00126	2984.61514	1704.05048W
45	1	1	1	43	0	0	0	0	42	1282.52790	-0.00206	3069.53314	1787.00318W

rms = 0.00033 cm⁻¹

2v₅ (Σ⁺) ← G.S. (Σ⁺)

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 0	0 0 0 0 1	1340.24284	-0.00056	1342.22645	1.98305
0 0 2 0 1	0 0 0 0 2	1338.26627	-0.00023	1344.21562	5.94912
0 0 2 0 2	0 0 0 0 3	1336.29596	0.00022	1348.19391	11.89816
0 0 2 0 3	0 0 0 0 4	1334.33076	-0.00037	1354.16122	19.83009
0 0 2 0 4	0 0 0 0 5	1332.37226	-0.00037	1362.11743	29.74480
0 0 2 0 5	0 0 0 0 6	1330.42012	-0.00007	1372.06234	41.64214
0 0 2 0 6	0 0 0 0 7	1328.47316	-0.00059	1383.99572	55.52197
0 0 2 0 7	0 0 0 0 8	1326.53367	0.00046	1397.91730	71.38408
0 0 2 0 8	0 0 0 0 9	1324.59826	-0.00022	1413.82675	89.22827
0 0 2 0 9	0 0 0 0 10	1322.66920	-0.00022	1431.72370	109.05428
0 0 2 0 10	0 0 0 0 11	1320.74510	-0.00080	1451.60774	130.86184
0 0 2 0 11	0 0 0 0 12	1318.82715	-0.00059	1473.47840	154.65066
0 0 2 0 12	0 0 0 0 13	1316.91530	-0.00094	1497.33518	180.42041

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0	0	2	0	36	0	0	0	0	35	1416.14781	0.00039	2663.67271	1247.52529
0	0	2	0	37	0	0	0	0	36	1418.19585	-0.00023	2736.89992	1318.70384
0	0	2	0	38	0	0	0	0	37	1420.24028	0.00032	2812.08731	1391.84735
0	0	2	0	39	0	0	0	0	38	1422.27934	0.00054	2889.23362	1466.95482
0	0	2	0	40	0	0	0	0	39	1424.31280	0.00041	2968.33759	1544.02520
0	0	2	0	41	0	0	0	0	40	1426.34049	-0.00002	3049.39796	1623.05745
0	0	2	0	42	0	0	0	0	41	1428.36324	0.00025	3132.41347	1704.05048
0	0	2	0	43	0	0	0	0	42	1430.37986	0.00019	3217.38286	1787.00318
0	0	2	0	44	0	0	0	0	43	1432.39049	0.00006	3304.30484	1871.91441
0	0	2	0	45	0	0	0	0	44	1434.39546	0.00032	3393.17815	1958.78301
0	0	2	0	46	0	0	0	0	45	1436.39346	-0.00025	3484.00150	2047.60779
0	0	2	0	47	0	0	0	0	46	1438.38575	-0.00033	3576.77361	2138.38752
0	0	2	0	48	0	0	0	0	47	1440.37228	0.00008	3671.49316	2231.12097
0	0	2	0	49	0	0	0	0	48	1442.35290	0.00088	3768.15887	2325.80685

rms = 0.00039 cm⁻¹

2v₅ (Δ) ← G.S. (Σ⁺)

v ₄ ' l ₄ ' V ₅ ' l ₅ ' J'	v ₄ '' l ₄ '' v ₅ '' l ₅ '' J''	OBS	OBS - CALC	E'	E''
0 0 2 2 36	0 0 0 0 37	1290.55715	-0.00022	2682.40472	1391.84735
0 0 2 2 35	0 0 0 0 36	1292.21495	-0.00034	2610.91913	1318.70384
0 0 2 2 34	0 0 0 0 35	1293.88745	-0.00037	2541.41311	1247.52529
0 0 2 2 33	0 0 0 0 34	1295.57450	-0.00018	2473.88734	1178.31267
0 0 2 2 32	0 0 0 0 33	1297.27564	0.00006	2408.34251	1111.06693
0 0 2 2 31	0 0 0 0 32	1298.99043	0.00021	2344.77921	1045.78899
0 0 2 2 30	0 0 0 0 31	1300.71869	0.00043	2283.19801	982.47976
0 0 2 2 29	0 0 0 0 30	1302.46019*	0.00084	2223.59944	921.14009
0 0 2 2 28	0 0 0 0 29	1304.21313	-0.00002	2165.98399	861.77083
0 0 2 2 27	0 0 0 0 28	1305.97949	0.00020	2110.35209	804.37280
0 0 2 2 26	0 0 0 0 27	1307.75705	-0.00034	2056.70417	748.94678
0 0 2 2 25	0 0 0 0 26	1309.54732	0.00025	2005.04061	695.49354
0 0 2 2 24	0 0 0 0 25	1311.34818	0.00023	1955.36175	644.01380
0 0 2 2 23	0 0 0 0 24	1313.15970*	0.00005	1907.66792	594.50827
0 0 2 2 22	0 0 0 0 23	1314.98231	0.00054	1861.95941	546.97764
0 0 2 2 21	0 0 0 0 22	1316.81416	0.00020	1818.23651	501.42254
0 0 2 2 20	0 0 0 0 21	1318.65567	-0.00016	1776.49946	457.84362
0 0 2 2 19	0 0 0 0 20	1320.50720	0.00017	1736.74850	416.24147
0 0 2 2 18	0 0 0 0 19	1322.36719	-0.00001	1698.98385	376.61665
0 0 2 2 17	0 0 0 0 18	1324.23624	0.00025	1663.20571	338.96972
0 0 2 2 16	0 0 0 0 17	1326.11294	-0.00014	1629.41426	303.30118
0 0 2 2 15	0 0 0 0 16	1327.99810	-0.00005	1597.60969	269.61154
0 0 2 2 14	0 0 0 0 15	1329.89080	-0.00011	1567.79214	237.90124
0 0 2 2 13	0 0 0 0 14	1331.79069	-0.00036	1539.96178	208.17072
0 0 2 2 12	0 0 0 0 13	1333.69864	0.00032	1514.11873	180.42041
0 0 2 2 11	0 0 0 0 12	1335.61122*	-0.00124	1490.26312	154.65066W
0 0 2 2 10	0 0 0 0 11	1337.53270*	-0.00053	1468.39508	130.86184
0 0 2 2 9	0 0 0 0 10	1339.46075	0.00033	1448.51470	109.05428
0 0 2 2 8	0 0 0 0 9	1341.39406	0.00025	1430.62208	89.22827
0 0 2 2 11	0 0 0 0 10	1381.20929	0.00045	1490.26312	109.05428
0 0 2 2 12	0 0 0 0 11	1383.25721	0.00032	1514.11873	130.86184
0 0 2 2 13	0 0 0 0 12	1385.30944*	-0.00168	1539.96178	154.65066W
0 0 2 2 14	0 0 0 0 13	1387.37224	0.00050	1567.79214	180.42041
0 0 2 2 15	0 0 0 0 14	1389.43869	-0.00027	1597.60969	208.17072
0 0 2 2 16	0 0 0 0 15	1391.51329	0.00026	1629.41426	237.90124
0 0 2 2 17	0 0 0 0 16	1393.59490	0.00073	1663.20571	269.61154
0 0 2 2 18	0 0 0 0 17	1395.68405*	0.00138	1698.98385	303.30118W
0 0 2 2 19	0 0 0 0 18	1397.77965	0.00087	1736.74850	338.96972
0 0 2 2 20	0 0 0 0 19	1399.88274	-0.00006	1776.49946	376.61665
0 0 2 2 21	0 0 0 0 20	1401.99518	0.00014	1818.23651	416.24147
0 0 2 2 22	0 0 0 0 21	1404.11572	-0.00007	1861.95941	457.84362
0 0 2 2 23	0 0 0 0 22	1406.24515	-0.00022	1907.66792	501.42254
0 0 2 2 24	0 0 0 0 23	1408.38390	-0.00021	1955.36175	546.97764
0 0 2 2 25	0 0 0 0 24	1410.53218	-0.00016	2005.04061	594.50827
0 0 2 2 26	0 0 0 0 25	1412.69034	-0.00004	2056.70417	644.01380
0 0 2 2 27	0 0 0 0 26	1414.85850	0.00008	2110.35209	695.49354

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0	0	2	2	28	0	0	0	0	27	1417.03721	0.00001	2165.98399	748.94678
0	0	2	2	29	0	0	0	0	28	1419.22663	-0.00001	2223.59944	804.37280
0	0	2	2	30	0	0	0	0	29	1421.42732	0.00014	2283.19801	861.77083
0	0	2	2	31	0	0	0	0	30	1423.63929	0.00017	2344.77921	921.14009
0	0	2	2	32	0	0	0	0	31	1425.86258	-0.00017	2408.34251	982.47976
0	0	2	2	33	0	0	0	0	32	1428.09817	-0.00018	2473.88734	1045.78899
0	0	2	2	34	0	0	0	0	33	1430.34626	0.00008	2541.41311	1111.06693
0	0	2	2	35	0	0	0	0	34	1432.60666	0.00019	2610.91913	1178.31267
0	0	2	2	36	0	0	0	0	35	1434.87959	0.00016	2682.40472	1247.52529
0	0	2	2	37	0	0	0	0	36	1437.16535	0.00008	2755.86911	1318.70384
0	0	2	2	38	0	0	0	0	37	1439.46434	0.00019	2831.31150	1391.84735
0	0	2	2	39	0	0	0	0	38	1441.77620	-0.00002	2908.73104	1466.95482
0	0	2	2	40	0	0	0	0	39	1444.10126	-0.00034	2988.12680	1544.02520
0	0	2	2	41	0	0	0	0	40	1446.43998	-0.00040	3069.49783	1623.05745
0	0	2	2	42	0	0	0	0	41	1448.79278	0.00014	3152.84312	1704.05048
0	0	2	2	43	0	0	0	0	42	1451.15842	0.00000	3238.16161	1787.00318
0	0	2	2	44	0	0	0	0	43	1453.53840	0.00065	3325.45217	1871.91441

rms = 0.00029 cm⁻¹

3v₄ (II) ← v₄ (II)

v ₄ ' l ₄ ' v ₅ ' l ₅ ' J'	v ₄ '' l ₄ '' v ₅ '' l ₅ '' J''	OBS	OBS - CALC	E'	E''
3 1 0 0 39	1 1 0 0 40	956.61880	0.00029	3098.63198	2142.01348
3 1 0 0 38	1 1 0 0 39	958.48954	-0.00006	3021.44478	2062.95519
3 1 0 0 37	1 1 0 0 38	960.36136	0.00003	2946.22055	1985.85922
3 1 0 0 36	1 1 0 0 37	962.23394	0.00027	2872.96032	1910.72665
3 1 0 0 35	1 1 0 0 36	964.10650	-0.00011	2801.66513	1837.55852
3 1 0 0 34	1 1 0 0 35	965.98039	0.00028	2732.33595	1766.35584
3 1 0 0 33	1 1 0 0 34	967.85387	-0.00030	2664.97378	1697.11961
3 1 0 0 32	1 1 0 0 33	969.72861	-0.00018	2599.57957	1629.85078
3 1 0 0 31	1 1 0 0 32	971.60381	-0.00016	2536.15427	1564.55030
3 1 0 0 30	1 1 0 0 31	973.47970	-0.00002	2474.69880	1501.21907
3 1 0 0 29	1 1 0 0 30	975.35610	0.00001	2415.21406	1439.85797
3 1 0 0 28	1 1 0 0 29	977.23306	-0.00005	2357.70096	1380.46786
3 1 0 0 27	1 1 0 0 28	979.11081	-0.00003	2302.16039	1323.04955
3 1 0 0 26	1 1 0 0 27	980.98929	-0.00009	2248.59323	1267.60385
3 1 0 0 25	1 1 0 0 26	982.86884	0.00004	2197.00034	1214.13154
3 1 0 0 24	1 1 0 0 25	984.74965	0.00040	2147.38259	1162.63334
3 1 0 0 23	1 1 0 0 24	986.63092	0.00007	2099.74084	1113.10999
3 1 0 0 22	1 1 0 0 23	988.51400	0.00023	2054.07593	1065.56217
3 1 0 0 21	1 1 0 0 22	990.39847	0.00028	2010.38873	1019.99053
3 1 0 0 20	1 1 0 0 21	992.28437	0.00003	1968.68006	976.39572
3 1 0 0 19	1 1 0 0 20	994.17275	0.00033	1928.95077	934.77834
3 1 0 0 18	1 1 0 0 19	996.06289	0.00018	1891.20168	895.13897
3 1 0 0 17	1 1 0 0 18	997.95526	-0.00020	1855.43362	857.47816
3 1 0 0 16	1 1 0 0 17	999.85096	0.00000	1821.64740	821.79644
3 1 0 0 15	1 1 0 0 16	1001.74967	0.00016	1789.84380	788.09430
3 1 0 0 14	1 1 0 0 15	1003.65120	-0.00021	1760.02361	756.37220
3 1 0 0 13	1 1 0 0 14	1005.55699	0.00001	1732.18758	726.63060
3 1 0 0 12	1 1 0 0 13	1007.46665	0.00011	1706.33645	698.86991
3 1 0 0 11	1 1 0 0 12	1009.38059	0.00020	1682.47090	673.09051
3 1 0 0 10	1 1 0 0 11	1011.29886	0.00000	1660.59161	649.29275
3 1 0 0 9	1 1 0 0 10	1013.22207	-0.00016	1640.69921	627.47699
3 1 0 0 8	1 1 0 0 9	1015.15089	0.00010	1622.79429	607.64350
3 1 0 0 7	1 1 0 0 8	1017.08510	0.00031	1606.87737	589.79258
3 1 0 0 6	1 1 0 0 7	1019.02461	0.00011	1592.94896	573.92447
3 1 0 0 5	1 1 0 0 6	1020.97014	0.00003	1581.00949	560.03938
3 1 0 0 4	1 1 0 0 5	1022.92169	-0.00012	1571.05934	548.13753
3 1 0 0 3	1 1 0 0 4	1024.87975	-0.00002	1563.09883	538.21906
3 1 0 0 2	1 1 0 0 3	1026.84444	0.00035	1557.12821	530.28412
3 1 0 0 1	1 1 0 0 2	1028.81514	0.00026	1553.14769	524.33282
3 1 0 0 2	1 1 0 0 1	1036.76290	-0.00007	1557.12821	520.36524
3 1 0 0 3	1 1 0 0 2	1038.76610	0.00009	1563.09883	524.33282
3 1 0 0 4	1 1 0 0 3	1040.77536	0.00014	1571.05934	530.28412
3 1 0 0 5	1 1 0 0 4	1042.78969	0.00011	1581.00949	538.21906

2	0	1	-1	8	1	-1	0	0	7	1209.81546	-0.00010	1783.98845	574.17289
2	0	1	-1	9	1	-1	0	0	8	1211.82581	0.00017	1801.93758	590.11194
2	0	1	-1	10	1	-1	0	0	9	1213.83628	0.00037	1821.87855	608.04264
2	0	1	-1	11	1	-1	0	0	10	1215.84619	0.00028	1843.81066	627.96474
2	0	1	-1	12	1	-1	0	0	11	1217.85563	0.00043	1867.73315	649.87795
2	0	1	-1	13	1	-1	0	0	12	1219.86353	0.00020	1893.64529	673.78196
2	0	1	-1	14	1	-1	0	0	13	1221.87042	0.00056	1921.54628	699.67642
2	0	1	-1	15	1	-1	0	0	14	1223.87454	0.00016	1951.43535	727.56097
2	0	1	-1	16	1	-1	0	0	15	1225.87753	0.00100	1983.31173	757.43520W
2	0	1	-1	17	1	-1	0	0	16	1227.87595	0.00000	2017.17464	789.29869

rms = 0.00029 cm⁻¹

$$2\nu_4 + \nu_5 (^1\Pi) \leftarrow \nu_4 (\Pi)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 1 -1 1	1 1 0 0 2	1200.12959	-0.00016	1724.46257	524.33282
2 2 1 -1 2	1 1 0 0 3	1198.16117	0.00015	1728.44514	530.28412
2 2 1 -1 3	1 1 0 0 4	1196.19983	-0.00016	1734.41904	538.21906
2 2 1 -1 4	1 1 0 0 5	1194.24692	0.00012	1742.38433	548.13753
2 2 1 -1 5	1 1 0 0 6	1192.30180	0.00012	1752.34107	560.03938
2 2 1 -1 6	1 1 0 0 7	1190.36488	0.00001	1764.28934	573.92447
2 2 1 -1 7	1 1 0 0 8	1188.43675	0.00007	1778.22926	589.79258
2 2 1 -1 8	1 1 0 0 9	1186.51757	0.00013	1794.16094	607.64350
2 2 1 -1 9	1 1 0 0 10	1184.60749	-0.00005	1812.08452	627.47699
2 2 1 -1 10	1 1 0 0 11	1182.70766	0.00025	1832.00016	649.29275
2 2 1 -1 11	1 1 0 0 12	1180.81755	0.00003	1853.90802	673.09051
2 2 1 -1 12	1 1 0 0 13	1178.93847	0.00009	1877.80829	698.86991
2 2 1 -1 13	1 1 0 0 14	1177.07076	0.00023	1903.70113	726.63060
2 2 1 -1 14	1 1 0 0 15	1175.21458	0.00004	1931.58675	756.37220
2 2 1 -1 15	1 1 0 0 16	1173.37101	-0.00002	1961.46532	788.09430
2 2 1 -1 16	1 1 0 0 17	1171.54086	0.00027	1993.33703	821.79644
2 2 1 -1 17	1 1 0 0 18	1169.72400	0.00012	2027.20204	857.47816
2 2 1 -1 18	1 1 0 0 19	1167.92162	0.00011	2063.06048	895.13897
2 2 1 -1 19	1 1 0 0 20	1166.13443	0.00032	2100.91245	934.77834
2 2 1 -1 20	1 1 0 0 21	1164.36228	-0.00001	2140.75802	976.39572
2 2 1 -1 21	1 1 0 0 22	1162.60715	0.00050	2182.59718	1019.99053
2 2 1 -1 22	1 1 0 0 23	1160.86739	-0.00032	2226.42988	1065.56217
2 2 1 -1 23	1 1 0 0 24	1159.14621	0.00021	2272.25599	1113.10999
2 2 1 -1 24	1 1 0 0 25	1157.44200	0.00003	2320.07531	1162.63334
2 2 1 -1 25	1 1 0 0 26	1155.75585	-0.00016	2369.88754	1214.13154
2 2 1 -1 26	1 1 0 0 27	1154.08870	0.00024	2421.69231	1267.60385
2 2 1 -1 27	1 1 0 0 28	1152.43977	0.00017	2475.48915	1323.04955
2 2 1 -1 28	1 1 0 0 29	1150.80998	0.00033	2531.27750	1380.46786
2 2 1 -1 29	1 1 0 0 30	1149.19895	0.00020	2589.05673	1439.85797
2 2 1 -1 30	1 1 0 0 31	1147.60718	0.00016	2648.82609	1501.21907
2 2 1 -1 31	1 1 0 0 32	1146.03484	0.00034	2710.58480	1564.55030
2 2 1 -1 32	1 1 0 0 33	1144.48157	0.00039	2774.33196	1629.85078
2 2 1 -1 33	1 1 0 0 34	1142.94771	0.00068	2840.06664	1697.11961
2 2 1 -1 34	1 1 0 0 35	1141.43168	-0.00029	2907.78781	1766.35584
2 2 1 -1 35	1 1 0 0 36	1139.93768*	0.00178	2977.49442	1837.55852W
2 2 1 -1 2	1 1 0 0 1	1208.07982	-0.00009	1728.44514	520.36524
2 2 1 -1 3	1 1 0 0 2	1210.08618	-0.00005	1734.41904	524.33282
2 2 1 -1 4	1 1 0 0 3	1212.09988	-0.00033	1742.38433	530.28412
2 2 1 -1 5	1 1 0 0 4	1214.12187	-0.00014	1752.34107	538.21906
2 2 1 -1 6	1 1 0 0 5	1216.15167	-0.00014	1764.28934	548.13753
2 2 1 -1 7	1 1 0 0 6	1218.18967	-0.00020	1778.22926	560.03938
2 2 1 -1 8	1 1 0 0 7	1220.23659	0.00012	1794.16094	573.92447
2 2 1 -1 9	1 1 0 0 8	1222.29190	-0.00004	1812.08452	589.79258
2 2 1 -1 10	1 1 0 0 9	1224.35665	-0.00001	1832.00016	607.64350
2 2 1 -1 11	1 1 0 0 10	1226.43090	-0.00014	1853.90802	627.47699
2 2 1 -1 12	1 1 0 0 11	1228.51550	-0.00003	1877.80829	649.29275
2 2 1 -1 13	1 1 0 0 12	1230.61085	0.00023	1903.70113	673.09051
2 2 1 -1 14	1 1 0 0 13	1232.71682	-0.00002	1931.58675	698.86991
2 2 1 -1 15	1 1 0 0 14	1234.83463	-0.00009	1961.46532	726.63060
2 2 1 -1 16	1 1 0 0 15	1236.96344	0.00023	1993.33703	756.37220

1	2	-2	1	1	13	1	-1	0	0	12	1230.76166	0.00013	1904.54349	673.78196
2	2	-2	1	1	14	1	-1	0	0	13	1232.88236	0.00006	1932.55872	699.67642
3	2	-2	1	1	15	1	-1	0	0	14	1235.01530	0.00016	1962.57611	727.56097
4	2	-2	1	1	16	1	-1	0	0	15	1237.16069	0.00008	1994.59581	757.43520
5	2	-2	1	1	17	1	-1	0	0	16	1239.31922	-0.00003	2028.61794	789.29869
6	2	-2	1	1	18	1	-1	0	0	17	1241.49161	0.00001	2064.64259	823.15099
7	2	-2	1	1	19	1	-1	0	0	18	1243.67828	0.00007	2102.66980	858.99160
8	2	-2	1	1	20	1	-1	0	0	19	1245.87952	-0.00005	2142.69958	896.82001
9	2	-2	1	1	21	1	-1	0	0	20	1248.09649	0.00031	2184.73187	936.63569
10	2	-2	1	1	22	1	-1	0	0	21	1250.32874	0.00025	2228.76654	978.43806
11	2	-2	1	1	23	1	-1	0	0	22	1252.57717	0.00028	2274.80341	1022.22652
12	2	-2	1	1	24	1	-1	0	0	23	1254.84204	0.00030	2322.84219	1068.00045
13	2	-2	1	1	25	1	-1	0	0	24	1257.12361	0.00026	2372.88254	1115.75919
14	2	-2	1	1	26	1	-1	0	0	25	1259.42274	0.00078	2424.92402	1165.50207
15	2	-2	1	1	27	1	-1	0	0	26	1261.73764	-0.00013	2478.96612	1217.22835
16	2	-2	1	1	28	1	-1	0	0	27	1264.07160	0.00069	2535.00823	1270.93732
17	2	-2	1	1	29	1	-1	0	0	28	1266.42230	0.00082	2593.04967	1326.62819
18	2	-2	1	1	30	1	-1	0	0	29	1268.78951	0.00000	2653.08968	1384.30018
19	2	-2	1	1	31	1	-1	0	0	30	1271.17511	0.00013	2715.12743	1443.95245
20	2	-2	1	1	32	1	-1	0	0	31	1273.57795	0.00008	2779.16202	1505.58415
21	2	-2	1	1	33	1	-1	0	0	32	1275.99802	-0.00005	2845.19248	1569.19441
22	2	-2	1	1	34	1	-1	0	0	33	1278.43511	-0.00036	2913.21778	1634.78230
23	2	-2	1	1	35	1	-1	0	0	34	1280.88994	0.00000	2983.23684	1702.34690
24	2	-2	1	1	36	1	-1	0	0	35	1283.36070	-0.00060	3055.24854	1771.88724
25	2	-2	1	1	37	1	-1	0	0	36	1285.84865	-0.00073	3129.25169	1843.40231
26	2	-2	1	1	38	1	-1	0	0	37	1288.35300	-0.00098	3205.24508	1916.89110
27	2	-2	1	1	39	1	-1	0	0	38	1290.87590*	0.00101	3283.22745	1992.35257W
28	2	-2	1	1	40	1	-1	0	0	39	1293.41160	-0.00030	3363.19751	2069.78561
29	2	-2	1	1	1	1	1	0	0	1	1204.10622	-0.00036	1724.47181	520.36524
30	2	-2	1	1	2	1	1	0	0	2	1204.14054	0.00048	1728.47288	524.33282
31	2	-2	1	1	3	1	1	0	0	3	1204.19054	0.00014	1734.47452	530.28412
32	2	-2	1	1	4	1	1	0	0	4	1204.25796	0.00022	1742.47680	538.21906
33	2	-2	1	1	5	1	1	0	0	5	1204.34188	-0.00038	1752.47978	548.13753
34	2	-2	1	1	6	1	1	0	0	6	1204.44430	0.00011	1764.48357	560.03938
35	2	-2	1	1	7	1	1	0	0	7	1204.56392	0.00012	1778.48827	573.92447
36	2	-2	1	1	8	1	1	0	0	8	1204.70127	-0.00015	1794.49400	589.79258
37	2	-2	1	1	9	1	1	0	0	9	1204.85717	-0.00024	1812.50091	607.64350
38	2	-2	1	1	10	1	1	0	0	10	1205.03204	-0.00012	1832.50915	627.47699
39	2	-2	1	1	11	1	1	0	0	11	1205.22620	0.00008	1854.51888	649.29275
40	2	-2	1	1	12	1	1	0	0	12	1205.43949	-0.00027	1878.53027	673.09051
41	2	-2	1	1	13	1	1	0	0	13	1205.67409	0.00051	1904.54349	698.86991

rms = 0.00027 cm⁻¹

$$2\nu_4 + \nu_5 (\Pi\Pi) \leftarrow \nu_5 (\Pi)$$

ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
2	0	1	1	32	0	0	1	1	33	973.96004	0.00021	2762.40757	1788.44775
2	0	1	1	31	0	0	1	1	32	975.77739	0.00041	2698.97215	1723.19517
2	0	1	1	30	0	0	1	1	31	977.58954	0.00012	2637.49992	1659.91050
2	0	1	1	29	0	0	1	1	30	979.39711	0.00016	2577.99156	1598.59460
2	0	1	1	28	0	0	1	1	29	981.20080	0.00134	2520.44778	1539.24832W
2	0	1	1	27	0	0	1	1	28	982.99704	0.00015	2464.86937	1481.87248
2	0	1	1	26	0	0	1	1	27	984.78939	0.00010	2411.25716	1426.46786
2	0	1	1	25	0	0	1	1	26	986.57656	-0.00029	2359.61208	1373.03523
2	0	1	1	24	0	0	1	1	25	988.35979	-0.00009	2309.93520	1321.57533
2	0	1	1	23	0	0	1	1	24	990.13874	-0.00013	2262.22772	1272.08885
2	0	1	1	22	0	0	1	1	23	991.91484	0.00036	2216.49097	1224.57649
2	0	1	1	21	0	0	1	1	22	993.68709	-0.00045	2172.72643	1179.03889
2	0	1	1	20	0	0	1	1	21	995.45933	0.00026	2130.93576	1135.47669
2	0	1	1	19	0	0	1	1	20	997.23013	-0.00009	2091.12070	1093.89049
2	0	1	1	18	0	0	1	1	19	999.00244	0.00018	2053.28311	1054.28084
2	0	1	1	17	0	0	1	1	18	1000.77573	-0.00083	2017.42488	1016.64832
2	0	1	1	16	0	0	1	1	17	1002.55470	0.00019	1983.54793	980.99342
2	0	1	1	15	0	0	1	1	16	1004.33755	0.00005	1951.65414	947.31664
2	0	1	1	14	0	0	1	1	14	1006.12489	0.00014	1921.74533	915.61845

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$$2\nu_4 + \nu_5 (^1\Pi) \leftarrow \nu_5 (\Pi)$$

ν_4'	ν_4''	ν_5'	ν_5''	J'	J''	OBS	OBS - CALC	E'	E''
2	2	1	-1	1	0	1040.70753	-0.00042	1724.46257	683.75462
2	2	1	-1	2	0	1038.74394	0.00020	1728.44514	689.70140
2	2	1	-1	3	0	1036.78883	0.00010	1734.41904	697.63032
2	2	1	-1	4	0	1034.84317	0.00010	1742.38433	707.54126
2	2	1	-1	5	0	1032.90701	0.00003	1752.34107	719.43409
2	2	1	-1	6	0	1030.97875*	-0.00195	1764.28934	733.30864W
2	2	1	-1	7	0	1029.06476	0.00023	1778.22926	749.16472
2	2	1	-1	8	0	1027.15899	0.00017	1794.16094	767.00212
2	2	1	-1	9	0	1025.26412	0.00019	1812.08452	786.82059
2	2	1	-1	10	0	1023.38025	-0.00006	1832.00016	808.61985
2	2	1	-1	11	0	1021.50872	0.00031	1853.90802	832.39961
2	2	1	-1	12	0	1019.64812	-0.00063	1877.80829	858.15954
2	2	1	-1	13	0	1017.80151	-0.00034	1903.70113	885.89928
2	2	1	-1	14	0	1015.96852	0.00022	1931.58675	915.61845
2	2	1	-1	15	0	1014.14874	0.00006	1961.46532	947.31664
2	2	1	-1	16	0	1012.34336	-0.00026	1993.33703	980.99342
2	2	1	-1	17	0	1010.55439	0.00067	2027.20204	1016.64832
2	2	1	-1	18	0	1008.77960	-0.00004	2063.06048	1054.28084
2	2	1	-1	19	0	1007.02290*	0.00093	2100.91245	1093.89049
2	2	1	-1	20	0	1005.28124	-0.00009	2140.75802	1135.47669
2	2	1	-1	21	0	1003.55790	-0.00039	2182.59718	1179.03889
2	2	1	-1	22	0	1001.85311	-0.00028	2226.42988	1224.57649
2	2	1	-1	2	0	1048.65679*	0.00170	1728.44514	679.79005W
2	2	1	-1	3	0	1050.66415	-0.00028	1734.41904	683.75462
2	2	1	-1	4	0	1052.68306	0.00013	1742.38433	689.70140
2	2	1	-1	5	0	1054.71091	0.00016	1752.34107	697.63032
2	2	1	-1	6	0	1056.74866	0.00058	1764.28934	707.54126
2	2	1	-1	7	0	1058.79544	0.00027	1778.22926	719.43409
2	2	1	-1	8	0	1060.85235	0.00005	1794.16094	733.30864
2	2	1	-1	9	0	1062.92081	0.00101	1812.08452	749.16472W
2	2	1	-1	10	0	1064.99824	0.00020	1832.00016	767.00212
2	2	1	-1	11	0	1067.08697	-0.00046	1853.90802	786.82059
2	2	1	-1	12	0	1069.18840	-0.00003	1877.80829	808.61985
2	2	1	-1	13	0	1071.30168	0.00016	1903.70113	832.39961
2	2	1	-1	14	0	1073.42670	-0.00051	1931.58675	858.15954
2	2	1	-1	15	0	1075.56624	0.00020	1961.46532	885.89928
2	2	1	-1	16	0	1077.71863	0.00004	1993.33703	915.61845
2	2	1	-1	17	0	1079.88523	-0.00017	2027.20204	947.31664
2	2	1	-1	18	0	1082.06670	-0.00036	2063.06048	980.99342
2	2	1	-1	19	0	1084.26382	-0.00032	2100.91245	1016.64832
2	2	1	-1	20	0	1086.47264*	-0.00453	2140.75802	1054.28084W
2	2	1	-1	21	0	1088.70690	0.00021	2182.59718	1093.89049
2	2	1	-1	22	0	1090.95315	-0.00004	2226.42988	1135.47669
2	2	1	-1	23	0	1093.21701	-0.00009	2272.25599	1179.03889
2	2	1	-1	24	0	1095.49936	0.00054	2320.07531	1224.57649
2	2	1	-1	25	0	1097.79777	-0.00092	2369.88754	1272.08885
2	-2	1	1	1	0	1040.69629	0.00025	1724.47181	683.77578
2	-2	1	1	2	0	1038.72906	-0.00011	1728.47288	689.74371
2	-2	1	1	3	0	1036.77372	0.00003	1734.47452	697.70083
2	-2	1	1	4	0	1034.82979	0.00002	1742.47680	707.64702
2	-2	1	1	5	0	1032.89797	0.00033	1752.47978	719.58215
2	-2	1	1	6	0	1030.97856*	0.00102	1764.48357	733.50603W
2	-2	1	1	7	0	1029.06992	0.00014	1778.48827	749.41849
2	-2	1	1	8	0	1027.17460	-0.00010	1794.49400	767.31930
2	-2	1	1	9	0	1025.29269	-0.00002	1812.50091	787.20820
2	-2	1	1	10	0	1023.42437	0.00014	1832.50915	809.08492
2	-2	1	1	11	0	1021.56985	0.00013	1854.51888	832.94916
2	-2	1	1	12	0	1019.72964	-0.00006	1878.53027	858.80057
2	-2	1	1	13	0	1017.90436	-0.00034	1904.54349	886.63880
2	-2	1	1	14	0	1016.09528	0.00001	1932.55872	916.46345
2	-2	1	1	15	0	1014.30173	-0.00026	1962.57611	948.27412

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1	2 -2 1 1 16	0 0 1 -1 17	1012.52502	-0.00044	1994.59581	982.07035
2	2 -2 1 1 17	0 0 1 -1 18	1010.76651	0.00024	2028.61794	1017.85167
3	2 -2 1 1 18	0 0 1 -1 19	1009.02393*	-0.00107	2064.64259	1055.61759W
4	2 -2 1 1 19	0 0 1 -1 20	1007.30239	0.00015	2102.66980	1095.36757
5	2 -2 1 1 20	0 0 1 -1 21	1005.59893	0.00040	2142.69958	1137.10105
6	2 -2 1 1 21	0 0 1 -1 22	1003.91437	-0.00004	2184.73187	1180.81746
7	2 -2 1 1 22	0 0 1 -1 23	1002.25057	0.00021	2228.76654	1226.51618
8	2 -2 1 1 23	0 0 1 -1 24	1000.60690	0.00006	2274.80341	1274.19657
9	2 -2 1 1 24	0 0 1 -1 25	998.98450	0.00028	2322.84219	1323.85797
10	2 -2 1 1 25	0 0 1 -1 26	997.38329	0.00043	2372.88254	1375.49968
11	2 -2 1 1 2	0 0 1 -1 1	1048.67590*	0.00013	1728.47288	679.79710
12	2 -2 1 1 3	0 0 1 -1 2	1050.69845	-0.00030	1734.47452	683.77578
13	2 -2 1 1 4	0 0 1 -1 3	1052.73330	0.00021	1742.47680	689.74371
14	2 -2 1 1 5	0 0 1 -1 4	1054.77905	0.00010	1752.47978	697.70083
15	2 -2 1 1 6	0 0 1 -1 5	1056.83554	-0.00101	1764.48357	707.64702W
16	2 -2 1 1 7	0 0 1 -1 6	1058.90403*	-0.00209	1778.48827	719.58215W
17	2 -2 1 1 8	0 0 1 -1 7	1060.98816	0.00019	1794.49400	733.50603
18	2 -2 1 1 9	0 0 1 -1 8	1063.08280	0.00038	1812.50091	749.41849
19	2 -2 1 1 10	0 0 1 -1 9	1065.18997	0.00012	1832.50915	767.31930
20	2 -2 1 1 11	0 0 1 -1 10	1067.31048	-0.00020	1854.51888	787.20820
21	2 -2 1 1 12	0 0 1 -1 11	1069.44512	-0.00023	1878.53027	809.08492
22	2 -2 1 1 13	0 0 1 -1 12	1071.59453	0.00019	1904.54349	832.94916
23	2 -2 1 1 14	0 0 1 -1 13	1073.75790	-0.00025	1932.55872	858.80057
24	2 -2 1 1 15	0 0 1 -1 14	1075.93714	-0.00017	1962.57611	886.63880
25	2 -2 1 1 16	0 0 1 -1 15	1078.13201	-0.00035	1994.59581	916.46345
26	2 -2 1 1 17	0 0 1 -1 16	1080.34385	0.00003	2028.61794	948.27412
27	2 -2 1 1 18	0 0 1 -1 17	1082.57215	-0.00009	2064.64259	982.07035
28	2 -2 1 1 19	0 0 1 -1 18	1084.81830	0.00017	2102.66980	1017.85167
29	2 -2 1 1 20	0 0 1 -1 19	1087.08215	0.00016	2142.69958	1055.61759
30	2 -2 1 1 21	0 0 1 -1 20	1089.36457	0.00027	2184.73187	1095.36757
31	2 -2 1 1 22	0 0 1 -1 21	1091.66585	0.00036	2228.76654	1137.10105
32	2 -2 1 1 23	0 0 1 -1 22	1093.98605	0.00010	2274.80341	1180.81746
33	2 -2 1 1 24	0 0 1 -1 23	1096.32620	0.00019	2322.84219	1226.51618
34	2 -2 1 1 25	0 0 1 -1 24	1098.68644	0.00047	2372.88254	1274.19657
35	2 -2 1 1 26	0 0 1 -1 25	1101.06653	0.00048	2424.92402	1323.85797
36	2 -2 1 1 27	0 0 1 -1 26	1103.46654	0.00010	2478.96612	1375.49968
37	2 -2 1 1 28	0 0 1 -1 27	1105.88772	0.00047	2535.00823	1429.12098
38	2 -2 1 1 29	0 0 1 -1 28	1108.32827	-0.00029	2593.04967	1484.72111
39	2 -2 1 1 30	0 0 1 -1 29	1110.79052	0.00015	2653.08968	1542.29931
40	2 -2 1 1 31	0 0 1 -1 30	1113.27247	-0.00020	2715.12743	1601.85477
41	2 -2 1 1 32	0 0 1 -1 31	1115.77450	-0.00088	2779.16202	1663.38664

rms = 0.00030 cm⁻¹

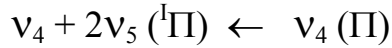
$v_4 + 2v_5 (^{\Pi\Pi}) \leftarrow v_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 2 0 1	1 1 0 0 2	1339.51684	-0.00025	1863.84991	524.33282
1 1 2 0 2	1 1 0 0 3	1337.54896	0.00022	1867.83286	530.28412
1 1 2 0 3	1 1 0 0 4	1335.58809	-0.00002	1873.80717	538.21906
1 1 2 0 4	1 1 0 0 5	1333.63526	0.00008	1881.77271	548.13753
1 1 2 0 5	1 1 0 0 6	1331.68968	-0.00023	1891.72929	560.03938
1 1 2 0 6	1 1 0 0 7	1329.75240	0.00016	1903.67670	573.92447
1 1 2 0 7	1 1 0 0 8	1327.82205	-0.00004	1917.61467	589.79258
1 1 2 0 8	1 1 0 0 9	1325.89933	-0.00004	1933.54287	607.64350
1 1 2 0 9	1 1 0 0 10	1323.98435	0.00038	1951.46095	627.47699
1 1 2 0 10	1 1 0 0 11	1322.07609	0.00034	1971.36850	649.29275
1 1 2 0 11	1 1 0 0 12	1320.17438	-0.00018	1993.26507	673.09051
1 1 2 0 12	1 1 0 0 13	1318.28025	0.00001	2017.15015	698.86991
1 1 2 0 13	1 1 0 0 14	1316.39240	-0.00019	2043.02319	726.63060
1 1 2 0 14	1 1 0 0 15	1314.51137	-0.00003	2070.88360	756.37220
1 1 2 0 15	1 1 0 0 16	1312.63644	0.00000	2100.73073	788.09430
1 1 2 0 16	1 1 0 0 17	1310.76749	0.00003	2132.56390	821.79644
1 1 2 0 17	1 1 0 0 18	1308.90426	0.00008	2166.38235	857.47816
1 1 2 0 18	1 1 0 0 19	1307.04636	0.00004	2202.18530	895.13897
1 1 2 0 19	1 1 0 0 20	1305.19450	-0.00002	2239.97191	934.77834

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1	-1	2	0	38	1	-1	0	0	37	1420.80652	0.00246	3337.69517	1916.89110W
1	-1	2	0	39	1	-1	0	0	38	1422.81713	0.00219	3415.16751	1992.35257W
1	-1	2	0	40	1	-1	0	0	39	1424.82437	0.00309	3494.60690	2069.78561W
1	-1	2	0	41	1	-1	0	0	40	1426.82576	0.00283	3576.01208	2149.18914W
1	-1	2	0	1	1	1	0	0	1	1343.49024	0.00005	1863.85543	520.36524
1	-1	2	0	2	1	1	0	0	2	1343.51662	0.00002	1867.84942	524.33282
1	-1	2	0	3	1	1	0	0	3	1343.55618	0.00001	1873.84028	530.28412
1	-1	2	0	4	1	1	0	0	4	1343.60886	0.00003	1881.82789	538.21906
1	-1	2	0	5	1	1	0	0	5	1343.67465	0.00012	1891.81206	548.13753
1	-1	2	0	6	1	1	0	0	6	1343.75320	0.00003	1903.79255	560.03938
1	-1	2	0	7	1	1	0	0	7	1343.84468	0.00004	1917.76910	573.92447
1	-1	2	0	8	1	1	0	0	8	1343.94871	-0.00010	1933.74139	589.79258
1	-1	2	0	9	1	1	0	0	9	1344.06563	0.00008	1951.70905	607.64350
1	-1	2	0	10	1	1	0	0	10	1344.19541*	0.00072	1971.67167	627.47699
1	-1	2	0	11	1	1	0	0	11	1344.33478*	-0.00127	1993.62880	649.29275W
1	-1	2	0	12	1	1	0	0	12	1344.49068	0.00123	2017.57995	673.09051W
1	-1	2	0	13	1	1	0	0	13	1344.65500	0.00033	2043.52458	698.86991
1	-1	2	0	14	1	1	0	0	14	1344.83116	-0.00034	2071.46210	726.63060
1	-1	2	0	15	1	1	0	0	15	1345.01968	-0.00002	2101.39190	756.37220
1	-1	2	0	16	1	1	0	0	16	1345.21858	-0.00044	2133.31332	788.09430
1	-1	2	0	17	1	1	0	0	17	1345.42848	-0.00072	2167.22564	821.79644
1	-1	2	0	18	1	1	0	0	18	1345.64964	-0.00034	2203.12814	857.47816
1	1	2	0	7	1	-1	0	0	7	1343.44222	0.00045	1917.61467	574.17289
1	1	2	0	8	1	-1	0	0	8	1343.43122	0.00029	1933.54287	590.11194
1	1	2	0	9	1	-1	0	0	9	1343.41878	0.00047	1951.46095	608.04264
1	1	2	0	10	1	-1	0	0	10	1343.40451	0.00075	1971.36850	627.96474
1	1	2	0	11	1	-1	0	0	11	1343.38645	-0.00067	1993.26507	649.87795
1	1	2	0	12	1	-1	0	0	12	1343.36871	0.00052	2017.15015	673.78196
1	1	2	0	13	1	-1	0	0	13	1343.34719	0.00042	2043.02319	699.67642
1	1	2	0	14	1	-1	0	0	14	1343.32314	0.00051	2070.88360	727.56097
1	1	2	0	15	1	-1	0	0	15	1343.29563	0.00010	2100.73073	757.43520

rms = 0.00035 cm⁻¹



v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
1	-1	2	2	20	1	1	0	0	21	1324.31102	0.00010	2300.70664	976.39572
1	-1	2	2	19	1	1	0	0	20	1326.09194	0.00035	2260.86993	934.77834
1	-1	2	2	18	1	1	0	0	19	1327.88660	0.00053	2223.02504	895.13897
1	-1	2	2	17	1	1	0	0	18	1329.69391	-0.00002	2187.17209	857.47816
1	-1	2	2	16	1	1	0	0	17	1331.51407	-0.00065	2153.31116	821.79644
1	-1	2	2	15	1	1	0	0	16	1333.34914	0.00116	2121.44228	788.09430W
1	-1	2	2	14	1	1	0	0	15	1335.19638*	0.00311	2091.56547	756.37220W
1	-1	2	2	13	1	1	0	0	14	1337.05026	0.00013	2063.68073	726.63060
1	-1	2	2	12	1	1	0	0	13	1338.91809	-0.00003	2037.78803	698.86991
1	-1	2	2	11	1	1	0	0	12	1340.79693	0.00010	2013.88734	673.09051
1	-1	2	2	10	1	1	0	0	11	1342.68536	-0.00049	1991.97861	649.29275
1	-1	2	2	9	1	1	0	0	10	1344.58495	0.00015	1972.06179	627.47699
1	-1	2	2	8	1	1	0	0	9	1346.49298	-0.00035	1954.13683	607.64350
1	-1	2	2	7	1	1	0	0	8	1348.41083	-0.00027	1938.20368	589.79258
1	-1	2	2	6	1	1	0	0	7	1350.33888	0.00105	1924.26229	573.92447W
1	-1	2	2	2	1	1	0	0	3	1358.13006	0.00065	1888.41352	530.28412
1	-1	2	2	1	1	1	0	0	2	1360.09376*	-0.00380	1884.43037	524.33282W
1	-1	2	2	2	1	1	0	0	1	1368.04889	0.00060	1888.41352	520.36524
1	-1	2	2	3	1	1	0	0	2	1370.05330	-0.00215	1894.38827	524.33282W
1	-1	2	2	4	1	1	0	0	3	1372.07048	-0.00002	1902.35462	530.28412
1	-1	2	2	5	1	1	0	0	4	1374.09347*	-0.00009	1912.31262	538.21906
1	-1	2	2	6	1	1	0	0	5	1376.12475	-0.00001	1924.26229	548.13753
1	-1	2	2	7	1	1	0	0	6	1378.16425	-0.00005	1938.20368	560.03938
1	-1	2	2	8	1	1	0	0	7	1380.21257	0.00021	1954.13683	573.92447
1	-1	2	2	9	1	1	0	0	8	1382.26924	0.00003	1972.06179	589.79258
1	-1	2	2	10	1	1	0	0	9	1384.33451	-0.00060	1991.97861	607.64350
1	-1	2	2	11	1	1	0	0	10	1386.41008	-0.00028	2013.88734	627.47699
1	-1	2	2	12	1	1	0	0	11	1388.49523	-0.00005	2037.78803	649.29275
1	-1	2	2	13	1	1	0	0	12	1390.58038	-0.00041	2063.68073	673.09051

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1	1	2	-2	29	1	-1	0	0	28	1423.76840	-0.00026	2750.39685	1326.62819
1	1	2	-2	30	1	-1	0	0	29	1425.95648	-0.00027	2810.25693	1384.30018
1	1	2	-2	31	1	-1	0	0	30	1428.15731	-0.00055	2872.11031	1443.95245
1	1	2	-2	32	1	-1	0	0	31	1430.37097	-0.00124	2935.95636	1505.58415W
1	1	2	-2	33	1	-1	0	0	32	1432.60593*	0.000592	3001.79442	1569.19441W
1	1	2	-2	34	1	-1	0	0	33	1434.84035	-0.00108	3069.62373	1634.78230W
1	1	2	-2	35	1	-1	0	0	34	1437.09540	-0.00121	3139.44351	1702.34690W
1	1	2	-2	36	1	-1	0	0	35	1439.36450	-0.00115	3211.25289	1771.88724W

rms = 0.00034 cm⁻¹

$$v_4 + 2v_5 (\text{II}\Pi) \leftarrow v_5 (\Pi)$$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
1	1	2	0	1	0	0	1	1	2	1180.09711*	0.00182	1863.84991	683.75462W
1	1	2	0	2	0	0	1	1	3	1178.13194*	0.00048	1867.83286	689.70140
1	1	2	0	3	0	0	1	1	4	1176.17681	-0.00004	1873.80717	697.63032
1	1	2	0	4	0	0	1	1	5	1174.23163	0.00018	1881.77271	707.54126
1	1	2	0	5	0	0	1	1	6	1172.29523	0.00002	1891.72929	719.43409
1	1	2	0	6	0	0	1	1	7	1170.36828	0.00022	1903.67670	733.30864
1	1	2	0	7	0	0	1	1	8	1168.44997	0.00003	1917.61467	749.16472
1	1	2	0	8	0	0	1	1	9	1166.54082	0.00007	1933.54287	767.00212
1	1	2	0	9	0	0	1	1	10	1164.64059	0.00023	1951.46095	786.82059
1	1	2	0	10	0	0	1	1	11	1162.74923	0.00058	1971.36850	808.61985
1	1	2	0	11	0	0	1	1	12	1160.86594*	0.00048	1993.26507	832.39961
1	1	2	0	12	0	0	1	1	13	1158.99112	0.00051	2017.15015	858.15954
1	1	2	0	13	0	0	1	1	14	1157.12441	0.00050	2043.02319	885.89928
1	1	2	0	14	0	0	1	1	15	1155.26566	0.00051	2070.88360	915.61845
1	1	2	0	15	0	0	1	1	16	1153.41469	0.00060	2100.73073	947.31664
1	1	2	0	16	0	0	1	1	17	1151.57116	0.00068	2132.56390	980.99342
1	1	2	0	17	0	0	1	1	18	1149.73481	0.00078	2166.38235	1016.64832
1	1	2	0	18	0	0	1	1	19	1147.90447	0.00002	2202.18530	1054.28084
1	1	2	0	19	0	0	1	1	20	1146.08203	0.00061	2239.97191	1093.89049
1	1	2	0	20	0	0	1	1	21	1144.26509	0.00050	2279.74129	1135.47669
1	1	2	0	21	0	0	1	1	22	1142.45411	0.00050	2321.49251	1179.03889
1	1	2	0	22	0	0	1	1	23	1140.64855	0.00046	2365.22458	1224.57649
1	1	2	0	23	0	0	1	1	24	1138.84734	-0.00029	2410.93648	1272.08885
1	1	2	0	24	0	0	1	1	25	1137.05222	0.00041	2458.62713	1321.57533
1	1	2	0	25	0	0	1	1	26	1135.25998	-0.00020	2508.29542	1373.03523
1	1	2	0	26	0	0	1	1	27	1133.47237	0.00006	2559.94017	1426.46786
1	1	2	0	27	0	0	1	1	28	1131.68733	-0.00039	2613.56020	1481.87248
1	1	2	0	28	0	0	1	1	29	1129.90580	-0.00013	2669.15425	1539.24832
1	1	2	0	2	0	0	1	1	1	1188.04252	-0.00029	1867.83286	679.79005
1	1	2	0	3	0	0	1	1	2	1190.05276	0.00021	1873.80717	683.75462
1	1	2	0	4	0	0	1	1	3	1192.07172	0.00042	1881.77271	689.70140
1	1	2	0	5	0	0	1	1	4	1194.09875	-0.00022	1891.72929	697.63032
1	1	2	0	6	0	0	1	1	5	1196.13565	0.00021	1903.67670	707.54126
1	1	2	0	7	0	0	1	1	6	1198.18103	0.00045	1917.61467	719.43409
1	1	2	0	8	0	0	1	1	7	1200.23486	0.00063	1933.54287	733.30864
1	1	2	0	9	0	0	1	1	8	1202.29659	0.00036	1951.46095	749.16472
1	1	2	0	10	0	0	1	1	9	1204.36693	0.00055	1971.36850	767.00212
1	1	2	0	11	0	0	1	1	10	1206.44434	-0.00014	1993.26507	786.82059
1	1	2	0	12	0	0	1	1	11	1208.53035	0.00006	2017.15015	808.61985
1	1	2	0	13	0	0	1	1	12	1210.62405	0.00047	2043.02319	832.39961
1	1	2	0	14	0	0	1	1	13	1212.72475	0.00069	2070.88360	858.15954
1	1	2	0	15	0	0	1	1	14	1214.83233	0.00088	2100.73073	885.89928
1	1	2	0	16	0	0	1	1	15	1216.94604	0.00059	2132.56390	915.61845
1	1	2	0	17	0	0	1	1	16	1219.06612	0.00041	2166.38235	947.31664
1	1	2	0	18	0	0	1	1	17	1221.19237	0.00049	2202.18530	980.99342
1	1	2	0	19	0	0	1	1	18	1223.32409	0.00050	2239.97191	1016.64832
1	1	2	0	20	0	0	1	1	19	1225.45978	-0.00066	2279.74129	1054.28084
1	1	2	0	21	0	0	1	1	20	1227.60238	0.00036	2321.49251	1093.89049
1	1	2	0	22	0	0	1	1	21	1229.74825	0.00036	2365.22458	1135.47669
1	1	2	0	23	0	0	1	1	22	1231.89796	0.00037	2410.93648	1179.03889
1	1	2	0	24	0	0	1	1	23	1234.05090	0.00026	2458.62713	1224.57649
1	1	2	0	25	0	0	1	1	24	1236.20384	0.00008	2508.29542	1272.08885

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1	1	1	2	0	26	0	0	1	1	25	1238.36479	-0.00006	2559.94017	1321.57533
	1	1	2	0	27	0	0	1	1	26	1240.52489	-0.00008	2613.56020	1373.03523
2	1	1	2	0	28	0	0	1	1	27	1242.68560	-0.00079	2669.15425	1426.46786
3	1	1	2	0	29	0	0	1	1	28	1244.84792	-0.00066	2726.72106	1481.87248
4	1	1	2	0	30	0	0	1	1	29	1247.01055	-0.00044	2786.25932	1539.24832
5	1	1	2	0	31	0	0	1	1	30	1249.17234	-0.00074	2847.76768	1598.59460
6	1	1	2	0	32	0	0	1	1	31	1251.33390	-0.00039	2911.24479	1659.91050
7	1	1	2	0	33	0	0	1	1	32	1253.49408	-0.00001	2976.68926	1723.19517
8	1	1	2	0	34	0	0	1	1	33	1255.65140	-0.00055	3044.09969	1788.44775
9	1	-1	2	0	1	0	0	1	-1	2	1180.07965	0.00000	1863.85543	683.77578
10	1	-1	2	0	2	0	0	1	-1	3	1178.10579	0.00008	1867.84942	689.74371
11	1	-1	2	0	3	0	0	1	-1	4	1176.13945	0.00000	1873.84028	697.70083
12	1	-1	2	0	4	0	0	1	-1	5	1174.18059	-0.00028	1881.82789	707.64702
13	1	-1	2	0	5	0	0	1	-1	6	1172.22956	-0.00035	1891.81206	719.58215
14	1	-1	2	0	6	0	0	1	-1	7	1170.28652	0.00000	1903.79255	733.50603
15	1	-1	2	0	7	0	0	1	-1	8	1168.35063	0.00002	1917.76910	749.41849
16	1	-1	2	0	8	0	0	1	-1	9	1166.42211	0.00002	1933.74139	767.31930
17	1	-1	2	0	9	0	0	1	-1	10	1164.50062	-0.00023	1951.70905	787.20820
18	1	-1	2	0	10	0	0	1	-1	11	1162.58653	-0.00022	1971.67167	809.08492
19	1	-1	2	0	11	0	0	1	-1	12	1160.67961	-0.00004	1993.62880	832.94916
20	1	-1	2	0	12	0	0	1	-1	13	1158.77907	-0.00032	2017.57995	858.80057
21	1	-1	2	0	13	0	0	1	-1	14	1156.88562	-0.00016	2043.52458	886.63880
22	1	-1	2	0	14	0	0	1	-1	15	1154.99858	-0.00007	2071.46210	916.46345
23	1	-1	2	0	15	0	0	1	-1	16	1153.11735	-0.00043	2101.39190	948.27412
24	1	-1	2	0	16	0	0	1	-1	17	1151.24247	-0.00050	2133.31332	982.07035
25	1	-1	2	0	17	0	0	1	-1	18	1149.37371	-0.00026	2167.22564	1017.85167
26	1	-1	2	0	18	0	0	1	-1	19	1147.51010	-0.00046	2203.12814	1055.61759
27	1	-1	2	0	19	0	0	1	-1	20	1145.65239	-0.00008	2241.02004	1095.36757
28	1	-1	2	0	20	0	0	1	-1	21	1143.79895	-0.00052	2280.90052	1137.10105
29	1	-1	2	0	21	0	0	1	-1	22	1141.95087	-0.00041	2322.76874	1180.81746
30	1	-1	2	0	22	0	0	1	-1	23	1140.10734	-0.00029	2366.62381	1226.51618
31	1	-1	2	0	23	0	0	1	-1	24	1138.26829	0.00003	2412.46483	1274.19657
32	1	-1	2	0	24	0	0	1	-1	25	1136.43324	0.00036	2460.29085	1323.85797
33	1	-1	2	0	25	0	0	1	-1	26	1134.60106	-0.00017	2510.10091	1375.49968
34	1	-1	2	0	26	0	0	1	-1	27	1132.77300	-0.00002	2561.89400	1429.12098
35	1	-1	2	0	2	0	0	1	-1	1	1188.05260	0.00029	1867.84942	679.79710
36	1	-1	2	0	3	0	0	1	-1	2	1190.06422	-0.00029	1873.84028	683.77578
37	1	-1	2	0	4	0	0	1	-1	3	1192.08388	-0.00030	1881.82789	689.74371
38	1	-1	2	0	5	0	0	1	-1	4	1194.11127	0.00004	1891.81206	697.70083
39	1	-1	2	0	6	0	0	1	-1	5	1196.14595	0.00042	1903.79255	707.64702
40	1	-1	2	0	7	0	0	1	-1	6	1198.18695	-0.00001	1917.76910	719.58215
41	1	-1	2	0	8	0	0	1	-1	7	1200.23486	-0.00050	1933.74139	733.50603
42	1	-1	2	0	9	0	0	1	-1	8	1202.29071	0.00015	1951.70905	749.41849
43	1	-1	2	0	10	0	0	1	-1	9	1204.35227	-0.00010	1971.67167	767.31930
44	1	-1	2	0	11	0	0	1	-1	10	1206.42024	-0.00036	1993.62880	787.20820
45	1	-1	2	0	12	0	0	1	-1	11	1208.49517	0.00014	2017.57995	809.08492
46	1	-1	2	0	13	0	0	1	-1	12	1210.57518	-0.00024	2043.52458	832.94916
47	1	-1	2	0	14	0	0	1	-1	13	1212.66144	-0.00010	2071.46210	858.80057
48	1	-1	2	0	15	0	0	1	-1	14	1214.75270	-0.00041	2101.39190	886.63880
49	1	-1	2	0	16	0	0	1	-1	15	1216.85008	0.00022	2133.31332	916.46345
50	1	-1	2	0	17	0	0	1	-1	16	1218.95155	0.00002	2167.22564	948.27412
51	1	-1	2	0	18	0	0	1	-1	17	1221.05759	-0.00020	2203.12814	982.07035
52	1	-1	2	0	19	0	0	1	-1	18	1223.16798	-0.00039	2241.02004	1017.85167
53	1	-1	2	0	20	0	0	1	-1	19	1225.28276	-0.00017	2280.90052	1055.61759
54	1	-1	2	0	21	0	0	1	-1	20	1227.40111	-0.00006	2322.76874	1095.36757
55	1	-1	2	0	22	0	0	1	-1	21	1229.52254	-0.00022	2366.62381	1137.10105
56	1	-1	2	0	23	0	0	1	-1	22	1231.64750	0.00013	2412.46483	1180.81746
57	1	-1	2	0	24	0	0	1	-1	23	1233.77513	0.00046	2460.29085	1226.51618
58	1	-1	2	0	25	0	0	1	-1	24	1235.90617	0.00183	2510.10091	1274.19657W
59	1	-1	2	0	26	0	0	1	-1	25	1238.03584	-0.00019	2561.89400	1323.85797
60	1	-1	2	0	27	0	0	1	-1	26	1240.16920	-0.00022	2615.66910	1375.49968

rms = 0.00037 cm⁻¹

$$v_4 + 2v_5 (^1\Pi) \leftarrow v_5 (^1\Pi)$$

	$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS – CALC	E'	E''
1	1 -1 2 2 34	0 0 1 1 35	1142.50963	0.00033	3067.36229	1924.85299
2	1 -1 2 2 33	0 0 1 1 34	1144.01746	0.00003	2999.68476	1855.66733
3	1 -1 2 2 32	0 0 1 1 33	1145.54404	0.00063	2933.99116	1788.44775
4	1 -1 2 2 31	0 0 1 1 32	1147.08807	0.00079	2870.28245	1723.19517
5	1 -1 2 2 30	0 0 1 1 31	1148.64955	0.00050	2808.55954	1659.91050
6	1 -1 2 2 29	0 0 1 1 30	1150.23021*	0.00151	2748.82330	1598.59460W
7	1 -1 2 2 28	0 0 1 1 29	1151.82664	0.00044	2691.07452	1539.24832
8	1 -1 2 2 27	0 0 1 1 28	1153.44139	-0.00006	2635.31393	1481.87248
9	1 -1 2 2 26	0 0 1 1 27	1155.07457	0.00023	2581.54220	1426.46786
10	1 -1 2 2 25	0 0 1 1 26	1156.72497	0.00027	2529.75993	1373.03523
11	1 -1 2 2 24	0 0 1 1 25	1158.39243	0.00011	2479.96765	1321.57533
12	1 -1 2 2 23	0 0 1 1 24	1160.07694	-0.00002	2432.16581	1272.08885
13	1 -1 2 2 22	0 0 1 1 23	1161.77818	-0.00015	2386.35482	1224.57649
14	1 -1 2 2 21	0 0 1 1 22	1163.49621	0.00010	2342.53501	1179.03889
15	1 -1 2 2 20	0 0 1 1 21	1165.23003	0.00008	2300.70664	1135.47669
16	1 -1 2 2 19	0 0 1 1 20	1166.97960	0.00016	2260.86993	1093.89049
17	1 -1 2 2 18	0 0 1 1 19	1168.74439	0.00019	2223.02504	1054.28084
18	1 -1 2 2 17	0 0 1 1 18	1170.52403	0.00025	2187.17209	1016.64832
19	1 -1 2 2 16	0 0 1 1 17	1172.31805	0.00031	2153.31116	980.99342
20	1 -1 2 2 15	0 0 1 1 16	1174.12593	0.00029	2121.44228	947.31664
21	1 -1 2 2 14	0 0 1 1 15	1175.94708	0.00006	2091.56547	915.61845
22	1 -1 2 2 13	0 0 1 1 14	1177.78130	-0.00015	2063.68073	885.89928
23	1 -1 2 2 12	0 0 1 1 13	1179.62869	0.00020	2037.78803	858.15954
24	1 -1 2 2 11	0 0 1 1 12	1181.48773	0.00000	2013.88734	832.39961
25	1 -1 2 2 10	0 0 1 1 11	1183.35889	0.00013	1991.97861	808.61985
26	1 -1 2 2 9	0 0 1 1 10	1185.24160	0.00040	1972.06179	786.82059
27	1 -1 2 2 8	0 0 1 1 9	1187.13484	0.00013	1954.13683	767.00212
28	1 -1 2 2 7	0 0 1 1 8	1189.03908	0.00012	1938.20368	749.16472
29	1 -1 2 2 6	0 0 1 1 7	1190.95364	-0.00001	1924.26229	733.30864
30	1 -1 2 2 5	0 0 1 1 6	1192.87857	0.00004	1912.31262	719.43409
31	1 -1 2 2 4	0 0 1 1 5	1194.81343	0.00007	1902.35462	707.54126
32	1 -1 2 2 3	0 0 1 1 4	1196.75793	-0.00002	1894.38827	697.63032
33	1 -1 2 2 2	0 0 1 1 3	1198.71259	0.00047	1888.41352	689.70140
34	1 -1 2 2 1	0 0 1 1 2	1200.67607	0.00031	1884.43037	683.75462
35	1 -1 2 2 2	0 0 1 1 1	1208.62320	-0.00027	1888.41352	679.79005
36	1 -1 2 2 3	0 0 1 1 2	1210.63304	-0.00061	1894.38827	683.75462
37	1 -1 2 2 4	0 0 1 1 3	1212.65352	0.00030	1902.35462	689.70140
38	1 -1 2 2 5	0 0 1 1 4	1214.68264	0.00034	1912.31262	697.63032
39	1 -1 2 2 6	0 0 1 1 5	1216.72139	0.00036	1924.26229	707.54126
40	1 -1 2 2 7	0 0 1 1 6	1218.76977	0.00018	1938.20368	719.43409
41	1 -1 2 2 8	0 0 1 1 7	1220.82840	0.00021	1954.13683	733.30864
42	1 -1 2 2 9	0 0 1 1 8	1222.89712	0.00005	1972.06179	749.16472
43	1 -1 2 2 10	0 0 1 1 9	1224.97697	0.00048	1991.97861	767.00212
44	1 -1 2 2 11	0 0 1 1 10	1227.06672	-0.00003	2013.88734	786.82059
45	1 -1 2 2 12	0 0 1 1 11	1229.16804	-0.00014	2037.78803	808.61985
46	1 -1 2 2 13	0 0 1 1 12	1231.28149	0.00037	2063.68073	832.39961
47	1 -1 2 2 14	0 0 1 1 13	1233.40601	0.00008	2091.56547	858.15954
48	1 -1 2 2 15	0 0 1 1 14	1235.54326	0.00026	2121.44228	885.89928
49	1 -1 2 2 16	0 0 1 1 15	1237.69241	-0.00030	2153.31116	915.61845
50	1 -1 2 2 17	0 0 1 1 16	1239.85551	0.00006	2187.17209	947.31664
51	1 -1 2 2 18	0 0 1 1 17	1242.03197	0.00035	2223.02504	980.99342
52	1 -1 2 2 19	0 0 1 1 18	1244.22181	0.00020	2260.86993	1016.64832
53	1 -1 2 2 20	0 0 1 1 19	1246.42579	0.00000	2300.70664	1054.28084
54	1 -1 2 2 21	0 0 1 1 20	1248.64425	-0.00027	2342.53501	1093.89049
55	1 -1 2 2 22	0 0 1 1 21	1250.87835	0.00022	2386.35482	1135.47669
56	1 -1 2 2 23	0 0 1 1 22	1253.12704	0.00012	2432.16581	1179.03889
57	1 -1 2 2 24	0 0 1 1 23	1255.39128	0.00012	2479.96765	1224.57649
58	1 -1 2 2 25	0 0 1 1 24	1257.67123	0.00015	2529.75993	1272.08885
59	1 -1 2 2 26	0 0 1 1 25	1259.96702	0.00014	2581.54220	1321.57533
60	1 -1 2 2 27	0 0 1 1 26	1262.27888	0.00018	2635.31393	1373.03523
	1 -1 2 2 28	0 0 1 1 27	1264.60693	0.00027	2691.07452	1426.46786
	1 -1 2 2 29	0 0 1 1 28	1266.95119	0.00037	2748.82330	1481.87248
	1 -1 2 2 30	0 0 1 1 29	1269.31150	0.00028	2808.55954	1539.24832
	1 -1 2 2 31	0 0 1 1 30	1271.68944*	0.00159	2870.28245	1598.59460W
	1 -1 2 2 32	0 0 1 1 31	1274.08288	0.00222	2933.99116	1659.91050W
	1 -1 2 2 33	0 0 1 1 32	1276.49033	0.00074	2999.68476	1723.19517
	1 -1 2 2 34	0 0 1 1 33	1278.91657	0.00209	3067.36229	1788.44775W

1	1	2	-2	1	0	0	1	1	1	1204.64294	-0.00072	1884.43371	679.79005
1	1	2	-2	2	0	0	1	1	2	1204.66836	-0.00055	1888.42353	683.75462
1	1	2	-2	3	0	0	1	1	3	1204.70680	-0.00007	1894.40827	689.70140
1	1	2	-2	4	0	0	1	1	4	1204.75773	0.00008	1902.38797	697.63032
1	1	2	-2	5	0	0	1	1	5	1204.82177	0.00038	1912.36265	707.54126
1	1	2	-2	6	0	0	1	1	6	1204.89858	0.00032	1924.33235	719.43409
1	1	2	-2	7	0	0	1	1	7	1204.98870	0.00023	1938.29711	733.30864
1	1	2	-2	8	0	0	1	1	8	1205.09243	0.00015	1954.25700	749.16472
1	1	2	-2	9	0	0	1	1	9	1205.20959	-0.00036	1972.21207	767.00212
1	-1	2	2	1	0	0	1	-1	1	1204.63393	0.00066	1884.43037	679.79710
1	-1	2	2	3	0	0	1	-1	3	1204.64402	-0.00053	1894.38827	689.74371
1	-1	2	2	4	0	0	1	-1	4	1204.65379	0.00000	1902.35462	697.70083
1	-1	2	2	5	0	0	1	-1	5	1204.66836*	0.00277	1912.31262	707.64702W
1	-1	2	2	6	0	0	1	-1	6	1204.68013	-0.00001	1924.26229	719.58215
1	-1	2	2	8	0	0	1	-1	8	1204.71891	0.00057	1954.13683	749.41849
1	-1	2	2	9	0	0	1	-1	9	1204.74263	0.00014	1972.06179	767.31930
1	-1	2	2	10	0	0	1	-1	10	1204.77059	0.00018	1991.97861	787.20820

rms = 0.00031 cm⁻¹3v₅ (II) ← v₅ (II)

<i>v</i> ₄ ' <i>l</i> ₄ ' <i>v</i> ₅ ' <i>l</i> ₅ ' <i>J</i> '	<i>v</i> ₄ " <i>l</i> ₄ " <i>v</i> ₅ " <i>l</i> ₅ " <i>J</i> "	OBS	OBS - CALC	E'	E''
0 0 3 1 1	0 0 1 1 2	1328.45439	0.00023	2012.20878	683.75462
0 0 3 1 2	0 0 1 1 3	1326.47768	0.00057	2016.17851	689.70140
0 0 3 1 3	0 0 1 1 4	1324.50249	-0.00020	2022.13301	697.63032
0 0 3 1 4	0 0 1 1 5	1322.53100	0.00008	2030.07218	707.54126
0 0 3 1 5	0 0 1 1 6	1320.56183	0.00003	2039.99589	719.43409
0 0 3 1 6	0 0 1 1 7	1318.59546	0.00015	2051.90395	733.30864
0 0 3 1 7	0 0 1 1 8	1316.63139	-0.00005	2065.79617	749.16472
0 0 3 1 8	0 0 1 1 9	1314.67021	0.00005	2081.67229	767.00212
0 0 3 1 9	0 0 1 1 10	1312.71127	-0.00018	2099.53204	786.82059
0 0 3 1 10	0 0 1 1 11	1310.75503	-0.00023	2119.37511	808.61985
0 0 3 1 11	0 0 1 1 12	1308.80152	-0.00003	2141.20116	832.39961
0 0 3 1 12	0 0 1 1 13	1306.85015	-0.00012	2165.00981	858.15954
0 0 3 1 13	0 0 1 1 14	1304.90124	-0.00012	2190.80064	885.89928
0 0 3 1 14	0 0 1 1 15	1302.95476	0.00000	2218.57321	915.61845
0 0 3 1 15	0 0 1 1 16	1301.01035	-0.00005	2248.32704	947.31664
0 0 3 1 16	0 0 1 1 17	1299.06806	-0.00015	2280.06163	980.99342
0 0 3 1 17	0 0 1 1 18	1297.12803	-0.00007	2313.77642	1016.64832
0 0 3 1 18	0 0 1 1 19	1295.18990	-0.00010	2349.47084	1054.28084
0 0 3 1 19	0 0 1 1 20	1293.25354	-0.00026	2387.14429	1093.89049
0 0 3 1 20	0 0 1 1 21	1291.31948	0.00005	2426.79612	1135.47669
0 0 3 1 21	0 0 1 1 22	1289.38688	0.00010	2468.42567	1179.03889
0 0 3 1 22	0 0 1 1 23	1287.45586	0.00011	2512.03224	1224.57649
0 0 3 1 23	0 0 1 1 24	1285.52636	0.00012	2557.61509	1272.08885
0 0 3 1 24	0 0 1 1 25	1283.59808	-0.00007	2605.17347	1321.57533
0 0 3 1 25	0 0 1 1 26	1281.67172	0.00037	2654.70659	1373.03523
0 0 3 1 26	0 0 1 1 27	1279.74586	0.00011	2706.21362	1426.46786
0 0 3 1 27	0 0 1 1 28	1277.82114	-0.00010	2759.69372	1481.87248
0 0 3 1 28	0 0 1 1 29	1275.89756	-0.00013	2815.14601	1539.24832
0 0 3 1 29	0 0 1 1 30	1273.97526	0.00027	2872.56959	1598.59460
0 0 3 1 30	0 0 1 1 31	1272.05327	0.00024	2931.96353	1659.91050
0 0 3 1 31	0 0 1 1 32	1270.13185	0.00014	2993.32688	1723.19517
0 0 3 1 32	0 0 1 1 33	1268.21126	0.00037	3056.65864	1788.44775
0 0 3 1 33	0 0 1 1 34	1266.28990	-0.00057	3121.95780	1855.66733
0 0 3 1 34	0 0 1 1 35	1264.37045	0.00010	3189.22334	1924.85299
0 0 3 1 35	0 0 1 1 36	1262.45060	0.00020	3258.45419	1996.00378
0 0 3 1 36	0 0 1 1 37	1260.53090	0.00037	3329.64926	2069.11873
0 0 3 1 37	0 0 1 1 38	1258.61056	-0.00006	3402.80744	2144.19682
0 0 3 1 38	0 0 1 1 39	1256.69029	-0.00029	3477.92760	2221.23702
0 0 3 1 39	0 0 1 1 40	1254.76900	-0.00131	3555.00858	2300.23827W
0 0 3 1 2	0 0 1 1 1	1336.38852	0.00006	2016.17851	679.79005
0 0 3 1 3	0 0 1 1 2	1338.37853	0.00014	2022.13301	683.75462
0 0 3 1 4	0 0 1 1 3	1340.37093	0.00015	2030.07218	689.70140
0 0 3 1 5	0 0 1 1 4	1339.99589	0.00015	2039.99589	697.63032

0	0	3	-1	10	0	0	1	1	10	1333.34973	-0.00097	2120.17129	786.82059
0	0	3	-1	11	0	0	1	1	11	1333.53843*	0.00188	2142.15640	808.61985W
0	0	3	-1	12	0	0	1	1	12	1333.73897	0.00008	2166.13850	832.39961
0	0	3	-1	13	0	0	1	1	13	1333.95846*	0.00086	2192.11714	858.15954
0	0	3	-1	15	0	0	1	1	15	1334.44299	-0.00066	2250.06210	915.61845
0	0	3	-1	16	0	0	1	1	16	1334.71231	0.00160	2282.02735	947.31664W

rms = 0.00027 cm⁻¹

3v₄ (Π) ← G.S. (Σ⁺)

<i>v</i> ₄ ' <i>l</i> ₄ ' <i>v</i> ₅ ' <i>l</i> ₅ ' <i>J</i> '	<i>v</i> ₄ '' <i>l</i> ₄ '' <i>v</i> ₅ '' <i>l</i> ₅ '' <i>J</i> ''	OBS	OBS - CALC	E'	E''
3 1 0 0 23	0 0 0 0 24	1505.23360	0.00103	2099.74084	594.50827W
3 1 0 0 22	0 0 0 0 23	1507.09800	-0.00030	2054.07593	546.97764
3 1 0 0 21	0 0 0 0 22	1508.96630*	0.00012	2010.38873	501.42254
3 1 0 0 20	0 0 0 0 21	1510.83640	-0.00004	1968.68006	457.84362
3 1 0 0 19	0 0 0 0 20	1512.70945	0.00015	1928.95077	416.24147
3 1 0 0 18	0 0 0 0 19	1514.58400	-0.00103	1891.20168	376.61665W
3 1 0 0 17	0 0 0 0 18	1516.46330	-0.00060	1855.43362	338.96972
3 1 0 0 16	0 0 0 0 17	1518.34630	0.00009	1821.64740	303.30118
3 1 0 0 15	0 0 0 0 16	1520.23170	-0.00057	1789.84380	269.61154
3 1 0 0 14	0 0 0 0 15	1522.12276	0.00039	1760.02361	237.90124
3 1 0 0 13	0 0 0 0 14	1524.01710	0.00024	1732.18758	208.17072
3 1 0 0 12	0 0 0 0 13	1525.91640	0.00036	1706.33645	180.42041
3 1 0 0 11	0 0 0 0 12	1527.81970	-0.00054	1682.47090	154.65066
3 1 0 0 10	0 0 0 0 11	1529.72790	-0.00187	1660.59161	130.86184W
3 1 0 0 9	0 0 0 0 10	1531.63909*	-0.00584	1640.69921	109.05428W
3 1 0 0 8	0 0 0 0 9	1533.56650	0.00048	1622.79429	89.22827
3 1 0 0 7	0 0 0 0 8	1535.49180*	-0.00149	1606.87737	71.38408W
3 1 0 0 6	0 0 0 0 7	1537.42750	0.00051	1592.94896	55.52197
3 1 0 0 5	0 0 0 0 6	1539.36720	-0.00015	1581.00949	41.64214
3 1 0 0 4	0 0 0 0 5	1541.31280	-0.00174	1571.05934	29.74480W
3 1 0 0 3	0 0 0 0 4	1543.26740	-0.00133	1563.09883	19.83009W
3 1 0 0 2	0 0 0 0 3	1545.23013	0.00008	1557.12821	11.89816
3 1 0 0 2	0 0 0 0 1	1555.14330*	-0.00186	1557.12821	1.98305W
3 1 0 0 3	0 0 0 0 2	1557.15000	0.00030	1563.09883	5.94912
3 1 0 0 4	0 0 0 0 3	1559.16200	0.00083	1571.05934	11.89816
3 1 0 0 5	0 0 0 0 4	1561.17980	0.00040	1581.00949	19.83009
3 1 0 0 6	0 0 0 0 5	1563.20630*	0.00214	1592.94896	29.74480W
3 1 0 0 7	0 0 0 0 6	1565.23510	-0.00013	1606.87737	41.64214
3 1 0 0 8	0 0 0 0 7	1567.27320	0.00088	1622.79429	55.52197
3 1 0 0 9	0 0 0 0 8	1569.31470	-0.00043	1640.69921	71.38408
3 1 0 0 10	0 0 0 0 9	1571.36280	-0.00054	1660.59161	89.22827
3 1 0 0 11	0 0 0 0 10	1573.41670	0.00008	1682.47090	109.05428
3 1 0 0 12	0 0 0 0 11	1575.47550	0.00090	1706.33645	130.86184
3 1 0 0 13	0 0 0 0 12	1577.53600	-0.00092	1732.18758	154.65066
3 1 0 0 14	0 0 0 0 13	1579.60180	-0.00141	1760.02361	180.42041W
3 1 0 0 15	0 0 0 0 14	1581.67360	0.00052	1789.84380	208.17072
3 1 0 0 16	0 0 0 0 15	1583.74490	-0.00126	1821.64740	237.90124W
3 1 0 0 17	0 0 0 0 16	1585.82130	-0.00079	1855.43362	269.61154
3 1 0 0 18	0 0 0 0 17	1587.90030	-0.00020	1891.20168	303.30118
3 -1 0 0 22	0 0 0 0 22	1557.03290	0.00192	2058.45353	501.42254W
3 -1 0 0 21	0 0 0 0 21	1556.56820	-0.00132	2014.41315	457.84362W
3 -1 0 0 20	0 0 0 0 20	1556.11780	-0.00158	1972.36084	416.24147W
3 -1 0 0 19	0 0 0 0 19	1555.68130	-0.00076	1932.29871	376.61665
3 -1 0 0 18	0 0 0 0 18	1555.25830	-0.00071	1894.22873	338.96972
3 -1 0 0 17	0 0 0 0 17	1554.85170	0.00011	1858.15277	303.30118
3 -1 0 0 16	0 0 0 0 16	1554.46020	-0.00084	1824.07257	269.61154
3 -1 0 0 15	0 0 0 0 15	1554.08836	-0.00015	1791.98975	237.90124
3 -1 0 0 14	0 0 0 0 14	1553.73535	0.00031	1761.90576	208.17072
3 -1 0 0 13	0 0 0 0 13	1553.40130	-0.00026	1733.82197	180.42041
3 -1 0 0 12	0 0 0 0 12	1553.08892	0.00001	1707.73957	154.65066
3 -1 0 0 11	0 0 0 0 11	1552.79769	-0.00014	1683.65967	130.86184
3 -1 0 0 10	0 0 0 0 10	1552.52958	0.00061	1661.58325	109.05428
3 -1 0 0 9	0 0 0 0 9	1552.28269	-0.00022	1641.51118	89.22827
3 -1 0 0 8	0 0 0 0 8	1552.04425	0.00023	1623.44425	71.38408

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3	-1	0	0	7	0	0	0	0	7	1551.86060	-0.00055	1607.38312	55.52197
3	-1	0	0	6	0	0	0	0	6	1551.68575	-0.00050	1593.32839	41.64214
3	-1	0	0	5	0	0	0	0	5	1551.53540	-0.00037	1581.28057	29.74480
3	-1	0	0	4	0	0	0	0	4	1551.40890	-0.00109	1571.24009	19.83009W
3	-1	0	0	3	0	0	0	0	3	1551.30820	-0.00092	1563.20728	11.89816
3	-1	0	0	2	0	0	0	0	2	1551.23230	-0.00102	1557.18244	5.94912W
3	-1	0	0	1	0	0	0	0	1	1551.18220*	-0.00052	1553.16577	1.98305

rms = 0.00050 cm⁻¹ $2\nu_4 + \nu_5 (\text{II}\Pi) \leftarrow G.S. (\Sigma^+)$

ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
2	0	1	1	21	0	0	0	0	22	1671.30320	-0.00069	2172.72643	501.42254
2	0	1	1	20	0	0	0	0	21	1673.09285	0.00071	2130.93576	457.84362
2	0	1	1	19	0	0	0	0	20	1674.87930	0.00007	2091.12070	416.24147
2	0	1	1	18	0	0	0	0	19	1676.66640	-0.00006	2053.28311	376.61665
2	0	1	1	17	0	0	0	0	18	1678.45480	-0.00036	2017.42488	338.96972
2	0	1	1	16	0	0	0	0	17	1680.24730	0.00055	1983.54793	303.30118
2	0	1	1	15	0	0	0	0	16	1682.04187	-0.00074	1951.65414	269.61154
2	0	1	1	14	0	0	0	0	15	1683.84402	-0.00007	1921.74533	237.90124
2	0	1	1	13	0	0	0	0	14	1685.65270	0.00021	1893.82321	208.17072
2	0	1	1	12	0	0	0	0	13	1687.46904	0.00006	1867.88938	180.42041
2	0	1	1	11	0	0	0	0	12	1689.29471	0.00006	1843.94531	154.65066
2	0	1	1	10	0	0	0	0	11	1691.13023	-0.00024	1821.99232	130.86184
2	0	1	1	9	0	0	0	0	10	1692.97749	0.00018	1802.03159	109.05428
2	0	1	1	8	0	0	0	0	9	1694.83564	-0.00027	1784.06418	89.22827
2	0	1	1	7	0	0	0	0	8	1696.70637	-0.00054	1768.09099	71.38408
2	0	1	1	6	0	0	0	0	7	1698.59136	0.00050	1754.11283	55.52197
2	0	1	1	5	0	0	0	0	6	1700.48770	-0.00051	1742.13035	41.64214
2	0	1	1	4	0	0	0	0	5	1702.39860	-0.00073	1732.14413	29.74480
2	0	1	1	3	0	0	0	0	4	1704.32340	-0.00113	1724.15462	19.83009W
2	0	1	1	2	0	0	0	0	3	1706.26360	-0.00042	1718.16218	11.89816
2	0	1	1	1	0	0	0	0	2	1708.21816	0.00021	1714.16707	5.94912
2	0	1	1	3	0	0	0	0	2	1718.20550	0.00000	1724.15462	5.94912
2	0	1	1	4	0	0	0	0	3	1720.24532	-0.00065	1732.14413	11.89816
2	0	1	1	5	0	0	0	0	4	1722.30052	0.00026	1742.13035	19.83009
2	0	1	1	6	0	0	0	0	5	1724.36804	0.00001	1754.11283	29.74480
2	0	1	1	7	0	0	0	0	6	1726.44930	0.00045	1768.09099	41.64214
2	0	1	1	8	0	0	0	0	7	1728.54167	-0.00054	1784.06418	55.52197
2	0	1	1	9	0	0	0	0	8	1730.64737	-0.00014	1802.03159	71.38408
2	0	1	1	10	0	0	0	0	9	1732.76367	-0.00038	1821.99232	89.22827
2	0	1	1	11	0	0	0	0	10	1734.89087	-0.00016	1843.94531	109.05428
2	0	1	1	12	0	0	0	0	11	1737.02780	0.00026	1867.88938	130.86184
2	0	1	1	13	0	0	0	0	12	1739.17249	-0.00006	1893.82321	154.65066
2	0	1	1	14	0	0	0	0	13	1741.32452	-0.00040	1921.74533	180.42041
2	0	1	1	15	0	0	0	0	14	1743.48260	-0.00082	1951.65414	208.17072
2	0	1	1	16	0	0	0	0	15	1745.64520	-0.00149	1983.54793	237.90124W
2	0	1	1	17	0	0	0	0	16	1747.81390	0.00055	2017.42488	269.61154
2	0	1	1	18	0	0	0	0	17	1749.98110	-0.00083	2053.28311	303.30118
2	0	1	1	19	0	0	0	0	18	1752.14950	-0.00148	2091.12070	338.96972W
2	0	1	-1	23	0	0	0	0	23	1715.04990	-0.00029	2262.02782	546.97764
2	0	1	-1	22	0	0	0	0	22	1714.83896	0.00033	2216.26118	501.42254
2	0	1	-1	21	0	0	0	0	21	1714.63236	-0.00072	2172.47670	457.84362
2	0	1	-1	20	0	0	0	0	20	1714.43332	-0.00030	2130.67509	416.24147
2	0	1	-1	19	0	0	0	0	19	1714.24023	-0.00018	2090.85706	376.61665
2	0	1	-1	18	0	0	0	0	18	1714.05374	0.00012	2053.02334	338.96972
2	0	1	-1	17	0	0	0	0	17	1713.87326	-0.00020	2017.17464	303.30118
2	0	1	-1	16	0	0	0	0	16	1713.70022	0.00003	1983.31173	269.61154
2	0	1	-1	15	0	0	0	0	15	1713.53421	0.00010	1951.43535	237.90124
2	0	1	-1	14	0	0	0	0	14	1713.37564	0.00009	1921.54628	208.17072
2	0	1	-1	13	0	0	0	0	13	1713.22479	-0.00009	1893.64529	180.42041
2	0	1	-1	12	0	0	0	0	12	1713.08219	-0.00030	1867.73315	154.65066
2	0	1	-1	11	0	0	0	0	11	1712.94878	-0.00003	1843.81066	130.86184
2	0	1	-1	10	0	0	0	0	10	1712.82429	0.00002	1821.87855	109.05428
2	0	1	-1	9	0	0	0	0	9	1712.70022	0.00002	1801.93758	89.22827

2	0	1	-1	8	0	0	0	0	8	1712.60425	-0.00012	1783.98845	71.38408
2	0	1	-1	7	0	0	0	0	7	1712.51018	0.00032	1768.03183	55.52197
2	0	1	-1	6	0	0	0	0	6	1712.42656	0.00037	1754.06834	41.64214
2	0	1	-1	5	0	0	0	0	5	1712.35344	-0.00029	1742.09853	29.74480
2	0	1	-1	4	0	0	0	0	4	1712.29296	0.00014	1732.12291	19.83009
2	0	1	-1	3	0	0	0	0	3	1712.24372	0.00000	1724.14189	11.89816
2	0	1	-1	2	0	0	0	0	2	1712.20753	0.00084	1718.15582	5.94912
2	0	1	-1	1	0	0	0	0	1	1712.18201	0.00011	1714.16495	1.98305

rms = 0.00039 cm⁻¹ $2\nu_4 + \nu_5 (^1\Pi) \leftarrow G.S. (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 1 -1 1	0 0 0 0 2	1718.51240	-0.00105	1724.46257	5.94912W
2 2 1 -1 2	0 0 0 0 3	1716.54590	-0.00108	1728.44514	11.89816W
2 2 1 -1 3	0 0 0 0 4	1714.58760	-0.00135	1734.41904	19.83009W
2 2 1 -1 4	0 0 0 0 5	1712.64002	0.00049	1742.38433	29.74480
2 2 1 -1 5	0 0 0 0 6	1710.69878	-0.00014	1752.34107	41.64214
2 2 1 -1 6	0 0 0 0 7	1708.76720	-0.00017	1764.28934	55.52197
2 2 1 -1 7	0 0 0 0 8	1706.84564	0.00047	1778.22926	71.38408
2 2 1 -1 8	0 0 0 0 9	1704.93234	-0.00033	1794.16094	89.22827
2 2 1 -1 9	0 0 0 0 10	1703.03026	0.00002	1812.08452	109.05428
2 2 1 -1 10	0 0 0 0 11	1701.13814	-0.00018	1832.00016	130.86184
2 2 1 -1 11	0 0 0 0 12	1699.25674	-0.00062	1853.90802	154.65066
2 2 1 -1 12	0 0 0 0 13	1697.38732	-0.00056	1877.80829	180.42041
2 2 1 -1 13	0 0 0 0 14	1695.52984	-0.00057	1903.70113	208.17072
2 2 1 -1 14	0 0 0 0 15	1693.68541	-0.00010	1931.58675	237.90124
2 2 1 -1 15	0 0 0 0 16	1691.85317	-0.00062	1961.46532	269.61154
2 2 1 -1 16	0 0 0 0 17	1690.03539	-0.00046	1993.33703	303.30118
2 2 1 -1 17	0 0 0 0 18	1688.23256	0.00024	2027.20204	338.96972
2 2 1 -1 18	0 0 0 0 19	1686.44347	-0.00036	2063.06048	376.61665
2 2 1 -1 19	0 0 0 0 20	1684.67092	-0.00006	2100.91245	416.24147
2 2 1 -1 20	0 0 0 0 21	1682.91368	-0.00071	2140.75802	457.84362
2 2 1 -1 21	0 0 0 0 22	1681.17487	0.00023	2182.59718	501.42254
2 2 1 -1 22	0 0 0 0 23	1679.45197	-0.00028	2226.42988	546.97764
2 2 1 -1 23	0 0 0 0 24	1677.74786	0.00014	2272.25599	594.50827
2 2 1 -1 24	0 0 0 0 25	1676.06127	-0.00024	2320.07531	644.01380
2 2 1 -1 25	0 0 0 0 26	1674.39307	-0.00094	2369.88754	695.49354
2 2 1 -1 26	0 0 0 0 27	1672.74407	-0.00146	2421.69231	748.94678W
2 2 1 -1 27	0 0 0 0 28	1671.11567	-0.00068	2475.48915	804.37280
2 2 1 -1 28	0 0 0 0 29	1669.51077	0.00410	2531.27750	861.77083W
2 2 1 -1 1	0 0 0 0 0	1724.46368	0.00111	1724.46257	0.00000W
2 2 1 -1 2	0 0 0 0 1	1726.45980	-0.00229	1728.44514	1.98305W
2 2 1 -1 3	0 0 0 0 2	1728.47043	0.00051	1734.41904	5.94912
2 2 1 -1 4	0 0 0 0 3	1730.48592	-0.00025	1742.38433	11.89816
2 2 1 -1 5	0 0 0 0 4	1732.51063	-0.00034	1752.34107	19.83009
2 2 1 -1 6	0 0 0 0 5	1734.54450	-0.00004	1764.28934	29.74480
2 2 1 -1 7	0 0 0 0 6	1736.58746	0.00035	1778.22926	41.64214
2 2 1 -1 8	0 0 0 0 7	1738.63901	0.00004	1794.16094	55.52197
2 2 1 -1 9	0 0 0 0 8	1740.70025	-0.00019	1812.08452	71.38408
2 2 1 -1 10	0 0 0 0 9	1742.77188	-0.00001	1832.00016	89.22827
2 2 1 -1 11	0 0 0 0 10	1744.85394	0.00019	1853.90802	109.05428
2 2 1 -1 12	0 0 0 0 11	1746.94630	-0.00014	1877.80829	130.86184
2 2 1 -1 13	0 0 0 0 12	1749.05065	0.00018	1903.70113	154.65066
2 2 1 -1 14	0 0 0 0 13	1751.16614	-0.00020	1931.58675	180.42041
2 2 1 -1 15	0 0 0 0 14	1753.29446	-0.00014	1961.46532	208.17072
2 2 1 -1 16	0 0 0 0 15	1755.43585	0.00005	1993.33703	237.90124
2 2 1 -1 17	0 0 0 0 16	1757.59087	0.00036	2027.20204	269.61154
2 2 1 -1 18	0 0 0 0 17	1759.75925	-0.00005	2063.06048	303.30118
2 2 1 -1 19	0 0 0 0 18	1761.94229	-0.00044	2100.91245	338.96972
2 2 1 -1 20	0 0 0 0 19	1764.14111	-0.00025	2140.75802	376.61665
2 2 1 -1 21	0 0 0 0 20	1766.35603	0.00032	2182.59718	416.24147
2 2 1 -1 22	0 0 0 0 21	1768.58640	0.00014	2226.42988	457.84362
2 2 1 -1 23	0 0 0 0 22	1770.83360	0.00015	2272.25599	501.42254
2 2 1 -1 24	0 0 0 0 23	1773.08900	0.00015	2320.07531	546.97764

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2	-2	1	1	1	0	0	0	0	1	1722.48808	-0.00068	1724.47181	1.98305
2	-2	1	1	2	0	0	0	0	2	1722.52377	0.00001	1728.47288	5.94912
2	-2	1	1	3	0	0	0	0	3	1722.57613	-0.00023	1734.47452	11.89816
2	-2	1	1	4	0	0	0	0	4	1722.64670	-0.00001	1742.47680	19.83009
2	-2	1	1	5	0	0	0	0	5	1722.73495	-0.00004	1752.47978	29.74480
2	-2	1	1	6	0	0	0	0	6	1722.84144	0.00001	1764.48357	41.64214
2	-2	1	1	7	0	0	0	0	7	1722.96620	-0.00010	1778.48827	55.52197
2	-2	1	1	8	0	0	0	0	8	1723.10995	0.00003	1794.49400	71.38408
2	-2	1	1	9	0	0	0	0	9	1723.27250	-0.00014	1812.50091	89.22827
2	-2	1	1	10	0	0	0	0	10	1723.45485	-0.00002	1832.50915	109.05428
2	-2	1	1	11	0	0	0	0	11	1723.65672	-0.00031	1854.51888	130.86184
2	-2	1	1	12	0	0	0	0	12	1723.87957	-0.00004	1878.53027	154.65066
2	-2	1	1	13	0	0	0	0	13	1724.12303	-0.00006	1904.54349	180.42041
2	-2	1	1	14	0	0	0	0	14	1724.38784	-0.00015	1932.55872	208.17072
2	-2	1	1	15	0	0	0	0	15	1724.67475	-0.00012	1962.57611	237.90124
2	-2	1	1	16	0	0	0	0	16	1724.98441	0.00013	1994.59581	269.61154
2	-2	1	1	17	0	0	0	0	17	1725.31680	0.00004	2028.61794	303.30118
2	-2	1	1	18	0	0	0	0	18	1725.67307	0.00020	2064.64259	338.96972
2	-2	1	1	19	0	0	0	0	19	1726.05306	-0.00009	2102.66980	376.61665
2	-2	1	1	20	0	0	0	0	20	1726.45980	0.00169	2142.69958	416.24147W
2	-2	1	1	21	0	0	0	0	21	1726.88769	-0.00056	2184.73187	457.84362
2	-2	1	1	22	0	0	0	0	22	1727.34297	-0.00103	2228.76654	501.42254W
2	-2	1	1	23	0	0	0	0	23	1727.82538	-0.00039	2274.80341	546.97764
2	-2	1	1	24	0	0	0	0	24	1728.33310	-0.00082	2322.84219	594.50827

rms = 0.00034 cm⁻¹ $v_4 + 2v_5 (^1\Pi) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 2 2 21	0 0 0 0 22	1841.11210	-0.00036	2342.53501	501.42254
1 -1 2 2 20	0 0 0 0 21	1842.86230	-0.00072	2300.70664	457.84362
1 -1 2 2 19	0 0 0 0 20	1844.62848	0.00002	2260.86993	416.24147
1 -1 2 2 18	0 0 0 0 19	1846.40833	-0.00006	2223.02504	376.61665
1 -1 2 2 17	0 0 0 0 18	1848.20244	0.00007	2187.17209	338.96972
1 -1 2 2 16	0 0 0 0 17	1850.00913	-0.00084	2153.31116	303.30118
1 -1 2 2 15	0 0 0 0 16	1851.83041	-0.00033	2121.44228	269.61154
1 -1 2 2 14	0 0 0 0 15	1853.66406	-0.00017	2091.56547	237.90124
1 -1 2 2 13	0 0 0 0 14	1855.50979	-0.00022	2063.68073	208.17072
1 -1 2 2 12	0 0 0 0 13	1857.36686	-0.00077	2037.78803	180.42041
1 -1 2 2 11	0 0 0 0 12	1859.23656	-0.00012	2013.88734	154.65066
1 -1 2 2 10	0 0 0 0 11	1861.11678	0.00001	1991.97861	130.86184
1 -1 2 2 9	0 0 0 0 10	1863.00746	-0.00005	1972.06179	109.05428
1 -1 2 2 8	0 0 0 0 9	1864.90879	0.00023	1954.13683	89.22827
1 -1 2 2 7	0 0 0 0 8	1866.81952	-0.00008	1938.20368	71.38408
1 -1 2 2 6	0 0 0 0 7	1868.74093	0.00061	1924.26229	55.52197
1 -1 2 2 5	0 0 0 0 6	1870.67011	-0.00036	1912.31262	41.64214
1 -1 2 2 4	0 0 0 0 5	1872.60930	-0.00052	1902.35462	29.74480
1 -1 2 2 3	0 0 0 0 4	1874.55780	-0.00037	1894.38827	19.83009
1 -1 2 2 2	0 0 0 0 3	1876.51460	-0.00076	1888.41352	11.89816
1 -1 2 2 1	0 0 0 0 2	1878.48100	-0.00025	1884.43037	5.94912
1 -1 2 2 1	0 0 0 0 0	1884.43075	0.00038	1884.43037	0.00000
1 -1 2 2 2	0 0 0 0 1	1886.43075	0.00028	1888.41352	1.98305
1 -1 2 2 3	0 0 0 0 2	1888.43967	0.00053	1894.38827	5.94912
1 -1 2 2 4	0 0 0 0 3	1890.45562	-0.00084	1902.35462	11.89816
1 -1 2 2 5	0 0 0 0 4	1892.48245	-0.00008	1912.31262	19.83009
1 -1 2 2 6	0 0 0 0 5	1894.51763	0.00014	1924.26229	29.74480
1 -1 2 2 7	0 0 0 0 6	1896.56153	-0.00001	1938.20368	41.64214
1 -1 2 2 8	0 0 0 0 7	1898.61495	0.00009	1954.13683	55.52197
1 -1 2 2 9	0 0 0 0 8	1900.67667*	-0.00103	1972.06179	71.38408W
1 -1 2 2 10	0 0 0 0 9	1902.75037	0.00003	1991.97861	89.22827
1 -1 2 2 11	0 0 0 0 10	1904.83274	-0.00032	2013.88734	109.05428
1 -1 2 2 12	0 0 0 0 11	1906.92613	-0.00006	2037.78803	130.86184
1 -1 2 2 13	0 0 0 0 12	1909.02998	-0.00009	2063.68073	154.65066
1 -1 2 2 14	0 0 0 0 13	1911.14485	-0.00022	2091.56547	180.42041
1 -1 2 2 15	0 0 0 0 14	1913.27072	-0.00082	2121.44228	208.17072

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1	1	-1	2	2	16	0	0	0	0	15	1915.40976	-0.00016	2153.31116	237.90124
2	1	-1	2	2	17	0	0	0	0	16	1917.55731*	-0.00325	2187.17209	269.61154W
3	1	-1	2	2	18	0	0	0	0	17	1919.72355	-0.00031	2223.02504	303.30118
4	1	-1	2	2	19	0	0	0	0	18	1921.90017	-0.00004	2260.86993	338.96972
5	1	-1	2	2	20	0	0	0	0	19	1924.08987	-0.00012	2300.70664	376.61665
6	1	-1	2	2	21	0	0	0	0	20	1926.29340	-0.00014	2342.53501	416.24147
7	1	-1	2	2	22	0	0	0	0	21	1928.51124	0.00004	2386.35482	457.84362
8	1	-1	2	2	23	0	0	0	0	22	1930.74340	0.00013	2432.16581	501.42254
9	1	-1	2	2	24	0	0	0	0	23	1932.98990	-0.00011	2479.96765	546.97764
10	1	-1	2	2	25	0	0	0	0	24	1935.25030	-0.00136	2529.75993	594.50827W
11	1	-1	2	2	26	0	0	0	0	25	1937.52770	-0.00071	2581.54220	644.01380
12	1	-1	2	2	27	0	0	0	0	26	1939.81960	-0.00080	2635.31393	695.49354
13	1	1	2	-2	4	0	0	0	0	4	1882.55809	0.00021	1902.38797	19.83009
14	1	1	2	-2	5	0	0	0	0	5	1882.61866	0.00081	1912.36265	29.74480
15	1	1	2	-2	6	0	0	0	0	6	1882.69037	0.00017	1924.33235	41.64214
16	1	1	2	-2	7	0	0	0	0	7	1882.77529	0.00015	1938.29711	55.52197
17	1	1	2	-2	8	0	0	0	0	8	1882.87303	0.00012	1954.25700	71.38408
18	1	1	2	-2	9	0	0	0	0	9	1882.98410	0.00030	1972.21207	89.22827
19	1	1	2	-2	10	0	0	0	0	10	1883.10805	-0.00008	1992.16240	109.05428
20	1	1	2	-2	11	0	0	0	0	11	1883.24639	0.00016	2014.10807	130.86184
21	1	1	2	-2	12	0	0	0	0	12	1883.39860	0.00010	2038.04916	154.65066
22	1	1	2	-2	13	0	0	0	0	13	1883.56533	-0.00002	2063.98575	180.42041
23	1	1	2	-2	14	0	0	0	0	14	1883.74724	0.00002	2091.91795	208.17072
24	1	1	2	-2	15	0	0	0	0	15	1883.94472	0.00012	2121.84584	237.90124
25	1	1	2	-2	16	0	0	0	0	16	1884.15814	0.00017	2153.76950	269.61154
26	1	1	2	-2	17	0	0	0	0	17	1884.38774	-0.00011	2187.68903	303.30118
27	1	1	2	-2	18	0	0	0	0	18	1884.63478	0.00001	2223.60449	338.96972
28	1	1	2	-2	19	0	0	0	0	19	1884.90192*	0.00265	2261.51593	376.61665W
29	1	1	2	-2	20	0	0	0	0	20	1885.18189	-0.00002	2301.42338	416.24147
30	1	1	2	-2	21	0	0	0	0	21	1885.48328	0.00007	2343.32683	457.84362
31	1	1	2	-2	22	0	0	0	0	22	1885.80365	-0.00007	2387.22627	501.42254
32	1	1	2	-2	23	0	0	0	0	23	1886.13745*	-0.00651	2433.12160	546.97764W
33	1	1	2	-2	24	0	0	0	0	24	1886.50429	-0.00015	2481.01271	594.50827
34	1	1	2	-2	25	0	0	0	0	25	1886.88587	0.00024	2530.89942	644.01380
35	1	1	2	-2	26	0	0	0	0	26	1887.28773	-0.00025	2582.78151	695.49354
36	1	1	2	-2	27	0	0	0	0	27	1887.71250	0.00059	2636.65870	748.94678
37	1	1	2	-2	28	0	0	0	0	28	1888.15740	-0.00041	2692.53061	804.37280
38	1	1	2	-2	29	0	0	0	0	29	1888.62600	-0.00002	2750.39685	861.77083
39	1	1	2	-2	30	0	0	0	0	30	1889.11630	-0.00054	2810.25693	921.14009

rms = 0.00035 cm⁻¹

3v₅ (Π) ← G.S. (Σ⁺)

	$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
46	0 0 3 1 1	0 0 0 0 2	2006.25984	0.00018	2012.20878	5.94912
47	0 0 3 1 2	0 0 0 0 3	2004.28082	0.00047	2016.17851	11.89816
48	0 0 3 1 3	0 0 0 0 4	2002.30291	-0.00001	2022.13301	19.83009
49	0 0 3 1 4	0 0 0 0 5	2000.32738	-0.00001	2030.07218	29.74480
50	0 0 3 1 5	0 0 0 0 6	1998.35393	0.00019	2039.99589	41.64214
51	0 0 3 1 6	0 0 0 0 7	1996.38185	-0.00013	2051.90395	55.52197
52	0 0 3 1 7	0 0 0 0 8	1994.41200	-0.00008	2065.79617	71.38408
53	0 0 3 1 8	0 0 0 0 9	1992.44426	0.00024	2081.67229	89.22827
54	0 0 3 1 9	0 0 0 0 10	1990.47762	-0.00014	2099.53204	109.05428
55	0 0 3 1 10	0 0 0 0 11	1988.51340	0.00013	2119.37511	130.86184
56	0 0 3 1 11	0 0 0 0 12	1986.55041	-0.00009	2141.20116	154.65066
57	0 0 3 1 12	0 0 0 0 13	1984.58953	0.00013	2165.00981	180.42041
58	0 0 3 1 13	0 0 0 0 14	1982.63003	0.00012	2190.80064	208.17072
59	0 0 3 1 14	0 0 0 0 15	1980.67206	0.00009	2218.57321	237.90124
60	0 0 3 1 15	0 0 0 0 16	1978.71537	-0.00014	2248.32704	269.61154
	0 0 3 1 16	0 0 0 0 17	1976.76067	0.00023	2280.06163	303.30118
	0 0 3 1 17	0 0 0 0 18	1974.80663	-0.00007	2313.77642	338.96972
	0 0 3 1 18	0 0 0 0 19	1972.85409	-0.00010	2349.47084	376.61665
	0 0 3 1 19	0 0 0 0 20	1970.90296	0.00014	2387.14429	416.24147
	0 0 3 1 20	0 0 0 0 21	1968.95246	-0.00004	2426.79612	457.84362
	0 0 3 1 21	0 0 0 0 22	1967.00196	-0.00004	2466.42567	501.42254

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0	0	3	-1	29	0	0	0	0	29	2017.02500	0.00004	2878.79579	861.77083
0	0	3	-1	30	0	0	0	0	30	2017.47020	0.00014	2938.61015	921.14009
0	0	3	-1	31	0	0	0	0	31	2017.92667	0.00020	3000.40622	982.47976
0	0	3	-1	32	0	0	0	0	32	2018.39453	0.00076	3064.18276	1045.78899
0	0	3	-1	33	0	0	0	0	33	2018.87110	-0.00044	3129.93847	1111.06693
0	0	3	-1	34	0	0	0	0	34	2019.37160	0.01227	3197.67199	1178.31267

rms = 0.00025 cm⁻¹

$$v_5(\text{II}) \leftarrow v_4(\text{II})$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	1 1 0 0 2	155.45724	0.00001	679.79005	524.33282
0 0 1 1 2	1 1 0 0 3	153.47038	-0.00012	683.75462	530.28412
0 0 1 1 3	1 1 0 0 4	151.48231	-0.00003	689.70140	538.21906
0 0 1 1 4	1 1 0 0 5	149.49279	0.00000	697.63032	548.13753
0 0 1 1 5	1 1 0 0 6	147.50187	-0.00001	707.54126	560.03938
0 0 1 1 6	1 1 0 0 7	145.50962	0.00000	719.43409	573.92447
0 0 1 1 7	1 1 0 0 8	143.51605	-0.00001	733.30864	589.79258
0 0 1 1 8	1 1 0 0 9	141.52121	-0.00001	749.16472	607.64350
0 0 1 1 9	1 1 0 0 10	139.52512	-0.00002	767.00212	627.47699
0 0 1 1 10	1 1 0 0 11	137.52783	-0.00001	786.82059	649.29275
0 0 1 1 11	1 1 0 0 12	135.52934	0.00000	808.61985	673.09051
0 0 1 1 12	1 1 0 0 13	133.52969	-0.00001	832.39961	698.86991
0 0 1 1 13	1 1 0 0 14	131.52893	-0.00001	858.15954	726.63060
0 0 1 1 14	1 1 0 0 15	129.52705	-0.00002	885.89928	756.37220
0 0 1 1 15	1 1 0 0 16	127.52411	-0.00004	915.61845	788.09430
0 0 1 1 16	1 1 0 0 17	125.52018	-0.00003	947.31664	821.79644
0 0 1 1 17	1 1 0 0 18	123.51521	-0.00004	980.99342	857.47816
0 0 1 1 18	1 1 0 0 19	121.50933	-0.00002	1016.64832	895.13897
0 0 1 1 19	1 1 0 0 20	119.50248	-0.00002	1054.28084	934.77834
0 0 1 1 20	1 1 0 0 21	117.49487	0.00011	1093.89049	976.39572
0 0 1 1 21	1 1 0 0 22	115.48617	0.00001	1135.47669	1019.99053
0 0 1 1 22	1 1 0 0 23	113.47672	-0.00001	1179.03889	1065.56217
0 0 1 1 23	1 1 0 0 24	111.46645	-0.00004	1224.57649	1113.10999
0 0 1 1 24	1 1 0 0 25	109.45552	0.00001	1272.08885	1162.63334
0 0 1 1 25	1 1 0 0 26	107.44379	0.00001	1321.57533	1214.13154
0 0 1 1 26	1 1 0 0 27	105.43131	-0.00007	1373.03523	1267.60385
0 0 1 1 27	1 1 0 0 28	103.41833	0.00002	1426.46786	1323.04955
0 0 1 1 28	1 1 0 0 29	101.40464	0.00001	1481.87248	1380.46786
0 0 1 1 29	1 1 0 0 30	99.39024	-0.00011	1539.24832	1439.85797
0 0 1 1 30	1 1 0 0 31	97.37556	0.00003	1598.59460	1501.21907
0 0 1 1 31	1 1 0 0 32	95.36017	-0.00003	1659.91050	1564.55030
0 0 1 1 32	1 1 0 0 33	93.34419	-0.00020	1723.19517	1629.85078
0 0 1 1 2	1 1 0 0 1	163.38939	0.00001	683.75462	520.36524
0 0 1 1 3	1 1 0 0 2	165.36862	0.00003	689.70140	524.33282
0 0 1 1 4	1 1 0 0 3	167.34621	0.00001	697.63032	530.28412
0 0 1 1 5	1 1 0 0 4	169.32223	0.00003	707.54126	538.21906
0 0 1 1 6	1 1 0 0 5	171.29658	0.00002	719.43409	548.13753
0 0 1 1 7	1 1 0 0 6	173.26932	0.00007	733.30864	560.03938
0 0 1 1 8	1 1 0 0 7	175.24028	0.00002	749.16472	573.92447
0 0 1 1 9	1 1 0 0 8	177.20958	0.00004	767.00212	589.79258
0 0 1 1 10	1 1 0 0 9	179.17711	0.00002	786.82059	607.64350
0 0 1 1 11	1 1 0 0 10	181.14291	0.00005	808.61985	627.47699
0 0 1 1 12	1 1 0 0 11	183.10689	0.00003	832.39961	649.29275
0 0 1 1 13	1 1 0 0 12	185.06906	0.00002	858.15954	673.09051
0 0 1 1 14	1 1 0 0 13	187.02940	0.00003	885.89928	698.86991
0 0 1 1 15	1 1 0 0 14	188.98787	0.00003	915.61845	726.63060
0 0 1 1 16	1 1 0 0 15	190.94447	0.00003	947.31664	756.37220
0 0 1 1 17	1 1 0 0 16	192.89914	0.00002	980.99342	788.09430
0 0 1 1 18	1 1 0 0 17	194.85191	0.00003	1016.64832	821.79644
0 0 1 1 19	1 1 0 0 18	196.80272	0.00004	1054.28084	857.47816
0 0 1 1 20	1 1 0 0 19	198.75155	0.00003	1093.89049	895.13897
0 0 1 1 21	1 1 0 0 20	200.69838	0.00003	1135.47669	934.77834
0 0 1 1 22	1 1 0 0 21	202.64342	0.00025	1179.03889	976.39572
0 0 1 1 23	1 1 0 0 22	204.57649	0.00025	1224.57649	1019.99053

1	0	0	1	-1	14	1	-1	0	0	13	186.96238	0.00001	886.63880	699.67642
2	0	0	1	-1	15	1	-1	0	0	14	188.90247	-0.00001	916.46345	727.56097
3	0	0	1	-1	16	1	-1	0	0	15	190.83892	0.00000	948.27412	757.43520
4	0	0	1	-1	17	1	-1	0	0	16	192.77165	-0.00001	982.07035	789.29869
5	0	0	1	-1	18	1	-1	0	0	17	194.70068	-0.00001	1017.85167	823.15099
6	0	0	1	-1	19	1	-1	0	0	18	196.62599	0.00000	1055.61759	858.99160
7	0	0	1	-1	20	1	-1	0	0	19	198.54756	0.00001	1095.36757	896.82001
8	0	0	1	-1	21	1	-1	0	0	20	200.46537	0.00001	1137.10105	936.63569
9	0	0	1	-1	22	1	-1	0	0	21	202.37949	0.00009	1180.81746	978.43806
10	0	0	1	-1	23	1	-1	0	0	22	204.28965	-0.00001	1226.51618	1022.22652
11	0	0	1	-1	24	1	-1	0	0	23	206.19613	0.00001	1274.19657	1068.00045
12	0	0	1	-1	25	1	-1	0	0	24	208.09884	0.00007	1323.85797	1115.75919
13	0	0	1	-1	26	1	-1	0	0	25	209.99761	0.00000	1375.49968	1165.50207
14	0	0	1	-1	27	1	-1	0	0	26	211.89264	0.00002	1429.12098	1217.22835
15	0	0	1	-1	28	1	-1	0	0	27	213.78381	0.00002	1484.72111	1270.93732
16	0	0	1	-1	29	1	-1	0	0	28	215.67115	0.00003	1542.29931	1326.62819
17	0	0	1	-1	30	1	-1	0	0	29	217.55463	0.00004	1601.85477	1384.30018
18	0	0	1	-1	31	1	-1	0	0	30	219.43420	0.00000	1663.38664	1443.95245
19	0	0	1	-1	32	1	-1	0	0	31	221.30998	0.00005	1726.89408	1505.58415
20	0	0	1	-1	33	1	-1	0	0	32	223.18184	0.00005	1792.37620	1569.19441
21	0	0	1	-1	34	1	-1	0	0	33	225.04980	0.00003	1859.83208	1634.78230
22	0	0	1	-1	35	1	-1	0	0	34	226.91391	0.00004	1929.26077	1702.34690
23	0	0	1	-1	36	1	-1	0	0	35	228.77397	-0.00011	2000.66131	1771.88724
24	0	0	1	-1	1	1	1	0	0	1	159.43188	0.00002	679.79710	520.36524
25	0	0	1	-1	2	1	1	0	0	2	159.44297	0.00001	683.77578	524.33282
26	0	0	1	-1	3	1	1	0	0	3	159.45962	0.00002	689.74371	530.28412
27	0	0	1	-1	4	1	1	0	0	4	159.48181	0.00003	697.70083	538.21906
28	0	0	1	-1	5	1	1	0	0	5	159.50950	0.00000	707.64702	548.13753
29	0	0	1	-1	6	1	1	0	0	6	159.54246*	-0.00030	719.58215	560.03938W
30	0	0	1	-1	7	1	1	0	0	7	159.58161	0.00004	733.50603	573.92447
31	0	0	1	-1	8	1	1	0	0	8	159.62588	-0.00003	749.41849	589.79258
32	0	0	1	-1	9	1	1	0	0	9	159.67575	-0.00005	767.31930	607.64350
33	0	0	1	-1	10	1	1	0	0	10	159.73350*	0.00228	787.20820	627.47699W
34	0	0	1	-1	11	1	1	0	0	11	159.79210	-0.00007	809.08492	649.29275
35	0	0	1	-1	12	1	1	0	0	12	159.85875	0.00010	832.94916	673.09051
36	0	0	1	-1	13	1	1	0	0	13	159.93055	-0.00011	858.80057	698.86991

rms = 0.000052 cm⁻¹

$$2\nu_5(\Sigma^+) \leftarrow \nu_4 + \nu_5(\Sigma^+)$$

	ν_4'	l_4'	ν_5'	l_5'	J'	ν_4''	l_4''	ν_5''	l_5''	J''	OBS	OBS - CALC	E'	E''
43	0	0	2	0	0	1	1	1	-1	1	139.73733	-0.00012	1342.22645	1202.48900
44	0	0	2	0	1	1	1	1	-1	2	137.74484	0.00007	1344.21562	1206.47085
45	0	0	2	0	2	1	1	1	-1	3	135.75008	-0.00007	1348.19391	1212.44377
46	0	0	2	0	3	1	1	1	-1	4	133.75337	0.00004	1354.16122	1220.40789
47	0	0	2	0	4	1	1	1	-1	5	131.75405	0.00006	1362.11743	1230.36343
48	0	0	2	0	5	1	1	1	-1	6	129.75175	0.00006	1372.06234	1242.31065
49	0	0	2	0	6	1	1	1	-1	7	127.74591	0.00003	1383.99572	1256.24984
50	0	0	2	0	7	1	1	1	-1	8	125.73588	-0.00005	1397.91730	1272.18137
51	0	0	2	0	8	1	1	1	-1	9	123.72110	-0.00004	1413.82675	1290.10561
52	0	0	2	0	9	1	1	1	-1	10	121.70082	0.00010	1431.72370	1310.02298
53	0	0	2	0	10	1	1	1	-1	11	119.67390	0.00009	1451.60774	1331.93393
54	0	0	2	0	11	1	1	1	-1	12	117.63954	0.00004	1473.47840	1355.83891
55	0	0	2	0	12	1	1	1	-1	13	115.59692	0.00009	1497.33518	1381.73835
56	0	0	2	0	13	1	1	1	-1	14	113.54488	0.00003	1523.17752	1409.63267
57	0	0	2	0	14	1	1	1	-1	15	111.48257	0.00000	1551.00481	1439.52224
58	0	0	2	0	15	1	1	1	-1	16	109.40918	0.00012	1580.81643	1471.40738
59	0	0	2	0	16	1	1	1	-1	17	107.32352	0.00013	1612.61167	1505.28829
60	0	0	2	0	17	1	1	1	-1	18	105.22480	0.00009	1646.38981	1541.16510
	0	0	2	0	18	1	1	1	-1	19	103.11213	-0.00011	1682.15007	1579.03782
	0	0	2	0	19	1	1	1	-1	20	100.98541	0.00014	1719.89163	1618.90635
	0	0	2	0	2	1	1	1	-1	1	145.70499	0.00008	1348.19391	1202.48900
	0	0	2	0	3	1	1	1	-1	2	147.69037	0.00000	1354.16122	1206.47085
	0	0	2	0	4	1	1	1	-1	3	149.67365	-0.00002	1362.11743	1212.44377
	0	0	2	0	5	1	1	1	-1	4	151.65693	0.00003	1372.06234	1220.40789

0	0	2	0	6	1	1	1	-1	5	153.63227	-0.00002	1383.99572	1230.36343
0	0	2	0	7	1	1	1	-1	6	155.60667	0.00002	1397.91730	1242.31065
0	0	2	0	8	1	1	1	-1	7	157.57710	0.00019	1413.82675	1256.24984
0	0	2	0	9	1	1	1	-1	8	159.54246	0.00013	1431.72370	1272.18137
0	0	2	0	10	1	1	1	-1	9	161.50216	0.00003	1451.60774	1290.10561
0	0	2	0	11	1	1	1	-1	10	163.45547	0.00005	1473.47840	1310.02298
0	0	2	0	12	1	1	1	-1	11	165.40128	0.00004	1497.33518	1331.93393
0	0	2	0	13	1	1	1	-1	12	167.33865	0.00004	1523.17752	1355.83891
0	0	2	0	14	1	1	1	-1	13	169.26657	0.00010	1551.00481	1381.73835
0	0	2	0	15	1	1	1	-1	14	171.18382	0.00006	1580.81643	1409.63267
0	0	2	0	16	1	1	1	-1	15	173.08947	0.00004	1612.61167	1439.52224
0	0	2	0	17	1	1	1	-1	16	174.98248	0.00005	1646.38981	1471.40738
0	0	2	0	18	1	1	1	-1	17	176.86188	0.00010	1682.15007	1505.28829
0	0	2	0	19	1	1	1	-1	18	178.72659	0.00007	1719.89163	1541.16510
0	0	2	0	20	1	1	1	-1	19	180.57581	0.00001	1759.61363	1579.03782
0	0	2	0	21	1	1	1	-1	20	182.40894	0.00012	1801.31517	1618.90635
0	0	2	0	22	1	1	1	-1	21	184.22491	0.00005	1844.99532	1660.77045
0	0	2	0	23	1	1	1	-1	22	186.02337	0.00005	1890.65309	1704.62977
0	0	2	0	24	1	1	1	-1	23	187.80370	0.00003	1938.28750	1750.48383
0	0	2	0	25	1	1	1	-1	24	189.56557	0.00015	1987.89749	1798.33206
0	0	2	0	26	1	1	1	-1	25	191.30822	0.00002	2039.48198	1848.17378
0	0	2	0	27	1	1	1	-1	26	193.03168	0.00002	2093.03990	1900.00824
0	0	2	0	28	1	1	1	-1	27	194.73527	-0.00022	2148.57010	1953.83461
0	0	2	0	29	1	1	1	-1	28	196.41921	-0.00025	2206.07144	2009.65198
0	0	2	0	30	1	1	1	-1	29	198.08326	-0.00008	2265.54275	2067.45942

rms = 0.000090 cm⁻¹

$2\nu_5(\Delta) \leftarrow \nu_4 + \nu_5(\Delta)$

ν_4'	ν_4''	ν_5'	ν_5''	J'	J''	OBS	OBS - CALC	E'	E''				
0	0	2	2	3	1	1	1	1	2	169.25597	0.00001	1370.97815	1201.72219
0	0	2	2	4	1	1	1	1	3	171.23605	-0.00011	1378.93084	1207.69469
0	0	2	2	5	1	1	1	1	4	173.21418	0.00005	1388.87163	1215.65751
0	0	2	2	6	1	1	1	1	5	175.19031	0.00005	1400.80048	1225.61022
0	0	2	2	7	1	1	1	1	6	177.16511	0.00008	1414.71732	1237.55228
0	0	2	2	8	1	1	1	1	7	179.13919	0.00016	1430.62208	1251.48305
0	0	2	2	9	1	1	1	1	8	181.11301	0.00008	1448.51470	1267.40177
0	0	2	2	10	1	1	1	1	9	183.08746	-0.00001	1468.39508	1285.30761
0	0	2	2	11	1	1	1	1	10	185.06350	0.00001	1490.26312	1305.19963
0	0	2	2	12	1	1	1	1	11	187.04192	0.00002	1514.11873	1327.07683
0	0	2	2	13	1	1	1	1	12	189.02368	0.00003	1539.96178	1350.93813
0	0	2	2	14	1	1	1	1	13	191.00976	0.00002	1567.79214	1376.78240
0	0	2	2	15	1	1	1	1	14	193.00120	0.00001	1597.60969	1404.60850
0	0	2	2	16	1	1	1	1	15	194.99900	0.00000	1629.41426	1434.41526
0	0	2	2	17	1	1	1	1	16	197.00420	0.00000	1663.20571	1466.20152
0	0	2	2	18	1	1	1	1	17	199.01767	-0.00004	1698.98385	1499.96614
0	0	2	2	19	1	1	1	1	18	201.04039	-0.00007	1736.74850	1535.70804
0	0	2	2	20	1	1	1	1	19	203.07319	-0.00007	1776.49946	1573.42620
0	0	2	2	21	1	1	1	1	20	205.11697	0.00009	1818.23651	1613.11962
0	0	2	2	22	1	1	1	1	21	207.17197	-0.00001	1861.95941	1654.78743
0	0	2	2	23	1	1	1	1	22	209.23917	0.00002	1907.66792	1698.42877
0	0	2	2	24	1	1	1	1	23	211.31888	0.00000	1955.36175	1744.04287
0	0	2	2	25	1	1	1	1	24	213.41158	-0.00003	2005.04061	1791.62900
0	0	2	2	26	1	1	1	1	25	215.51779	0.00009	2056.70417	1841.18647
0	0	2	2	27	1	1	1	1	26	217.63748	0.00001	2110.35209	1892.71462
0	0	2	2	28	1	1	1	1	27	219.77137	0.00019	2165.98399	1946.21281
0	0	2	2	29	1	1	1	1	28	221.91921	0.00018	2223.59944	2001.68041
0	0	2	2	30	1	1	1	1	29	224.08137	0.00013	2283.19801	2059.11678
0	0	2	2	2	1	1	1	1	3	157.31885	-0.00006	1365.01359	1207.69469
0	0	2	2	3	1	1	1	1	4	155.32064	0.00000	1370.97815	1215.65751
0	0	2	2	4	1	1	1	1	5	153.32068	0.00006	1378.93084	1225.61022
0	0	2	2	5	1	1	1	1	6	151.31925	-0.00010	1388.87163	1237.55228
0	0	2	2	6	1	1	1	1	7	149.31748	0.00005	1400.80048	1251.48305
0	0	2	2	7	1	1	1	1	8	147.31559	0.00005	1414.71732	1267.40177
0	0	2	2	8	1	1	1	1	9	145.31372	0.00005	1430.62208	1285.30761

0	0	2	-2	15	1	-1	1	-1	16	131.16353	-0.00003	1597.56645	1466.40289
0	0	2	-2	16	1	-1	1	-1	17	129.14014	-0.00007	1629.35868	1500.21846
0	0	2	-2	17	1	-1	1	-1	18	127.11570	-0.00009	1663.13533	1536.01954
0	0	2	-2	18	1	-1	1	-1	19	125.09025	-0.00010	1698.89591	1573.80556
0	0	2	-2	19	1	-1	1	-1	20	123.06383	-0.00013	1736.63994	1613.57597
0	0	2	-2	20	1	-1	1	-1	21	121.03631	-0.00037	1776.36688	1655.33020
0	0	2	-2	21	1	-1	1	-1	22	119.00860	0.00007	1818.07617	1699.06765
0	0	2	-2	22	1	-1	1	-1	23	116.97951	-0.00004	1861.76724	1744.78769
0	0	2	-2	23	1	-1	1	-1	24	114.94969	-0.00008	1907.43947	1792.48970
0	0	2	-2	2	1	1	1	1	2	163.29139	0.00000	1365.01357	1201.72219
0	0	2	-2	3	1	1	1	1	3	163.28333	-0.00004	1370.97805	1207.69469
0	0	2	-2	4	1	1	1	1	4	163.27289	-0.00017	1378.93057	1215.65751
0	0	2	-2	5	1	1	1	1	5	163.26071	-0.00007	1388.87100	1225.61022
0	0	2	-2	6	1	1	1	1	6	163.24675	-0.00018	1400.79921	1237.55228
0	0	2	-2	7	1	1	1	1	7	163.23219	0.00021	1414.71503	1251.48305
0	0	2	-2	8	1	1	1	1	8	163.21652	0.00002	1430.61827	1267.40177
0	0	2	-2	9	1	1	1	1	9	163.20159*	0.00049	1448.50870	1285.30761
0	0	2	-2	10	1	1	1	1	10	163.18586*	-0.00060	1468.38608	1305.19963W
0	0	2	-2	11	1	1	1	1	11	163.17306	-0.00025	1490.25013	1327.07683
0	0	2	-2	12	1	1	1	1	12	163.16206	-0.00035	1514.10054	1350.93813

rms = 0.00013 cm⁻¹

$$v_4 + v_5 (\Sigma^+) \leftarrow 2v_4 (\Sigma^+)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	2 0 0 0 1	164.56916	0.00023	1200.49810	1035.92917
1 1 1 -1 1	2 0 0 0 2	162.57244	0.00022	1202.48900	1039.91679
1 1 1 -1 2	2 0 0 0 3	160.57314	0.00018	1206.47085	1045.89789
1 1 1 -1 3	2 0 0 0 4	158.57178	0.00011	1212.44377	1053.87209
1 1 1 -1 4	2 0 0 0 5	156.56914	0.00013	1220.40789	1063.83887
1 1 1 -1 5	2 0 0 0 6	154.56590	0.00006	1230.36343	1075.79759
1 1 1 -1 6	2 0 0 0 7	152.56325	0.00007	1242.31065	1089.74746
1 1 1 -1 7	2 0 0 0 8	150.56219	-0.00004	1256.24984	1105.68761
1 1 1 -1 8	2 0 0 0 9	148.56437	0.00002	1272.18137	1123.61701
1 1 1 -1 9	2 0 0 0 10	146.57100	-0.00004	1290.10561	1143.53456
1 1 1 -1 10	2 0 0 0 11	144.58388	-0.00003	1310.02298	1165.43907
1 1 1 -1 11	2 0 0 0 12	142.60461	-0.00007	1331.93393	1189.32925
1 1 1 -1 12	2 0 0 0 13	140.63508	-0.00003	1355.83891	1215.20380
1 1 1 -1 13	2 0 0 0 14	138.67691	-0.00007	1381.73835	1243.06138
1 1 1 -1 14	2 0 0 0 15	136.73193	-0.00009	1409.63267	1272.90065
1 1 1 -1 15	2 0 0 0 16	134.80182	-0.00009	1439.52224	1304.72033
1 1 1 -1 16	2 0 0 0 17	132.88807	-0.00012	1471.40738	1338.51918
1 1 1 -1 17	2 0 0 0 18	130.99215	-0.00010	1505.28829	1374.29604
1 1 1 -1 18	2 0 0 0 19	129.11505	-0.00020	1541.16510	1412.04985
1 1 1 -1 19	2 0 0 0 20	127.25801	-0.00019	1579.03782	1451.77962
1 1 1 -1 20	2 0 0 0 21	125.42186	0.00001	1618.90635	1493.48450
1 1 1 -1 21	2 0 0 0 22	123.60678	0.00001	1660.77045	1537.16368
1 1 1 -1 22	2 0 0 0 23	121.81339	0.00008	1704.62977	1582.81646
1 1 1 -1 23	2 0 0 0 24	120.04162	-0.00002	1750.48383	1630.44219
1 1 1 -1 1	2 0 0 0 0	168.55386	0.00015	1202.48900	1033.93529
1 1 1 -1 2	2 0 0 0 1	170.54182	0.00014	1206.47085	1035.92917
1 1 1 -1 3	2 0 0 0 2	172.52715	0.00017	1212.44377	1039.91679
1 1 1 -1 4	2 0 0 0 3	174.51017	0.00017	1220.40789	1045.89789
1 1 1 -1 5	2 0 0 0 4	176.49149	0.00015	1230.36343	1053.87209
1 1 1 -1 6	2 0 0 0 5	178.47191	0.00013	1242.31065	1063.83887
1 1 1 -1 7	2 0 0 0 6	180.45235	0.00009	1256.24984	1075.79759
1 1 1 -1 8	2 0 0 0 7	182.43398	0.00008	1272.18137	1089.74746
1 1 1 -1 9	2 0 0 0 8	184.41804	0.00004	1290.10561	1105.68761
1 1 1 -1 10	2 0 0 0 9	186.40600	0.00003	1310.02298	1123.61701
1 1 1 -1 11	2 0 0 0 10	188.39937	0.00001	1331.93393	1143.53456
1 1 1 -1 12	2 0 0 0 11	190.39984	0.00000	1355.83891	1165.43907
1 1 1 -1 13	2 0 0 0 12	192.40906	-0.00004	1381.73835	1189.32925
1 1 1 -1 14	2 0 0 0 13	194.42876	-0.00011	1409.63267	1215.20380
1 1 1 -1 15	2 0 0 0 14	196.46078	-0.00008	1439.52224	1243.06138
1 1 1 -1 16	2 0 0 0 15	198.49486	-0.00004	1471.40738	1272.90065

1	1	1	-1	17	2	0	0	0	16	200.56784	-0.00011	1505.28829	1304.72033
1	1	1	-1	18	2	0	0	0	17	202.64600	0.00009	1541.16510	1338.51918
1	1	1	-1	19	2	0	0	0	18	204.74167	-0.00012	1579.03782	1374.29604
2	1	1	1	-1	20	2	0	0	19	206.85638	-0.00013	1618.90635	1412.04985
3	1	1	1	-1	21	2	0	0	20	208.99072	-0.00011	1660.77045	1451.77962
4	1	1	1	-1	22	2	0	0	21	211.14512	-0.00015	1704.62977	1493.48450
5	1	1	1	-1	23	2	0	0	22	213.32014	0.00000	1750.48383	1537.16368
6	1	1	1	-1	24	2	0	0	23	215.51550	-0.00010	1798.33206	1582.81646
7	1	1	1	-1	25	2	0	0	24	217.73151	-0.00008	1848.17378	1630.44219
8	1	1	1	-1	26	2	0	0	25	219.96783	-0.00016	1900.00824	1680.04024
9	1	1	1	-1	27	2	0	0	26	222.22486	0.00031	1953.83461	1731.61005
10	1	1	1	-1	28	2	0	0	27	224.50086	-0.00009	2009.65198	1785.15104
11	1	1	1	-1	29	2	0	0	28	226.79691	0.00013	2067.45942	1840.66263

rms = 0.00012 cm⁻¹

$$v_4 + v_5 (\Delta) \leftarrow 2v_4 (\Delta)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 3	2 2 0 0 2	162.99424	0.00014	1207.69469	1044.70059
1 1 1 1 4	2 2 0 0 3	164.97687	-0.00005	1215.65751	1050.68059
1 1 1 1 5	2 2 0 0 4	166.95596	-0.00001	1225.61022	1058.65425
1 1 1 1 6	2 2 0 0 5	168.93039	-0.00002	1237.55228	1068.62187
1 1 1 1 7	2 2 0 0 6	170.89922	-0.00003	1251.48305	1080.58379
1 1 1 1 8	2 2 0 0 7	172.86133	0.00002	1267.40177	1094.54045
1 1 1 1 9	2 2 0 0 8	174.81530	0.00003	1285.30761	1110.49234
1 1 1 1 10	2 2 0 0 9	176.75967	0.00002	1305.19963	1128.43999
1 1 1 1 11	2 2 0 0 10	178.69288	0.00004	1327.07683	1148.38399
1 1 1 1 12	2 2 0 0 11	180.61321	0.00006	1350.93813	1170.32497
1 1 1 1 13	2 2 0 0 12	182.51889	0.00005	1376.78240	1194.26357
1 1 1 1 14	2 2 0 0 13	184.40815	0.00004	1404.60850	1220.20039
1 1 1 1 15	2 2 0 0 14	186.27927	0.00004	1434.41526	1248.13603
1 1 1 1 16	2 2 0 0 15	188.13061	0.00010	1466.20152	1278.07100
1 1 1 1 17	2 2 0 0 16	189.96043	0.00003	1499.96614	1310.00574
1 1 1 1 18	2 2 0 0 17	191.76756	0.00006	1535.70804	1343.94054
1 1 1 1 19	2 2 0 0 18	193.55061	0.00001	1573.42620	1379.87559
1 1 1 1 20	2 2 0 0 19	195.30873	0.00003	1613.11962	1417.81092
1 1 1 1 21	2 2 0 0 20	197.04104	0.00000	1654.78743	1457.74639
1 1 1 1 22	2 2 0 0 21	198.74705	0.00000	1698.42877	1499.68172
1 1 1 1 23	2 2 0 0 22	200.42638	0.00000	1744.04287	1543.61649
1 1 1 1 24	2 2 0 0 23	202.07883	-0.00002	1791.62900	1589.55014
1 1 1 1 25	2 2 0 0 24	203.70431	-0.00016	1841.18647	1637.48199
1 1 1 1 26	2 2 0 0 25	205.30331	-0.00004	1892.71462	1687.41127
1 1 1 1 27	2 2 0 0 26	206.87555	-0.00015	1946.21281	1739.33712
1 1 1 1 28	2 2 0 0 27	208.42215*	0.00034	2001.68041	1793.25860
1 1 1 1 29	2 2 0 0 28	209.94173	-0.00032	2059.11678	1849.17473
1 1 1 1 30	2 2 0 0 29	211.43618	-0.00059	2118.52125	1907.08448W
1 1 1 1 31	2 2 0 0 30	212.90628	-0.00012	2179.89318	1966.98678
1 1 1 1 2	2 2 0 0 3	151.04207	0.00047	1201.72219	1050.68059
1 1 1 1 3	2 2 0 0 4	149.04058	0.00015	1207.69469	1058.65425
1 1 1 1 4	2 2 0 0 5	147.03562	-0.00002	1215.65751	1068.62187
1 1 1 1 5	2 2 0 0 6	145.02639	-0.00003	1225.61022	1080.58379
1 1 1 1 6	2 2 0 0 7	143.01179	-0.00003	1237.55228	1094.54045
1 1 1 1 7	2 2 0 0 8	140.99067	-0.00004	1251.48305	1110.49234
1 1 1 1 8	2 2 0 0 9	138.96189	0.00011	1267.40177	1128.43999
1 1 1 1 9	2 2 0 0 10	136.92359	-0.00002	1285.30761	1148.38399
1 1 1 1 10	2 2 0 0 11	134.87459	-0.00006	1305.19963	1170.32497
1 1 1 1 11	2 2 0 0 12	132.81324	-0.00002	1327.07683	1194.26357
1 1 1 1 12	2 2 0 0 13	130.73773	0.00000	1350.93813	1220.20039
1 1 1 1 13	2 2 0 0 14	128.64635	-0.00002	1376.78240	1248.13603
1 1 1 1 14	2 2 0 0 15	126.53748	-0.00002	1404.60850	1278.07100
1 1 1 1 15	2 2 0 0 16	124.40953	0.00001	1434.41526	1310.00574
1 1 1 1 16	2 2 0 0 17	122.26095	-0.00002	1466.20152	1343.94054
1 1 1 1 17	2 2 0 0 18	120.09049	-0.00006	1499.96614	1379.87559
1 1 1 1 18	2 2 0 0 19	117.89707	-0.00006	1535.70804	1417.81092
1 1 1 1 19	2 2 0 0 20	115.71399	0.00001	1573.42620	1457.74639

1	1	-1	1	-1	22	2	-2	0	0	23	110.57840	0.00010	1699.06765	1588.48935
	1	-1	1	-1	23	2	-2	0	0	24	108.52689	-0.00010	1744.78769	1636.26071
2	1	-1	1	-1	24	2	-2	0	0	25	106.47294	-0.00010	1792.48970	1686.01666
3	1	-1	1	-1	25	2	-2	0	0	26	104.41660	0.00007	1842.17301	1737.75648
4	1	-1	1	-1	26	2	-2	0	0	27	102.35785	0.00034	1893.83694	1791.47943
5	1	-1	1	-1	27	2	-2	0	0	28	100.29611	0.00007	1947.48076	1847.18472
6	1	-1	1	-1	28	2	-2	0	0	29	98.23216	-0.00003	2003.10374	1904.87155
7	1	1	1	1	2	2	-2	0	0	2	157.02161	-0.00010	1201.72219	1044.70049
8	1	1	1	1	3	2	-2	0	0	3	157.01446	-0.00014	1207.69469	1050.68009
9	1	1	1	1	4	2	-2	0	0	4	157.00446	-0.00030	1215.65751	1058.65275
10	1	1	1	1	5	2	-2	0	0	5	156.99177	-0.00009	1225.61022	1068.61835
11	1	1	1	1	6	2	-2	0	0	6	156.97549	-0.00002	1237.55228	1080.57677
12	1	1	1	1	7	2	-2	0	0	7	156.95509	-0.00014	1251.48305	1094.52781
13	1	1	1	1	8	2	-2	0	0	8	156.93052	0.00003	1267.40177	1110.47128
14	1	1	1	1	9	2	-2	0	0	9	156.90063*	-0.00002	1285.30761	1128.40695
15	1	1	1	1	10	2	-2	0	0	10	156.86519	0.00013	1305.19963	1148.33456
16	1	1	1	1	11	2	-2	0	0	11	156.82349	0.00049	1327.07683	1170.25382

rms = 0.00014 cm⁻¹2v₄(Σ⁺) ← v₅(Π)

v ₄ '	l ₄ '	v ₅ '	l ₅ '	J'	v ₄ ''	l ₄ ''	v ₅ ''	l ₅ ''	J''	OBS	OBS - CALC	E'	E''
2	0	0	0	2	0	0	1	1	3	350.21502	-0.00037	1039.91679	689.70140
2	0	0	0	3	0	0	1	1	4	348.26764	0.00007	1045.89789	697.63032
2	0	0	0	4	0	0	1	1	5	346.33073	-0.00011	1053.87209	707.54126
2	0	0	0	5	0	0	1	1	6	344.40466	-0.00013	1063.83887	719.43409
2	0	0	0	6	0	0	1	1	7	342.48904	0.00009	1075.79759	733.30864
2	0	0	0	7	0	0	1	1	8	340.58281	0.00007	1089.74746	749.16472
2	0	0	0	8	0	0	1	1	9	338.68566	0.00018	1105.68761	767.00212
2	0	0	0	9	0	0	1	1	10	336.79691	0.00049	1123.61701	786.82059
2	0	0	0	10	0	0	1	1	11	334.91516	0.00045	1143.53456	808.61985
2	0	0	0	11	0	0	1	1	12	333.04003	0.00058	1165.43907	832.39961
2	0	0	0	12	0	0	1	1	13	331.17026	0.00055	1189.32925	858.15954
2	0	0	0	13	0	0	1	1	14	329.30440	-0.00012	1215.20380	885.89928
2	0	0	0	14	0	0	1	1	15	327.44313	0.00021	1243.06138	915.61845
2	0	0	0	15	0	0	1	1	16	325.58390	-0.00011	1272.90065	947.31664
2	0	0	0	16	0	0	1	1	17	323.72728	0.00037	1304.72033	980.99342
2	0	0	0	17	0	0	1	1	18	321.87147	0.00060	1338.51918	1016.64832
2	0	0	0	18	0	0	1	1	19	320.01536	0.00016	1374.29604	1054.28084
2	0	0	0	19	0	0	1	1	20	318.16001	0.00065	1412.04985	1093.89049
2	0	0	0	20	0	0	1	1	21	316.30287	-0.00006	1451.77962	1135.47669
2	0	0	0	21	0	0	1	1	22	314.44570	0.00010	1493.48450	1179.03889
2	0	0	0	22	0	0	1	1	23	312.58740	0.00021	1537.16368	1224.57649
2	0	0	0	2	0	0	1	-1	2	356.14140	0.00039	1039.91679	683.77578
2	0	0	0	3	0	0	1	-1	3	356.15438	0.00020	1045.89789	689.74371
2	0	0	0	4	0	0	1	-1	4	356.17125	-0.00001	1053.87209	697.70083
2	0	0	0	5	0	0	1	-1	5	356.19210	0.00025	1063.83887	707.64702
2	0	0	0	6	0	0	1	-1	6	356.21551	0.00007	1075.79759	719.58215
2	0	0	0	7	0	0	1	-1	7	356.24172	0.00029	1089.74746	733.50603
2	0	0	0	8	0	0	1	-1	8	356.26924	0.00013	1105.68761	749.41849
2	0	0	0	9	0	0	1	-1	9	356.29780	0.00009	1123.61701	767.31930
2	0	0	0	10	0	0	1	-1	10	356.32650	0.00014	1143.53456	787.20820
2	0	0	0	11	0	0	1	-1	11	356.35429	0.00015	1165.43907	809.08492
2	0	0	0	12	0	0	1	-1	12	356.38038	0.00029	1189.32925	832.94916
2	0	0	0	13	0	0	1	-1	13	356.40325	0.00002	1215.20380	858.80057
2	0	0	0	14	0	0	1	-1	14	356.42284	0.00026	1243.06138	886.63880
2	0	0	0	15	0	0	1	-1	15	356.43732	0.00012	1272.90065	916.46345
2	0	0	0	16	0	0	1	-1	16	356.44648	0.00026	1304.72033	948.27412
2	0	0	0	17	0	0	1	-1	17	356.44966*	0.00083	1338.51918	982.07035
2	0	0	0	18	0	0	1	-1	18	356.44440	0.00003	1374.29604	1017.85167
2	0	0	0	19	0	0	1	-1	19	356.43225	0.00000	1412.04985	1055.61759
2	0	0	0	20	0	0	1	-1	20	356.41239	0.00034	1451.77962	1095.36757
2	0	0	0	21	0	0	1	-1	21	356.38329	-0.00015	1493.48450	1137.10105
2	0	0	0	22	0	0	1	-1	22	356.34623	0.00000	1537.16368	1180.81746
2	0	0	0	23	0	0	1	-1	23	356.30109	0.00019	1582.81646	1226.51618

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rms = 0.00027 cm⁻¹ $\nu_4 + 2\nu_5 (\Phi) \leftarrow 2\nu_4 + \nu_5 (\Phi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''	
1	1 1 2 2 15	2 2 1 1 16	128.63908	-0.00001	2115.65882	1987.01973
2	1 1 2 2 14	2 2 1 1 15	130.69696	-0.00006	2085.78481	1955.08779
3	1 1 2 2 13	2 2 1 1 14	132.74731	-0.00005	2057.89941	1925.15205
4	1 1 2 2 12	2 2 1 1 13	134.79078	-0.00013	2032.00319	1897.21228
5	1 1 2 2 11	2 2 1 1 12	136.82801	-0.00041	2008.09670	1871.26829
6	1 1 2 2 10	2 2 1 1 11	138.86048	-0.00006	1986.18048	1847.31994
7	1 1 2 2 9	2 2 1 1 10	140.88818	0.00031	1966.25501	1825.36714
8	1 1 2 2 7	2 2 1 1 8	144.93028	0.00023	1932.37810	1787.44806
9	1 1 2 2 6	2 2 1 1 7	146.94599	0.00033	1918.42746	1771.48179
10	1 1 2 2 5	2 2 1 1 6	148.95778	-0.00026	1906.46914	1757.51111
11	1 1 2 2 4	2 2 1 1 5	150.96758	0.00020	1896.50344	1745.53606
12	1 1 2 2 3	2 2 1 1 4	152.97514	0.00126	1888.53059	1735.55671W
13	1 1 2 2 4	2 2 1 1 3	168.93051*	0.00021	1896.50344	1727.57314
14	1 1 2 2 5	2 2 1 1 4	170.91285*	0.00042	1906.46914	1735.55671
15	1 1 2 2 6	2 2 1 1 5	172.89154	0.00014	1918.42746	1745.53606
16	1 1 2 2 7	2 2 1 1 6	174.86690	-0.00009	1932.37810	1757.51111
17	1 1 2 2 8	2 2 1 1 7	176.83800*	-0.00095	1948.32074	1771.48179
18	1 1 2 2 9	2 2 1 1 8	178.80733	0.00038	1966.25501	1787.44806
19	1 1 2 2 10	2 2 1 1 9	180.77085	0.00022	1986.18048	1805.40985
20	1 1 2 2 11	2 2 1 1 10	182.72944	-0.00013	2008.09670	1825.36714
21	1 1 2 2 12	2 2 1 1 11	184.68300	-0.00025	2032.00319	1847.31994
22	1 1 2 2 13	2 2 1 1 12	186.63155	0.00043	2057.89941	1871.26829
23	1 1 2 2 14	2 2 1 1 13	188.57256	0.00003	2085.78481	1897.21228
24	1 1 2 2 15	2 2 1 1 14	190.50700*	0.00023	2115.65882	1925.15205
25	1 1 2 2 16	2 2 1 1 15	192.43344	0.00041	2147.52082	1955.08779
26	1 1 2 2 17	2 2 1 1 16	194.35058	0.00010	2181.37021	1987.01973
27	1 1 2 2 18	2 2 1 1 17	196.25842	0.00018	2217.20636	2020.94812
28	1 1 2 2 19	2 2 1 1 18	198.15552	0.00009	2255.02864	2056.87321
29	1 1 2 2 20	2 2 1 1 19	200.04148	0.00031	2294.83643	2094.79526
30	1 1 2 2 21	2 2 1 1 20	201.91508	0.00040	2336.62911	2134.71443
31	1 1 2 2 22	2 2 1 1 21	203.77527	0.00002	2380.40608	2176.63083
32	1 1 2 2 23	2 2 1 1 22	205.62271	0.00040	2426.16675	2220.54443
33	1 -1 2 -2 3	2 2 1 1 3	160.95773	0.00028	1888.53059	1727.57314
34	1 -1 2 -2 4	2 2 1 1 4	160.94689	0.00016	1896.50344	1735.55671
35	1 -1 2 -2 5	2 2 1 1 5	160.93321	0.00013	1906.46914	1745.53606
36	1 -1 2 -2 6	2 2 1 1 6	160.91655	0.00022	1918.42744	1757.51111
37	1 -1 2 -2 7	2 2 1 1 7	160.89668	0.00042	1932.37805	1771.48179
38	1 -1 2 -2 8	2 2 1 1 8	160.87296	0.00038	1948.32063	1787.44806
39	1 -1 2 -2 10	2 2 1 1 10	160.81265	-0.00029	1986.18007	1825.36714
40	1 -1 2 -2 17	2 -2 1 -1 18	124.59490	0.00017	2181.36119	2056.76646
41	1 -1 2 -2 16	2 -2 1 -1 17	126.64433	0.00017	2147.51449	2020.87032
42	1 -1 2 -2 14	2 -2 1 -1 15	130.73233	-0.00020	2085.78191	1955.04938
43	1 -1 2 -2 13	2 -2 1 -1 14	132.77144	0.00007	2057.89753	1925.12616
44	1 -1 2 -2 12	2 -2 1 -1 13	134.80668	0.00004	2032.00201	1897.19537
45	1 -1 2 -2 11	2 -2 1 -1 12	136.83837	0.00002	2008.09600	1871.25765
46	1 -1 2 -2 10	2 -2 1 -1 11	138.86681	0.00026	1986.18007	1847.31352
47	1 -1 2 -2 9	2 -2 1 -1 10	140.89175	0.00042	1966.25479	1825.36346
48	1 -1 2 -2 8	2 -2 1 -1 9	142.91297	0.00020	1948.32063	1805.40786
49	1 -1 2 -2 7	2 -2 1 -1 8	144.93029	-0.00070	1932.37805	1787.44706
50	1 -1 2 -2 6	2 -2 1 -1 7	146.94597	-0.00013	1918.42744	1771.48134
51	1 -1 2 -2 5	2 -2 1 -1 6	148.95777	-0.00044	1906.46914	1757.51093
52	1 -1 2 -2 4	2 -2 1 -1 5	150.96758	0.00014	1896.50344	1745.53600
53	1 -1 2 -2 6	2 -2 1 -1 5	172.89153	0.00009	1918.42744	1745.53600
54	1 -1 2 -2 7	2 -2 1 -1 6	174.86697	-0.00016	1932.37805	1757.51093
55	1 -1 2 -2 8	2 -2 1 -1 7	176.83940*	0.00011	1948.32063	1771.48134
56	1 -1 2 -2 9	2 -2 1 -1 8	178.80734	-0.00039	1966.25479	1787.44706
57	1 -1 2 -2 10	2 -2 1 -1 9	180.77192	-0.00029	1986.18007	1805.40786
58	1 -1 2 -2 11	2 -2 1 -1 10	182.73216	-0.00038	2008.09600	1825.36346
59	1 -1 2 -2 12	2 -2 1 -1 11	184.68820	-0.00029	2032.00201	1847.31352
60	1 -1 2 -2 13	2 -2 1 -1 12	186.63155	-0.00042	2057.89753	1871.25765

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1	1	-1	2	-2	14	2	-2	1	-1	13	188.58626	-0.00028	2085.78191	1897.19537
	1	-1	2	-2	15	2	-2	1	-1	14	190.52808	-0.00024	2115.65447	1925.12616
2	1	-1	2	-2	16	2	-2	1	-1	15	192.46514	0.00003	2147.51449	1955.04938
3	1	-1	2	-2	17	2	-2	1	-1	16	194.39677	-0.00006	2181.36119	1986.96435
4	1	-1	2	-2	18	2	-2	1	-1	17	196.32340	-0.00005	2217.19377	2020.87032
5	1	-1	2	-2	19	2	-2	1	-1	18	198.24502	0.00007	2255.01141	2056.76646
6	1	-1	2	-2	20	2	-2	1	-1	19	200.16159	0.00023	2294.81323	2094.65187
7	1	-1	2	-2	21	2	-2	1	-1	20	202.07244	-0.00029	2336.59836	2134.52563
8	1	-1	2	-2	22	2	-2	1	-1	21	203.97890	-0.00024	2380.36588	2176.38674
9	1	-1	2	-2	23	2	-2	1	-1	22	205.88082	0.00014	2426.11489	2220.23421
10	1	-1	2	-2	25	2	-2	1	-1	24	209.66973	0.00013	2523.55362	2313.88402
11	1	1	2	2	3	2	-2	1	-1	3	160.95773	0.00028	1888.53059	1727.57314
12	1	1	2	2	4	2	-2	1	-1	4	160.94689	0.00015	1896.50344	1735.55670
13	1	1	2	2	5	2	-2	1	-1	5	160.93321	0.00006	1906.46914	1745.53600
14	1	1	2	2	6	2	-2	1	-1	6	160.91655	0.00002	1918.42746	1757.51093
15	1	1	2	2	7	2	-2	1	-1	7	160.89668	-0.00008	1932.37810	1771.48134
16	1	1	2	2	8	2	-2	1	-1	8	160.87409	0.00041	1948.32074	1787.44706

rms = 0.00025 cm⁻¹

$$2\nu_4 + \nu_5 (^1\Pi) \leftarrow 3\nu_4 (\Pi)$$

ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''	
25	2	2	1	-1	2	3	1	0	0	3	165.34610	-0.00022	1728.44514	1563.09883
26	2	2	1	-1	3	3	1	0	0	4	163.36015	0.00044	1734.41904	1571.05934
27	2	2	1	-1	4	3	1	0	0	5	161.37471	-0.00013	1742.38433	1581.00949
28	2	2	1	-1	5	3	1	0	0	6	159.39210	0.00000	1752.34107	1592.94896
29	2	2	1	-1	6	3	1	0	0	7	157.41233	0.00036	1764.28934	1606.87737
30	2	2	1	-1	7	3	1	0	0	8	155.43514	0.00017	1778.22926	1622.79429
31	2	2	1	-1	8	3	1	0	0	9	153.46149	-0.00024	1794.16094	1640.69921
32	2	2	1	-1	9	3	1	0	0	10	151.49288	-0.00003	1812.08452	1660.59161
33	2	2	1	-1	10	3	1	0	0	11	149.52833*	-0.00093	1832.00016	1682.47090
34	2	2	1	-1	11	3	1	0	0	12	147.57183	0.00025	1853.90802	1706.33645
35	2	2	1	-1	12	3	1	0	0	13	145.62091	0.00021	1877.80829	1732.18758
36	2	2	1	-1	13	3	1	0	0	14	143.67753	0.00001	1903.70113	1760.02361
37	2	2	1	-1	14	3	1	0	0	15	141.74299	0.00004	1931.58675	1789.84380
38	2	2	1	-1	15	3	1	0	0	16	139.81759	-0.00034	1961.46532	1821.64740
39	2	2	1	-1	16	3	1	0	0	17	137.90345	0.00004	1993.33703	1855.43362
40	2	2	1	-1	17	3	1	0	0	18	136.00087	0.00051	2027.20204	1891.20168
41	2	2	1	-1	18	3	1	0	0	19	134.10968	-0.00003	2063.06048	1928.95077
42	2	2	1	-1	19	3	1	0	0	20	132.23248	0.00009	2100.91245	1968.68006
43	2	2	1	-1	2	3	1	0	0	1	175.29788	0.00043	1728.44514	1553.14769
44	2	2	1	-1	3	3	1	0	0	2	177.29095	0.00012	1734.41904	1557.12821
45	2	2	1	-1	4	3	1	0	0	3	179.28510	-0.00040	1742.38433	1563.09883
46	2	2	1	-1	5	3	1	0	0	4	181.28186	0.00013	1752.34107	1571.05934
47	2	2	1	-1	6	3	1	0	0	5	183.27993	0.00008	1764.28934	1581.00949
48	2	2	1	-1	7	3	1	0	0	6	185.28076	0.00047	1778.22926	1592.94896
49	2	2	1	-1	8	3	1	0	0	7	187.28373	0.00016	1794.16094	1606.87737
50	2	2	1	-1	9	3	1	0	0	8	189.29065	0.00041	1812.08452	1622.79429
51	2	2	1	-1	10	3	1	0	0	9	191.30083	-0.00012	1832.00016	1640.69921
52	2	2	1	-1	11	3	1	0	0	10	193.31611	-0.00030	1853.90802	1660.59161
53	2	2	1	-1	12	3	1	0	0	11	195.33759	0.00021	1877.80829	1682.47090
54	2	2	1	-1	13	3	1	0	0	12	197.36450	-0.00018	1903.70113	1706.33645
55	2	2	1	-1	14	3	1	0	0	13	199.39922	0.00006	1931.58675	1732.18758
56	2	2	1	-1	15	3	1	0	0	14	201.44140*	-0.00031	1961.46532	1760.02361
57	2	2	1	-1	16	3	1	0	0	15	203.49337	0.00014	1993.33703	1789.84380
58	2	2	1	-1	17	3	1	0	0	16	205.55478	0.00014	2027.20204	1821.64740
59	2	2	1	-1	18	3	1	0	0	17	207.62737*	0.00051	2063.06048	1855.43362
60	2	2	1	-1	19	3	1	0	0	18	209.71090	0.00013	2100.91245	1891.20168
	2	2	1	-1	20	3	1	0	0	19	211.80742	0.00017	2140.75802	1928.95077
	2	-2	1	1	1	3	1	0	0	1	171.32398	-0.00014	1724.47181	1553.14769
	2	-2	1	1	2	3	-1	0	0	3	165.26573	0.00014	1728.47288	1563.20728
	2	-2	1	1	3	3	-1	0	0	4	163.23492	0.00048	1734.47452	1571.24009
	2	-2	1	1	4	3	-1	0	0	5	161.19642	0.00019	1742.47680	1581.28057
	2	-2	1	1	5	3	-1	0	0	6	159.15131	-0.00008	1752.47978	1593.32839
	2	-2	1	1	6	3	-1	0	0	7	157.10400	0.00000	1764.48357	1607.38312

1	2	-2	1	1	7	3	-1	0	0	8	155.04401	-0.00001	1778.48827	1623.44425
2	2	-2	1	1	8	3	-1	0	0	9	152.98282	0.00000	1794.49400	1641.51118
3	2	-2	1	1	9	3	-1	0	0	10	150.91770	0.00004	1812.50091	1661.58325
4	2	-2	1	1	10	3	-1	0	0	11	148.84957	0.00009	1832.50915	1683.65967
5	2	-2	1	1	11	3	-1	0	0	12	146.77919	-0.00012	1854.51888	1707.73957
6	2	-2	1	1	12	3	-1	0	0	13	144.70856	0.00026	1878.53027	1733.82197
7	2	-2	1	1	13	3	-1	0	0	14	142.63762	-0.00011	1904.54349	1761.90576
8	2	-2	1	1	14	3	-1	0	0	15	140.56907	0.00010	1932.55872	1791.98975
9	2	-2	1	1	15	3	-1	0	0	16	138.50370	0.00016	1962.57611	1824.07257
10	2	-2	1	1	16	3	-1	0	0	17	136.44337*	0.00033	1994.59581	1858.15277
11	2	-2	1	1	2	3	-1	0	0	1	175.30690	-0.00021	1728.47288	1553.16577
12	2	-2	1	1	3	3	-1	0	0	2	177.29252	0.00044	1734.47452	1557.18244
13	2	-2	1	1	4	3	-1	0	0	3	179.26982	0.00031	1742.47680	1563.20728
14	2	-2	1	1	5	3	-1	0	0	4	181.23984	0.00014	1752.47978	1571.24009
15	2	-2	1	1	6	3	-1	0	0	5	183.20309	0.00009	1764.48357	1581.28057
16	2	-2	1	1	7	3	-1	0	0	6	185.16013	0.00025	1778.48827	1593.32839
17	2	-2	1	1	8	3	-1	0	0	7	187.11076	-0.00012	1794.49400	1607.38312
18	2	-2	1	1	9	3	-1	0	0	8	189.05705*	0.00039	1812.50091	1623.44425
19	2	-2	1	1	10	3	-1	0	0	9	190.99783	-0.00013	1832.50915	1641.51118
20	2	-2	1	1	11	3	-1	0	0	10	192.93569	0.00006	1854.51888	1661.58325
21	2	-2	1	1	12	3	-1	0	0	11	194.87054	-0.00006	1878.53027	1683.65967
22	2	-2	1	1	14	3	-1	0	0	13	198.73625*	-0.00050	1932.55872	1733.82197
23	2	-2	1	1	15	3	-1	0	0	14	200.67023	-0.00012	1962.57611	1761.90576
24	2	-2	1	1	16	3	-1	0	0	15	202.60628	0.00022	1994.59581	1791.98975
25	2	-2	1	1	17	3	-1	0	0	16	204.54565	0.00028	2028.61794	1824.07257
26	2	-2	1	1	18	3	-1	0	0	17	206.48962	-0.00020	2064.64259	1858.15277

rms = 0.00023 cm⁻¹

$$v_4 + v_5 (\Delta) \leftarrow 2v_4 (\Sigma^+)$$

v_4'	l_4'	v_5'	l_5'	J'	v_4''	l_4''	v_5''	l_5''	J''	OBS	OBS - CALC	E'	E''
1	1	1	1	8	2	0	0	0	9	143.78462	-0.00014	1267.40177	1123.61701
2	1	1	1	9	2	0	0	0	10	141.77280	-0.00024	1285.30761	1143.53456
3	1	1	1	10	2	0	0	0	11	139.76079	0.00023	1305.19963	1165.43907
4	1	1	1	11	2	0	0	0	12	137.74740	-0.00018	1327.07683	1189.32925
5	1	1	1	12	2	0	0	0	13	135.73443	0.00010	1350.93813	1215.20380
6	1	1	1	13	2	0	0	0	14	133.72091	-0.00012	1376.78240	1243.06138
7	1	1	1	14	2	0	0	0	15	131.70787	0.00002	1404.60850	1272.90065
8	1	1	1	15	2	0	0	0	16	129.69475	-0.00018	1434.41526	1304.72033
9	1	1	1	16	2	0	0	0	17	127.68229	-0.00004	1466.20152	1338.51918
10	1	1	1	17	2	0	0	0	18	125.67021	0.00011	1499.96614	1374.29604
11	1	1	1	18	2	0	0	0	19	123.65842	0.00022	1535.70804	1412.04985
12	1	1	1	19	2	0	0	0	20	121.64674	0.00017	1573.42620	1451.77962
13	1	1	1	20	2	0	0	0	21	119.63504*	-0.00009	1613.11962	1493.48450
14	1	1	1	21	2	0	0	0	22	117.62373	-0.00002	1654.78743	1537.16368
15	1	1	1	22	2	0	0	0	23	115.61249	0.00018	1698.42877	1582.81646
16	1	1	1	23	2	0	0	0	24	113.60089	0.00021	1744.04287	1630.44219
17	1	1	1	24	2	0	0	0	25	111.58897	0.00022	1791.62900	1680.04024
18	1	1	1	25	2	0	0	0	26	109.57690*	0.00049	1841.18647	1731.61005
19	1	1	1	26	2	0	0	0	27	107.56395	0.00037	1892.71462	1785.15104
20	1	1	1	9	2	0	0	0	8	179.62002	0.00002	1285.30761	1105.68761
21	1	1	1	10	2	0	0	0	9	181.58256	-0.00006	1305.19963	1123.61701
22	1	1	1	11	2	0	0	0	10	183.54200	-0.00026	1327.07683	1143.53456
23	1	1	1	12	2	0	0	0	11	185.49915	0.00009	1350.93813	1165.43907
24	1	1	1	13	2	0	0	0	12	187.45337	0.00022	1376.78240	1189.32925
25	1	1	1	14	2	0	0	0	13	189.40479	0.00009	1404.60850	1215.20380
26	1	1	1	15	2	0	0	0	14	191.35383	-0.00005	1434.41526	1243.06138
27	1	1	1	16	2	0	0	0	15	193.30110	0.00024	1466.20152	1272.90065
28	1	1	1	17	2	0	0	0	16	195.24588	0.00007	1499.96614	1304.72033
29	1	1	1	18	2	0	0	0	17	197.18906	0.00020	1535.70804	1338.51918
30	1	1	1	19	2	0	0	0	18	199.13053	0.00038	1573.42620	1374.29604
31	1	1	1	20	2	0	0	0	19	201.07004	0.00026	1613.11962	1412.04985
32	1	1	1	21	2	0	0	0	20	203.00793	0.00012	1654.78743	1451.77962
33	1	1	1	22	2	0	0	0	21	204.94463	0.00036	1698.42877	1493.48450
34	1	1	1	23	2	0	0	0	22	206.88132	-0.00020	1744.04287	1537.16368

1	1	1	1	24	2	0	0	0	23	208.81272	0.00019	1791.62900	1582.81646
1	1	1	1	25	2	0	0	0	24	210.74455	0.00027	1841.18647	1630.44219
2	1	1	1	26	2	0	0	0	25	212.67473	0.00035	1892.71462	1680.04024
3	1	1	1	27	2	0	0	0	26	214.60305	0.00029	1946.21281	1731.61005
4	1	1	1	28	2	0	0	0	27	216.52966	0.00029	2001.68041	1785.15104
5	1	1	1	29	2	0	0	0	28	218.45446	0.00032	2059.11678	1840.66263
6	1	1	1	30	2	0	0	0	29	220.37722	0.00021	2118.52125	1898.14425
7	1	1	1	31	2	0	0	0	30	222.29827	0.00037	2179.89318	1957.59528
8	1	1	1	32	2	0	0	0	31	224.21666	-0.00009	2243.23185	2019.01510
9	1	1	1	33	2	0	0	0	32	226.13361	0.00009	2308.53656	2082.40305

rms = 0.00022 cm⁻¹

$$v_4 + v_5 (\Sigma^+) \leftarrow 2v_4 (\Delta)$$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 8	2 2 0 0 9	143.74137	-0.00001	1272.18137	1128.43999
1 1 1 -1 9	2 2 0 0 10	141.72122*	-0.00039	1290.10561	1148.38399
1 1 1 -1 10	2 2 0 0 11	139.69734*	-0.00067	1310.02298	1170.32497W
1 1 1 -1 11	2 2 0 0 12	137.67065	0.00028	1331.93393	1194.26357
1 1 1 -1 12	2 2 0 0 13	135.63864	0.00012	1355.83891	1220.20039
1 1 1 -1 13	2 2 0 0 14	133.60255	0.00023	1381.73835	1248.13603
1 1 1 -1 14	2 2 0 0 15	131.56157	-0.00010	1409.63267	1278.07100
1 1 1 -1 15	2 2 0 0 16	129.51659	0.00008	1439.52224	1310.00574
1 1 1 -1 16	2 2 0 0 17	127.46718	0.00035	1471.40738	1343.94054
1 1 1 -1 17	2 2 0 0 18	125.41292	0.00023	1505.28829	1379.87559
1 1 1 -1 18	2 2 0 0 19	123.35415	-0.00003	1541.16510	1417.81092
1 1 1 -1 19	2 2 0 0 20	121.29146	0.00002	1579.03782	1457.74639
1 1 1 -1 20	2 2 0 0 21	119.22481	0.00018	1618.90635	1499.68172
1 1 1 -1 21	2 2 0 0 22	117.15348	-0.00048	1660.77045	1543.61649
1 1 1 -1 22	2 2 0 0 23	115.07999	0.00036	1704.62977	1589.55014
1 1 1 -1 23	2 2 0 0 24	113.00189	0.00005	1750.48383	1637.48199
1 1 1 -1 24	2 2 0 0 25	110.92082	0.00003	1798.33206	1687.41127
1 1 1 -1 25	2 2 0 0 26	108.83662	-0.00004	1848.17378	1739.33712
1 1 1 -1 26	2 2 0 0 27	106.74914	-0.00050	1900.00824	1793.25860W
1 1 1 -1 27	2 2 0 0 28	104.65965	-0.00023	1953.83461	1849.17473
1 1 1 -1 9	2 2 0 0 8	179.61302	-0.00025	1290.10561	1110.49234
1 1 1 -1 10	2 2 0 0 9	181.58268	-0.00032	1310.02298	1128.43999
1 1 1 -1 11	2 2 0 0 10	183.54999	0.00005	1331.93393	1148.38399
1 1 1 -1 12	2 2 0 0 11	185.51407	0.00014	1355.83891	1170.32497
1 1 1 -1 13	2 2 0 0 12	187.47503	0.00025	1381.73835	1194.26357
1 1 1 -1 14	2 2 0 0 13	189.43232	0.00004	1409.63267	1220.20039
1 1 1 -1 15	2 2 0 0 14	191.38626*	0.00004	1439.52224	1248.13603
1 1 1 -1 16	2 2 0 0 15	193.33647	0.00010	1471.40738	1278.07100
1 1 1 -1 17	2 2 0 0 16	195.28254	-0.00001	1505.28829	1310.00574
1 1 1 -1 18	2 2 0 0 17	197.22440	-0.00016	1541.16510	1343.94054
1 1 1 -1 19	2 2 0 0 18	199.16214	-0.00009	1579.03782	1379.87559
1 1 1 -1 20	2 2 0 0 19	201.09532	-0.00011	1618.90635	1417.81092
1 1 1 -1 21	2 2 0 0 20	203.02396	-0.00010	1660.77045	1457.74639
1 1 1 -1 22	2 2 0 0 21	204.94808	0.00003	1704.62977	1499.68172
1 1 1 -1 23	2 2 0 0 22	206.86725	-0.00009	1750.48383	1543.61649
1 1 1 -1 24	2 2 0 0 23	208.78174	-0.00018	1798.33206	1589.55014
1 1 1 -1 25	2 2 0 0 24	210.69158	-0.00021	1848.17378	1637.48199
1 1 1 -1 26	2 2 0 0 25	212.59684	-0.00013	1900.00824	1687.41127
1 1 1 -1 27	2 2 0 0 26	214.49739	-0.00010	1953.83461	1739.33712
1 1 1 -1 28	2 2 0 0 27	216.39311	-0.00027	2009.65198	1793.25860
1 1 1 -1 29	2 2 0 0 28	218.28448	-0.00021	2067.45942	1849.17473
1 1 1 -1 30	2 2 0 0 29	220.17190	0.00046	2127.25592	1907.08448
1 1 1 -1 31	2 2 0 0 30	222.05368	0.00000	2189.04046	1966.98678
1 1 1 -1 32	2 2 0 0 31	223.93163	0.00018	2252.81197	2028.88052
1 1 1 -1 33	2 2 0 0 32	225.80500	0.00022	2318.56937	2092.76459
1 1 1 -1 34	2 2 0 0 33	227.67422	0.00053	2386.31153	2158.63783W
1 1 1 -1 35	2 2 0 0 34	229.53833	0.00011	2456.03731	2226.49908

rms = 0.00020 cm⁻¹

$2\nu_5(\Sigma^+) \leftarrow \nu_4 + \nu_5(\Delta)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 11	1 1 1 1 12	122.54059	0.00031	1473.47840	1350.93813
0 0 2 0 12	1 1 1 1 13	120.55298	0.00020	1497.33518	1376.78240
0 0 2 0 13	1 1 1 1 14	118.56900	-0.00001	1523.17752	1404.60850
0 0 2 0 14	1 1 1 1 15	116.58907*	-0.00049	1551.00481	1434.41526
0 0 2 0 15	1 1 1 1 16	114.61511	0.00020	1580.81643	1466.20152
0 0 2 0 16	1 1 1 1 17	112.64539	-0.00014	1612.61167	1499.96614
0 0 2 0 17	1 1 1 1 18	110.68185	0.00008	1646.38981	1535.70804
0 0 2 0 18	1 1 1 1 19	108.72383	-0.00004	1682.15007	1573.42620
0 0 2 0 16	1 1 1 1 15	178.19688*	0.00047	1612.61167	1434.41526
0 0 2 0 17	1 1 1 1 16	180.18834	0.00004	1646.38981	1466.20152
0 0 2 0 18	1 1 1 1 17	182.18395	0.00002	1682.15007	1499.96614
0 0 2 0 19	1 1 1 1 18	184.18349	-0.00009	1719.89163	1535.70804
0 0 2 0 20	1 1 1 1 19	186.18760	0.00017	1759.61363	1573.42620
0 0 2 0 21	1 1 1 1 20	188.19515*	-0.00039	1801.31517	1613.11962
0 0 2 0 22	1 1 1 1 21	190.20775	-0.00014	1844.99532	1654.78743
0 0 2 0 23	1 1 1 1 22	192.22425	-0.00008	1890.65309	1698.42877
0 0 2 0 24	1 1 1 1 23	194.24477	0.00014	1938.28750	1744.04287
0 0 2 0 25	1 1 1 1 24	196.26858	0.00009	1987.89749	1791.62900
0 0 2 0 26	1 1 1 1 25	198.29551	-0.00001	2039.48198	1841.18647
0 0 2 0 27	1 1 1 1 26	200.32526	-0.00002	2093.03990	1892.71462
0 0 2 0 28	1 1 1 1 27	202.35743	0.00015	2148.57010	1946.21281
0 0 2 0 29	1 1 1 1 28	204.39122	0.00019	2206.07144	2001.68041
0 0 2 0 30	1 1 1 1 29	206.42620	0.00022	2265.54275	2059.11678

rms = 0.00014 cm⁻¹

 Rotational transitions in the $G.S.(\Sigma^+)$, $\nu_4(\Pi)$ and $\nu_5(\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 0 0 1	0 0 0 0 0	1.98306*	0.000009	1.98305	0.000000W
0 0 0 0 3	0 0 0 0 2	5.94904	0.000001	11.89816	5.94912
0 0 0 0 6	0 0 0 0 5	11.89735	0.000002	41.64214	29.74480
0 0 0 0 7	0 0 0 0 6	13.87983	0.000001	55.52197	41.64214
0 0 0 0 8	0 0 0 0 7	15.86212	0.000001	71.38408	55.52197
0 0 0 0 9	0 0 0 0 8	17.84419	0.000001	89.22827	71.38408
0 0 0 0 10	0 0 0 0 9	19.82601	-0.000001	109.05428	89.22827
0 0 0 0 11	0 0 0 0 10	21.80756	0.000000	130.86184	109.05428
1 1 0 0 2	1 1 0 0 1	3.96758	0.000002	524.33282	520.36524
1 1 0 0 6	1 1 0 0 5	11.90186	0.000001	560.03938	548.13753
1 1 0 0 7	1 1 0 0 6	13.88508	-0.000001	573.92447	560.03938
1 -1 0 0 2	1 -1 0 0 1	3.98533	0.000001	524.35945	520.37411
1 -1 0 0 6	1 -1 0 0 5	11.95508	-0.000001	560.22573	548.27064
1 -1 0 0 7	1 -1 0 0 6	13.94717	0.000000	574.17289	560.22573
0 0 1 1 2	0 0 1 1 1	3.96457	0.000001	683.75462	679.79005
0 0 1 1 3	0 0 1 1 2	5.94679	0.000003	689.70140	683.75462
0 0 1 1 6	0 0 1 1 5	11.89283	0.000000	719.43409	707.54126
0 0 1 1 7	0 0 1 1 6	13.87455	0.000000	733.30864	719.43409
0 0 1 -1 2	0 0 1 -1 1	3.97867	0.000000	683.77578	679.79710
0 0 1 -1 3	0 0 1 -1 2	5.96794	-0.000001	689.74371	683.77578
0 0 1 -1 6	0 0 1 -1 5	11.93512	-0.000002	719.58215	707.64702
0 0 1 -1 7	0 0 1 -1 6	13.92388	-0.000005	733.50603	719.58215

rms = 0.000002 cm⁻¹