The infrared spectrum of $^{13}\text{C}_2\text{HD}$ between 100 and 2100 cm^{-1} : a global fit for the bending states up to $v_4 + v_5 = 3$.

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**The infrared spectrum of $^{13}\text{C}_2\text{HD}$ between 100
and 2100 cm^{-1} : a global fit for the bending
states up to $\nu_4 + \nu_5 = 3$**

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Abstract

The fundamental bending ro-vibrational bands and a number of overtone, combination and hot bands of $^{13}\text{C}_2\text{HD}$ have been recorded by Fourier transform infrared spectroscopy (FTIR) in the range 450–2100 cm^{-1} . In addition, the $\nu_5 \leftarrow \nu_4$ band, centred at 164.65 cm^{-1} , has been identified in a spectrum of $^{13}\text{C}_2\text{H}_2$. The data have been analysed simultaneously in a global fit that has provided very accurate rotational and vibrational parameters for the ground and for the vibrationally excited states.

Keywords

$\text{H}^{13}\text{C}^{13}\text{CD}$

High-resolution Fourier Transform Infrared Spectroscopy

Bending vibrations

Fundamental bands

Combination, Overtone, Hot bands

Global analysis

Introduction

Spectroscopic investigations on partially deuterated acetylene isotopologues have been mainly devoted to the $^{12}\text{C}_2\text{HD}$ molecule. High resolution studies provided an accurate characterization of a large number of vibrational states in the bending and stretching fundamental and overtone regions. Recently, the detection of the molecule in Titan's atmosphere by the CIRS instrument mounted on CASSINI spacecraft stimulated the measurement of intensities of several bands and a new global analysis of the bending region [1 and references therein]. $\text{H}^{12}\text{C}^{13}\text{CD}$ and $\text{H}^{13}\text{C}^{12}\text{CD}$ have been the subject of less numerous investigations [2-5].

To our knowledge, only two experimental works were published on $^{13}\text{C}_2\text{HD}$ [2,6]. The authors in Ref. [2] detected the $\nu_5 \leftarrow \text{GS}$ and $\nu_3 \leftarrow \text{GS}$ fundamentals, with band origins at 674 cm^{-1} and 2548 cm^{-1} , respectively, and the $\nu_3 + \nu_4 \leftarrow \nu_4$ and $\nu_3 + \nu_5 \leftarrow \nu_5$ hot bands, with origins at 2533 cm^{-1} and 2545 cm^{-1} , respectively. We have systematically re-investigated the $450\text{--}6500\text{ cm}^{-1}$ spectral range by Infrared Fourier Transform Spectroscopy (FTIR). Because of the great number of lines observed, only the bands below 2000 cm^{-1} and involving the bending modes are reported in this paper, leaving the rest for a further

publication. The most important bands within this range are the bending fundamentals, ν_4 and ν_5 , and the CC stretching fundamental, ν_2 . As usual, a number of hot, overtone and combination bands are easily observed. In addition, the $\nu_5 \leftarrow \nu_4$ hot band centred at 164.65 cm^{-1} has been identified as an impurity in the far infrared spectrum of $^{13}\text{C}_2\text{H}_2$.

The recording was carried out with a 50% pure sample of $^{13}\text{C}_2\text{HD}$ synthesized in Venice (see experimental section). Some interfering bands due to $^{13}\text{C}_2\text{H}_2$, $^{13}\text{C}_2\text{D}_2$ and C_2H_4 were present in the observed spectra.

Forty-nine bands, of which only 9 cold bands, were detected and analysed. Vibrational excitations up to $\nu_{\text{tot}} = \nu_4 + \nu_5 = 3$, with the exception of $\nu_4 = 3$, $\ell_4 = \pm 3$ were observed.

Experimental details

$^{13}\text{C}_2\text{HD}$ was prepared, on a 20-mmol scale, in a two-step reaction following the procedure reported in [7].

In the first reaction step, a solution of $^{13}\text{C}_2$ -monolithium acetylide, $\text{Li}^{13}\text{C}_2\text{H}$, was prepared by the reaction of $^{13}\text{C}_2\text{H}_2$ (^{13}C 99.5 %, Isotec) in anhydrous tetrahydrofuran (THF) with n-butyllithium solution (1.6 M in hexanes, Aldrich) at -80°C . In the second step, $^{13}\text{C}_2\text{HD}$ was obtained by adding acetic acid-OD (D 99.12%, Isotec) in anhydrous THF to the solution of $\text{Li}^{13}\text{C}_2\text{H}$ at -80°C . $^{13}\text{C}_2\text{HD}$ was separated from the reaction mixture by several bulb-to-bulb distillations. The final sample was trapped from -107 to -96°C (2-methylbutane/liquid nitrogen slush bath). The composition of the sample, determined by both FTIR and NMR spectroscopic analysis, was ~50% $^{13}\text{C}_2\text{HD}$, ~35% $^{13}\text{C}_2\text{H}_2$ and ~15% $^{13}\text{C}_2\text{D}_2$. The yield of the species $^{13}\text{C}_2\text{HD}$, based on the starting $^{13}\text{C}_2\text{H}_2$, was estimated to be about 35%.

Although a number of exploratory syntheses of $^{12}\text{C}_2\text{HD}$ has been made prior to the preparation of $^{13}\text{C}_2\text{HD}$, we were not able to replicate the result reported in [7]. The difficulty of obtaining pure C_2HD , free from C_2H_2 and C_2D_2 , has already been reported in [8]. Several spectra were recorded at pressures between 1 and 10 Torr. We mostly used a multipass absorption cell with an effective pathlength of 10 m, but also a 0.18 m long cell. By adjusting these parameters we avoided saturation for the strong bands and detected the weak ones with a reasonable S/N ratio.

The spectra were recorded with a Bomem DA.3 spectrometer equipped with a Globar source, KBr beamsplitter, HgCdTe and InSb detectors. The resolution ranged between 0.004 and 0.008 cm^{-1} . Several hundreds of scans, up to 1000, were co-added in order to improve the quality of the spectra.

Spectra of a $^{13}\text{C}_2\text{H}_2$ sample, containing $^{13}\text{C}_2\text{HD}$ as an impurity, were recorded in the region 50–200 cm^{-1} at 0.003 cm^{-1} resolution at the Steacie Institute for Molecular Sciences in Ottawa with a modified Bomem DA3.002. Optical path length was 18 m and pressure 200 Pa.

Results and discussion

In figures 1 and 2 some examples of the recorded spectra are illustrated. Figure 1 shows the spectral region around the Q-branch of the $\nu_5 \leftarrow \text{GS}$ fundamental band. Figure 2 shows some combination bands at higher energies.

Most of the bands were assigned rather easily and several tens of lines could be identified for each band. The ν_4 spectral region shows a low S/N ratio, if compared with the rest of the spectrum. This is mainly due to the poor performance of our HgCdTe detector below 550 cm^{-1} . This is also the reason why we couldn't detect the $3\nu_4(\Phi) \leftarrow 2\nu_4(\Delta)$ transition, while the corresponding band for the ν_5 bending mode has been observed. The $\nu_4=3(\Phi)$ component is the only state not identified in our search.

[insert Figures 1 and 2 about here]

Table 1 collects all the analysed bands together with the symmetry of the vibrational states involved in the transitions, the band centre, the observed range of J'' values for the various subbands, the number of fitted and

assigned lines and the RMS error resulting from the simultaneous least-squares analysis described below.

[insert Table 1 about here]

Among the 49 bands detected, three of them were observed only through their dominant Q -branch, being the P and R branches too weak or overlapped. These are:

$2\nu_4 + \nu_5 (^1\Pi) \leftarrow 2\nu_4 (\Sigma^+)$, $\nu_4 + 2\nu_5 (^1\Pi) \leftarrow \nu_4 + \nu_5 (\Sigma^+)$ and $3\nu_4 (\Pi) \leftarrow 2\nu_4 (\Delta)$.

The unambiguous assignment of the Q -branch lines was assisted by the knowledge of the energies of the states involved in the transitions from the analysis of other bands.

In the region below 800 cm^{-1} the highest J -transition detected was the $R(43)$ of the fundamental $\nu_5 \leftarrow \text{GS}$ band. Above 800 cm^{-1} the $2\nu_5 \leftarrow \text{GS}$ overtone band was the most extended, with observed transitions up to $P(48)$ and $R(48)$.

Initially, the transition wavenumbers for each band were fitted separately to the upper state ro-vibrational parameters, in order to check the correctness of the assignments and to extend the data set. The data were analysed using the basic Hamiltonian of a linear molecule, with centrifugal distortion corrections up to the sextic

term. For the bending modes, the ℓ -doubling energy contributions containing q_v and q_v^J coefficients were included in the model.

The ro-vibrational energy term values are given by

$$T^0(v, J) = G_v^0 + B_v J(J+1) - D_v [J(J+1)]^2 \mp \frac{1}{2} \{ q_v [J(J+1)] + q_v^J [J(J+1)]^2 \} \quad (1)$$

with the $-$ and $+$ signs related to the e and f levels, respectively, and $G_v^0 = G_v^0 - B_v k^2 - D_v k^4$, with G_v^0 the pure vibrational term value and $k = \ell_4 + \ell_5$.

The band centre is defined as

$$\nu_c = G_v^0 - B_v k^2 - D_v k^4 - (G_{v''}^0 - B_{v''} k^2 - D_{v''} k^4) \quad (2)$$

where G_v^0 and $G_{v''}^0$ represent the purely vibrational energy of the upper and lower state.

Identical unitary weights were assigned to all the transitions, except for the overlapped or very weak lines, which were given zero weight. The values of the spectroscopic parameters of the lower states were kept constrained. Those for the ground state were determined from the simultaneous fit of ground state combination differences

calculated using P and R transitions of the ν_4 and ν_5 bands. The values for the $\nu_4=1$, $\nu_5=1$, $\nu_4=2$, $\nu_4=\nu_5=1$ and $\nu_5=2$ states, were obtained from the fits of the corresponding bands from the ground state.

After having identified all possible transitions in the various bands of the spectra, a simultaneous fit of all the experimental data was performed. The model Hamiltonian adopted for the global analysis is the one used for $^{12}\text{C}_2\text{HD}$ [9]. It represents an extension up to three quanta of excitation, $\nu_{\text{tot}}=3$, of the Hamiltonian for a molecule with two bending vibrations [10]. The energies of the ro-vibrational levels of the transitions were obtained by diagonalizing the appropriate energy matrix containing the following vibration (G^0) and rotation (F) diagonal contributions :

$$\begin{aligned}
 G^0(\nu_4, \ell_4, \nu_5, \ell_5) = & \omega_4^0 \nu_4 + \omega_5^0 \nu_5 + x_{44}^0 (\nu_4)^2 + x_{45}^0 \nu_4 \nu_5 + x_{55}^0 (\nu_5)^2 + g_{44}^0 (\ell_4)^2 \\
 & + g_{45}^0 \ell_4 \ell_5 + g_{55}^0 (\ell_5)^2 + y_{444}^0 (\nu_4)^3 + y_{445}^0 (\nu_4)^2 \nu_5 + y_{455}^0 \nu_4 (\nu_5)^2 + y_{555}^0 (\nu_5)^3 \\
 & + y_4^{44} \nu_4 (\ell_4)^2 + y_4^{45} \nu_4 \ell_4 \ell_5 + y_4^{55} \nu_4 (\ell_5)^2 + y_5^{44} \nu_5 (\ell_4)^2 + y_5^{45} \nu_5 \ell_4 \ell_5 + y_5^{55} \nu_5 (\ell_5)^2 \quad (3)
 \end{aligned}$$

$$\begin{aligned}
F(v_4, \ell_4, v_5, \ell_5) = & [B_0 - \alpha_4 v_4 - \alpha_5 v_5 + \gamma_{44}(v_4)^2 + \gamma_{45} v_4 v_5 + \gamma_{55}(v_5)^2 + \gamma^{44}(\ell_4)^2 + \\
& \gamma^{45} \ell_4 \ell_5 + \gamma^{55}(\ell_5)^2 + \gamma_{444}(v_4)^3 + \gamma_{445}(v_4)^2 v_5 + \gamma_{455} v_4 (v_5)^2 + \gamma_{555}(v_5)^3 + \gamma^{44} v_4 (\ell_4)^2 + \\
& \gamma^{45} v_4 \ell_4 \ell_5 + \gamma^{55} v_4 (\ell_5)^2 + \gamma^{44} v_5 (\ell_4)^2 + \gamma^{45} v_5 \ell_4 \ell_5 + \gamma^{55} v_5 (\ell_5)^2][M - k^2] - [D_0 + \\
& \beta_4 v_4 + \beta_5 v_5 + \delta_{44}(v_4)^2 + \delta_{45} v_4 v_5 + \delta_{55}(v_5)^2 + \delta^{44}(\ell_4)^2 + \delta^{45} \ell_4 \ell_5 + \delta^{55}(\ell_5)^2][M - \\
& k^2]^2 + [H_0 + h_4 v_4 + h_5 v_5][M - k^2]^3
\end{aligned} \quad (4)$$

Vibrational and rotational ℓ -type resonances are expressed by off-diagonal matrix elements [9,10] containing the following parameters:

$$r_{45} = r_{45}^0 + r_{445}(v_4 + 1) + r_{455}(v_5 + 1) + r_{45}^J M \quad (5)$$

$$q_t = q_t^0 + q_{tt} v_t + q_{tt'} v_{t'} + q_t^J M + q_t^k (k \pm 1)^2 \quad (6)$$

$$\rho_t = \rho_t^0 + \rho_{tt} v_t + \rho_{tt'} v_{t'} + \rho_t^J M \quad (7)$$

and ρ_{45}^0 ,

with $M = J(J + 1)$, $t, t' = 4$ or 5 and $k = l_4 + l_5$.

All together, 4342 line wavenumbers out of 4894 assigned transitions, were considered in the final cycle of the

global fit, giving a set of 58 well-determined parameters listed in Table 2. The remaining 552 lines were excluded from the fit because they were overlapped or exceeded the chosen limit for rejection, equal to 0.001 cm^{-1} . In Table 3 the vibrational term values G_c^0 of the observed k -substates are reported.

[insert Tables 2 and 3 about here]

As expected, the results in Table 2 show strong similarities with those of our recent work on $^{12}\text{C}_2\text{HD}$ [9] in terms of dataset and fitted parameters. However, it is interesting to point out that there is a sizable difference concerning the anharmonicity coefficient x_{44}^0 . The experimental value for this constant is $-0.142681(264) \text{ cm}^{-1}$ for $^{12}\text{C}_2\text{HD}$ and $0.010493(259) \text{ cm}^{-1}$ for $^{13}\text{C}_2\text{HD}$. If compared to the value for the most abundant species $^{12}\text{C}_2\text{H}_2$, $3.15781(44) \text{ cm}^{-1}$ [11], two anomalies are evident: x_{44}^0 is negative for $^{12}\text{C}_2\text{HD}$ and two orders of magnitude smaller for $^{13}\text{C}_2\text{HD}$. The most recent theoretical work in the literature [12] agrees with the negative value for $^{12}\text{C}_2\text{HD}$ (-0.286 cm^{-1}) but no calculations for $^{13}\text{C}_2\text{HD}$ are reported. The authors emphasize that the bending motions, particularly ν_4 , are fairly difficult to

describe theoretically, being extremely sensitive to the basis set. Therefore, the calculated values for the anharmonicity constants x_{44}^0 , x_{45}^0 and g_{44}^0 strongly depend on the choice of the basis set. Experimental values for these constants are available in the literature for all isotopologues, except for the mixed species $\text{H}^{13}\text{C}^{12}\text{CD}$ and $\text{H}^{12}\text{C}^{13}\text{CD}$, for which only $x_{44}^0 - g_{44}^0$ was determined from the fits [4], and for $\text{D}^{13}\text{C}^{12}\text{CD}$. These species are being investigated in our laboratory in Bologna. With respect to Ref. [4], we expect to identify a larger number of infrared bands involving the bending modes of the mixed partially deuterated molecules. Their analysis would provide a set of spectroscopic parameters of the same quality as the one presented in this work, and, hopefully, the separate determination of x_{44}^0 and g_{44}^0 . More detailed comments about the anharmonicity constants for different isotopologues of acetylene will be reported in a further paper, when more data will be available.

Tables with the full list of transition wavenumbers, quantum numbers and residuals from the fits are deposited with the British Library under the Supplementary Publications scheme. The tables are also available from the authors.

Conclusions

The infrared spectrum of $^{13}\text{C}_2\text{HD}$ has been recorded in the 450-2000 cm^{-1} spectral region. All the fundamental bands and a number of overtone, combination and hot bands involving excitations of the bending states up to $\nu_4 + \nu_5 = 3$ have been detected. Nearly 5000 assigned transitions were analysed in a global rotation-vibration fit, yielding a set of 58 spectroscopic parameters.

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References

- [1] A. Jolly, Y. Benilan, E. Cané, L. Fusina, F. Tamassia, A. Fayt, S. Robert, M. Herman, *JQSRT.*, **109**, 2846 (2008).
- [2] S. Ghersetti, A. Baldacci, S. Giorgianni, R. H. Barnes, K. Narahari Rao, *Gazz. Chim. It.*, **105**, 875 (1975).
- [3] J. L. Hardwick, Z. T. Martin, M. J. Pilkenton, E. N. Wolf, *J. Mol. Spectrosc.*, **243**, 10 (2007).
- [4] L. Fusina, E. Cané, F. Tamassia, G. Di Lonardo, *Mol. Phys.*, **105**, 2321 (2007).
- [5] G. Cazzoli, C. Puzzarini, L. Fusina, F. Tamassia *J.Mol.Spectrosc.*, **247**, 115 (2008).
- [6] K. A. Mohamed, *Indian J. Pure Appl. Phys.*, **26**, 705 (1998).
- [7] L. Lompa-Krzymien, L.C. Leitch, *Synthesis*, **2**, 124 (1976).
- [8] K. Kim, W.T. King, *J. Mol. Struct.*, **57**, 201 (1979).
- [9] L. Fusina, E. Cané, F. Tamassia, G. Di Lonardo, *Mol. Phys.*, **103**, 3263 (2005).
- [10] M. Herman, T. R. Huet, Y. Kabbady, J. Vander Auwera, *Mol. Phys.*, **72**, 75 (1991).
- [11] S. Robert, M. Herman, J. Vander Auwera, G. Di Lonardo, L. Fusina, G. Blanquet, M. Lepere, A. Fayt, *Mol. Phys.*, **105**, 559 (2007).

[12] J. M. L. Martin, T. J. Lee, P. R. Taylor, *J. Chem. Phys.*, **108**, 676 (1998).

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Table Captions

Table 1

Bands of $^{13}\text{C}_2\text{HD}$ included in the least-squares fitting procedure.

Table 2

Spectroscopic parameters (in cm^{-1}) for $^{13}\text{C}_2\text{HD}$ resulting from the simultaneous fit of all subbands involving levels up to $\nu_4+\nu_5=3$.

Table 3

Vibrational term values, G_v^0 , (in cm^{-1}) of the observed k -substates in $^{13}\text{C}_2\text{HD}$.

Captions for figures

Figure 1.

A portion of the infrared spectrum of $^{13}\text{C}_2\text{HD}$ around the Q -branch of the ν_5 fundamental band. The origins of a number of bands are shown: $\nu_4+\nu_5(\Delta)\leftarrow\nu_4(\Pi)$, $\nu_c=673.8763\text{ cm}^{-1}$; $\nu_4+\nu_5(\Sigma^-)\leftarrow\nu_4(\Pi)$, $\nu_c=674.1592\text{ cm}^{-1}$; $\nu_5(\Pi)\leftarrow\text{GS}(\Sigma^+)$, $\nu_c=674.2363\text{ cm}^{-1}$; $\nu_4+2\nu_5(\Phi)\leftarrow\nu_4+\nu_5(\Delta)$, $\nu_c=677.3190\text{ cm}^{-1}$; $2\nu_5(\Delta)\leftarrow\nu_5(\Pi)$, $\nu_c=677.6629\text{ cm}^{-1}$; $\nu_4+\nu_5(\Sigma^+)\leftarrow\nu_4(\Pi)$, $\nu_c=677.8273\text{ cm}^{-1}$; $\nu_4+2\nu_5(^1\Pi)\leftarrow\nu_4+\nu_5(\Sigma^+)$, $\nu_c=678.1794\text{ cm}^{-1}$. Experimental conditions: pressure 280 Pa, absorption path length 0.18 m, resolution 0.004 cm^{-1} , 480 scans.

Figure 2.

The Q -branches of the $2\nu_4+\nu_5(^1\Pi)\leftarrow\text{GS}(\Sigma^+)$ ($\nu_c=1691.4204\text{ cm}^{-1}$) and $2\nu_4+\nu_5(^1\Pi)\leftarrow\text{GS}(\Sigma^+)$ ($\nu_c=1700.4628\text{ cm}^{-1}$) infrared bands of $^{13}\text{C}_2\text{HD}$. Experimental conditions: pressure 1.33 kPa, absorption path length 10 m, resolution 0.006 cm^{-1} , 800 scans.

Supplementary materials

Molecular Physics: Supplementary Materials (79 pp) for the paper

The infrared spectrum of ¹³C₂HD between 100 and 2100 cm⁻¹: a global fit for the bending states up to ν₄ + ν₅ = 3

by
Luciano Fusina, Filippo Tamassia, Gianfranco Di Lonardo and Alessandro Baldan

Table of the vibration-rotation lines used in the global vibration-rotation fit in ¹³C₂HD

Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm⁻¹) for the bands involving bending states up to ν₄ + ν₅ = 3 of ¹³C₂HD ^a (79 pp)

ν₄(Π) ← G.S. (Σ⁺)

ν ₄ '	ℓ ₄ '	ν ₅ '	ℓ ₅ '	J'	ν ₄ ''	ℓ ₄ ''	ν ₅ ''	ℓ ₅ ''	J''	OBS	OBS – CALC	G'	G''
1	1	0	0	1	0	0	0	0	2	505.78405	-0.00027	511.48627	5.70195
1	1	0	0	2	0	0	0	0	3	503.88436	-0.00013	515.28830	11.40382
1	1	0	0	3	0	0	0	0	4	501.98505	-0.00005	520.99129	19.00619
1	1	0	0	4	0	0	0	0	5	500.08613	-0.00005	528.59515	28.50898
1	1	0	0	5	0	0	0	0	6	498.18767	-0.00008	538.09979	39.91204
1	1	0	0	6	0	0	0	0	7	496.28974	-0.00010	549.50508	53.21523
1	1	0	0	7	0	0	0	0	8	494.39245	-0.00003	562.81086	68.41838
1	1	0	0	8	0	0	0	0	9	492.49590	0.00022	578.01697	85.52129
1	1	0	0	9	0	0	0	0	10	490.59942	-0.00004	595.12319	104.52373
1	1	0	0	10	0	0	0	0	11	488.70381	-0.00004	614.12929	125.42544
1	1	0	0	11	0	0	0	0	12	486.80885	-0.00002	635.03503	148.22616
1	1	0	0	12	0	0	0	0	13	484.91457	0.00002	657.84012	172.92558
1	1	0	0	13	0	0	0	0	14	483.02094	0.00005	682.54427	199.52337
1	1	0	0	14	0	0	0	0	15	481.12852*	0.00059	709.14713	228.01920
1	1	0	0	15	0	0	0	0	16	479.23573	0.00005	737.64836	258.41268
1	1	0	0	16	0	0	0	0	17	477.34427	0.00010	768.04757	290.70340
1	1	0	0	17	0	0	0	0	18	475.45347	0.00006	800.34436	324.89096
1	1	0	0	18	0	0	0	0	19	473.56357	0.00015	834.53830	360.97488
1	1	0	0	19	0	0	0	0	20	471.67476*	0.00054	870.62893	398.95471
1	1	0	0	20	0	0	0	0	21	469.78586	0.00003	908.61577	438.82993
1	1	0	0	21	0	0	0	0	22	467.89844	0.00017	948.49830	480.60003
1	1	0	0	22	0	0	0	0	23	466.01166	0.00010	990.27601	524.26445
1	1	0	0	23	0	0	0	0	24	464.12586	0.00015	1033.94833	569.82262
1	1	0	0	24	0	0	0	0	25	462.24084	0.00009	1079.51468	617.27393
1	1	0	0	25	0	0	0	0	26	460.35700	0.00032	1126.97445	666.61777
1	1	0	0	26	0	0	0	0	27	458.47358	0.00005	1176.32701	717.85348
1	1	0	0	27	0	0	0	0	28	456.59110	-0.00021	1227.57169	770.98038
1	1	0	0	28	0	0	0	0	29	454.70999	-0.00005	1280.70782	825.99778
1	1	0	0	29	0	0	0	0	30	452.82980	0.00007	1335.73468	882.90495
1	1	0	0	30	0	0	0	0	31	450.95056	0.00017	1392.65154	941.70115
1	1	0	0	31	0	0	0	0	32	449.07200	-0.00006	1451.45764	1002.38559
1	1	0	0	32	0	0	0	0	33	447.19344	0.00000	1517.73441	1074.73441
1	1	0	0	33	0	0	0	0	34	445.31488	0.00000	1574.73441	1129.41599

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1	1	0	0	1	0	0	0	0	511.48625	-0.00002	511.48627	0.00000
1	1	0	0	2	0	0	0	1	513.38759	-0.00006	515.28830	1.90066
1	1	0	0	3	0	0	0	2	515.28931	-0.00003	520.99129	5.70195
1	1	0	0	4	0	0	0	3	517.19129	-0.00005	528.59515	11.40382
1	1	0	0	5	0	0	0	4	519.09356	-0.00004	538.09979	19.00619
1	1	0	0	6	0	0	0	5	520.99607	-0.00003	549.50508	28.50898
1	1	0	0	7	0	0	0	6	522.89879	-0.00003	562.81086	39.91204
1	1	0	0	8	0	0	0	7	524.80172	-0.00001	578.01697	53.21523
1	1	0	0	9	0	0	0	8	526.70477	-0.00003	595.12319	68.41838
1	1	0	0	10	0	0	0	9	528.60795	-0.00005	614.12929	85.52129
1	1	0	0	11	0	0	0	10	530.51131	0.00001	635.03503	104.52373
1	1	0	0	12	0	0	0	11	532.41471	0.00003	657.84012	125.42544
1	1	0	0	13	0	0	0	12	534.31809	-0.00002	682.54427	148.22616
1	1	0	0	14	0	0	0	13	536.22160	0.00005	709.14713	172.92558
1	1	0	0	15	0	0	0	14	538.12489	-0.00009	737.64836	199.52337
1	1	0	0	16	0	0	0	15	540.02839	0.00002	768.04757	228.01920
1	1	0	0	17	0	0	0	16	541.93167	-0.00002	800.34436	258.41268
1	1	0	0	18	0	0	0	17	543.83490	0.00000	834.53830	290.70340
1	1	0	0	19	0	0	0	18	545.73791	-0.00006	870.62893	324.89096
1	1	0	0	20	0	0	0	19	547.64104	0.00016	908.61577	360.97488
1	1	0	0	21	0	0	0	20	549.54374	0.00014	948.49830	398.95471
1	1	0	0	22	0	0	0	21	551.44613	0.00005	990.27601	438.82993
1	1	0	0	23	0	0	0	22	553.34825	-0.00005	1033.94833	480.60003
1	1	0	0	24	0	0	0	23	555.25032	0.00009	1079.51468	524.26445
1	1	0	0	25	0	0	0	24	557.15175	-0.00008	1126.97445	569.82262
1	1	0	0	26	0	0	0	25	559.05302	-0.00005	1176.32701	617.27393
1	1	0	0	27	0	0	0	26	560.95372	-0.00020	1227.57169	666.61777
1	1	0	0	28	0	0	0	27	562.85441	0.00007	1280.70782	717.85348
1	1	0	0	29	0	0	0	28	564.75442	0.00012	1335.73468	770.98038
1	1	0	0	30	0	0	0	29	566.65402	0.00026	1392.65154	825.99778
1	1	0	0	31	0	0	0	30	568.55324	0.00055	1451.45764	882.90495
1	1	0	0	32	0	0	0	31	570.45121	0.00015	1512.15220	941.70115
1	1	0	0	33	0	0	0	32	572.34941	0.00059	1574.73441	1002.38559
1	1	0	0	34	0	0	0	33	574.24547*	-0.00048	1639.20342	1064.95747
1	1	0	0	35	0	0	0	34	576.14323	0.00083	1705.55838	1129.41599
1	1	0	0	36	0	0	0	35	578.03838	0.00024	1773.79841	1195.76027
1	1	0	0	37	0	0	0	36	579.93342	0.00028	1843.92260	1263.98946
1	1	0	0	38	0	0	0	37	581.82836	0.00101	1915.93000	1334.10264W
1	1	0	0	39	0	0	0	38	583.72001	-0.00074	1989.81965	1406.09891
1	-1	0	0	1	0	0	0	1	509.59383	-0.00007	511.49456	1.90066
1	-1	0	0	2	0	0	0	2	509.61118	-0.00004	515.31316	5.70195
1	-1	0	0	3	0	0	0	3	509.63714	-0.00005	521.04101	11.40382
1	-1	0	0	4	0	0	0	4	509.67178	-0.00004	528.67801	19.00619
1	-1	0	0	5	0	0	0	5	509.71505	-0.00005	538.22407	28.50898
1	-1	0	0	6	0	0	0	6	509.76698	-0.00004	549.67906	39.91204
1	-1	0	0	7	0	0	0	7	509.82752	-0.00005	563.04281	53.21523
1	-1	0	0	8	0	0	0	8	509.89670	-0.00005	578.31514	68.41838
1	-1	0	0	9	0	0	0	9	509.97455	-0.00001	595.49585	85.52129
1	-1	0	0	10	0	0	0	10	510.06095	-0.00002	614.58469	104.52373
1	-1	0	0	11	0	0	0	11	510.15600	0.00002	635.58142	125.42544
1	-1	0	0	12	0	0	0	12	510.25954	-0.00004	658.48573	148.22616
1	-1	0	0	13	0	0	0	13	510.37169	-0.00005	683.29732	172.92558
1	-1	0	0	14	0	0	0	14	510.49242	-0.00005	710.01584	199.52337
1	-1	0	0	15	0	0	0	15	510.62168	-0.00005	738.64093	228.01920
1	-1	0	0	16	0	0	0	16	510.75943	-0.00009	769.17220	258.41268
1	-1	0	0	17	0	0	0	17	510.90578	-0.00004	801.60923	290.70340
1	-1	0	0	18	0	0	0	18	511.06055	-0.00006	835.95156	324.89096
1	-1	0	0	19	0	0	0	19	511.22380	-0.00006	872.19874	360.97488
1	-1	0	0	20	0	0	0	20	511.39541	-0.00015	910.35027	398.95471
1	-1	0	0	21	0	0	0	21	511.57563	-0.00005	950.40561	438.82993
1	-1	0	0	22	0	0	0	22	511.76411	-0.00009	992.36423	480.60003
1	-1	0	0	23	0	0	0	23	511.96102	-0.00008	1036.22555	524.26445
1	-1	0	0	24	0	0	0	24	512.16622	-0.00012	1081.98896	569.82262
1	-1	0	0	25	0	0	0	25	512.37979	-0.00012	1129.65384	617.27393
1	-1	0	0	26	0	0	0	26	512.60160	-0.00017	1179.21954	666.61777
1	-1	0	0	27	0	0	0	27	512.83172	-0.00018	1230.68537	717.85348
1	-1	0	0	28	0	0	0	28	513.07005	-0.00021	1284.05064	770.98038
1	-1	0	0	29	0	0	0	29	513.31655	-0.00027	1339.31460	825.99778
1	-1	0	0	30	0	0	0	30	513.57169	-0.00014	1396.47651	882.90495

1	-1	0	0	31	0	0	0	0	31	513.83427	-0.00015	1455.53557	941.70115
1	-1	0	0	32	0	0	0	0	32	514.10521	-0.00018	1516.49098	1002.38559
1	-1	0	0	33	0	0	0	0	33	514.38445	0.00002	1579.34190	1064.95747
1	-1	0	0	34	0	0	0	0	34	514.67132	-0.00017	1644.08748	1129.41599
1	-1	0	0	36	0	0	0	0	36	515.26924	-0.00031	1779.25901	1263.98946
1	-1	0	0	37	0	0	0	0	37	515.58055	0.00008	1849.68311	1334.10264
1	-1	0	0	38	0	0	0	0	38	515.89946	0.00021	1921.99816	1406.09891

rms = 0.00018 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	G'	G''
0 0 1 1 1	0 0 0 0 2	670.43408	-0.00010	676.13613	5.70195
0 0 1 1 2	0 0 0 0 3	668.53177	-0.00009	679.93567	11.40382
0 0 1 1 3	0 0 0 0 4	666.62874	0.00000	685.63493	19.00619
0 0 1 1 4	0 0 0 0 5	664.72474	-0.00010	693.23382	28.50898
0 0 1 1 5	0 0 0 0 6	662.82029	0.00009	702.73224	39.91204
0 0 1 1 6	0 0 0 0 7	660.91409*	-0.00075	714.13007	53.21523
0 0 1 1 7	0 0 0 0 8	659.00868	-0.00010	727.42716	68.41838
0 0 1 1 8	0 0 0 0 9	657.10196	-0.00008	742.62333	85.52129
0 0 1 1 9	0 0 0 0 10	655.19440	-0.00026	759.71839	104.52373
0 0 1 1 10	0 0 0 0 11	653.28657	-0.00008	778.71209	125.42544
0 0 1 1 11	0 0 0 0 12	651.37803	-0.00002	799.60420	148.22616
0 0 1 1 12	0 0 0 0 13	649.46861	-0.00026	822.39444	172.92558
0 0 1 1 13	0 0 0 0 14	647.55904	-0.00010	847.08251	199.52337
0 0 1 1 14	0 0 0 0 15	645.64867	-0.00021	873.66808	228.01920
0 0 1 1 15	0 0 0 0 16	643.73806	-0.00006	902.15079	258.41268
0 0 1 1 16	0 0 0 0 17	641.82682	-0.00006	932.53028	290.70340
0 0 1 1 17	0 0 0 0 18	639.91516	-0.00003	964.80614	324.89096
0 0 1 1 18	0 0 0 0 19	638.00322	0.00016	998.97795	360.97488
0 0 1 1 19	0 0 0 0 20	636.09050	-0.00003	1035.04524	398.95471
0 0 1 1 20	0 0 0 0 21	634.17751	-0.00011	1073.00756	438.82993
0 0 1 1 21	0 0 0 0 22	632.26444	0.00009	1112.86438	480.60003
0 0 1 1 22	0 0 0 0 23	630.35084	0.00009	1154.61520	524.26445
0 0 1 1 23	0 0 0 0 24	628.43705	0.00022	1198.25945	569.82262
0 0 1 1 24	0 0 0 0 25	626.52251	-0.00012	1243.79656	617.27393
0 0 1 1 25	0 0 0 0 26	624.60790	-0.00026	1291.22593	666.61777
0 0 1 1 26	0 0 0 0 27	622.69345	0.00000	1340.54693	717.85348
0 0 1 1 27	0 0 0 0 28	620.77800	-0.00053	1391.75891	770.98038
0 0 1 1 28	0 0 0 0 29	618.86334	-0.00007	1444.86119	825.99778
0 0 1 1 29	0 0 0 0 30	616.94810	-0.00002	1499.85307	882.90495
0 0 1 1 30	0 0 0 0 31	615.03260	-0.00008	1556.73383	941.70115
0 0 1 1 31	0 0 0 0 32	613.11712	0.00000	1615.50271	1002.38559
0 0 1 1 32	0 0 0 0 33	611.20120	-0.00026	1676.15894	1064.95747
0 0 1 1 33	0 0 0 0 34	609.28565	-0.00007	1738.70171	1129.41599
0 0 1 1 34	0 0 0 0 35	607.36965	-0.00027	1803.13019	1195.76027
0 0 1 1 35	0 0 0 0 36	605.45418	0.00008	1869.44355	1263.98946
0 0 1 1 36	0 0 0 0 37	603.53783	-0.00043	1937.64090	1334.10264
0 0 1 1 37	0 0 0 0 38	601.62271	0.00028	2007.72134	1406.09891
0 0 1 1 38	0 0 0 0 39	599.70609	-0.00055	2079.68394	1479.97730
0 0 1 1 39	0 0 0 0 40	597.79067	-0.00024	2153.52776	1555.73685
0 0 1 1 40	0 0 0 0 41	595.87522	-0.00004	2229.25182	1633.37656
0 0 1 1 41	0 0 0 0 42	593.95873	-0.00098	2306.85512	1712.89541
0 0 1 1 42	0 0 0 0 43	592.04366	-0.00063	2386.33663	1794.29235
0 0 1 1 43	0 0 0 0 44	590.12939	0.00038	2467.69531	1877.56630
0 0 1 1 44	0 0 0 0 45	588.21483	0.00093	2550.93008	1962.71617
0 0 1 1 45	0 0 0 0 46	586.29903	0.00004	2636.03983	2049.74085
0 0 1 1 1	0 0 0 0 0	676.13618	0.00005	676.13613	0.00000
0 0 1 1 2	0 0 0 0 1	678.03482	-0.00020	679.93567	1.90066
0 0 1 1 3	0 0 0 0 2	679.93290	-0.00008	685.63493	5.70195

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0	0	1	1	4	0	0	0	0	3	681.83001	0.00001	693.23382	11.40382
0	0	1	1	5	0	0	0	0	4	683.72597	-0.00008	702.73224	19.00619
0	0	1	1	6	0	0	0	0	5	685.62104	-0.00006	714.13007	28.50898
0	0	1	1	7	0	0	0	0	6	687.51501	-0.00011	727.42716	39.91204
0	0	1	1	8	0	0	0	0	7	689.40804	-0.00006	742.62333	53.21523
0	0	1	1	9	0	0	0	0	8	691.29989	-0.00011	759.71839	68.41838
0	0	1	1	10	0	0	0	0	9	693.19074	-0.00006	778.71209	85.52129
0	0	1	1	11	0	0	0	0	10	695.08046	-0.00002	799.60420	104.52373
0	0	1	1	12	0	0	0	0	11	696.96899	-0.00002	822.39444	125.42544
0	0	1	1	13	0	0	0	0	12	698.85648	0.00013	847.08251	148.22616
0	0	1	1	14	0	0	0	0	13	700.74251	0.00001	873.66808	172.92558
0	0	1	1	15	0	0	0	0	14	702.62739	-0.00003	902.15079	199.52337
0	0	1	1	16	0	0	0	0	15	704.51109	0.00001	932.53028	228.01920
0	0	1	1	17	0	0	0	0	16	706.39339	-0.00008	964.80614	258.41268
0	0	1	1	18	0	0	0	0	17	708.27445	-0.00009	998.97795	290.70340
0	0	1	1	19	0	0	0	0	18	710.15440	0.00011	1035.04524	324.89096
0	0	1	1	20	0	0	0	0	19	712.03271	0.00004	1073.00756	360.97488
0	0	1	1	21	0	0	0	0	20	713.90977	0.00009	1112.86438	398.95471
0	0	1	1	22	0	0	0	0	21	715.78537	0.00010	1154.61520	438.82993
0	0	1	1	23	0	0	0	0	22	717.65945	0.00003	1198.25945	480.60003
0	0	1	1	24	0	0	0	0	23	719.53208	-0.00003	1243.79656	524.26445
0	0	1	1	25	0	0	0	0	24	721.40328	-0.00003	1291.22593	569.82262
0	0	1	1	26	0	0	0	0	25	723.27310	0.00010	1340.54693	617.27393
0	0	1	1	27	0	0	0	0	26	725.14110	-0.00004	1391.75891	666.61777
0	0	1	1	28	0	0	0	0	27	727.00800	0.00029	1444.86119	717.85348
0	0	1	1	29	0	0	0	0	28	728.87216	-0.00053	1499.85307	770.98038
0	0	1	1	30	0	0	0	0	29	730.73520	-0.00085	1556.73383	825.99778
0	0	1	1	31	0	0	0	0	30	732.59770	-0.00006	1615.50271	882.90495
0	0	1	1	32	0	0	0	0	31	734.45800	0.00021	1676.15894	941.70115
0	0	1	1	33	0	0	0	0	32	736.31620	0.00008	1738.70171	1002.38559
0	0	1	1	34	0	0	0	0	33	738.17255	-0.00017	1803.13019	1064.95747
0	0	1	1	35	0	0	0	0	34	740.02724	-0.00033	1869.44355	1129.41599
0	0	1	1	36	0	0	0	0	35	741.88088	0.00025	1937.64090	1195.76027
0	0	1	1	37	0	0	0	0	36	743.73144	-0.00044	2007.72134	1263.98946
0	0	1	1	38	0	0	0	0	37	745.58131	0.00001	2079.68394	1334.10264
0	0	1	1	39	0	0	0	0	38	747.42835	-0.00051	2153.52776	1406.09891
0	0	1	1	40	0	0	0	0	39	749.27481	0.00029	2229.25182	1479.97730
0	0	1	1	41	0	0	0	0	40	751.11814	-0.00013	2306.85512	1555.73685
0	0	1	1	42	0	0	0	0	41	752.95968	-0.00039	2386.33663	1633.37656
0	0	1	1	43	0	0	0	0	42	754.79938*	-0.00052	2467.69531	1712.89541
0	0	1	1	44	0	0	0	0	43	756.63784	0.00011	2550.93008	1794.29235
0	0	1	-1	1	0	0	0	0	1	674.24191	-0.00008	676.14265	1.90066
0	0	1	-1	2	0	0	0	0	2	674.25319	-0.00010	679.95524	5.70195
0	0	1	-1	3	0	0	0	0	3	674.27014	-0.00010	685.67405	11.40382
0	0	1	-1	4	0	0	0	0	4	674.29276	-0.00007	693.29902	19.00619
0	0	1	-1	5	0	0	0	0	5	674.32077	-0.00029	702.83004	28.50898
0	0	1	-1	6	0	0	0	0	6	674.35485	-0.00009	714.26698	39.91204
0	0	1	-1	7	0	0	0	0	7	674.39415	-0.00031	727.60969	53.21523
0	0	1	-1	8	0	0	0	0	8	674.43967	0.00006	742.85799	68.41838
0	0	1	-1	9	0	0	0	0	9	674.49036	-0.00003	760.01168	85.52129
0	0	1	-1	10	0	0	0	0	10	674.54659	-0.00020	779.07052	104.52373
0	0	1	-1	11	0	0	0	0	11	674.60881	-0.00001	800.03426	125.42544
0	0	1	-1	12	0	0	0	0	12	674.67638	-0.00008	822.90261	148.22616
0	0	1	-1	13	0	0	0	0	13	674.74968	-0.00003	847.67528	172.92558
0	0	1	-1	14	0	0	0	0	14	674.82856	0.00000	874.35193	199.52337
0	0	1	-1	15	0	0	0	0	15	674.91294	-0.00006	902.93220	228.01920
0	0	1	-1	16	0	0	0	0	16	675.00288	-0.00015	933.41570	258.41268
0	0	1	-1	17	0	0	0	0	17	675.09860	-0.00003	965.80204	290.70340
0	0	1	-1	18	0	0	0	0	18	675.19973	-0.00008	1000.09076	324.89096
0	0	1	-1	19	0	0	0	0	19	675.30644	-0.00010	1036.28142	360.97488
0	0	1	-1	20	0	0	0	0	20	675.41854	-0.00028	1074.37353	398.95471
0	0	1	-1	21	0	0	0	0	21	675.53647	-0.00017	1114.36658	438.82993
0	0	1	-1	22	0	0	0	0	22	675.65875*	-0.00124	1156.26002	480.60003W
0	0	1	-1	23	0	0	0	0	23	675.78863	-0.00023	1200.05331	524.26445
0	0	1	-1	24	0	0	0	0	24	675.92318	-0.00004	1245.74584	569.82262
0	0	1	-1	25	0	0	0	0	25	676.06287	-0.00021	1293.33701	617.27393
0	0	1	-1	26	0	0	0	0	26	676.20814	-0.00027	1342.82618	666.61777
0	0	1	-1	27	0	0	0	0	27	676.35892	-0.00029	1394.21269	717.85348
0	0	1	-1	28	0	0	0	0	28	676.51523	-0.00023	1447.49584	770.98038

0	0	1	-1	29	0	0	0	0	29	676.67697	-0.00017	1502.67492	825.99778
0	0	1	-1	30	0	0	0	0	30	676.84420	-0.00004	1559.74920	882.90495
0	0	1	-1	31	0	0	0	0	31	677.01652	-0.00023	1618.71789	941.70115
0	0	1	-1	32	0	0	0	0	32	677.19452	-0.00012	1679.58023	1002.38559
0	0	1	-1	33	0	0	0	0	33	677.37750	-0.00040	1742.33538	1064.95747
0	0	1	-1	34	0	0	0	0	34	677.56637	-0.00015	1806.98250	1129.41599
0	0	1	-1	37	0	0	0	0	37	678.16436	0.00007	2012.26694	1334.10264
0	0	1	-1	39	0	0	0	0	39	678.58942	0.00019	2158.56653	1479.97730

rms = 0.00024 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
0 0 1 1 1	1 1 0 0 2	160.84768	-0.00015	676.13613	515.28830
0 0 1 1 2	1 1 0 0 3	158.94462	0.00024	679.93567	520.99129
0 0 1 1 3	1 1 0 0 4	157.04001	0.00023	685.63493	528.59515
0 0 1 1 4	1 1 0 0 5	155.13411	0.00008	693.23382	538.09979
0 0 1 1 5	1 1 0 0 6	153.22744	0.00028	702.73224	549.50508
0 0 1 1 6	1 1 0 0 7	151.31907	-0.00014	714.13007	562.81086
0 0 1 1 7	1 1 0 0 8	149.41030	0.00011	727.42716	578.01697
0 0 1 1 8	1 1 0 0 9	147.50025	0.00010	742.62333	595.12319
0 0 1 1 9	1 1 0 0 10	145.58922	0.00013	759.71839	614.12929
0 0 1 1 10	1 1 0 0 11	143.67715	0.00009	778.71209	635.03503
0 0 1 1 11	1 1 0 0 12	141.76419	0.00011	799.60420	657.84012
0 0 1 1 12	1 1 0 0 13	139.85022	0.00004	822.39444	682.54427
0 0 1 1 13	1 1 0 0 14	137.93547	0.00009	847.08251	709.14713
0 0 1 1 14	1 1 0 0 15	136.02002	0.00030	873.66808	737.64836
0 0 1 1 15	1 1 0 0 16	134.10331	0.00009	902.15079	768.04757
0 0 1 1 17	1 1 0 0 18	130.26790	0.00006	964.80614	834.53830
0 0 1 1 18	1 1 0 0 19	128.34907	0.00005	998.97795	870.62893
0 0 1 1 19	1 1 0 0 20	126.42956	0.00008	1035.04524	908.61577
0 0 1 1 20	1 1 0 0 21	124.50954	0.00029	1073.00756	948.49830
0 0 1 1 21	1 1 0 0 22	122.58843	0.00006	1112.86438	990.27601
0 0 1 1 22	1 1 0 0 23	120.66715	0.00028	1154.61520	1033.94833
0 0 1 1 23	1 1 0 0 24	118.74489	0.00012	1198.25945	1079.51468
0 0 1 1 24	1 1 0 0 25	116.82228	0.00017	1243.79656	1126.97445
0 0 1 1 25	1 1 0 0 26	114.89871	-0.00022	1291.22593	1176.32701
0 0 1 1 2	1 1 0 0 1	168.44986	0.00046	679.93567	511.48627
0 0 1 1 3	1 1 0 0 2	170.36045*	0.01382	685.63493	515.28830W
0 0 1 1 4	1 1 0 0 3	172.24273	0.00020	693.23382	520.99129
0 0 1 1 5	1 1 0 0 4	174.13726	0.00017	702.73224	528.59515
0 0 1 1 7	1 1 0 0 6	177.92232	0.00024	727.42716	549.50508
0 0 1 1 8	1 1 0 0 7	179.81251	0.00004	742.62333	562.81086
0 0 1 1 9	1 1 0 0 8	181.70173	0.00031	759.71839	578.01697
0 0 1 1 10	1 1 0 0 9	183.58916	0.00025	778.71209	595.12319
0 0 1 1 11	1 1 0 0 10	185.47531	0.00040	799.60420	614.12929
0 0 1 1 12	1 1 0 0 11	187.35963	0.00022	822.39444	635.03503
0 0 1 1 13	1 1 0 0 12	189.24273	0.00034	847.08251	657.84012
0 0 1 1 14	1 1 0 0 13	191.12410	0.00029	873.66808	682.54427
0 0 1 1 15	1 1 0 0 14	193.00399	0.00033	902.15079	709.14713
0 0 1 1 16	1 1 0 0 15	194.88238	0.00046	932.53028	737.64836
0 0 1 1 17	1 1 0 0 16	196.75900	0.00043	964.80614	768.04757
0 0 1 1 18	1 1 0 0 17	198.63371	0.00013	998.97795	800.34436
0 0 1 1 19	1 1 0 0 18	200.50700	0.00006	1035.04524	834.53830
0 0 1 1 1	1 -1 0 0 1	164.64155	-0.00002	676.13613	511.49456
0 0 1 1 2	1 -1 0 0 2	164.62299	0.00048	679.93567	515.31316
0 0 1 1 3	1 -1 0 0 3	164.59396	0.00004	685.63493	521.04101
0 0 1 -1 1	1 -1 0 0 2	160.82981	0.00032	676.14265	515.31316
0 0 1 -1 2	1 -1 0 0 3	158.91126*	-0.00297	679.95524	521.04101W
0 0 1 -1 3	1 -1 0 0 4	156.99620	0.00016	685.67405	528.67801
0 0 1 -1 4	1 -1 0 0 5	155.07505	0.00010	693.29902	538.22407
0 0 1 -1 5	1 -1 0 0 6	153.15112	0.00014	702.83004	549.67906
0 0 1 -1 6	1 -1 0 0 7	151.22435	0.00018	714.26698	563.04281
0 0 1 -1 7	1 -1 0 0 8	149.29467	0.00012	727.60969	578.31514
0 0 1 -1 8	1 -1 0 0 9	147.37599	0.00012	742.85799	595.49585

0	0	1	-1	9	1	-1	0	0	10	145.42706	0.00008	760.01168	614.58469
0	0	1	-1	10	1	-1	0	0	11	143.48921	0.00011	779.07052	635.58142
0	0	1	-1	11	1	-1	0	0	12	141.54836	-0.00016	800.03426	658.48573
0	0	1	-1	12	1	-1	0	0	13	139.60537	0.00008	822.90261	683.29732
0	0	1	-1	13	1	-1	0	0	14	137.65943	-0.00001	847.67528	710.01584
0	0	1	-1	14	1	-1	0	0	15	135.71003*	-0.00097	874.35193	738.64093
0	0	1	-1	15	1	-1	0	0	16	133.75990	-0.00010	902.93220	769.17220
0	0	1	-1	17	1	-1	0	0	18	129.85049	0.00002	965.80204	835.95156
0	0	1	-1	18	1	-1	0	0	19	127.89203	0.00001	1000.09076	872.19874
0	0	1	-1	19	1	-1	0	0	20	125.93126	0.00010	1036.28142	910.35027
0	0	1	-1	20	1	-1	0	0	21	123.96786	-0.00006	1074.37353	950.40561
0	0	1	-1	21	1	-1	0	0	22	122.00214	-0.00021	1114.36658	992.36423
0	0	1	-1	22	1	-1	0	0	23	120.03447	0.00000	1156.26002	1036.22555
0	0	1	-1	23	1	-1	0	0	24	118.06410	-0.00024	1200.05331	1081.98896
0	0	1	-1	24	1	-1	0	0	25	116.09212	0.00012	1245.74584	1129.65384
0	0	1	-1	25	1	-1	0	0	26	114.11787	0.00040	1293.33701	1179.21954
0	0	1	-1	2	1	-1	0	0	1	168.46065	-0.00003	679.95524	511.49456
0	0	1	-1	3	1	-1	0	0	2	170.36104*	0.00015	685.67405	515.31316
0	0	1	-1	4	1	-1	0	0	3	172.25829	0.00028	693.29902	521.04101
0	0	1	-1	5	1	-1	0	0	4	174.15231	0.00028	702.83004	528.67801
0	0	1	-1	6	1	-1	0	0	5	176.04313	0.00022	714.26698	538.22407
0	0	1	-1	7	1	-1	0	0	6	177.93081	0.00017	727.60969	549.67906
0	0	1	-1	8	1	-1	0	0	7	179.81396*	-0.00123	742.85799	563.04281W
0	0	1	-1	9	1	-1	0	0	8	181.69677	0.00023	760.01168	578.31514
0	0	1	-1	10	1	-1	0	0	9	183.57486	0.00019	779.07052	595.49585
0	0	1	-1	11	1	-1	0	0	10	185.44987	0.00031	800.03426	614.58469
0	0	1	-1	12	1	-1	0	0	11	187.32145	0.00025	822.90261	635.58142
0	0	1	-1	13	1	-1	0	0	12	189.18984	0.00029	847.67528	658.48573
0	0	1	-1	14	1	-1	0	0	13	191.05477	0.00016	874.35193	683.29732
0	0	1	-1	15	1	-1	0	0	14	192.91643	0.00007	902.93220	710.01584
0	0	1	-1	16	1	-1	0	0	15	194.77505	0.00028	933.41570	738.64093
0	0	1	-1	17	1	-1	0	0	16	196.63005	0.00021	965.80204	769.17220
0	0	1	-1	18	1	-1	0	0	17	198.48176	0.00022	1000.09076	801.60923
0	0	1	-1	19	1	-1	0	0	18	200.33043	0.00057	1036.28142	835.95156
0	0	1	-1	1	1	1	0	0	1	164.65658	0.00020	676.14265	511.48627
0	0	1	-1	2	1	1	0	0	2	164.66689	-0.00004	679.95524	515.28830

rms = 0.00022 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 0 0 0 0	1 1 0 0 1	505.36430*	-0.00082	1016.85139	511.48627
2 0 0 0 1	1 1 0 0 2	503.47264	-0.00055	1018.76149	515.28830
2 0 0 0 2	1 1 0 0 3	501.59035	0.00005	1022.58159	520.99129
2 0 0 0 3	1 1 0 0 4	499.71643	0.00015	1028.31143	528.59515
2 0 0 0 4	1 1 0 0 5	497.85125	0.00040	1035.95064	538.09979
2 0 0 0 5	1 1 0 0 6	495.99366	-0.00001	1045.49875	549.50508
2 0 0 0 6	1 1 0 0 7	494.14417	-0.00011	1056.95515	562.81086
2 0 0 0 7	1 1 0 0 8	492.30244	0.00031	1070.31910	578.01697
2 0 0 0 8	1 1 0 0 9	490.46686	0.00028	1085.58977	595.12319
2 0 0 0 9	1 1 0 0 10	488.63695	0.00003	1102.76621	614.12929
2 0 0 0 10	1 1 0 0 11	486.81323*	0.00088	1121.84738	635.03503
2 0 0 0 11	1 1 0 0 12	484.99178	-0.00026	1142.83216	657.84012
2 0 0 0 12	1 1 0 0 13	483.17512	0.00003	1165.71936	682.54427
2 0 0 0 13	1 1 0 0 14	481.36076	0.00015	1190.50774	709.14713
2 0 0 0 14	1 1 0 0 15	479.54765	-0.00005	1217.19606	737.64836
2 0 0 0 15	1 1 0 0 16	477.73558	0.00007	1245.78308	768.04757
2 0 0 0 16	1 1 0 0 17	475.92339	0.00015	1276.26760	800.34436
2 0 0 0 17	1 1 0 0 18	474.11045	0.00027	1308.64848	834.53830
2 0 0 0 18	1 1 0 0 19	472.29548	-0.00025	1342.92466	870.62893
2 0 0 0 19	1 1 0 0 20	470.47942	0.00004	1379.09514	908.61577
2 0 0 0 20	1 1 0 0 21	468.66049	-0.00026	1417.15906	948.49830
2 0 0 0 21	1 1 0 0 22	466.83934	-0.00025	1457.11560	990.27601

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

1	2	0	0	0	22	1	1	0	0	23	465.01566	-0.00007	1498.96407	1033.94833
2	2	0	0	0	23	1	1	0	0	24	463.18911	-0.00002	1542.70381	1079.51468
3	2	0	0	0	24	1	1	0	0	25	461.35952	-0.00027	1588.33424	1126.97445
4	2	0	0	0	25	1	1	0	0	26	459.52772	-0.00008	1635.85480	1176.32701
5	2	0	0	0	26	1	1	0	0	27	457.69238	-0.00091	1685.26498	1227.57169
6	2	0	0	0	27	1	1	0	0	28	455.85571	-0.00073	1736.56425	1280.70782
7	2	0	0	0	2	1	1	0	0	1	511.09625*	0.00093	1022.58159	511.48627
8	2	0	0	0	3	1	1	0	0	2	513.02280	-0.00033	1028.31143	515.28830
9	2	0	0	0	4	1	1	0	0	3	514.95949	0.00013	1035.95064	520.99129
10	2	0	0	0	5	1	1	0	0	4	516.90355	-0.00005	1045.49875	528.59515
11	2	0	0	0	6	1	1	0	0	5	518.85534	-0.00001	1056.95515	538.09979
12	2	0	0	0	7	1	1	0	0	6	520.81419	0.00017	1070.31910	549.50508
13	2	0	0	0	8	1	1	0	0	7	522.77887	-0.00003	1085.58977	562.81086
14	2	0	0	0	9	1	1	0	0	8	524.74939	0.00015	1102.76621	578.01697
15	2	0	0	0	10	1	1	0	0	9	526.72417	-0.00003	1121.84738	595.12319
16	2	0	0	0	11	1	1	0	0	10	528.70300	0.00013	1142.83216	614.12929
17	2	0	0	0	12	1	1	0	0	11	530.68448	0.00015	1165.71936	635.03503
18	2	0	0	0	13	1	1	0	0	12	532.66778	0.00016	1190.50774	657.84012
19	2	0	0	0	14	1	1	0	0	13	534.65184	0.00005	1217.19606	682.54427
20	2	0	0	0	15	1	1	0	0	14	536.63617	0.00022	1245.78308	709.14713
21	2	0	0	0	16	1	1	0	0	15	538.61918	-0.00006	1276.26760	737.64836
22	2	0	0	0	17	1	1	0	0	16	540.60109	0.00018	1308.64848	768.04757
23	2	0	0	0	18	1	1	0	0	17	542.58066	0.00037	1342.92466	800.34436
24	2	0	0	0	19	1	1	0	0	18	544.55685	0.00001	1379.09514	834.53830
25	2	0	0	0	20	1	1	0	0	19	546.52979	-0.00034	1417.15906	870.62893
26	2	0	0	0	21	1	1	0	0	20	548.49955	-0.00029	1457.11560	908.61577
27	2	0	0	0	22	1	1	0	0	21	550.46538	-0.00038	1498.96407	948.49830
28	2	0	0	0	23	1	1	0	0	22	552.42807	0.00027	1542.70381	990.27601
29	2	0	0	0	24	1	1	0	0	23	554.38632	0.00042	1588.33424	1033.94833
30	2	0	0	0	25	1	1	0	0	24	556.34007	-0.00005	1635.85480	1079.51468
31	2	0	0	0	26	1	1	0	0	25	558.29026	-0.00027	1685.26498	1126.97445
32	2	0	0	0	27	1	1	0	0	26	560.23755	0.00030	1736.56425	1176.32701
33	2	0	0	0	28	1	1	0	0	27	562.18061	0.00019	1789.75210	1227.57169
34	2	0	0	0	29	1	1	0	0	28	564.12050	0.00031	1844.82800	1280.70782
35	2	0	0	0	30	1	1	0	0	29	566.05629	-0.00043	1901.79140	1335.73468
36	2	0	0	0	31	1	1	0	0	30	567.98950	-0.00067	1960.64171	1392.65154
37	2	0	0	0	32	1	1	0	0	31	569.92028	-0.00042	2021.37834	1451.45764
38	2	0	0	0	33	1	1	0	0	32	571.84781	-0.00063	2084.00064	1512.15220
39	2	0	0	0	34	1	1	0	0	33	573.77294	-0.00060	2148.50794	1574.73441
40	2	0	0	0	35	1	1	0	0	34	575.69473	-0.00139	2214.89954	1639.20342W
41	2	0	0	0	8	1	-1	0	0	8	507.27536*	0.00073	1085.58977	578.31514
42	2	0	0	0	9	1	-1	0	0	9	507.27034	-0.00002	1102.76621	595.49585
43	2	0	0	0	10	1	-1	0	0	10	507.26282	0.00013	1121.84738	614.58469
44	2	0	0	0	11	1	-1	0	0	11	507.25090	0.00016	1142.83216	635.58142
45	2	0	0	0	12	1	-1	0	0	12	507.23377	0.00014	1165.71936	658.48573
46	2	0	0	0	13	1	-1	0	0	13	507.21039	-0.00003	1190.50774	683.29732
47	2	0	0	0	14	1	-1	0	0	14	507.18021	-0.00001	1217.19606	710.01584
48	2	0	0	0	15	1	-1	0	0	15	507.14234	0.00019	1245.78308	738.64093
49	2	0	0	0	16	1	-1	0	0	16	507.09535	-0.00005	1276.26760	769.17220
50	2	0	0	0	17	1	-1	0	0	17	507.03944	0.00018	1308.64848	801.60923
51	2	0	0	0	18	1	-1	0	0	18	506.97316	0.00007	1342.92466	835.95156
52	2	0	0	0	19	1	-1	0	0	19	506.89630	-0.00010	1379.09514	872.19874
53	2	0	0	0	20	1	-1	0	0	20	506.80889	0.00010	1417.15906	910.35027
54	2	0	0	0	21	1	-1	0	0	21	506.70951	-0.00048	1457.11560	950.40561
55	2	0	0	0	22	1	-1	0	0	22	506.59997	0.00014	1498.96407	992.36423
56	2	0	0	0	23	1	-1	0	0	23	506.47884*	0.00058	1542.70381	1036.22555
57	2	0	0	0	24	1	-1	0	0	24	506.34556	0.00028	1588.33424	1081.98896
58	2	0	0	0	25	1	-1	0	0	25	506.20062	-0.00034	1635.85480	1129.65384

rms = 0.00028 cm⁻¹

$2\nu_4(\Delta) \leftarrow \nu_4(\Pi)$

ν_4'	ℓ_4'	V_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	G'	G''
2	2	0	0	2	1	1	0	0	3	505.99028	0.00063	1026.98094	520.99129
2	2	0	0	3	1	1	0	0	4	505.99028	0.00063	1032.70973	528.59515

1	2	2	0	0	4	1	1	0	0	5	502.24893	0.00029	1040.34843	538.09979
2	2	2	0	0	5	1	1	0	0	6	500.39203	-0.00021	1049.89732	549.50508
3	2	2	0	0	6	1	1	0	0	7	498.54613	0.00024	1061.35675	562.81086
4	2	2	0	0	7	1	1	0	0	8	496.71018	0.00003	1074.72712	578.01697
5	2	2	0	0	8	1	1	0	0	9	494.88584	0.00014	1090.00889	595.12319
6	2	2	0	0	9	1	1	0	0	10	493.07287	-0.00043	1107.20259	614.12929
7	2	2	0	0	10	1	1	0	0	11	491.27362	-0.00014	1126.30879	635.03503
8	2	2	0	0	11	1	1	0	0	12	489.48782	-0.00013	1147.32807	657.84012
9	2	2	0	0	12	1	1	0	0	13	487.71665	-0.00014	1170.26105	682.54427
10	2	2	0	0	13	1	1	0	0	14	485.96136	0.00017	1195.10832	709.14713
11	2	2	0	0	14	1	1	0	0	15	484.22240	0.00032	1221.87043	737.64836
12	2	2	0	0	15	1	1	0	0	16	482.50035	0.00004	1250.54788	768.04757
13	2	2	0	0	16	1	1	0	0	17	480.79634	-0.00038	1281.14108	800.34436
14	2	2	0	0	17	1	1	0	0	18	479.11137	-0.00065	1313.65031	834.53830
15	2	2	0	0	18	1	1	0	0	19	477.44832	0.00150	1348.07575	870.62893W
16	2	2	0	0	19	1	1	0	0	20	475.80214	0.00049	1384.41742	908.61577
17	2	2	0	0	2	1	1	0	0	1	515.49489	0.00022	1026.98094	511.48627
18	2	2	0	0	3	1	1	0	0	2	517.42158	0.00016	1032.70973	515.28830
19	2	2	0	0	4	1	1	0	0	3	519.35736	0.00022	1040.34843	520.99129
20	2	2	0	0	5	1	1	0	0	4	521.30242	0.00025	1049.89732	528.59515
21	2	2	0	0	6	1	1	0	0	5	523.25699	0.00003	1061.35675	538.09979
22	2	2	0	0	7	1	1	0	0	6	525.22212	0.00008	1074.72712	549.50508
23	2	2	0	0	8	1	1	0	0	7	527.19814	0.00011	1090.00889	562.81086
24	2	2	0	0	9	1	1	0	0	8	529.18568	0.00005	1107.20259	578.01697
25	2	2	0	0	10	1	1	0	0	9	531.18577	0.00017	1126.30879	595.12319
26	2	2	0	0	11	1	1	0	0	10	533.19868	-0.00010	1147.32807	614.12929
27	2	2	0	0	12	1	1	0	0	11	535.22577	-0.00025	1170.26105	635.03503
28	2	2	0	0	13	1	1	0	0	12	537.26833	0.00013	1195.10832	657.84012
29	2	2	0	0	14	1	1	0	0	13	539.32666	0.00049	1221.87043	682.54427
30	2	2	0	0	15	1	1	0	0	14	541.40105	0.00030	1250.54788	709.14713
31	2	2	0	0	16	1	1	0	0	15	543.49291	0.00019	1281.14108	737.64836
32	2	2	0	0	17	1	1	0	0	16	545.60267	-0.00007	1313.65031	768.04757
33	2	2	0	0	18	1	1	0	0	17	547.73177	0.00038	1348.07575	800.34436
34	2	2	0	0	19	1	1	0	0	18	549.87903	-0.00009	1384.41742	834.53830
35	2	2	0	0	20	1	1	0	0	19	552.04634	0.00008	1422.67519	870.62893
36	2	2	0	0	21	1	1	0	0	20	554.23367	0.00064	1462.84880	908.61577
37	2	2	0	0	22	1	1	0	0	21	556.43949	-0.00005	1504.93784	948.49830
38	2	2	0	0	23	1	1	0	0	22	558.66653	0.00073	1548.94181	990.27601
39	2	2	0	0	24	1	1	0	0	23	560.91308	0.00135	1594.86006	1033.94833W
40	2	2	0	0	2	1	-1	0	0	2	511.66906*	0.00128	1026.98094	515.31316W
41	2	2	0	0	3	1	-1	0	0	3	511.66906	0.00034	1032.70973	521.04101
42	2	2	0	0	4	1	-1	0	0	4	511.66906*	-0.00136	1040.34843	528.67801W
43	2	2	0	0	5	1	-1	0	0	5	511.67313	-0.00012	1049.89732	538.22407
44	2	2	0	0	6	1	-1	0	0	6	511.67797	0.00027	1061.35675	549.67906
45	2	2	0	0	7	1	-1	0	0	7	511.68435	0.00004	1074.72712	563.04281
46	2	2	0	0	8	1	-1	0	0	8	511.69358	-0.00017	1090.00889	578.31514
47	2	2	0	0	9	1	-1	0	0	9	511.70686	0.00012	1107.20259	595.49585
48	2	2	0	0	10	1	-1	0	0	10	511.72423	0.00014	1126.30879	614.58469
49	2	2	0	0	11	1	-1	0	0	11	511.74668	0.00002	1147.32807	635.58142
50	2	2	0	0	12	1	-1	0	0	12	511.77536	0.00004	1170.26105	658.48573
51	2	2	0	0	13	1	-1	0	0	13	511.81103	0.00003	1195.10832	683.29732
52	2	2	0	0	14	1	-1	0	0	14	511.85464	0.00005	1221.87043	710.01584
53	2	2	0	0	15	1	-1	0	0	15	511.90666	-0.00029	1250.54788	738.64093
54	2	2	0	0	16	1	-1	0	0	16	511.96913	0.00025	1281.14108	769.17220
55	2	2	0	0	17	1	-1	0	0	17	512.04120	0.00011	1313.65031	801.60923
56	2	2	0	0	18	1	-1	0	0	18	512.12434	0.00015	1348.07575	835.95156
57	2	2	0	0	19	1	-1	0	0	19	512.21872	0.00005	1384.41742	872.19874
58	2	2	0	0	20	1	-1	0	0	20	512.32602*	0.00110	1422.67519	910.35027W
59	2	2	0	0	21	1	-1	0	0	21	512.44334	0.00016	1462.84880	950.40561
60	2	2	0	0	22	1	-1	0	0	22	512.57436	0.00075	1504.93784	992.36423
	2	2	0	0	23	1	-1	0	0	23	512.71641	0.00015	1548.94181	1036.22555
	2	2	0	0	24	1	-1	0	0	24	512.87125	0.00015	1594.86006	1081.98896
	2	2	0	0	25	1	-1	0	0	25	513.03824	0.00021	1642.69188	1129.65384
	2	2	0	0	26	1	-1	0	0	26	513.21732	0.00040	1692.43646	1179.21954
	2	2	0	0	27	1	-1	0	0	27	513.40787	0.00030	1744.09294	1230.68537
	2	2	0	0	28	1	-1	0	0	28	513.60972	-0.00006	1797.66042	1284.05064
	2	-2	0	0	2	1	-1	0	0	3	505.94133*	0.00149	1026.98084	521.04101W
	2	-2	0	0	3	1	-1	0	0	4	504.03090	-0.00034	1032.70925	528.67801
	2	-2	0	0	4	1	-1	0	0	5	502.12306	0.00013	1040.34700	538.22407

1	2	-2	0	0	5	1	-1	0	0	6	500.21541	0.00047	1049.89400	549.67906
2	2	-2	0	0	6	1	-1	0	0	7	498.30730	0.00001	1061.35010	563.04281
3	2	-2	0	0	7	1	-1	0	0	8	496.40022	0.00022	1074.71514	578.31514
4	2	-2	0	0	8	1	-1	0	0	9	494.49282	-0.00029	1089.98896	595.49585
5	2	-2	0	0	9	1	-1	0	0	10	492.58669	0.00007	1107.17132	614.58469
6	2	-2	0	0	10	1	-1	0	0	11	490.68068	0.00010	1126.26199	635.58142
7	2	-2	0	0	11	1	-1	0	0	12	488.77528	0.00029	1147.26072	658.48573
8	2	-2	0	0	12	1	-1	0	0	13	486.86990	0.00002	1170.16720	683.29732
9	2	-2	0	0	13	1	-1	0	0	14	484.96530	0.00002	1194.98112	710.01584
10	2	-2	0	0	14	1	-1	0	0	15	483.06085	-0.00035	1221.70214	738.64093
11	2	-2	0	0	15	1	-1	0	0	16	481.15769	0.00001	1250.32988	769.17220
12	2	-2	0	0	16	1	-1	0	0	17	479.25447	-0.00026	1280.86395	801.60923
13	2	-2	0	0	17	1	-1	0	0	18	477.35241	0.00005	1313.30393	835.95156
14	2	-2	0	0	18	1	-1	0	0	19	475.44980	-0.00082	1347.64936	872.19874
15	2	-2	0	0	19	1	-1	0	0	20	473.54973	0.00023	1383.89977	910.35027
16	2	-2	0	0	20	1	-1	0	0	21	471.64844	-0.00060	1422.05465	950.40561
17	2	-2	0	0	21	1	-1	0	0	22	469.74922	-0.00004	1462.11349	992.36423
18	2	-2	0	0	22	1	-1	0	0	23	467.84922	-0.00095	1504.07572	1036.22555
19	2	-2	0	0	23	1	-1	0	0	24	465.95120	-0.00059	1547.94075	1081.98896
20	2	-2	0	0	24	1	-1	0	0	25	464.05383	-0.00032	1593.70799	1129.65384
21	2	-2	0	0	2	1	-1	0	0	1	515.48639	0.00010	1026.98084	511.49456
22	2	-2	0	0	3	1	-1	0	0	2	517.39664	0.00055	1032.70925	515.31316
23	2	-2	0	0	4	1	-1	0	0	3	519.30624	0.00024	1040.34700	521.04101
24	2	-2	0	0	5	1	-1	0	0	4	521.21596	-0.00002	1049.89400	528.67801
25	2	-2	0	0	6	1	-1	0	0	5	523.12617	0.00015	1061.35010	538.22407
26	2	-2	0	0	7	1	-1	0	0	6	525.03615	0.00006	1074.71514	549.67906
27	2	-2	0	0	8	1	-1	0	0	7	526.94643	0.00028	1089.98896	563.04281
28	2	-2	0	0	9	1	-1	0	0	8	528.85634	0.00016	1107.17132	578.31514
29	2	-2	0	0	10	1	-1	0	0	9	530.76599	-0.00016	1126.26199	595.49585
30	2	-2	0	0	11	1	-1	0	0	10	532.67618	0.00016	1147.26072	614.58469
31	2	-2	0	0	12	1	-1	0	0	11	534.58580	0.00002	1170.16720	635.58142
32	2	-2	0	0	13	1	-1	0	0	12	536.49515	-0.00024	1194.98112	658.48573
33	2	-2	0	0	14	1	-1	0	0	13	538.40508	0.00026	1221.70214	683.29732
34	2	-2	0	0	15	1	-1	0	0	14	540.31384	-0.00020	1250.32988	710.01584
35	2	-2	0	0	16	1	-1	0	0	15	542.22289	-0.00013	1280.86395	738.64093
36	2	-2	0	0	17	1	-1	0	0	16	544.13134	-0.00039	1313.30393	769.17220
37	2	-2	0	0	18	1	-1	0	0	17	546.04022	0.00009	1347.64936	801.60923
38	2	-2	0	0	19	1	-1	0	0	18	547.94812	-0.00009	1383.89977	835.95156
39	2	-2	0	0	20	1	-1	0	0	19	549.85585	-0.00006	1422.05465	872.19874
40	2	-2	0	0	21	1	-1	0	0	20	551.76300	-0.00022	1462.11349	910.35027
41	2	-2	0	0	22	1	-1	0	0	21	553.67072*	0.00062	1504.07572	950.40561
42	2	-2	0	0	23	1	-1	0	0	22	555.57594	-0.00058	1547.94075	992.36423
43	2	-2	0	0	24	1	-1	0	0	23	557.48197	-0.00047	1593.70799	1036.22555
44	2	-2	0	0	25	1	-1	0	0	24	559.38816	0.00032	1641.37680	1081.98896
45	2	-2	0	0	26	1	-1	0	0	25	561.29324	0.00057	1690.94652	1129.65384
46	2	-2	0	0	27	1	-1	0	0	26	563.19681	-0.00010	1742.41645	1179.21954
47	2	-2	0	0	28	1	-1	0	0	27	565.10027	-0.00025	1795.78589	1230.68537
48	2	-2	0	0	29	1	-1	0	0	28	567.00350	0.00004	1851.05410	1284.05064
49	2	-2	0	0	30	1	-1	0	0	29	568.90616	0.00045	1908.22031	1339.31460
50	2	-2	0	0	31	1	-1	0	0	30	570.80995*	0.00273	1967.28373	1396.47651W
51	2	-2	0	0	32	1	-1	0	0	31	572.70823	0.00026	2028.24354	1455.53557
52	2	-2	0	0	33	1	-1	0	0	32	574.60905	0.00114	2091.09889	1516.49098W
53	2	-2	0	0	2	1	1	0	0	2	511.69358*	0.00104	1026.98084	515.28830W
54	2	-2	0	0	3	1	1	0	0	3	511.71831	0.00035	1032.70925	520.99129
55	2	-2	0	0	4	1	1	0	0	4	511.75209	0.00024	1040.34700	528.59515
56	2	-2	0	0	5	1	1	0	0	5	511.79442	0.00021	1049.89400	538.09979
57	2	-2	0	0	6	1	1	0	0	6	511.84464*	-0.00038	1061.35010	549.50508
58	2	-2	0	0	7	1	1	0	0	7	511.90372*	-0.00056	1074.71514	562.81086
59	2	-2	0	0	8	1	1	0	0	8	511.97214	0.00015	1089.98896	578.01697
60	2	-2	0	0	9	1	1	0	0	9	512.04812	-0.00001	1107.17132	595.12319
	2	-2	0	0	10	1	1	0	0	10	512.13284	0.00014	1126.26199	614.12929
	2	-2	0	0	11	1	1	0	0	11	512.22570	0.00001	1147.26072	635.03503
	2	-2	0	0	12	1	1	0	0	12	512.32664	-0.00044	1170.16720	657.84012
	2	-2	0	0	13	1	1	0	0	13	512.43681	-0.00004	1194.98112	682.54427
	2	-2	0	0	14	1	1	0	0	14	512.55509	0.00008	1221.70214	709.14713
	2	-2	0	0	15	1	1	0	0	15	512.68131	-0.00021	1250.32988	737.64836
	2	-2	0	0	16	1	1	0	0	16	512.81610	-0.00028	1280.86395	768.04757
	2	-2	0	0	17	1	1	0	0	17	512.95934	-0.00023	1313.30393	800.34436
	2	-2	0	0	18	1	1	0	0	18	513.11076	-0.00039	1347.64936	834.53830

2	-2	0	0	19	1	1	0	0	19	513.27048	-0.00036	1383.89977	870.62893
2	-2	0	0	20	1	1	0	0	20	513.43881	-0.00008	1422.05465	908.61577
2	-2	0	0	21	1	1	0	0	21	513.61490	-0.00028	1462.11349	948.49830
2	-2	0	0	22	1	1	0	0	22	513.79946	-0.00024	1504.07572	990.27601
2	-2	0	0	23	1	1	0	0	23	513.99205	-0.00037	1547.94075	1033.94833
2	-2	0	0	24	1	1	0	0	24	514.19275	-0.00056	1593.70799	1079.51468
2	-2	0	0	25	1	1	0	0	25	514.40253	0.00018	1641.37680	1126.97445
2	-2	0	0	26	1	1	0	0	26	514.61940	-0.00011	1690.94652	1176.32701
2	-2	0	0	27	1	1	0	0	27	514.84523	0.00047	1742.41645	1227.57169
2	-2	0	0	28	1	1	0	0	28	515.07795	-0.00013	1795.78589	1280.70782
2	-2	0	0	29	1	1	0	0	29	515.31936	-0.00006	1851.05410	1335.73468
2	-2	0	0	30	1	1	0	0	30	515.57034*	0.00157	1908.22031	1392.65154W
2	-2	0	0	31	1	1	0	0	31	515.82586	-0.00023	1967.28373	1451.45764
2	-2	0	0	32	1	1	0	0	32	516.09199	0.00066	2028.24354	1512.15220
2	-2	0	0	33	1	1	0	0	33	516.36378	-0.00070	2091.09889	1574.73441

rms = 0.00031 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 1 -1 0	1 1 0 0 1	675.92263*	-0.00367	1187.41257	511.48627W
1 1 1 -1 1	1 1 0 0 2	674.03127	-0.00046	1189.32003	515.28830
1 1 1 -1 2	1 1 0 0 3	672.14360	-0.00013	1193.13502	520.99129
1 1 1 -1 3	1 1 0 0 4	670.26216	-0.00033	1198.85764	528.59515
1 1 1 -1 4	1 1 0 0 5	668.38825	-0.00004	1206.48808	538.09979
1 1 1 -1 5	1 1 0 0 6	666.52149	0.00002	1216.02655	549.50508
1 1 1 -1 6	1 1 0 0 7	664.66246	-0.00001	1227.47333	562.81086
1 1 1 -1 7	1 1 0 0 8	662.81196	0.00015	1240.82878	578.01697
1 1 1 -1 8	1 1 0 0 9	660.96934	-0.00073	1256.09326	595.12319
1 1 1 -1 9	1 1 0 0 10	659.13768	-0.00023	1273.26720	614.12929
1 1 1 -1 10	1 1 0 0 11	657.31595	-0.00008	1292.35106	635.03503
1 1 1 -1 11	1 1 0 0 12	655.50490	-0.00029	1313.34532	657.84012
1 1 1 -1 12	1 1 0 0 13	653.70611	-0.00006	1336.25044	682.54427
1 1 1 -1 13	1 1 0 0 14	651.91946	-0.00030	1361.06689	709.14713
1 1 1 -1 14	1 1 0 0 15	650.14620	-0.00053	1387.79509	737.64836
1 1 1 -1 15	1 1 0 0 16	648.38754	-0.00029	1416.43541	768.04757
1 1 1 -1 16	1 1 0 0 17	646.64350	-0.00026	1446.98812	800.34436
1 1 1 -1 17	1 1 0 0 18	644.91494	-0.00018	1479.45342	834.53830
1 1 1 -1 18	1 1 0 0 19	643.20197	-0.00048	1513.83138	870.62893
1 1 1 -1 19	1 1 0 0 20	641.50611	-0.00007	1550.12195	908.61577
1 1 1 -1 20	1 1 0 0 21	639.82640	-0.00025	1588.32496	948.49830
1 1 1 -1 21	1 1 0 0 22	638.16420	0.00010	1628.44012	990.27601
1 1 1 -1 22	1 1 0 0 23	636.51841	-0.00027	1670.46701	1033.94833
1 1 1 -1 23	1 1 0 0 24	634.89026	-0.00019	1714.40513	1079.51468
1 1 1 -1 24	1 1 0 0 25	633.27971	0.00030	1760.25386	1126.97445
1 1 1 -1 25	1 1 0 0 26	631.68561	0.00009	1808.01252	1176.32701
1 1 1 -1 26	1 1 0 0 27	630.10922	0.00056	1857.68035	1227.57169
1 1 1 -1 27	1 1 0 0 28	628.54886	0.00013	1909.25654	1280.70782
1 1 1 -1 28	1 1 0 0 29	627.00362*	-0.00193	1962.74023	1335.73468W
1 1 1 -1 30	1 1 0 0 31	623.97035	0.00154	2075.42646	1451.45764W
1 1 1 -1 31	1 1 0 0 32	622.47577	0.00086	2134.62711	1512.15220
1 1 1 -1 32	1 1 0 0 33	620.99729	0.00022	2195.73148	1574.73441
1 1 1 -1 2	1 1 0 0 1	681.64820	-0.00055	1193.13502	511.48627
1 1 1 -1 3	1 1 0 0 2	683.56923	-0.00011	1198.85764	515.28830
1 1 1 -1 4	1 1 0 0 3	685.49668	-0.00011	1206.48808	520.99129
1 1 1 -1 5	1 1 0 0 4	687.43196*	0.00057	1216.02655	528.59515
1 1 1 -1 6	1 1 0 0 5	689.37173*	-0.00181	1227.47333	538.09979W
1 1 1 -1 7	1 1 0 0 6	691.32403	0.00033	1240.82878	549.50508
1 1 1 -1 8	1 1 0 0 7	693.28270	0.00030	1256.09326	562.81086
1 1 1 -1 9	1 1 0 0 8	695.25004	-0.00020	1273.26720	578.01697
1 1 1 -1 10	1 1 0 0 9	697.22780	-0.00008	1292.35106	595.12319
1 1 1 -1 11	1 1 0 0 10	699.21608	0.00005	1313.34532	614.12929
1 1 1 -1 12	1 1 0 0 11	701.21492	-0.00049	1336.25044	635.03503
1 1 1 -1 13	1 1 0 0 12	703.22655	-0.00021	1361.06689	657.84012
1 1 1 -1 14	1 1 0 0 13	705.24000	-0.00009	1387.79509	682.54427

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45	1	1	1	-1	15	1	1	0	0	14	707.28814	-0.00014	1416.43541	709.14713
	1	1	1	-1	16	1	1	0	0	15	709.33948	-0.00028	1446.98812	737.64836
	1	1	1	-1	17	1	1	0	0	16	711.40572	-0.00013	1479.45342	768.04757
	1	1	1	-1	18	1	1	0	0	17	713.48680	-0.00022	1513.83138	800.34436
	1	1	1	-1	19	1	1	0	0	18	715.58363	-0.00002	1550.12195	834.53830
	1	1	1	-1	20	1	1	0	0	19	717.69540	-0.00063	1588.32496	870.62893
	1	1	1	-1	21	1	1	0	0	20	719.82399	-0.00036	1628.44012	908.61577
	1	1	1	-1	22	1	1	0	0	21	721.96836	-0.00035	1670.46701	948.49830
	1	1	1	-1	23	1	1	0	0	22	724.12917	0.00006	1714.40513	990.27601
	1	1	1	-1	24	1	1	0	0	23	726.30544	-0.00009	1760.25386	1033.94833
	1	1	1	-1	25	1	1	0	0	24	728.49797	0.00013	1808.01252	1079.51468
	1	1	1	-1	26	1	1	0	0	25	730.70526	-0.00064	1857.68035	1126.97445
	1	1	1	-1	27	1	1	0	0	26	732.92948	-0.00006	1909.25654	1176.32701
	1	1	1	-1	28	1	1	0	0	27	735.16932	0.00078	1962.74023	1227.57169
	1	1	1	-1	29	1	1	0	0	28	737.42260*	-0.00009	2018.13051	1280.70782
	1	1	1	-1	1	1	-1	0	0	1	677.82529	-0.00019	1189.32003	511.49456
	1	1	1	-1	2	1	-1	0	0	2	677.82199	0.00013	1193.13502	515.31316
	1	1	1	-1	3	1	-1	0	0	3	677.81645	-0.00019	1198.85764	521.04101
	1	1	1	-1	4	1	-1	0	0	4	677.80961	-0.00045	1206.48808	528.67801
	1	1	1	-1	5	1	-1	0	0	5	677.80228	-0.00019	1216.02655	538.22407
	1	1	1	-1	6	1	-1	0	0	6	677.79410	-0.00018	1227.47333	549.67906
	1	1	1	-1	7	1	-1	0	0	7	677.78620	0.00023	1240.82878	563.04281
	1	1	1	-1	8	1	-1	0	0	8	677.77775	-0.00037	1256.09326	578.31514
	1	1	1	-1	9	1	-1	0	0	9	677.77037*	-0.00098	1273.26720	595.49585
	1	1	1	-1	10	1	-1	0	0	10	677.76456*	-0.00181	1292.35106	614.58469W
	1	1	1	-1	11	1	-1	0	0	11	677.76456*	0.00066	1313.34532	635.58142
	1	1	1	-1	12	1	-1	0	0	12	677.76456	-0.00015	1336.25044	658.48573
	1	1	1	-1	13	1	-1	0	0	13	677.77037*	0.00080	1361.06689	683.29732
	1	1	1	-1	14	1	-1	0	0	14	677.77912	-0.00013	1387.79509	710.01584
	1	1	1	-1	15	1	-1	0	0	15	677.79410	-0.00037	1416.43541	738.64093
	1	1	1	-1	16	1	-1	0	0	16	677.81514	-0.00078	1446.98812	769.17220
	1	1	1	-1	17	1	-1	0	0	17	677.84391	-0.00029	1479.45342	801.60923
	1	1	1	-1	18	1	-1	0	0	18	677.87964	-0.00018	1513.83138	835.95156
	1	1	1	-1	19	1	-1	0	0	19	677.92258	-0.00063	1550.12195	872.19874
	1	1	1	-1	20	1	-1	0	0	20	677.97471	0.00002	1588.32496	910.35027
	1	1	1	-1	21	1	-1	0	0	21	678.03482	0.00032	1628.44012	950.40561
	1	1	1	-1	22	1	-1	0	0	22	678.10261	-0.00017	1670.46701	992.36423
	1	1	1	-1	23	1	-1	0	0	23	678.17950	-0.00008	1714.40513	1036.22555
	1	1	1	-1	24	1	-1	0	0	24	678.26530	0.00040	1760.25386	1081.98896
	1	1	1	-1	25	1	-1	0	0	25	678.35873	0.00005	1808.01252	1129.65384
	1	1	1	-1	26	1	-1	0	0	26	678.46057	-0.00024	1857.68035	1179.21954
	1	1	1	-1	27	1	-1	0	0	27	678.57104	-0.00013	1909.25654	1230.68537
	1	1	1	-1	28	1	-1	0	0	28	678.68957	-0.00002	1962.74023	1284.05064
	1	1	1	-1	29	1	-1	0	0	29	678.81601	0.00010	2018.13051	1339.31460
	1	1	1	-1	30	1	-1	0	0	30	678.94996	0.00001	2075.42646	1396.47651
	1	1	1	-1	31	1	-1	0	0	31	679.09099	-0.00055	2134.62711	1455.53557
	1	1	1	-1	32	1	-1	0	0	32	679.23880*	-0.00170	2195.73148	1516.49098W
	1	1	1	-1	33	1	-1	0	0	33	679.39740	0.00074	2258.73857	1579.34190W

rms = 0.00033 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 -1 1 1 0	1 -1 0 0 1	672.24978	-0.00009	1183.74443	511.49456
1 -1 1 1 1	1 -1 0 0 2	670.33861	-0.00020	1185.65198	515.31316
1 -1 1 1 2	1 -1 0 0 3	668.42618	0.00012	1189.46706	521.04101
1 -1 1 1 3	1 -1 0 0 4	666.51154	-0.00012	1195.18967	528.67801
1 -1 1 1 4	1 -1 0 0 5	664.59574	0.00005	1202.81976	538.22407
1 -1 1 1 5	1 -1 0 0 6	662.67829	0.00004	1212.35731	549.67906
1 -1 1 1 6	1 -1 0 0 7	660.75991	0.00048	1223.80224	563.04281
1 -1 1 1 7	1 -1 0 0 8	658.83999	0.00063	1237.15450	578.31514
1 -1 1 1 8	1 -1 0 0 9	656.91800	-0.00016	1252.41400	595.49585
1 -1 1 1 9	1 -1 0 0 10	654.99581	-0.00015	1269.58065	614.58469
1 -1 1 1 10	1 -1 0 0 11	653.07279	-0.00012	1288.65432	635.58142
1 -1 1 1 11	1 -1 0 0 12	651.14977	-0.00009	1309.63487	658.48573

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1	-1	1	1	12	1	-1	0	0	13	649.22486	0.00008	1332.52210	683.29732
1	-1	1	1	13	1	-1	0	0	14	647.29995	-0.00001	1357.31580	710.01584
1	-1	1	1	14	1	-1	0	0	15	645.37462	-0.00015	1384.01571	738.64093
1	-1	1	1	15	1	-1	0	0	16	643.44932	0.00000	1412.62152	769.17220
1	-1	1	1	16	1	-1	0	0	17	641.52351	-0.00015	1443.13289	801.60923
1	-1	1	1	17	1	-1	0	0	18	639.59808	0.00022	1475.54942	835.95156
1	-1	1	1	18	1	-1	0	0	19	637.67192	-0.00003	1509.87069	872.19874
1	-1	1	1	19	1	-1	0	0	20	635.74575	-0.00021	1546.09623	910.35027
1	-1	1	1	20	1	-1	0	0	21	633.81949	-0.00041	1584.22551	950.40561
1	-1	1	1	21	1	-1	0	0	22	631.89386	0.00007	1624.25802	992.36423
1	-1	1	1	22	1	-1	0	0	23	629.96765	0.00003	1666.19317	1036.22555
1	-1	1	1	23	1	-1	0	0	24	628.04144	0.00003	1710.03037	1081.98896
1	-1	1	1	24	1	-1	0	0	25	626.11486	-0.00029	1755.76899	1129.65384
1	-1	1	1	25	1	-1	0	0	26	624.18814	-0.00071	1803.40839	1179.21954
1	-1	1	1	26	1	-1	0	0	27	622.26185	-0.00066	1852.94788	1230.68537
1	-1	1	1	27	1	-1	0	0	28	620.33633	0.00020	1904.38677	1284.05064
1	-1	1	1	28	1	-1	0	0	29	618.41016	0.00044	1957.72433	1339.31460
1	-1	1	1	29	1	-1	0	0	30	616.48391	0.00062	2012.95980	1396.47651
1	-1	1	1	30	1	-1	0	0	31	614.55735	0.00050	2070.09242	1455.53557
1	-1	1	1	31	1	-1	0	0	32	612.63098	0.00058	2129.12138	1516.49098
1	-1	1	1	32	1	-1	0	0	33	610.70415	0.00019	2190.04587	1579.34190
1	-1	1	1	33	1	-1	0	0	34	608.77775	0.00021	2252.86502	1644.08748
1	-1	1	1	34	1	-1	0	0	35	606.85077	-0.00039	2317.57798	1710.72682
1	-1	1	1	35	1	-1	0	0	36	604.92446	-0.00036	2384.18383	1779.25901
1	-1	1	1	36	1	-1	0	0	37	602.99662	-0.00194	2452.68167	1849.68311W
1	-1	1	1	37	1	-1	0	0	38	601.07297	0.00060	2523.07053	1921.99816
1	-1	1	1	38	1	-1	0	0	39	599.14785	0.00156	2595.34945	1996.20316W
1	-1	1	1	2	1	-1	0	0	1	677.97413*	0.00162	1189.46706	511.49456W
1	-1	1	1	3	1	-1	0	0	2	679.87666	0.00015	1195.18967	515.31316
1	-1	1	1	4	1	-1	0	0	3	681.77906	0.00030	1202.81976	521.04101
1	-1	1	1	5	1	-1	0	0	4	683.67935	0.00006	1212.35731	528.67801
1	-1	1	1	6	1	-1	0	0	5	685.57821	0.00004	1223.80224	538.22407
1	-1	1	1	7	1	-1	0	0	6	687.47580	0.00036	1237.15450	549.67906
1	-1	1	1	8	1	-1	0	0	7	689.37140	0.00020	1252.41400	563.04281
1	-1	1	1	9	1	-1	0	0	8	691.26597	0.00046	1269.58065	578.31514
1	-1	1	1	10	1	-1	0	0	9	693.15881	0.00033	1288.65432	595.49585
1	-1	1	1	11	1	-1	0	0	10	695.04972	-0.00045	1309.63487	614.58469
1	-1	1	1	12	1	-1	0	0	11	696.94119	0.00051	1332.52210	635.58142
1	-1	1	1	13	1	-1	0	0	12	698.83001	-0.00006	1357.31580	658.48573
1	-1	1	1	14	1	-1	0	0	13	700.71847	0.00008	1384.01571	683.29732
1	-1	1	1	15	1	-1	0	0	14	702.60539	-0.00029	1412.62152	710.01584
1	-1	1	1	16	1	-1	0	0	15	704.49193	-0.00003	1443.13289	738.64093
1	-1	1	1	17	1	-1	0	0	16	706.37760	0.00038	1475.54942	769.17220
1	-1	1	1	18	1	-1	0	0	17	708.26170	0.00023	1509.87069	801.60923
1	-1	1	1	19	1	-1	0	0	18	710.14540	0.00074	1546.09623	835.95156
1	-1	1	1	20	1	-1	0	0	19	712.02702	0.00025	1584.22551	872.19874
1	-1	1	1	21	1	-1	0	0	20	713.90884*	0.00109	1624.25802	910.35027W
1	-1	1	1	22	1	-1	0	0	21	715.78513*	-0.00243	1666.19317	950.40561W
1	-1	1	1	23	1	-1	0	0	22	717.66695	0.00081	1710.03037	992.36423
1	-1	1	1	24	1	-1	0	0	23	719.54334	-0.00011	1755.76899	1036.22555
1	-1	1	1	25	1	-1	0	0	24	721.41920	-0.00023	1803.40839	1081.98896
1	-1	1	1	26	1	-1	0	0	25	723.29392	-0.00012	1852.94788	1129.65384
1	-1	1	1	27	1	-1	0	0	26	725.16711	-0.00012	1904.38677	1179.21954
1	-1	1	1	28	1	-1	0	0	27	727.03869	-0.00026	1957.72433	1230.68537
1	-1	1	1	30	1	-1	0	0	29	730.77592*	-0.00190	2070.09242	1339.31460W
1	-1	1	1	31	1	-1	0	0	30	732.64546	0.00058	2129.12138	1396.47651
1	-1	1	1	32	1	-1	0	0	31	734.51037	0.00007	2190.04587	1455.53557
1	-1	1	1	33	1	-1	0	0	32	736.37423	0.00019	2252.86502	1516.49098
1	-1	1	1	34	1	-1	0	0	33	738.23681	0.00074	2317.57798	1579.34190
1	-1	1	1	35	1	-1	0	0	34	740.09644	0.00009	2384.18383	1644.08748
1	-1	1	1	36	1	-1	0	0	35	741.95470	-0.00015	2452.68167	1710.72682
1	-1	1	1	37	1	-1	0	0	36	743.81175	0.00023	2523.07053	1779.25901
1	-1	1	1	38	1	-1	0	0	37	745.66637	0.00003	2595.34945	1849.68311
1	-1	1	1	2	1	1	0	0	2	674.17872	-0.00004	1189.46706	515.28830
1	-1	1	1	3	1	1	0	0	3	674.19848	0.00010	1195.18967	520.99129
1	-1	1	1	4	1	1	0	0	4	674.22500	0.00039	1202.81976	528.59515
1	-1	1	1	5	1	1	0	0	5	674.25771	0.00020	1212.35731	538.09979
1	-1	1	1	6	1	1	0	0	6	674.29756	0.00040	1223.80224	549.50508
1	-1	1	1	7	1	1	0	0	7	674.34308	0.00056	1237.15450	562.81086

1	1	-1	1	1	9	1	1	0	0	9	674.45740	-0.00007	1269.58065	595.12319
2	1	-1	1	1	10	1	1	0	0	10	674.52475	-0.00028	1288.65432	614.12929
3	1	-1	1	1	11	1	1	0	0	11	674.59975	-0.00009	1309.63487	635.03503
4	1	-1	1	1	12	1	1	0	0	12	674.68209	0.00012	1332.52210	657.84012
5	1	-1	1	1	13	1	1	0	0	13	674.77144	-0.00009	1357.31580	682.54427
6	1	-1	1	1	14	1	1	0	0	14	674.86865	0.00007	1384.01571	709.14713
7	1	-1	1	1	15	1	1	0	0	15	674.97339	0.00023	1412.62152	737.64836
8	1	-1	1	1	16	1	1	0	0	16	675.08524	-0.00008	1443.13289	768.04757
9	1	-1	1	1	17	1	1	0	0	17	675.20539	0.00033	1475.54942	800.34436
10	1	-1	1	1	18	1	1	0	0	18	675.33239	0.00000	1509.87069	834.53830
11	1	-1	1	1	19	1	1	0	0	19	675.46724	-0.00006	1546.09623	870.62893
12	1	-1	1	1	20	1	1	0	0	20	675.60963	-0.00012	1584.22551	908.61577
13	1	-1	1	1	21	1	1	0	0	21	675.76000	0.00029	1624.25802	948.49830
14	1	-1	1	1	22	1	1	0	0	22	676.08220	0.00016	1710.03037	1033.94833
15	1	-1	1	1	23	1	1	0	0	23	676.25400	-0.00031	1755.76899	1079.51468
16	1	-1	1	1	24	1	1	0	0	24	676.43416	0.00022	1803.40839	1126.97445
17	1	-1	1	1	25	1	1	0	0	25	676.62075	-0.00013	1852.94788	1176.32701
18	1	-1	1	1	26	1	1	0	0	26	676.81529	0.00021	1904.38677	1227.57169
19	1	-1	1	1	27	1	1	0	0	27	677.01691*	0.00040	1957.72433	1280.70782
20	1	-1	1	1	28	1	1	0	0	28	677.22425	-0.00087	2012.95980	1335.73468
21	1	-1	1	1	29	1	1	0	0	29				

rms = 0.00032 cm⁻¹

lf

$$V_4 + V_5 (\Delta) \leftarrow V_4 (\Pi)$$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	G'	G''
1	1	1	1	2	1	1	0	0	3	668.19285	0.00016	1189.18398	520.99129
2	1	1	1	3	1	1	0	0	4	666.31068	-0.00026	1194.90609	528.59515
3	1	1	1	4	1	1	0	0	5	664.43521	-0.00006	1202.53506	538.09979
4	1	1	1	5	1	1	0	0	6	662.56575	0.00037	1212.07046	549.50508
5	1	1	1	6	1	1	0	0	7	660.70072	-0.00016	1223.51174	562.81086
6	1	1	1	7	1	1	0	0	8	658.84044	-0.00084	1236.85825	578.01697
7	1	1	1	8	1	1	0	0	9	656.98580	-0.00026	1252.10924	595.12319
8	1	1	1	9	1	1	0	0	10	655.13445	-0.00014	1269.26388	614.12929
9	1	1	1	10	1	1	0	0	11	653.28661	0.00041	1288.32123	635.03503
10	1	1	1	11	1	1	0	0	12	651.44007	-0.00011	1309.28031	657.84012
11	1	1	1	12	1	1	0	0	13	649.59574	-0.00005	1332.14005	682.54427
12	1	1	1	13	1	1	0	0	14	647.75224	-0.00001	1356.89938	709.14713
13	1	1	1	14	1	1	0	0	15	645.90915	0.00031	1383.55720	737.64836
14	1	1	1	15	1	1	0	0	16	644.06468	-0.00016	1412.11241	768.04757
15	1	1	1	16	1	1	0	0	17	642.21898	-0.00060	1442.56394	800.34436
16	1	1	1	17	1	1	0	0	18	640.37237	-0.00011	1474.91078	834.53830
17	1	1	1	18	1	1	0	0	19	638.52268	-0.00036	1509.15197	870.62893
18	1	1	1	19	1	1	0	0	20	636.67068	-0.00016	1545.28661	908.61577
19	1	1	1	20	1	1	0	0	21	634.81598	0.00040	1583.31388	948.49830
20	1	1	1	21	1	1	0	0	22	632.95728	0.00025	1623.23305	990.27601
21	1	1	1	22	1	1	0	0	23	631.09513	0.00005	1665.04341	1033.94833
22	1	1	1	23	1	1	0	0	24	629.22946	-0.00020	1708.74434	1079.51468
23	1	1	1	24	1	1	0	0	25	627.36064	-0.00017	1754.33526	1126.97445
24	1	1	1	25	1	1	0	0	26	625.48928	0.00069	1801.81559	1176.32701
25	1	1	1	26	1	1	0	0	27	623.61257	-0.00054	1851.18480	1227.57169
26	1	1	1	27	1	1	0	0	28	621.73412	-0.00040	1902.44233	1280.70782
27	1	1	1	28	1	1	0	0	29	619.85365	0.00067	1955.58766	1335.73468
28	1	1	1	29	1	1	0	0	30	617.96940	0.00073	2010.62021	1392.65154
29	1	1	1	30	1	1	0	0	31	616.08154	-0.00023	2067.53942	1451.45764
30	1	1	1	31	1	1	0	0	32	614.19224	-0.00023	2126.34468	1512.15220
31	1	1	1	32	1	1	0	0	33	612.30097	0.00002	2187.03535	1574.73441
32	1	1	1	33	1	1	0	0	34	610.40722	-0.00015	2249.61079	1639.20342
33	1	1	1	34	1	1	0	0	35	608.51236	0.00044	2314.07030	1705.55838
34	1	1	1	35	1	1	0	0	36	606.61441	-0.00033	2380.41315	1773.79841
35	1	1	1	36	1	1	0	0	37	604.71566	-0.00032	2448.63858	1843.92260
36	1	1	1	37	1	1	0	0	38	602.81732*	0.00152	2518.74579	1915.93000W
37	1	1	1	38	1	1	0	0	39	600.91564	0.00133	2590.73397	1989.81965W
38	1	1	1	39	1	1	0	0	40	599.01053	-0.00112	2664.60223	2065.59058W
39	1	1	1	2	1	1	0	0	1	677.69639*	-0.00132	1189.18398	511.48627W
40	1	1	1	3	1	1	0	0	2			1189.18398	515.28830

1	1	1	1	4	1	1	0	0	3	681.54365	-0.00012	1202.53506	520.99129
2	1	1	1	5	1	1	0	0	4	683.47494	-0.00037	1212.07046	528.59515
3	1	1	1	6	1	1	0	0	5	685.41221	0.00026	1223.51174	538.09979
4	1	1	1	7	1	1	0	0	6	687.35309	-0.00008	1236.85825	549.50508
5	1	1	1	8	1	1	0	0	7	689.29832	-0.00006	1252.10924	562.81086
6	1	1	1	9	1	1	0	0	8	691.24695	0.00004	1269.26388	578.01697
7	1	1	1	10	1	1	0	0	9	693.19799	-0.00006	1288.32123	595.12319
8	1	1	1	11	1	1	0	0	10	695.15098	-0.00004	1309.28031	614.12929
9	1	1	1	12	1	1	0	0	11	697.10504	0.00002	1332.14005	635.03503
10	1	1	1	13	1	1	0	0	12	699.05910	-0.00016	1356.89938	657.84012
11	1	1	1	14	1	1	0	0	13	701.01321	0.00028	1383.55720	682.54427
12	1	1	1	15	1	1	0	0	14	702.96530	0.00002	1412.11241	709.14713
13	1	1	1	16	1	1	0	0	15	704.91575	0.00016	1442.56394	737.64836
14	1	1	1	17	1	1	0	0	16	706.86341	0.00020	1474.91078	768.04757
15	1	1	1	18	1	1	0	0	17	708.80680*	-0.00081	1509.15197	800.34436
16	1	1	1	19	1	1	0	0	18	710.74905	0.00074	1545.28661	834.53830
17	1	1	1	20	1	1	0	0	19	712.68478	-0.00017	1583.31388	870.62893
18	1	1	1	21	1	1	0	0	20	714.61690	-0.00038	1623.23305	908.61577
19	1	1	1	22	1	1	0	0	21	716.54534	0.00023	1665.04341	948.49830
20	1	1	1	23	1	1	0	0	22	718.46848	0.00015	1708.74434	990.27601
21	1	1	1	24	1	1	0	0	23	720.38683	-0.00010	1754.33526	1033.94833
22	1	1	1	25	1	1	0	0	24	722.30089	-0.00002	1801.81559	1079.51468
23	1	1	1	26	1	1	0	0	25	724.21033	-0.00002	1851.18480	1126.97445
24	1	1	1	27	1	1	0	0	26	726.11511	-0.00022	1902.44233	1176.32701
25	1	1	1	28	1	1	0	0	27	728.01543	-0.00054	1955.58766	1227.57169
26	1	1	1	29	1	1	0	0	28	729.91246	0.00007	2010.62021	1280.70782
27	1	1	1	30	1	1	0	0	29	731.80657*	0.00183	2067.53942	1335.73468W
28	1	1	1	31	1	1	0	0	30	733.69217	-0.00096	2126.34468	1392.65154
29	1	1	1	32	1	1	0	0	31	735.57734	-0.00037	2187.03535	1451.45764
30	1	1	1	33	1	1	0	0	32	737.45896	0.00037	2249.61079	1512.15220
31	1	1	1	34	1	1	0	0	33	739.33617	0.00027	2314.07030	1574.73441
32	1	1	1	35	1	1	0	0	34	741.21025	0.00052	2380.41315	1639.20342
33	1	1	1	36	1	1	0	0	35	743.07944	-0.00076	2448.63858	1705.55838
34	1	1	1	37	1	1	0	0	36	744.94751	0.00013	2518.74579	1773.79841
35	1	1	1	38	1	1	0	0	37	746.81119	-0.00018	2590.73397	1843.92260
36	1	1	1	39	1	1	0	0	38	748.66870*	-0.00354	2664.60223	1915.93000W
37	1	1	1	40	1	1	0	0	39	750.52996	-0.00008	2740.34970	1989.81965
38	1	1	1	41	1	1	0	0	40	752.38500	0.00015	2817.97543	2065.59058
39	1	1	1	2	1	-1	0	0	2	673.87052	-0.00029	1189.18398	515.31316
40	1	1	1	3	1	-1	0	0	3	673.86496	-0.00012	1194.90609	521.04101
41	1	1	1	4	1	-1	0	0	4	673.85703	-0.00002	1202.53506	528.67801
42	1	1	1	5	1	-1	0	0	5	673.84639	0.00000	1212.07046	538.22407
43	1	1	1	6	1	-1	0	0	6	673.83281	0.00013	1223.51174	549.67906
44	1	1	1	7	1	-1	0	0	7	673.81516	-0.00028	1236.85825	563.04281
45	1	1	1	8	1	-1	0	0	8	673.79404	-0.00006	1252.10924	578.31514
46	1	1	1	9	1	-1	0	0	9	673.76808	0.00005	1269.26388	595.49585
47	1	1	1	10	1	-1	0	0	10	673.73677	0.00023	1288.32123	614.58469
48	1	1	1	11	1	-1	0	0	11	673.69896	0.00007	1309.28031	635.58142
49	1	1	1	12	1	-1	0	0	12	673.65424	-0.00008	1332.14005	658.48573
50	1	1	1	13	1	-1	0	0	13	673.60197	-0.00010	1356.89938	683.29732
51	1	1	1	14	1	-1	0	0	14	673.54153	0.00017	1383.55720	710.01584
52	1	1	1	15	1	-1	0	0	15	673.47158	0.00010	1412.11241	738.64093
53	1	1	1	16	1	-1	0	0	16	673.39195	0.00021	1442.56394	769.17220
54	1	1	1	17	1	-1	0	0	17	673.30162	0.00006	1474.91078	801.60923
55	1	1	1	18	1	-1	0	0	18	673.20025	-0.00015	1509.15197	835.95156
56	1	1	1	19	1	-1	0	0	19	673.08839	0.00053	1545.28661	872.19874
57	1	1	1	20	1	-1	0	0	20	672.96352	-0.00010	1583.31388	910.35027
58	1	1	1	21	1	-1	0	0	21	672.82790	0.00047	1623.23305	950.40561
59	1	1	1	22	1	-1	0	0	22	672.67944	0.00026	1665.04341	992.36423
60	1	1	1	23	1	-1	0	0	23	672.51913	0.00033	1708.74434	1036.22555
	1	1	1	24	1	-1	0	0	24	672.34610	-0.00020	1754.33526	1081.98896
	1	1	1	25	1	-1	0	0	25	672.16249	0.00074	1801.81559	1129.65384
	1	1	1	26	1	-1	0	0	26	671.96543	0.00018	1851.18480	1179.21954
	1	1	1	27	1	-1	0	0	27	671.75712	0.00016	1902.44233	1230.68537
	1	1	1	28	1	-1	0	0	28	671.53774	0.00072	1955.58766	1284.05064
	1	1	1	29	1	-1	0	0	29	671.30681	0.00120	2010.62021	1339.31460W
	1	1	1	30	1	-1	0	0	30	671.06300	0.00009	2067.53942	1396.47651
	1	1	1	31	1	-1	0	0	31	670.81073	0.00162	2126.34468	1455.53557W
	1	1	1	32	1	-1	0	0	32	670.54612*	0.00175	2187.03535	1516.49098W

1	1	1	1	33	1	-1	0	0	33	670.26817	-0.00072	2249.61079	1579.34190
	1	1	1	34	1	-1	0	0	34	669.98335	0.00053	2314.07030	1644.08748
2	1	1	1	35	1	-1	0	0	35	669.68801	0.00168	2380.41315	1710.72682W
3	1	-1	1	-1	2	1	-1	0	3	668.14186	-0.00118	1189.18404	521.04101W
4	1	-1	1	-1	3	1	-1	0	4	666.22815	-0.00026	1194.90643	528.67801
5	1	-1	1	-1	4	1	-1	0	5	664.31232	0.00032	1202.53608	538.22407
6	1	-1	1	-1	5	1	-1	0	6	662.39379	0.00002	1212.07282	549.67906
7	1	-1	1	-1	6	1	-1	0	7	660.47352	-0.00014	1223.51646	563.04281
8	1	-1	1	-1	7	1	-1	0	8	658.54891	-0.00270	1236.86675	578.31514W
9	1	-1	1	-1	8	1	-1	0	9	656.62892	0.00137	1252.12340	595.49585W
10	1	-1	1	-1	9	1	-1	0	10	654.70171	0.00032	1269.28609	614.58469
11	1	-1	1	-1	10	1	-1	0	11	652.77262	-0.00044	1288.35448	635.58142
12	1	-1	1	-1	11	1	-1	0	12	650.84215	-0.00032	1309.32820	658.48573
13	1	-1	1	-1	12	1	-1	0	13	648.90974	0.00021	1332.20685	683.29732
14	1	-1	1	-1	13	1	-1	0	14	646.97380	-0.00040	1356.99004	710.01584
15	1	-1	1	-1	14	1	-1	0	15	645.03659	0.00018	1383.67734	738.64093
16	1	-1	1	-1	15	1	-1	0	16	643.09664	0.00051	1412.26833	769.17220
17	1	-1	1	-1	16	1	-1	0	17	641.15346	0.00011	1442.76257	801.60923
18	1	-1	1	-1	17	1	-1	0	18	639.20798	-0.00009	1475.15963	835.95156
19	1	-1	1	-1	18	1	-1	0	19	637.26038	0.00007	1509.45905	872.19874
20	1	-1	1	-1	19	1	-1	0	20	635.31074	0.00065	1545.66036	910.35027
21	1	-1	1	-1	20	1	-1	0	21	633.35723	-0.00023	1583.76307	950.40561
22	1	-1	1	-1	21	1	-1	0	22	631.40191	-0.00055	1623.76670	992.36423
23	1	-1	1	-1	22	1	-1	0	23	629.44452	-0.00063	1665.67070	1036.22555
24	1	-1	1	-1	23	1	-1	0	24	627.48498	-0.00060	1709.47454	1081.98896
25	1	-1	1	-1	24	1	-1	0	25	625.52369	-0.00012	1755.17765	1129.65384
26	1	-1	1	-1	2	1	-1	0	1	677.68980	0.00031	1189.18404	511.49456
27	1	-1	1	-1	3	1	-1	0	2	679.59313	-0.00013	1194.90643	515.31316
28	1	-1	1	-1	4	1	-1	0	3	681.49500	-0.00007	1202.53608	521.04101
29	1	-1	1	-1	5	1	-1	0	4	683.39483	0.00002	1212.07282	528.67801
30	1	-1	1	-1	6	1	-1	0	5	685.29294	0.00055	1223.51646	538.22407
31	1	-1	1	-1	7	1	-1	0	6	687.18735	-0.00034	1236.86675	549.67906
32	1	-1	1	-1	8	1	-1	0	7	689.08002	-0.00057	1252.12340	563.04281
33	1	-1	1	-1	9	1	-1	0	8	690.97082	-0.00013	1269.28609	578.31514
34	1	-1	1	-1	10	1	-1	0	9	692.85872	0.00009	1288.35448	595.49585
35	1	-1	1	-1	11	1	-1	0	10	694.74291	-0.00059	1309.32820	614.58469
36	1	-1	1	-1	12	1	-1	0	11	696.62550	0.00007	1332.20685	635.58142
37	1	-1	1	-1	13	1	-1	0	12	698.50432	0.00001	1356.99004	658.48573
38	1	-1	1	-1	14	1	-1	0	13	700.38068	0.00066	1383.67734	683.29732
39	1	-1	1	-1	15	1	-1	0	14	702.25265	0.00016	1412.26833	710.01584
40	1	-1	1	-1	16	1	-1	0	15	704.12178	0.00014	1442.76257	738.64093
41	1	-1	1	-1	17	1	-1	0	16	705.98749	0.00006	1475.15963	769.17220
42	1	-1	1	-1	18	1	-1	0	17	707.85011	0.00029	1509.45905	801.60923
43	1	-1	1	-1	19	1	-1	0	18	709.70897	0.00018	1545.66036	835.95156
44	1	-1	1	-1	20	1	-1	0	19	711.56468	0.00035	1583.76307	872.19874
45	1	-1	1	-1	21	1	-1	0	20	713.41634	-0.00009	1623.76670	910.35027
46	1	-1	1	-1	22	1	-1	0	21	715.26478	-0.00031	1665.67070	950.40561
47	1	-1	1	-1	23	1	-1	0	22	717.11061	0.00030	1709.47454	992.36423
48	1	-1	1	-1	24	1	-1	0	23	718.95236	0.00026	1755.17765	1036.22555
49	1	-1	1	-1	25	1	-1	0	24	720.78994	-0.00052	1802.77942	1081.98896
50	1	-1	1	-1	26	1	-1	0	25	722.62611	0.00073	1852.27923	1129.65384
51	1	-1	1	-1	27	1	-1	0	26	724.45744	0.00056	1903.67642	1179.21954
52	1	-1	1	-1	28	1	-1	0	27	726.28568	0.00072	1956.97033	1230.68537
53	1	-1	1	-1	29	1	-1	0	28	728.11481*	0.00521	2012.16024	1284.05064W
54	1	-1	1	-1	30	1	-1	0	29	729.93073	-0.00008	2069.24541	1339.31460
55	1	-1	1	-1	2	1	1	0	2	673.89565	-0.00009	1189.18404	515.28830
56	1	-1	1	-1	3	1	1	0	3	673.91513	-0.00001	1194.90643	520.99129
57	1	-1	1	-1	4	1	1	0	4	673.94070	-0.00022	1202.53608	528.59515
58	1	-1	1	-1	5	1	1	0	5	673.97297	-0.00006	1212.07282	538.09979
59	1	-1	1	-1	6	1	1	0	6	674.01138	-0.00001	1223.51646	549.50508
60	1	-1	1	-1	7	1	1	0	7	674.05585	-0.00004	1236.86675	562.81086
	1	-1	1	-1	8	1	1	0	8	674.10631	-0.00012	1252.12340	578.01697
	1	-1	1	-1	9	1	1	0	9	674.16305	0.00015	1269.28609	595.12319
	1	-1	1	-1	10	1	1	0	10	674.22500	-0.00019	1288.35448	614.12929
	1	-1	1	-1	11	1	1	0	11	674.29295	-0.00022	1309.32820	635.03503
	1	-1	1	-1	12	1	1	0	12	674.36665	-0.00008	1332.20685	657.84012
	1	-1	1	-1	13	1	1	0	13	674.44457*	-0.00120	1356.99004	682.54427W
	1	-1	1	-1	14	1	1	0	14	674.53033	0.00012	1383.67734	709.14713
	1	-1	1	-1	15	1	1	0	15	674.61998	0.00001	1412.26833	737.64836

1	-1	1	-1	16	1	1	0	0	16	674.71491	-0.00009	1442.76257	768.04757
2	-1	1	-1	17	1	1	0	0	17	674.81527	0.00000	1475.15963	800.34436
3	-1	1	-1	18	1	1	0	0	18	674.92065	-0.00010	1509.45905	834.53830
4	-1	1	-1	19	1	1	0	0	19	675.03134	-0.00009	1545.66036	870.62893
5	-1	1	-1	20	1	1	0	0	20	675.14745	0.00014	1583.76307	908.61577
6	-1	1	-1	21	1	1	0	0	21	675.26847	0.00008	1623.76670	948.49830
7	-1	1	-1	22	1	1	0	0	22	675.39462	-0.00007	1665.67070	990.27601
8	-1	1	-1	23	1	1	0	0	23	675.52629	0.00008	1709.47454	1033.94833
9	-1	1	-1	24	1	1	0	0	24	675.66211	-0.00086	1755.17765	1079.51468
10	-1	1	-1	25	1	1	0	0	25	675.80473	-0.00024	1802.77942	1126.97445
11	-1	1	-1	26	1	1	0	0	26	675.95186	-0.00036	1852.27923	1176.32701
12	-1	1	-1	27	1	1	0	0	27	676.10417	-0.00057	1903.67642	1227.57169
13	-1	1	-1	28	1	1	0	0	28	676.26227	-0.00024	1956.97033	1280.70782
14	-1	1	-1	29	1	1	0	0	29	676.42520	-0.00036	2012.16024	1335.73468
15	-1	1	-1	30	1	1	0	0	30	676.59375	-0.00012	2069.24541	1392.65154
16	-1	1	-1	31	1	1	0	0	31	676.76720	-0.00025	2128.22510	1451.45764
17	-1	1	-1	32	1	1	0	0	32	676.94620	-0.00010	2189.09850	1512.15220
18	-1	1	-1	33	1	1	0	0	33	677.12996	-0.00044	2251.86480	1574.73441
19	-1	1	-1	34	1	1	0	0	34	677.32048	0.00073	2316.52317	1639.20342

rms = 0.00034 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 1 -1 5	0 0 1 1 6	501.89462	-0.00185	1216.02655	714.13007W
1 1 1 -1 6	0 0 1 1 7	500.04692	0.00075	1227.47333	727.42716
1 1 1 -1 7	0 0 1 1 8	498.20590	0.00046	1240.82878	742.62333
1 1 1 -1 8	0 0 1 1 9	496.37547	0.00060	1256.09326	759.71839
1 1 1 -1 9	0 0 1 1 10	494.55541	0.00030	1273.26720	778.71209
1 1 1 -1 10	0 0 1 1 11	492.74590	-0.00096	1292.35106	799.60420
1 1 1 -1 11	0 0 1 1 12	490.95166	0.00079	1313.34532	822.39444
1 1 1 -1 12	0 0 1 1 13	489.16839	0.00046	1336.25044	847.08251
1 1 1 -1 13	0 0 1 1 14	487.39800	-0.00081	1361.06689	873.66808
1 1 1 -1 14	0 0 1 1 15	485.64545	0.00115	1387.79509	902.15079W
1 1 1 -1 7	0 0 1 1 6	526.69930	0.00059	1240.82878	714.13007
1 1 1 -1 8	0 0 1 1 7	528.66631	0.00021	1256.09326	727.42716
1 1 1 -1 9	0 0 1 1 8	530.64622*	0.00235	1273.26720	742.62333W
1 1 1 -1 10	0 0 1 1 9	532.63216	-0.00052	1292.35106	759.71839
1 1 1 -1 11	0 0 1 1 10	534.63319	-0.00003	1313.34532	778.71209
1 1 1 -1 12	0 0 1 1 11	536.64753*	0.00130	1336.25044	799.60420W
1 1 1 -1 13	0 0 1 1 12	538.67222	-0.00022	1361.06689	822.39444
1 1 1 -1 14	0 0 1 1 13	540.71273	0.00015	1387.79509	847.08251
1 1 1 -1 15	0 0 1 1 14	542.76810	0.00077	1416.43541	873.66808
1 1 1 -1 16	0 0 1 1 15	544.83806	0.00073	1446.98812	902.15079
1 1 1 -1 17	0 0 1 1 16	546.92504*	0.00190	1479.45342	932.53028W
1 1 1 -1 18	0 0 1 1 17	549.02426	-0.00098	1513.83138	964.80614
1 1 1 -1 19	0 0 1 1 18	551.14377	-0.00023	1550.12195	998.97795
1 1 1 -1 20	0 0 1 1 19	553.27802*	-0.00170	1588.32496	1035.04524W
1 1 1 -1 21	0 0 1 1 20	555.43189	-0.00067	1628.44012	1073.00756
1 1 1 -1 22	0 0 1 1 21	557.60492*	0.00229	1670.46701	1112.86438W
1 1 1 -1 23	0 0 1 1 22	559.79010	0.00017	1714.40513	1154.61520
1 1 1 -1 5	0 0 1 -1 5	513.19673	0.00022	1216.02655	702.83004
1 1 1 -1 6	0 0 1 -1 6	513.20690	0.00055	1227.47333	714.26698
1 1 1 -1 7	0 0 1 -1 7	513.21804*	-0.00105	1240.82878	727.60969W
1 1 1 -1 8	0 0 1 -1 8	513.23454	-0.00073	1256.09326	742.85799
1 1 1 -1 9	0 0 1 -1 9	513.25554	0.00001	1273.26720	760.01168
1 1 1 -1 10	0 0 1 -1 10	513.28038	-0.00017	1292.35106	779.07052
1 1 1 -1 11	0 0 1 -1 11	513.31087	-0.00019	1313.34532	800.03426
1 1 1 -1 12	0 0 1 -1 12	513.34775	-0.00007	1336.25044	822.90261
1 1 1 -1 13	0 0 1 -1 13	513.39153	-0.00008	1361.06689	847.67528
1 1 1 -1 14	0 0 1 -1 14	513.44338	0.00022	1387.79509	874.35193
1 1 1 -1 15	0 0 1 -1 15	513.50317	-0.00004	1416.43541	902.93220
1 1 1 -1 16	0 0 1 -1 16	513.57169	-0.00073	1446.98812	933.41570
1 1 1 -1 17	0 0 1 -1 17	513.65160	0.00022	1479.45342	965.80204
1 1 1 -1 18	0 0 1 -1 18	513.73138	0.00073	1513.83138	1000.09076

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1 2 3	1	1	1	-1	19	0	0	1	-1	19	513.84006	-0.00047	1550.12195	1036.28142
	1	1	1	-1	20	0	0	1	-1	20	513.95159	0.00016	1588.32496	1074.37353
	1	1	1	-1	23	0	0	1	-1	23	514.35233	0.00051	1714.40513	1200.05331
	1	1	1	-1	24	0	0	1	-1	24	514.50655	-0.00147	1760.25386	1245.74584W

rms = 0.00050 cm⁻¹

$V_4 + V_5 (\Sigma^-) \leftarrow V_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 -1 1 1 2	0 0 1 -1 3	503.79311	0.00010	1189.46706	685.67405
1 -1 1 1 3	0 0 1 -1 4	501.89462*	0.00397	1195.18967	693.29902W
1 -1 1 1 4	0 0 1 -1 5	499.99242*	0.00269	1202.81976	702.83004W
1 -1 1 1 5	0 0 1 -1 6	498.09029	-0.00003	1212.35731	714.26698
1 -1 1 1 6	0 0 1 -1 7	496.19272	0.00017	1223.80224	727.60969
1 -1 1 1 7	0 0 1 -1 8	494.29597	-0.00054	1237.15450	742.85799
1 -1 1 1 8	0 0 1 -1 9	492.40183	-0.00050	1252.41400	760.01168
1 -1 1 1 9	0 0 1 -1 10	490.50958	-0.00056	1269.58065	779.07052
1 -1 1 1 10	0 0 1 -1 11	488.62046	0.00039	1288.65432	800.03426
1 -1 1 1 11	0 0 1 -1 12	486.73281	0.00056	1309.63487	822.90261
1 -1 1 1 12	0 0 1 -1 13	484.84770	0.00089	1332.52210	847.67528
1 -1 1 1 13	0 0 1 -1 14	482.96419	0.00032	1357.31580	874.35193
1 -1 1 1 14	0 0 1 -1 15	481.08388	0.00037	1384.01571	902.93220
1 -1 1 1 4	0 0 1 -1 3	517.14655	0.00084	1202.81976	685.67405
1 -1 1 1 6	0 0 1 -1 5	520.97287	0.00067	1223.80224	702.83004
1 -1 1 1 7	0 0 1 -1 6	522.88655	-0.00097	1237.15450	714.26698
1 -1 1 1 8	0 0 1 -1 7	524.80163	-0.00268	1252.41400	727.60969W
1 -1 1 1 10	0 0 1 -1 9	528.64069	-0.00196	1288.65432	760.01168W
1 -1 1 1 11	0 0 1 -1 10	530.56622	0.00187	1309.63487	779.07052W
1 -1 1 1 12	0 0 1 -1 11	532.48710	-0.00074	1332.52210	800.03426
1 -1 1 1 13	0 0 1 -1 12	534.41324	0.00006	1357.31580	822.90261
1 -1 1 1 14	0 0 1 -1 13	536.33979	-0.00063	1384.01571	847.67528
1 -1 1 1 15	0 0 1 -1 14	538.27035	0.00076	1412.62152	874.35193
1 -1 1 1 16	0 0 1 -1 15	540.20113	0.00044	1443.13289	902.93220
1 -1 1 1 5	0 0 1 1 5	509.62515	0.00009	1212.35731	702.73224
1 -1 1 1 6	0 0 1 1 6	509.67178	-0.00039	1223.80224	714.13007
1 -1 1 1 7	0 0 1 1 7	509.72739	0.00005	1237.15450	727.42716
1 -1 1 1 8	0 0 1 1 8	509.79059	-0.00008	1252.41400	742.62333
1 -1 1 1 9	0 0 1 1 9	509.86250	0.00023	1269.58065	759.71839
1 -1 1 1 10	0 0 1 1 10	509.94212	-0.00011	1288.65432	778.71209
1 -1 1 1 11	0 0 1 1 11	510.03078	0.00012	1309.63487	799.60420
1 -1 1 1 12	0 0 1 1 12	510.12773	0.00008	1332.52210	822.39444
1 -1 1 1 13	0 0 1 1 13	510.23312	-0.00017	1357.31580	847.08251
1 -1 1 1 14	0 0 1 1 14	510.34759	-0.00004	1384.01571	873.66808
1 -1 1 1 15	0 0 1 1 15	510.47048	-0.00025	1412.62152	902.15079
1 -1 1 1 16	0 0 1 1 16	510.60317	0.00056	1443.13289	932.53028
1 -1 1 1 17	0 0 1 1 17	510.74299	-0.00029	1475.54942	964.80614
1 -1 1 1 18	0 0 1 1 18	510.89285	0.00010	1509.87069	998.97795
1 -1 1 1 19	0 0 1 1 19	511.05084	-0.00014	1546.09623	1035.04524
1 -1 1 1 20	0 0 1 1 20	511.21735	-0.00061	1584.22551	1073.00756

rms = 0.00046 cm⁻¹

$V_4 + V_5 (\Delta) \leftarrow V_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 1 1 5	0 0 1 1 6	497.94092	0.00053	1212.07046	714.13007
1 1 1 1 6	0 0 1 1 7	496.08463	0.00005	1223.51174	727.42716
1 1 1 1 7	0 0 1 1 8	494.23447	-0.00045	1236.85825	742.62333
1 1 1 1 8	0 0 1 1 9	492.39106	0.00020	1252.10924	759.71839
1 1 1 1 9	0 0 1 1 10	490.55161	-0.00018	1269.26388	778.71209
1 1 1 1 10	0 0 1 1 11	488.71726	0.00023	1288.32123	799.60420

1	1	1	1	11	0	0	1	1	12	486.88473*	-0.00113	1309.28031	822.39444W
2	1	1	1	1	12	0	0	1	1	13	485.05621	-0.00133	847.08251W
3	1	1	1	1	13	0	0	1	1	14	483.23158	0.00027	873.66808
4	1	1	1	1	14	0	0	1	1	15	481.40525	-0.00116	902.15079W
5	1	1	1	1	15	0	0	1	1	16	479.58251	0.00038	932.53028
6	1	1	1	1	16	0	0	1	1	17	477.75758	-0.00022	964.80614
7	1	1	1	1	4	0	0	1	1	3	516.89948	-0.00066	685.63493
8	1	1	1	1	5	0	0	1	1	4	518.83631	-0.00033	693.23382
9	1	1	1	1	6	0	0	1	1	5	520.77991	0.00041	702.73224
10	1	1	1	1	7	0	0	1	1	6	522.72797	-0.00021	714.13007
11	1	1	1	1	8	0	0	1	1	7	524.68201	-0.00007	727.42716
12	1	1	1	1	9	0	0	1	1	8	526.64014	-0.00041	742.62333
13	1	1	1	1	10	0	0	1	1	9	528.60222	-0.00063	759.71839
14	1	1	1	1	11	0	0	1	1	10	530.56847	0.00026	778.71209
15	1	1	1	1	12	0	0	1	1	11	532.53621	0.00036	799.60420
16	1	1	1	1	13	0	0	1	1	12	534.50449	-0.00045	822.39444
17	1	1	1	1	14	0	0	1	1	13	536.47501	0.00032	847.08251
18	1	1	1	1	15	0	0	1	1	14	538.44453	0.00020	873.66808
19	1	1	1	1	16	0	0	1	1	15	540.41346	0.00031	902.15079
20	1	1	1	1	17	0	0	1	1	16	542.38062	0.00012	932.53028
21	1	1	1	1	18	0	0	1	1	17	544.34549	-0.00034	964.80614
22	1	1	1	1	19	0	0	1	1	18	546.30783	-0.00083	998.97795
23	1	1	1	1	20	0	0	1	1	19	548.26835	-0.00029	1035.04524
24	1	1	1	1	21	0	0	1	1	20	550.22574	0.00025	1073.00756
25	1	1	1	1	22	0	0	1	1	21	552.17893	-0.00010	1112.86438
26	1	1	1	1	23	0	0	1	1	22	554.12969	0.00055	1154.61520
27	1	1	1	1	24	0	0	1	1	23	556.07634	0.00053	1198.25945
28	1	1	1	1	25	0	0	1	1	24	558.01825	-0.00078	1243.79656
29	1	1	1	1	26	0	0	1	1	25	559.95881	-0.00005	1291.22593
30	1	1	1	1	27	0	0	1	1	26	561.89594	0.00054	1340.54693
31	1	1	1	1	3	0	0	1	-1	3	509.23173	-0.00031	685.67405
32	1	1	1	1	4	0	0	1	-1	4	509.23698*	0.00094	693.29902
33	1	1	1	1	5	0	0	1	-1	5	509.23980*	-0.00062	702.83004
34	1	1	1	1	6	0	0	1	-1	6	509.24585*	0.00109	714.26698W
35	1	1	1	1	7	0	0	1	-1	7	509.24585*	-0.00271	727.60969W
36	1	1	1	1	8	0	0	1	-1	8	509.25147*	0.00022	742.85799
37	1	1	1	1	9	0	0	1	-1	9	509.25147*	-0.00073	760.01168
38	1	1	1	1	10	0	0	1	-1	10	509.25147*	0.00075	779.07052
39	1	1	1	1	11	0	0	1	-1	11	509.24585	-0.00020	800.03426
40	1	1	1	1	12	0	0	1	-1	12	509.23698	-0.00046	822.90261
41	1	1	1	1	13	0	0	1	-1	13	509.22465	0.00055	847.67528
42	1	1	1	1	14	0	0	1	-1	14	509.20496	-0.00031	874.35193
43	1	1	1	1	15	0	0	1	-1	15	509.18073	0.00052	902.93220
44	1	1	1	1	16	0	0	1	-1	16	509.14891	0.00067	933.41570
45	1	1	1	1	17	0	0	1	-1	17	509.10856	-0.00019	965.80204
46	1	1	1	1	18	0	0	1	-1	18	509.06150	0.00030	1000.09076
47	1	1	1	1	19	0	0	1	-1	19	509.00482	-0.00036	1036.28142
48	1	1	1	1	20	0	0	1	-1	20	508.94112	0.00077	1074.37353
49	1	-1	1	-1	4	0	0	1	-1	5	499.70552	-0.00052	702.83004
50	1	-1	1	-1	5	0	0	1	-1	6	497.80605	0.00021	714.26698
51	1	-1	1	-1	6	0	0	1	-1	7	495.90668	-0.00009	727.60969
52	1	-1	1	-1	7	0	0	1	-1	8	494.00810	-0.00066	742.85799
53	1	-1	1	-1	8	0	0	1	-1	9	492.11149	-0.00023	760.01168
54	1	-1	1	-1	9	0	0	1	-1	10	490.21599	0.00042	779.07052
55	1	-1	1	-1	10	0	0	1	-1	11	488.32056	0.00034	800.03426
56	1	-1	1	-1	11	0	0	1	-1	12	486.42527	-0.00031	822.90261
57	1	-1	1	-1	12	0	0	1	-1	13	484.53149	-0.00008	847.67528
58	1	-1	1	-1	13	0	0	1	-1	14	482.63775	-0.00036	874.35193
59	1	-1	1	-1	14	0	0	1	-1	15	480.74599	0.00085	902.93220
60	1	-1	1	-1	15	0	0	1	-1	16	478.85401	0.00138	933.41570W
	1	-1	1	-1	16	0	0	1	-1	17	476.95970	-0.00084	965.80204
	1	-1	1	-1	17	0	0	1	-1	18	475.06959	0.00072	1000.09076
	1	-1	1	-1	18	0	0	1	-1	19	473.17680	-0.00082	1036.28142
	1	-1	1	-1	19	0	0	1	-1	20	471.28655	-0.00027	1074.37353
	1	-1	1	-1	20	0	0	1	-1	21	469.39731	0.00081	1114.36658
	1	-1	1	-1	21	0	0	1	-1	22	467.50641	-0.00026	1156.26002
	1	-1	1	-1	22	0	0	1	-1	23	465.61614	-0.00126	1200.05331W
	1	-1	1	-1	23	0	0	1	-1	24	463.72447	-0.00423	1245.74584W
	1	-1	1	-1	24	0	0	1	-1	25	461.84157*	0.00093	1293.33701

1	1	-1	1	-1	25	0	0	1	-1	26	459.95312	-0.00012	1802.77942	1342.82618
2	1	-1	1	-1	4	0	0	1	-1	3	516.86164	-0.00038	1202.53608	685.67405
3	1	-1	1	-1	5	0	0	1	-1	4	518.77375	-0.00005	1212.07282	693.29902
4	1	-1	1	-1	6	0	0	1	-1	5	520.68659	0.00016	1223.51646	702.83004
5	1	-1	1	-1	7	0	0	1	-1	6	522.59955	-0.00022	1236.86675	714.26698
6	1	-1	1	-1	8	0	0	1	-1	7	524.51417	0.00046	1252.12340	727.60969
7	1	-1	1	-1	9	0	0	1	-1	8	526.42891*	0.00081	1269.28609	742.85799
8	1	-1	1	-1	10	0	0	1	-1	9	528.34278	-0.00002	1288.35448	760.01168
9	1	-1	1	-1	11	0	0	1	-1	10	530.25813	0.00045	1309.32820	779.07052
10	1	-1	1	-1	12	0	0	1	-1	11	532.17329*	0.00069	1332.20685	800.03426
11	1	-1	1	-1	13	0	0	1	-1	12	534.08710	-0.00033	1356.99004	822.90261
12	1	-1	1	-1	14	0	0	1	-1	13	536.00210	0.00004	1383.67734	847.67528
13	1	-1	1	-1	15	0	0	1	-1	14	537.91663	0.00023	1412.26833	874.35193
14	1	-1	1	-1	16	0	0	1	-1	15	539.83005	-0.00033	1442.76257	902.93220
15	1	-1	1	-1	17	0	0	1	-1	16	541.74360	-0.00033	1475.15963	933.41570
16	1	-1	1	-1	18	0	0	1	-1	17	543.65757	0.00056	1509.45905	965.80204
17	1	-1	1	-1	19	0	0	1	-1	18	545.56910	-0.00049	1545.66036	1000.09076
18	1	-1	1	-1	20	0	0	1	-1	19	547.48145	-0.00020	1583.76307	1036.28142
19	1	-1	1	-1	21	0	0	1	-1	20	549.39233	-0.00083	1623.76670	1074.37353
20	1	-1	1	-1	22	0	0	1	-1	21	551.30384	-0.00029	1665.67070	1114.36658
21	1	-1	1	-1	23	0	0	1	-1	22	553.21476	0.00024	1709.47454	1156.26002
22	1	-1	1	-1	24	0	0	1	-1	23	555.12517	0.00083	1755.17765	1200.05331
23	1	-1	1	-1	25	0	0	1	-1	24	557.03364	0.00006	1802.77942	1245.74584
24	1	-1	1	-1	26	0	0	1	-1	25	558.94220	-0.00001	1852.27923	1293.33701
25	1	-1	1	-1	27	0	0	1	-1	26	560.85032	0.00008	1903.67642	1342.82618
26	1	-1	1	-1	28	0	0	1	-1	27	562.75782	0.00018	1956.97033	1394.21269
27	1	-1	1	-1	3	0	0	1	1	3	509.27191	0.00041	1194.90643	685.63493
28	1	-1	1	-1	4	0	0	1	1	4	509.30201	-0.00025	1202.53608	693.23382
29	1	-1	1	-1	6	0	0	1	1	6	509.38673	0.00034	1223.51646	714.13007
30	1	-1	1	-1	7	0	0	1	1	7	509.44053*	0.00094	1236.86675	727.42716
31	1	-1	1	-1	8	0	0	1	1	8	509.50015	0.00009	1252.12340	742.62333
32	1	-1	1	-1	9	0	0	1	1	9	509.56742	-0.00028	1269.28609	759.71839
33	1	-1	1	-1	10	0	0	1	1	10	509.64243	0.00004	1288.35448	778.71209
34	1	-1	1	-1	12	0	0	1	1	12	509.81196	-0.00045	1332.20685	822.39444
35	1	-1	1	-1	13	0	0	1	1	13	509.90711	-0.00042	1356.99004	847.08251
36	1	-1	1	-1	14	0	0	1	1	14	510.00843	-0.00083	1383.67734	873.66808
37	1	-1	1	-1	15	0	0	1	1	15	510.11631*	-0.00123	1412.26833	902.15079W
38	1	-1	1	-1	16	0	0	1	1	16	510.23281	0.00052	1442.76257	932.53028

rms = 0.00043 cm⁻¹

2v₅ (Σ⁺) ← v₅ (Π)

v ₄ '	l ₄ '	v ₅ '	l ₅ '	J'	v ₄ ''	l ₄ ''	v ₅ ''	l ₅ ''	J''	OBS	OBS – CALC	G'	G''
0	0	2	0	0	0	0	1	1	1	659.17205	-0.00032	1335.30850	676.13613
0	0	2	0	1	0	0	1	1	2	657.27896	0.00016	1337.21447	679.93567
0	0	2	0	2	0	0	1	1	3	655.39130	-0.00015	1341.02637	685.63493
0	0	2	0	3	0	0	1	1	4	653.51031	0.00000	1346.74412	693.23382
0	0	2	0	4	0	0	1	1	5	651.63513	-0.00022	1354.36759	702.73224
0	0	2	0	5	0	0	1	1	6	649.76666	0.00011	1363.89662	714.13007
0	0	2	0	6	0	0	1	1	7	647.90391	0.00007	1375.33100	727.42716
0	0	2	0	7	0	0	1	1	8	646.04650	-0.00064	1388.67047	742.62333
0	0	2	0	8	0	0	1	1	9	644.19611	-0.00026	1403.91476	759.71839
0	0	2	0	9	0	0	1	1	10	642.35134	-0.00009	1421.06352	778.71209
0	0	2	0	10	0	0	1	1	11	640.51191	-0.00027	1440.11639	799.60420
0	0	2	0	11	0	0	1	1	12	638.67828	-0.00022	1461.07294	822.39444
0	0	2	0	12	0	0	1	1	13	636.84963	-0.00059	1483.93273	847.08251
0	0	2	0	13	0	0	1	1	14	635.02725	0.00008	1508.69525	873.66808
0	0	2	0	14	0	0	1	1	15	633.20906	-0.00011	1535.35996	902.15079
0	0	2	0	15	0	0	1	1	16	631.39568	-0.00033	1563.92630	932.53028
0	0	2	0	16	0	0	1	1	17	629.58760	0.00011	1594.39363	964.80614
0	0	2	0	17	0	0	1	1	18	627.78331	-0.00004	1626.76130	998.97795
0	0	2	0	18	0	0	1	1	19	625.98319	-0.00017	1661.02860	1035.04524
0	0	2	0	19	0	0	1	1	20	624.18731	0.00005	1697.19482	1073.00756
0	0	2	0	20	0	0	1	1	21	622.39494	0.00017	1735.25916	1112.86438
0	0	2	0	21	0	0	1	1	22	620.60257	0.00029	1775.22081	1154.61520

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0	0	2	0	22	0	0	1	1	23	618.81924	-0.00025	1817.07894	1198.25945
0	0	2	0	23	0	0	1	1	24	617.03562	-0.00048	1860.83266	1243.79656
0	0	2	0	24	0	0	1	1	25	615.25399	-0.00114	1906.48106	1291.22593W
0	0	2	0	25	0	0	1	1	26	613.47615	-0.00010	1954.02319	1340.54693
0	0	2	0	26	0	0	1	1	27	611.69924	0.00008	2003.45808	1391.75891
0	0	2	0	27	0	0	1	1	28	609.92372	0.00019	2054.78472	1444.86119
0	0	2	0	28	0	0	1	1	29	608.14929	0.00026	2108.00210	1499.85307
0	0	2	0	29	0	0	1	1	30	606.37517	-0.00016	2163.10916	1556.73383
0	0	2	0	30	0	0	1	1	31	604.60245	0.00033	2220.10483	1615.50271
0	0	2	0	31	0	0	1	1	32	602.82928	0.00019	2278.98802	1676.15894
0	0	2	0	32	0	0	1	1	33	601.05599	0.00007	2339.75763	1738.70171
0	0	2	0	33	0	0	1	1	34	599.28183	-0.00050	2402.41252	1803.13019
0	0	2	0	34	0	0	1	1	35	597.50803	0.00001	2466.95157	1869.44355
0	0	2	0	35	0	0	1	1	36	595.73285	0.00011	2533.37364	1937.64090
0	0	2	0	36	0	0	1	1	37	593.95873	0.00252	2601.67755	2007.72134W
0	0	2	0	37	0	0	1	1	38	592.17952	0.00130	2671.86216	2079.68394W
0	0	2	0	2	0	0	1	1	1	664.89036	0.00011	1341.02637	676.13613
0	0	2	0	3	0	0	1	1	2	666.80800	-0.00045	1346.74412	679.93567
0	0	2	0	4	0	0	1	1	3	668.73242	-0.00025	1354.36759	685.63493
0	0	2	0	5	0	0	1	1	4	670.66271	-0.00009	1363.89662	693.23382
0	0	2	0	6	0	0	1	1	5	672.59861	-0.00015	1375.33100	702.73224
0	0	2	0	7	0	0	1	1	6	674.54517*	0.00477	1388.67047	714.13007W
0	0	2	0	8	0	0	1	1	7	676.48757	-0.00003	1403.91476	727.42716
0	0	2	0	9	0	0	1	1	8	678.44023	0.00004	1421.06352	742.62333
0	0	2	0	10	0	0	1	1	9	680.39785	-0.00015	1440.11639	759.71839
0	0	2	0	11	0	0	1	1	10	682.36099	0.00014	1461.07294	778.71209
0	0	2	0	12	0	0	1	1	11	684.32819	-0.00033	1483.93273	799.60420
0	0	2	0	13	0	0	1	1	12	686.30059	-0.00021	1508.69525	822.39444
0	0	2	0	14	0	0	1	1	13	688.27727	-0.00018	1535.35996	847.08251
0	0	2	0	15	0	0	1	1	14	690.25799	-0.00023	1563.92630	873.66808
0	0	2	0	16	0	0	1	1	15	692.24274	-0.00009	1594.39363	902.15079
0	0	2	0	17	0	0	1	1	16	694.23095	-0.00006	1626.76130	932.53028
0	0	2	0	18	0	0	1	1	17	696.22214	-0.00032	1661.02860	964.80614
0	0	2	0	19	0	0	1	1	18	698.21636	-0.00051	1697.19482	998.97795
0	0	2	0	20	0	0	1	1	19	700.21367	-0.00024	1735.25916	1035.04524
0	0	2	0	21	0	0	1	1	20	702.21316	-0.00010	1775.22081	1073.00756
0	0	2	0	22	0	0	1	1	21	704.21413	-0.00043	1817.07894	1112.86438
0	0	2	0	23	0	0	1	1	22	706.21703	-0.00043	1860.83266	1154.61520
0	0	2	0	24	0	0	1	1	23	708.22083	-0.00078	1906.48106	1198.25945
0	0	2	0	25	0	0	1	1	24	710.22620	-0.00042	1954.02319	1243.79656
0	0	2	0	26	0	0	1	1	25	712.23261	0.00047	2003.45808	1291.22593
0	0	2	0	27	0	0	1	1	26	714.23950*	0.00171	2054.78472	1340.54693W
0	0	2	0	28	0	0	1	1	27	716.24291	-0.00028	2108.00210	1391.75891
0	0	2	0	29	0	0	1	1	28	718.24818	0.00021	2163.10916	1444.86119
0	0	2	0	30	0	0	1	1	29	720.25180	0.00004	2220.10483	1499.85307
0	0	2	0	4	0	0	1	-1	4	661.06978*	0.00121	1354.36759	693.29902W
0	0	2	0	5	0	0	1	-1	5	661.06750*	0.00092	1363.89662	702.83004
0	0	2	0	6	0	0	1	-1	6	661.06417	0.00015	1375.33100	714.26698
0	0	2	0	7	0	0	1	-1	7	661.06123	0.00045	1388.67047	727.60969
0	0	2	0	8	0	0	1	-1	8	661.05681	0.00004	1403.91476	742.85799
0	0	2	0	9	0	0	1	-1	9	661.05218	0.00034	1421.06352	760.01168
0	0	2	0	10	0	0	1	-1	10	661.04571	-0.00016	1440.11639	779.07052
0	0	2	0	11	0	0	1	-1	11	661.03855	-0.00013	1461.07294	800.03426
0	0	2	0	12	0	0	1	-1	12	661.03000	-0.00011	1483.93273	822.90261
0	0	2	0	13	0	0	1	-1	13	661.01975	-0.00021	1508.69525	847.67528
0	0	2	0	14	0	0	1	-1	14	661.00783	-0.00020	1535.35996	874.35193
0	0	2	0	15	0	0	1	-1	15	660.99406	-0.00004	1563.92630	902.93220
0	0	2	0	16	0	0	1	-1	16	660.97765	-0.00027	1594.39363	933.41570
0	0	2	0	17	0	0	1	-1	17	660.95895	-0.00031	1626.76130	965.80204
0	0	2	0	18	0	0	1	-1	18	660.93773	-0.00011	1661.02860	1000.09076
0	0	2	0	20	0	0	1	-1	20	660.88550	-0.00012	1735.25916	1074.37353
0	0	2	0	21	0	0	1	-1	21	660.85424	0.00000	1775.22081	1114.36658
0	0	2	0	22	0	0	1	-1	22	660.81920	0.00028	1817.07894	1156.26002
0	0	2	0	23	0	0	1	-1	23	660.77902	-0.00033	1860.83266	1200.05331
0	0	2	0	24	0	0	1	-1	24	660.73575	0.00053	1906.48106	1245.74584
0	0	2	0	25	0	0	1	-1	25	660.68608	-0.00009	1954.02319	1293.33701
0	0	2	0	26	0	0	1	-1	26	660.63180	-0.00009	2003.45808	1342.82618
0	0	2	0	27	0	0	1	-1	27	660.57198	-0.00005	2054.78472	1394.21269
0	0	2	0	28	0	0	1	-1	28	660.50600	-0.00026	2108.00210	1447.49584

1	0	0	2	0	29	0	0	1	-1	29	660.43376	-0.00048	2163.10916	1502.67492
2	0	0	2	0	30	0	0	1	-1	30	660.35586	0.00023	2220.10483	1559.74920
3	0	0	2	0	31	0	0	1	-1	31	660.27025	0.00012	2278.98802	1618.71789
4	0	0	2	0	32	0	0	1	-1	32	660.17633	-0.00107	2339.75763	1679.58023W
5	0	0	2	0	33	0	0	1	-1	33	660.07778	0.00063	2402.41252	1742.33538
6	0	0	2	0	34	0	0	1	-1	34	659.96709*	-0.00198	2466.95157	1806.98250W
7	0	0	2	0	35	0	0	1	-1	35	659.85318	0.00028	2533.37364	1873.52074
8	0	0	2	0	36	0	0	1	-1	36	659.72888	0.00051	2601.67755	1941.94919
9	0	0	2	0	37	0	0	1	-1	37	659.59569	0.00046	2671.86216	2012.26694
10	0	0	2	0	38	0	0	1	-1	38	659.45330	0.00004	2743.92630	2084.47304

rms = 0.00028 cm⁻¹

2ν₅ (Δ) ← ν₅ (Π)

ν ₄ '	ℓ ₄ '	ν ₅ '	ℓ ₅ '	J'	ν ₄ "	ℓ ₄ "	ν ₅ "	ℓ ₅ "	J''	OBS	OBS - CALC	G'	G''
0	0	2	2	3	0	0	1	1	4	670.09560	-0.00018	1363.32960	693.23382
0	0	2	2	4	0	0	1	1	5	668.21789	0.00039	1370.94974	702.73224
0	0	2	2	5	0	0	1	1	6	666.34445	-0.00032	1380.47484	714.13007
0	0	2	2	6	0	0	1	1	7	664.47760	-0.00010	1391.90486	727.42716
0	0	2	2	7	0	0	1	1	8	662.61630	-0.00009	1405.23972	742.62333
0	0	2	2	8	0	0	1	1	9	660.75990*	-0.00109	1420.47938	759.71839W
0	0	2	2	9	0	0	1	1	10	658.91128	-0.00036	1437.62374	778.71209
0	0	2	2	10	0	0	1	1	11	657.06871	0.00020	1456.67272	799.60420
0	0	2	2	11	0	0	1	1	12	655.23178	0.00001	1477.62621	822.39444
0	0	2	2	12	0	0	1	1	13	653.40149	-0.00012	1500.48412	847.08251
0	0	2	2	13	0	0	1	1	14	651.57802	-0.00023	1525.24633	873.66808
0	0	2	2	14	0	0	1	1	15	649.76176	-0.00015	1551.91270	902.15079
0	0	2	2	15	0	0	1	1	16	647.95266	-0.00015	1580.48310	932.53028
0	0	2	2	16	0	0	1	1	17	646.15090	-0.00033	1610.95737	964.80614
0	0	2	2	17	0	0	1	1	18	644.35704	-0.00038	1643.33536	998.97795
0	0	2	2	18	0	0	1	1	19	642.57161	-0.00004	1677.61689	1035.04524
0	0	2	2	19	0	0	1	1	20	640.79394	-0.00028	1713.80178	1073.00756
0	0	2	2	20	0	0	1	1	21	639.02561	0.00017	1751.88982	1112.86438
0	0	2	2	21	0	0	1	1	22	637.26540	-0.00021	1791.88081	1154.61520
0	0	2	2	22	0	0	1	1	23	635.51514	0.00009	1833.77451	1198.25945
0	0	2	2	23	0	0	1	1	24	633.77332	-0.00078	1877.57067	1243.79656
0	0	2	2	24	0	0	1	1	25	632.04251	-0.00058	1923.26903	1291.22593
0	0	2	2	25	0	0	1	1	26	630.32262	0.00025	1970.86930	1340.54693
0	0	2	2	26	0	0	1	1	27	628.61250	0.00023	2020.37118	1391.75891
0	0	2	2	27	0	0	1	1	28	626.91238	-0.00076	2071.77433	1444.86119
0	0	2	2	28	0	0	1	1	29	625.22477	-0.00056	2125.07841	1499.85307
0	0	2	2	29	0	0	1	1	30	623.54980*	0.00062	2180.28301	1556.73383
0	0	2	2	30	0	0	1	1	31	621.88448	-0.00055	2237.38774	1615.50271
0	0	2	2	31	0	0	1	1	32	620.23286	-0.00035	2296.39214	1676.15894
0	0	2	2	32	0	0	1	1	33	618.59337	-0.00066	2357.29574	1738.70171
0	0	2	2	33	0	0	1	1	34	616.96910	0.00128	2420.09801	1803.13019W
0	0	2	2	34	0	0	1	1	35	615.35581	0.00095	2484.79841	1869.44355
0	0	2	2	2	0	0	1	1	1	681.47824	-0.00009	1357.61446	676.13613
0	0	2	2	3	0	0	1	1	2	683.39483	0.00090	1363.32960	679.93567
0	0	2	2	4	0	0	1	1	3	685.31441	-0.00040	1370.94974	685.63493
0	0	2	2	5	0	0	1	1	4	687.24129	0.00027	1380.47484	693.23382
0	0	2	2	6	0	0	1	1	5	689.17285	0.00023	1391.90486	702.73224
0	0	2	2	7	0	0	1	1	6	691.10984	0.00019	1405.23972	714.13007
0	0	2	2	8	0	0	1	1	7	693.05279	0.00057	1420.47938	727.42716
0	0	2	2	9	0	0	1	1	8	695.00079	0.00039	1437.62374	742.62333
0	0	2	2	10	0	0	1	1	9	696.95476	0.00043	1456.67272	759.71839
0	0	2	2	11	0	0	1	1	10	698.91419	0.00007	1477.62621	778.71209
0	0	2	2	12	0	0	1	1	11	700.87993	0.00001	1500.48412	799.60420
0	0	2	2	13	0	0	1	1	12	702.85190	0.00002	1525.24633	822.39444
0	0	2	2	15	0	0	1	1	14	706.81517	0.00015	1580.48310	873.66808
0	0	2	2	16	0	0	1	1	15	708.80629	-0.00029	1610.95737	902.15079
0	0	2	2	17	0	0	1	1	16	710.80490	-0.00018	1643.33536	932.53028
0	0	2	2	18	0	0	1	1	17	712.81071	-0.00004	1677.61689	964.80614
0	0	2	2	19	0	0	1	1	18	714.82376	-0.00007	1713.80178	998.97795
0	0	2	2	20	0	0	1	1	19	716.83700	0.00000	1751.88982	1035.04524

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0	0	2	2	21	0	0	1	1	20	718.87319	-0.00006	1791.88081	1073.00756
0	0	2	2	22	0	0	1	1	21	720.90994	-0.00018	1833.77451	1112.86438
0	0	2	2	23	0	0	1	1	22	722.95529	-0.00018	1877.57067	1154.61520
0	0	2	2	24	0	0	1	1	23	725.00951	-0.00006	1923.26903	1198.25945
0	0	2	2	25	0	0	1	1	24	727.07297	0.00023	1970.86930	1243.79656
0	0	2	2	26	0	0	1	1	25	729.14487	-0.00038	2020.37118	1291.22593
0	0	2	2	27	0	0	1	1	26	731.22712	-0.00028	2071.77433	1340.54693
0	0	2	2	28	0	0	1	1	27	733.31938	-0.00011	2125.07841	1391.75891
0	0	2	2	29	0	0	1	1	28	735.42198	0.00016	2180.28301	1444.86119
0	0	2	2	30	0	0	1	1	29	737.53428	-0.00038	2237.38774	1499.85307
0	0	2	2	31	0	0	1	1	30	739.65709*	-0.00122	2296.39214	1556.73383W
0	0	2	2	32	0	0	1	1	31	741.79321	0.00018	2357.29574	1615.50271
0	0	2	2	33	0	0	1	1	32	743.93968	0.00060	2420.09801	1676.15894
0	0	2	2	34	0	0	1	1	33	746.09738	0.00067	2484.79841	1738.70171
0	0	2	2	35	0	0	1	1	34	748.26634	0.00019	2551.39634	1803.13019
0	0	2	2	36	0	0	1	1	35	750.44826	0.00064	2619.89117	1869.44355
0	0	2	2	37	0	0	1	1	36	752.64118	-0.00013	2690.28221	1937.64090
0	0	2	2	3	0	0	1	-1	3	677.65599	0.00044	1363.32960	685.67405
0	0	2	2	4	0	0	1	-1	4	677.65110	0.00038	1370.94974	693.29902
0	0	2	2	8	0	0	1	-1	8	677.62197*	0.00058	1420.47938	742.85799
0	0	2	2	9	0	0	1	-1	9	677.61210	0.00004	1437.62374	760.01168
0	0	2	2	10	0	0	1	-1	10	677.60164	-0.00056	1456.67272	779.07052
0	0	2	2	11	0	0	1	-1	11	677.59241	0.00045	1477.62621	800.03426
0	0	2	2	12	0	0	1	-1	12	677.58173	0.00022	1500.48412	822.90261
0	0	2	2	13	0	0	1	-1	13	677.57103	-0.00002	1525.24633	847.67528
0	0	2	2	14	0	0	1	-1	14	677.56099	0.00022	1551.91270	874.35193
0	0	2	2	15	0	0	1	-1	15	677.55133	0.00043	1580.48310	902.93220
0	0	2	2	16	0	0	1	-1	16	677.54190	0.00023	1610.95737	933.41570
0	0	2	2	17	0	0	1	-1	17	677.53317	-0.00016	1643.33536	965.80204
0	0	2	2	18	0	0	1	-1	18	677.52554	-0.00059	1677.61689	1000.09076
0	0	2	2	19	0	0	1	-1	19	677.51992	-0.00044	1713.80178	1036.28142
0	0	2	2	20	0	0	1	-1	20	677.51646	0.00017	1751.88982	1074.37353
0	0	2	-2	2	0	0	1	-1	3	671.94100*	0.00061	1357.61444	685.67405
0	0	2	-2	3	0	0	1	-1	4	670.03095	0.00045	1363.32952	693.29902
0	0	2	-2	4	0	0	1	-1	5	668.12020	0.00074	1370.94950	702.83004
0	0	2	-2	5	0	0	1	-1	6	666.20713	-0.00018	1380.47429	714.26698
0	0	2	-2	6	0	0	1	-1	7	664.29394	-0.00012	1391.90376	727.60969
0	0	2	-2	7	0	0	1	-1	8	662.37952	-0.00023	1405.23774	742.85799
0	0	2	-2	8	0	0	1	-1	9	660.46440	0.00000	1420.47607	760.01168
0	0	2	-2	9	0	0	1	-1	10	658.54859	0.00056	1437.61854	779.07052
0	0	2	-2	10	0	0	1	-1	11	656.63040	-0.00027	1456.66492	800.03426
0	0	2	-2	11	0	0	1	-1	12	654.71221	-0.00013	1477.61496	822.90261
0	0	2	-2	12	0	0	1	-1	13	652.79360	0.00052	1500.46836	847.67528
0	0	2	-2	13	0	0	1	-1	14	650.87303	0.00013	1525.22483	874.35193
0	0	2	-2	14	0	0	1	-1	15	648.95200	0.00016	1551.88404	902.93220
0	0	2	-2	15	0	0	1	-1	16	647.03017	0.00025	1580.44562	933.41570
0	0	2	-2	16	0	0	1	-1	17	645.10727	0.00011	1610.90919	965.80204
0	0	2	-2	17	0	0	1	-1	18	643.18425	0.00066	1643.27435	1000.09076
0	0	2	-2	18	0	0	1	-1	19	641.25978	0.00054	1677.54066	1036.28142
0	0	2	-2	19	0	0	1	-1	20	639.33438	0.00026	1713.70766	1074.37353
0	0	2	-2	20	0	0	1	-1	21	637.40816	-0.00012	1751.77486	1114.36658
0	0	2	-2	21	0	0	1	-1	22	635.48184	0.00011	1791.74175	1156.26002
0	0	2	-2	22	0	0	1	-1	23	633.55492	0.00042	1833.60781	1200.05331
0	0	2	-2	23	0	0	1	-1	24	631.62637	-0.00024	1877.37245	1245.74584
0	0	2	-2	24	0	0	1	-1	25	629.69792	-0.00018	1923.03511	1293.33701
0	0	2	-2	25	0	0	1	-1	26	627.76884	-0.00014	1970.59516	1342.82618
0	0	2	-2	26	0	0	1	-1	27	625.83946	0.00018	2020.05197	1394.21269
0	0	2	-2	27	0	0	1	-1	28	623.90894	-0.00010	2071.40488	1447.49584
0	0	2	-2	28	0	0	1	-1	29	621.97884	0.00058	2124.65319	1502.67492
0	0	2	-2	29	0	0	1	-1	30	620.04782	0.00083	2179.79618	1559.74920
0	0	2	-2	30	0	0	1	-1	31	618.11534	0.00010	2236.83314	1618.71789
0	0	2	-2	31	0	0	1	-1	32	616.18237	-0.00068	2295.76327	1679.58023
0	0	2	-2	32	0	0	1	-1	33	614.24984	-0.00059	2356.58580	1742.33538
0	0	2	-2	33	0	0	1	-1	34	612.31751	0.00010	2419.29991	1806.98250
0	0	2	-2	34	0	0	1	-1	35	610.38467	0.00065	2483.90476	1873.52074
0	0	2	-2	35	0	0	1	-1	36	608.45066	0.00037	2550.39948	1941.94919
0	0	2	-2	36	0	0	1	-1	37	606.51563	-0.00061	2618.78318	2012.26694
0	0	2	-2	2	0	0	1	-1	1	681.47175	-0.00004	1357.61444	676.14265
0	0	2	-2	3	0	0	1	-1	2	683.37456	0.00038	1363.32952	679.95524

1	0	0	2	-2	4	0	0	1	-1	3	685.27496	-0.00049	1370.94950	685.67405
2	0	0	2	-2	5	0	0	1	-1	4	687.17513	-0.00014	1380.47429	693.29902
3	0	0	2	-2	6	0	0	1	-1	5	689.07410	0.00038	1391.90376	702.83004
4	0	0	2	-2	7	0	0	1	-1	6	690.97082	0.00006	1405.23774	714.26698
5	0	0	2	-2	8	0	0	1	-1	7	692.86640	0.00002	1420.47607	727.60969
6	0	0	2	-2	9	0	0	1	-1	8	694.76069	0.00014	1437.61854	742.85799
7	0	0	2	-2	10	0	0	1	-1	9	696.65327	0.00002	1456.66492	760.01168
8	0	0	2	-2	11	0	0	1	-1	10	698.54451	0.00007	1477.61496	779.07052
9	0	0	2	-2	12	0	0	1	-1	11	700.43407	-0.00003	1500.46836	800.03426
10	0	0	2	-2	13	0	0	1	-1	12	702.32252	0.00030	1525.22483	822.90261
11	0	0	2	-2	14	0	0	1	-1	13	704.20961	0.00085	1551.88404	847.67528
12	0	0	2	-2	15	0	0	1	-1	14	706.09418	0.00049	1580.44562	874.35193
13	0	0	2	-2	16	0	0	1	-1	15	707.97700	0.00000	1610.90919	902.93220
14	0	0	2	-2	17	0	0	1	-1	16	709.85906	0.00041	1643.27435	933.41570
15	0	0	2	-2	18	0	0	1	-1	17	711.73903	0.00041	1677.54066	965.80204
16	0	0	2	-2	19	0	0	1	-1	18	713.61685	-0.00004	1713.70766	1000.09076
17	0	0	2	-2	20	0	0	1	-1	19	715.49340	-0.00003	1751.77486	1036.28142
18	0	0	2	-2	21	0	0	1	-1	20	717.36828	0.00006	1791.74175	1074.37353
19	0	0	2	-2	22	0	0	1	-1	21	719.24117	-0.00006	1833.60781	1114.36658
20	0	0	2	-2	23	0	0	1	-1	22	721.11262	0.00019	1877.37245	1156.26002
21	0	0	2	-2	24	0	0	1	-1	23	722.98173	-0.00007	1923.03511	1200.05331
22	0	0	2	-2	25	0	0	1	-1	24	724.84928	-0.00004	1970.59516	1245.74584
23	0	0	2	-2	26	0	0	1	-1	25	726.71477	-0.00019	2020.05197	1293.33701
24	0	0	2	-2	27	0	0	1	-1	26	728.57906*	0.00037	2071.40488	1342.82618
25	0	0	2	-2	28	0	0	1	-1	27	730.43960*	-0.00090	2124.65319	1394.21269
26	0	0	2	-2	29	0	0	1	-1	28	732.29976	-0.00058	2179.79618	1447.49584
27	0	0	2	-2	30	0	0	1	-1	29	734.15820	-0.00001	2236.83314	1502.67492
28	0	0	2	-2	31	0	0	1	-1	30	736.01350	-0.00058	2295.76327	1559.74920
29	0	0	2	-2	32	0	0	1	-1	31	737.86852	0.00061	2356.58580	1618.71789
30	0	0	2	-2	33	0	0	1	-1	32	739.71942	-0.00027	2419.29991	1679.58023
31	0	0	2	-2	34	0	0	1	-1	33	741.56959	0.00021	2483.90476	1742.33538
32	0	0	2	-2	35	0	0	1	-1	34	743.41731	0.00033	2550.39948	1806.98250
33	0	0	2	-2	37	0	0	1	-1	36	747.10563	-0.00012	2689.05494	1941.94919
34	0	0	2	-2	38	0	0	1	-1	37	748.94990	0.00301	2761.21382	2012.26694W
35	0	0	2	-2	39	0	0	1	-1	38	750.78621	0.00040	2835.25885	2084.47304
36	0	0	2	-2	40	0	0	1	-1	39	752.62270	0.00019	2911.18905	2158.56653
37	0	0	2	-2	41	0	0	1	-1	40	754.45642	-0.00054	2989.00338	2234.54642
38	0	0	2	-2	2	0	0	1	1	2	677.67882	0.00005	1357.61444	679.93567
39	0	0	2	-2	3	0	0	1	1	3	677.69464	0.00005	1363.32952	685.63493
40	0	0	2	-2	4	0	0	1	1	4	677.71579	0.00010	1370.94950	693.23382
41	0	0	2	-2	5	0	0	1	1	5	677.74216	0.00011	1380.47429	702.73224
42	0	0	2	-2	7	0	0	1	1	7	677.81130*	0.00072	1405.23774	727.42716
43	0	0	2	-2	8	0	0	1	1	8	677.85306	0.00032	1420.47607	742.62333
44	0	0	2	-2	9	0	0	1	1	9	677.90029	0.00013	1437.61854	759.71839
45	0	0	2	-2	10	0	0	1	1	10	677.95300	0.00017	1456.66492	778.71209
46	0	0	2	-2	11	0	0	1	1	11	678.01077	0.00002	1477.61496	799.60420
47	0	0	2	-2	12	0	0	1	1	12	678.07389	-0.00003	1500.46836	822.39444
48	0	0	2	-2	13	0	0	1	1	13	678.14226	-0.00006	1525.22483	847.08251
49	0	0	2	-2	14	0	0	1	1	14	678.21589	-0.00007	1551.88404	873.66808
50	0	0	2	-2	15	0	0	1	1	15	678.29496	0.00013	1580.44562	902.15079
51	0	0	2	-2	16	0	0	1	1	16	678.37887	-0.00004	1610.90919	932.53028
52	0	0	2	-2	17	0	0	1	1	17	678.46800	-0.00021	1643.27435	964.80614
53	0	0	2	-2	18	0	0	1	1	18	678.56256	-0.00015	1677.54066	998.97795
54	0	0	2	-2	19	0	0	1	1	19	678.66220	-0.00021	1713.70766	1035.04524
55	0	0	2	-2	20	0	0	1	1	20	678.76717	-0.00013	1751.77486	1073.00756
56	0	0	2	-2	21	0	0	1	1	21	678.87724	-0.00013	1791.74175	1112.86438
57	0	0	2	-2	22	0	0	1	1	22	678.99190	-0.00071	1833.60781	1154.61520
58	0	0	2	-2	23	0	0	1	1	23	679.11249	-0.00051	1877.37245	1198.25945
59	0	0	2	-2	24	0	0	1	1	24	679.23803	-0.00052	1923.03511	1243.79656
60	0	0	2	-2	25	0	0	1	1	25	679.36902	-0.00021	1970.59516	1291.22593
	0	0	2	-2	26	0	0	1	1	26	679.50462	-0.00042	2020.05197	1340.54693
	0	0	2	-2	27	0	0	1	1	27	679.64570	-0.00027	2071.40488	1391.75891
	0	0	2	-2	28	0	0	1	1	28	679.79151	-0.00048	2124.65319	1444.86119
	0	0	2	-2	29	0	0	1	1	29	679.94263	-0.00048	2179.79618	1499.85307
	0	0	2	-2	30	0	0	1	1	30	680.09911	-0.00019	2236.83314	1556.73383
	0	0	2	-2	31	0	0	1	1	31	680.26047	-0.00009	2295.76327	1615.50271
	0	0	2	-2	32	0	0	1	1	32	680.42626	-0.00061	2356.58580	1676.15894
	0	0	2	-2	33	0	0	1	1	33	680.59768	-0.00053	2419.29991	1738.70171
	0	0	2	-2	34	0	0	1	1	34	680.77312	-0.00145	2483.90476	1803.13019W

0 0 2 -2 35 0 0 1 1 35 680.95624 0.00031 2550.39948 1869.44355

rms = 0.00036 cm⁻¹

$2\nu_4 + \nu_5 (\text{II } \Pi) \leftarrow 2\nu_4 (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 0 1 1 1	2 0 0 0 2	670.75476*	0.00265	1693.33369	1022.58159W
2 0 1 1 2	2 0 0 0 3	668.84915	0.00031	1697.16027	1028.31143
2 0 1 1 3	2 0 0 0 4	666.94947	0.00019	1702.89992	1035.95064
2 0 1 1 4	2 0 0 0 5	665.05311	-0.00055	1710.55241	1045.49875
2 0 1 1 5	2 0 0 0 6	663.16271	0.00045	1720.11740	1056.95515
2 0 1 1 6	2 0 0 0 7	661.27524	-0.00012	1731.59446	1070.31910
2 0 1 1 7	2 0 0 0 8	659.39319	-0.00009	1744.98305	1085.58977
2 0 1 1 8	2 0 0 0 9	657.51647	0.00013	1760.28255	1102.76621
2 0 1 1 9	2 0 0 0 10	655.64490	0.00006	1777.49222	1121.84738
2 0 1 1 10	2 0 0 0 11	653.77925	0.00022	1796.61120	1142.83216
2 0 1 1 11	2 0 0 0 12	651.91985	0.00072	1817.63849	1165.71936
2 0 1 1 12	2 0 0 0 13	650.06533	0.00009	1840.57298	1190.50774
2 0 1 1 13	2 0 0 0 14	648.21761	0.00025	1865.41342	1217.19606
2 0 1 1 14	2 0 0 0 15	646.37566	0.00032	1892.15842	1245.78308
2 0 1 1 15	2 0 0 0 16	644.53890	0.00003	1920.80648	1276.26760
2 0 1 1 16	2 0 0 0 17	642.70758	0.00011	1951.35596	1308.64848
2 0 1 1 17	2 0 0 0 18	640.87996	-0.00053	1983.80515	1342.92466
2 0 1 1 18	2 0 0 0 19	639.05744	0.00033	2018.15225	1379.09514
2 0 1 1 19	2 0 0 0 20	637.23675	0.00033	2054.39547	1417.15906
2 0 1 1 20	2 0 0 0 21	635.41748	0.00008	2092.53300	1457.11560
2 0 1 1 21	2 0 0 0 22	633.59929	0.00027	2132.56309	1498.96407
2 0 1 1 22	2 0 0 0 23	631.78031	0.00002	2174.48410	1542.70381
2 0 1 1 23	2 0 0 0 24	629.96058	0.00032	2218.29450	1588.33424
2 0 1 1 24	2 0 0 0 25	628.13866	0.00054	2263.99292	1635.85480
2 0 1 1 25	2 0 0 0 26	626.31290	-0.00025	2311.57813	1685.26498
2 0 1 1 26	2 0 0 0 27	624.48660	0.00178	2361.04907	1736.56425W
2 0 1 1 1	2 0 0 0 0	676.48757*	0.00526	1693.33369	1016.85139W
2 0 1 1 2	2 0 0 0 1	678.39955	0.00078	1697.16027	1018.76149
2 0 1 1 3	2 0 0 0 2	680.31807	-0.00027	1702.89992	1022.58159
2 0 1 1 4	2 0 0 0 3	682.24142	0.00043	1710.55241	1028.31143
2 0 1 1 5	2 0 0 0 4	684.16623	-0.00053	1720.11740	1035.95064
2 0 1 1 6	2 0 0 0 5	686.09788*	0.00218	1731.59446	1045.49875W
2 0 1 1 7	2 0 0 0 6	688.02764	-0.00026	1744.98305	1056.95515
2 0 1 1 8	2 0 0 0 7	689.96327	-0.00019	1760.28255	1070.31910
2 0 1 1 9	2 0 0 0 8	691.90249	0.00004	1777.49222	1085.58977
2 0 1 1 10	2 0 0 0 9	693.84444	-0.00054	1796.61120	1102.76621
2 0 1 1 11	2 0 0 0 10	695.79060	-0.00050	1817.63849	1121.84738
2 0 1 1 12	2 0 0 0 11	697.74040	-0.00041	1840.57298	1142.83216
2 0 1 1 13	2 0 0 0 12	699.69446	0.00040	1865.41342	1165.71936
2 0 1 1 14	2 0 0 0 13	701.65018	-0.00050	1892.15842	1190.50774
2 0 1 1 15	2 0 0 0 14	703.61008	-0.00034	1920.80648	1217.19606
2 0 1 1 16	2 0 0 0 15	705.57285	-0.00003	1951.35596	1245.78308
2 0 1 1 17	2 0 0 0 16	707.53762	0.00008	1983.80515	1276.26760
2 0 1 1 18	2 0 0 0 17	709.50345	-0.00032	2018.15225	1308.64848
2 0 1 1 19	2 0 0 0 18	711.47054	-0.00028	2054.39547	1342.92466
2 0 1 1 20	2 0 0 0 19	713.43756	-0.00030	2092.53300	1379.09514
2 0 1 1 21	2 0 0 0 20	715.40460	0.00057	2132.56309	1417.15906
2 0 1 1 22	2 0 0 0 21	717.36828	-0.00022	2174.48410	1457.11560
2 0 1 1 23	2 0 0 0 22	719.33029	-0.00014	2218.29450	1498.96407
2 0 1 1 24	2 0 0 0 23	721.28904	-0.00007	2263.99292	1542.70381
2 0 1 1 25	2 0 0 0 24	723.24245	-0.00145	2311.57813	1588.33424W
2 0 1 -1 1	2 0 0 0 1	674.57208*	0.00176	1693.33182	1018.76149W
2 0 1 -1 2	2 0 0 0 2	674.57208	-0.00096	1697.15463	1022.58159
2 0 1 -1 3	2 0 0 0 3	674.57780	0.00058	1702.88865	1028.31143
2 0 1 -1 4	2 0 0 0 4	674.58305	0.00007	1710.53362	1035.95064
2 0 1 -1 5	2 0 0 0 5	674.58988	-0.00060	1720.08923	1045.49875
2 0 1 -1 9	2 0 0 0 9	674.64240	-0.00046	1777.40907	1102.76621
2 0 1 -1 10	2 0 0 0 10	674.66388	0.00063	1796.51064	1121.84738
2 0 1 -1 11	2 0 0 0 11	674.67517	0.00059	1817.51959	1142.83216

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2	0	1	-1	12	2	0	0	0	12	674.71502*	-0.00084	1840.43522	1165.71936
2	0	1	-1	13	2	0	0	0	13	674.74859	-0.00051	1865.25684	1190.50774
2	0	1	-1	14	2	0	0	0	14	674.78702	-0.00063	1891.98370	1217.19606
2	0	1	-1	15	2	0	0	0	15	674.82730*	-0.00472	1920.61510	1245.78308W
2	0	1	-1	16	2	0	0	0	16	674.88243	-0.00027	1951.15030	1276.26760
2	0	1	-1	17	2	0	0	0	17	674.93954	-0.00057	1983.58860	1308.64848
2	0	1	-1	18	2	0	0	0	18	675.00208*	-0.00254	2017.92928	1342.92466W
2	0	1	-1	19	2	0	0	0	19	675.07646	-0.00005	2054.17165	1379.09514
2	0	1	-1	20	2	0	0	0	20	675.15651	0.00053	2092.31503	1417.15906
2	0	1	-1	21	2	0	0	0	21	675.24345	0.00029	2132.35877	1457.11560
2	0	1	-1	22	2	0	0	0	22	675.33853	0.00041	2174.30219	1498.96407
2	0	1	-1	23	2	0	0	0	23	675.44127	0.00043	2218.14465	1542.70381

rms = 0.00040 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 -2 1 1 3	2 0 0 0 3	683.64742	-0.00026	1711.95911	1028.31143
2 -2 1 1 4	2 0 0 0 4	683.67257	-0.00024	1719.62345	1035.95064
2 -2 1 1 5	2 0 0 0 5	683.70486	-0.00043	1729.20404	1045.49875
2 -2 1 1 6	2 0 0 0 6	683.74603	0.00018	1740.70099	1056.95515
2 -2 1 1 7	2 0 0 0 7	683.79534	0.00001	1754.11443	1070.31910
2 -2 1 1 8	2 0 0 0 8	683.85423	-0.00049	1769.44449	1085.58977
2 -2 1 1 9	2 0 0 0 9	683.92510	-0.00004	1786.69135	1102.76621
2 -2 1 1 10	2 0 0 0 10	684.00626	-0.00154	1805.85519	1121.84738W
2 -2 1 1 11	2 0 0 0 11	684.10518	0.00115	1826.93619	1142.83216W
2 -2 1 1 12	2 0 0 0 12	684.21651	0.00131	1849.93456	1165.71936W
2 -2 1 1 13	2 0 0 0 13	684.34303	0.00027	1874.85050	1190.50774
2 -2 1 1 14	2 0 0 0 14	684.48870	0.00054	1901.68422	1217.19606
2 -2 1 1 15	2 0 0 0 15	684.65038*	-0.00244	1930.43590	1245.78308W
2 -2 1 1 16	2 0 0 0 16	684.83881	0.00069	1961.10572	1276.26760
2 -2 1 1 17	2 0 0 0 17	685.04691	0.00157	1993.69383	1308.64848W
2 -2 1 1 18	2 0 0 0 18	685.27556	-0.00012	2028.20034	1342.92466

rms = 0.00036 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 2 1 -1 3	2 2 0 0 4	671.55980	-0.00007	1711.90830	1040.34843
2 2 1 -1 4	2 2 0 0 5	669.64189	0.00044	1719.53877	1049.89732
2 2 1 -1 5	2 2 0 0 6	667.72029	0.00004	1729.07700	1061.35675
2 2 1 -1 6	2 2 0 0 7	665.79596	-0.00003	1740.52311	1074.72712
2 2 1 -1 7	2 2 0 0 8	663.86763	-0.00069	1753.87721	1090.00889
2 2 1 -1 8	2 2 0 0 9	661.93580*	-0.00105	1769.13944	1107.20259W
2 2 1 -1 9	2 2 0 0 10	660.00085	-0.00032	1786.30996	1126.30879
2 2 1 -1 10	2 2 0 0 11	658.06128	0.00039	1805.38896	1147.32807
2 2 1 -1 11	2 2 0 0 12	656.11560	0.00003	1826.37662	1170.26105
2 2 1 -1 12	2 2 0 0 13	654.16494	0.00011	1849.27315	1195.10832
2 2 1 -1 13	2 2 0 0 14	652.20908	0.00075	1874.07876	1221.87043
2 2 1 -1 14	2 2 0 0 15	650.24619	0.00041	1900.79367	1250.54788
2 2 1 -1 15	2 2 0 0 16	648.27626	-0.00074	1929.41808	1281.14108
2 2 1 -1 16	2 2 0 0 17	646.30200	0.00012	1959.95219	1313.65031
2 2 1 -1 17	2 2 0 0 18	644.32101	0.00057	1992.39619	1348.07575
2 2 1 -1 18	2 2 0 0 19	642.33402	0.00122	2026.75022	1384.41742W
2 2 1 -1 19	2 2 0 0 20	640.33903	-0.00017	2063.01439	1422.67519
2 2 1 -1 20	2 2 0 0 21	638.33910	-0.00086	2101.18875	1462.84880
2 2 1 -1 21	2 2 0 0 22	636.33465	-0.00083	2141.27332	1504.93784
2 2 1 -1 5	2 2 0 0 4	688.72929	0.00072	1729.07700	1040.34843
2 2 1 -1 6	2 2 0 0 5	690.62557	-0.00021	1740.52311	1049.89732
2 2 1 -1 7	2 2 0 0 6	692.51946*	-0.00100	1753.87721	1061.35675

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2	2	1	-1	8	2	2	0	0	7	694.41212	-0.00020	1769.13944	1074.72712
2	2	1	-1	9	2	2	0	0	8	696.30159	0.00052	1786.30996	1090.00889
2	2	1	-1	10	2	2	0	0	9	698.18601	-0.00036	1805.38896	1107.20259
2	2	1	-1	11	2	2	0	0	10	700.06763	-0.00020	1826.37662	1126.30879
2	2	1	-1	12	2	2	0	0	11	701.94494	-0.00014	1849.27315	1147.32807
2	2	1	-1	13	2	2	0	0	12	703.81815	0.00044	1874.07876	1170.26105
2	2	1	-1	14	2	2	0	0	13	705.68601	0.00066	1900.79367	1195.10832
2	2	1	-1	15	2	2	0	0	14	707.54188	-0.00576	1929.41808	1221.87043W
2	2	1	-1	16	2	2	0	0	15	709.40430	-0.00001	1959.95219	1250.54788
2	2	1	-1	17	2	2	0	0	16	711.25515	0.00004	1992.39619	1281.14108
2	2	1	-1	18	2	2	0	0	17	713.09978	-0.00012	2026.75022	1313.65031
2	2	1	-1	19	2	2	0	0	18	714.93868	0.00005	2063.01439	1348.07575
2	2	1	-1	20	2	2	0	0	19	716.77170	0.00036	2101.18875	1384.41742
2	-2	1	1	3	2	-2	0	0	4	671.61193	-0.00017	1711.95911	1040.34700
2	-2	1	1	4	2	-2	0	0	5	669.72650*	-0.00296	1719.62345	1049.89400W
2	-2	1	1	5	2	-2	0	0	6	667.85406	0.00011	1729.20404	1061.35010
2	-2	1	1	6	2	-2	0	0	7	665.98631	0.00046	1740.70099	1074.71514
2	-2	1	1	7	2	-2	0	0	8	664.12529	-0.00018	1754.11443	1089.98896
2	-2	1	1	8	2	-2	0	0	9	662.27354	0.00037	1769.44449	1107.17132
2	-2	1	1	9	2	-2	0	0	10	660.42968	0.00032	1786.69135	1126.26199
2	-2	1	1	10	2	-2	0	0	11	658.59471	0.00024	1805.85519	1147.26072
2	-2	1	1	11	2	-2	0	0	12	656.76900	0.00001	1826.93619	1170.16720
2	-2	1	1	12	2	-2	0	0	13	654.95373	0.00029	1849.93456	1194.98112
2	-2	1	1	13	2	-2	0	0	14	653.14919	0.00082	1874.85050	1221.70214
2	-2	1	1	14	2	-2	0	0	15	651.35386	-0.00048	1901.68422	1250.32988
2	-2	1	1	15	2	-2	0	0	16	649.57266	0.00071	1930.43590	1280.86395
2	-2	1	1	16	2	-2	0	0	17	647.80226	0.00047	1961.10572	1313.30393
2	-2	1	1	17	2	-2	0	0	18	646.04731	0.00284	1993.69383	1347.64936W
2	-2	1	1	18	2	-2	0	0	19	644.30016	-0.00041	2028.20034	1383.89977
2	-2	1	1	19	2	-2	0	0	20	642.57210*	0.00143	2064.62532	1422.05465W
2	-2	1	1	20	2	-2	0	0	21	640.85612	0.00081	2102.96880	1462.11349
2	-2	1	1	5	2	-2	0	0	4	688.85735	0.00031	1729.20404	1040.34700
2	-2	1	1	6	2	-2	0	0	5	690.80697	-0.00003	1740.70099	1049.89400
2	-2	1	1	7	2	-2	0	0	6	692.76281	-0.00152	1754.11443	1061.35010W
2	-2	1	1	8	2	-2	0	0	7	694.72895	-0.00040	1769.44449	1074.71514
2	-2	1	1	9	2	-2	0	0	8	696.70189	-0.00051	1786.69135	1089.98896
2	-2	1	1	10	2	-2	0	0	9	698.68338	-0.00049	1805.85519	1107.17132
2	-2	1	1	11	2	-2	0	0	10	700.67446	0.00026	1826.93619	1126.26199
2	-2	1	1	12	2	-2	0	0	11	702.67422	0.00038	1849.93456	1147.26072
2	-2	1	1	13	2	-2	0	0	12	704.68357	0.00027	1874.85050	1170.16720
2	-2	1	1	14	2	-2	0	0	13	706.70307	-0.00003	1901.68422	1194.98112
2	-2	1	1	15	2	-2	0	0	14	708.73378	0.00002	1930.43590	1221.70214
2	-2	1	1	16	2	-2	0	0	15	710.77578	-0.00006	1961.10572	1250.32988
2	-2	1	1	17	2	-2	0	0	16	712.83019	0.00031	1993.69383	1280.86395
2	-2	1	1	18	2	-2	0	0	17	714.89687	0.00046	2028.20034	1313.30393
2	-2	1	1	19	2	-2	0	0	18	716.97660*	0.00063	2064.62532	1347.64936
2	-2	1	1	20	2	-2	0	0	19	719.07046	0.00143	2102.96880	1383.89977W
2	-2	1	1	3	2	2	0	0	3	679.24911	-0.00027	1711.95911	1032.70973
2	-2	1	1	4	2	2	0	0	4	679.27604	0.00102	1719.62345	1040.34843W
2	-2	1	1	5	2	2	0	0	5	679.30686	0.00014	1729.20404	1049.89732
2	-2	1	1	6	2	2	0	0	6	679.34233*	-0.00191	1740.70099	1061.35675W
2	-2	1	1	7	2	2	0	0	7	679.38670	-0.00061	1754.11443	1074.72712
2	-2	1	1	8	2	2	0	0	8	679.43536	-0.00024	1769.44449	1090.00889
2	-2	1	1	9	2	2	0	0	9	679.48847	-0.00029	1786.69135	1107.20259
2	-2	1	1	10	2	2	0	0	10	679.54681	0.00041	1805.85519	1126.30879
2	-2	1	1	11	2	2	0	0	11	679.60854	0.00042	1826.93619	1147.32807
2	-2	1	1	12	2	2	0	0	12	679.67276	-0.00075	1849.93456	1170.26105
2	-2	1	1	13	2	2	0	0	13	679.74046*	-0.00172	1874.85050	1195.10832W
2	-2	1	1	14	2	2	0	0	14	679.81358	-0.00021	1901.68422	1221.87043
2	-2	1	1	15	2	2	0	0	15	679.88838	0.00036	1930.43590	1250.54788
2	-2	1	1	16	2	2	0	0	16	679.96416	-0.00048	1961.10572	1281.14108
2	-2	1	1	17	2	2	0	0	17	680.04259	-0.00092	1993.69383	1313.65031
2	-2	1	1	18	2	2	0	0	18	680.12482	0.00023	2028.20034	1348.07575
2	-2	1	1	19	2	2	0	0	19	680.20820	0.00029	2064.62532	1384.41742
2	-2	1	1	20	2	2	0	0	20	680.29388	0.00027	2102.96880	1422.67519
2	-2	1	1	21	2	2	0	0	21	680.38296*	0.00104	2143.23071	1462.84880W
2	-2	1	1	22	2	2	0	0	22	680.47296	-0.00016	2185.41096	1504.93784
2	-2	1	1	23	2	2	0	0	23	680.56776	0.00021	2229.50936	1548.94181
2	-2	1	1	24	2	2	0	0	24	680.65568	0.00011	2275.52563	1594.86006

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2	-2	1	1	25	2	2	0	0	25	680.76780	0.00024	2323.45944	1642.69188
2	-2	1	1	26	2	2	0	0	26	680.87405	0.00016	2373.31035	1692.43646
2	-2	1	1	27	2	2	0	0	27	680.98602	0.00111	2425.07785	1744.09294W
2	-2	1	1	28	2	2	0	0	28	681.10016	-0.00078	2478.76136	1797.66042
2	-2	1	1	29	2	2	0	0	29	681.22259	0.00032	2534.36020	1853.13793

rms = 0.00042 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	G'	G''
2 2 1 1 4	2 2 0 0 5	663.94628*	0.00265	1713.84096	1049.89732W
2 2 1 1 5	2 2 0 0 6	662.04298	0.00009	1723.39964	1061.35675
2 2 1 1 6	2 2 0 0 7	660.14282	0.00004	1734.86989	1074.72712
2 2 1 1 7	2 2 0 0 8	658.24303	0.00029	1748.25163	1090.00889
2 2 1 1 8	2 2 0 0 9	656.34154	-0.00064	1763.54477	1107.20259
2 2 1 1 9	2 2 0 0 10	654.44112	0.00063	1780.74928	1126.30879
2 2 1 1 10	2 2 0 0 11	652.53715	0.00012	1799.86510	1147.32807
2 2 1 1 11	2 2 0 0 12	650.63123	0.00005	1820.89223	1170.26105
2 2 1 1 12	2 2 0 0 13	648.72254	0.00015	1843.83071	1195.10832
2 2 1 1 13	2 2 0 0 14	646.81085	0.00068	1868.68060	1221.87043
2 2 1 1 14	2 2 0 0 15	644.89430	0.00014	1895.44204	1250.54788
2 2 1 1 15	2 2 0 0 16	642.97462	0.00049	1924.11521	1281.14108
2 2 1 1 16	2 2 0 0 17	641.04984	-0.00017	1954.70033	1313.65031
2 2 1 1 17	2 2 0 0 18	639.12164	-0.00026	1987.19766	1348.07575
2 2 1 1 18	2 2 0 0 19	637.19029	0.00024	2021.60747	1384.41742
2 2 1 1 19	2 2 0 0 20	635.25450	-0.00034	2057.93003	1422.67519
2 2 1 1 20	2 2 0 0 21	633.31657	-0.00019	2096.16555	1462.84880
2 2 1 1 21	2 2 0 0 22	631.37623	-0.00011	2136.31418	1504.93784
2 2 1 1 22	2 2 0 0 23	629.43126	-0.00288	2178.37595	1548.94181W
2 2 1 1 23	2 2 0 0 24	627.48782	-0.00288	2222.35076	1594.86006W
2 2 1 1 24	2 2 0 0 25	625.54525	-0.00126	2268.23838	1642.69188W
2 2 1 1 25	2 2 0 0 26	623.60260	0.00064	2316.03842	1692.43646
2 2 1 1 26	2 2 0 0 27	621.65757	0.00017	2365.75035	1744.09294
2 2 1 1 27	2 2 0 0 28	619.71328	0.00021	2417.37349	1797.66042
2 2 1 1 28	2 2 0 0 29	617.76973	0.00058	2470.90708	1853.13793
2 2 1 1 3	2 2 0 0 2	679.21266	-0.00030	1706.19390	1026.98094
2 2 1 1 4	2 2 0 0 3	681.13138	0.00015	1713.84096	1032.70973
2 2 1 1 5	2 2 0 0 4	683.05232	0.00111	1723.39964	1040.34843W
2 2 1 1 6	2 2 0 0 5	684.97148*	-0.00109	1734.86989	1049.89732W
2 2 1 1 7	2 2 0 0 6	686.89513	0.00025	1748.25163	1061.35675
2 2 1 1 8	2 2 0 0 7	688.81803	0.00037	1763.54477	1074.72712
2 2 1 1 9	2 2 0 0 8	690.73982	-0.00057	1780.74928	1090.00889
2 2 1 1 10	2 2 0 0 9	692.66227	-0.00024	1799.86510	1107.20259
2 2 1 1 11	2 2 0 0 10	694.58327	-0.00017	1820.89223	1126.30879
2 2 1 1 12	2 2 0 0 11	696.50229	-0.00034	1843.83071	1147.32807
2 2 1 1 13	2 2 0 0 12	698.41932	-0.00023	1868.68060	1170.26105
2 2 1 1 14	2 2 0 0 13	700.33223*	-0.00149	1895.44204	1195.10832W
2 2 1 1 15	2 2 0 0 14	702.24469	-0.00008	1924.11521	1221.87043
2 2 1 1 16	2 2 0 0 15	704.15246	0.00002	1954.70033	1250.54788
2 2 1 1 17	2 2 0 0 16	706.05638	-0.00020	1987.19766	1281.14108
2 2 1 1 18	2 2 0 0 17	707.95703	-0.00012	2021.60747	1313.65031
2 2 1 1 19	2 2 0 0 18	709.85339*	-0.00089	2057.93003	1348.07575
2 2 1 1 20	2 2 0 0 19	711.74793	-0.00020	2096.16555	1384.41742
2 2 1 1 21	2 2 0 0 20	713.63856	-0.00043	2136.31418	1422.67519
2 2 1 1 22	2 2 0 0 21	715.52663	-0.00052	2178.37595	1462.84880
2 2 1 1 23	2 2 0 0 22	717.41263	-0.00029	2222.35076	1504.93784
2 2 1 1 24	2 2 0 0 23	719.29639	-0.00018	2268.23838	1548.94181
2 2 1 1 25	2 2 0 0 24	721.17782	-0.00054	2316.03842	1594.86006
2 2 1 1 26	2 2 0 0 25	723.05929	0.00082	2365.75035	1642.69188
2 2 1 1 27	2 2 0 0 26	724.93708	0.00004	2417.37349	1692.43646
2 2 1 1 28	2 2 0 0 27	726.81326	-0.00088	2470.90708	1744.09294
2 2 1 1 3	2 -2 0 0 3	673.48331	-0.00134	1706.19390	1032.70925W
2 2 1 1 4	2 -2 0 0 4	673.49263	-0.00132	1713.84096	1040.34700W
2 2 1 1 5	2 -2 0 0 5	673.50593	0.00028	1723.39964	1049.89400
2 2 1 1 6	2 -2 0 0 6	673.51925	0.00034	1734.86989	1061.35010

1	2	2	1	1	7	2	-2	0	0	7	673.53582	-0.00066	1748.25163	1074.71514
2	2	2	1	1	8	2	-2	0	0	8	673.55613	0.00031	1763.54477	1089.98896
3	2	2	1	1	9	2	-2	0	0	9	673.57810	0.00014	1780.74928	1107.17132
4	2	2	1	1	10	2	-2	0	0	10	673.60181*	-0.00130	1799.86510	1126.26199W
5	2	2	1	1	11	2	-2	0	0	11	673.63150	-0.00002	1820.89223	1147.26072
6	2	2	1	1	12	2	-2	0	0	12	673.66378	0.00027	1843.83071	1170.16720
7	2	2	1	1	13	2	-2	0	0	13	673.69885	-0.00063	1868.68060	1194.98112
8	2	-2	1	-1	3	2	-2	0	0	4	665.84640	-0.00050	1706.19390	1040.34700
9	2	-2	1	-1	4	2	-2	0	0	5	663.94628	-0.00066	1713.84094	1049.89400
10	2	-2	1	-1	5	2	-2	0	0	6	662.04782*	-0.00167	1723.39959	1061.35010W
11	2	-2	1	-1	6	2	-2	0	0	7	660.15471	0.00014	1734.86972	1074.71514
12	2	-2	1	-1	7	2	-2	0	0	8	658.26195	-0.00029	1748.25119	1089.98896
13	2	-2	1	-1	8	2	-2	0	0	9	656.37410	0.00160	1763.54382	1107.17132W
14	2	-2	1	-1	9	2	-2	0	0	10	654.48556	0.00018	1780.74737	1126.26199
15	2	-2	1	-1	10	2	-2	0	0	11	652.60137	0.00052	1799.86157	1147.26072
16	2	-2	1	-1	11	2	-2	0	0	12	650.71932	0.00045	1820.88607	1170.16720
17	2	-2	1	-1	12	2	-2	0	0	13	648.83998	0.00061	1843.82049	1194.98112
18	2	-2	1	-1	13	2	-2	0	0	14	646.96161*	-0.00061	1868.66436	1221.70214
19	2	-2	1	-1	14	2	-2	0	0	15	645.08795	0.00068	1895.41715	1250.32988
20	2	-2	1	-1	15	2	-2	0	0	16	643.21496	0.00065	1924.07827	1280.86395
21	2	-2	1	-1	16	2	-2	0	0	17	641.34340	0.00027	1954.64705	1313.30393
22	2	-2	1	-1	17	2	-2	0	0	18	639.47369	0.00026	1987.12279	1347.64936
23	2	-2	1	-1	18	2	-2	0	0	19	637.60531	0.00039	2021.50469	1383.89977
24	2	-2	1	-1	19	2	-2	0	0	20	635.73644	-0.00083	2057.79192	1422.05465
25	2	-2	1	-1	20	2	-2	0	0	21	633.87101	0.00087	2095.98363	1462.11349
26	2	-2	1	-1	21	2	-2	0	0	22	632.00313	-0.00005	2136.07890	1504.07572
27	2	-2	1	-1	22	2	-2	0	0	23	630.13634	0.00028	2178.07681	1547.94075
28	2	-2	1	-1	23	2	-2	0	0	24	628.26781	-0.00064	2221.97644	1593.70799
29	2	-2	1	-1	24	2	-2	0	0	25	626.39962	-0.00041	2267.77684	1641.37680
30	2	-2	1	-1	25	2	-2	0	0	26	624.53110	0.00055	2315.47707	1690.94652
31	2	-2	1	-1	26	2	-2	0	0	27	622.66157	0.00182	2365.07620	1742.41645W
32	2	-2	1	-1	3	2	-2	0	0	2	679.21266	-0.00040	1706.19390	1026.98084
33	2	-2	1	-1	4	2	-2	0	0	3	681.13138	-0.00031	1713.84094	1032.70925
34	2	-2	1	-1	5	2	-2	0	0	4	683.05272	0.00014	1723.39959	1040.34700
35	2	-2	1	-1	6	2	-2	0	0	5	684.97148*	-0.00424	1734.86972	1049.89400W
36	2	-2	1	-1	7	2	-2	0	0	6	686.90051	-0.00059	1748.25119	1061.35010
37	2	-2	1	-1	8	2	-2	0	0	7	688.82846	-0.00022	1763.54382	1074.71514
38	2	-2	1	-1	9	2	-2	0	0	8	690.75773	-0.00069	1780.74737	1089.98896
39	2	-2	1	-1	10	2	-2	0	0	9	692.69052	0.00027	1799.86157	1107.17132
40	2	-2	1	-1	11	2	-2	0	0	10	694.62455	0.00047	1820.88607	1126.26199
41	2	-2	1	-1	12	2	-2	0	0	11	696.56013	0.00036	1843.82049	1147.26072
42	2	-2	1	-1	13	2	-2	0	0	12	698.49769	0.00053	1868.66436	1170.16720
43	2	-2	1	-1	14	2	-2	0	0	13	700.43436*	-0.00166	1895.41715	1194.98112W
44	2	-2	1	-1	15	2	-2	0	0	14	702.37525	-0.00088	1924.07827	1221.70214
45	2	-2	1	-1	16	2	-2	0	0	15	704.31676	-0.00041	1954.64705	1250.32988
46	2	-2	1	-1	17	2	-2	0	0	16	706.25839	-0.00045	1987.12279	1280.86395
47	2	-2	1	-1	18	2	-2	0	0	17	708.20041	-0.00035	2021.50469	1313.30393
48	2	-2	1	-1	19	2	-2	0	0	18	710.14342	0.00085	2057.79192	1347.64936
49	2	-2	1	-1	20	2	-2	0	0	19	712.08310	-0.00076	2095.98363	1383.89977
50	2	-2	1	-1	21	2	-2	0	0	20	714.02406	-0.00018	2136.07890	1422.05465
51	2	-2	1	-1	22	2	-2	0	0	21	715.96295	-0.00037	2178.07681	1462.11349
52	2	-2	1	-1	23	2	-2	0	0	22	717.89997*	-0.00075	2221.97644	1504.07572
53	2	-2	1	-1	24	2	-2	0	0	23	719.83608	0.00000	2267.77684	1547.94075
54	2	-2	1	-1	25	2	-2	0	0	24	721.76956	0.00049	2315.47707	1593.70799
55	2	-2	1	-1	26	2	-2	0	0	25	723.69841	-0.00099	2365.07620	1641.37680
56	2	-2	1	-1	27	2	-2	0	0	26	725.62721	0.00040	2416.57332	1690.94652
57	2	-2	1	-1	3	2	2	0	0	3	673.48331	-0.00086	1706.19390	1032.70973
58	2	-2	1	-1	4	2	2	0	0	4	673.49263	0.00012	1713.84094	1040.34843
59	2	-2	1	-1	5	2	2	0	0	5	673.50297	0.00071	1723.39959	1049.89732
60	2	-2	1	-1	6	2	2	0	0	6	673.51288	-0.00009	1734.86972	1061.35675
	2	-2	1	-1	7	2	2	0	0	7	673.52418	0.00010	1748.25119	1074.72712
	2	-2	1	-1	8	2	2	0	0	8	673.53582	0.00089	1763.54382	1090.00889

rms = 0.00046 cm⁻¹

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

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
1 -1 2 0 3	1 1 1 -1 3	658.57389	0.00074	1857.43079	1198.85764
1 -1 2 0 4	1 1 1 -1 4	658.59421	-0.00076	1865.08304	1206.48808
1 -1 2 0 5	1 1 1 -1 5	658.62113	-0.00037	1874.64805	1216.02655
1 -1 2 0 6	1 1 1 -1 6	658.65151	-0.00075	1886.12559	1227.47333
1 -1 2 0 7	1 1 1 -1 7	658.68653	-0.00013	1899.51544	1240.82878
1 -1 2 0 8	1 1 1 -1 8	658.72342	-0.00061	1914.81729	1256.09326
1 -1 2 0 9	1 1 1 -1 9	658.76310	-0.00052	1932.03082	1273.26720
1 -1 2 0 10	1 1 1 -1 10	658.80482	0.00023	1951.15566	1292.35106
1 -1 2 0 12	1 1 1 -1 12	658.88773	0.00060	1995.13757	1336.25044
1 -1 2 0 13	1 1 1 -1 13	658.92590	-0.00093	2019.99372	1361.06689
1 -1 2 0 14	1 1 1 -1 14	658.96401	-0.00019	2046.75929	1387.79509
1 -1 2 0 15	1 1 1 -1 15	658.99868*	0.00036	2075.43373	1416.43541
1 -1 2 0 16	1 1 1 -1 16	659.02674	-0.00157	2106.01643	1446.98812W
1 -1 2 0 18	1 1 1 -1 18	659.07177	-0.00089	2172.90404	1513.83138
1 -1 2 0 19	1 1 1 -1 19	659.07695*	-0.00865	2209.20755	1550.12195W
rms = 0.00062 cm ⁻¹					

$v_4 + 2v_5 (^1\Pi) \leftarrow v_4 + v_5 (\Sigma^+)$					
$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
1 -1 2 2 1	1 1 1 -1 2	674.36616*	0.00115	1867.50003	1193.13502W
1 -1 2 2 2	1 1 1 -1 3	672.45766	-0.00090	1871.31621	1198.85764
1 -1 2 2 3	1 1 1 -1 4	670.55441	0.00199	1877.04050	1206.48808W
1 -1 2 2 4	1 1 1 -1 5	668.64555	-0.00083	1884.67293	1216.02655
1 -1 2 2 5	1 1 1 -1 6	666.74047	0.00027	1894.21354	1227.47333
1 -1 2 2 6	1 1 1 -1 7	664.83157	-0.00202	1905.66237	1240.82878W
1 -1 2 2 7	1 1 1 -1 8	662.92614	-0.00007	1919.01947	1256.09326
1 -1 2 2 8	1 1 1 -1 9	661.01976*	0.00205	1934.28491	1273.26720W
1 -1 2 2 9	1 1 1 -1 10	659.10675	-0.00093	1951.45875	1292.35106
1 -1 2 2 10	1 1 1 -1 11	657.19537	-0.00037	1970.54106	1313.34532
1 -1 2 2 11	1 1 1 -1 12	655.27993	-0.00154	1991.53191	1336.25044W
1 -1 2 2 12	1 1 1 -1 13	653.36430	-0.00018	2014.43136	1361.06689
1 -1 2 2 13	1 1 1 -1 14	651.44008*	-0.00433	2039.23950	1387.79509W
1 -1 2 2 14	1 1 1 -1 15	649.52081	-0.00015	2065.95636	1416.43541
1 -1 2 2 15	1 1 1 -1 16	647.59370	-0.00019	2094.58201	1446.98812
1 -1 2 2 16	1 1 1 -1 17	645.66297	-0.00006	2125.11645	1479.45342
1 -1 2 2 17	1 1 1 -1 18	643.72603*	-0.00229	2157.55970	1513.83138W
1 -1 2 2 18	1 1 1 -1 19	641.79116	0.00139	2191.91172	1550.12195W
1 -1 2 2 19	1 1 1 -1 20	639.84770	0.00020	2228.17246	1588.32496
1 -1 2 2 20	1 1 1 -1 21	637.90241	0.00073	2266.34179	1628.44012
1 -1 2 2 1	1 1 1 -1 0	680.08832	0.00086	1867.50003	1187.41257
1 -1 2 2 2	1 1 1 -1 1	681.99746	0.00129	1871.31621	1189.32003W
1 -1 2 2 3	1 1 1 -1 2	683.90555	0.00007	1877.04050	1193.13502
1 -1 2 2 4	1 1 1 -1 3	685.81504	-0.00024	1884.67293	1198.85764
1 -1 2 2 5	1 1 1 -1 4	687.72485	-0.00061	1894.21354	1206.48808
1 -1 2 2 6	1 1 1 -1 5	689.63594	0.00012	1905.66237	1216.02655
1 -1 2 2 7	1 1 1 -1 6	691.54651	0.00037	1919.01947	1227.47333
1 -1 2 2 8	1 1 1 -1 7	693.45735	0.00122	1934.28491	1240.82878W
1 -1 2 2 9	1 1 1 -1 8	695.36584	0.00035	1951.45875	1256.09326
1 -1 2 2 10	1 1 1 -1 9	697.27370	-0.00015	1970.54106	1273.26720
1 -1 2 2 11	1 1 1 -1 10	699.18109	0.00025	1991.53191	1292.35106
1 -1 2 2 12	1 1 1 -1 11	701.08630	0.00025	2014.43136	1313.34532
1 -1 2 2 13	1 1 1 -1 12	702.98897	-0.00009	2039.23950	1336.25044
1 -1 2 2 14	1 1 1 -1 13	704.88969	0.00021	2065.95636	1361.06689
1 -1 2 2 15	1 1 1 -1 14	706.78730	0.00038	2094.58201	1387.79509
1 -1 2 2 16	1 1 1 -1 15	708.68186	0.00081	2125.11645	1416.43541
1 -1 2 2 17	1 1 1 -1 16	710.57126	-0.00032	2157.55970	1446.98812
1 -1 2 2 18	1 1 1 -1 17	712.45803	-0.00027	2191.91172	1479.45342
1 -1 2 2 19	1 1 1 -1 18	714.34444*	0.00336	2228.17246	1513.83138W
1 -1 2 2 20	1 1 1 -1 19	716.21972	-0.00012	2266.34179	1550.12195
1 -1 2 2 21	1 1 1 -1 20	718.09439	-0.00022	2306.41957	1588.32496
1 -1 2 2 22	1 1 1 -1 21	719.96560	0.00013	2348.40558	1628.44012

1	1	-1	2	2	23	1	1	1	-1	22	721.83184	-0.00071	2392.29956	1670.46701
2	1	1	2	-2	3	1	1	1	-1	3	678.19904	-0.00015	1877.05683	1198.85764
3	1	1	2	-2	4	1	1	1	-1	4	678.21593*	0.00385	1884.70016	1206.48808W
4	1	1	2	-2	5	1	1	1	-1	5	678.22768	-0.00016	1894.25438	1216.02655
5	1	1	2	-2	6	1	1	1	-1	6	678.24660	0.00037	1905.71956	1227.47333
6	1	1	2	-2	7	1	1	1	-1	7	678.26517*	-0.00181	1919.09576	1240.82878W
7	1	1	2	-2	10	1	1	1	-1	10	678.34046	0.00036	1970.69116	1292.35106
8	1	1	2	-2	11	1	1	1	-1	11	678.36708	0.00019	1991.71220	1313.34532
9	1	1	2	-2	12	1	1	1	-1	12	678.39427	0.00001	2014.64470	1336.25044
10	1	1	2	-2	13	1	1	1	-1	13	678.42318*	0.00131	2039.48875	1361.06689W
11	1	1	2	-2	14	1	1	1	-1	14	678.44952	0.00012	2066.24449	1387.79509
12	1	1	2	-2	15	1	1	1	-1	15	678.47692	0.00031	2094.91201	1416.43541
13	1	1	2	-2	16	1	1	1	-1	16	678.50305	-0.00026	2125.49143	1446.98812
14	1	1	2	-2	17	1	1	1	-1	17	678.52928	-0.00014	2157.98284	1479.45342
15	1	1	2	-2	18	1	1	1	-1	18	678.55521	0.00026	2192.38633	1513.83138
16	1	1	2	-2	19	1	1	1	-1	19	678.58032	0.00030	2228.70197	1550.12195
17	1	1	2	-2	20	1	1	1	-1	20	678.60108*	-0.00374	2266.92978	1588.32496W
18	1	1	2	-2	21	1	1	1	-1	21	678.62988	0.00022	2307.06978	1628.44012
19	1	1	2	-2	22	1	1	1	-1	22	678.65549	0.00057	2349.12193	1670.46701
20	1	1	2	-2	23	1	1	1	-1	23	678.68126	0.00022	2393.08616	1714.40513
21	1	1	2	-2	24	1	1	1	-1	24	678.70743	-0.00106	2438.96235	1760.25386W
22	1	1	2	-2	25	1	1	1	-1	25	678.73784	0.00004	2486.75032	1808.01252

rms = 0.00040 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	G'	G''
1 -1 2 0 1	1 -1 1 1 2	658.39967*	0.00157	1847.86517	1189.46706W
1 -1 2 0 2	1 -1 1 1 3	656.50097	-0.00082	1851.69146	1195.18967
1 -1 2 0 3	1 -1 1 1 4	654.61068	-0.00035	1857.43079	1202.81976
1 -1 2 0 4	1 -1 1 1 5	652.72578	0.00004	1865.08304	1212.35731
1 -1 2 0 5	1 -1 1 1 6	650.84316*	-0.00265	1874.64805	1223.80224W
1 -1 2 0 6	1 -1 1 1 7	648.97136	0.00027	1886.12559	1237.15450
1 -1 2 0 7	1 -1 1 1 8	647.10166	0.00023	1899.51544	1252.41400
1 -1 2 0 8	1 -1 1 1 9	645.23695	0.00031	1914.81729	1269.58065
1 -1 2 0 9	1 -1 1 1 10	643.37682	0.00033	1932.03082	1288.65432
1 -1 2 0 10	1 -1 1 1 11	641.52385*	0.00306	1951.15566	1309.63487W
1 -1 2 0 11	1 -1 1 1 12	639.66829	-0.00100	1972.19139	1332.52210W
1 -1 2 0 12	1 -1 1 1 13	637.82163	-0.00015	1995.13757	1357.31580
1 -1 2 0 13	1 -1 1 1 14	635.97827	0.00026	2019.99372	1384.01571
1 -1 2 0 14	1 -1 1 1 15	634.13754	-0.00023	2046.75929	1412.62152
1 -1 2 0 15	1 -1 1 1 16	632.30085	0.00001	2075.43373	1443.13289
1 -1 2 0 16	1 -1 1 1 17	630.46722	0.00021	2106.01643	1475.54942
1 -1 2 0 17	1 -1 1 1 18	628.63580	-0.00027	2138.50676	1509.87069
1 -1 2 0 18	1 -1 1 1 19	626.80793	0.00012	2172.90404	1546.09623
1 -1 2 0 19	1 -1 1 1 20	624.98176	-0.00028	2209.20755	1584.22551
1 -1 2 0 20	1 -1 1 1 21	623.15857	0.00002	2247.41657	1624.25802
1 -1 2 0 21	1 -1 1 1 22	621.33732	0.00019	2287.53030	1666.19317
1 -1 2 0 22	1 -1 1 1 23	619.52052	0.00295	2329.54794	1710.03037W
1 -1 2 0 23	1 -1 1 1 24	617.70051	0.00085	2373.46866	1755.76899
1 -1 2 0 24	1 -1 1 1 25	615.88353	0.00034	2419.29158	1803.40839
1 -1 2 0 25	1 -1 1 1 26	614.06729	-0.00065	2467.01582	1852.94788
1 -1 2 0 1	1 -1 1 1 0	664.12066*	-0.00008	1847.86517	1183.74443
1 -1 2 0 6	1 -1 1 1 5	673.76931*	0.00102	1886.12559	1212.35731W
1 -1 2 0 7	1 -1 1 1 6	675.71314	-0.00006	1899.51544	1223.80224
1 -1 2 0 8	1 -1 1 1 7	677.65665*	-0.00614	1914.81729	1237.15450W
1 -1 2 0 9	1 -1 1 1 8	679.61754*	0.00073	1932.03082	1252.41400
1 -1 2 0 10	1 -1 1 1 9	681.57478	-0.00022	1951.15566	1269.58065
1 -1 2 0 11	1 -1 1 1 10	683.53742	0.00035	1972.19139	1288.65432
1 -1 2 0 12	1 -1 1 1 11	685.50176	-0.00095	1995.13757	1309.63487
1 -1 2 0 13	1 -1 1 1 12	687.47517*	0.00355	2019.99372	1332.52210W
1 -1 2 0 14	1 -1 1 1 13	689.44359	0.00010	2046.75929	1357.31580
1 -1 2 0 15	1 -1 1 1 14	691.41793	-0.00009	2075.43373	1384.01571
1 -1 2 0 16	1 -1 1 1 15	693.39451	-0.00040	2106.01643	1412.62152
1 -1 2 0 17	1 -1 1 1 16	695.37150	0.00000	2138.50676	1443.13289

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

1	1	-1	2	0	18	1	-1	1	1	17	697.35478	0.00017	2172.90404	1475.54942
2	1	-1	2	0	19	1	-1	1	1	18	699.33698	0.00012	2209.20755	1509.87069
3	1	-1	2	0	20	1	-1	1	1	19	701.32059	0.00025	2247.41657	1546.09623
4	1	-1	2	0	21	1	-1	1	1	20	703.30488	0.00010	2287.53030	1584.22551
5	1	-1	2	0	22	1	-1	1	1	21	705.28654*	-0.00338	2329.54794	1624.25802W
6	1	-1	2	0	23	1	-1	1	1	22	707.27437	-0.00112	2373.46866	1666.19317W
7	1	-1	2	0	24	1	-1	1	1	23	709.26201	0.00080	2419.29158	1710.03037
8	1	-1	2	0	25	1	-1	1	1	24	711.24619	-0.00064	2467.01582	1755.76899
9	1	1	2	0	12	1	-1	1	1	12	662.18360	0.00079	1994.70491	1332.52210
10	1	1	2	0	13	1	-1	1	1	13	662.17432	0.00112	2019.48900	1357.31580W
11	1	1	2	0	14	1	-1	1	1	14	662.16141	0.00015	2046.17697	1384.01571
12	1	1	2	0	15	1	-1	1	1	15	662.14722	0.00050	2074.76824	1412.62152
13	1	1	2	0	16	1	-1	1	1	16	662.13038*	0.00109	2105.26218	1443.13289W
14	1	1	2	0	17	1	-1	1	1	17	662.10993*	0.00123	2137.65812	1475.54942W
15	1	1	2	0	18	1	-1	1	1	18	662.08571	0.00104	2171.95536	1509.87069W
16	1	1	2	0	19	1	-1	1	1	19	662.05807	0.00115	2208.15315	1546.09623W
17	1	1	2	0	20	1	-1	1	1	20	662.02571	0.00055	2246.25067	1584.22551
18	1	1	2	0	21	1	-1	1	1	21	661.99063	0.00155	2286.24710	1624.25802W
19	1	1	2	0	22	1	-1	1	1	22	661.94774	-0.00063	2328.14154	1666.19317
20	1	1	2	0	23	1	-1	1	1	23	661.90210*	-0.00062	2371.93309	1710.03037

rms = 0.00043 cm⁻¹

21	$v_4 + 2v_5 (^1\Pi) \leftarrow v_4 + v_5 (\Sigma^-)$													
22														
23														
24														
25														
26	v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	G'	G''
27														
28	1	1	2	-2	1	1	-1	1	1	2	678.03446*	-0.00123	1867.50275	1189.46706W
29	1	1	2	-2	2	1	-1	1	1	3	676.13572*	0.00101	1871.32438	1195.18967W
30	1	1	2	-2	3	1	-1	1	1	4	674.22511*	-0.01196	1877.05683	1202.81976W
31	1	1	2	-2	4	1	-1	1	1	5	672.34130*	-0.00155	1884.70016	1212.35731W
32	1	1	2	-2	5	1	-1	1	1	6	670.45096	-0.00119	1894.25438	1223.80224W
33	1	1	2	-2	6	1	-1	1	1	7	668.56482	-0.00025	1905.71956	1237.15450
34	1	1	2	-2	7	1	-1	1	1	8	666.68178	0.00003	1919.09576	1252.41400
35	1	1	2	-2	8	1	-1	1	1	9	664.80244	0.00006	1934.38303	1269.58065
36	1	1	2	-2	9	1	-1	1	1	10	662.92684	-0.00031	1951.58147	1288.65432
37	1	1	2	-2	10	1	-1	1	1	11	661.05677*	0.00047	1970.69116	1309.63487
38	1	1	2	-2	11	1	-1	1	1	12	659.19035	0.00024	1991.71220	1332.52210
39	1	1	2	-2	12	1	-1	1	1	13	657.32986	0.00096	2014.64470	1357.31580
40	1	1	2	-2	13	1	-1	1	1	14	655.47254	-0.00051	2039.48875	1384.01571
41	1	1	2	-2	14	1	-1	1	1	15	653.62292	-0.00005	2066.24449	1412.62152
42	1	1	2	-2	15	1	-1	1	1	16	651.77924	0.00012	2094.91201	1443.13289
43	1	1	2	-2	16	1	-1	1	1	17	649.94239	0.00039	2125.49143	1475.54942
44	1	1	2	-2	17	1	-1	1	1	18	648.11208	-0.00007	2157.98284	1509.87069
45	1	1	2	-2	18	1	-1	1	1	19	646.29012	0.00001	2192.38633	1546.09623
46	1	1	2	-2	19	1	-1	1	1	20	644.47665	0.00020	2228.70197	1584.22551
47	1	1	2	-2	1	1	-1	1	1	0	683.75843	0.00010	1867.50275	1183.74443
48	1	1	2	-2	2	1	-1	1	1	1	685.67337	0.00097	1871.32438	1185.65198
49	1	1	2	-2	3	1	-1	1	1	2	687.58947	-0.00030	1877.05683	1189.46706
50	1	1	2	-2	4	1	-1	1	1	3	689.51046	-0.00003	1884.70016	1195.18967
51	1	1	2	-2	5	1	-1	1	1	4	691.43501	0.00039	1894.25438	1202.81976
52	1	1	2	-2	6	1	-1	1	1	5	693.36269	0.00043	1905.71956	1212.35731
53	1	1	2	-2	7	1	-1	1	1	6	695.29466	0.00114	1919.09576	1223.80224W
54	1	1	2	-2	8	1	-1	1	1	7	697.22780	-0.00074	1934.38303	1237.15450
55	1	1	2	-2	9	1	-1	1	1	8	699.16724	-0.00023	1951.58147	1252.41400
56	1	1	2	-2	10	1	-1	1	1	9	701.10980	-0.00071	1970.69116	1269.58065
57	1	1	2	-2	11	1	-1	1	1	10	703.05916*	0.00128	1991.71220	1288.65432W
58	1	1	2	-2	12	1	-1	1	1	11	705.01083	0.00100	2014.64470	1309.63487
59	1	1	2	-2	13	1	-1	1	1	12	706.96735	0.00069	2039.48875	1332.52210
60	1	1	2	-2	14	1	-1	1	1	13	708.92844	-0.00025	2066.24449	1357.31580
	1	1	2	-2	15	1	-1	1	1	14	710.89722	0.00091	2094.91201	1384.01571
	1	1	2	-2	16	1	-1	1	1	15	712.86934	-0.00057	2125.49143	1412.62152
	1	1	2	-2	17	1	-1	1	1	16	714.85013	0.00018	2157.98284	1443.13289
	1	1	2	-2	18	1	-1	1	1	17	716.85047*	0.01356	2192.38633	1475.54942W
	1	1	2	-2	19	1	-1	1	1	18	718.83081	-0.00046	2228.70197	1509.87069
	1	1	2	-2	20	1	-1	1	1	19	720.83295	-0.00060	2266.92978	1546.09623
	1	-1	2	2	6	1	-1	1	1	20	722.80509	0.00055	2305.66237	1584.22551

1	-1	2	2	7	1	-1	1	1	7	681.86535	0.00038	1919.01947	1237.15450
2	-1	2	2	8	1	-1	1	1	8	681.87069	-0.00022	1934.28491	1252.41400
3	-1	2	2	9	1	-1	1	1	9	681.87793	-0.00017	1951.45875	1269.58065
4	-1	2	2	10	1	-1	1	1	10	681.88693	0.00020	1970.54106	1288.65432
5	-1	2	2	11	1	-1	1	1	11	681.89698	-0.00006	1991.53191	1309.63487
6	-1	2	2	12	1	-1	1	1	12	681.90920	-0.00007	2014.43136	1332.52210
7	-1	2	2	13	1	-1	1	1	13	681.92353	-0.00017	2039.23950	1357.31580
8	-1	2	2	14	1	-1	1	1	14	681.94026	-0.00040	2065.95636	1384.01571
9	-1	2	2	15	1	-1	1	1	15	681.96046	-0.00003	2094.58201	1412.62152
10	-1	2	2	16	1	-1	1	1	16	681.98434	0.00078	2125.11645	1443.13289
11	-1	2	2	17	1	-1	1	1	17	682.00923*	-0.00105	2157.55970	1475.54942W
12	-1	2	2	18	1	-1	1	1	18	682.04133	0.00030	2191.91172	1509.87069
13	-1	2	2	19	1	-1	1	1	19	682.07574	-0.00049	2228.17246	1546.09623
14	-1	2	2	20	1	-1	1	1	20	682.11422*	-0.00206	2266.34179	1584.22551W
15	-1	2	2	21	1	-1	1	1	21	682.16172	0.00017	2306.41957	1624.25802
16	-1	2	2	22	1	-1	1	1	22	682.21262*	0.00021	2348.40558	1666.19317
17	-1	2	2	23	1	-1	1	1	23	682.26999	0.00080	2392.29956	1710.03037
18	-1	2	2	24	1	-1	1	1	24	682.33276	0.00059	2438.10116	1755.76899

rms = 0.00047 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 2 0 1	1 1 1 1 2	658.67175*	-0.00388	1847.85961	1189.18398W
1 1 2 0 2	1 1 1 1 3	656.76899	0.00029	1851.67479	1194.90609
1 1 2 0 3	1 1 1 1 4	654.86336	0.00096	1857.39746	1202.53506
1 1 2 0 4	1 1 1 1 5	652.95818	0.00114	1865.02750	1212.07046W
1 1 2 0 5	1 1 1 1 6	651.05360	0.00060	1874.56474	1223.51174
1 1 2 0 6	1 1 1 1 7	649.15103	0.00030	1886.00898	1236.85825
1 1 2 0 7	1 1 1 1 8	647.24989	-0.00085	1899.35999	1252.10924
1 1 2 0 8	1 1 1 1 9	645.35366	0.00008	1914.61746	1269.26388
1 1 2 0 9	1 1 1 1 10	643.45902*	-0.00083	1931.78108	1288.32123
1 1 2 0 10	1 1 1 1 11	641.56993	-0.00024	1950.85047	1309.28031
1 1 2 0 11	1 1 1 1 12	639.68571	0.00053	1971.82524	1332.14005
1 1 2 0 12	1 1 1 1 13	637.80615	0.00063	1994.70491	1356.89938
1 1 2 0 13	1 1 1 1 14	635.93253	0.00073	2019.48900	1383.55720
1 1 2 0 14	1 1 1 1 15	634.06580	0.00124	2046.17697	1412.11241W
1 1 2 0 15	1 1 1 1 16	632.20495	0.00066	2074.76824	1442.56394
1 1 2 0 16	1 1 1 1 17	630.34991	-0.00148	2105.26218	1474.91078W
1 1 2 0 17	1 1 1 1 18	628.50702	0.00086	2137.65812	1509.15197
1 1 2 0 18	1 1 1 1 19	626.66916	0.00040	2171.95536	1545.28661
1 1 2 0 19	1 1 1 1 20	624.84024	0.00098	2208.15315	1583.31388
1 1 2 0 20	1 1 1 1 21	623.01828	0.00066	2246.25067	1623.23305
1 1 2 0 21	1 1 1 1 22	621.20370	0.00001	2286.24710	1665.04341
1 1 2 0 22	1 1 1 1 23	619.39817	0.00097	2328.14154	1708.74434
1 1 2 0 23	1 1 1 1 24	617.59860	0.00077	2371.93309	1754.33526
1 1 2 0 24	1 1 1 1 25	615.80739	0.00221	2417.62077	1801.81559W
1 1 2 0 25	1 1 1 1 26	614.01996	0.00118	2465.20357	1851.18480W
1 1 2 0 4	1 1 1 1 3	670.12058	-0.00083	1865.02750	1194.90609
1 1 2 0 5	1 1 1 1 4	672.03011	0.00043	1874.56474	1202.53506
1 1 2 0 6	1 1 1 1 5	673.94059*	0.00207	1886.00898	1212.07046W
1 1 2 0 7	1 1 1 1 6	675.84883	0.00058	1899.35999	1223.51174
1 1 2 0 8	1 1 1 1 7	677.76488*	0.00567	1914.61746	1236.85825W
1 1 2 0 9	1 1 1 1 8	679.67276	0.00092	1931.78108	1252.10924
1 1 2 0 10	1 1 1 1 9	681.58594	-0.00066	1950.85047	1269.26388
1 1 2 0 11	1 1 1 1 10	683.50593*	0.00193	1971.82524	1288.32123W
1 1 2 0 12	1 1 1 1 11	685.42706*	0.00246	1994.70491	1309.28031W
1 1 2 0 13	1 1 1 1 12	687.35311	0.00416	2019.48900	1332.14005W
1 1 2 0 14	1 1 1 1 13	689.27791	0.00033	2046.17697	1356.89938
1 1 2 0 15	1 1 1 1 14	691.21174	0.00070	2074.76824	1383.55720
1 1 2 0 16	1 1 1 1 15	693.15855*	0.00878	2105.26218	1412.11241W
1 1 2 0 17	1 1 1 1 16	695.09427	0.00009	2137.65812	1442.56394
1 1 2 0 18	1 1 1 1 17	697.04539	0.00081	2171.95536	1474.91078
1 1 2 0 19	1 1 1 1 18	699.00119	0.00001	2208.15315	1509.15197
1 1 2 0 20	1 1 1 1 19	700.94651	0.00046	2246.25067	1545.28661W

1	1	1	2	0	21	1	1	1	1	20	702.93418*	0.00097	2286.24710	1583.31388
2	1	1	2	0	22	1	1	1	1	21	704.90839	-0.00011	2328.14154	1623.23305
3	1	1	2	0	23	1	1	1	1	22	706.89132	0.00164	2371.93309	1665.04341W
4	1	1	2	0	24	1	1	1	1	23	708.84852*	-0.02790	2417.62077	1708.74434W
5	1	-1	2	0	1	1	-1	1	-1	2	658.68340	0.00228	1847.86517	1189.18404W
6	1	-1	2	0	2	1	-1	1	-1	3	656.78468	-0.00035	1851.69146	1194.90643
7	1	-1	2	0	3	1	-1	1	-1	4	654.89497	0.00026	1857.43079	1202.53608
8	1	-1	2	0	4	1	-1	1	-1	5	653.01001	-0.00021	1865.08304	1212.07282
9	1	-1	2	0	5	1	-1	1	-1	6	651.13211	0.00053	1874.64805	1223.51646
10	1	-1	2	0	6	1	-1	1	-1	7	649.26022	0.00138	1886.12559	1236.86675W
11	1	-1	2	0	7	1	-1	1	-1	8	647.39100	-0.00104	1899.51544	1252.12340W
12	1	-1	2	0	8	1	-1	1	-1	9	645.53082	-0.00038	1914.81729	1269.28609
13	1	-1	2	0	9	1	-1	1	-1	10	643.67607	-0.00027	1932.03082	1288.35448
14	1	-1	2	0	10	1	-1	1	-1	11	641.83075*	0.00329	1951.15566	1309.32820W
15	1	-1	2	0	11	1	-1	1	-1	12	639.98348	-0.00106	1972.19139	1332.20685W
16	1	-1	2	0	12	1	-1	1	-1	13	638.14755	0.00002	1995.13757	1356.99004
17	1	-1	2	0	13	1	-1	1	-1	14	636.31674	0.00037	2019.99372	1383.67734
18	1	-1	2	0	14	1	-1	1	-1	15	634.49089	-0.00007	2046.75929	1412.26833
19	1	-1	2	0	15	1	-1	1	-1	16	632.67271	0.00156	2075.43373	1442.76257W
20	1	-1	2	0	16	1	-1	1	-1	17	630.85760	0.00080	2106.01643	1475.15963
21	1	-1	2	0	4	1	-1	1	-1	3	670.17627	-0.00035	1865.08304	1194.90643
22	1	-1	2	0	5	1	-1	1	-1	4	672.11201	0.00004	1874.64805	1202.53608
23	1	-1	2	0	6	1	-1	1	-1	5	674.05574*	0.00297	1886.12559	1212.07282W
24	1	-1	2	0	7	1	-1	1	-1	6	675.99536*	-0.00361	1899.51544	1223.51646W
25	1	-1	2	0	8	1	-1	1	-1	7	677.95281*	0.00227	1914.81729	1236.86675W
26	1	-1	2	0	9	1	-1	1	-1	8	679.90751	0.00009	1932.03082	1252.12340
27	1	-1	2	0	10	1	-1	1	-1	9	681.87068	0.00111	1951.15566	1269.28609W
28	1	-1	2	0	11	1	-1	1	-1	10	683.83627	-0.00064	1972.19139	1288.35448
29	1	-1	2	0	12	1	-1	1	-1	11	685.81046	0.00108	1995.13757	1309.32820W
30	1	-1	2	0	13	1	-1	1	-1	12	687.78630	-0.00056	2019.99372	1332.20685
31	1	-1	2	0	14	1	-1	1	-1	13	689.76952	0.00027	2046.75929	1356.99004
32	1	-1	2	0	15	1	-1	1	-1	14	691.75657	0.00018	2075.43373	1383.67734
33	1	-1	2	0	5	1	1	1	1	5	662.57832	0.00074	1874.64805	1212.07046
34	1	-1	2	0	6	1	1	1	1	6	662.61685	0.00300	1886.12559	1223.51174W
35	1	-1	2	0	7	1	1	1	1	7	662.65816	0.00097	1899.51544	1236.85825
36	1	-1	2	0	8	1	1	1	1	8	662.70908	0.00103	1914.81729	1252.10924W
37	1	-1	2	0	9	1	1	1	1	9	662.76693	-0.00001	1932.03082	1269.26388
38	1	-1	2	0	10	1	1	1	1	10	662.81371*	-0.02071	1951.15566	1288.32123W
39	1	-1	2	0	11	1	1	1	1	11	662.91133	0.00025	1972.19139	1309.28031
40	1	-1	2	0	12	1	1	1	1	12	662.99384	-0.00368	1995.13757	1332.14005W
41	1	-1	2	0	13	1	1	1	1	13	663.09414	-0.00019	2019.99372	1356.89938
42	1	-1	2	0	14	1	1	1	1	14	663.20177	-0.00032	2046.75929	1383.55720
43	1	-1	2	0	15	1	1	1	1	15	663.32094	-0.00038	2075.43373	1412.11241
44	1	-1	2	0	16	1	1	1	1	16	663.45245	-0.00004	2106.01643	1442.56394
45	1	-1	2	0	17	1	1	1	1	17	663.59609	0.00011	2138.50676	1474.91078
46	1	-1	2	0	18	1	1	1	1	18	663.75215	0.00008	2172.90404	1509.15197
47	1	-1	2	0	19	1	1	1	1	19	663.92081	-0.00014	2209.20755	1545.28661

rms = 0.00053 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
1 1 2 2 3	1 1 1 1 4	669.70297	0.00066	1872.23737	1202.53506
1 1 2 2 4	1 1 1 1 5	667.80340*	-0.00107	1879.87493	1212.07046W
1 1 2 2 5	1 1 1 1 6	665.91036	0.00058	1889.42152	1223.51174
1 1 2 2 6	1 1 1 1 7	664.01842	-0.00024	1900.87691	1236.85825
1 1 2 2 7	1 1 1 1 8	662.13077	-0.00080	1914.24081	1252.10924
1 1 2 2 8	1 1 1 1 9	660.24884	-0.00019	1929.51291	1269.26388
1 1 2 2 9	1 1 1 1 10	658.37182	0.00022	1946.69283	1288.32123
1 1 2 2 10	1 1 1 1 11	656.50011	0.00024	1965.78018	1309.28031
1 1 2 2 11	1 1 1 1 12	654.63491	0.00048	1986.77449	1332.14005
1 1 2 2 12	1 1 1 1 13	652.77627*	0.00037	2009.67528	1356.89938
1 1 2 2 13	1 1 1 1 14	650.92509	0.00023	2034.48206	1383.55720
1 1 2 2 14	1 1 1 1 15	649.08247	0.00062	2061.19426	1412.11241
1 1 2 2 15	1 1 1 1 16	647.24085	0.00091	2089.81134	1442.56394

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1	1	2	2	16	1	1	1	1	17	645.42170	-0.00022	2120.33270	1474.91078
1	1	2	2	17	1	1	1	1	18	643.60645	0.00065	2152.75777	1509.15197
1	1	2	2	18	1	1	1	1	19	641.80060*	0.00128	2187.08593	1545.28661W
1	1	2	2	19	1	1	1	1	20	640.00209	-0.00062	2223.31659	1583.31388
1	1	2	2	20	1	1	1	1	21	638.21636	0.00023	2261.44918	1623.23305
1	1	2	2	21	1	1	1	1	22	636.43936	-0.00033	2301.48310	1665.04341
1	1	2	2	22	1	1	1	1	23	634.67284	-0.00062	2343.41781	1708.74434
1	1	2	2	23	1	1	1	1	24	632.91784	0.00033	2387.25277	1754.33526
1	1	2	2	24	1	1	1	1	25	631.16995	-0.00193	2432.98747	1801.81559W
1	1	2	2	3	1	1	1	1	2	683.05272	-0.00068	1872.23737	1189.18398
1	1	2	2	4	1	1	1	1	3	684.96900	0.00016	1879.87493	1194.90609
1	1	2	2	5	1	1	1	1	4	686.88585	-0.00061	1889.42152	1202.53506
1	1	2	2	6	1	1	1	1	5	688.80606	-0.00039	1900.87691	1212.07046
1	1	2	2	7	1	1	1	1	6	690.72975	0.00068	1914.24081	1223.51174
1	1	2	2	8	1	1	1	1	7	692.65447	-0.00019	1929.51291	1236.85825
1	1	2	2	9	1	1	1	1	8	694.58327	-0.00032	1946.69283	1252.10924
1	1	2	2	10	1	1	1	1	9	696.51597	-0.00033	1965.78018	1269.26388
1	1	2	2	11	1	1	1	1	10	698.45336	0.00011	1986.77449	1288.32123
1	1	2	2	12	1	1	1	1	11	700.39492	-0.00006	2009.67528	1309.28031
1	1	2	2	13	1	1	1	1	12	702.34152	-0.00048	2034.48206	1332.14005
1	1	2	2	14	1	1	1	1	13	704.29534	0.00046	2061.19426	1356.89938
1	1	2	2	15	1	1	1	1	14	706.25467	0.00053	2089.81134	1383.55720
1	1	2	2	16	1	1	1	1	15	708.22083	0.00054	2120.33270	1412.11241
1	1	2	2	17	1	1	1	1	16	710.19377	-0.00005	2152.75777	1442.56394
1	1	2	2	18	1	1	1	1	17	712.17492	-0.00022	2187.08593	1474.91078
1	1	2	2	19	1	1	1	1	18	714.16431	-0.00032	2223.31659	1509.15197
1	1	2	2	20	1	1	1	1	19	716.16245	-0.00012	2261.44918	1545.28661
1	1	2	2	21	1	1	1	1	20	718.16965	0.00043	2301.48310	1583.31388
1	1	2	2	22	1	1	1	1	21	720.18493	0.00017	2343.41781	1623.23305
1	1	2	2	23	1	1	1	1	22	722.20965	0.00029	2387.25277	1665.04341
1	1	2	2	24	1	1	1	1	23	724.24391	0.00079	2432.98747	1708.74434
1	1	2	2	3	1	-1	1	-1	3	677.33063	-0.00032	1872.23737	1194.90643
1	1	2	2	4	1	-1	1	-1	4	677.33853	-0.00032	1879.87493	1202.53608
1	1	2	2	5	1	-1	1	-1	5	677.34995*	0.00126	1889.42152	1212.07282W
1	1	2	2	6	1	-1	1	-1	6	677.35988	-0.00056	1900.87691	1223.51646
1	1	2	2	7	1	-1	1	-1	7	677.37779*	0.00373	1914.24081	1236.86675W
1	1	2	2	8	1	-1	1	-1	8	677.38910	-0.00041	1929.51291	1252.12340
1	1	2	2	9	1	-1	1	-1	9	677.40662	-0.00013	1946.69283	1269.28609
1	1	2	2	10	1	-1	1	-1	10	677.42859*	0.00289	1965.78018	1288.35448W
1	1	2	2	11	1	-1	1	-1	11	677.44613	-0.00016	1986.77449	1309.32820
1	1	2	2	12	1	-1	1	-1	12	677.46827	-0.00016	2009.67528	1332.20685
1	1	2	2	13	1	-1	1	-1	13	677.49265	0.00063	2034.48206	1356.99004
1	-1	2	-2	3	1	-1	1	-1	4	669.70159	0.00029	1872.23737	1202.53608
1	-1	2	-2	4	1	-1	1	-1	5	667.80340*	0.00130	1879.87493	1212.07282W
1	-1	2	-2	5	1	-1	1	-1	6	665.90340*	-0.00165	1889.42151	1223.51646W
1	-1	2	-2	6	1	-1	1	-1	7	664.00998	-0.00016	1900.87689	1236.86675
1	-1	2	-2	7	1	-1	1	-1	8	662.11725	-0.00012	1914.24077	1252.12340
1	-1	2	-2	8	1	-1	1	-1	9	660.22644	-0.00028	1929.51281	1269.28609
1	-1	2	-2	9	1	-1	1	-1	10	658.33589*	-0.00227	1946.69264	1288.35448W
1	-1	2	-2	10	1	-1	1	-1	11	656.45201	0.00040	1965.77980	1309.32820
1	-1	2	-2	11	1	-1	1	-1	12	654.56705	0.00006	1986.77384	1332.20685
1	-1	2	-2	12	1	-1	1	-1	13	652.68481	0.00064	2009.67421	1356.99004
1	-1	2	-2	13	1	-1	1	-1	14	650.80355	0.00056	2034.48033	1383.67734
1	-1	2	-2	14	1	-1	1	-1	15	648.92274	-0.00053	2061.19160	1412.26833
1	-1	2	-2	15	1	-1	1	-1	16	647.04369	-0.00109	2089.80736	1442.76257W
1	-1	2	-2	16	1	-1	1	-1	17	645.16725	-0.00001	2120.32690	1475.15963
1	-1	2	-2	17	1	-1	1	-1	18	643.29036	-0.00009	2152.74950	1509.45905
1	-1	2	-2	18	1	-1	1	-1	19	641.41427	0.00023	2187.07439	1545.66036
1	-1	2	-2	19	1	-1	1	-1	20	639.54564*	0.00791	2223.30081	1583.76307W
1	-1	2	-2	21	1	-1	1	-1	22	635.78317	-0.00108	2301.45495	1665.67070W
1	-1	2	-2	3	1	-1	1	-1	2	683.05272	-0.00061	1872.23737	1189.18404
1	-1	2	-2	4	1	-1	1	-1	3	684.96863*	0.00013	1879.87493	1194.90643
1	-1	2	-2	5	1	-1	1	-1	4	686.88585	0.00041	1889.42151	1202.53608
1	-1	2	-2	6	1	-1	1	-1	5	688.80511*	0.00105	1900.87689	1212.07282W
1	-1	2	-2	7	1	-1	1	-1	6	690.72503	0.00073	1914.24077	1223.51646
1	-1	2	-2	8	1	-1	1	-1	7	692.64608	0.00002	1929.51281	1236.86675
1	-1	2	-2	9	1	-1	1	-1	8	694.56900	-0.00024	1946.69264	1252.12340
1	-1	2	-2	10	1	-1	1	-1	9	696.49386	0.00014	1965.77980	1269.28609
1	-1	2	-2	11	1	-1	1	-1	10	698.41971	0.00035	1986.77384	1288.35448

1	1	-1	2	-2	12	1	-1	1	-1	11	700.34649	0.00048	2009.67421	1309.32820
2	1	-1	2	-2	13	1	-1	1	-1	12	702.27392	0.00044	2034.48033	1332.20685
3	1	-1	2	-2	14	1	-1	1	-1	13	704.20150	-0.00006	2061.19160	1356.99004
4	1	-1	2	-2	15	1	-1	1	-1	14	706.13015	0.00013	2089.80736	1383.67734
5	1	-1	2	-2	16	1	-1	1	-1	15	708.05828	-0.00029	2120.32690	1412.26833
6	1	-1	2	-2	17	1	-1	1	-1	16	709.98700	0.00008	2152.74950	1442.76257
7	1	-1	2	-2	18	1	-1	1	-1	17	711.91419	-0.00057	2187.07439	1475.15963
8	1	-1	2	-2	19	1	-1	1	-1	18	713.84194	0.00018	2223.30081	1509.45905
9	1	-1	2	-2	20	1	-1	1	-1	19	715.76739	-0.00019	2261.42793	1545.66036
10	1	-1	2	-2	21	1	-1	1	-1	20	717.69541*	0.00353	2301.45495	1583.76307W
11	1	-1	2	-2	22	1	-1	1	-1	21	719.61450	0.00016	2343.38104	1623.76670
12	1	-1	2	-2	23	1	-1	1	-1	22	721.53395	-0.00071	2387.20536	1665.67070
13	1	-1	2	-2	24	1	-1	1	-1	23	723.45186*	-0.00067	2432.92708	1709.47454
14	1	-1	2	-2	25	1	-1	1	-1	24	725.36723	-0.00048	2480.54536	1755.17765
15	1	-1	2	-2	3	1	1	1	1	3	677.33063	-0.00065	1872.23737	1194.90609
16	1	-1	2	-2	4	1	1	1	1	4	677.33853	-0.00133	1879.87493	1202.53506W
17	1	-1	2	-2	5	1	1	1	1	5	677.34995	-0.00110	1889.42151	1212.07046W
18	1	-1	2	-2	6	1	1	1	1	6	677.36568	0.00053	1900.87689	1223.51174
19	1	-1	2	-2	7	1	1	1	1	7	677.38244	-0.00008	1914.24077	1236.85825
20	1	-1	2	-2	8	1	1	1	1	8	677.40351	-0.00006	1929.51281	1252.10924
21	1	-1	2	-2	9	1	1	1	1	9	677.42859	-0.00017	1946.69264	1269.26388
22	1	-1	2	-2	10	1	1	1	1	10	677.45867	0.00010	1965.77980	1288.32123
23	1	-1	2	-2	11	1	1	1	1	11	677.49266	-0.00087	1986.77384	1309.28031
24	1	-1	2	-2	12	1	1	1	1	12	677.53297*	-0.00118	2009.67421	1332.14005W
25	1	-1	2	-2	13	1	1	1	1	13	677.58170	0.00075	2034.48033	1356.89938

rms = 0.00042 cm⁻¹

3v₄ (Π) ← 2v₄ (Σ⁺)

v ₄ '	l ₄ '	v ₅ '	l ₅ '	J'	v ₄ ''	l ₄ ''	v ₅ ''	l ₅ ''	J''	OBS	OBS - CALC	G'	G''
3	1	0	0	1	2	0	0	0	2	505.24187	0.00071	1527.82275	1022.58159
3	1	0	0	2	2	0	0	0	3	503.32273	-0.00143	1531.63559	1028.31143W
3	1	0	0	3	2	0	0	0	4	501.40360	-0.00045	1537.35469	1035.95064
3	1	0	0	4	2	0	0	0	5	499.48075	-0.00037	1544.97988	1045.49875
3	1	0	0	5	2	0	0	0	6	497.55447	-0.00128	1554.51090	1056.95515W
3	1	0	0	6	2	0	0	0	7	495.62754	-0.00083	1565.94747	1070.31910
3	1	0	0	7	2	0	0	0	8	493.69961	0.00015	1579.28923	1085.58977
3	1	0	0	8	2	0	0	0	9	491.76939	-0.00016	1594.53577	1102.76621
3	1	0	0	9	2	0	0	0	10	489.83925	0.00000	1611.68663	1121.84738
3	1	0	0	10	2	0	0	0	11	487.90936	0.00020	1630.74133	1142.83216
3	1	0	0	11	2	0	0	0	12	485.98014	0.00020	1651.69930	1165.71936
3	1	0	0	12	2	0	0	0	13	484.05176	-0.00048	1674.55997	1190.50774
3	1	0	0	13	2	0	0	0	14	482.12690	0.00023	1699.32273	1217.19606
3	1	0	0	14	2	0	0	0	15	480.20292	-0.00091	1725.98691	1245.78308
3	1	0	0	15	2	0	0	0	16	478.28460	0.00036	1754.55184	1276.26760
3	1	0	0	16	2	0	0	0	17	476.36701	-0.00133	1785.01683	1308.64848W
3	1	0	0	1	2	0	0	0	0	510.96978	-0.00159	1527.82275	1016.85139W
3	1	0	0	2	2	0	0	0	1	512.87186	-0.00224	1531.63559	1018.76149W
3	1	0	0	3	2	0	0	0	2	514.77238	-0.00072	1537.35469	1022.58159
3	1	0	0	4	2	0	0	0	3	516.66678	-0.00167	1544.97988	1028.31143W
3	1	0	0	5	2	0	0	0	4	518.55888	-0.00138	1554.51090	1035.95064W
3	1	0	0	6	2	0	0	0	5	520.44723	-0.00149	1565.94747	1045.49875W
3	1	0	0	7	2	0	0	0	6	522.33437	0.00029	1579.28923	1056.95515
3	1	0	0	8	2	0	0	0	7	524.21514	-0.00153	1594.53577	1070.31910W
3	1	0	0	9	2	0	0	0	8	526.09737	0.00050	1611.68663	1085.58977
3	1	0	0	10	2	0	0	0	9	527.97506	-0.00006	1630.74133	1102.76621
3	1	0	0	11	2	0	0	0	10	529.85145	-0.00047	1651.69930	1121.84738
3	1	0	0	12	2	0	0	0	11	531.72761	-0.00020	1674.55997	1142.83216
3	1	0	0	13	2	0	0	0	12	533.60232	-0.00105	1699.32273	1165.71936W
3	1	0	0	14	2	0	0	0	13	535.47988	0.00071	1725.98691	1190.50774
3	1	0	0	15	2	0	0	0	14	537.35595	0.00017	1754.55184	1217.19606
3	1	0	0	16	2	0	0	0	15	539.23323	-0.00052	1785.01683	1245.78308
3	1	0	0	17	2	0	0	0	16	541.11416	0.00061	1817.38115	1276.26760
3	1	0	0	18	2	0	0	0	17	542.99636	0.00077	1851.64407	1308.64848
3	1	0	0	19	2	0	0	0	18	544.87857	0.00085	1887.80485	1342.92466W

3	1	0	0	20	2	0	0	0	19	546.76816	0.00058	1925.86272	1379.09514
3	1	0	0	21	2	0	0	0	20	548.65706	-0.00081	1965.81693	1417.15906
3	1	0	0	22	2	0	0	0	21	550.55044	-0.00065	2007.66669	1457.11560
3	1	0	0	23	2	0	0	0	22	552.44924	0.00206	2051.41124	1498.96407W
3	1	0	0	24	2	0	0	0	23	554.34745*	0.00146	2097.04980	1542.70381W
3	1	0	0	25	2	0	0	0	24	556.24770	0.00036	2144.58158	1588.33424
3	1	0	0	26	2	0	0	0	25	558.15103	0.00004	2194.00579	1635.85480
3	1	0	0	28	2	0	0	0	27	561.96505	0.00096	2298.52834	1736.56425
3	-1	0	0	1	2	0	0	0	1	509.07686	-0.00125	1527.83961	1018.76149W
3	-1	0	0	2	2	0	0	0	2	509.10632	0.00176	1531.68615	1022.58159W
3	-1	0	0	3	2	0	0	0	3	509.14614	0.00176	1537.45581	1028.31143W
3	-1	0	0	4	2	0	0	0	4	509.19898*	0.00123	1545.14839	1035.95064W
3	-1	0	0	5	2	0	0	0	5	509.26463	-0.00026	1554.76364	1045.49875
3	-1	0	0	6	2	0	0	0	6	509.34776*	0.00168	1566.30123	1056.95515W
3	-1	0	0	7	2	0	0	0	7	509.44062	-0.00104	1579.76075	1070.31910W
3	-1	0	0	8	2	0	0	0	8	509.55287	0.00089	1595.14175	1085.58977
3	-1	0	0	9	2	0	0	0	9	509.67947*	0.00201	1612.44367	1102.76621W
3	-1	0	0	10	2	0	0	0	10	509.81800	-0.00049	1631.66587	1121.84738
3	-1	0	0	11	2	0	0	0	11	509.97464	-0.00084	1652.80764	1142.83216
3	-1	0	0	12	2	0	0	0	12	510.14773	-0.00106	1675.86815	1165.71936W
3	-1	0	0	13	2	0	0	0	13	510.33879	0.00004	1700.84649	1190.50774
3	-1	0	0	14	2	0	0	0	14	510.54387	-0.00170	1727.74163	1217.19606W
3	-1	0	0	15	2	0	0	0	15	510.76975*	0.00039	1756.55244	1245.78308
3	-1	0	0	16	2	0	0	0	16	511.01143	0.00138	1787.27765	1276.26760W
3	-1	0	0	17	2	0	0	0	17	511.26868	0.00127	1819.91590	1308.64848W
3	-1	0	0	18	2	0	0	0	18	511.54017	-0.00084	1854.46566	1342.92466
3	-1	0	0	19	2	0	0	0	19	511.82868	-0.00150	1890.92532	1379.09514W
3	-1	0	0	20	2	0	0	0	20	512.13350	-0.00056	1929.29312	1417.15906
3	-1	0	0	21	2	0	0	0	21	512.45214	0.00055	1969.56720	1457.11560
3	-1	0	0	22	2	0	0	0	22	512.78147	-0.00006	2011.74560	1498.96407
3	-1	0	0	23	2	0	0	0	23	513.12192	-0.00057	2055.82629	1542.70381
3	-1	0	0	24	2	0	0	0	24	513.47590	0.00291	2101.80723	1588.33424W

rms = 0.00054 cm⁻¹

$3\nu_4(\Pi) \leftarrow 2\nu_4(\Delta)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
3 -1 0 0 5	2 2 0 0 5	504.86702	0.00071	1554.76364	1049.89732
3 -1 0 0 6	2 2 0 0 6	504.94273	-0.00174	1566.30123	1061.35675W
3 -1 0 0 7	2 2 0 0 7	505.03070	-0.00294	1579.76075	1074.72712W
3 -1 0 0 8	2 2 0 0 8	505.12748	-0.00538	1595.14175	1090.00889W
3 -1 0 0 9	2 2 0 0 9	505.24187	0.00079	1612.44367	1107.20259
3 -1 0 0 11	2 2 0 0 11	505.48100	0.00143	1652.80764	1147.32807W
3 -1 0 0 12	2 2 0 0 12	505.60699	-0.00011	1675.86815	1170.26105
3 -1 0 0 13	2 2 0 0 13	505.74013	0.00196	1700.84649	1195.10832W
3 -1 0 0 14	2 2 0 0 14	505.87102	-0.00018	1727.74163	1221.87043
3 -1 0 0 15	2 2 0 0 15	506.00538	0.00083	1756.55244	1250.54788
3 -1 0 0 16	2 2 0 0 16	506.13723	0.00066	1787.27765	1281.14108
3 -1 0 0 17	2 2 0 0 17	506.26598	0.00040	1819.91590	1313.65031
3 -1 0 0 18	2 2 0 0 18	506.39016	0.00025	1854.46566	1348.07575
3 -1 0 0 19	2 2 0 0 19	506.50856	0.00066	1890.92532	1384.41742
3 -1 0 0 20	2 2 0 0 20	506.61762	-0.00031	1929.29312	1422.67519
3 1 0 0 4	2 -2 0 0 4	504.63230	-0.00057	1544.97988	1040.34700
3 1 0 0 5	2 -2 0 0 5	504.61611	-0.00079	1554.51090	1049.89400
3 1 0 0 6	2 -2 0 0 6	504.59543	-0.00194	1565.94747	1061.35010W
3 1 0 0 7	2 -2 0 0 7	504.57360	-0.00048	1579.28923	1074.71514
3 1 0 0 8	2 -2 0 0 8	504.54603	-0.00078	1594.53577	1089.98896
3 1 0 0 9	2 -2 0 0 9	504.51615	0.00084	1611.68663	1107.17132
3 1 0 0 10	2 -2 0 0 10	504.47875	-0.00058	1630.74133	1126.26199
3 1 0 0 11	2 -2 0 0 11	504.43853	-0.00005	1651.69930	1147.26072
3 1 0 0 12	2 -2 0 0 12	504.39462	0.00185	1674.55997	1170.16720W
3 1 0 0 13	2 -2 0 0 13	504.34154	-0.00007	1699.32273	1194.98112
3 1 0 0 14	2 -2 0 0 14	504.28378	-0.00099	1725.98691	1221.70214
3 1 0 0 15	2 -2 0 0 15	504.22232	0.00036	1754.55184	1250.32988
3 1 0 0 17	2 -2 0 0 17	504.11731	0.00099	1781.738115	1313.30393

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3	1	0	0	18	2	-2	0	0	18	503.99645	0.00173	1851.64407	1347.64936W
3	1	0	0	20	2	-2	0	0	20	503.80767	-0.00040	1925.86272	1422.05465
3	1	0	0	21	2	-2	0	0	21	503.70323	-0.00021	1965.81693	1462.11349
3	1	0	0	22	2	-2	0	0	22	503.59622	0.00524	2007.66669	1504.07572W
rms = 0.00056 cm ⁻¹													
3v ₅ (Π) ← 2v ₅ (Σ ⁺)													
v ₄ ' l ₄ ' v ₅ ' l ₅ ' J'					v ₄ '' l ₄ '' v ₅ '' l ₅ '' J''					OBS	OBS – CALC	G'	G''
0	0	3	1	1	0	0	2	0	2	660.80360	-0.00069	2001.83066	1341.02637
0	0	3	1	2	0	0	2	0	3	658.88724	-0.00295	2005.63431	1346.74412W
0	0	3	1	3	0	0	2	0	4	656.97229	0.00018	2011.33970	1354.36759
0	0	3	1	4	0	0	2	0	5	655.05076	0.00063	2018.94675	1363.89662
0	0	3	1	5	0	0	2	0	6	653.12483	0.00051	2028.45531	1375.33100
0	0	3	1	6	0	0	2	0	7	651.19505	0.00027	2039.86525	1388.67047
0	0	3	1	7	0	0	2	0	8	649.26037	-0.00123	2053.17636	1403.91476W
0	0	3	1	8	0	0	2	0	9	647.32478	-0.00013	2068.38843	1421.06352
0	0	3	1	9	0	0	2	0	10	645.38484	0.00002	2085.50121	1440.11639
0	0	3	1	10	0	0	2	0	11	643.44131	-0.00016	2104.51441	1461.07294
0	0	3	1	11	0	0	2	0	12	641.49375*	-0.00125	2125.42773	1483.93273W
0	0	3	1	12	0	0	2	0	13	639.54564	0.00008	2148.24081	1508.69525
0	0	3	1	13	0	0	2	0	14	637.59259	-0.00073	2172.95328	1535.35996
0	0	3	1	14	0	0	2	0	15	635.63879	0.00034	2199.56474	1563.92630
0	0	3	1	15	0	0	2	0	16	633.68160	0.00047	2228.07476	1594.39363
0	0	3	1	16	0	0	2	0	17	631.72128	-0.00029	2258.48287	1626.76130
0	0	3	1	17	0	0	2	0	18	629.75953	-0.00044	2290.78857	1661.02860
0	0	3	1	18	0	0	2	0	19	627.79554	-0.00099	2324.99134	1697.19482
0	0	3	1	19	0	0	2	0	20	625.83102	-0.00046	2361.09064	1735.25916
0	0	3	1	20	0	0	2	0	21	623.86509	0.00004	2399.08587	1775.22081
0	0	3	1	21	0	0	2	0	22	621.89686	-0.00062	2438.97642	1817.07894
0	0	3	1	22	0	0	2	0	23	619.92828	-0.00073	2480.76167	1860.83266
0	0	3	1	23	0	0	2	0	24	617.96911*	0.00923	2524.44094	1906.48106W
0	0	3	1	24	0	0	2	0	25	615.99058	0.00024	2570.01353	1954.02319
0	0	3	1	25	0	0	2	0	26	614.01997	-0.00069	2617.47873	2003.45808
0	0	3	1	26	0	0	2	0	27	612.04982	-0.00125	2666.83579	2054.78472W
0	0	3	1	1	0	0	2	0	0	666.52149*	-0.00067	2001.83066	1335.30850
0	0	3	1	2	0	0	2	0	1	668.41955	-0.00029	2005.63431	1337.21447
0	0	3	1	3	0	0	2	0	2	670.31277	-0.00056	2011.33970	1341.02637
0	0	3	1	4	0	0	2	0	3	672.20198	-0.00064	2018.94675	1346.74412
0	0	3	1	5	0	0	2	0	4	674.08745	-0.00027	2028.45531	1354.36759
0	0	3	1	6	0	0	2	0	5	675.96850	-0.00013	2039.86525	1363.89662
0	0	3	1	7	0	0	2	0	6	677.84398*	-0.00138	2053.17636	1375.33100W
0	0	3	1	8	0	0	2	0	7	679.71879	0.00083	2068.38843	1388.67047
0	0	3	1	9	0	0	2	0	8	681.58594	-0.00051	2085.50121	1403.91476
0	0	3	1	10	0	0	2	0	9	683.45044	-0.00045	2104.51441	1421.06352
0	0	3	1	11	0	0	2	0	10	685.31480*	0.00346	2125.42773	1440.11639W
0	0	3	1	12	0	0	2	0	11	687.16798	0.00011	2148.24081	1461.07294
0	0	3	1	13	0	0	2	0	12	689.02108	0.00053	2172.95328	1483.93273
0	0	3	1	14	0	0	2	0	13	690.86970	0.00020	2199.56474	1508.69525
0	0	3	1	15	0	0	2	0	14	692.71465	-0.00015	2228.07476	1535.35996
0	0	3	1	16	0	0	2	0	15	694.55640	-0.00017	2258.48287	1563.92630
0	0	3	1	17	0	0	2	0	16	696.39500	0.00006	2290.78857	1594.39363
0	0	3	1	18	0	0	2	0	17	698.22954	-0.00051	2324.99134	1626.76130
0	0	3	1	19	0	0	2	0	18	700.06227	0.00024	2361.09064	1661.02860
0	0	3	1	20	0	0	2	0	19	701.89122	0.00017	2399.08587	1697.19482
0	0	3	1	21	0	0	2	0	20	703.71707	-0.00020	2438.97642	1735.25916
0	0	3	1	22	0	0	2	0	21	705.54182	0.00097	2480.76167	1775.22081
0	0	3	1	23	0	0	2	0	22	707.36176	-0.00023	2524.44094	1817.07894
0	0	3	1	24	0	0	2	0	23	709.18135	0.00048	2570.01353	1860.83266
0	0	3	1	25	0	0	2	0	24	710.99783	0.00016	2617.47873	1906.48106
0	0	3	-1	1	0	0	2	0	1	664.62980	0.00022	2001.84405	1337.21447
0	0	3	-1	2	0	0	2	0	2	664.64785	-0.00025	2005.67447	1341.02637
0	0	3	-1	3	0	0	2	0	3	664.67577	-0.00013	2011.42003	1346.74412
0	0	3	-1	4	0	0	2	0	4	664.71323	0.00021	2019.08062	1354.36759
0	0	3	-1	5	0	0	2	0	5	664.75175	0.00028	2028.65611	1363.89662

0	0	3	-1	6	0	0	2	0	6	664.81527	-0.00007	2040.14634	1375.33100
0	0	3	-1	7	0	0	2	0	7	664.88173	0.00109	2053.55111	1388.67047W
0	0	3	-1	8	0	0	2	0	8	664.95543	-0.00001	2068.87020	1403.91476
0	0	3	-1	9	0	0	2	0	9	665.03971	-0.00011	2086.10334	1421.06352
0	0	3	-1	10	0	0	2	0	10	665.13354	-0.00032	2105.25025	1440.11639
0	0	3	-1	11	0	0	2	0	11	665.23734	-0.00030	2126.31058	1461.07294
0	0	3	-1	12	0	0	2	0	12	665.35112	-0.00013	2149.28398	1483.93273
0	0	3	-1	13	0	0	2	0	13	665.47479	-0.00001	2174.17005	1508.69525
0	0	3	-1	14	0	0	2	0	14	665.60863	0.00024	2200.96836	1535.35996
0	0	3	-1	15	0	0	2	0	15	665.75251	0.00036	2229.67844	1563.92630
0	0	3	-1	16	0	0	2	0	16	665.90665	0.00047	2260.29981	1594.39363
0	0	3	-1	17	0	0	2	0	17	666.07106	0.00045	2292.83191	1626.76130
0	0	3	-1	18	0	0	2	0	18	666.24552	-0.00006	2327.27418	1661.02860
0	0	3	-1	19	0	0	2	0	19	666.43094	-0.00027	2363.62602	1697.19482
0	0	3	-1	20	0	0	2	0	20	666.62669*	-0.00094	2401.88678	1735.25916
0	0	3	-1	21	0	0	2	0	21	666.83557	0.00060	2442.05578	1775.22081
0	0	3	-1	22	0	0	2	0	22	667.05388	0.00051	2484.13231	1817.07894
0	0	3	-1	23	0	0	2	0	23	667.28283	-0.00012	2528.11561	1860.83266
0	0	3	-1	24	0	0	2	0	24	667.52407	0.00024	2574.00488	1906.48106
0	0	3	-1	25	0	0	2	0	25	667.77693	0.00081	2621.79931	1954.02319

rms = 0.00042 cm⁻¹

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
0 0 3 1 1	0 0 2 2 2	644.21635	0.00015	2001.83066	1357.61446
0 0 3 1 2	0 0 2 2 3	642.30673	0.00202	2005.63431	1363.32960W
0 0 3 1 3	0 0 2 2 4	640.38910	-0.00086	2011.33970	1370.94974
0 0 3 1 4	0 0 2 2 5	638.47167	-0.00023	2018.94675	1380.47484
0 0 3 1 5	0 0 2 2 6	636.54971	-0.00075	2028.45531	1391.90486
0 0 3 1 6	0 0 2 2 7	634.62516	-0.00036	2039.86525	1405.23972
0 0 3 1 7	0 0 2 2 8	632.69621	-0.00077	2053.17636	1420.47938
0 0 3 1 8	0 0 2 2 9	630.76501	0.00031	2068.38843	1437.62374
0 0 3 1 9	0 0 2 2 10	628.82928	0.00079	2085.50121	1456.67272
0 0 3 1 10	0 0 2 2 11	626.88848	0.00028	2104.51441	1477.62621
0 0 3 1 11	0 0 2 2 12	624.94342	-0.00018	2125.42773	1500.48412
0 0 3 1 12	0 0 2 2 13	622.99595	0.00147	2148.24081	1525.24633W
0 0 3 1 13	0 0 2 2 14	621.04144	0.00086	2172.95328	1551.91270
0 0 3 1 14	0 0 2 2 15	619.08245	0.00080	2199.56474	1580.48310
0 0 3 1 15	0 0 2 2 16	617.11762	0.00023	2228.07476	1610.95737
0 0 3 1 16	0 0 2 2 17	615.14435*	-0.00316	2258.48287	1643.33536W
0 0 3 1 17	0 0 2 2 18	613.16979	-0.00189	2290.78857	1677.61689W
0 0 3 1 7	0 0 2 2 6	661.27524*	0.00374	2053.17636	1391.90486W
0 0 3 1 8	0 0 2 2 7	663.14817	-0.00054	2068.38843	1405.23972
0 0 3 1 9	0 0 2 2 8	665.02211	0.00028	2085.50121	1420.47938
0 0 3 1 10	0 0 2 2 9	666.89082	0.00015	2104.51441	1437.62374
0 0 3 1 11	0 0 2 2 10	668.75497	-0.00004	2125.42773	1456.67272
0 0 3 1 12	0 0 2 2 11	670.61685*	0.00226	2148.24081	1477.62621W
0 0 3 1 13	0 0 2 2 12	672.47019*	0.00103	2172.95328	1500.48412W
0 0 3 1 2	0 0 2 -2 2	648.01964	-0.00023	2005.63431	1357.61444
0 0 3 1 3	0 0 2 -2 3	648.01134*	0.00116	2011.33970	1363.32952W
0 0 3 1 4	0 0 2 -2 4	647.99715	-0.00009	2018.94675	1370.94950
0 0 3 1 5	0 0 2 -2 5	647.98116	0.00014	2028.45531	1380.47429
0 0 3 1 6	0 0 2 -2 6	647.96212*	0.00063	2039.86525	1391.90376
0 0 3 1 7	0 0 2 -2 7	647.93821	-0.00041	2053.17636	1405.23774
0 0 3 1 8	0 0 2 -2 8	647.91144	-0.00092	2068.38843	1420.47607
0 0 3 1 9	0 0 2 -2 9	647.88355	0.00088	2085.50121	1437.61854
0 0 3 1 10	0 0 2 -2 10	647.84997	0.00048	2104.51441	1456.66492
0 0 3 1 11	0 0 2 -2 11	647.81279	0.00002	2125.42773	1477.61496
0 0 3 1 12	0 0 2 -2 12	647.77213	-0.00031	2148.24081	1500.46836
0 0 3 1 13	0 0 2 -2 13	647.72901	0.00056	2172.95328	1525.22483
0 0 3 1 14	0 0 2 -2 14	647.68022	-0.00049	2199.56474	1551.88404
0 0 3 1 15	0 0 2 -2 15	647.62939	0.00025	2228.07476	1580.44562
0 0 3 1 17	0 0 2 -2 17	647.51354	-0.00068	2290.78857	1643.27435
0 0 3 1 18	0 0 2 -2 18	647.49134	0.00024	2299.99134	1677.54066

1	0	0	3	1	19	0	0	2	-2	19	647.38135	-0.00163	2361.09064	1713.70766W
2	0	0	3	1	21	0	0	2	-2	21	647.23512	0.00045	2438.97642	1791.74175
3	0	0	3	-1	1	0	0	2	-2	2	644.22940	-0.00021	2001.84405	1357.61444
4	0	0	3	-1	2	0	0	2	-2	3	642.35176*	0.00681	2005.67447	1363.32952W
5	0	0	3	-1	3	0	0	2	-2	4	640.47180	0.00128	2011.42003	1370.94950W
6	0	0	3	-1	4	0	0	2	-2	5	638.60656	0.00024	2019.08062	1380.47429
7	0	0	3	-1	5	0	0	2	-2	6	636.75355	0.00120	2028.65611	1391.90376W
8	0	0	3	-1	6	0	0	2	-2	7	634.90919	0.00060	2040.14634	1405.23774
9	0	0	3	-1	7	0	0	2	-2	8	633.07507	0.00003	2053.55111	1420.47607
10	0	0	3	-1	8	0	0	2	-2	9	631.25228	0.00062	2068.87020	1437.61854
11	0	0	3	-1	9	0	0	2	-2	10	629.43533*	-0.00309	2086.10334	1456.66492W
12	0	0	3	-1	10	0	0	2	-2	11	627.63518	-0.00011	2105.25025	1477.61496
13	0	0	3	-1	11	0	0	2	-2	12	625.84023*	-0.00199	2126.31058	1500.46836W
14	0	0	3	-1	12	0	0	2	-2	13	624.05899	-0.00015	2149.28398	1525.22483
15	0	0	3	-1	13	0	0	2	-2	14	622.28623	0.00022	2174.17005	1551.88404
16	0	0	3	-1	14	0	0	2	-2	15	620.52522*	0.00248	2200.96836	1580.44562W
17	0	0	3	-1	15	0	0	2	-2	16	618.76947	0.00022	2229.67844	1610.90919
18	0	0	3	-1	17	0	0	2	-2	18	615.29023	-0.00102	2292.83191	1677.54066W
19	0	0	3	-1	18	0	0	2	-2	19	613.56658	0.00005	2327.27418	1713.70766
20	0	0	3	-1	19	0	0	2	-2	20	611.85217	0.00101	2363.62602	1751.77486W
21	0	0	3	-1	6	0	0	2	-2	5	659.67517	0.00312	2040.14634	1380.47429W
22	0	0	3	-1	7	0	0	2	-2	6	661.64631	-0.00105	2053.55111	1391.90376W
23	0	0	3	-1	8	0	0	2	-2	7	663.63294	0.00048	2068.87020	1405.23774
24	0	0	3	-1	9	0	0	2	-2	8	665.62762	0.00035	2086.10334	1420.47607
25	0	0	3	-1	10	0	0	2	-2	9	667.63174	0.00004	2105.25025	1437.61854
26	0	0	3	-1	11	0	0	2	-2	10	669.64190*	-0.00375	2126.31058	1456.66492W
27	0	0	3	-1	12	0	0	2	-2	11	671.67003	0.00101	2149.28398	1477.61496W
28	0	0	3	-1	2	0	0	2	2	2	648.05959	-0.00042	2005.67447	1357.61446
29	0	0	3	-1	3	0	0	2	2	3	648.09004	-0.00039	2011.42003	1363.32960
30	0	0	3	-1	4	0	0	2	2	4	648.13111	0.00023	2019.08062	1370.94974
31	0	0	3	-1	5	0	0	2	2	5	648.18188	0.00062	2028.65611	1380.47484
32	0	0	3	-1	6	0	0	2	2	6	648.24380*	0.00232	2040.14634	1391.90486W
33	0	0	3	-1	7	0	0	2	2	7	648.31153	0.00014	2053.55111	1405.23972
34	0	0	3	-1	8	0	0	2	2	8	648.38827	-0.00255	2068.87020	1420.47938W
35	0	0	3	-1	9	0	0	2	2	9	648.47998	0.00037	2086.10334	1437.62374
36	0	0	3	-1	10	0	0	2	2	10	648.57730	-0.00023	2105.25025	1456.67272
37	0	0	3	-1	11	0	0	2	2	11	648.68506	0.00070	2126.31058	1477.62621
38	0	0	3	-1	12	0	0	2	2	12	648.80039	0.00054	2149.28398	1500.48412
39	0	0	3	-1	13	0	0	2	2	13	648.92423	0.00051	2174.17005	1525.24633
40	0	0	3	-1	14	0	0	2	2	14	649.05645	0.00079	2200.96836	1551.91270
41	0	0	3	-1	15	0	0	2	2	15	649.19123	-0.00412	2229.67844	1580.48310W
42	0	0	3	-1	16	0	0	2	2	16	649.34181	-0.00062	2260.29981	1610.95737
43	0	0	3	-1	18	0	0	2	2	18	649.65732	0.00003	2327.27418	1677.61689
44	0	0	3	-1	19	0	0	2	2	19	649.82472	0.00048	2363.62602	1713.80178
45	0	0	3	-1	20	0	0	2	2	20	649.99675	-0.00021	2401.88678	1751.88982
46	0	0	3	-1	21	0	0	2	2	21	650.17556	0.00059	2442.05578	1791.88081

rms = 0.00047 cm⁻¹

3v₅ (Φ) ← 2v₅ (Δ)

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
0 0 3 3 3	0 0 2 2 4	673.76814*	0.00057	2044.71731	1370.94974
0 0 3 3 4	0 0 2 2 5	671.86969	0.00073	2052.34380	1380.47484
0 0 3 3 5	0 0 2 2 6	669.97264	0.00074	2061.87676	1391.90486
0 0 3 3 6	0 0 2 2 7	668.07774	0.00137	2073.31609	1405.23972W
0 0 3 3 7	0 0 2 2 8	666.18268	0.00038	2086.66168	1420.47938
0 0 3 3 8	0 0 2 2 9	664.29414*	0.00449	2101.91339	1437.62374W
0 0 3 3 9	0 0 2 2 10	662.39428*	-0.00405	2119.07105	1456.67272W
0 0 3 3 10	0 0 2 2 11	660.50717	-0.00110	2138.13448	1477.62621W
0 0 3 3 11	0 0 2 2 12	658.61749	-0.00188	2159.10350	1500.48412W
0 0 3 3 12	0 0 2 2 13	656.73106	-0.00048	2181.97786	1525.24633
0 0 3 3 13	0 0 2 2 14	654.84396	-0.00069	2206.75735	1551.91270
0 0 3 3 14	0 0 2 2 15	652.95818	-0.00040	2233.44168	1580.48310
0 0 3 3 15	0 0 2 2 16	651.07341	0.00020	2262.03058	1610.95737
0 0 3 3 16	0 0 2 2 17	649.18864	0.00092	2292.52375	1643.33536

1	0	0	3	3	17	0	0	2	2	18	647.30426	0.00030	2324.92085	1677.61689
2	0	0	3	3	18	0	0	2	2	19	645.41950	-0.00026	2359.22154	1713.80178
3	0	0	3	3	19	0	0	2	2	20	643.53609	0.00047	2395.42544	1751.88982
4	0	0	3	3	20	0	0	2	2	21	641.65278	0.00141	2433.53218	1791.88081W
5	0	0	3	3	21	0	0	2	2	22	639.76533	-0.00148	2473.54132	1833.77451W
6	0	0	3	3	22	0	0	2	2	23	637.88319	0.00143	2515.45243	1877.57067W
7	0	0	3	3	23	0	0	2	2	24	635.99663	0.00061	2559.26505	1923.26903
8	0	0	3	3	3	0	0	2	2	2	687.10253	-0.00032	2044.71731	1357.61446
9	0	0	3	3	4	0	0	2	2	3	689.01422	0.00002	2052.34380	1363.32960
10	0	0	3	3	5	0	0	2	2	4	690.92680	-0.00022	2061.87676	1370.94974
11	0	0	3	3	6	0	0	2	2	5	692.84138	0.00013	2073.31609	1380.47484
12	0	0	3	3	7	0	0	2	2	6	694.75834	0.00152	2086.66168	1391.90486W
13	0	0	3	3	8	0	0	2	2	7	696.67415	0.00049	2101.91339	1405.23972
14	0	0	3	3	9	0	0	2	2	8	698.59221	0.00054	2119.07105	1420.47938
15	0	0	3	3	10	0	0	2	2	9	700.51060	-0.00015	2138.13448	1437.62374
16	0	0	3	3	11	0	0	2	2	10	702.43078	0.00000	2159.10350	1456.67272
17	0	0	3	3	12	0	0	2	2	11	704.35114	-0.00051	2181.97786	1477.62621
18	0	0	3	3	13	0	0	2	2	12	706.27281	-0.00041	2206.75735	1500.48412
19	0	0	3	3	14	0	0	2	2	13	708.19567	0.00032	2233.44168	1525.24633
20	0	0	3	3	15	0	0	2	2	14	710.11732	-0.00056	2262.03058	1551.91270
21	0	0	3	3	16	0	0	2	2	15	712.05009*	0.00944	2292.52375	1580.48310W
22	0	0	3	3	17	0	0	2	2	16	713.96357	0.00009	2324.92085	1610.95737
23	0	0	3	3	18	0	0	2	2	17	715.88662	0.00044	2359.22154	1643.33536
24	0	0	3	3	19	0	0	2	2	18	717.81280*	0.00425	2395.42544	1677.61689W
25	0	0	3	3	20	0	0	2	2	19	719.73072	0.00033	2433.53218	1713.80178
26	0	0	3	3	21	0	0	2	2	20	721.65238	0.00089	2473.54132	1751.88982
27	0	0	3	3	22	0	0	2	2	21	723.57193	0.00031	2515.45243	1791.88081
28	0	0	3	3	23	0	0	2	2	22	725.48996	-0.00058	2559.26505	1833.77451
29	0	0	3	3	3	0	0	2	-2	3	681.38631	-0.00148	2044.71731	1363.32952W
30	0	0	3	3	4	0	0	2	-2	4	681.39407	-0.00023	2052.34380	1370.94950
31	0	0	3	3	5	0	0	2	-2	5	681.40217	-0.00030	2061.87676	1380.47429
32	0	0	3	3	6	0	0	2	-2	6	681.41152	-0.00082	2073.31609	1391.90376
33	0	0	3	3	7	0	0	2	-2	7	681.42341	-0.00053	2086.66168	1405.23774
34	0	0	3	3	8	0	0	2	-2	8	681.43676	-0.00055	2101.91339	1420.47607
35	0	0	3	3	9	0	0	2	-2	9	681.45273	0.00023	2119.07105	1437.61854
36	0	0	3	3	10	0	0	2	-2	10	681.47207*	0.00251	2138.13448	1456.66492W
37	0	0	3	3	11	0	0	2	-2	11	681.49483*	0.00629	2159.10350	1477.61496W
38	0	0	3	3	12	0	0	2	-2	12	681.50975	0.00025	2181.97786	1500.46836
39	0	0	3	3	13	0	0	2	-2	13	681.53260	0.00009	2206.75735	1525.22483
40	0	0	3	3	14	0	0	2	-2	14	681.55759	-0.00005	2233.44168	1551.88404
41	0	0	3	3	15	0	0	2	-2	15	681.58575	0.00079	2262.03058	1580.44562
42	0	0	3	3	16	0	0	2	-2	16	681.61444	-0.00011	2292.52375	1610.90919
43	0	0	3	3	17	0	0	2	-2	17	681.64747	0.00097	2324.92085	1643.27435
44	0	0	3	3	18	0	0	2	-2	18	681.68047	-0.00041	2359.22154	1677.54066
45	0	0	3	3	19	0	0	2	-2	19	681.71842	0.00063	2395.42544	1713.70766
46	0	0	3	3	20	0	0	2	-2	20	681.75766	0.00034	2433.53218	1751.77486
47	0	0	3	-3	3	0	0	2	-2	4	673.76814*	0.00033	2044.71731	1370.94950
48	0	0	3	-3	4	0	0	2	-2	5	671.86969	0.00018	2052.34380	1380.47429
49	0	0	3	-3	5	0	0	2	-2	6	669.97263	-0.00038	2061.87676	1391.90376
50	0	0	3	-3	6	0	0	2	-2	7	668.07774	-0.00061	2073.31610	1405.23774
51	0	0	3	-3	7	0	0	2	-2	8	666.18524	-0.00038	2086.66169	1420.47607
52	0	0	3	-3	8	0	0	2	-2	9	664.29414*	-0.00072	2101.91340	1437.61854
53	0	0	3	-3	9	0	0	2	-2	10	662.40670	0.00054	2119.07108	1456.66492
54	0	0	3	-3	10	0	0	2	-2	11	660.51930	-0.00029	2138.13455	1477.61496
55	0	0	3	-3	11	0	0	2	-2	12	658.63416	-0.00109	2159.10361	1500.46836W
56	0	0	3	-3	12	0	0	2	-2	13	656.75364	0.00042	2181.97805	1525.22483
57	0	0	3	-3	13	0	0	2	-2	14	654.87414	0.00054	2206.75764	1551.88404
58	0	0	3	-3	14	0	0	2	-2	15	652.99646	-0.00006	2233.44214	1580.44562
59	0	0	3	-3	15	0	0	2	-2	16	651.12163	-0.00045	2262.03127	1610.90919
60	0	0	3	-3	16	0	0	2	-2	17	649.25117	0.00077	2292.52476	1643.27435
	0	0	3	-3	17	0	0	2	-2	18	647.38135	-0.00028	2324.92229	1677.54066
	0	0	3	-3	18	0	0	2	-2	19	645.51610	0.00020	2359.22356	1713.70766
	0	0	3	-3	19	0	0	2	-2	20	643.65371	0.00034	2395.42823	1751.77486
	0	0	3	-3	20	0	0	2	-2	21	641.79661	0.00242	2433.53595	1791.74175W
	0	0	3	-3	21	0	0	2	-2	22	639.94124	0.00270	2473.54635	1833.60781W
	0	0	3	-3	22	0	0	2	-2	23	638.08583	-0.00077	2515.45906	1877.37245
	0	0	3	-3	3	0	0	2	-2	2	687.10253	-0.00034	2044.71731	1357.61444
	0	0	3	-3	4	0	0	2	-2	3	689.01422	-0.00006	2052.34380	1363.32952
	0	0	3	-3	5	0	0	2	-2	4	690.92680	-0.00046	2061.87676	1370.94950

1	0	0	3	-3	6	0	0	2	-2	5	692.84138	-0.00042	2073.31610	1380.47429
2	0	0	3	-3	7	0	0	2	-2	6	694.75834	0.00041	2086.66169	1391.90376
3	0	0	3	-3	8	0	0	2	-2	7	696.67481	-0.00085	2101.91340	1405.23774
4	0	0	3	-3	9	0	0	2	-2	8	698.59351	-0.00150	2119.07108	1420.47607W
5	0	0	3	-3	10	0	0	2	-2	9	700.51530	-0.00070	2138.13455	1437.61854
6	0	0	3	-3	11	0	0	2	-2	10	702.43850	-0.00018	2159.10361	1456.66492
7	0	0	3	-3	12	0	0	2	-2	11	704.36298	-0.00011	2181.97805	1477.61496
8	0	0	3	-3	13	0	0	2	-2	12	706.28971	0.00043	2206.75764	1500.46836
9	0	0	3	-3	14	0	0	2	-2	13	708.22083*	0.00352	2233.44214	1525.22483W
10	0	0	3	-3	15	0	0	2	-2	14	710.14478*	-0.00245	2262.03127	1551.88404W
11	0	0	3	-3	16	0	0	2	-2	15	712.07947	0.00033	2292.52476	1580.44562
12	0	0	3	-3	17	0	0	2	-2	16	714.01396	0.00086	2324.92229	1610.90919
13	0	0	3	-3	18	0	0	2	-2	17	715.94880	-0.00041	2359.22356	1643.27435
14	0	0	3	-3	19	0	0	2	-2	18	717.88705	-0.00052	2395.42823	1677.54066
15	0	0	3	-3	20	0	0	2	-2	19	719.83539*	0.00710	2433.53595	1713.70766W
16	0	0	3	-3	21	0	0	2	-2	20	721.77037	-0.00112	2473.54635	1751.77486W
17	0	0	3	-3	22	0	0	2	-2	21	723.71742	0.00012	2515.45906	1791.74175
18	0	0	3	-3	3	0	0	2	2	3	681.38946	0.00175	2044.71731	1363.32960W
19	0	0	3	-3	4	0	0	2	2	4	681.39407	0.00001	2052.34380	1370.94974
20	0	0	3	-3	5	0	0	2	2	5	681.40217	0.00025	2061.87676	1380.47484
21	0	0	3	-3	6	0	0	2	2	6	681.41152	0.00028	2073.31610	1391.90486
22	0	0	3	-3	7	0	0	2	2	7	681.42341	0.00145	2086.66169	1405.23972W
23	0	0	3	-3	8	0	0	2	2	8	681.43351	-0.00051	2101.91340	1420.47938
24	0	0	3	-3	9	0	0	2	2	9	681.44753	0.00019	2119.07108	1437.62374
25	0	0	3	-3	10	0	0	2	2	10	681.46088	-0.00095	2138.13455	1456.67272
26	0	0	3	-3	11	0	0	2	2	11	681.47825	0.00086	2159.10361	1477.62621
27	0	0	3	-3	12	0	0	2	2	12	681.49481	0.00088	2181.97805	1500.48412
28	0	0	3	-3	13	0	0	2	2	13	681.50975	-0.00156	2206.75764	1525.24633W
29	0	0	3	-3	14	0	0	2	2	14	681.54379*	0.01435	2233.44214	1551.91270W
30	0	0	3	-3	15	0	0	2	2	15	681.54379	-0.00439	2262.03127	1580.48310W
31	0	0	3	-3	16	0	0	2	2	16	681.56657	-0.00082	2292.52476	1610.95737
32	0	0	3	-3	17	0	0	2	2	17	681.58594	-0.00099	2324.92229	1643.33536
33	0	0	3	-3	18	0	0	2	2	18	681.60588	-0.00079	2359.22356	1677.61689
34	0	0	3	-3	19	0	0	2	2	19	681.62608	-0.00037	2395.42823	1713.80178
35	0	0	3	-3	20	0	0	2	2	20	681.64687	0.00075	2433.53595	1751.88982
36	0	0	3	-3	21	0	0	2	2	21	681.66552	-0.00002	2473.54635	1791.88081

rms = 0.00050 cm⁻¹

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

ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	G'	G''
2	0	0	0	0	0	0	0	0	1	1014.95064	-0.00009	1016.85139	1.90066
2	0	0	0	1	0	0	0	0	2	1013.05955	0.00000	1018.76149	5.70195
2	0	0	0	2	0	0	0	0	3	1011.17772	-0.00005	1022.58159	11.40382
2	0	0	0	3	0	0	0	0	4	1009.30522	-0.00002	1028.31143	19.00619
2	0	0	0	4	0	0	0	0	5	1007.44172	0.00005	1035.95064	28.50898
2	0	0	0	5	0	0	0	0	6	1005.58679	0.00008	1045.49875	39.91204
2	0	0	0	6	0	0	0	0	7	1003.73994	0.00003	1056.95515	53.21523
2	0	0	0	7	0	0	0	0	8	1001.90072	0.00001	1070.31910	68.41838
2	0	0	0	8	0	0	0	0	9	1000.06851	0.00003	1085.58977	85.52129
2	0	0	0	9	0	0	0	0	10	998.24280	0.00031	1102.76621	104.52373
2	0	0	0	10	0	0	0	0	11	996.42216	0.00021	1121.84738	125.42544
2	0	0	0	11	0	0	0	0	12	994.60618	0.00017	1142.83216	148.22616
2	0	0	0	12	0	0	0	0	13	992.79391	0.00013	1165.71936	172.92558
2	0	0	0	13	0	0	0	0	14	990.98449	0.00013	1190.50774	199.52337
2	0	0	0	14	0	0	0	0	15	989.17702	0.00016	1217.19606	228.01920
2	0	0	0	15	0	0	0	0	16	987.37061	0.00021	1245.78308	258.41268
2	0	0	0	16	0	0	0	0	17	985.56430	0.00010	1276.26760	290.70340
2	0	0	0	17	0	0	0	0	18	983.75762	0.00009	1308.64848	324.89096
2	0	0	0	18	0	0	0	0	19	981.94966	-0.00011	1342.92466	360.97488
2	0	0	0	19	0	0	0	0	20	980.14040	-0.00003	1379.09514	398.95471
2	0	0	0	20	0	0	0	0	21	978.32912	0.00000	1417.15906	438.82993
2	0	0	0	21	0	0	0	0	22	976.51556	-0.00001	1457.11560	480.60003
2	0	0	0	22	0	0	0	0	23	974.69952	-0.00010	1498.96407	524.26445
2	0	0	0	23	0	0	0	0	24	972.88348	-0.00002	1542.70381	569.82262

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

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2	0	0	0	24	0	0	0	0	25	971.06028	-0.00002	1588.33424	617.27393
2	0	0	0	25	0	0	0	0	26	969.23719	0.00016	1635.85480	666.61777
2	0	0	0	26	0	0	0	0	27	967.41125	-0.00025	1685.26498	717.85348
2	0	0	0	27	0	0	0	0	28	965.58351	-0.00036	1736.56425	770.98038
2	0	0	0	28	0	0	0	0	29	963.75380	-0.00052	1789.75210	825.99778
2	0	0	0	29	0	0	0	0	30	961.92265	-0.00040	1844.82800	882.90495
2	0	0	0	30	0	0	0	0	31	960.08999	-0.00026	1901.79140	941.70115
2	0	0	0	31	0	0	0	0	32	958.25579	-0.00033	1960.64171	1002.38559
2	0	0	0	32	0	0	0	0	33	956.42068	-0.00018	2021.37834	1064.95747
2	0	0	0	33	0	0	0	0	34	954.58446	-0.00020	2084.00064	1129.41599
2	0	0	0	34	0	0	0	0	35	952.74752	-0.00015	2148.50794	1195.76027
2	0	0	0	35	0	0	0	0	36	950.90981	-0.00027	2214.89954	1263.98946
2	0	0	0	36	0	0	0	0	37	949.07194	-0.00009	2283.17467	1334.10264
2	0	0	0	37	0	0	0	0	38	947.23364	-0.00001	2353.33256	1406.09891
2	0	0	0	38	0	0	0	0	39	945.39512	0.00004	2425.37239	1479.97730
2	0	0	0	39	0	0	0	0	40	943.55685	0.00041	2499.29329	1555.73685
2	0	0	0	40	0	0	0	0	41	941.71777	-0.00005	2575.09439	1633.37656
2	0	0	0	41	0	0	0	0	42	939.88513*	0.00580	2652.77474	1712.89541W
2	0	0	0	42	0	0	0	0	43	938.04133	0.00028	2732.33340	1794.29235
2	0	0	0	43	0	0	0	0	44	936.20304	-0.00002	2813.76936	1877.56630
2	0	0	0	44	0	0	0	0	45	934.36608	0.00066	2897.08160	1962.71617
2	0	0	0	45	0	0	0	0	46	932.53120	0.00299	2982.26906	2049.74085W
2	0	0	0	2	0	0	0	0	1	1020.68108	0.00015	1022.58159	1.90066
2	0	0	0	3	0	0	0	0	2	1022.60944	-0.00004	1028.31143	5.70195
2	0	0	0	4	0	0	0	0	3	1024.54690	0.00007	1035.95064	11.40382
2	0	0	0	5	0	0	0	0	4	1026.49270	0.00014	1045.49875	19.00619
2	0	0	0	6	0	0	0	0	5	1028.44637	0.00020	1056.95515	28.50898
2	0	0	0	7	0	0	0	0	6	1030.40720	0.00014	1070.31910	39.91204
2	0	0	0	8	0	0	0	0	7	1032.37473	0.00020	1085.58977	53.21523
2	0	0	0	9	0	0	0	0	8	1034.34795	0.00012	1102.76621	68.41838
2	0	0	0	10	0	0	0	0	9	1036.32623	0.00014	1121.84738	85.52129
2	0	0	0	11	0	0	0	0	10	1038.30866	0.00022	1142.83216	104.52373
2	0	0	0	12	0	0	0	0	11	1040.29420	0.00028	1165.71936	125.42544
2	0	0	0	13	0	0	0	0	12	1042.28196	0.00038	1190.50774	148.22616
2	0	0	0	14	0	0	0	0	13	1044.27080	0.00032	1217.19606	172.92558
2	0	0	0	15	0	0	0	0	14	1046.25993	0.00022	1245.78308	199.52337
2	0	0	0	16	0	0	0	0	15	1048.24852	0.00012	1276.26760	228.01920
2	0	0	0	17	0	0	0	0	16	1050.23602	0.00021	1308.64848	258.41268
2	0	0	0	18	0	0	0	0	17	1052.22152	0.00027	1342.92466	290.70340
2	0	0	0	19	0	0	0	0	18	1054.20429	0.00010	1379.09514	324.89096
2	0	0	0	20	0	0	0	0	19	1056.18417	0.00000	1417.15906	360.97488
2	0	0	0	21	0	0	0	0	20	1058.16114	0.00025	1457.11560	398.95471
2	0	0	0	22	0	0	0	0	21	1060.13404	-0.00009	1498.96407	438.82993
2	0	0	0	23	0	0	0	0	22	1062.10358	-0.00020	1542.70381	480.60003
2	0	0	0	24	0	0	0	0	23	1064.06961	-0.00018	1588.33424	524.26445
2	0	0	0	25	0	0	0	0	24	1066.03212	-0.00006	1635.85480	569.82262
2	0	0	0	26	0	0	0	0	25	1067.99088	-0.00017	1685.26498	617.27393
2	0	0	0	27	0	0	0	0	26	1069.94582	-0.00066	1736.56425	666.61777
2	0	0	0	28	0	0	0	0	27	1071.89838	-0.00025	1789.75210	717.85348
2	0	0	0	29	0	0	0	0	28	1073.84704	-0.00058	1844.82800	770.98038
2	0	0	0	30	0	0	0	0	29	1075.79317	-0.00044	1901.79140	825.99778
2	0	0	0	31	0	0	0	0	30	1077.73644	-0.00032	1960.64171	882.90495
2	0	0	0	32	0	0	0	0	31	1079.67657	-0.00062	2021.37834	941.70115
2	0	0	0	33	0	0	0	0	32	1081.61455	-0.00051	2084.00064	1002.38559
2	0	0	0	34	0	0	0	0	33	1083.54990	-0.00057	2148.50794	1064.95747
2	0	0	0	35	0	0	0	0	34	1085.48315	-0.00040	2214.89954	1129.41599
2	0	0	0	36	0	0	0	0	35	1087.41405	-0.00035	2283.17467	1195.76027
2	0	0	0	37	0	0	0	0	36	1089.34285	-0.00025	2353.33256	1263.98946
2	0	0	0	38	0	0	0	0	37	1091.26948	-0.00026	2425.37239	1334.10264
2	0	0	0	39	0	0	0	0	38	1093.19386	-0.00052	2499.29329	1406.09891
2	0	0	0	40	0	0	0	0	39	1095.11634	-0.00074	2575.09439	1479.97730
2	0	0	0	41	0	0	0	0	40	1097.03853	0.00064	2652.77474	1555.73685
2	0	0	0	42	0	0	0	0	41	1098.95694	0.00011	2732.33340	1633.37656
2	0	0	0	43	0	0	0	0	42	1100.87428	0.00033	2813.76936	1712.89541
2	0	0	0	44	0	0	0	0	43	1102.78977	0.00052	2897.08160	1794.29235
2	0	0	0	45	0	0	0	0	44	1104.70240	-0.00036	2982.26906	1877.56630
2	0	0	0	46	0	0	0	0	45	1106.61590	0.00142	3069.33065	1962.71617W

rms = 0.00029 cm⁻¹URL: <http://mc.manuscriptcentral.com/tandf/tpmh>

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

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
2 2 0 0 4	0 0 0 0 5	1011.84070	0.00125	1040.34843	28.50898W
2 2 0 0 5	0 0 0 0 6	1009.98613	0.00085	1049.89732	39.91204
2 2 0 0 6	0 0 0 0 7	1008.14179	0.00027	1061.35675	53.21523
2 2 0 0 7	0 0 0 0 8	1006.30948*	0.00075	1074.72712	68.41838
2 2 0 0 8	0 0 0 0 9	1004.48717	-0.00043	1090.00889	85.52129
2 2 0 0 9	0 0 0 0 10	1002.67870	-0.00017	1107.20259	104.52373
2 2 0 0 10	0 0 0 0 11	1000.88355	0.00020	1126.30879	125.42544
2 2 0 0 11	0 0 0 0 12	999.10163	-0.00029	1147.32807	148.22616
2 2 0 0 12	0 0 0 0 13	997.33532	-0.00016	1170.26105	172.92558
2 2 0 0 13	0 0 0 0 14	995.58494	-0.00001	1195.10832	199.52337
2 2 0 0 14	0 0 0 0 15	993.85106	-0.00017	1221.87043	228.01920
2 2 0 0 15	0 0 0 0 16	992.13527	0.00006	1250.54788	258.41268
2 2 0 0 16	0 0 0 0 17	990.43777	0.00009	1281.14108	290.70340
2 2 0 0 17	0 0 0 0 18	988.75982	0.00046	1313.65031	324.89096
2 2 0 0 18	0 0 0 0 19	987.10115	0.00028	1348.07575	360.97488
2 2 0 0 19	0 0 0 0 20	985.46305	0.00034	1384.41742	398.95471
2 2 0 0 20	0 0 0 0 21	983.84565	0.00040	1422.67519	438.82993
2 2 0 0 21	0 0 0 0 22	982.24832	-0.00044	1462.84880	480.60003
2 2 0 0 22	0 0 0 0 23	980.67281	-0.00058	1504.93784	524.26445
2 2 0 0 23	0 0 0 0 24	979.11961	0.00042	1548.94181	569.82262
2 2 0 0 24	0 0 0 0 25	977.58570	-0.00043	1594.86006	617.27393
2 2 0 0 25	0 0 0 0 26	976.07411	0.00000	1642.69188	666.61777
2 2 0 0 26	0 0 0 0 27	974.58301	0.00003	1692.43646	717.85348
2 2 0 0 27	0 0 0 0 28	973.11271	0.00015	1744.09294	770.98038
2 2 0 0 28	0 0 0 0 29	971.66292	0.00028	1797.66042	825.99778
2 2 0 0 29	0 0 0 0 30	970.23345	0.00047	1853.13793	882.90495
2 2 0 0 30	0 0 0 0 31	968.82343	0.00007	1910.52450	941.70115
2 2 0 0 31	0 0 0 0 32	967.43362	0.00010	1969.81911	1002.38559
2 2 0 0 32	0 0 0 0 33	966.06334	0.00009	2031.02072	1064.95747
2 2 0 0 33	0 0 0 0 34	964.71256	0.00026	2094.12829	1129.41599
2 2 0 0 34	0 0 0 0 35	963.38038	-0.00008	2159.14073	1195.76027
2 2 0 0 35	0 0 0 0 36	962.06756	0.00005	2226.05697	1263.98946
2 2 0 0 36	0 0 0 0 37	960.77329	0.00005	2294.87589	1334.10264
2 2 0 0 37	0 0 0 0 38	959.49718	-0.00029	2365.59637	1406.09891
2 2 0 0 38	0 0 0 0 39	958.24022	0.00023	2438.21729	1479.97730
2 2 0 0 39	0 0 0 0 40	957.00093	0.00030	2512.73749	1555.73685
2 2 0 0 40	0 0 0 0 41	955.77920	-0.00002	2589.15579	1633.37656
2 2 0 0 41	0 0 0 0 42	954.57530	-0.00030	2667.47101	1712.89541
2 2 0 0 42	0 0 0 0 43	953.38905	-0.00055	2747.68195	1794.29235
2 2 0 0 43	0 0 0 0 44	952.22138	0.00031	2829.78737	1877.56630
2 2 0 0 44	0 0 0 0 45	951.06985	-0.00001	2913.78604	1962.71617
2 2 0 0 6	0 0 0 0 5	1032.84777	-0.00001	1061.35675	28.50898
2 2 0 0 7	0 0 0 0 6	1034.81563	0.00055	1074.72712	39.91204
2 2 0 0 8	0 0 0 0 7	1036.79385	0.00019	1090.00889	53.21523
2 2 0 0 9	0 0 0 0 8	1038.78446	0.00025	1107.20259	68.41838
2 2 0 0 10	0 0 0 0 9	1040.78768	0.00018	1126.30879	85.52129
2 2 0 0 11	0 0 0 0 10	1042.80457	0.00022	1147.32807	104.52373
2 2 0 0 12	0 0 0 0 11	1044.83550	-0.00012	1170.26105	125.42544
2 2 0 0 13	0 0 0 0 12	1046.88225	0.00008	1195.10832	148.22616
2 2 0 0 14	0 0 0 0 13	1048.94498	0.00012	1221.87043	172.92558
2 2 0 0 15	0 0 0 0 14	1051.02458	0.00007	1250.54788	199.52337
2 2 0 0 16	0 0 0 0 15	1053.12191	0.00003	1281.14108	228.01920
2 2 0 0 17	0 0 0 0 16	1055.23418*	-0.00346	1313.65031	258.41268W
2 2 0 0 18	0 0 0 0 17	1057.37223	-0.00012	1348.07575	290.70340
2 2 0 0 19	0 0 0 0 18	1059.52716	0.00070	1384.41742	324.89096
2 2 0 0 20	0 0 0 0 19	1061.70035	0.00005	1422.67519	360.97488
2 2 0 0 21	0 0 0 0 20	1063.89425	0.00016	1462.84880	398.95471
2 2 0 0 22	0 0 0 0 21	1066.10757	-0.00034	1504.93784	438.82993
2 2 0 0 23	0 0 0 0 22	1068.34242	0.00064	1548.94181	480.60003
2 2 0 0 24	0 0 0 0 23	1070.59628	0.00067	1594.86006	524.26445
2 2 0 0 25	0 0 0 0 24	1072.86948	0.00022	1642.69188	569.82262

2	2	0	0	26	0	0	0	0	25	1075.16261	0.00009	1692.43646	617.27393
2	2	0	0	27	0	0	0	0	26	1077.47517	0.00000	1744.09294	666.61777
2	2	0	0	28	0	0	0	0	27	1079.80698	0.00004	1797.66042	717.85348
2	2	0	0	29	0	0	0	0	28	1082.15743	-0.00012	1853.13793	770.98038
2	2	0	0	30	0	0	0	0	29	1084.52684	0.00012	1910.52450	825.99778
2	2	0	0	31	0	0	0	0	30	1086.91425	0.00009	1969.81911	882.90495
2	2	0	0	32	0	0	0	0	31	1089.31951	-0.00007	2031.02072	941.70115
2	2	0	0	33	0	0	0	0	32	1091.74278	0.00008	2094.12829	1002.38559
2	2	0	0	34	0	0	0	0	33	1094.18321	-0.00005	2159.14073	1064.95747
2	2	0	0	35	0	0	0	0	34	1096.64064	-0.00034	2226.05697	1129.41599
2	2	0	0	36	0	0	0	0	35	1099.11512	-0.00050	2294.87589	1195.76027
2	2	0	0	37	0	0	0	0	36	1101.60630	-0.00062	2365.59637	1263.98946
2	2	0	0	38	0	0	0	0	37	1104.11531	0.00066	2438.21729	1334.10264
2	2	0	0	39	0	0	0	0	38	1106.63800	-0.00058	2512.73749	1406.09891
2	2	0	0	40	0	0	0	0	39	1109.17904	0.00055	2589.15579	1479.97730
2	2	0	0	41	0	0	0	0	40	1111.73443	0.00027	2667.47101	1555.73685
2	2	0	0	42	0	0	0	0	41	1114.30474	-0.00064	2747.68195	1633.37656
2	2	0	0	43	0	0	0	0	42	1116.88732*	-0.00464	2829.78737	1712.89541W
2	2	0	0	44	0	0	0	0	43	1119.49357	-0.00012	2913.78604	1794.29235
2	2	0	0	45	0	0	0	0	44	1122.11001	-0.00037	2999.67668	1877.56630

rms = 0.00033 cm⁻¹

$V_4 + V_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 1 -1 0	0 0 0 0 1	1185.51213	0.00022	1187.41257	1.90066
1 1 1 -1 1	0 0 0 0 2	1183.61842	0.00033	1189.32003	5.70195
1 1 1 -1 2	0 0 0 0 3	1181.73117	-0.00003	1193.13502	11.40382
1 1 1 -1 3	0 0 0 0 4	1179.85142	-0.00003	1198.85764	19.00619
1 1 1 -1 4	0 0 0 0 5	1177.97912	0.00002	1206.48808	28.50898
1 1 1 -1 5	0 0 0 0 6	1176.11434	-0.00017	1216.02655	39.91204
1 1 1 -1 6	0 0 0 0 7	1174.25812	0.00002	1227.47333	53.21523
1 1 1 -1 7	0 0 0 0 8	1172.41048	0.00009	1240.82878	68.41838
1 1 1 -1 8	0 0 0 0 9	1170.57203	0.00006	1256.09326	85.52129
1 1 1 -1 9	0 0 0 0 10	1168.74345	-0.00003	1273.26720	104.52373
1 1 1 -1 10	0 0 0 0 11	1166.92554	-0.00009	1292.35106	125.42544
1 1 1 -1 11	0 0 0 0 12	1165.11899	-0.00017	1313.34532	148.22616
1 1 1 -1 12	0 0 0 0 13	1163.32481	-0.00005	1336.25044	172.92558
1 1 1 -1 13	0 0 0 0 14	1161.54358	0.00007	1361.06689	199.52337
1 1 1 -1 14	0 0 0 0 15	1159.77567	-0.00022	1387.79509	228.01920
1 1 1 -1 15	0 0 0 0 16	1158.02251	-0.00022	1416.43541	258.41268
1 1 1 -1 16	0 0 0 0 17	1156.28466	-0.00006	1446.98812	290.70340
1 1 1 -1 17	0 0 0 0 18	1154.56247	0.00001	1479.45342	324.89096
1 1 1 -1 18	0 0 0 0 19	1152.85647	-0.00003	1513.83138	360.97488
1 1 1 -1 19	0 0 0 0 20	1151.16734	0.00010	1550.12195	398.95471
1 1 1 -1 20	0 0 0 0 21	1149.49480	-0.00023	1588.32496	438.82993
1 1 1 -1 21	0 0 0 0 22	1147.84009	0.00001	1628.44012	480.60003
1 1 1 -1 22	0 0 0 0 23	1146.20226	-0.00030	1670.46701	524.26445
1 1 1 -1 23	0 0 0 0 24	1144.58234	-0.00017	1714.40513	569.82262
1 1 1 -1 24	0 0 0 0 25	1142.97985	-0.00008	1760.25386	617.27393
1 1 1 -1 25	0 0 0 0 26	1141.39431	-0.00044	1808.01252	666.61777
1 1 1 -1 26	0 0 0 0 27	1139.82687	-0.00001	1857.68035	717.85348
1 1 1 -1 27	0 0 0 0 28	1138.27607	-0.00009	1909.25654	770.98038
1 1 1 -1 28	0 0 0 0 29	1136.74231	-0.00014	1962.74023	825.99778
1 1 1 -1 29	0 0 0 0 30	1135.22525	-0.00031	2018.13051	882.90495
1 1 1 -1 30	0 0 0 0 31	1133.72499	-0.00032	2075.42646	941.70115
1 1 1 -1 31	0 0 0 0 32	1132.24178	0.00026	2134.62711	1002.38559
1 1 1 -1 32	0 0 0 0 33	1130.77404	0.00004	2195.73148	1064.95747
1 1 1 -1 33	0 0 0 0 34	1129.32288	0.00030	2258.73857	1129.41599
1 1 1 -1 34	0 0 0 0 35	1127.88740	0.00032	2323.64735	1195.76027
1 1 1 -1 35	0 0 0 0 36	1126.46740	0.00007	2390.45679	1263.98946
1 1 1 -1 36	0 0 0 0 37	1125.06411	0.00094	2459.16581	1334.10264
1 1 1 -1 37	0 0 0 0 38	1123.67532	0.00087	2529.77336	1406.09891
1 1 1 -1 38	0 0 0 0 39	1122.30181	0.00079	2602.27832	1479.97730
1 1 1 -1 39	0 0 0 0 40	1120.94250	0.00066	2676.67960	1555.73685

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

1	1	1	-1	40	0	0	0	0	41	1119.59952	0.00003	2752.97605	1633.37656
2	1	1	1	-1	41	0	0	0	0	42	1118.27126	0.00013	2831.16654
3	1	1	1	-1	42	0	0	0	0	43	1116.95795	0.00041	2911.24989
4	1	1	1	-1	43	0	0	0	0	44	1115.65947	0.00086	2993.22491
5	1	1	1	-1	44	0	0	0	0	45	1114.37574	0.00151	3077.09040
6	1	1	1	-1	1	0	0	0	0	0	1189.32044	0.00041	1189.32003
7	1	1	1	-1	2	0	0	0	0	1	1191.23453	0.00017	1193.13502
8	1	1	1	-1	3	0	0	0	0	2	1193.15567	-0.00003	1198.85764
9	1	1	1	-1	4	0	0	0	0	3	1195.08430	0.00004	1206.48808
10	1	1	1	-1	5	0	0	0	0	4	1197.02046	0.00011	1216.02655
11	1	1	1	-1	6	0	0	0	0	5	1198.96433	-0.00003	1227.47333
12	1	1	1	-1	7	0	0	0	0	6	1200.91675	0.00001	1240.82878
13	1	1	1	-1	8	0	0	0	0	7	1202.87813	0.00011	1256.09326
14	1	1	1	-1	9	0	0	0	0	8	1204.84879	-0.00003	1273.26720
15	1	1	1	-1	10	0	0	0	0	9	1206.82982	0.00005	1292.35106
16	1	1	1	-1	11	0	0	0	0	10	1208.82154	-0.00005	1313.34532
17	1	1	1	-1	12	0	0	0	0	11	1210.82491	-0.00009	1336.25044
18	1	1	1	-1	13	0	0	0	0	12	1212.84077	0.00004	1361.06689
19	1	1	1	-1	14	0	0	0	0	13	1214.86958	0.00007	1387.79509
20	1	1	1	-1	15	0	0	0	0	14	1216.91215	0.00012	1416.43541
21	1	1	1	-1	16	0	0	0	0	15	1218.96910	0.00018	1446.98812
22	1	1	1	-1	17	0	0	0	0	16	1221.04094	0.00020	1479.45342
23	1	1	1	-1	18	0	0	0	0	17	1223.12818	0.00020	1513.83138
24	1	1	1	-1	19	0	0	0	0	18	1225.23098	-0.00001	1550.12195
25	1	1	1	-1	20	0	0	0	0	19	1227.35000	-0.00008	1588.32496
26	1	1	1	-1	21	0	0	0	0	20	1229.48542	0.00001	1628.44012
27	1	1	1	-1	22	0	0	0	0	21	1231.63725	0.00017	1670.46701
28	1	1	1	-1	23	0	0	0	0	22	1233.80513	0.00003	1714.40513
29	1	1	1	-1	24	0	0	0	0	23	1235.98933	-0.00008	1760.25386
30	1	1	1	-1	25	0	0	0	0	24	1238.19011	0.00021	1808.01252
31	1	1	1	-1	26	0	0	0	0	25	1240.40632	-0.00010	1857.68035
32	1	1	1	-1	27	0	0	0	0	26	1242.63840	-0.00037	1909.25654
33	1	1	1	-1	28	0	0	0	0	27	1244.88670	-0.00005	1962.74023
34	1	1	1	-1	29	0	0	0	0	28	1247.15022	0.00009	2018.13051
35	1	1	1	-1	30	0	0	0	0	29	1249.42868	0.00001	2075.42646
36	1	1	1	-1	31	0	0	0	0	30	1251.72215	0.00000	2134.62711
37	1	1	1	-1	32	0	0	0	0	31	1254.03032	-0.00001	2195.73148
38	1	1	1	-1	33	0	0	0	0	32	1256.35294	-0.00004	2258.73857
39	1	1	1	-1	34	0	0	0	0	33	1258.69014	0.00026	2323.64735
40	1	1	1	-1	35	0	0	0	0	34	1261.04111	0.00031	2390.45679
41	1	1	1	-1	36	0	0	0	0	35	1263.40583	0.00029	2459.16581
42	1	1	1	-1	37	0	0	0	0	36	1265.78424	0.00034	2529.77336
43	1	1	1	-1	38	0	0	0	0	37	1268.17646	0.00078	2602.27832
44	1	1	1	-1	39	0	0	0	0	38	1270.58116	0.00047	2676.67960
45	1	1	1	-1	40	0	0	0	0	39	1272.99678	-0.00197	2752.97605
46	1	1	1	-1	41	0	0	0	0	40	1275.43031	0.00062	2831.16654
47	1	1	1	-1	42	0	0	0	0	41	1277.87460	0.00128	2911.24989
48	1	1	1	-1	43	0	0	0	0	42	1280.32862	-0.00088	2993.22491
49	1	1	1	-1	44	0	0	0	0	43	1282.79846	0.00041	3077.09040

rms = 0.00030 cm⁻¹

50
51
52 $v_4 + v_5 (\Delta) \leftarrow G.S. (\Sigma^+)$
53

	v_4'	ι_4'	v_5'	ι_5'	J'	v_4''	ι_4''	v_5''	ι_5''	J''	OBS	OBS – CALC	G'	G''
54														
55														
56	1	1	1	1	6	0	0	0	0	7	1170.29616	-0.00035	1223.51174	53.21523
57	1	1	1	1	7	0	0	0	0	8	1168.43966	-0.00020	1236.85825	68.41838
58	1	1	1	1	8	0	0	0	0	9	1166.58850	0.00055	1252.10924	85.52129
59	1	1	1	1	9	0	0	0	0	10	1164.73993	-0.00022	1269.26388	104.52373
60	1	1	1	1	10	0	0	0	0	11	1162.89583	0.00004	1288.32123	125.42544
	1	1	1	1	11	0	0	0	0	12	1161.05463	0.00048	1309.28031	148.22616
	1	1	1	1	12	0	0	0	0	13	1159.21449	0.00001	1332.14005	172.92558
	1	1	1	1	13	0	0	0	0	14	1157.37638	0.00037	1356.89938	199.52337
	1	1	1	1	14	0	0	0	0	15	1155.53816	0.00016	1383.55720	228.01920
	1	1	1	1	15	0	0	0	0	16	1153.70007	0.00034	1412.11241	258.41268
	1	1	1	1	16	0	0	0	0	17	1151.86192	0.00042	1442.56394	290.70340

1	1	1	1	17	0	0	0	0	18	1150.02019	0.00036	1474.91078	324.89096
2	1	1	1	18	0	0	0	0	19	1148.17745	0.00037	1509.15197	360.97488
3	1	1	1	19	0	0	0	0	20	1146.33123	-0.00067	1545.28661	398.95471
4	1	1	1	20	0	0	0	0	21	1144.48487	0.00092	1583.31388	438.82993
5	1	1	1	21	0	0	0	0	22	1142.63326	0.00025	1623.23305	480.60003
6	1	1	1	22	0	0	0	0	23	1140.77922	0.00026	1665.04341	524.26445
7	1	1	1	23	0	0	0	0	24	1138.92225	0.00052	1708.74434	569.82262
8	1	1	1	24	0	0	0	0	25	1137.06170	0.00037	1754.33526	617.27393
9	1	1	1	25	0	0	0	0	26	1135.19802	0.00020	1801.81559	666.61777
10	1	1	1	26	0	0	0	0	27	1133.33156	0.00024	1851.18480	717.85348
11	1	1	1	27	0	0	0	0	28	1131.46244	0.00049	1902.44233	770.98038
12	1	1	1	28	0	0	0	0	29	1129.58999	0.00011	1955.58766	825.99778
13	1	1	1	29	0	0	0	0	30	1127.71559	0.00033	2010.62021	882.90495
14	1	1	1	30	0	0	0	0	31	1125.83864	0.00037	2067.53942	941.70115
15	1	1	1	31	0	0	0	0	32	1123.95906	-0.00003	2126.34468	1002.38559
16	1	1	1	32	0	0	0	0	33	1122.07829	0.00041	2187.03535	1064.95747
17	1	1	1	33	0	0	0	0	34	1120.19475	-0.00006	2249.61079	1129.41599
18	1	1	1	34	0	0	0	0	35	1118.31011	0.00008	2314.07030	1195.76027
19	1	1	1	35	0	0	0	0	36	1116.42379	0.00010	2380.41315	1263.98946
20	1	1	1	36	0	0	0	0	37	1114.53577	-0.00017	2448.63858	1334.10264
21	1	1	1	37	0	0	0	0	38	1112.64683	-0.00006	2518.74579	1406.09891
22	1	1	1	38	0	0	0	0	39	1110.75642	-0.00024	2590.73397	1479.97730
23	1	1	1	39	0	0	0	0	40	1108.86543	0.00005	2664.60223	1555.73685
24	1	1	1	40	0	0	0	0	41	1106.97268	-0.00046	2740.34970	1633.37656
25	1	1	1	7	0	0	0	0	6	1196.94618	-0.00003	1236.85825	39.91204
26	1	1	1	8	0	0	0	0	7	1198.89416	0.00015	1252.10924	53.21523
27	1	1	1	9	0	0	0	0	8	1200.84581	0.00032	1269.26388	68.41838
28	1	1	1	10	0	0	0	0	9	1202.80035	0.00041	1288.32123	85.52129
29	1	1	1	11	0	0	0	0	10	1204.75708	0.00050	1309.28031	104.52373
30	1	1	1	12	0	0	0	0	11	1206.71499	0.00038	1332.14005	125.42544
31	1	1	1	13	0	0	0	0	12	1208.67363	0.00040	1356.89938	148.22616
32	1	1	1	14	0	0	0	0	13	1210.63185	0.00023	1383.55720	172.92558
33	1	1	1	15	0	0	0	0	14	1212.58938	0.00034	1412.11241	199.52337
34	1	1	1	16	0	0	0	0	15	1214.54522	0.00048	1442.56394	228.01920
35	1	1	1	17	0	0	0	0	16	1216.49862	0.00051	1474.91078	258.41268
36	1	1	1	18	0	0	0	0	17	1218.44884	0.00028	1509.15197	290.70340
37	1	1	1	20	0	0	0	0	19	1222.33967	0.00067	1583.31388	360.97488
38	1	1	1	21	0	0	0	0	20	1224.27856	0.00022	1623.23305	398.95471
39	1	1	1	22	0	0	0	0	21	1226.21418	0.00070	1665.04341	438.82993
40	1	1	1	23	0	0	0	0	22	1228.14468	0.00037	1708.74434	480.60003
41	1	1	1	24	0	0	0	0	23	1230.07122	0.00041	1754.33526	524.26445
42	1	1	1	25	0	0	0	0	24	1231.99321	0.00024	1801.81559	569.82262
43	1	1	1	26	0	0	0	0	25	1233.91177	0.00091	1851.18480	617.27393
44	1	1	1	27	0	0	0	0	26	1235.82487	0.00031	1902.44233	666.61777
45	1	1	1	28	0	0	0	0	27	1237.73446	0.00028	1955.58766	717.85348
46	1	1	1	29	0	0	0	0	28	1239.64011	0.00028	2010.62021	770.98038
47	1	1	1	30	0	0	0	0	29	1241.54181	0.00017	2067.53942	825.99778
48	1	1	1	31	0	0	0	0	30	1243.43989	0.00017	2126.34468	882.90495
49	1	1	1	32	0	0	0	0	31	1245.33423	0.00002	2187.03535	941.70115
50	1	1	1	33	0	0	0	0	32	1247.22509	-0.00012	2249.61079	1002.38559
51	1	1	1	34	0	0	0	0	33	1249.11274	-0.00009	2314.07030	1064.95747
52	1	1	1	35	0	0	0	0	34	1250.99813	0.00097	2380.41315	1129.41599
53	1	1	1	36	0	0	0	0	35	1252.87806	-0.00025	2448.63858	1195.76027
54	1	1	1	37	0	0	0	0	36	1254.75606	-0.00028	2518.74579	1263.98946
55	1	1	1	38	0	0	0	0	37	1256.63114	-0.00018	2590.73397	1334.10264
56	1	1	1	39	0	0	0	0	38	1258.50287	-0.00046	2664.60223	1406.09891
57	1	1	1	40	0	0	0	0	39	1260.37274	0.00034	2740.34970	1479.97730
58	1	1	1	41	0	0	0	0	40	1262.23841	-0.00017	2817.97543	1555.73685
59	1	1	1	42	0	0	0	0	41	1264.10215	0.00024	2897.47848	1633.37656

rms = 0.00037 cm⁻¹

$$2\nu_5(\Sigma^+) \leftarrow G.S.(\Sigma^+)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
0 0 2 0 0	0 0 0 0 0	1150.02019	0.00036	35.30850	1.90066

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60	0	0	2	0	1	0	0	0	0	2	1331.51278	0.00025	1337.21447	5.70195
	0	0	2	0	2	0	0	0	0	3	1329.62264	0.00008	1341.02637	11.40382
	0	0	2	0	3	0	0	0	0	4	1327.73822	0.00029	1346.74412	19.00619
	0	0	2	0	4	0	0	0	0	5	1325.85876	0.00014	1354.36759	28.50898
	0	0	2	0	5	0	0	0	0	6	1323.98154*	-0.00304	1363.89662	39.91204W
	0	0	2	0	6	0	0	0	0	7	1322.11586	0.00010	1375.33100	53.21523
	0	0	2	0	7	0	0	0	0	8	1320.25209	0.00000	1388.67047	68.41838
	0	0	2	0	8	0	0	0	0	9	1318.39348	0.00001	1403.91476	85.52129
	0	0	2	0	9	0	0	0	0	10	1316.53975	-0.00005	1421.06352	104.52373
	0	0	2	0	10	0	0	0	0	11	1314.69130	0.00035	1440.11639	125.42544
	0	0	2	0	11	0	0	0	0	12	1312.84698	0.00020	1461.07294	148.22616
	0	0	2	0	12	0	0	0	0	13	1311.00726	0.00011	1483.93273	172.92558
	0	0	2	0	13	0	0	0	0	14	1309.17192	0.00005	1508.69525	199.52337
	0	0	2	0	14	0	0	0	0	15	1307.34096	0.00020	1535.35996	228.01920
	0	0	2	0	15	0	0	0	0	16	1305.51366	0.00004	1563.92630	258.41268
	0	0	2	0	16	0	0	0	0	17	1303.69028	0.00006	1594.39363	290.70340
	0	0	2	0	17	0	0	0	0	18	1301.87053	0.00019	1626.76130	324.89096
	0	0	2	0	18	0	0	0	0	19	1300.05386	0.00014	1661.02860	360.97488
	0	0	2	0	19	0	0	0	0	20	1298.24011	0.00000	1697.19482	398.95471
	0	0	2	0	20	0	0	0	0	21	1296.42947	0.00025	1735.25916	438.82993
	0	0	2	0	21	0	0	0	0	22	1294.62090	0.00012	1775.22081	480.60003
	0	0	2	0	22	0	0	0	0	23	1292.81380	-0.00069	1817.07894	524.26445
	0	0	2	0	23	0	0	0	0	24	1291.01008	0.00004	1860.83266	569.82262
	0	0	2	0	24	0	0	0	0	25	1289.20729	0.00017	1906.48106	617.27393
	0	0	2	0	25	0	0	0	0	26	1287.40553	0.00011	1954.02319	666.61777
	0	0	2	0	26	0	0	0	0	27	1285.60396	-0.00064	2003.45808	717.85348
	0	0	2	0	27	0	0	0	0	28	1283.80456	0.00022	2054.78472	770.98038
	0	0	2	0	28	0	0	0	0	29	1282.00441	0.00009	2108.00210	825.99778
	0	0	2	0	29	0	0	0	0	30	1280.20436	0.00015	2163.10916	882.90495
	0	0	2	0	30	0	0	0	0	31	1278.40325	-0.00043	2220.10483	941.70115
	0	0	2	0	31	0	0	0	0	32	1276.60227	-0.00017	2278.98802	1002.38559
	0	0	2	0	32	0	0	0	0	33	1274.80008	-0.00007	2339.75763	1064.95747
	0	0	2	0	33	0	0	0	0	34	1272.99678	0.00024	2402.41252	1129.41599
	0	0	2	0	34	0	0	0	0	35	1271.19153	0.00023	2466.95157	1195.76027
	0	0	2	0	35	0	0	0	0	36	1269.38420	0.00002	2533.37364	1263.98946
	0	0	2	0	36	0	0	0	0	37	1267.57513	0.00022	2601.67755	1334.10264
	0	0	2	0	37	0	0	0	0	38	1265.76337	0.00011	2671.86216	1406.09891
	0	0	2	0	38	0	0	0	0	39	1263.94899	-0.00001	2743.92630	1479.97730
	0	0	2	0	39	0	0	0	0	40	1262.13201	0.00008	2817.86878	1555.73685
	0	0	2	0	40	0	0	0	0	41	1260.31217	0.00030	2893.68843	1633.37656
	0	0	2	0	41	0	0	0	0	42	1258.48885	0.00019	2971.38407	1712.89541
	0	0	2	0	42	0	0	0	0	43	1256.66258	0.00042	3050.95450	1794.29235
	0	0	2	0	43	0	0	0	0	44	1254.83163	-0.00061	3132.39854	1877.56630
	0	0	2	0	44	0	0	0	0	45	1252.99859	-0.00023	3215.71499	1962.71617
	0	0	2	0	45	0	0	0	0	46	1251.16130	-0.00050	3300.90265	2049.74085
	0	0	2	0	46	0	0	0	0	47	1249.32134	0.00021	3387.96030	2138.63917
	0	0	2	0	47	0	0	0	0	48	1247.47661	-0.00015	3476.88675	2229.40999
	0	0	2	0	1	0	0	0	0	0	1337.21497	0.00050	1337.21447	0.00000
	0	0	2	0	2	0	0	0	0	1	1339.12611	0.00039	1341.02637	1.90066
	0	0	2	0	3	0	0	0	0	2	1341.04256	0.00038	1346.74412	5.70195
	0	0	2	0	4	0	0	0	0	3	1342.96404	0.00026	1354.36759	11.40382
	0	0	2	0	5	0	0	0	0	4	1344.89062	0.00019	1363.89662	19.00619
	0	0	2	0	6	0	0	0	0	5	1346.82223	0.00021	1375.33100	28.50898
	0	0	2	0	7	0	0	0	0	6	1348.75868	0.00025	1388.67047	39.91204
	0	0	2	0	8	0	0	0	0	7	1350.69955	0.00003	1403.91476	53.21523
	0	0	2	0	9	0	0	0	0	8	1352.64480	-0.00034	1421.06352	68.41838
	0	0	2	0	10	0	0	0	0	9	1354.59526	0.00016	1440.11639	85.52129
	0	0	2	0	11	0	0	0	0	10	1356.54933	0.00011	1461.07294	104.52373
	0	0	2	0	12	0	0	0	0	11	1358.50645	-0.00084	1483.93273	125.42544
	0	0	2	0	13	0	0	0	0	12	1360.46903	-0.00006	1508.69525	148.22616
	0	0	2	0	14	0	0	0	0	13	1362.43453	0.00014	1535.35996	172.92558
	0	0	2	0	15	0	0	0	0	14	1364.40307	0.00015	1563.92630	199.52337
	0	0	2	0	16	0	0	0	0	15	1366.37454	0.00011	1594.39363	228.01920
	0	0	2	0	17	0	0	0	0	16	1368.34898	0.00036	1626.76130	258.41268
	0	0	2	0	18	0	0	0	0	17	1370.32529	0.00009	1661.02860	290.70340
	0	0	2	0	19	0	0	0	0	18	1372.30409	0.00023	1697.19482	324.89096
	0	0	2	0	20	0	0	0	0	19	1374.28444	0.00017	1735.25916	360.97488
	0	0	2	0	21	0	0	0	0	20	1376.26622	0.00012	1775.22081	398.95471
	0	0	2	0	22	0	0	0	0	21	1378.25085*	0.00184	1817.07894	438.82993W

0	0	2	0	23	0	0	0	0	22	1380.23294	0.00031	1860.83266	480.60003
0	0	2	0	24	0	0	0	0	23	1382.21702	0.00041	1906.48106	524.26445
0	0	2	0	25	0	0	0	0	24	1384.20076	0.00019	1954.02319	569.82262
0	0	2	0	26	0	0	0	0	25	1386.18447	0.00033	2003.45808	617.27393
0	0	2	0	27	0	0	0	0	26	1388.16720	0.00025	2054.78472	666.61777
0	0	2	0	28	0	0	0	0	27	1390.14879	0.00017	2108.00210	717.85348
0	0	2	0	29	0	0	0	0	28	1392.12914	0.00036	2163.10916	770.98038
0	0	2	0	30	0	0	0	0	29	1394.10719	0.00014	2220.10483	825.99778
0	0	2	0	31	0	0	0	0	30	1396.08307	0.00000	2278.98802	882.90495
0	0	2	0	32	0	0	0	0	31	1398.05742	0.00094	2339.75763	941.70115
0	0	2	0	33	0	0	0	0	32	1400.02685	-0.00008	2402.41252	1002.38559
0	0	2	0	34	0	0	0	0	33	1401.99401	-0.00009	2466.95157	1064.95747
0	0	2	0	35	0	0	0	0	34	1403.95762	-0.00003	2533.37364	1129.41599
0	0	2	0	36	0	0	0	0	35	1405.91719	-0.00009	2601.67755	1195.76027
0	0	2	0	37	0	0	0	0	36	1407.87261	-0.00010	2671.86216	1263.98946
0	0	2	0	38	0	0	0	0	37	1409.82359	-0.00007	2743.92630	1334.10264
0	0	2	0	39	0	0	0	0	38	1411.76976	-0.00011	2817.86878	1406.09891
0	0	2	0	40	0	0	0	0	39	1413.71108	-0.00005	2893.68843	1479.97730
0	0	2	0	41	0	0	0	0	40	1415.64742	0.00020	2971.38407	1555.73685
0	0	2	0	42	0	0	0	0	41	1417.57782	-0.00012	3050.95450	1633.37656
0	0	2	0	43	0	0	0	0	42	1419.50275	-0.00038	3132.39854	1712.89541
0	0	2	0	44	0	0	0	0	43	1421.42214	-0.00050	3215.71499	1794.29235
0	0	2	0	45	0	0	0	0	44	1423.33675	0.00040	3300.90265	1877.56630
0	0	2	0	46	0	0	0	0	45	1425.24392	-0.00021	3387.96030	1962.71617
0	0	2	0	47	0	0	0	0	46	1427.14583	-0.00007	3476.88675	2049.74085
0	0	2	0	48	0	0	0	0	47	1429.04145	-0.00013	3567.68076	2138.63917
0	0	2	0	49	0	0	0	0	48	1430.92949	-0.00163	3660.34111	2229.40999W

rms = 0.00028 cm⁻¹

$2\nu_5(\Delta) \leftarrow G.S.(\Sigma^+)$

$\nu_4' \ell_4' V_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
0 0 2 2 11	0 0 0 0 12	1329.40010	0.00004	1477.62621	148.22616
0 0 2 2 12	0 0 0 0 13	1327.55736	-0.00119	1500.48412	172.92558W
0 0 2 2 13	0 0 0 0 14	1325.72326	0.00031	1525.24633	199.52337
0 0 2 2 14	0 0 0 0 15	1323.89436	0.00086	1551.91270	228.01920
0 0 2 2 15	0 0 0 0 16	1322.07083	0.00041	1580.48310	258.41268
0 0 2 2 16	0 0 0 0 17	1320.25457	0.00060	1610.95737	290.70340
0 0 2 2 17	0 0 0 0 18	1318.44361	-0.00080	1643.33536	324.89096
0 0 2 2 18	0 0 0 0 19	1316.64215	0.00014	1677.61689	360.97488
0 0 2 2 19	0 0 0 0 20	1314.84662	-0.00045	1713.80178	398.95471
0 0 2 2 20	0 0 0 0 21	1313.06005	0.00016	1751.88982	438.82993
0 0 2 2 21	0 0 0 0 22	1311.28144	0.00066	1791.88081	480.60003
0 0 2 2 22	0 0 0 0 23	1309.51025	0.00020	1833.77451	524.26445
0 0 2 2 23	0 0 0 0 24	1307.74820	0.00015	1877.57067	569.82262
0 0 2 2 24	0 0 0 0 25	1305.99521	0.00012	1923.26903	617.27393
0 0 2 2 25	0 0 0 0 26	1304.25164	0.00011	1970.86930	666.61777
0 0 2 2 26	0 0 0 0 27	1302.51777	0.00007	2020.37118	717.85348
0 0 2 2 27	0 0 0 0 28	1300.79402	0.00007	2071.77433	770.98038
0 0 2 2 28	0 0 0 0 29	1299.08024	-0.00038	2125.07841	825.99778
0 0 2 2 29	0 0 0 0 30	1297.37889	0.00083	2180.28301	882.90495
0 0 2 2 30	0 0 0 0 31	1295.68612*	-0.00047	2237.38774	941.70115
0 0 2 2 31	0 0 0 0 32	1294.00625	-0.00030	2296.39214	1002.38559
0 0 2 2 32	0 0 0 0 33	1292.33796	-0.00030	2357.29574	1064.95747
0 0 2 2 33	0 0 0 0 34	1290.68195	-0.00008	2420.09801	1129.41599
0 0 2 2 34	0 0 0 0 35	1289.03833	0.00019	2484.79841	1195.76027
0 0 2 2 35	0 0 0 0 36	1287.40583	-0.00106	2551.39634	1263.98946W
0 0 2 2 36	0 0 0 0 37	1285.78807	-0.00046	2619.89117	1334.10264
0 0 2 2 37	0 0 0 0 38	1284.18281	-0.00050	2690.28221	1406.09891
0 0 2 2 38	0 0 0 0 39	1282.59083	-0.00062	2762.56875	1479.97730
0 0 2 2 39	0 0 0 0 40	1281.01360	0.00044	2836.75002	1555.73685
0 0 2 2 11	0 0 0 0 10	1373.10323	0.00074	1477.62621	104.52373
0 0 2 2 12	0 0 0 0 11	1375.05927	0.00058	1500.48412	125.42544
0 0 2 2 13	0 0 0 0 12	1377.01988	-0.00029	1525.24633	148.22616
0 0 2 2 14	0 0 0 0 13	1379.00000	0.00000	1551.91270	172.92558

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

1	0	0	2	2	15	0	0	0	0	14	1380.95811	-0.00161	1580.48310	199.52337W
2	0	0	2	2	16	0	0	0	0	15	1382.93833	0.00016	1610.95737	228.01920
3	0	0	2	2	17	0	0	0	0	16	1384.92227	-0.00042	1643.33536	258.41268
4	0	0	2	2	18	0	0	0	0	17	1386.91398	0.00049	1677.61689	290.70340
5	0	0	2	2	19	0	0	0	0	18	1388.91130	0.00047	1713.80178	324.89096
6	0	0	2	2	20	0	0	0	0	19	1390.91537	0.00043	1751.88982	360.97488
7	0	0	2	2	21	0	0	0	0	20	1392.92600	-0.00010	1791.88081	398.95471
8	0	0	2	2	22	0	0	0	0	21	1394.94467	0.00010	1833.77451	438.82993
9	0	0	2	2	23	0	0	0	0	22	1396.97102	0.00038	1877.57067	480.60003
10	0	0	2	2	24	0	0	0	0	23	1399.00483	0.00025	1923.26903	524.26445
11	0	0	2	2	25	0	0	0	0	24	1401.04667	-0.00001	1970.86930	569.82262
12	0	0	2	2	26	0	0	0	0	25	1403.09768	0.00043	2020.37118	617.27393
13	0	0	2	2	27	0	0	0	0	26	1405.15682	0.00026	2071.77433	666.61777
14	0	0	2	2	28	0	0	0	0	27	1407.22496	0.00003	2125.07841	717.85348
15	0	0	2	2	29	0	0	0	0	28	1409.30270	0.00007	2180.28301	770.98038
16	0	0	2	2	30	0	0	0	0	29	1411.38990	-0.00006	2237.38774	825.99778
17	0	0	2	2	31	0	0	0	0	30	1413.48716	-0.00003	2296.39214	882.90495
18	0	0	2	2	32	0	0	0	0	31	1415.59420	-0.00039	2357.29574	941.70115
19	0	0	2	2	33	0	0	0	0	32	1417.71266	0.00023	2420.09801	1002.38559
20	0	0	2	2	34	0	0	0	0	33	1419.84066	-0.00028	2484.79841	1064.95747
21	0	0	2	2	35	0	0	0	0	34	1421.97990	-0.00046	2551.39634	1129.41599
22	0	0	2	2	36	0	0	0	0	35	1424.12991	-0.00099	2619.89117	1195.76027
23	0	0	2	2	37	0	0	0	0	36	1426.29256	-0.00020	2690.28221	1263.98946
24	0	0	2	2	38	0	0	0	0	37	1428.46679	0.00068	2762.56875	1334.10264
25	0	0	2	2	39	0	0	0	0	38	1430.65137	0.00026	2836.75002	1406.09891
26	0	0	2	2	40	0	0	0	0	39	1432.84786	-0.00003	2912.82519	1479.97730
27	0	0	2	2	41	0	0	0	0	40	1435.05705	0.00048	2990.79342	1555.73685
28	0	0	2	2	42	0	0	0	0	41	1437.27652	-0.00072	3070.65380	1633.37656
29	0	0	2	2	43	0	0	0	0	42	1439.50999	0.00003	3152.40537	1712.89541
30	0	0	2	2	44	0	0	0	0	43	1441.75485	0.00007	3236.04713	1794.29235

$$\text{rms} = 0.00043 \text{ cm}^{-1}$$

$$3v_4(\Pi) \leftarrow v_4(\Pi)$$

	v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	G'	G''
36	3	1	0	0	1	1	1	0	0	2	1012.53478	0.00033	1527.82275	515.28830
37	3	1	0	0	2	1	1	0	0	3	1010.64470	0.00040	1531.63559	520.99129
38	3	1	0	0	3	1	1	0	0	4	1008.75957	0.00003	1537.35469	528.59515
39	3	1	0	0	4	1	1	0	0	5	1006.88004	-0.00004	1544.97988	538.09979
40	3	1	0	0	5	1	1	0	0	6	1005.00556	-0.00026	1554.51090	549.50508
41	3	1	0	0	6	1	1	0	0	7	1003.13679	0.00019	1565.94747	562.81086
42	3	1	0	0	7	1	1	0	0	8	1001.27194	-0.00032	1579.28923	578.01697
43	3	1	0	0	8	1	1	0	0	9	999.41226	-0.00032	1594.53577	595.12319
44	3	1	0	0	9	1	1	0	0	10	997.55804*	0.00070	1611.68663	614.12929
45	3	1	0	0	10	1	1	0	0	11	995.70594	-0.00036	1630.74133	635.03503
46	3	1	0	0	11	1	1	0	0	12	993.85898	-0.00020	1651.69930	657.84012
47	3	1	0	0	12	1	1	0	0	13	992.01573	0.00002	1674.55997	682.54427
48	3	1	0	0	13	1	1	0	0	14	990.17535	-0.00025	1699.32273	709.14713
49	3	1	0	0	14	1	1	0	0	15	988.33845	-0.00010	1725.98691	737.64836
50	3	1	0	0	15	1	1	0	0	16	986.50385	-0.00042	1754.55184	768.04757
51	3	1	0	0	16	1	1	0	0	17	984.67237	-0.00010	1785.01683	800.34436
52	3	1	0	0	17	1	1	0	0	18	982.84292	0.00007	1817.38115	834.53830
53	3	1	0	0	18	1	1	0	0	19	981.01510	-0.00005	1851.64407	870.62893
54	3	1	0	0	19	1	1	0	0	20	979.18879	-0.00029	1887.80485	908.61577
55	3	1	0	0	20	1	1	0	0	21	977.36422	-0.00020	1925.86272	948.49830
56	3	1	0	0	21	1	1	0	0	22	975.54060	-0.00031	1965.81693	990.27601
57	3	1	0	0	22	1	1	0	0	23	973.71846	0.00010	2007.66669	1033.94833
58	3	1	0	0	23	1	1	0	0	24	971.89674	0.00018	2051.41124	1079.51468
59	3	1	0	0	24	1	1	0	0	25	970.07560	0.00025	2097.04980	1126.97445
60	3	1	0	0	25	1	1	0	0	26	968.25457	0.00000	2144.58158	1176.32701
	3	1	0	0	26	1	1	0	0	27	966.43392	-0.00018	2194.00579	1227.57169
	3	1	0	0	27	1	1	0	0	28	964.61386	0.00003	2245.32165	1280.70782
	3	1	0	0	28	1	1	0	0	29	962.79388	0.00022	2298.52834	1335.73468
	3	1	0	0	29	1	1	0	0	30	960.97376	0.00023	2353.62507	1392.65154
	3	1	0	0	30	1	1	0	0	31	959.15369	0.00010	2410.61102	1451.45764

3	1	0	0	31	1	1	0	0	32	957.33321	0.00004	2469.48537	1512.15220
3	1	0	0	32	1	1	0	0	33	955.51290	0.00003	2530.24728	1574.73441
3	1	0	0	33	1	1	0	0	34	953.69277	0.00029	2592.89590	1639.20342
3	1	0	0	34	1	1	0	0	35	951.87217	0.00019	2657.43036	1705.55838
3	1	0	0	35	1	1	0	0	36	950.05222	0.00084	2723.84979	1773.79841
3	1	0	0	36	1	1	0	0	37	948.23065	-0.00005	2792.15329	1843.92260
3	1	0	0	37	1	1	0	0	38	946.41004	0.00010	2862.33994	1915.93000
3	1	0	0	38	1	1	0	0	39	944.59064	0.00149	2934.40881	1989.81965W
3	1	0	0	39	1	1	0	0	40	942.76928	0.00094	3008.35893	2065.59058
3	1	0	0	2	1	1	0	0	1	1020.14915	-0.00017	1531.63559	511.48627
3	1	0	0	3	1	1	0	0	2	1022.06607	-0.00032	1537.35469	515.28830
3	1	0	0	4	1	1	0	0	3	1023.98864	0.00005	1544.97988	520.99129
3	1	0	0	5	1	1	0	0	4	1025.91573	-0.00002	1554.51090	528.59515
3	1	0	0	6	1	1	0	0	5	1027.84729	-0.00039	1565.94747	538.09979
3	1	0	0	7	1	1	0	0	6	1029.78410	-0.00005	1579.28923	549.50508
3	1	0	0	8	1	1	0	0	7	1031.72498	0.00008	1594.53577	562.81086
3	1	0	0	9	1	1	0	0	8	1033.66956	-0.00011	1611.68663	578.01697
3	1	0	0	10	1	1	0	0	9	1035.61828	0.00014	1630.74133	595.12319
3	1	0	0	11	1	1	0	0	10	1037.56996	-0.00005	1651.69930	614.12929
3	1	0	0	12	1	1	0	0	11	1039.52489	-0.00005	1674.55997	635.03503
3	1	0	0	13	1	1	0	0	12	1041.48239	-0.00021	1699.32273	657.84012
3	1	0	0	14	1	1	0	0	13	1043.44253	-0.00011	1725.98691	682.54427
3	1	0	0	15	1	1	0	0	14	1045.40484	0.00013	1754.55184	709.14713
3	1	0	0	16	1	1	0	0	15	1047.36843	-0.00004	1785.01683	737.64836
3	1	0	0	17	1	1	0	0	16	1049.33367	0.00009	1817.38115	768.04757
3	1	0	0	18	1	1	0	0	17	1051.29938	-0.00033	1851.64407	800.34436
3	1	0	0	19	1	1	0	0	18	1053.26645	-0.00010	1887.80485	834.53830
3	1	0	0	20	1	1	0	0	19	1055.23408	0.00029	1925.86272	870.62893
3	1	0	0	21	1	1	0	0	20	1057.20140	0.00024	1965.81693	908.61577
3	1	0	0	22	1	1	0	0	21	1059.16838	-0.00001	2007.66669	948.49830
3	1	0	0	23	1	1	0	0	22	1061.13519	-0.00004	2051.41124	990.27601
3	1	0	0	24	1	1	0	0	23	1063.10142	-0.00005	2097.04980	1033.94833
3	1	0	0	25	1	1	0	0	24	1065.06700	0.00010	2144.58158	1079.51468
3	1	0	0	26	1	1	0	0	25	1067.03180	0.00046	2194.00579	1126.97445
3	1	0	0	27	1	1	0	0	26	1068.99463	-0.00001	2245.32165	1176.32701
3	1	0	0	28	1	1	0	0	27	1070.95664	-0.00001	2298.52834	1227.57169
3	1	0	0	29	1	1	0	0	28	1072.91724	-0.00002	2353.62507	1280.70782
3	1	0	0	30	1	1	0	0	29	1074.87606	-0.00029	2410.61102	1335.73468
3	1	0	0	31	1	1	0	0	30	1076.83367	-0.00016	2469.48537	1392.65154
3	1	0	0	32	1	1	0	0	31	1078.78936	-0.00028	2530.24728	1451.45764
3	1	0	0	33	1	1	0	0	32	1080.74342	-0.00028	2592.89590	1512.15220
3	1	0	0	34	1	1	0	0	33	1082.69581	-0.00015	2657.43036	1574.73441
3	1	0	0	35	1	1	0	0	34	1084.64668	0.00031	2723.84979	1639.20342
3	1	0	0	36	1	1	0	0	35	1086.59544	0.00053	2792.15329	1705.55838
3	1	0	0	37	1	1	0	0	36	1088.54118	-0.00035	2862.33994	1773.79841
3	1	0	0	38	1	1	0	0	37	1090.48614	-0.00007	2934.40881	1843.92260
3	1	0	0	39	1	1	0	0	38	1092.43064	0.00171	3008.35893	1915.93000W
3	1	0	0	40	1	1	0	0	39	1094.36981	0.00014	3084.18932	1989.81965
3	1	0	0	41	1	1	0	0	40	1096.31260	0.00419	3161.89900	2065.59058W
3	1	0	0	42	1	1	0	0	41	1098.24666	0.00152	3241.48691	2143.24177W
3	1	0	0	1	1	-1	0	0	1	1016.32839	0.00019	1527.82275	511.49456
3	1	0	0	2	1	-1	0	0	2	1016.32202	-0.00041	1531.63559	515.31316
3	1	0	0	3	1	-1	0	0	3	1016.31368	0.00000	1537.35469	521.04101
3	1	0	0	4	1	-1	0	0	4	1016.30151	-0.00035	1544.97988	528.67801
3	1	0	0	5	1	-1	0	0	5	1016.28696	0.00013	1554.51090	538.22407
3	1	0	0	6	1	-1	0	0	6	1016.26798	-0.00043	1565.94747	549.67906
3	1	0	0	7	1	-1	0	0	7	1016.24647	0.00005	1579.28923	563.04281
3	1	0	0	8	1	-1	0	0	8	1016.22126	0.00063	1594.53577	578.31514
3	1	0	0	9	1	-1	0	0	9	1016.19026	-0.00053	1611.68663	595.49585
3	1	0	0	10	1	-1	0	0	10	1016.15655	-0.00008	1630.74133	614.58469
3	1	0	0	11	1	-1	0	0	11	1016.11808	0.00020	1651.69930	635.58142
3	1	0	0	12	1	-1	0	0	12	1016.07435	0.00011	1674.55997	658.48573
3	1	0	0	13	1	-1	0	0	13	1016.02519	-0.00022	1699.32273	683.29732
3	1	0	0	14	1	-1	0	0	14	1015.97119*	0.00012	1725.98691	710.01584
3	1	0	0	15	1	-1	0	0	15	1015.91025	-0.00066	1754.55184	738.64093
3	-1	0	0	1	1	-1	0	0	2	1012.52632	-0.00013	1527.83961	515.31316
3	-1	0	0	2	1	-1	0	0	3	1010.64470	-0.00044	1531.68615	521.04101
3	-1	0	0	3	1	-1	0	0	4	1008.77780	0.00000	1537.45581	528.67801
3	-1	0	0	4	1	-1	0	0	5	1006.82410	0.00022	1545.14839	538.22407

1	3	-1	0	0	5	1	-1	0	0	6	1005.08434	-0.00024	1554.76364	549.67906
2	3	-1	0	0	6	1	-1	0	0	7	1003.25809	-0.00033	1566.30123	563.04281
3	3	-1	0	0	7	1	-1	0	0	8	1001.44550	-0.00011	1579.76075	578.31514
4	3	-1	0	0	8	1	-1	0	0	9	999.64585	-0.00005	1595.14175	595.49585
5	3	-1	0	0	9	1	-1	0	0	10	997.85894	-0.00004	1612.44367	614.58469
6	3	-1	0	0	10	1	-1	0	0	11	996.08453	0.00007	1631.66587	635.58142
7	3	-1	0	0	11	1	-1	0	0	12	994.32208	0.00017	1652.80764	658.48573
8	3	-1	0	0	12	1	-1	0	0	13	992.57116	0.00033	1675.86815	683.29732
9	3	-1	0	0	13	1	-1	0	0	14	990.83078	0.00013	1700.84649	710.01584
10	3	-1	0	0	14	1	-1	0	0	15	989.10100	0.00030	1727.74163	738.64093
11	3	-1	0	0	15	1	-1	0	0	16	987.38028	0.00004	1756.55244	769.17220
12	3	-1	0	0	16	1	-1	0	0	17	985.66887	0.00044	1787.27765	801.60923
13	3	-1	0	0	17	1	-1	0	0	18	983.96476	0.00042	1819.91590	835.95156
14	3	-1	0	0	18	1	-1	0	0	19	982.26760	0.00068	1854.46566	872.19874
15	3	-1	0	0	19	1	-1	0	0	20	980.57536	0.00031	1890.92532	910.35027
16	3	-1	0	0	20	1	-1	0	0	21	978.88793	0.00042	1929.29312	950.40561
17	3	-1	0	0	21	1	-1	0	0	22	977.20323	0.00027	1969.56720	992.36423
18	3	-1	0	0	22	1	-1	0	0	23	975.52035	0.00030	2011.74560	1036.22555
19	3	-1	0	0	23	1	-1	0	0	24	973.83750	0.00017	2055.82629	1081.98896
20	3	-1	0	0	24	1	-1	0	0	25	972.15280	-0.00058	2101.80723	1129.65384
21	3	-1	0	0	25	1	-1	0	0	26	970.46716	0.00037	2149.68633	1179.21954
22	3	-1	0	0	26	1	-1	0	0	27	968.77635	0.00014	2199.46159	1230.68537
23	3	-1	0	0	27	1	-1	0	0	28	967.08059	0.00017	2251.13106	1284.05064
24	3	-1	0	0	28	1	-1	0	0	29	965.37845	0.00013	2304.69292	1339.31460
25	3	-1	0	0	29	1	-1	0	0	30	963.66908	0.00005	2360.14554	1396.47651
26	3	-1	0	0	30	1	-1	0	0	31	961.95155	-0.00031	2417.48743	1455.53557
27	3	-1	0	0	31	1	-1	0	0	32	960.22625	-0.00009	2476.71732	1516.49098
28	3	-1	0	0	32	1	-1	0	0	33	958.49187	-0.00034	2537.83412	1579.34190
29	3	-1	0	0	33	1	-1	0	0	34	956.74920	-0.00023	2600.83691	1644.08748
30	3	-1	0	0	34	1	-1	0	0	35	954.99799	-0.00011	2665.72492	1710.72682
31	3	-1	0	0	35	1	-1	0	0	36	953.23846	-0.00003	2732.49750	1779.25901
32	3	-1	0	0	36	1	-1	0	0	37	951.47065	-0.00032	2801.15408	1849.68311
33	3	-1	0	0	37	1	-1	0	0	38	949.69605	0.00006	2871.69415	1921.99816
34	3	-1	0	0	38	1	-1	0	0	39	947.91368	-0.00037	2944.11722	1996.20316
35	3	-1	0	0	2	1	-1	0	0	1	1020.19146	-0.00014	1531.68615	511.49456
36	3	-1	0	0	3	1	-1	0	0	2	1022.14255	-0.00010	1537.45581	515.31316
37	3	-1	0	0	4	1	-1	0	0	3	1024.10760	0.00022	1545.14839	521.04101
38	3	-1	0	0	5	1	-1	0	0	4	1026.08567	0.00004	1554.76364	528.67801
39	3	-1	0	0	6	1	-1	0	0	5	1028.07723	0.00008	1566.30123	538.22407
40	3	-1	0	0	7	1	-1	0	0	6	1030.08165	-0.00005	1579.76075	549.67906
41	3	-1	0	0	8	1	-1	0	0	7	1032.09877	-0.00018	1595.14175	563.04281
42	3	-1	0	0	9	1	-1	0	0	8	1034.12866	0.00013	1612.44367	578.31514
43	3	-1	0	0	10	1	-1	0	0	9	1036.17034	0.00031	1631.66587	595.49585
44	3	-1	0	0	11	1	-1	0	0	10	1038.22290	-0.00005	1652.80764	614.58469
45	3	-1	0	0	12	1	-1	0	0	11	1040.28676	0.00003	1675.86815	635.58142
46	3	-1	0	0	13	1	-1	0	0	12	1042.36084	0.00008	1700.84649	658.48573
47	3	-1	0	0	14	1	-1	0	0	13	1044.44491	0.00060	1727.74163	683.29732
48	3	-1	0	0	15	1	-1	0	0	14	1046.53678	0.00018	1756.55244	710.01584
49	3	-1	0	0	16	1	-1	0	0	15	1048.63709	0.00037	1787.27765	738.64093
50	3	-1	0	0	17	1	-1	0	0	16	1050.74404	0.00034	1819.91590	769.17220
51	3	-1	0	0	18	1	-1	0	0	17	1052.85684	0.00040	1854.46566	801.60923
52	3	-1	0	0	19	1	-1	0	0	18	1054.97469	0.00093	1890.92532	835.95156
53	3	-1	0	0	20	1	-1	0	0	19	1057.09519	0.00081	1929.29312	872.19874
54	3	-1	0	0	21	1	-1	0	0	20	1059.21736	0.00043	1969.56720	910.35027
55	3	-1	0	0	22	1	-1	0	0	21	1061.34035	0.00037	2011.74560	950.40561
56	3	-1	0	0	23	1	-1	0	0	22	1063.46250	0.00044	2055.82629	992.36423
57	3	-1	0	0	24	1	-1	0	0	23	1065.58192	0.00024	2101.80723	1036.22555
58	3	-1	0	0	25	1	-1	0	0	24	1067.69680	-0.00057	2149.68633	1081.98896
59	3	-1	0	0	26	1	-1	0	0	25	1069.80805	0.00031	2199.46159	1129.65384
60	3	-1	0	0	27	1	-1	0	0	26	1071.91147	-0.00004	2251.13106	1179.21954
	3	-1	0	0	28	1	-1	0	0	27	1074.00752	-0.00003	2304.69292	1230.68537
	3	-1	0	0	29	1	-1	0	0	28	1076.09475	-0.00015	2360.14554	1284.05064
	3	-1	0	0	30	1	-1	0	0	29	1078.17266	-0.00017	2417.48743	1339.31460
	3	-1	0	0	31	1	-1	0	0	30	1080.24042	-0.00039	2476.71732	1396.47651
	3	-1	0	0	32	1	-1	0	0	31	1082.29827	-0.00028	2537.83412	1455.53557
	3	-1	0	0	33	1	-1	0	0	32	1084.34551	-0.00042	2600.83691	1516.49098
	3	-1	0	0	34	1	-1	0	0	33	1086.38316	0.00015	2665.72492	1579.34190
	3	-1	0	0	35	1	-1	0	0	34	1088.41048	0.00046	2732.49750	1644.08748
	3	-1	0	0	36	1	-1	0	0	35	1090.42668	0.00059	2801.15408	1710.72682

3	-1	0	0	37	1	-1	0	0	36	1092.43559	0.00045	2871.69415	1779.25901
3	-1	0	0	38	1	-1	0	0	37	1094.43417	0.00006	2944.11722	1849.68311
3	-1	0	0	39	1	-1	0	0	38	1096.42461	-0.00003	3018.42279	1921.99816
3	-1	0	0	40	1	-1	0	0	39	1098.40723	0.00002	3094.61038	1996.20316
3	-1	0	0	41	1	-1	0	0	40	1100.38263	0.00031	3172.67942	2072.29710
3	-1	0	0	1	1	1	0	0	1	1016.35307	-0.00027	1527.83961	511.48627
3	-1	0	0	2	1	1	0	0	2	1016.39803	0.00018	1531.68615	515.28830
3	-1	0	0	3	1	1	0	0	3	1016.46452	0.00000	1537.45581	520.99129
3	-1	0	0	4	1	1	0	0	4	1016.55250	-0.00074	1545.14839	528.59515
3	-1	0	0	5	1	1	0	0	5	1016.66383	-0.00002	1554.76364	538.09979
3	-1	0	0	6	1	1	0	0	6	1016.79520	-0.00095	1566.30123	549.50508
3	-1	0	0	7	1	1	0	0	7	1016.94975	-0.00014	1579.76075	562.81086
3	-1	0	0	8	1	1	0	0	8	1017.12504	0.00025	1595.14175	578.01697
3	-1	0	0	9	1	1	0	0	9	1017.32068	0.00019	1612.44367	595.12319
3	-1	0	0	10	1	1	0	0	10	1017.53714	0.00056	1631.66587	614.12929
3	-1	0	0	11	1	1	0	0	11	1017.77280	0.00019	1652.80764	635.03503
3	-1	0	0	12	1	1	0	0	12	1018.02785	-0.00018	1675.86815	657.84012
3	-1	0	0	13	1	1	0	0	13	1018.30178	-0.00044	1700.84649	682.54427
3	-1	0	0	14	1	1	0	0	14	1018.59412	-0.00038	1727.74163	709.14713
3	-1	0	0	15	1	1	0	0	15	1018.90366	-0.00042	1756.55244	737.64836
3	-1	0	0	16	1	1	0	0	16	1019.23166	0.00158	1787.27765	768.04757W
3	-1	0	0	17	1	1	0	0	17	1019.56948*	-0.00206	1819.91590	800.34436W

rms = 0.00031 cm⁻¹

$$2\nu_4 + \nu_5 (^{\Pi}\Pi) \leftarrow \nu_4 (\Pi)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 0 1 1 1	1 1 0 0 2	1178.04300*	-0.00239	1693.33369	515.28830W
2 0 1 1 2	1 1 0 0 3	1176.16859	-0.00039	1697.16027	520.99129
2 0 1 1 3	1 1 0 0 4	1174.30447	-0.00030	1702.89992	528.59515
2 0 1 1 4	1 1 0 0 5	1172.45312	0.00050	1710.55241	538.09979
2 0 1 1 5	1 1 0 0 6	1170.61228	-0.00004	1720.11740	549.50508
2 0 1 1 6	1 1 0 0 7	1168.78341	-0.00018	1731.59446	562.81086
2 0 1 1 7	1 1 0 0 8	1166.96575	-0.00033	1744.98305	578.01697
2 0 1 1 8	1 1 0 0 9	1165.15929	-0.00008	1760.28255	595.12319
2 0 1 1 9	1 1 0 0 10	1163.36282	-0.00011	1777.49222	614.12929
2 0 1 1 10	1 1 0 0 11	1161.57604	-0.00013	1796.61120	635.03503
2 0 1 1 11	1 1 0 0 12	1159.79827	-0.00009	1817.63849	657.84012
2 0 1 1 12	1 1 0 0 13	1158.02279*	-0.00592	1840.57298	682.54427W
2 0 1 1 13	1 1 0 0 14	1156.26613	-0.00016	1865.41342	709.14713
2 0 1 1 14	1 1 0 0 15	1154.51000	-0.00006	1892.15842	737.64836
2 0 1 1 15	1 1 0 0 16	1152.75921	0.00030	1920.80648	768.04757
2 0 1 1 16	1 1 0 0 17	1151.01156	-0.00004	1951.35596	800.34436
2 0 1 1 17	1 1 0 0 18	1149.26697	0.00012	1983.80515	834.53830
2 0 1 1 18	1 1 0 0 19	1147.52095*	-0.00238	2018.15225	870.62893W
2 0 1 1 19	1 1 0 0 20	1145.77928	-0.00043	2054.39547	908.61577
2 0 1 1 20	1 1 0 0 21	1144.03441	-0.00028	2092.53300	948.49830
2 0 1 1 21	1 1 0 0 22	1142.28701	-0.00007	2132.56309	990.27601
2 0 1 1 22	1 1 0 0 23	1140.53580	0.00004	2174.48410	1033.94833
2 0 1 1 23	1 1 0 0 24	1138.77981	-0.00001	2218.29450	1079.51468
2 0 1 1 24	1 1 0 0 25	1137.01827	-0.00020	2263.99292	1126.97445
2 0 1 1 25	1 1 0 0 26	1135.25117	0.00004	2311.57813	1176.32701
2 0 1 1 26	1 1 0 0 27	1133.47718	-0.00020	2361.04907	1227.57169
2 0 1 1 27	1 1 0 0 28	1131.69730	0.00031	2412.40481	1280.70782
2 0 1 1 28	1 1 0 0 29	1129.90938	-0.00046	2465.64452	1335.73468
2 0 1 1 29	1 1 0 0 30	1128.11583	-0.00012	2520.76749	1392.65154
2 0 1 1 30	1 1 0 0 31	1126.31478	-0.00066	2577.77308	1451.45764
2 0 1 1 31	1 1 0 0 32	1124.50802	-0.00047	2636.66069	1512.15220
2 0 1 1 32	1 1 0 0 33	1122.69509	-0.00026	2697.42976	1574.73441
2 0 1 1 33	1 1 0 0 34	1120.87631	0.00000	2760.07973	1639.20342
2 0 1 1 34	1 1 0 0 35	1119.05260	0.00094	2824.61004	1705.55838
2 0 1 1 35	1 1 0 0 36	1117.22258	0.00086	2891.02013	1773.79841
2 0 1 1 36	1 1 0 0 37	1115.38650	-0.00032	2959.30942	1843.92260
2 0 1 1 37	1 1 0 0 38	1113.54833	0.00105	3029.47728	1915.93000W
2 0 1 1 38	1 1 0 0 39	1111.71016	-0.00158	3101.52306	1989.81965

1	2	0	1	1	2	1	1	0	0	1	1185.67407	0.00007	1697.16027	511.48627
2	2	0	1	1	3	1	1	0	0	2	1187.61183	0.00021	1702.89992	515.28830
3	2	0	1	1	4	1	1	0	0	3	1189.56087	-0.00026	1710.55241	520.99129
4	2	0	1	1	5	1	1	0	0	4	1191.52259	0.00034	1720.11740	528.59515
5	2	0	1	1	6	1	1	0	0	5	1193.49537	0.00071	1731.59446	538.09979
6	2	0	1	1	7	1	1	0	0	6	1195.47856	0.00059	1744.98305	549.50508
7	2	0	1	1	8	1	1	0	0	7	1197.47169	0.00000	1760.28255	562.81086
8	2	0	1	1	9	1	1	0	0	8	1199.47504	-0.00022	1777.49222	578.01697
9	2	0	1	1	10	1	1	0	0	9	1201.48786	-0.00015	1796.61120	595.12319
10	2	0	1	1	11	1	1	0	0	10	1203.50937	0.00017	1817.63849	614.12929
11	2	0	1	1	12	1	1	0	0	11	1205.53802	0.00007	1840.57298	635.03503
12	2	0	1	1	13	1	1	0	0	12	1207.57314	-0.00015	1865.41342	657.84012
13	2	0	1	1	14	1	1	0	0	13	1209.61422	0.00007	1892.15842	682.54427
14	2	0	1	1	15	1	1	0	0	14	1211.65940	0.00005	1920.80648	709.14713
15	2	0	1	1	16	1	1	0	0	15	1213.70798	0.00038	1951.35596	737.64836
16	2	0	1	1	17	1	1	0	0	16	1215.75801	0.00044	1983.80515	768.04757
17	2	0	1	1	18	1	1	0	0	17	1217.80787	-0.00002	2018.15225	800.34436
18	2	0	1	1	19	1	1	0	0	18	1219.85700	-0.00017	2054.39547	834.53830
19	2	0	1	1	20	1	1	0	0	19	1221.90425	0.00018	2092.53300	870.62893
20	2	0	1	1	21	1	1	0	0	20	1223.94706	-0.00026	2132.56309	908.61577
21	2	0	1	1	22	1	1	0	0	21	1225.98570	-0.00009	2174.48410	948.49830
22	2	0	1	1	23	1	1	0	0	22	1228.01834	-0.00015	2218.29450	990.27601
23	2	0	1	1	24	1	1	0	0	23	1230.04460	0.00001	2263.99292	1033.94833
24	2	0	1	1	25	1	1	0	0	24	1232.06318	-0.00027	2311.57813	1079.51468
25	2	0	1	1	26	1	1	0	0	25	1234.07458	-0.00004	2361.04907	1126.97445
26	2	0	1	1	27	1	1	0	0	26	1236.07761	-0.00019	2412.40481	1176.32701
27	2	0	1	1	28	1	1	0	0	27	1238.07265	-0.00018	2465.64452	1227.57169
28	2	0	1	1	29	1	1	0	0	28	1240.05934	-0.00034	2520.76749	1280.70782
29	2	0	1	1	30	1	1	0	0	29	1242.03839	-0.00001	2577.77308	1335.73468
30	2	0	1	1	31	1	1	0	0	30	1244.00911	-0.00004	2636.66069	1392.65154
31	2	0	1	1	32	1	1	0	0	31	1245.97164	-0.00048	2697.42976	1451.45764
32	2	0	1	1	33	1	1	0	0	32	1247.92747	-0.00005	2760.07973	1512.15220
33	2	0	1	1	34	1	1	0	0	33	1249.87680*	0.00117	2824.61004	1574.73441W
34	2	0	1	1	35	1	1	0	0	34	1251.81686	0.00015	2891.02013	1639.20342
35	2	0	1	1	36	1	1	0	0	35	1253.75165	0.00061	2959.30942	1705.55838
36	2	0	1	1	37	1	1	0	0	36	1255.67982	0.00095	3029.47728	1773.79841
37	2	0	1	1	38	1	1	0	0	37	1257.60106	0.00059	3101.52306	1843.92260
38	2	0	1	1	39	1	1	0	0	38	1259.51636	0.00027	3175.44608	1915.93000
39	2	0	1	-1	1	1	-1	0	0	2	1178.01902	0.00037	1693.33182	515.31316
40	2	0	1	-1	2	1	-1	0	0	3	1176.11437	0.00074	1697.15463	521.04101
41	2	0	1	-1	3	1	-1	0	0	4	1174.20993	-0.00071	1702.88865	528.67801
42	2	0	1	-1	4	1	-1	0	0	5	1172.30916	-0.00039	1710.53362	538.22407
43	2	0	1	-1	5	1	-1	0	0	6	1170.40997	-0.00020	1720.08923	549.67906
44	2	0	1	-1	6	1	-1	0	0	7	1168.51173	-0.00053	1731.55507	563.04281
45	2	0	1	-1	7	1	-1	0	0	8	1166.61554	0.00000	1744.93068	578.31514
46	2	0	1	-1	8	1	-1	0	0	9	1164.71943	-0.00026	1760.21554	595.49585
47	2	0	1	-1	9	1	-1	0	0	10	1162.82410	-0.00027	1777.40907	614.58469
48	2	0	1	-1	10	1	-1	0	0	11	1160.92944	0.00022	1796.51064	635.58142
49	2	0	1	-1	11	1	-1	0	0	12	1159.03355	-0.00030	1817.51959	658.48573
50	2	0	1	-1	12	1	-1	0	0	13	1157.13865	0.00075	1840.43522	683.29732
51	2	0	1	-1	13	1	-1	0	0	14	1155.24070	-0.00029	1865.25684	710.01584
52	2	0	1	-1	14	1	-1	0	0	15	1153.34319	0.00042	1891.98370	738.64093
53	2	0	1	-1	15	1	-1	0	0	16	1151.44132	-0.00158	1920.61510	769.17220W
54	2	0	1	-1	16	1	-1	0	0	17	1149.54138	0.00030	1951.15030	801.60923
55	2	0	1	-1	17	1	-1	0	0	18	1147.63699	-0.00004	1983.58860	835.95156
56	2	0	1	-1	18	1	-1	0	0	19	1145.72986	-0.00067	2017.92928	872.19874
57	2	0	1	-1	19	1	-1	0	0	20	1143.82009	-0.00129	2054.17165	910.35027W
58	2	0	1	-1	20	1	-1	0	0	21	1141.90964	0.00022	2092.31503	950.40561
59	2	0	1	-1	21	1	-1	0	0	22	1139.99313	-0.00140	2132.35877	992.36423W
60	2	0	1	-1	22	1	-1	0	0	23	1138.07550	-0.00114	2174.30219	1036.22555W
	2	0	1	-1	2	1	-1	0	0	1	1185.66286	0.00278	1697.15463	511.49456W
	2	0	1	-1	3	1	-1	0	0	2	1187.57622	0.00073	1702.88865	515.31316
	2	0	1	-1	4	1	-1	0	0	3	1189.49197	-0.00065	1710.53362	521.04101
	2	0	1	-1	5	1	-1	0	0	4	1191.41037	-0.00085	1720.08923	528.67801
	2	0	1	-1	6	1	-1	0	0	5	1193.33132	0.00032	1731.55507	538.22407
	2	0	1	-1	7	1	-1	0	0	6	1195.25172	0.00009	1744.93068	549.67906
	2	0	1	-1	8	1	-1	0	0	7	1197.17242	-0.00032	1760.21554	563.04281
	2	0	1	-1	9	1	-1	0	0	8	1199.09433	0.00040	1777.40907	578.31514
	2	0	1	-1	10	1	-1	0	0	9	1201.01485	0.00006	1796.51064	595.49585

2	0	1	-1	11	1	-1	0	0	10	1202.93398*	-0.00091	1817.51959	614.58469
2	0	1	-1	12	1	-1	0	0	11	1204.85248	-0.00132	1840.43522	635.58142W
2	0	1	-1	13	1	-1	0	0	12	1206.77341	0.00231	1865.25684	658.48573W
2	0	1	-1	14	1	-1	0	0	13	1208.68684	0.00046	1891.98370	683.29732
2	0	1	-1	15	1	-1	0	0	14	1210.60009	0.00083	1920.61510	710.01584
2	0	1	-1	16	1	-1	0	0	15	1212.50898	-0.00039	1951.15030	738.64093
2	0	1	-1	17	1	-1	0	0	16	1214.41590	-0.00050	1983.58860	769.17220
2	0	1	-1	18	1	-1	0	0	17	1216.31939	-0.00066	2017.92928	801.60923
2	0	1	-1	19	1	-1	0	0	18	1218.21965	-0.00043	2054.17165	835.95156
2	0	1	-1	20	1	-1	0	0	19	1220.11661	0.00032	2092.31503	872.19874
2	0	1	-1	21	1	-1	0	0	20	1222.00770	-0.00080	2132.35877	910.35027
2	0	1	-1	22	1	-1	0	0	21	1223.89787	0.00129	2174.30219	950.40561W
2	0	1	-1	23	1	-1	0	0	22	1225.78135	0.00093	2218.14465	992.36423
2	0	1	-1	24	1	-1	0	0	23	1227.65929	-0.00067	2263.88551	1036.22555

rms = 0.00040 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	G'	G''
2 2 1 -1 1	1 1 0 0 2	1187.08240	0.00033	1702.37037	515.28830
2 2 1 -1 2	1 1 0 0 3	1185.19421	-0.00003	1706.18553	520.99129
2 2 1 -1 3	1 1 0 0 4	1183.31311	-0.00004	1711.90830	528.59515
2 2 1 -1 4	1 1 0 0 5	1181.43920	0.00022	1719.53877	538.09979
2 2 1 -1 5	1 1 0 0 6	1179.57192	0.00000	1729.07700	549.50508
2 2 1 -1 6	1 1 0 0 7	1177.71206	-0.00019	1740.52311	562.81086
2 2 1 -1 7	1 1 0 0 8	1175.86019	-0.00005	1753.87721	578.01697
2 2 1 -1 8	1 1 0 0 9	1174.01659	0.00034	1769.13944	595.12319
2 2 1 -1 9	1 1 0 0 10	1172.18029	-0.00038	1786.30996	614.12929
2 2 1 -1 10	1 1 0 0 11	1170.35408	0.00015	1805.38896	635.03503
2 2 1 -1 11	1 1 0 0 12	1168.53632	-0.00018	1826.37662	657.84012
2 2 1 -1 12	1 1 0 0 13	1166.72874	-0.00015	1849.27315	682.54427
2 2 1 -1 13	1 1 0 0 14	1164.93175	0.00012	1874.07876	709.14713
2 2 1 -1 14	1 1 0 0 15	1163.14540	0.00009	1900.79367	737.64836
2 2 1 -1 15	1 1 0 0 16	1161.37034	-0.00017	1929.41808	768.04757
2 2 1 -1 16	1 1 0 0 17	1159.60786	0.00003	1959.95219	800.34436
2 2 1 -1 17	1 1 0 0 18	1157.85783	-0.00006	1992.39619	834.53830
2 2 1 -1 18	1 1 0 0 19	1156.12130	0.00001	2026.75022	870.62893
2 2 1 -1 19	1 1 0 0 20	1154.39867	0.00005	2063.01439	908.61577
2 2 1 -1 20	1 1 0 0 21	1152.69035	-0.00010	2101.18875	948.49830
2 2 1 -1 21	1 1 0 0 22	1150.99724	-0.00007	2141.27332	990.27601
2 2 1 -1 22	1 1 0 0 23	1149.31976	0.00007	2183.26802	1033.94833
2 2 1 -1 23	1 1 0 0 24	1147.65780	-0.00022	2227.17270	1079.51468
2 2 1 -1 24	1 1 0 0 25	1146.01264	-0.00005	2272.98715	1126.97445
2 2 1 -1 25	1 1 0 0 26	1144.38389	-0.00014	2320.71103	1176.32701
2 2 1 -1 26	1 1 0 0 27	1142.77225	-0.00003	2370.34397	1227.57169
2 2 1 -1 27	1 1 0 0 28	1141.17769	0.00003	2421.88547	1280.70782
2 2 1 -1 28	1 1 0 0 29	1139.60037	0.00008	2475.33497	1335.73468
2 2 1 -1 29	1 1 0 0 30	1138.04002	-0.00025	2530.69181	1392.65154
2 2 1 -1 30	1 1 0 0 31	1136.49816	0.00054	2587.95527	1451.45764
2 2 1 -1 31	1 1 0 0 32	1134.97189	-0.00046	2647.12455	1512.15220
2 2 1 -1 32	1 1 0 0 33	1133.46417	-0.00022	2708.19879	1574.73441
2 2 1 -1 33	1 1 0 0 34	1131.97419	0.00052	2771.17709	1639.20342
2 2 1 -1 34	1 1 0 0 35	1130.49969	-0.00039	2836.05847	1705.55838
2 2 1 -1 35	1 1 0 0 36	1129.04476	0.00125	2902.84192	1773.79841W
2 2 1 -1 36	1 1 0 0 37	1127.60429	0.00050	2971.52639	1843.92260
2 2 1 -1 37	1 1 0 0 38	1126.18022	-0.00057	3042.11078	1915.93000
2 2 1 -1 38	1 1 0 0 39	1124.77374	-0.00060	3114.59399	1989.81965
2 2 1 -1 2	1 1 0 0 1	1194.69904	-0.00022	1706.18553	511.48627
2 2 1 -1 3	1 1 0 0 2	1196.62006	0.00006	1711.90830	515.28830
2 2 1 -1 4	1 1 0 0 3	1198.54740	-0.00008	1719.53877	520.99129
2 2 1 -1 5	1 1 0 0 4	1200.48187	0.00002	1729.07700	528.59515
2 2 1 -1 6	1 1 0 0 5	1202.42297	-0.00035	1740.52311	538.09979
2 2 1 -1 7	1 1 0 0 6	1204.37206	-0.00007	1753.87721	549.50508
2 2 1 -1 8	1 1 0 0 7	1206.32864	0.00007	1769.13944	562.81086
2 2 1 -1 9	1 1 0 0 8	1208.29186	0.00000	1786.30996	578.01697

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

1	2	2	1	-1	10	1	1	0	0	9	1210.26557	-0.00021	1805.38896	595.12319
2	2	2	1	-1	11	1	1	0	0	10	1212.24712	-0.00021	1826.37662	614.12929
3	2	2	1	-1	12	1	1	0	0	11	1214.23819	0.00007	1849.27315	635.03503
4	2	2	1	-1	13	1	1	0	0	12	1216.23838	-0.00026	1874.07876	657.84012
5	2	2	1	-1	14	1	1	0	0	13	1218.24941	0.00001	1900.79367	682.54427
6	2	2	1	-1	15	1	1	0	0	14	1220.27160	0.00065	1929.41808	709.14713
7	2	2	1	-1	16	1	1	0	0	15	1222.30420	0.00037	1959.95219	737.64836
8	2	2	1	-1	17	1	1	0	0	16	1224.34877	0.00015	1992.39619	768.04757
9	2	2	1	-1	18	1	1	0	0	17	1226.40597	0.00011	2026.75022	800.34436
10	2	2	1	-1	19	1	1	0	0	18	1228.47595	-0.00014	2063.01439	834.53830
11	2	2	1	-1	20	1	1	0	0	19	1230.55984	0.00001	2101.18875	870.62893
12	2	2	1	-1	21	1	1	0	0	20	1232.65757	0.00001	2141.27332	908.61577
13	2	2	1	-1	22	1	1	0	0	21	1234.76960	-0.00012	2183.26802	948.49830
14	2	2	1	-1	23	1	1	0	0	22	1236.89669	0.00000	2227.17270	990.27601
15	2	2	1	-1	24	1	1	0	0	23	1239.03893	0.00012	2272.98715	1033.94833
16	2	2	1	-1	25	1	1	0	0	24	1241.19627	-0.00008	2320.71103	1079.51468
17	2	2	1	-1	26	1	1	0	0	25	1243.36938	-0.00014	2370.34397	1126.97445
18	2	2	1	-1	27	1	1	0	0	26	1245.55852	0.00005	2421.88547	1176.32701
19	2	2	1	-1	28	1	1	0	0	27	1247.76331	0.00003	2475.33497	1227.57169
20	2	2	1	-1	29	1	1	0	0	28	1249.98397	-0.00002	2530.69181	1280.70782
21	2	2	1	-1	30	1	1	0	0	29	1252.22075	0.00016	2587.95527	1335.73468
22	2	2	1	-1	31	1	1	0	0	30	1254.47274	-0.00027	2647.12455	1392.65154
23	2	2	1	-1	32	1	1	0	0	31	1256.74164	0.00049	2708.19879	1451.45764
24	2	2	1	-1	33	1	1	0	0	32	1259.02251*	-0.00238	2771.17709	1512.15220W
25	2	2	1	-1	34	1	1	0	0	33	1261.32399	-0.00007	2836.05847	1574.73441
26	2	2	1	-1	35	1	1	0	0	34	1263.63961	0.00111	2902.84192	1639.20342W
27	2	2	1	-1	36	1	1	0	0	35	1265.96843	0.00043	2971.52639	1705.55838
28	2	2	1	-1	37	1	1	0	0	36	1268.31325	0.00088	3042.11078	1773.79841
29	2	2	1	-1	38	1	1	0	0	37	1270.67227	0.00088	3114.59399	1843.92260
30	2	2	1	-1	1	1	-1	0	0	1	1190.87570*	-0.00012	1702.37037	511.49456
31	2	2	1	-1	2	1	-1	0	0	2	1190.87324*	0.00088	1706.18553	515.31316
32	2	2	1	-1	3	1	-1	0	0	3	1190.86756	0.00026	1711.90830	521.04101
33	2	2	1	-1	4	1	-1	0	0	4	1190.86060	-0.00016	1719.53877	528.67801
34	2	2	1	-1	5	1	-1	0	0	5	1190.85294	0.00001	1729.07700	538.22407
35	2	2	1	-1	6	1	-1	0	0	6	1190.84402	-0.00003	1740.52311	549.67906
36	2	2	1	-1	7	1	-1	0	0	7	1190.83446	0.00006	1753.87721	563.04281
37	2	2	1	-1	8	1	-1	0	0	8	1190.82457	0.00027	1769.13944	578.31514
38	2	2	1	-1	9	1	-1	0	0	9	1190.81391	-0.00021	1786.30996	595.49585
39	2	2	1	-1	10	1	-1	0	0	10	1190.80385	-0.00042	1805.38896	614.58469
40	2	2	1	-1	11	1	-1	0	0	11	1190.79537	0.00017	1826.37662	635.58142
41	2	2	1	-1	12	1	-1	0	0	12	1190.78779	0.00037	1849.27315	658.48573
42	2	-2	1	1	1	1	-1	0	0	2	1187.06680	0.00112	1702.37884	515.31316W
43	2	-2	1	1	2	1	-1	0	0	3	1185.16970	-0.00022	1706.21093	521.04101
44	2	-2	1	1	3	1	-1	0	0	4	1183.28190	0.00080	1711.95911	528.67801
45	2	-2	1	1	4	1	-1	0	0	5	1181.40013	0.00075	1719.62345	538.22407
46	2	-2	1	1	5	1	-1	0	0	6	1179.52500	0.00001	1729.20404	549.67906
47	2	-2	1	1	6	1	-1	0	0	7	1177.65787	-0.00032	1740.70099	563.04281
48	2	-2	1	1	7	1	-1	0	0	8	1175.79942	0.00013	1754.11443	578.31514
49	2	-2	1	1	8	1	-1	0	0	9	1173.94901	0.00037	1769.44449	595.49585
50	2	-2	1	1	9	1	-1	0	0	10	1172.10638	-0.00028	1786.69135	614.58469
51	2	-2	1	1	10	1	-1	0	0	11	1170.27362	-0.00015	1805.85519	635.58142
52	2	-2	1	1	11	1	-1	0	0	12	1168.45060	0.00014	1826.93619	658.48573
53	2	-2	1	1	12	1	-1	0	0	13	1166.63752	0.00028	1849.93456	683.29732
54	2	-2	1	1	13	1	-1	0	0	14	1164.83440	-0.00026	1874.85050	710.01584
55	2	-2	1	1	14	1	-1	0	0	15	1163.04340	0.00011	1901.68422	738.64093
56	2	-2	1	1	15	1	-1	0	0	16	1161.26393	0.00023	1930.43590	769.17220
57	2	-2	1	1	16	1	-1	0	0	17	1159.49658	0.00009	1961.10572	801.60923
58	2	-2	1	1	17	1	-1	0	0	18	1157.74273	0.00046	1993.69383	835.95156
59	2	-2	1	1	18	1	-1	0	0	19	1156.00182	0.00022	2028.20034	872.19874
60	2	-2	1	1	19	1	-1	0	0	20	1154.27546	0.00040	2064.62532	910.35027
	2	-2	1	1	20	1	-1	0	0	21	1152.56342	0.00024	2102.96880	950.40561
	2	-2	1	1	21	1	-1	0	0	22	1150.86713	0.00065	2143.23071	992.36423
	2	-2	1	1	22	1	-1	0	0	23	1149.18571	0.00030	2185.41096	1036.22555
	2	-2	1	1	23	1	-1	0	0	24	1147.52162	0.00122	2229.50936	1081.98896W
	2	-2	1	1	24	1	-1	0	0	25	1145.87200	0.00021	2275.52563	1129.65384
	2	-2	1	1	25	1	-1	0	0	26	1144.23986	-0.00004	2323.45944	1179.21954
	2	-2	1	1	26	1	-1	0	0	27	1142.62528	0.00031	2373.31035	1230.68537
	2	-2	1	1	27	1	-1	0	0	28	1141.02734	0.00013	2425.07785	1284.05064
	2	-2	1	1	28	1	-1	0	0	29	1139.44689	0.00014	2478.76136	1339.31460

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2	-2	1	1	29	1	-1	0	0	30	1137.88357	-0.00012	2534.36020	1396.47651
2	-2	1	1	30	1	-1	0	0	31	1136.33846	0.00038	2591.87365	1455.53557
2	-2	1	1	31	1	-1	0	0	32	1134.80957	-0.00034	2651.30089	1516.49098
2	-2	1	1	32	1	-1	0	0	33	1133.29915	-0.00002	2712.64107	1579.34190
2	-2	1	1	33	1	-1	0	0	34	1131.80564	-0.00015	2775.89327	1644.08748
2	-2	1	1	34	1	-1	0	0	35	1130.32876	-0.00093	2841.05651	1710.72682
2	-2	1	1	35	1	-1	0	0	36	1128.86989	-0.00088	2908.12977	1779.25901
2	-2	1	1	36	1	-1	0	0	37	1127.42642	-0.00247	2977.11201	1849.68311W
2	-2	1	1	37	1	-1	0	0	38	1125.99967	-0.00427	3048.00210	1921.99816W
2	-2	1	1	2	1	-1	0	0	1	1194.71643	0.00006	1706.21093	511.49456
2	-2	1	1	3	1	-1	0	0	2	1196.64660	0.00065	1711.95911	515.31316
2	-2	1	1	4	1	-1	0	0	3	1198.58230	-0.00014	1719.62345	521.04101
2	-2	1	1	5	1	-1	0	0	4	1200.52604	0.00001	1729.20404	528.67801
2	-2	1	1	6	1	-1	0	0	5	1202.47685	-0.00007	1740.70099	538.22407
2	-2	1	1	7	1	-1	0	0	6	1204.43520	-0.00017	1754.11443	549.67906
2	-2	1	1	8	1	-1	0	0	7	1206.40182	0.00013	1769.44449	563.04281
2	-2	1	1	9	1	-1	0	0	8	1208.37591	-0.00030	1786.69135	578.31514
2	-2	1	1	10	1	-1	0	0	9	1210.35921	-0.00013	1805.85519	595.49585
2	-2	1	1	11	1	-1	0	0	10	1212.35102	-0.00048	1826.93619	614.58469
2	-2	1	1	12	1	-1	0	0	11	1214.35314	0.00000	1849.93456	635.58142
2	-2	1	1	13	1	-1	0	0	12	1216.36469	-0.00008	1874.85050	658.48573
2	-2	1	1	14	1	-1	0	0	13	1218.38743	0.00053	1901.68422	683.29732
2	-2	1	1	15	1	-1	0	0	14	1220.42037	0.00031	1930.43590	710.01584
2	-2	1	1	16	1	-1	0	0	15	1222.46555	0.00076	1961.10572	738.64093
2	-2	1	1	17	1	-1	0	0	16	1224.52244	0.00081	1993.69383	769.17220
2	-2	1	1	18	1	-1	0	0	17	1226.59151	0.00040	2028.20034	801.60923
2	-2	1	1	19	1	-1	0	0	18	1228.67410	0.00034	2064.62532	835.95156
2	-2	1	1	20	1	-1	0	0	19	1230.77150	0.00145	2102.96880	872.19874W
2	-2	1	1	21	1	-1	0	0	20	1232.88080	0.00035	2143.23071	910.35027
2	-2	1	1	22	1	-1	0	0	21	1235.00597	0.00062	2185.41096	950.40561
2	-2	1	1	23	1	-1	0	0	22	1237.14530	0.00017	2229.50936	992.36423
2	-2	1	1	24	1	-1	0	0	23	1239.30012	0.00004	2275.52563	1036.22555
2	-2	1	1	25	1	-1	0	0	24	1241.47072	0.00024	2323.45944	1081.98896
2	-2	1	1	26	1	-1	0	0	25	1243.65682	0.00031	2373.31035	1129.65384
2	-2	1	1	27	1	-1	0	0	26	1245.85841	0.00010	2425.07785	1179.21954
2	-2	1	1	28	1	-1	0	0	27	1248.07594	-0.00004	2478.76136	1230.68537
2	-2	1	1	29	1	-1	0	0	28	1250.30961	0.00005	2534.36020	1284.05064
2	-2	1	1	30	1	-1	0	0	29	1252.55952	0.00048	2591.87365	1339.31460
2	-2	1	1	31	1	-1	0	0	30	1254.82412	-0.00027	2651.30089	1396.47651
2	-2	1	1	32	1	-1	0	0	31	1257.10548	-0.00002	2712.64107	1455.53557
2	-2	1	1	33	1	-1	0	0	32	1259.40211	-0.00018	2775.89327	1516.49098
2	-2	1	1	34	1	-1	0	0	33	1261.71403	-0.00057	2841.05651	1579.34190
2	-2	1	1	35	1	-1	0	0	34	1264.04231	0.00001	2908.12977	1644.08748
2	-2	1	1	36	1	-1	0	0	35	1266.38466	-0.00053	2977.11201	1710.72682
2	-2	1	1	37	1	-1	0	0	36	1268.74245	-0.00064	3048.00210	1779.25901
2	-2	1	1	38	1	-1	0	0	37	1271.11553	-0.00029	3120.79893	1849.68311
2	-2	1	1	1	1	1	0	0	1	1190.89259	0.00002	1702.37884	511.48627
2	-2	1	1	2	1	1	0	0	2	1190.92247	-0.00015	1706.21093	515.28830
2	-2	1	1	3	1	1	0	0	3	1190.96769	-0.00013	1711.95911	520.99129
2	-2	1	1	4	1	1	0	0	4	1191.02800	-0.00030	1719.62345	528.59515
2	-2	1	1	5	1	1	0	0	5	1191.10415	-0.00010	1729.20404	538.09979
2	-2	1	1	6	1	1	0	0	6	1191.19612	0.00021	1740.70099	549.50508
2	-2	1	1	7	1	1	0	0	7	1191.30377	0.00021	1754.11443	562.81086
2	-2	1	1	8	1	1	0	0	8	1191.42657	-0.00096	1769.44449	578.01697
2	-2	1	1	9	1	1	0	0	9	1191.56815	-0.00002	1786.69135	595.12319
2	-2	1	1	10	1	1	0	0	10	1191.72479	-0.00111	1805.85519	614.12929W
2	-2	1	1	11	1	1	0	0	11	1191.90066	-0.00050	1826.93619	635.03503
2	-2	1	1	12	1	1	0	0	12	1192.09354	-0.00090	1849.93456	657.84012
2	-2	1	1	13	1	1	0	0	13	1192.30639	0.00015	1874.85050	682.54427
2	-2	1	1	14	1	1	0	0	14	1192.53616	-0.00093	1901.68422	709.14713
2	-2	1	1	15	1	1	0	0	15	1192.78717	-0.00037	1930.43590	737.64836

rms = 0.00034 cm⁻¹

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

	$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
1	2 0 1 1 1	0 0 1 1 2	1013.39836	0.00034	1693.33369	679.93567
2	2 0 1 1 2	0 0 1 1 3	1011.52521	-0.00013	1697.16027	685.63493
3	2 0 1 1 3	0 0 1 1 4	1009.66603	-0.00008	1702.89992	693.23382
4	2 0 1 1 4	0 0 1 1 5	1007.81979	-0.00038	1710.55241	702.73224
5	2 0 1 1 5	0 0 1 1 6	1005.98735	0.00002	1720.11740	714.13007
6	2 0 1 1 6	0 0 1 1 7	1004.16718	-0.00011	1731.59446	727.42716
7	2 0 1 1 7	0 0 1 1 8	1002.35955	-0.00017	1744.98305	742.62333
8	2 0 1 1 8	0 0 1 1 9	1000.56475	0.00058	1760.28255	759.71839
9	2 0 1 1 9	0 0 1 1 10	998.78011	-0.00002	1777.49222	778.71209
10	2 0 1 1 10	0 0 1 1 11	997.00697	-0.00002	1796.61120	799.60420
11	2 0 1 1 11	0 0 1 1 12	995.24406	0.00002	1817.63849	822.39444
12	2 0 1 1 12	0 0 1 1 13	993.49032	-0.00015	1840.57298	847.08251
13	2 0 1 1 13	0 0 1 1 14	991.74526	-0.00008	1865.41342	873.66808
14	2 0 1 1 14	0 0 1 1 15	990.00767	0.00004	1892.15842	902.15079
15	2 0 1 1 15	0 0 1 1 16	988.27640	0.00021	1920.80648	932.53028
16	2 0 1 1 16	0 0 1 1 17	986.54977	-0.00005	1951.35596	964.80614
17	2 0 1 1 17	0 0 1 1 18	984.82710	-0.00010	1983.80515	998.97795
18	2 0 1 1 18	0 0 1 1 19	983.10716	0.00015	2018.15225	1035.04524
19	2 0 1 1 19	0 0 1 1 20	981.38781	-0.00010	2054.39547	1073.00756
20	2 0 1 1 20	0 0 1 1 21	979.66850	-0.00011	2092.53300	1112.86438
21	2 0 1 1 21	0 0 1 1 22	977.94831	0.00042	2132.56309	1154.61520
22	2 0 1 1 22	0 0 1 1 23	976.22465	0.00000	2174.48410	1198.25945
23	2 0 1 1 23	0 0 1 1 24	974.49798	0.00004	2218.29450	1243.79656
24	2 0 1 1 24	0 0 1 1 25	972.76675	-0.00024	2263.99292	1291.22593
25	2 0 1 1 25	0 0 1 1 26	971.03126	0.00006	2311.57813	1340.54693
26	2 0 1 1 26	0 0 1 1 27	969.29019	0.00003	2361.04907	1391.75891
27	2 0 1 1 27	0 0 1 1 28	967.54379	0.00017	2412.40481	1444.86119
28	2 0 1 1 28	0 0 1 1 29	965.79124	-0.00021	2465.64452	1499.85307
29	2 0 1 1 29	0 0 1 1 30	964.03353	-0.00013	2520.76749	1556.73383
30	2 0 1 1 30	0 0 1 1 31	962.27062	0.00025	2577.77308	1615.50271
31	2 0 1 1 31	0 0 1 1 32	960.50174	-0.00002	2636.66069	1676.15894
32	2 0 1 1 32	0 0 1 1 33	958.72815	0.00010	2697.42976	1738.70171
33	2 0 1 1 2	0 0 1 1 1	1021.02536	0.00122	1697.16027	676.13613W
34	2 0 1 1 3	0 0 1 1 2	1022.96425	0.00000	1702.89992	679.93567
35	2 0 1 1 4	0 0 1 1 3	1024.91720	-0.00029	1710.55241	685.63493
36	2 0 1 1 5	0 0 1 1 4	1026.88345	-0.00013	1720.11740	693.23382
37	2 0 1 1 6	0 0 1 1 5	1028.86157	-0.00065	1731.59446	702.73224
38	2 0 1 1 7	0 0 1 1 6	1030.85303	0.00005	1744.98305	714.13007
39	2 0 1 1 8	0 0 1 1 7	1032.85531	-0.00008	1760.28255	727.42716
40	2 0 1 1 9	0 0 1 1 8	1034.86895	0.00006	1777.49222	742.62333
41	2 0 1 1 10	0 0 1 1 9	1036.89272	-0.00009	1796.61120	759.71839
42	2 0 1 1 11	0 0 1 1 10	1038.92648	0.00009	1817.63849	778.71209
43	2 0 1 1 12	0 0 1 1 11	1040.96897	0.00020	1840.57298	799.60420
44	2 0 1 1 13	0 0 1 1 12	1043.01906	0.00009	1865.41342	822.39444
45	2 0 1 1 14	0 0 1 1 13	1045.07601	0.00010	1892.15842	847.08251
46	2 0 1 1 15	0 0 1 1 14	1047.13850	0.00010	1920.80648	873.66808
47	2 0 1 1 16	0 0 1 1 15	1049.20513	-0.00003	1951.35596	902.15079
48	2 0 1 1 17	0 0 1 1 16	1051.27506	0.00020	1983.80515	932.53028
49	2 0 1 1 18	0 0 1 1 17	1053.34605	-0.00006	2018.15225	964.80614
50	2 0 1 1 19	0 0 1 1 18	1055.41754	0.00001	2054.39547	998.97795
51	2 0 1 1 20	0 0 1 1 19	1057.48784	0.00009	2092.53300	1035.04524
52	2 0 1 1 21	0 0 1 1 20	1059.55536	-0.00017	2132.56309	1073.00756
53	2 0 1 1 22	0 0 1 1 21	1061.61979	0.00008	2174.48410	1112.86438
54	2 0 1 1 23	0 0 1 1 22	1063.67926	-0.00004	2218.29450	1154.61520
55	2 0 1 1 24	0 0 1 1 23	1065.73337	-0.00010	2263.99292	1198.25945
56	2 0 1 1 25	0 0 1 1 24	1067.78126	-0.00031	2311.57813	1243.79656
57	2 0 1 1 26	0 0 1 1 25	1069.82270	-0.00044	2361.04907	1291.22593
58	2 0 1 1 27	0 0 1 1 26	1071.85772	-0.00016	2412.40481	1340.54693
59	2 0 1 1 28	0 0 1 1 27	1073.88505	-0.00056	2465.64452	1391.75891
60	2 0 1 1 29	0 0 1 1 28	1075.90648	0.00018	2520.76749	1444.86119
	2 0 1 1 30	0 0 1 1 29	1077.91981	-0.00020	2577.77308	1499.85307
	2 0 1 1 31	0 0 1 1 30	1079.92670	-0.00016	2636.66069	1556.73383
	2 0 1 1 32	0 0 1 1 31	1081.92679	-0.00026	2697.42976	1615.50271
	2 0 1 1 33	0 0 1 1 32	1083.92023	-0.00056	2760.07973	1676.15894
	2 0 1 1 34	0 0 1 1 33	1085.90846	0.00013	2824.61004	1738.70171
	2 0 1 1 35	0 0 1 1 34	1087.89056	0.00062	2891.02013	1803.13019
	2 0 1 1 36	0 0 1 1 35	1089.86659	0.00077	2959.30942	1869.44355

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2	0	1	1	1	0	0	1	-1	1	1017.19092	-0.00012	1693.33369	676.14265
2	0	1	1	2	0	0	1	-1	2	1017.20485	-0.00018	1697.16027	679.95524
2	0	1	1	3	0	0	1	-1	3	1017.22648	0.00061	1702.89992	685.67405
2	0	1	1	4	0	0	1	-1	4	1017.25357	0.00018	1710.55241	693.29902
2	0	1	1	5	0	0	1	-1	5	1017.28783	0.00047	1720.11740	702.83004
2	0	1	1	6	0	0	1	-1	6	1017.32734	-0.00013	1731.59446	714.26698
2	0	1	1	7	0	0	1	-1	7	1017.36989*	-0.00347	1744.98305	727.60969W
2	0	1	1	8	0	0	1	-1	8	1017.42482	0.00026	1760.28255	742.85799
2	0	1	-1	1	0	0	1	-1	2	1013.37676	0.00018	1693.33182	679.95524
2	0	1	-1	2	0	0	1	-1	3	1011.47995	-0.00063	1697.15463	685.67405
2	0	1	-1	3	0	0	1	-1	4	1009.58856*	-0.00107	1702.88865	693.29902W
2	0	1	-1	4	0	0	1	-1	5	1007.70341	-0.00018	1710.53362	702.83004
2	0	1	-1	5	0	0	1	-1	6	1005.82196	-0.00029	1720.08923	714.26698
2	0	1	-1	6	0	0	1	-1	7	1003.94538	0.00000	1731.55507	727.60969
2	0	1	-1	7	0	0	1	-1	8	1002.07145*	-0.00124	1744.93068	742.85799W
2	0	1	-1	8	0	0	1	-1	9	1000.20379	-0.00008	1760.21554	760.01168
2	0	1	-1	9	0	0	1	-1	10	998.33840	-0.00015	1777.40907	779.07052
2	0	1	-1	10	0	0	1	-1	11	996.47639	0.00001	1796.51064	800.03426
2	0	1	-1	11	0	0	1	-1	12	994.61706	0.00009	1817.51959	822.90261
2	0	1	-1	12	0	0	1	-1	13	992.75996	0.00002	1840.43522	847.67528
2	0	1	-1	13	0	0	1	-1	14	990.90512	0.00021	1865.25684	874.35193
2	0	1	-1	14	0	0	1	-1	15	989.05169	0.00018	1891.98370	902.93220
2	0	1	-1	15	0	0	1	-1	16	987.19946	0.00006	1920.61510	933.41570
2	0	1	-1	16	0	0	1	-1	17	985.34860	0.00033	1951.15030	965.80204
2	0	1	-1	17	0	0	1	-1	18	983.49804	0.00021	1983.58860	1000.09076
2	0	1	-1	18	0	0	1	-1	19	981.64804	0.00019	2017.92928	1036.28142
2	0	1	-1	19	0	0	1	-1	20	979.79839	0.00028	2054.17165	1074.37353
2	0	1	-1	20	0	0	1	-1	21	977.94831	-0.00015	2092.31503	1114.36658
2	0	1	-1	21	0	0	1	-1	22	976.09913	0.00039	2132.35877	1156.26002
2	0	1	-1	22	0	0	1	-1	23	974.24915	0.00027	2174.30219	1200.05331
2	0	1	-1	23	0	0	1	-1	24	972.39887	0.00006	2218.14465	1245.74584
2	0	1	-1	24	0	0	1	-1	25	970.54857	0.00008	2263.88551	1293.33701
2	0	1	-1	25	0	0	1	-1	26	968.69806	0.00014	2311.52410	1342.82618
2	0	1	-1	26	0	0	1	-1	27	966.84722	0.00012	2361.05979	1394.21269
2	0	1	-1	27	0	0	1	-1	28	964.99616	0.00011	2412.49189	1447.49584
2	0	1	-1	28	0	0	1	-1	29	963.14452	-0.00031	2465.81975	1502.67492
2	0	1	-1	29	0	0	1	-1	30	961.29340	-0.00007	2521.04267	1559.74920
2	0	1	-1	30	0	0	1	-1	31	959.44188	-0.00016	2578.15994	1618.71789
2	0	1	-1	31	0	0	1	-1	32	957.59021	-0.00039	2637.17082	1679.58023
2	0	1	-1	32	0	0	1	-1	33	955.73859	-0.00061	2698.07457	1742.33538
2	0	1	-1	33	0	0	1	-1	34	953.88724	-0.00068	2760.87042	1806.98250
2	0	1	-1	34	0	0	1	-1	35	952.03568	-0.00113	2825.55755	1873.52074W
2	0	1	-1	35	0	0	1	-1	36	950.18585	-0.00010	2892.13513	1941.94919
2	0	1	-1	2	0	0	1	-1	1	1021.01167	-0.00031	1697.15463	676.14265
2	0	1	-1	3	0	0	1	-1	2	1022.93344	0.00002	1702.88865	679.95524
2	0	1	-1	4	0	0	1	-1	3	1024.85949	-0.00008	1710.53362	685.67405
2	0	1	-1	5	0	0	1	-1	4	1026.79031	0.00010	1720.08923	693.29902
2	0	1	-1	6	0	0	1	-1	5	1028.72505	0.00002	1731.55507	702.83004
2	0	1	-1	7	0	0	1	-1	6	1030.66370	0.00000	1744.93068	714.26698
2	0	1	-1	8	0	0	1	-1	7	1032.60592	0.00007	1760.21554	727.60969
2	0	1	-1	9	0	0	1	-1	8	1034.55125	0.00017	1777.40907	742.85799
2	0	1	-1	10	0	0	1	-1	9	1036.49901	0.00005	1796.51064	760.01168
2	0	1	-1	11	0	0	1	-1	10	1038.44917	0.00010	1817.51959	779.07052
2	0	1	-1	12	0	0	1	-1	11	1040.40110	0.00013	1840.43522	800.03426
2	0	1	-1	13	0	0	1	-1	12	1042.35483	0.00061	1865.25684	822.90261
2	0	1	-1	14	0	0	1	-1	13	1044.30838	-0.00004	1891.98370	847.67528
2	0	1	-1	15	0	0	1	-1	14	1046.26351	0.00034	1920.61510	874.35193
2	0	1	-1	16	0	0	1	-1	15	1048.21825	0.00014	1951.15030	902.93220
2	0	1	-1	17	0	0	1	-1	16	1050.17310	0.00021	1983.58860	933.41570
2	0	1	-1	18	0	0	1	-1	17	1052.12753	0.00029	2017.92928	965.80204
2	0	1	-1	19	0	0	1	-1	18	1054.08120	0.00032	2054.17165	1000.09076
2	0	1	-1	20	0	0	1	-1	19	1056.03364	0.00003	2092.31503	1036.28142
2	0	1	-1	21	0	0	1	-1	20	1057.98545	0.00022	2132.35877	1074.37353
2	0	1	-1	22	0	0	1	-1	21	1059.93608	0.00047	2174.30219	1114.36658
2	0	1	-1	23	0	0	1	-1	22	1061.88483	0.00020	2218.14465	1156.26002
2	0	1	-1	24	0	0	1	-1	23	1063.83238	0.00018	2263.88551	1200.05331
2	0	1	-1	25	0	0	1	-1	24	1065.77841	0.00015	2311.52410	1245.74584
2	0	1	-1	26	0	0	1	-1	25	1067.72316	0.00039	2361.05979	1293.33701
2	0	1	-1	27	0	0	1	-1	26	1069.66543	0.00028	2412.49189	1342.82618

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1	2	0	1	-1	28	0	0	1	-1	27	1071.60766	0.00060	2465.81975	1394.21269
2	2	0	1	-1	29	0	0	1	-1	28	1073.54730	0.00047	2521.04267	1447.49584
3	2	0	1	-1	30	0	0	1	-1	29	1075.48518	0.00017	2578.15994	1502.67492
4	2	0	1	-1	31	0	0	1	-1	30	1077.42185	0.00022	2637.17082	1559.74920
5	2	0	1	-1	32	0	0	1	-1	31	1079.35708	0.00040	2698.07457	1618.71789
6	2	0	1	-1	33	0	0	1	-1	32	1081.28941	-0.00078	2760.87042	1679.58023
7	2	0	1	-1	34	0	0	1	-1	33	1083.22205	-0.00012	2825.55755	1742.33538
8	2	0	1	-1	35	0	0	1	-1	34	1085.15219	-0.00044	2892.13513	1806.98250
9	2	0	1	-1	36	0	0	1	-1	35	1087.08085	-0.00074	2960.60232	1873.52074
10	2	0	1	-1	37	0	0	1	-1	36	1089.00879	-0.00025	3030.95823	1941.94919
11	2	0	1	-1	1	0	0	1	1	1	1017.19706*	0.00137	1693.33182	676.13613W
12	2	0	1	-1	2	0	0	1	1	2	1017.21875	-0.00021	1697.15463	679.93567
13	2	0	1	-1	3	0	0	1	1	3	1017.25357	-0.00015	1702.88865	685.63493
14	2	0	1	-1	4	0	0	1	1	4	1017.29953	-0.00028	1710.53362	693.23382
15	2	0	1	-1	5	0	0	1	1	5	1017.35694	-0.00005	1720.08923	702.73224
16	2	0	1	-1	6	0	0	1	1	6	1017.42482	-0.00018	1731.55507	714.13007
17	2	0	1	-1	7	0	0	1	1	7	1017.50381	0.00029	1744.93068	727.42716
18	2	0	1	-1	8	0	0	1	1	8	1017.59218	-0.00003	1760.21554	742.62333
19	2	0	1	-1	9	0	0	1	1	9	1017.69004	-0.00064	1777.40907	759.71839

rms = 0.00028 cm⁻¹

2v₄ + v₅ (¹Π) ← v₅ (Π)

v ₄ '	l ₄ '	v ₅ '	l ₅ '	J'	v ₄ ''	l ₄ ''	v ₅ ''	l ₅ ''	J''	OBS	OBS - CALC	G'	G''
2	2	1	-1	1	0	0	1	1	2	1022.43459	-0.00011	1702.37037	679.93567
2	2	1	-1	2	0	0	1	1	3	1020.55074	0.00014	1706.18553	685.63493
2	2	1	-1	3	0	0	1	1	4	1018.67479	0.00030	1711.90830	693.23382
2	2	1	-1	4	0	0	1	1	5	1016.80716	0.00063	1719.53877	702.73224
2	2	1	-1	5	0	0	1	1	6	1014.95043*	0.00350	1729.07700	714.13007W
2	2	1	-1	7	0	0	1	1	8	1011.25515	0.00128	1753.87721	742.62333W
2	2	1	-1	8	0	0	1	1	9	1009.42082	-0.00023	1769.13944	759.71839
2	2	1	-1	9	0	0	1	1	10	1007.59769	-0.00018	1786.30996	778.71209
2	2	1	-1	10	0	0	1	1	11	1005.78613	0.00137	1805.38896	799.60420W
2	2	1	-1	11	0	0	1	1	12	1003.98202	-0.00016	1826.37662	822.39444
2	2	1	-1	12	0	0	1	1	13	1002.19043	-0.00021	1849.27315	847.08251
2	2	1	-1	13	0	0	1	1	14	1000.41132	0.00064	1874.07876	873.66808
2	2	1	-1	14	0	0	1	1	15	998.64259	-0.00028	1900.79367	902.15079
2	2	1	-1	15	0	0	1	1	16	996.88744	-0.00036	1929.41808	932.53028
2	2	1	-1	16	0	0	1	1	17	995.14436	-0.00169	1959.95219	964.80614W
2	2	1	-1	17	0	0	1	1	18	993.41756	-0.00068	1992.39619	998.97795
2	2	1	-1	18	0	0	1	1	19	991.70515	0.00018	2026.75022	1035.04524
2	2	1	-1	19	0	0	1	1	20	990.00766	0.00083	2063.01439	1073.00756
2	2	1	-1	20	0	0	1	1	21	988.32359	-0.00078	2101.18875	1112.86438
2	2	1	-1	21	0	0	1	1	22	986.65773	-0.00039	2141.27332	1154.61520
2	2	1	-1	22	0	0	1	1	23	985.00732	-0.00125	2183.26802	1198.25945W
2	2	1	-1	23	0	0	1	1	24	983.37587	-0.00027	2227.17270	1243.79656
2	2	1	-1	24	0	0	1	1	25	981.76044	-0.00077	2272.98715	1291.22593
2	2	1	-1	25	0	0	1	1	26	980.16268	-0.00142	2320.71103	1340.54693W
2	2	1	-1	4	0	0	1	1	3	1033.90498*	0.00114	1719.53877	685.63493W
2	2	1	-1	6	0	0	1	1	5	1037.79125	0.00038	1740.52311	702.73224
2	2	1	-1	7	0	0	1	1	6	1039.74697	-0.00016	1753.87721	714.13007
2	2	1	-1	8	0	0	1	1	7	1041.71214	-0.00014	1769.13944	727.42716
2	2	1	-1	9	0	0	1	1	8	1043.68665	0.00002	1786.30996	742.62333
2	2	1	-1	10	0	0	1	1	9	1045.67040	-0.00018	1805.38896	759.71839
2	2	1	-1	11	0	0	1	1	10	1047.66465	0.00012	1826.37662	778.71209
2	2	1	-1	12	0	0	1	1	11	1049.66907	0.00012	1849.27315	799.60420
2	2	1	-1	13	0	0	1	1	12	1051.68441	0.00009	1874.07876	822.39444
2	2	1	-1	14	0	0	1	1	13	1053.71077	-0.00039	1900.79367	847.08251
2	2	1	-1	15	0	0	1	1	14	1055.74936	-0.00064	1929.41808	873.66808
2	2	1	-1	16	0	0	1	1	15	1057.80092	-0.00048	1959.95219	902.15079
2	2	1	-1	17	0	0	1	1	16	1059.86588	-0.00003	1992.39619	932.53028
2	2	1	-1	18	0	0	1	1	17	1061.94422	0.00014	2026.75022	964.80614
2	2	1	-1	19	0	0	1	1	18	1064.03651	0.00007	2063.01439	998.97795
2	2	1	-1	20	0	0	1	1	19	1066.14189*	-0.00162	2101.18875	1035.04524W
2	2	1	-1	21	0	0	1	1	20	1068.25727	-0.00078	2141.27332	1073.00756

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2	2	1	-1	22	0	0	1	1	21	1070.40412	0.00048	2183.26802	1112.86438
2	2	1	-1	23	0	0	1	1	22	1072.55609	-0.00141	2227.17270	1154.61520W
2	2	1	-1	24	0	0	1	1	23	1074.72661	-0.00108	2272.98715	1198.25945W
2	2	1	-1	25	0	0	1	1	24	1076.91342	-0.00105	2320.71103	1243.79656W
2	2	1	-1	26	0	0	1	1	25	1079.11777	-0.00027	2370.34397	1291.22593
2	2	1	-1	27	0	0	1	1	26	1081.33904	0.00050	2421.88547	1340.54693
2	2	1	-1	28	0	0	1	1	27	1083.57651	0.00045	2475.33497	1391.75891
2	-2	1	1	1	0	0	1	-1	2	1022.42334	-0.00026	1702.37884	679.95524
2	-2	1	1	2	0	0	1	-1	3	1020.53609	-0.00078	1706.21093	685.67405
2	-2	1	1	3	0	0	1	-1	4	1018.66074	0.00065	1711.95911	693.29902
2	-2	1	1	4	0	0	1	-1	5	1016.79520*	0.00179	1719.62345	702.83004W
2	-2	1	1	5	0	0	1	-1	6	1014.93709	0.00003	1729.20404	714.26698
2	-2	1	1	6	0	0	1	-1	7	1013.09162	0.00032	1740.70099	727.60969
2	-2	1	1	7	0	0	1	-1	8	1011.25516	-0.00128	1754.11443	742.85799W
2	-2	1	1	8	0	0	1	-1	9	1009.43222	-0.00060	1769.44449	760.01168
2	-2	1	1	9	0	0	1	-1	10	1007.62072	-0.00012	1786.69135	779.07052
2	-2	1	1	10	0	0	1	-1	11	1005.82195	0.00102	1805.85519	800.03426W
2	-2	1	1	11	0	0	1	-1	12	1004.03373	0.00015	1826.93619	822.90261
2	-2	1	1	12	0	0	1	-1	13	1002.25491*	-0.00437	1849.93456	847.67528W
2	-2	1	1	13	0	0	1	-1	14	1000.49861	0.00004	1874.85050	874.35193
2	-2	1	1	14	0	0	1	-1	15	998.75276	0.00074	1901.68422	902.93220
2	-2	1	1	15	0	0	1	-1	16	997.02019	-0.00001	1930.43590	933.41570
2	-2	1	1	16	0	0	1	-1	17	995.30410	0.00042	1961.10572	965.80204
2	-2	1	1	17	0	0	1	-1	18	993.60286	-0.00021	1993.69383	1000.09076
2	-2	1	1	18	0	0	1	-1	19	991.91961	0.00069	2028.20034	1036.28142
2	-2	1	1	19	0	0	1	-1	20	990.25198	0.00019	2064.62532	1074.37353
2	-2	1	1	20	0	0	1	-1	21	988.60537*	0.00315	2102.96880	1114.36658W
2	-2	1	1	21	0	0	1	-1	22	986.97075	0.00006	2143.23071	1156.26002
2	-2	1	1	22	0	0	1	-1	23	985.35720	-0.00046	2185.41096	1200.05331
2	-2	1	1	23	0	0	1	-1	24	983.76031*	-0.00321	2229.50936	1245.74584W
2	-2	1	1	24	0	0	1	-1	25	982.19028*	0.00166	2275.52563	1293.33701W
2	-2	1	1	25	0	0	1	-1	26	980.63348	0.00022	2323.45944	1342.82618
2	-2	1	1	26	0	0	1	-1	27	979.09728	-0.00038	2373.31035	1394.21269
2	-2	1	1	27	0	0	1	-1	28	977.58090*	-0.00111	2425.07785	1447.49584W
2	-2	1	1	28	0	0	1	-1	29	976.08540	-0.00103	2478.76136	1502.67492W
2	-2	1	1	29	0	0	1	-1	30	974.61085	-0.00015	2534.36020	1559.74920
2	-2	1	1	30	0	0	1	-1	31	973.15554	-0.00021	2591.87365	1618.71789
2	-2	1	1	31	0	0	1	-1	32	971.71953	-0.00114	2651.30089	1679.58023W
2	-2	1	1	32	0	0	1	-1	33	970.30516	-0.00054	2712.64107	1742.33538
2	-2	1	1	33	0	0	1	-1	34	968.91011	-0.00066	2775.89327	1806.98250
2	-2	1	1	2	0	0	1	-1	1	1030.06936	0.00108	1706.21093	676.14265W
2	-2	1	1	3	0	0	1	-1	2	1032.00540	0.00153	1711.95911	679.95524W
2	-2	1	1	4	0	0	1	-1	3	1033.95230*	0.00290	1719.62345	685.67405W
2	-2	1	1	5	0	0	1	-1	4	1035.90449	-0.00053	1729.20404	693.29902
2	-2	1	1	6	0	0	1	-1	5	1037.87092	-0.00003	1740.70099	702.83004
2	-2	1	1	7	0	0	1	-1	6	1039.84749	0.00004	1754.11443	714.26698
2	-2	1	1	8	0	0	1	-1	7	1041.83512	0.00032	1769.44449	727.60969
2	-2	1	1	9	0	0	1	-1	8	1043.83361	0.00025	1786.69135	742.85799
2	-2	1	1	10	0	0	1	-1	9	1045.84377	0.00026	1805.85519	760.01168
2	-2	1	1	11	0	0	1	-1	10	1047.86607	0.00040	1826.93619	779.07052
2	-2	1	1	12	0	0	1	-1	11	1049.90042	0.00011	1849.93456	800.03426
2	-2	1	1	13	0	0	1	-1	12	1051.94838	0.00049	1874.85050	822.90261
2	-2	1	1	14	0	0	1	-1	13	1054.00860	-0.00034	1901.68422	847.67528
2	-2	1	1	15	0	0	1	-1	14	1056.08385	-0.00012	1930.43590	874.35193
2	-2	1	1	16	0	0	1	-1	15	1058.17326	-0.00026	1961.10572	902.93220
2	-2	1	1	17	0	0	1	-1	16	1060.27644*	-0.00169	1993.69383	933.41570W
2	-2	1	1	18	0	0	1	-1	17	1062.39819	-0.00011	2028.20034	965.80204
2	-2	1	1	19	0	0	1	-1	18	1064.53461	0.00005	2064.62532	1000.09076
2	-2	1	1	20	0	0	1	-1	19	1066.68740	0.00003	2102.96880	1036.28142
2	-2	1	1	21	0	0	1	-1	20	1068.85740	0.00022	2143.23071	1074.37353
2	-2	1	1	23	0	0	1	-1	22	1073.25035*	0.00101	2229.50936	1156.26002W
2	-2	1	1	24	0	0	1	-1	23	1075.47210	-0.00023	2275.52563	1200.05331
2	-2	1	1	25	0	0	1	-1	24	1077.71376	0.00016	2323.45944	1245.74584
2	-2	1	1	26	0	0	1	-1	25	1079.97371	0.00037	2373.31035	1293.33701
2	-2	1	1	27	0	0	1	-1	26	1082.25131	-0.00036	2425.07785	1342.82618
2	-2	1	1	28	0	0	1	-1	27	1084.55104*	0.00237	2478.76136	1394.21269W
2	-2	1	1	29	0	0	1	-1	28	1086.86449	0.00013	2534.36020	1447.49584
2	-2	1	1	30	0	0	1	-1	29	1089.19859	-0.00013	2591.87365	1502.67492
2	-2	1	1	31	0	0	1	-1	30	1091.55141	0.00039	2651.30089	1559.74920

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2	-2	1	1	32	0	0	1	-1	31	1093.92305	-0.00013	2712.64107	1618.71789
2	-2	1	1	33	0	0	1	-1	32	1096.31320	0.00016	2775.89327	1679.58023
2	-2	1	1	34	0	0	1	-1	33	1098.72082	-0.00031	2841.05651	1742.33538
2	-2	1	1	35	0	0	1	-1	34	1101.14745	0.00018	2908.12977	1806.98250

rms = 0.00037 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	G'	G''
1 1 2 0 1	1 1 0 0 2	1332.57162	0.00031	1847.85961	515.28830
1 1 2 0 2	1 1 0 0 3	1330.68339	-0.00011	1851.67479	520.99129
1 1 2 0 3	1 1 0 0 4	1328.80214	-0.00017	1857.39746	528.59515
1 1 2 0 4	1 1 0 0 5	1326.92814	0.00043	1865.02750	538.09979
1 1 2 0 5	1 1 0 0 6	1325.05973	0.00007	1874.56474	549.50508
1 1 2 0 6	1 1 0 0 7	1323.19806	-0.00006	1886.00898	562.81086
1 1 2 0 7	1 1 0 0 8	1321.34311	0.00009	1899.35999	578.01697
1 1 2 0 8	1 1 0 0 9	1319.49525	0.00098	1914.61746	595.12319
1 1 2 0 9	1 1 0 0 10	1317.65211	0.00032	1931.78108	614.12929
1 1 2 0 10	1 1 0 0 11	1315.81518	-0.00026	1950.85047	635.03503
1 1 2 0 11	1 1 0 0 12	1313.98520	0.00009	1971.82524	657.84012
1 1 2 0 12	1 1 0 0 13	1312.16073	0.00009	1994.70491	682.54427
1 1 2 0 13	1 1 0 0 14	1310.34219	0.00032	2019.48900	709.14713
1 1 2 0 14	1 1 0 0 15	1308.52797	-0.00064	2046.17697	737.64836
1 1 2 0 15	1 1 0 0 16	1306.72072	0.00005	2074.76824	768.04757
1 1 2 0 16	1 1 0 0 17	1304.91844	0.00062	2105.26218	800.34436
1 1 2 0 17	1 1 0 0 18	1303.12006	0.00024	2137.65812	834.53830
1 1 2 0 18	1 1 0 0 19	1301.32681	0.00037	2171.95536	870.62893
1 1 2 0 19	1 1 0 0 20	1299.53755	0.00017	2208.15315	908.61577
1 1 2 0 20	1 1 0 0 21	1297.75260	0.00024	2246.25067	948.49830
1 1 2 0 21	1 1 0 0 22	1295.97125	0.00017	2286.24710	990.27601
1 1 2 0 22	1 1 0 0 23	1294.19357	0.00036	2328.14154	1033.94833
1 1 2 0 23	1 1 0 0 24	1292.41902	0.00061	2371.93309	1079.51468
1 1 2 0 24	1 1 0 0 25	1290.64658	0.00026	2417.62077	1126.97445
1 1 2 0 25	1 1 0 0 26	1288.87690	0.00033	2465.20357	1176.32701
1 1 2 0 26	1 1 0 0 27	1287.10899	0.00022	2514.68046	1227.57169
1 1 2 0 27	1 1 0 0 28	1285.34265	0.00011	2566.05036	1280.70782
1 1 2 0 28	1 1 0 0 29	1283.57769	0.00022	2619.31215	1335.73468
1 1 2 0 29	1 1 0 0 30	1281.81264	-0.00050	2674.46468	1392.65154
1 1 2 0 30	1 1 0 0 31	1280.04888	-0.00026	2731.50678	1451.45764
1 1 2 0 31	1 1 0 0 32	1278.28410	-0.00094	2790.43724	1512.15220
1 1 2 0 32	1 1 0 0 33	1276.52030	-0.00013	2851.25484	1574.73441
1 1 2 0 33	1 1 0 0 34	1274.75513	0.00024	2913.95831	1639.20342
1 1 2 0 34	1 1 0 0 35	1272.98744	-0.00056	2978.54639	1705.55838
1 1 2 0 35	1 1 0 0 36	1271.21860	-0.00077	3045.01779	1773.79841
1 1 2 0 36	1 1 0 0 37	1269.44809	-0.00052	3113.37120	1843.92260
1 1 2 0 37	1 1 0 0 38	1267.67537	0.00003	3183.60533	1915.93000
1 1 2 0 38	1 1 0 0 39	1265.89999	0.00079	3255.71885	1989.81965
1 1 2 0 39	1 1 0 0 40	1264.11891	-0.00096	3329.71045	2065.59058
1 1 2 0 40	1 1 0 0 41	1262.33356	-0.00346	3405.57880	2143.24177W
1 1 2 0 2	1 1 0 0 1	1340.18877	0.00025	1851.67479	511.48627
1 1 2 0 3	1 1 0 0 2	1342.10906	-0.00010	1857.39746	515.28830
1 1 2 0 4	1 1 0 0 3	1344.03918*	0.00297	1865.02750	520.99129W
1 1 2 0 5	1 1 0 0 4	1345.96925	-0.00034	1874.56474	528.59515
1 1 2 0 6	1 1 0 0 5	1347.91014	0.00095	1886.00898	538.09979
1 1 2 0 7	1 1 0 0 6	1349.85496	0.00005	1899.35999	549.50508
1 1 2 0 8	1 1 0 0 7	1351.80652	-0.00008	1914.61746	562.81086
1 1 2 0 9	1 1 0 0 8	1353.76354	-0.00057	1931.78108	578.01697
1 1 2 0 10	1 1 0 0 9	1355.72728	-0.00001	1950.85047	595.12319
1 1 2 0 11	1 1 0 0 10	1357.69548	-0.00046	1971.82524	614.12929
1 1 2 0 12	1 1 0 0 11	1359.66959	-0.00029	1994.70491	635.03503
1 1 2 0 13	1 1 0 0 12	1361.64884	-0.00004	2019.48900	657.84012
1 1 2 0 14	1 1 0 0 13	1363.63248	-0.00022	2046.17697	682.54427
1 1 2 0 15	1 1 0 0 14	1365.62067	-0.00044	2074.76824	709.14713
1 1 2 0 16	1 1 0 0 15	1367.61389	0.00007	2105.26218	737.64836
1 1 2 0 17	1 1 0 0 16	1369.60711	0.00000	2137.65812	768.04757

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1	1	2	0	18	1	1	0	0	17	1371.61133	0.00033	2171.95536	800.34436
1	1	2	0	19	1	1	0	0	18	1373.61514	0.00029	2208.15315	834.53830
1	1	2	0	20	1	1	0	0	19	1375.62213	0.00039	2246.25067	870.62893
1	1	2	0	21	1	1	0	0	20	1377.63159	0.00026	2286.24710	908.61577
1	1	2	0	22	1	1	0	0	21	1379.64326	0.00002	2328.14154	948.49830
1	1	2	0	23	1	1	0	0	22	1381.65728	0.00020	2371.93309	990.27601
1	1	2	0	24	1	1	0	0	23	1383.67264*	0.00021	2417.62077	1033.94833
1	1	2	0	25	1	1	0	0	24	1385.68887	-0.00002	2465.20357	1079.51468
1	1	2	0	26	1	1	0	0	25	1387.70611	0.00010	2514.68046	1126.97445
1	1	2	0	27	1	1	0	0	26	1389.72342	0.00007	2566.05036	1176.32701
1	1	2	0	28	1	1	0	0	27	1391.74071	0.00025	2619.31215	1227.57169
1	1	2	0	29	1	1	0	0	28	1393.75704	0.00018	2674.46468	1280.70782
1	1	2	0	30	1	1	0	0	29	1395.77210	0.00000	2731.50678	1335.73468
1	1	2	0	31	1	1	0	0	30	1397.78549*	-0.00021	2790.43724	1392.65154
1	1	2	0	32	1	1	0	0	31	1399.79695	-0.00024	2851.25484	1451.45764
1	1	2	0	33	1	1	0	0	32	1401.80580	-0.00031	2913.95831	1512.15220
1	1	2	0	34	1	1	0	0	33	1403.81161	-0.00037	2978.54639	1574.73441
1	1	2	0	35	1	1	0	0	34	1405.81368	-0.00069	3045.01779	1639.20342
1	1	2	0	36	1	1	0	0	35	1407.81222	-0.00060	3113.37120	1705.55838
1	1	2	0	37	1	1	0	0	36	1409.80608	-0.00084	3183.60533	1773.79841
1	1	2	0	38	1	1	0	0	37	1411.79527	-0.00099	3255.71885	1843.92260
1	1	2	0	39	1	1	0	0	38	1413.77975	-0.00070	3329.71045	1915.93000
1	1	2	0	40	1	1	0	0	39	1415.75768	-0.00146	3405.57880	1989.81965W
1	1	2	0	41	1	1	0	0	40	1417.73055	-0.00144	3483.32257	2065.59058W
1	1	2	0	42	1	1	0	0	41	1419.69655	-0.00214	3562.94046	2143.24177W
1	1	2	0	1	1	-1	0	0	1	1336.36475	-0.00030	1847.85961	511.49456
1	1	2	0	2	1	-1	0	0	2	1336.36224*	0.00061	1851.67479	515.31316
1	1	2	0	3	1	-1	0	0	3	1336.35663	0.00018	1857.39746	521.04101
1	1	2	0	4	1	-1	0	0	4	1336.34923	-0.00025	1865.02750	528.67801
1	1	2	0	5	1	-1	0	0	5	1336.34114	0.00047	1874.56474	538.22407
1	1	2	0	6	1	-1	0	0	6	1336.32971	-0.00022	1886.00898	549.67906
1	1	2	0	7	1	-1	0	0	7	1336.31739	0.00021	1899.35999	563.04281
1	1	2	0	8	1	-1	0	0	8	1336.30297	0.00065	1914.61746	578.31514
1	1	2	0	9	1	-1	0	0	9	1336.28554	0.00031	1931.78108	595.49585
1	1	2	0	10	1	-1	0	0	10	1336.26566	-0.00012	1950.85047	614.58469
1	1	2	0	11	1	-1	0	0	11	1336.24408	0.00026	1971.82524	635.58142
1	1	2	0	12	1	-1	0	0	12	1336.21918	0.00000	1994.70491	658.48573
1	1	2	0	13	1	-1	0	0	13	1336.19220	0.00052	2019.48900	683.29732
1	1	2	0	14	1	-1	0	0	14	1336.16041	-0.00072	2046.17697	710.01584
1	1	2	0	15	1	-1	0	0	15	1336.12725	-0.00005	2074.76824	738.64093
1	1	2	0	16	1	-1	0	0	16	1336.08876	-0.00122	2105.26218	769.17220W
1	1	2	0	17	1	-1	0	0	17	1336.04837	-0.00053	2137.65812	801.60923
1	1	2	0	18	1	-1	0	0	18	1336.00448	0.00068	2171.95536	835.95156
1	1	2	0	19	1	-1	0	0	19	1335.95422	-0.00018	2208.15315	872.19874
1	1	2	0	20	1	-1	0	0	20	1335.89930	-0.00110	2246.25067	910.35027W
1	-1	2	0	1	1	-1	0	0	2	1332.55216	0.00016	1847.86517	515.31316
1	-1	2	0	2	1	-1	0	0	3	1330.65058	0.00013	1851.69146	521.04101
1	-1	2	0	3	1	-1	0	0	4	1328.75335	0.00057	1857.43079	528.67801
1	-1	2	0	4	1	-1	0	0	5	1326.85908	0.00011	1865.08304	538.22407
1	-1	2	0	5	1	-1	0	0	6	1324.96921	0.00022	1874.64805	549.67906
1	-1	2	0	6	1	-1	0	0	7	1323.08266	-0.00013	1886.12559	563.04281
1	-1	2	0	7	1	-1	0	0	8	1321.20010	-0.00020	1899.51544	578.31514
1	-1	2	0	8	1	-1	0	0	9	1319.32063	-0.00081	1914.81729	595.49585
1	-1	2	0	9	1	-1	0	0	10	1317.44697	0.00085	1932.03082	614.58469
1	-1	2	0	10	1	-1	0	0	11	1315.57412	-0.00012	1951.15566	635.58142
1	-1	2	0	11	1	-1	0	0	12	1313.70519	-0.00047	1972.19139	658.48573
1	-1	2	0	12	1	-1	0	0	13	1311.83985	-0.00040	1995.13757	683.29732
1	-1	2	0	13	1	-1	0	0	14	1309.97804	0.00017	2019.99372	710.01584
1	-1	2	0	14	1	-1	0	0	15	1308.11831	-0.00005	2046.75929	738.64093
1	-1	2	0	15	1	-1	0	0	16	1306.26141	-0.00012	2075.43373	769.17220
1	-1	2	0	16	1	-1	0	0	17	1304.40691	-0.00030	2106.01643	801.60923
1	-1	2	0	17	1	-1	0	0	18	1302.55485	-0.00035	2138.50676	835.95156
1	-1	2	0	18	1	-1	0	0	19	1300.70522	-0.00008	2172.90404	872.19874
1	-1	2	0	19	1	-1	0	0	20	1298.85699	-0.00030	2209.20755	910.35027
1	-1	2	0	20	1	-1	0	0	21	1297.01080	-0.00015	2247.41657	950.40561
1	-1	2	0	21	1	-1	0	0	22	1295.16585	-0.00021	2287.53030	992.36423
1	-1	2	0	22	1	-1	0	0	23	1293.32193	-0.00046	2329.54794	1036.22555
1	-1	2	0	23	1	-1	0	0	24	1291.47931	-0.00039	2373.46866	1081.98896
1	-1	2	0	24	1	-1	0	0	25	1289.63758	-0.00016	2419.29158	1129.65384

1	1	-1	2	0	25	1	-1	0	0	26	1287.79613	-0.00015	2467.01582	1179.21954
2	1	-1	2	0	26	1	-1	0	0	27	1285.95473	-0.00035	2516.64046	1230.68537
3	1	-1	2	0	27	1	-1	0	0	28	1284.11369	-0.00021	2568.16454	1284.05064
4	1	-1	2	0	28	1	-1	0	0	29	1282.27233	-0.00016	2621.58710	1339.31460
5	1	-1	2	0	29	1	-1	0	0	30	1280.43038	-0.00026	2676.90715	1396.47651
6	1	-1	2	0	30	1	-1	0	0	31	1278.58760	-0.00051	2734.12368	1455.53557
7	1	-1	2	0	31	1	-1	0	0	32	1276.74450	-0.00018	2793.23566	1516.49098
8	1	-1	2	0	32	1	-1	0	0	33	1274.90036	0.00022	2854.24204	1579.34190
9	1	-1	2	0	33	1	-1	0	0	34	1273.05469	0.00040	2917.14177	1644.08748
10	1	-1	2	0	34	1	-1	0	0	35	1271.20688	-0.00005	2981.93375	1710.72682
11	1	-1	2	0	35	1	-1	0	0	36	1269.35843	0.00055	3048.61689	1779.25901
12	1	-1	2	0	36	1	-1	0	0	37	1267.50758	0.00060	3117.19009	1849.68311
13	1	-1	2	0	37	1	-1	0	0	38	1265.65516	0.00109	3187.65223	1921.99816W
14	1	-1	2	0	38	1	-1	0	0	39	1263.79860	-0.00040	3260.00217	1996.20316
15	1	-1	2	0	39	1	-1	0	0	40	1261.94239	0.00074	3334.23876	2072.29710
16	1	-1	2	0	40	1	-1	0	0	41	1260.08281	0.00091	3410.36084	2150.27894
17	1	-1	2	0	2	1	-1	0	0	1	1340.19668	-0.00022	1851.69146	511.49456
18	1	-1	2	0	3	1	-1	0	0	2	1342.11773	0.00010	1857.43079	515.31316
19	1	-1	2	0	4	1	-1	0	0	3	1344.04094	-0.00109	1865.08304	521.04101W
20	1	-1	2	0	5	1	-1	0	0	4	1345.96925	-0.00078	1874.64805	528.67801
21	1	-1	2	0	6	1	-1	0	0	5	1347.90178	0.00026	1886.12559	538.22407
22	1	-1	2	0	7	1	-1	0	0	6	1349.83678	0.00040	1899.51544	549.67906
23	1	-1	2	0	8	1	-1	0	0	7	1351.77441	-0.00007	1914.81729	563.04281
24	1	-1	2	0	9	1	-1	0	0	8	1353.71614	0.00046	1932.03082	578.31514
25	1	-1	2	0	10	1	-1	0	0	9	1355.65925	-0.00056	1951.15566	595.49585
26	1	-1	2	0	11	1	-1	0	0	10	1357.60728	0.00058	1972.19139	614.58469
27	1	-1	2	0	12	1	-1	0	0	11	1359.55565	-0.00050	1995.13757	635.58142
28	1	-1	2	0	13	1	-1	0	0	12	1361.50715	-0.00083	2019.99372	658.48573
29	1	-1	2	0	14	1	-1	0	0	13	1363.46232	0.00035	2046.75929	683.29732
30	1	-1	2	0	15	1	-1	0	0	14	1365.41753	-0.00036	2075.43373	710.01584
31	1	-1	2	0	16	1	-1	0	0	15	1367.37521	-0.00029	2106.01643	738.64093
32	1	-1	2	0	17	1	-1	0	0	16	1369.33415	-0.00041	2138.50676	769.17220
33	1	-1	2	0	18	1	-1	0	0	17	1371.29414	-0.00067	2172.90404	801.60923
34	1	-1	2	0	19	1	-1	0	0	18	1373.25571	-0.00028	2209.20755	835.95156
35	1	-1	2	0	20	1	-1	0	0	19	1375.21747	-0.00035	2247.41657	872.19874
36	1	-1	2	0	21	1	-1	0	0	20	1377.17994	-0.00009	2287.53030	910.35027
37	1	-1	2	0	22	1	-1	0	0	21	1379.14199	-0.00034	2329.54794	950.40561
38	1	-1	2	0	23	1	-1	0	0	22	1381.10387	-0.00056	2373.46866	992.36423
39	1	-1	2	0	24	1	-1	0	0	23	1383.06522	-0.00081	2419.29158	1036.22555
40	1	-1	2	0	25	1	-1	0	0	24	1385.02638	-0.00048	2467.01582	1081.98896
41	1	-1	2	0	26	1	-1	0	0	25	1386.98615	-0.00046	2516.64046	1129.65384
42	1	-1	2	0	27	1	-1	0	0	26	1388.94473	-0.00026	2568.16454	1179.21954
43	1	-1	2	0	28	1	-1	0	0	27	1390.90135	-0.00037	2621.58710	1230.68537
44	1	-1	2	0	29	1	-1	0	0	28	1392.85633	-0.00018	2676.90715	1284.05064
45	1	-1	2	0	30	1	-1	0	0	29	1394.80875	-0.00033	2734.12368	1339.31460
46	1	-1	2	0	31	1	-1	0	0	30	1396.75901	-0.00014	2793.23566	1396.47651
47	1	-1	2	0	32	1	-1	0	0	31	1398.70652	0.00005	2854.24204	1455.53557
48	1	-1	2	0	33	1	-1	0	0	32	1400.65075	-0.00004	2917.14177	1516.49098
49	1	-1	2	0	34	1	-1	0	0	33	1402.59098	-0.00086	2981.93375	1579.34190
50	1	-1	2	0	35	1	-1	0	0	34	1404.52880	-0.00061	3048.61689	1644.08748
51	1	-1	2	0	36	1	-1	0	0	35	1406.46311	-0.00017	3117.19009	1710.72682
52	1	-1	2	0	37	1	-1	0	0	36	1408.39339	0.00017	3187.65223	1779.25901
53	1	-1	2	0	38	1	-1	0	0	37	1410.31968	0.00062	3260.00217	1849.68311
54	1	-1	2	0	39	1	-1	0	0	38	1412.24156	0.00096	3334.23876	1921.99816
55	1	-1	2	0	40	1	-1	0	0	39	1414.15876	0.00108	3410.36084	1996.20316W
56	1	-1	2	0	41	1	-1	0	0	40	1416.07110	0.00096	3488.36724	2072.29710
57	1	-1	2	0	42	1	-1	0	0	41	1417.97953	0.00168	3568.25679	2150.27894W
58	1	-1	2	0	1	1	1	0	0	1	1336.37897	0.00007	1847.86517	511.48627
59	1	-1	2	0	2	1	1	0	0	2	1336.40340	0.00024	1851.69146	515.28830
60	1	-1	2	0	3	1	1	0	0	3	1336.43941	-0.00009	1857.43079	520.99129
	1	-1	2	0	4	1	1	0	0	4	1336.48811	0.00022	1865.08304	528.59515
	1	-1	2	0	5	1	1	0	0	5	1336.54804	-0.00021	1874.64805	538.09979
	1	-1	2	0	6	1	1	0	0	6	1336.62087	0.00036	1886.12559	549.50508
	1	-1	2	0	7	1	1	0	0	7	1336.70464	0.00007	1899.51544	562.81086
	1	-1	2	0	8	1	1	0	0	8	1336.80038	0.00006	1914.81729	578.01697
	1	-1	2	0	9	1	1	0	0	9	1336.90784	0.00021	1932.03082	595.12319
	1	-1	2	0	10	1	1	0	0	10	1337.02602	-0.00034	1951.15566	614.12929
	1	-1	2	0	11	1	1	0	0	11	1337.15652	0.00016	1972.19139	635.03503
	1	-1	2	0	12	1	1	0	0	12	1337.29768	0.00023	1995.13757	657.84012

1	-1	2	0	13	1	1	0	0	13	1337.44834	-0.00111	2019.99372	682.54427W
2	-1	2	0	14	1	1	0	0	14	1337.61180	-0.00036	2046.75929	709.14713
3	-1	2	0	15	1	1	0	0	15	1337.78476	-0.00061	2075.43373	737.64836
4	-1	2	0	16	1	1	0	0	16	1337.96849	-0.00037	2106.01643	768.04757
5	-1	2	0	17	1	1	0	0	17	1338.16149	-0.00091	2138.50676	800.34436
6	-1	2	0	18	1	1	0	0	18	1338.36599	0.00025	2172.90404	834.53830

rms = 0.00042 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 -1 2 2 1	1 1 0 0 2	1352.21184	0.00011	1867.50003	515.28830
1 -1 2 2 2	1 1 0 0 3	1350.32606*	0.00114	1871.31621	520.99129W
1 -1 2 2 3	1 1 0 0 4	1348.44531	-0.00004	1877.04050	528.59515
1 -1 2 2 4	1 1 0 0 5	1346.57348	0.00034	1884.67293	538.09979
1 -1 2 2 5	1 1 0 0 6	1344.70845	-0.00001	1894.21354	549.50508
1 -1 2 2 6	1 1 0 0 7	1342.85141	-0.00009	1905.66237	562.81086
1 -1 2 2 7	1 1 0 0 8	1341.00177	-0.00073	1919.01947	578.01697
1 -1 2 2 8	1 1 0 0 9	1339.16211	0.00039	1934.28491	595.12319
1 -1 2 2 9	1 1 0 0 10	1337.32915	-0.00031	1951.45875	614.12929
1 -1 2 2 10	1 1 0 0 11	1335.50506	-0.00097	1970.54106	635.03503
1 -1 2 2 11	1 1 0 0 12	1333.69142	-0.00036	1991.53191	657.84012
1 -1 2 2 12	1 1 0 0 13	1331.88676	-0.00034	2014.43136	682.54427
1 -1 2 2 13	1 1 0 0 14	1330.09294	0.00057	2039.23950	709.14713
1 -1 2 2 14	1 1 0 0 15	1328.30824	0.00023	2065.95636	737.64836
1 -1 2 2 15	1 1 0 0 16	1326.53565	0.00121	2094.58201	768.04757W
1 -1 2 2 16	1 1 0 0 17	1324.77257	0.00048	2125.11645	800.34436
1 -1 2 2 17	1 1 0 0 18	1323.02135	-0.00005	2157.55970	834.53830
1 -1 2 2 18	1 1 0 0 19	1321.28173	-0.00107	2191.91172	870.62893W
1 -1 2 2 19	1 1 0 0 20	1319.55717	0.00048	2228.17246	908.61577
1 -1 2 2 20	1 1 0 0 21	1317.84340	-0.00009	2266.34179	948.49830
1 -1 2 2 21	1 1 0 0 22	1316.14354	-0.00002	2306.41957	990.27601
1 -1 2 2 22	1 1 0 0 23	1314.45581	-0.00144	2348.40558	1033.94833W
1 -1 2 2 2	1 1 0 0 1	1359.83060	0.00066	1871.31621	511.48627
1 -1 2 2 3	1 1 0 0 2	1361.75209	-0.00011	1877.04050	515.28830
1 -1 2 2 4	1 1 0 0 3	1363.68137	-0.00027	1884.67293	520.99129
1 -1 2 2 5	1 1 0 0 4	1365.62067*	0.00229	1894.21354	528.59515W
1 -1 2 2 6	1 1 0 0 5	1367.56297	0.00040	1905.66237	538.09979
1 -1 2 2 7	1 1 0 0 6	1369.51371	-0.00068	1919.01947	549.50508
1 -1 2 2 8	1 1 0 0 7	1371.47359	-0.00046	1934.28491	562.81086
1 -1 2 2 9	1 1 0 0 8	1373.44121	-0.00057	1951.45875	578.01697
1 -1 2 2 10	1 1 0 0 9	1375.41762	-0.00025	1970.54106	595.12319
1 -1 2 2 11	1 1 0 0 10	1377.40263	0.00001	1991.53191	614.12929
1 -1 2 2 12	1 1 0 0 11	1379.39663	0.00030	2014.43136	635.03503
1 -1 2 2 13	1 1 0 0 12	1381.39925	-0.00012	2039.23950	657.84012
1 -1 2 2 14	1 1 0 0 13	1383.41227	0.00017	2065.95636	682.54427
1 -1 2 2 15	1 1 0 0 14	1385.43480	-0.00008	2094.58201	709.14713
1 -1 2 2 16	1 1 0 0 15	1387.46840	0.00031	2125.11645	737.64836
1 -1 2 2 17	1 1 0 0 16	1389.51177	-0.00036	2157.55970	768.04757
1 -1 2 2 18	1 1 0 0 17	1391.56800	0.00064	2191.91172	800.34436
1 -1 2 2 19	1 1 0 0 18	1393.63406	-0.00010	2228.17246	834.53830
1 -1 2 2 20	1 1 0 0 19	1395.71342	0.00056	2266.34179	870.62893
1 -1 2 2 21	1 1 0 0 20	1397.80460	0.00080	2306.41957	908.61577
1 -1 2 2 22	1 1 0 0 21	1399.90885	0.00157	2348.40558	948.49830W
1 -1 2 2 23	1 1 0 0 22	1402.02316	-0.00038	2392.29956	990.27601
1 -1 2 2 24	1 1 0 0 23	1404.15470	0.00187	2438.10116	1033.94833W
1 -1 2 2 25	1 1 0 0 24	1406.29608	0.00076	2485.81000	1079.51468
1 1 2 -2 1	1 -1 0 0 2	1352.18985	0.00026	1867.50275	515.31316
1 1 2 -2 2	1 -1 0 0 3	1350.28317	-0.00020	1871.32438	521.04101
1 1 2 -2 3	1 -1 0 0 4	1348.37980*	0.00098	1877.05683	528.67801
1 1 2 -2 4	1 -1 0 0 5	1346.47636	0.00028	1884.70016	538.22407
1 1 2 -2 5	1 -1 0 0 6	1344.57828*	0.00295	1894.25438	549.67906W
1 1 2 -2 6	1 -1 0 0 7	1342.67667	-0.00009	1905.71956	563.04281
1 1 2 -2 7	1 -1 0 0 8	1340.78112	0.00050	1919.09576	578.31514
1 1 2 -2 8	1 -1 0 0 9	1338.88661	-0.00025	1934.38303	595.49585

1	1	1	2	-2	9	1	-1	0	0	10	1336.99667	-0.00011	1951.58147	614.58469
2	1	1	2	-2	10	1	-1	0	0	11	1335.10978	0.00004	1970.69116	635.58142
3	1	1	2	-2	11	1	-1	0	0	12	1333.22601	-0.00046	1991.71220	658.48573
4	1	1	2	-2	12	1	-1	0	0	13	1331.34742	0.00004	2014.64470	683.29732
5	1	1	2	-2	13	1	-1	0	0	14	1329.47292	0.00001	2039.48875	710.01584
6	1	1	2	-2	14	1	-1	0	0	15	1327.60376	0.00021	2066.24449	738.64093
7	1	1	2	-2	15	1	-1	0	0	16	1325.73855*	-0.00126	2094.91201	769.17220W
8	1	1	2	-2	16	1	-1	0	0	17	1323.88489*	0.00269	2125.49143	801.60923W
9	1	1	2	-2	17	1	-1	0	0	18	1322.03073	-0.00055	2157.98284	835.95156
10	1	1	2	-2	18	1	-1	0	0	19	1320.18758	-0.00001	2192.38633	872.19874
11	1	1	2	-2	19	1	-1	0	0	20	1318.35162	-0.00008	2228.70197	910.35027
12	1	1	2	-2	20	1	-1	0	0	21	1316.52528*	0.00111	2266.92978	950.40561W
13	1	1	2	-2	21	1	-1	0	0	22	1314.70548	-0.00006	2307.06978	992.36423
14	1	1	2	-2	22	1	-1	0	0	23	1312.89673	0.00035	2349.12193	1036.22555
15	1	1	2	-2	23	1	-1	0	0	24	1311.09727	0.00007	2393.08616	1081.98896
16	1	1	2	-2	24	1	-1	0	0	25	1309.30870	0.00019	2438.96235	1129.65384
17	1	1	2	-2	25	1	-1	0	0	26	1307.53132	0.00054	2486.75032	1179.21954
18	1	1	2	-2	26	1	-1	0	0	27	1305.76363	-0.00084	2536.44985	1230.68537
19	1	1	2	-2	27	1	-1	0	0	28	1304.01064	0.00065	2588.06063	1284.05064
20	1	1	2	-2	2	1	-1	0	0	1	1359.83060	0.00078	1871.32438	511.49456
21	1	1	2	-2	3	1	-1	0	0	2	1361.74369	0.00002	1877.05683	515.31316
22	1	1	2	-2	4	1	-1	0	0	3	1363.65888	-0.00027	1884.70016	521.04101
23	1	1	2	-2	5	1	-1	0	0	4	1365.57682	0.00045	1894.25438	528.67801
24	1	1	2	-2	6	1	-1	0	0	5	1367.49580	0.00031	1905.71956	538.22407
25	1	1	2	-2	7	1	-1	0	0	6	1369.41625	-0.00045	1919.09576	549.67906
26	1	1	2	-2	8	1	-1	0	0	7	1371.34046	0.00023	1934.38303	563.04281
27	1	1	2	-2	9	1	-1	0	0	8	1373.26680*	0.00047	1951.58147	578.31514
28	1	1	2	-2	10	1	-1	0	0	9	1375.19545	0.00013	1970.69116	595.49585
29	1	1	2	-2	11	1	-1	0	0	10	1377.12777	0.00026	1991.71220	614.58469
30	1	1	2	-2	12	1	-1	0	0	11	1379.06330	0.00002	2014.64470	635.58142
31	1	1	2	-2	13	1	-1	0	0	12	1381.00256	-0.00046	2039.48875	658.48573
32	1	1	2	-2	14	1	-1	0	0	13	1382.94747	0.00030	2066.24449	683.29732
33	1	1	2	-2	15	1	-1	0	0	14	1384.89628	0.00011	2094.91201	710.01584
34	1	1	2	-2	16	1	-1	0	0	15	1386.85047	-0.00003	2125.49143	738.64093
35	1	1	2	-2	17	1	-1	0	0	16	1388.81053	-0.00011	2157.98284	769.17220
36	1	1	2	-2	18	1	-1	0	0	17	1390.77693	-0.00018	2192.38633	801.60923
37	1	1	2	-2	19	1	-1	0	0	18	1392.75019	-0.00021	2228.70197	835.95156
38	1	1	2	-2	20	1	-1	0	0	19	1394.73095	-0.00009	2266.92978	872.19874
39	1	1	2	-2	21	1	-1	0	0	20	1396.71897	-0.00054	2307.06978	910.35027
40	1	1	2	-2	22	1	-1	0	0	21	1398.71540	-0.00092	2349.12193	950.40561
41	1	1	2	-2	23	1	-1	0	0	22	1400.72224	0.00031	2393.08616	992.36423
42	1	1	2	-2	24	1	-1	0	0	23	1402.73680	0.00000	2438.96235	1036.22555
43	1	1	2	-2	25	1	-1	0	0	24	1404.76178	0.00042	2486.75032	1081.98896
44	1	1	2	-2	26	1	-1	0	0	25	1406.79619	0.00019	2536.44985	1129.65384
45	1	1	2	-2	27	1	-1	0	0	26	1408.84142	0.00033	2588.06063	1179.21954
46	1	1	2	-2	28	1	-1	0	0	27	1410.89715	0.00020	2641.58233	1230.68537
47	1	1	2	-2	29	1	-1	0	0	28	1412.96386	-0.00004	2697.01454	1284.05064
48	1	1	2	-2	30	1	-1	0	0	29	1415.04098	-0.00120	2754.35678	1339.31460W
49	1	1	2	-2	31	1	-1	0	0	30	1417.13143	-0.00060	2813.60854	1396.47651
50	1	1	2	-2	32	1	-1	0	0	31	1419.23341	-0.00025	2874.76923	1455.53557
51	1	1	2	-2	33	1	-1	0	0	32	1421.34637	-0.00086	2937.83821	1516.49098
52	1	1	2	-2	34	1	-1	0	0	33	1423.47065	-0.00223	3002.81478	1579.34190W
53	1	1	2	-2	35	1	-1	0	0	34	1425.60996	-0.00077	3069.69821	1644.08748
54	1	1	2	-2	36	1	-1	0	0	35	1427.76079	-0.00007	3138.48768	1710.72682
55	1	1	2	-2	37	1	-1	0	0	36	1429.91997*	-0.00337	3209.18235	1779.25901W
56	1	1	2	-2	38	1	-1	0	0	37	1432.09633	-0.00189	3281.78133	1849.68311W

rms = 0.00040 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
1 1 2 0 1	0 0 1 1 2	1167.92320	-0.00074	1847.85961	679.93567
1 1 2 0 2	0 0 1 1 3	1166.03972	-0.00014	1851.67479	685.63493
1 1 2 0 3	0 0 1 1 4	1164.16367	0.00003	1857.39746	693.23382
1 1 2 0 4	0 0 1 1 5	1162.28762	0.00000	1863.02750	702.73224

1	1	1	2	0	5	0	0	1	1	6	1160.43456	-0.00011	1874.56474	714.13007
2	1	1	2	0	6	0	0	1	1	7	1158.58157	-0.00025	1886.00898	727.42716
3	1	1	2	0	7	0	0	1	1	8	1156.73692	0.00027	1899.35999	742.62333
4	1	1	2	0	8	0	0	1	1	9	1154.89904	-0.00003	1914.61746	759.71839
5	1	1	2	0	9	0	0	1	1	10	1153.06939	0.00040	1931.78108	778.71209
6	1	1	2	0	10	0	0	1	1	11	1151.24642	0.00015	1950.85047	799.60420
7	1	1	2	0	11	0	0	1	1	12	1149.43108	0.00029	1971.82524	822.39444
8	1	1	2	0	12	0	0	1	1	13	1147.62274	0.00034	1994.70491	847.08251
9	1	1	2	0	13	0	0	1	1	14	1145.82127	0.00035	2019.48900	873.66808
10	1	1	2	0	14	0	0	1	1	15	1144.02647	0.00029	2046.17697	902.15079
11	1	1	2	0	15	0	0	1	1	16	1142.23782	-0.00013	2074.76824	932.53028
12	1	1	2	0	16	0	0	1	1	17	1140.45625	0.00021	2105.26218	964.80614
13	1	1	2	0	17	0	0	1	1	18	1138.68037	0.00019	2137.65812	998.97795
14	1	1	2	0	18	0	0	1	1	19	1136.91023	0.00011	2171.95536	1035.04524
15	1	1	2	0	19	0	0	1	1	20	1135.14615	0.00056	2208.15315	1073.00756
16	1	1	2	0	20	0	0	1	1	21	1133.38654	0.00026	2246.25067	1112.86438
17	1	1	2	0	21	0	0	1	1	22	1131.63256	0.00066	2286.24710	1154.61520
18	1	1	2	0	22	0	0	1	1	23	1129.88241	0.00032	2328.14154	1198.25945
19	1	1	2	0	23	0	0	1	1	24	1128.13656	0.00003	2371.93309	1243.79656
20	1	1	2	0	24	0	0	1	1	25	1126.39529	0.00046	2417.62077	1291.22593
21	1	1	2	0	25	0	0	1	1	26	1124.65681	0.00017	2465.20357	1340.54693
22	1	1	2	0	26	0	0	1	1	27	1122.92164	0.00009	2514.68046	1391.75891
23	1	1	2	0	27	0	0	1	1	28	1121.18969	0.00052	2566.05036	1444.86119
24	1	1	2	0	28	0	0	1	1	29	1119.45926	0.00019	2619.31215	1499.85307
25	1	1	2	0	29	0	0	1	1	30	1117.73034	-0.00051	2674.46468	1556.73383
26	1	1	2	0	30	0	0	1	1	31	1116.00315	-0.00092	2731.50678	1615.50271
27	1	1	2	0	31	0	0	1	1	32	1114.27924	0.00093	2790.43724	1676.15894
28	1	1	2	0	32	0	0	1	1	33	1112.55265	-0.00048	2851.25484	1738.70171
29	1	1	2	0	33	0	0	1	1	34	1110.82792	-0.00019	2913.95831	1803.13019
30	1	1	2	0	34	0	0	1	1	35	1109.10139	-0.00144	2978.54639	1869.44355W
31	1	1	2	0	35	0	0	1	1	36	1107.37581	-0.00108	3045.01779	1937.64090W
32	1	1	2	0	2	0	0	1	1	1	1175.53894	0.00028	1851.67479	676.13613
33	1	1	2	0	3	0	0	1	1	2	1177.46222	0.00043	1857.39746	679.93567
34	1	1	2	0	4	0	0	1	1	3	1179.39292	0.00035	1865.02750	685.63493
35	1	1	2	0	5	0	0	1	1	4	1181.33098	0.00006	1874.56474	693.23382
36	1	1	2	0	6	0	0	1	1	5	1183.28080*	0.00406	1886.00898	702.73224W
37	1	1	2	0	7	0	0	1	1	6	1185.22997	0.00006	1899.35999	714.13007
38	1	1	2	0	8	0	0	1	1	7	1187.19015	-0.00015	1914.61746	727.42716
39	1	1	2	0	9	0	0	1	1	8	1189.15804	0.00029	1931.78108	742.62333
40	1	1	2	0	10	0	0	1	1	9	1191.13221	0.00012	1950.85047	759.71839
41	1	1	2	0	11	0	0	1	1	10	1193.11331	0.00017	1971.82524	778.71209
42	1	1	2	0	12	0	0	1	1	11	1195.10183	0.00113	1994.70491	799.60420W
43	1	1	2	0	13	0	0	1	1	12	1197.09345	-0.00111	2019.48900	822.39444W
44	1	1	2	0	14	0	0	1	1	13	1199.09433	-0.00013	2046.17697	847.08251
45	1	1	2	0	15	0	0	1	1	14	1201.10038	0.00022	2074.76824	873.66808
46	1	1	2	0	16	0	0	1	1	15	1203.11151	0.00013	2105.26218	902.15079
47	1	1	2	0	17	0	0	1	1	16	1205.12835	0.00051	2137.65812	932.53028
48	1	1	2	0	18	0	0	1	1	17	1207.14939	0.00017	2171.95536	964.80614
49	1	1	2	0	19	0	0	1	1	18	1209.17562	0.00042	2208.15315	998.97795
50	1	1	2	0	20	0	0	1	1	19	1211.20561	0.00018	2246.25067	1035.00756
51	1	1	2	0	21	0	0	1	1	20	1213.24006	0.00052	2286.24710	1073.04524
52	1	1	2	0	22	0	0	1	1	21	1215.27706	-0.00010	2328.14154	1112.86438
53	1	1	2	0	23	0	0	1	1	22	1217.31829	0.00040	2371.93309	1154.61520
54	1	1	2	0	24	0	0	1	1	23	1219.36164	0.00033	2417.62077	1198.25945
55	1	1	2	0	25	0	0	1	1	24	1221.40703	0.00002	2465.20357	1243.79656
56	1	1	2	0	26	0	0	1	1	25	1223.45473	0.00020	2514.68046	1291.22593
57	1	1	2	0	27	0	0	1	1	26	1225.50364	0.00021	2566.05036	1340.54693
58	1	1	2	0	28	0	0	1	1	27	1227.55334	0.00010	2619.31215	1391.75891
59	1	1	2	0	29	0	0	1	1	28	1229.60392	0.00043	2674.46468	1444.86119
60	1	1	2	0	30	0	0	1	1	29	1231.65330	-0.00041	2731.50678	1499.85307
	1	1	2	0	31	0	0	1	1	30	1233.70351	0.00010	2790.43724	1556.73383
	1	1	2	0	32	0	0	1	1	31	1235.75147	-0.00066	2851.25484	1615.50271
	1	1	2	0	33	0	0	1	1	32	1237.79879	-0.00058	2913.95831	1676.15894
	1	1	2	0	34	0	0	1	1	33	1239.84094*	-0.00374	2978.54639	1738.70171W
	1	1	2	0	35	0	0	1	1	34	1241.88719	-0.00040	3045.01779	1803.13019
	1	1	2	0	36	0	0	1	1	35	1243.92651	-0.00114	3113.37120	1869.44355W
	1	-1	2	0	1	0	0	1	-1	2	1167.90981	-0.00012	1847.86517	679.95524
	1	-1	2	0	2	0	0	1	-1	3	1166.01666	-0.00075	1851.69146	685.67405
	1	-1	2	0	3	0	0	1	-1	3	1164.13132	-0.00045	1857.43079	693.29902

1	1	-1	2	0	4	0	0	1	-1	5	1162.25296	-0.00004	1865.08304	702.83004
2	1	-1	2	0	5	0	0	1	-1	6	1160.38063	-0.00043	1874.64805	714.26698
3	1	-1	2	0	6	0	0	1	-1	7	1158.51584	-0.00006	1886.12559	727.60969
4	1	-1	2	0	7	0	0	1	-1	8	1156.65761	0.00016	1899.51544	742.85799
5	1	-1	2	0	8	0	0	1	-1	9	1154.80576	0.00015	1914.81729	760.01168
6	1	-1	2	0	9	0	0	1	-1	10	1152.96038	0.00008	1932.03082	779.07052
7	1	-1	2	0	10	0	0	1	-1	11	1151.12141	0.00001	1951.15566	800.03426
8	1	-1	2	0	11	0	0	1	-1	12	1149.28852	-0.00026	1972.19139	822.90261
9	1	-1	2	0	12	0	0	1	-1	13	1147.46210	-0.00019	1995.13757	847.67528
10	1	-1	2	0	13	0	0	1	-1	14	1145.64122	-0.00057	2019.99372	874.35193
11	1	-1	2	0	14	0	0	1	-1	15	1143.82767	0.00058	2046.75929	902.93220
12	1	-1	2	0	15	0	0	1	-1	16	1142.01838	0.00035	2075.43373	933.41570
13	1	-1	2	0	16	0	0	1	-1	17	1140.21429	-0.00011	2106.01643	965.80204
14	1	-1	2	0	17	0	0	1	-1	18	1138.41571	-0.00029	2138.50676	1000.09076
15	1	-1	2	0	18	0	0	1	-1	19	1136.62280	0.00019	2172.90404	1036.28142
16	1	-1	2	0	19	0	0	1	-1	20	1134.83365	-0.00037	2209.20755	1074.37353
17	1	-1	2	0	20	0	0	1	-1	21	1133.04963	-0.00036	2247.41657	1114.36658
18	1	-1	2	0	21	0	0	1	-1	22	1131.26989	-0.00038	2287.53030	1156.26002
19	1	-1	2	0	22	0	0	1	-1	23	1129.49399	-0.00064	2329.54794	1200.05331
20	1	-1	2	0	23	0	0	1	-1	24	1127.72322	0.00040	2373.46866	1245.74584
21	1	-1	2	0	24	0	0	1	-1	25	1125.95439	-0.00018	2419.29158	1293.33701
22	1	-1	2	0	25	0	0	1	-1	26	1124.19018	0.00054	2467.01582	1342.82618
23	1	-1	2	0	26	0	0	1	-1	27	1122.42732	-0.00045	2516.64046	1394.21269
24	1	-1	2	0	27	0	0	1	-1	28	1120.66882	0.00012	2568.16454	1447.49584
25	1	-1	2	0	28	0	0	1	-1	29	1118.91234	0.00017	2621.58710	1502.67492
26	1	-1	2	0	29	0	0	1	-1	30	1117.15796	0.00001	2676.90715	1559.74920
27	1	-1	2	0	30	0	0	1	-1	31	1115.40326	-0.00252	2734.12368	1618.71789W
28	1	-1	2	0	31	0	0	1	-1	32	1113.65648	0.00105	2793.23566	1679.58023W
29	1	-1	2	0	2	0	0	1	-1	1	1175.54921	0.00040	1851.69146	676.14265
30	1	-1	2	0	3	0	0	1	-1	2	1177.47577	0.00021	1857.43079	679.95524
31	1	-1	2	0	4	0	0	1	-1	3	1179.40911	0.00012	1865.08304	685.67405
32	1	-1	2	0	5	0	0	1	-1	4	1181.34938	0.00036	1874.64805	693.29902
33	1	-1	2	0	6	0	0	1	-1	5	1183.29491	-0.00064	1886.12559	702.83004
34	1	-1	2	0	7	0	0	1	-1	6	1185.24877	0.00031	1899.51544	714.26698
35	1	-1	2	0	8	0	0	1	-1	7	1187.20743	-0.00017	1914.81729	727.60969
36	1	-1	2	0	9	0	0	1	-1	8	1189.17237	-0.00046	1932.03082	742.85799
37	1	-1	2	0	10	0	0	1	-1	9	1191.14440	0.00042	1951.15566	760.01168
38	1	-1	2	0	11	0	0	1	-1	10	1193.12108	0.00021	1972.19139	779.07052
39	1	-1	2	0	12	0	0	1	-1	11	1195.10183	-0.00149	1995.13757	800.03426W
40	1	-1	2	0	13	0	0	1	-1	12	1197.09238	0.00128	2019.99372	822.90261W
41	1	-1	2	0	14	0	0	1	-1	13	1199.08337	-0.00064	2046.75929	847.67528
42	1	-1	2	0	15	0	0	1	-1	14	1201.08152	-0.00028	2075.43373	874.35193
43	1	-1	2	0	16	0	0	1	-1	15	1203.08330	-0.00093	2106.01643	902.93220
44	1	-1	2	0	17	0	0	1	-1	16	1205.09115	0.00009	2138.50676	933.41570
45	1	-1	2	0	18	0	0	1	-1	17	1207.10159	-0.00041	2172.90404	965.80204
46	1	-1	2	0	19	0	0	1	-1	18	1209.11665	-0.00014	2209.20755	1000.09076
47	1	-1	2	0	20	0	0	1	-1	19	1211.13458	-0.00056	2247.41657	1036.28142
48	1	-1	2	0	21	0	0	1	-1	20	1213.15641	-0.00035	2287.53030	1074.37353
49	1	-1	2	0	22	0	0	1	-1	21	1215.18145	0.00009	2329.54794	1114.36658
50	1	-1	2	0	23	0	0	1	-1	22	1217.20762	-0.00102	2373.46866	1156.26002W
51	1	-1	2	0	24	0	0	1	-1	23	1219.23798	-0.00030	2419.29158	1200.05331
52	1	-1	2	0	25	0	0	1	-1	24	1221.26983	-0.00015	2467.01582	1245.74584
53	1	-1	2	0	26	0	0	1	-1	25	1223.30282	-0.00062	2516.64046	1293.33701
54	1	-1	2	0	27	0	0	1	-1	26	1225.33787	-0.00048	2568.16454	1342.82618
55	1	-1	2	0	28	0	0	1	-1	27	1227.37348	-0.00093	2621.58710	1394.21269
56	1	-1	2	0	29	0	0	1	-1	28	1229.41111	-0.00020	2676.90715	1447.49584
57	1	-1	2	0	30	0	0	1	-1	29	1231.44913	0.00037	2734.12368	1502.67492
58	1	-1	2	0	31	0	0	1	-1	30	1233.48602	-0.00044	2793.23566	1559.74920
59	1	-1	2	0	32	0	0	1	-1	31	1235.52509	0.00094	2854.24204	1618.71789

rms = 0.00039 cm⁻¹

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

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	G'	G''
1 -1 2 2 1	0 0 1 -1 5	1162.25296	-0.00004	1865.08304	702.83004

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1	-1	2	2	2	0	0	1	1	3	1185.68129	0.00001	1871.31621	685.63493
1	-1	2	2	3	0	0	1	1	4	1183.80680	0.00012	1877.04050	693.23382
1	-1	2	2	4	0	0	1	1	5	1181.94080	0.00011	1884.67293	702.73224
1	-1	2	2	5	0	0	1	1	6	1180.08359	0.00013	1894.21354	714.13007
1	-1	2	2	6	0	0	1	1	7	1178.23524	0.00004	1905.66237	727.42716
1	-1	2	2	7	0	0	1	1	8	1176.39617	0.00003	1919.01947	742.62333
1	-1	2	2	8	0	0	1	1	9	1174.56672	0.00020	1934.28491	759.71839
1	-1	2	2	9	0	0	1	1	10	1172.74665	-0.00001	1951.45875	778.71209
1	-1	2	2	10	0	0	1	1	11	1170.93691	0.00006	1970.54106	799.60420
1	-1	2	2	11	0	0	1	1	12	1169.13753	0.00007	1991.53191	822.39444
1	-1	2	2	12	0	0	1	1	13	1167.34879	-0.00006	2014.43136	847.08251
1	-1	2	2	13	0	0	1	1	14	1165.57142	0.00000	2039.23950	873.66808
1	-1	2	2	14	0	0	1	1	15	1163.80562	0.00005	2065.95636	902.15079
1	-1	2	2	15	0	0	1	1	16	1162.05146	-0.00027	2094.58201	932.53028
1	-1	2	2	16	0	0	1	1	17	1160.31029	-0.00002	2125.11645	964.80614
1	-1	2	2	17	0	0	1	1	18	1158.58185	0.00010	2157.55970	998.97795
1	-1	2	2	18	0	0	1	1	19	1156.86648	0.00000	2191.91172	1035.04524
1	-1	2	2	19	0	0	1	1	20	1155.16467	-0.00023	2228.17246	1073.00756
1	-1	2	2	20	0	0	1	1	21	1153.47759	0.00018	2266.34179	1112.86438
1	-1	2	2	21	0	0	1	1	22	1151.80418	-0.00019	2306.41957	1154.61520
1	-1	2	2	22	0	0	1	1	23	1150.14582	-0.00031	2348.40558	1198.25945
1	-1	2	2	23	0	0	1	1	24	1148.50292	-0.00007	2392.29956	1243.79656
1	-1	2	2	24	0	0	1	1	25	1146.87536	0.00013	2438.10116	1291.22593
1	-1	2	2	25	0	0	1	1	26	1145.26328	0.00021	2485.81000	1340.54693
1	-1	2	2	26	0	0	1	1	27	1143.66675	0.00006	2535.42560	1391.75891
1	-1	2	2	27	0	0	1	1	28	1142.08650	0.00024	2586.94745	1444.86119
1	-1	2	2	28	0	0	1	1	29	1140.52187	0.00000	2640.37494	1499.85307
1	-1	2	2	29	0	0	1	1	30	1138.97359	0.00000	2695.70742	1556.73383
1	-1	2	2	30	0	0	1	1	31	1137.44188	0.00042	2752.94417	1615.50271
1	-1	2	2	31	0	0	1	1	32	1135.92516	-0.00033	2812.08442	1676.15894
1	-1	2	2	32	0	0	1	1	33	1134.42516	-0.00048	2873.12735	1738.70171
1	-1	2	2	33	0	0	1	1	34	1132.94206*	0.00018	2936.07207	1803.13019
1	-1	2	2	34	0	0	1	1	35	1131.47393	-0.00020	3000.91768	1869.44355
1	-1	2	2	2	0	0	1	1	1	1195.18088	0.00080	1871.31621	676.13613
1	-1	2	2	3	0	0	1	1	2	1197.10346*	-0.00137	1877.04050	679.93567W
1	-1	2	2	4	0	0	1	1	3	1199.03829	0.00029	1884.67293	685.63493
1	-1	2	2	5	0	0	1	1	4	1200.97999	0.00027	1894.21354	693.23382
1	-1	2	2	6	0	0	1	1	5	1202.93007	-0.00006	1905.66237	702.73224
1	-1	2	2	7	0	0	1	1	6	1204.88957	0.00017	1919.01947	714.13007
1	-1	2	2	8	0	0	1	1	7	1206.85768	-0.00007	1934.28491	727.42716
1	-1	2	2	9	0	0	1	1	8	1208.83560	0.00018	1951.45875	742.62333
1	-1	2	2	10	0	0	1	1	9	1210.82380*	0.00113	1970.54106	759.71839W
1	-1	2	2	11	0	0	1	1	10	1212.81990	0.00009	1991.53191	778.71209
1	-1	2	2	12	0	0	1	1	11	1214.82726	0.00010	2014.43136	799.60420
1	-1	2	2	13	0	0	1	1	12	1216.84510	0.00005	2039.23950	822.39444
1	-1	2	2	14	0	0	1	1	13	1218.87379	-0.00006	2065.95636	847.08251
1	-1	2	2	15	0	0	1	1	14	1220.91382	-0.00011	2094.58201	873.66808
1	-1	2	2	16	0	0	1	1	15	1222.96567	0.00001	2125.11645	902.15079
1	-1	2	2	17	0	0	1	1	16	1225.02947	0.00005	2157.55970	932.53028
1	-1	2	2	18	0	0	1	1	17	1227.10569	0.00011	2191.91172	964.80614
1	-1	2	2	19	0	0	1	1	18	1229.19460	0.00009	2228.17246	998.97795
1	-1	2	2	20	0	0	1	1	19	1231.29646	-0.00009	2266.34179	1035.04524
1	-1	2	2	21	0	0	1	1	20	1233.41203	0.00002	2306.41957	1073.00756
1	-1	2	2	22	0	0	1	1	21	1235.54130	0.00010	2348.40558	1112.86438
1	-1	2	2	23	0	0	1	1	22	1237.68428	-0.00008	2392.29956	1154.61520
1	-1	2	2	24	0	0	1	1	23	1239.84183	0.00012	2438.10116	1198.25945
1	-1	2	2	25	0	0	1	1	24	1242.01339	-0.00004	2485.81000	1243.79656
1	-1	2	2	26	0	0	1	1	25	1244.19910	-0.00057	2535.42560	1291.22593
1	-1	2	2	27	0	0	1	1	26	1246.40032	-0.00020	2586.94745	1340.54693
1	-1	2	2	28	0	0	1	1	27	1248.61597	-0.00006	2640.37494	1391.75891
1	-1	2	2	29	0	0	1	1	28	1250.84634	0.00011	2695.70742	1444.86119
1	-1	2	2	30	0	0	1	1	29	1253.09149	0.00039	2752.94417	1499.85307
1	-1	2	2	31	0	0	1	1	30	1255.35066	0.00007	2812.08442	1556.73383
1	-1	2	2	32	0	0	1	1	31	1257.62482	0.00018	2873.12735	1615.50271
1	-1	2	2	33	0	0	1	1	32	1259.91349	0.00035	2936.07207	1676.15894
1	-1	2	2	34	0	0	1	1	33	1262.21556	-0.00041	3000.91768	1738.70171
1	-1	2	2	35	0	0	1	1	34	1264.53306	0.00005	3067.66320	1803.13019
1	-1	2	2	36	0	0	1	1	35	1266.86455	0.00045	3136.30765	1869.44355
1	-1	2	2	1	0	0	1	1	1	1191.35832	0.00004	1867.50003	676.14265

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60	1	-1	2	2	3	0	0	1	-1	3	1191.36656	0.00011	1877.04050	685.67405
	1	-1	2	2	4	0	0	1	-1	4	1191.37482	0.00091	1884.67293	693.29902
	1	-1	2	2	5	0	0	1	-1	5	1191.38381	0.00031	1894.21354	702.83004
	1	-1	2	2	6	0	0	1	-1	6	1191.39588	0.00050	1905.66237	714.26698
	1	-1	2	2	8	0	0	1	-1	8	1191.42691	-0.00001	1934.28491	742.85799
	1	-1	2	2	9	0	0	1	-1	9	1191.44738	0.00031	1951.45875	760.01168
	1	1	2	-2	1	0	0	1	-1	2	1187.54752	0.00000	1867.50275	679.95524
	1	1	2	-2	2	0	0	1	-1	3	1185.65067	0.00035	1871.32438	685.67405
	1	1	2	-2	3	0	0	1	-1	4	1183.75790	0.00009	1877.05683	693.29902
	1	1	2	-2	4	0	0	1	-1	5	1181.87009	-0.00003	1884.70016	702.83004
	1	1	2	-2	5	0	0	1	-1	6	1179.98738	-0.00002	1894.25438	714.26698
	1	1	2	-2	6	0	0	1	-1	7	1178.11012	0.00025	1905.71956	727.60969
	1	1	2	-2	7	0	0	1	-1	8	1176.23790	0.00013	1919.09576	742.85799
	1	1	2	-2	8	0	0	1	-1	9	1174.37163	0.00027	1934.38303	760.01168
	1	1	2	-2	9	0	0	1	-1	10	1172.51099	0.00003	1951.58147	779.07052
	1	1	2	-2	10	0	0	1	-1	11	1170.65722	0.00031	1970.69116	800.03426
	1	1	2	-2	11	0	0	1	-1	12	1168.80939	-0.00020	1991.71220	822.90261
	1	1	2	-2	12	0	0	1	-1	13	1166.96924	-0.00017	2014.64470	847.67528
	1	1	2	-2	13	0	0	1	-1	14	1165.13682	0.00000	2039.48875	874.35193
	1	1	2	-2	14	0	0	1	-1	15	1163.31256	0.00027	2066.24449	902.93220
	1	1	2	-2	15	0	0	1	-1	16	1161.49632	0.00001	2094.91201	933.41570
	1	1	2	-2	16	0	0	1	-1	17	1159.68938	-0.00001	2125.49143	965.80204
	1	1	2	-2	17	0	0	1	-1	18	1157.89196	-0.00012	2157.98284	1000.09076
	1	1	2	-2	18	0	0	1	-1	19	1156.10499	0.00008	2192.38633	1036.28142
	1	1	2	-2	19	0	0	1	-1	20	1154.32853	0.00010	2228.70197	1074.37353
	1	1	2	-2	20	0	0	1	-1	21	1152.56342	0.00022	2266.92978	1114.36658
	1	1	2	-2	21	0	0	1	-1	22	1150.80983	0.00008	2307.06978	1156.26002
	1	1	2	-2	22	0	0	1	-1	23	1149.06867	0.00005	2349.12193	1200.05331
	1	1	2	-2	23	0	0	1	-1	24	1147.34026	-0.00006	2393.08616	1245.74584
	1	1	2	-2	24	0	0	1	-1	25	1145.62540	0.00006	2438.96235	1293.33701
	1	1	2	-2	25	0	0	1	-1	26	1143.92428	0.00014	2486.75032	1342.82618
	1	1	2	-2	26	0	0	1	-1	27	1142.23769	0.00053	2536.44985	1394.21269
	1	1	2	-2	27	0	0	1	-1	28	1140.56483	0.00004	2588.06063	1447.49584
	1	1	2	-2	28	0	0	1	-1	29	1138.90736	-0.00005	2641.58233	1502.67492
	1	1	2	-2	29	0	0	1	-1	30	1137.26533	-0.00001	2697.01454	1559.74920
	1	1	2	-2	30	0	0	1	-1	31	1135.63915	0.00026	2754.35678	1618.71789
	1	1	2	-2	31	0	0	1	-1	32	1134.02833	0.00001	2813.60854	1679.58023
	1	1	2	-2	32	0	0	1	-1	33	1132.43409	0.00023	2874.76923	1742.33538
	1	1	2	-2	2	0	0	1	-1	1	1195.18088	-0.00085	1871.32438	676.14265
	1	1	2	-2	3	0	0	1	-1	2	1197.10233	0.00073	1877.05683	679.95524
	1	1	2	-2	4	0	0	1	-1	3	1199.02601	-0.00010	1884.70016	685.67405
	1	1	2	-2	5	0	0	1	-1	4	1200.95559	0.00023	1894.25438	693.29902
	1	1	2	-2	6	0	0	1	-1	5	1202.88946	-0.00007	1905.71956	702.83004
	1	1	2	-2	7	0	0	1	-1	6	1204.82886	0.00008	1919.09576	714.26698
	1	1	2	-2	8	0	0	1	-1	7	1206.77341	0.00007	1934.38303	727.60969
	1	1	2	-2	9	0	0	1	-1	8	1208.72347	-0.00001	1951.58147	742.85799
	1	1	2	-2	10	0	0	1	-1	9	1210.67950	0.00001	1970.69116	760.01168
	1	1	2	-2	11	0	0	1	-1	10	1212.64175	0.00006	1991.71220	779.07052
	1	1	2	-2	12	0	0	1	-1	11	1214.61059	0.00015	2014.64470	800.03426
	1	1	2	-2	13	0	0	1	-1	12	1216.58607	-0.00007	2039.48875	822.90261
	1	1	2	-2	14	0	0	1	-1	13	1218.56915	-0.00006	2066.24449	847.67528
	1	1	2	-2	15	0	0	1	-1	14	1220.56007	-0.00001	2094.91201	874.35193
	1	1	2	-2	16	0	0	1	-1	15	1222.55926	0.00003	2125.49143	902.93220
	1	1	2	-2	17	0	0	1	-1	16	1224.56711	-0.00003	2157.98284	933.41570
	1	1	2	-2	18	0	0	1	-1	17	1226.58429	-0.00001	2192.38633	965.80204
	1	1	2	-2	19	0	0	1	-1	18	1228.61108	-0.00012	2228.70197	1000.09076
	1	1	2	-2	20	0	0	1	-1	19	1230.64839	0.00004	2266.92978	1036.28142
	1	1	2	-2	21	0	0	1	-1	20	1232.69622	-0.00002	2307.06978	1074.37353
	1	1	2	-2	22	0	0	1	-1	21	1234.75529	-0.00006	2349.12193	1114.36658
	1	1	2	-2	23	0	0	1	-1	22	1236.82609	-0.00005	2393.08616	1156.26002
	1	1	2	-2	24	0	0	1	-1	23	1238.90904	-0.00001	2438.96235	1200.05331
	1	1	2	-2	25	0	0	1	-1	24	1241.00472	0.00024	2486.75032	1245.74584
	1	1	2	-2	26	0	0	1	-1	25	1243.11289	0.00006	2536.44985	1293.33701
	1	1	2	-2	27	0	0	1	-1	26	1245.23422	-0.00023	2588.06063	1342.82618
	1	1	2	-2	28	0	0	1	-1	27	1247.36959	-0.00005	2641.58233	1394.21269
	1	1	2	-2	29	0	0	1	-1	28	1249.51871	0.00001	2697.01454	1447.49584
	1	1	2	-2	30	0	0	1	-1	29	1251.68521	0.00335	2754.35678	1502.67492W
	1	1	2	-2	31	0	0	1	-1	30	1253.85978	0.00043	2813.60854	1559.74920
	1	1	2	-2	32	0	0	1	-1	31	1256.05193	0.00059	2874.76923	1618.71789

1	1	2	-2	33	0	0	1	-1	32	1258.25779	-0.00019	2937.83821	1679.58023
1	1	2	-2	34	0	0	1	-1	33	1260.47945	0.00004	3002.81478	1742.33538
1	1	2	-2	35	0	0	1	-1	34	1262.71726	0.00156	3069.69821	1806.98250W
1	1	2	-2	36	0	0	1	-1	35	1264.96687	-0.00007	3138.48768	1873.52074
1	1	2	-2	37	0	0	1	-1	36	1267.23329	0.00013	3209.18235	1941.94919
1	1	2	-2	1	0	0	1	1	1	1191.36656	-0.00006	1867.50275	676.13613
1	1	2	-2	2	0	0	1	1	2	1191.38838	-0.00032	1871.32438	679.93567
1	1	2	-2	3	0	0	1	1	3	1191.42311*	0.00120	1877.05683	685.63493W
1	1	2	-2	4	0	0	1	1	4	1191.46711	0.00077	1884.70016	693.23382
1	1	2	-2	5	0	0	1	1	5	1191.52210	-0.00004	1894.25438	702.73224
1	1	2	-2	6	0	0	1	1	6	1191.58819	-0.00130	1905.71956	714.13007W
1	1	2	-2	7	0	0	1	1	7	1191.66969	0.00109	1919.09576	727.42716W
1	1	2	-2	8	0	0	1	1	8	1191.75901	-0.00069	1934.38303	742.62333
1	1	2	-2	9	0	0	1	1	9	1191.86392	0.00083	1951.58147	759.71839

rms = 0.00027 cm⁻¹

$3\nu_5(\Pi) \leftarrow \nu_5(\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
0 0 3 1 1	0 0 1 1 2	1321.89521	0.00022	2001.83066	679.93567
0 0 3 1 2	0 0 1 1 3	1319.99954	0.00016	2005.63431	685.63493
0 0 3 1 3	0 0 1 1 4	1318.10619	0.00031	2011.33970	693.23382
0 0 3 1 4	0 0 1 1 5	1316.21435	-0.00015	2018.94675	702.73224
0 0 3 1 5	0 0 1 1 6	1314.32536	0.00012	2028.45531	714.13007
0 0 3 1 6	0 0 1 1 7	1312.43795	-0.00014	2039.86525	727.42716
0 0 3 1 7	0 0 1 1 8	1310.55337	0.00034	2053.17636	742.62333
0 0 3 1 8	0 0 1 1 9	1308.67020	0.00015	2068.38843	759.71839
0 0 3 1 9	0 0 1 1 10	1306.78923	0.00011	2085.50121	778.71209
0 0 3 1 10	0 0 1 1 11	1304.90994	-0.00027	2104.51441	799.60420
0 0 3 1 11	0 0 1 1 12	1303.03340	0.00012	2125.42773	822.39444
0 0 3 1 12	0 0 1 1 13	1301.15854	0.00024	2148.24081	847.08251
0 0 3 1 13	0 0 1 1 14	1299.28534	0.00014	2172.95328	873.66808
0 0 3 1 14	0 0 1 1 15	1297.41414	0.00019	2199.56474	902.15079
0 0 3 1 15	0 0 1 1 16	1295.54454	0.00006	2228.07476	932.53028
0 0 3 1 16	0 0 1 1 17	1293.67684	0.00011	2258.48287	964.80614
0 0 3 1 17	0 0 1 1 18	1291.81008	-0.00054	2290.78857	998.97795
0 0 3 1 18	0 0 1 1 19	1289.94584	-0.00026	2324.99134	1035.04524
0 0 3 1 19	0 0 1 1 20	1288.08274	-0.00034	2361.09064	1073.00756
0 0 3 1 20	0 0 1 1 21	1286.22112	-0.00036	2399.08587	1112.86438
0 0 3 1 21	0 0 1 1 22	1284.36088	-0.00034	2438.97642	1154.61520
0 0 3 1 22	0 0 1 1 23	1282.50213	-0.00009	2480.76167	1198.25945
0 0 3 1 23	0 0 1 1 24	1280.64419	-0.00018	2524.44094	1243.79656
0 0 3 1 24	0 0 1 1 25	1278.78767	0.00007	2570.01353	1291.22593
0 0 3 1 25	0 0 1 1 26	1276.93180	0.00000	2617.47873	1340.54693
0 0 3 1 26	0 0 1 1 27	1275.07686	-0.00002	2666.83579	1391.75891
0 0 3 1 27	0 0 1 1 28	1273.22296	0.00022	2718.08394	1444.86119
0 0 3 1 28	0 0 1 1 29	1271.36955	0.00026	2771.22236	1499.85307
0 0 3 1 29	0 0 1 1 30	1269.51671	0.00030	2826.25024	1556.73383
0 0 3 1 30	0 0 1 1 31	1267.66408	0.00006	2883.16673	1615.50271
0 0 3 1 31	0 0 1 1 32	1265.81241	0.00041	2941.97094	1676.15894
0 0 3 1 32	0 0 1 1 33	1263.96053	0.00027	3002.66197	1738.70171
0 0 3 1 33	0 0 1 1 34	1262.10944	0.00074	3065.23889	1803.13019
0 0 3 1 34	0 0 1 1 35	1260.25856	0.00135	3129.70076	1869.44355W
0 0 3 1 35	0 0 1 1 36	1258.40726	0.00156	3196.04660	1937.64090W
0 0 3 1 36	0 0 1 1 37	1256.55361	-0.00046	3264.27541	2007.72134
0 0 3 1 37	0 0 1 1 38	1254.70262	0.00040	3334.38617	2079.68394
0 0 3 1 38	0 0 1 1 39	1252.84943	-0.00063	3406.37783	2153.52776
0 0 3 1 39	0 0 1 1 40	1250.99702	-0.00048	3480.24932	2229.25182
0 0 3 1 40	0 0 1 1 41	1249.14459	0.00014	3555.99957	2306.85512
0 0 3 1 41	0 0 1 1 42	1247.29279	0.00198	3633.62745	2386.33663W
0 0 3 1 42	0 0 1 1 43	1245.43620	-0.00032	3713.13182	2467.69531
0 0 3 1 2	0 0 1 1 1	1329.49808	-0.00010	2005.63431	676.13613
0 0 3 1 3	0 0 1 1 2	1331.40397	-0.00006	2011.33970	679.93567
0 0 3 1 4	0 0 1 1 3	1333.31132	-0.00050	2018.94675	685.63493
0 0 3 1 5	0 0 1 1 4	1335.21867	0.00000	2028.45531	693.23382

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

1	0	0	3	1	6	0	0	1	1	5	1337.13241	-0.00060	2039.86525	702.73224
2	0	0	3	1	7	0	0	1	1	6	1339.04609	-0.00020	2053.17636	714.13007
3	0	0	3	1	8	0	0	1	1	7	1340.96164	0.00037	2068.38843	727.42716
4	0	0	3	1	9	0	0	1	1	8	1342.87771	-0.00017	2085.50121	742.62333
5	0	0	3	1	10	0	0	1	1	9	1344.79625	0.00022	2104.51441	759.71839
6	0	0	3	1	11	0	0	1	1	10	1346.71571	0.00008	2125.42773	778.71209
7	0	0	3	1	12	0	0	1	1	11	1348.63639	-0.00021	2148.24081	799.60420
8	0	0	3	1	13	0	0	1	1	12	1350.55895	0.00011	2172.95328	822.39444
9	0	0	3	1	14	0	0	1	1	13	1352.48205	-0.00018	2199.56474	847.08251
10	0	0	3	1	15	0	0	1	1	14	1354.40714	0.00046	2228.07476	873.66808
11	0	0	3	1	16	0	0	1	1	15	1356.33223	0.00016	2258.48287	902.15079
12	0	0	3	1	17	0	0	1	1	16	1358.25809	-0.00020	2290.78857	932.53028
13	0	0	3	1	18	0	0	1	1	17	1360.18479	-0.00041	2324.99134	964.80614
14	0	0	3	1	19	0	0	1	1	18	1362.11298	0.00029	2361.09064	998.97795
15	0	0	3	1	20	0	0	1	1	19	1364.04033	-0.00029	2399.08587	1035.04524
16	0	0	3	1	21	0	0	1	1	20	1365.96864	-0.00023	2438.97642	1073.00756
17	0	0	3	1	22	0	0	1	1	21	1367.89712	-0.00016	2480.76167	1112.86438
18	0	0	3	1	23	0	0	1	1	22	1369.82584	0.00010	2524.44094	1154.61520
19	0	0	3	1	24	0	0	1	1	23	1371.75385	-0.00023	2570.01353	1198.25945
20	0	0	3	1	25	0	0	1	1	24	1373.68213	-0.00004	2617.47873	1243.79656
21	0	0	3	1	26	0	0	1	1	25	1375.61001	0.00015	2666.83579	1291.22593
22	0	0	3	1	27	0	0	1	1	26	1377.53698	-0.00002	2718.08394	1340.54693
23	0	0	3	1	28	0	0	1	1	27	1379.46315	-0.00030	2771.22236	1391.75891
24	0	0	3	1	29	0	0	1	1	28	1381.38903	-0.00002	2826.25024	1444.86119
25	0	0	3	1	30	0	0	1	1	29	1383.31313	-0.00052	2883.16673	1499.85307
26	0	0	3	1	31	0	0	1	1	30	1385.23704	-0.00007	2941.97094	1556.73383
27	0	0	3	1	32	0	0	1	1	31	1387.15928	0.00002	3002.66197	1615.50271
28	0	0	3	1	33	0	0	1	1	32	1389.08019	0.00023	3065.23889	1676.15894
29	0	0	3	1	34	0	0	1	1	33	1390.99938	0.00032	3129.70076	1738.70171
30	0	0	3	1	35	0	0	1	1	34	1392.91646	0.00005	3196.04660	1803.13019
31	0	0	3	1	36	0	0	1	1	35	1394.82915	-0.00271	3264.27541	1869.44355W
32	0	0	3	1	37	0	0	1	1	36	1396.74546	0.00019	3334.38617	1937.64090
33	0	0	3	1	38	0	0	1	1	37	1398.65701	0.00052	3406.37783	2007.72134
34	0	0	3	1	39	0	0	1	1	38	1400.56562	0.00024	3480.24932	2079.68394
35	0	0	3	1	40	0	0	1	1	39	1402.47111	-0.00069	3555.99957	2153.52776
36	0	0	3	1	41	0	0	1	1	40	1404.37561	-0.00001	3633.62745	2229.25182
37	0	0	3	1	42	0	0	1	1	41	1406.27709	0.00038	3713.13182	2306.85512
38	0	0	3	1	43	0	0	1	1	42	1408.17494	0.00002	3794.51155	2386.33663
39	0	0	3	1	44	0	0	1	1	43	1410.07068	0.00054	3877.76545	2467.69531
40	0	0	3	1	1	0	0	1	-1	1	1325.68780	-0.00021	2001.83066	676.14265
41	0	0	3	1	2	0	0	1	-1	2	1325.67917	0.00010	2005.63431	679.95524
42	0	0	3	1	3	0	0	1	-1	3	1325.66574	0.00009	2011.33970	685.67405
43	0	0	3	1	4	0	0	1	-1	4	1325.64804	0.00032	2018.94675	693.29902
44	0	0	3	1	5	0	0	1	-1	5	1325.62555	0.00028	2028.45531	702.83004
45	0	0	3	1	6	0	0	1	-1	6	1325.59824	-0.00003	2039.86525	714.26698
46	0	0	3	1	7	0	0	1	-1	7	1325.56637	-0.00030	2053.17636	727.60969
47	0	0	3	1	8	0	0	1	-1	8	1325.53048	0.00004	2068.38843	742.85799
48	0	0	3	1	9	0	0	1	-1	9	1325.48993	0.00040	2085.50121	760.01168
49	0	0	3	1	10	0	0	1	-1	10	1325.44341	-0.00048	2104.51441	779.07052
50	0	0	3	1	11	0	0	1	-1	11	1325.39324	-0.00023	2125.42773	800.03426
51	0	0	3	1	12	0	0	1	-1	12	1325.33795	-0.00024	2148.24081	822.90261
52	0	0	3	1	13	0	0	1	-1	13	1325.27747	-0.00053	2172.95328	847.67528
53	0	0	3	1	14	0	0	1	-1	14	1325.21262	-0.00019	2199.56474	874.35193
54	0	0	3	1	15	0	0	1	-1	15	1325.14178	-0.00078	2228.07476	902.93220
55	0	0	3	1	18	0	0	1	-1	18	1324.90042	-0.00016	2324.99134	1000.09076
56	0	0	3	-1	1	0	0	1	-1	2	1321.88868	-0.00013	2001.84405	679.95524
57	0	0	3	-1	2	0	0	1	-1	3	1320.00038	-0.00004	2005.67447	685.67405
58	0	0	3	-1	3	0	0	1	-1	4	1318.12008*	-0.00093	2011.42003	693.29902
59	0	0	3	-1	4	0	0	1	-1	5	1316.25088	0.00030	2019.08062	702.83004
60	0	0	3	-1	5	0	0	1	-1	6	1314.38892	-0.00021	2028.65611	714.26698
	0	0	3	-1	6	0	0	1	-1	7	1312.53700	0.00035	2040.14634	727.60969
	0	0	3	-1	7	0	0	1	-1	8	1310.69334	0.00022	2053.55111	742.85799
	0	0	3	-1	8	0	0	1	-1	9	1308.85842	-0.00010	2068.87020	760.01168
	0	0	3	-1	9	0	0	1	-1	10	1307.03289	0.00006	2086.10334	779.07052
	0	0	3	-1	10	0	0	1	-1	11	1305.21625	0.00026	2105.25025	800.03426
	0	0	3	-1	11	0	0	1	-1	12	1303.40794	-0.00002	2126.31058	822.90261
	0	0	3	-1	12	0	0	1	-1	13	1301.60885	0.00016	2149.28398	847.67528
	0	0	3	-1	13	0	0	1	-1	14	1299.81844	0.00032	2174.17005	874.35193
	0	0	3	-1	14	0	0	1	-1	15	1298.03642	0.00026	2200.96836	902.93220

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0	0	3	-1	15	0	0	1	-1	16	1296.26266	-0.00008	2229.67844	933.41570
0	0	3	-1	16	0	0	1	-1	17	1294.49783	0.00006	2260.29981	965.80204
0	0	3	-1	17	0	0	1	-1	18	1292.74132	0.00017	2292.83191	1000.09076
0	0	3	-1	18	0	0	1	-1	19	1290.99288	0.00012	2327.27418	1036.28142
0	0	3	-1	19	0	0	1	-1	20	1289.25277	0.00028	2363.62602	1074.37353
0	0	3	-1	20	0	0	1	-1	21	1287.52014	-0.00006	2401.88678	1114.36658
0	0	3	-1	21	0	0	1	-1	22	1285.79577	0.00001	2442.05578	1156.26002
0	0	3	-1	22	0	0	1	-1	23	1284.07902	0.00002	2484.13231	1200.05331
0	0	3	-1	23	0	0	1	-1	24	1282.36967	-0.00010	2528.11561	1245.74584
0	0	3	-1	24	0	0	1	-1	25	1280.66806	0.00019	2574.00488	1293.33701
0	0	3	-1	25	0	0	1	-1	26	1278.97306	-0.00006	2621.79931	1342.82618
0	0	3	-1	26	0	0	1	-1	27	1277.28527	-0.00004	2671.49800	1394.21269
0	0	3	-1	27	0	0	1	-1	28	1275.60437	0.00015	2723.10006	1447.49584
0	0	3	-1	28	0	0	1	-1	29	1273.92947	-0.00014	2776.60454	1502.67492
0	0	3	-1	29	0	0	1	-1	30	1272.26117	-0.00006	2832.01043	1559.74920
0	0	3	-1	30	0	0	1	-1	31	1270.59895	0.00014	2889.31671	1618.71789
0	0	3	-1	31	0	0	1	-1	32	1268.94197	-0.00010	2948.52229	1679.58023
0	0	3	-1	32	0	0	1	-1	33	1267.29041	-0.00028	3009.62607	1742.33538
0	0	3	-1	33	0	0	1	-1	34	1265.64394	-0.00043	3072.62687	1806.98250
0	0	3	-1	34	0	0	1	-1	35	1264.00241	-0.00035	3137.52349	1873.52074
0	0	3	-1	35	0	0	1	-1	36	1262.36557	0.00007	3204.31469	1941.94919
0	0	3	-1	36	0	0	1	-1	37	1260.73166	-0.00056	3272.99916	2012.26694
0	0	3	-1	37	0	0	1	-1	38	1259.10189	-0.00063	3343.57556	2084.47304
0	0	3	-1	38	0	0	1	-1	39	1257.47552	-0.00046	3416.04251	2158.56653
0	0	3	-1	39	0	0	1	-1	40	1255.85212	-0.00005	3490.39859	2234.54642
0	0	3	-1	40	0	0	1	-1	41	1254.23197	0.00133	3566.64232	2312.41168W
0	0	3	-1	2	0	0	1	-1	1	1329.53156	-0.00026	2005.67447	676.14265
0	0	3	-1	3	0	0	1	-1	2	1331.46464	-0.00015	2011.42003	679.95524
0	0	3	-1	4	0	0	1	-1	3	1333.40615	-0.00041	2019.08062	685.67405
0	0	3	-1	5	0	0	1	-1	4	1335.35770	0.00061	2028.65611	693.29902
0	0	3	-1	6	0	0	1	-1	5	1337.31582	-0.00048	2040.14634	702.83004
0	0	3	-1	7	0	0	1	-1	6	1339.28472	0.00059	2053.55111	714.26698
0	0	3	-1	8	0	0	1	-1	7	1341.26004	-0.00047	2068.87020	727.60969
0	0	3	-1	9	0	0	1	-1	8	1343.24611	0.00076	2086.10334	742.85799
0	0	3	-1	10	0	0	1	-1	9	1345.23876	0.00019	2105.25025	760.01168
0	0	3	-1	11	0	0	1	-1	10	1347.23998	-0.00008	2126.31058	779.07052
0	0	3	-1	12	0	0	1	-1	11	1349.25047	0.00075	2149.28398	800.03426
0	0	3	-1	13	0	0	1	-1	12	1351.26772	0.00029	2174.17005	822.90261
0	0	3	-1	14	0	0	1	-1	13	1353.29330	0.00023	2200.96836	847.67528
0	0	3	-1	15	0	0	1	-1	14	1355.32723	0.00072	2229.67844	874.35193
0	0	3	-1	16	0	0	1	-1	15	1357.36822	0.00061	2260.29981	902.93220
0	0	3	-1	17	0	0	1	-1	16	1359.41611	-0.00010	2292.83191	933.41570
0	0	3	-1	18	0	0	1	-1	17	1361.47290	0.00075	2327.27418	965.80204
0	0	3	-1	19	0	0	1	-1	18	1363.53530	0.00004	2363.62602	1000.09076
0	0	3	-1	20	0	0	1	-1	19	1365.60537	0.00001	2401.88678	1036.28142
0	0	3	-1	21	0	0	1	-1	20	1367.68221	-0.00004	2442.05578	1074.37353
0	0	3	-1	22	0	0	1	-1	21	1369.76480	-0.00093	2484.13231	1114.36658
0	0	3	-1	23	0	0	1	-1	22	1371.85553	-0.00006	2528.11561	1156.26002
0	0	3	-1	24	0	0	1	-1	23	1373.95148	-0.00010	2574.00488	1200.05331
0	0	3	-1	25	0	0	1	-1	24	1376.05335	-0.00012	2621.79931	1245.74584
0	0	3	-1	26	0	0	1	-1	25	1378.16075	-0.00024	2671.49800	1293.33701
0	0	3	-1	27	0	0	1	-1	26	1380.27362	-0.00026	2723.10006	1342.82618
0	0	3	-1	28	0	0	1	-1	27	1382.39156	-0.00029	2776.60454	1394.21269
0	0	3	-1	29	0	0	1	-1	28	1384.51446	-0.00013	2832.01043	1447.49584
0	0	3	-1	30	0	0	1	-1	29	1386.64175	-0.00003	2889.31671	1502.67492
0	0	3	-1	31	0	0	1	-1	30	1388.77287	-0.00023	2948.52229	1559.74920
0	0	3	-1	32	0	0	1	-1	31	1390.90852	0.00034	3009.62607	1618.71789
0	0	3	-1	33	0	0	1	-1	32	1393.04638	-0.00027	3072.62687	1679.58023
0	0	3	-1	34	0	0	1	-1	33	1395.18808	-0.00004	3137.52349	1742.33538
0	0	3	-1	35	0	0	1	-1	34	1397.33275	0.00056	3204.31469	1806.98250
0	0	3	-1	36	0	0	1	-1	35	1399.47837	-0.00005	3272.99916	1873.52074
0	0	3	-1	37	0	0	1	-1	36	1401.62660	0.00023	3343.57556	1941.94919
0	0	3	-1	38	0	0	1	-1	37	1403.77583	0.00025	3416.04251	2012.26694
0	0	3	-1	39	0	0	1	-1	38	1405.92566	0.00011	3490.39859	2084.47304
0	0	3	-1	40	0	0	1	-1	39	1408.07610	0.00031	3566.64232	2158.56653
0	0	3	-1	41	0	0	1	-1	40	1410.22713	0.00137	3644.77218	2234.54642W
0	0	3	-1	42	0	0	1	-1	41	1412.37582	0.00088	3724.78662	2312.41168
0	0	3	-1	43	0	0	1	-1	42	1414.52534	0.00258	3806.68403	2392.16127W
0	0	3	-1	1	0	0	1	-1	1	1325.70775	0.00017	2001.84405	676.13613

0	0	3	-1	2	0	0	1	1	2	1325.73865	-0.00015	2005.67447	679.93567
0	0	3	-1	3	0	0	1	1	3	1325.78493	-0.00017	2011.42003	685.63493
0	0	3	-1	4	0	0	1	1	4	1325.84685	0.00005	2019.08062	693.23382
0	0	3	-1	5	0	0	1	1	5	1325.92385	-0.00002	2028.65611	702.73224
0	0	3	-1	6	0	0	1	1	6	1326.01593	-0.00033	2040.14634	714.13007
0	0	3	-1	9	0	0	1	1	9	1326.38501	0.00005	2086.10334	759.71839
0	0	3	-1	10	0	0	1	1	10	1326.53659	-0.00156	2105.25025	778.71209W
0	0	3	-1	11	0	0	1	1	11	1326.70653	0.00016	2126.31058	799.60420
0	0	3	-1	12	0	0	1	1	12	1326.88835*	-0.00118	2149.28398	822.39444W
0	0	3	-1	13	0	0	1	1	13	1327.08666	-0.00087	2174.17005	847.08251

rms = 0.00032 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	G'	G"
3 1 0 0 3	0 0 0 0 4	1518.34848	-0.00002	1537.35469	19.00619
3 1 0 0 4	0 0 0 0 5	1516.46606*	-0.00484	1544.97988	28.50898W
3 1 0 0 5	0 0 0 0 6	1514.59995	0.00109	1554.51090	39.91204W
3 1 0 0 6	0 0 0 0 7	1512.73175	-0.00048	1565.94747	53.21523
3 1 0 0 7	0 0 0 0 8	1510.87223	0.00139	1579.28923	68.41838W
3 1 0 0 8	0 0 0 0 9	1509.01364	-0.00084	1594.53577	85.52129
3 1 0 0 9	0 0 0 0 10	1507.16334	0.00043	1611.68663	104.52373
3 1 0 0 10	0 0 0 0 11	1505.31666	0.00077	1630.74133	125.42544
3 1 0 0 11	0 0 0 0 12	1503.47320	0.00005	1651.69930	148.22616
3 1 0 0 12	0 0 0 0 13	1501.63300	-0.00140	1674.55997	172.92558W
3 1 0 0 13	0 0 0 0 14	1499.80066*	0.00131	1699.32273	199.52337W
3 1 0 0 14	0 0 0 0 15	1497.96798	0.00027	1725.98691	228.01920
3 1 0 0 15	0 0 0 0 16	1496.13751	-0.00165	1754.55184	258.41268W
3 1 0 0 16	0 0 0 0 17	1494.31345	0.00002	1785.01683	290.70340
3 1 0 0 17	0 0 0 0 18	1492.49036	0.00017	1817.38115	324.89096
3 1 0 0 18	0 0 0 0 19	1490.66875	-0.00044	1851.64407	360.97488
3 1 0 0 19	0 0 0 0 20	1488.85035	0.00021	1887.80485	398.95471
3 1 0 0 20	0 0 0 0 21	1487.03267	-0.00012	1925.86272	438.82993
3 1 0 0 21	0 0 0 0 22	1485.21681	-0.00009	1965.81693	480.60003
3 1 0 0 22	0 0 0 0 23	1483.40292	0.00068	2007.66669	524.26445
3 1 0 0 23	0 0 0 0 24	1481.58781	-0.00081	2051.41124	569.82262
3 1 0 0 4	0 0 0 0 3	1533.57574	-0.00032	1544.97988	11.40382
3 1 0 0 5	0 0 0 0 4	1535.50440	-0.00031	1554.51090	19.00619
3 1 0 0 6	0 0 0 0 5	1537.43771	-0.00078	1565.94747	28.50898
3 1 0 0 7	0 0 0 0 6	1539.37726	0.00007	1579.28923	39.91204
3 1 0 0 8	0 0 0 0 7	1541.32108	0.00055	1594.53577	53.21523
3 1 0 0 9	0 0 0 0 8	1543.26834	0.00009	1611.68663	68.41838
3 1 0 0 10	0 0 0 0 9	1545.22004	0.00000	1630.74133	85.52129
3 1 0 0 11	0 0 0 0 10	1547.17540	-0.00018	1651.69930	104.52373
3 1 0 0 12	0 0 0 0 11	1549.13350	-0.00104	1674.55997	125.42544W
3 1 0 0 13	0 0 0 0 12	1551.09522	-0.00135	1699.32273	148.22616W
3 1 0 0 14	0 0 0 0 13	1553.06135	0.00002	1725.98691	172.92558
3 1 0 0 15	0 0 0 0 14	1555.02811	-0.00036	1754.55184	199.52337
3 1 0 0 16	0 0 0 0 15	1556.99755	-0.00008	1785.01683	228.01920
3 1 0 0 17	0 0 0 0 16	1558.97161	0.00314	1817.38115	258.41268W
3 1 0 0 18	0 0 0 0 17	1560.94076	0.00009	1851.64407	290.70340
3 -1 0 0 1	0 0 0 0 1	1525.93974	0.00079	1527.83961	1.90066
3 -1 0 0 2	0 0 0 0 2	1525.98497	0.00076	1531.68615	5.70195
3 -1 0 0 3	0 0 0 0 3	1526.05278	0.00078	1537.45581	11.40382
3 -1 0 0 4	0 0 0 0 4	1526.14181	-0.00039	1545.14839	19.00619
3 -1 0 0 5	0 0 0 0 5	1526.25472	0.00006	1554.76364	28.50898
3 -1 0 0 6	0 0 0 0 6	1526.38838	-0.00081	1566.30123	39.91204
3 -1 0 0 7	0 0 0 0 7	1526.54525	-0.00027	1579.76075	53.21523
3 -1 0 0 8	0 0 0 0 8	1526.72382	0.00045	1595.14175	68.41838
3 -1 0 0 9	0 0 0 0 9	1526.92223	-0.00015	1612.44367	85.52129
3 -1 0 0 10	0 0 0 0 10	1527.14092	-0.00123	1631.66587	104.52373W
3 -1 0 0 11	0 0 0 0 11	1527.38250	0.00030	1652.80764	125.42544
3 -1 0 0 12	0 0 0 0 12	1527.64247	0.00047	1675.86815	148.22616
3 -1 0 0 13	0 0 0 0 13	1527.91986	-0.00105	1700.84649	172.92558W
3 -1 0 0 14	0 0 0 0 14	1527.74163	0.00000	1727.74163	199.52337

3	-1	0	0	15	0	0	0	0	15	1528.53454	0.00130	1756.55244	228.01920W
3	-1	0	0	16	0	0	0	0	16	1528.86498	0.00000	1787.27765	258.41268
3	-1	0	0	17	0	0	0	0	17	1529.21264	0.00015	1819.91590	290.70340
3	-1	0	0	18	0	0	0	0	18	1529.57362	-0.00109	1854.46566	324.89096W
3	-1	0	0	19	0	0	0	0	19	1529.95037	-0.00007	1890.92532	360.97488

rms = 0.00044 cm⁻¹

$2\nu_4 + \nu_5 (\text{II} \Pi) \leftarrow G.S. (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	G'	G''
2 0 1 1 1	0 0 0 0 2	1687.62945	-0.00230	1693.33369	5.70195W
2 0 1 1 2	0 0 0 0 3	1685.75640	-0.00005	1697.16027	11.40382
2 0 1 1 3	0 0 0 0 4	1683.89375	0.00002	1702.89992	19.00619
2 0 1 1 4	0 0 0 0 5	1682.04308	-0.00036	1710.55241	28.50898
2 0 1 1 5	0 0 0 0 6	1680.20504	-0.00032	1720.11740	39.91204
2 0 1 1 6	0 0 0 0 7	1678.37956	0.00034	1731.59446	53.21523
2 0 1 1 7	0 0 0 0 8	1676.56484	0.00017	1744.98305	68.41838
2 0 1 1 8	0 0 0 0 9	1674.76103	-0.00023	1760.28255	85.52129
2 0 1 1 9	0 0 0 0 10	1672.96826	-0.00024	1777.49222	104.52373
2 0 1 1 10	0 0 0 0 11	1671.18607	0.00031	1796.61120	125.42544
2 0 1 1 11	0 0 0 0 12	1669.41310	0.00077	1817.63849	148.22616
2 0 1 1 12	0 0 0 0 13	1667.64736	-0.00004	1840.57298	172.92558
2 0 1 1 13	0 0 0 0 14	1665.88977	-0.00027	1865.41342	199.52337
2 0 1 1 14	0 0 0 0 15	1664.13832	-0.00090	1892.15842	228.01920
2 0 1 1 15	0 0 0 0 16	1662.39432	0.00052	1920.80648	258.41268
2 0 1 1 16	0 0 0 0 17	1660.65244	-0.00011	1951.35596	290.70340
2 0 1 1 17	0 0 0 0 18	1658.91487	0.00068	1983.80515	324.89096
2 0 1 1 18	0 0 0 0 19	1657.17808	0.00071	2018.15225	360.97488
2 0 1 1 1	0 0 0 0 0	1693.33337	-0.00032	1693.33369	0.00000
2 0 1 1 2	0 0 0 0 1	1695.25924	-0.00037	1697.16027	1.90066
2 0 1 1 3	0 0 0 0 2	1697.19661	-0.00137	1702.89992	5.70195W
2 0 1 1 4	0 0 0 0 3	1699.14823	-0.00037	1710.55241	11.40382
2 0 1 1 5	0 0 0 0 4	1701.11095	-0.00026	1720.11740	19.00619
2 0 1 1 6	0 0 0 0 5	1703.08557	0.00009	1731.59446	28.50898
2 0 1 1 7	0 0 0 0 6	1705.07193	0.00092	1744.98305	39.91204
2 0 1 1 8	0 0 0 0 7	1707.06857	0.00125	1760.28255	53.21523W
2 0 1 1 9	0 0 0 0 8	1709.07434	0.00050	1777.49222	68.41838
2 0 1 1 10	0 0 0 0 9	1711.08981	-0.00010	1796.61120	85.52129
2 0 1 1 11	0 0 0 0 10	1713.11484	0.00008	1817.63849	104.52373
2 0 1 1 12	0 0 0 0 11	1715.15622*	0.00868	1840.57298	125.42544W
2 0 1 1 13	0 0 0 0 12	1717.18747	0.00021	1865.41342	148.22616
2 0 1 1 14	0 0 0 0 13	1719.23280	-0.00004	1892.15842	172.92558
2 0 1 1 15	0 0 0 0 14	1721.28295	-0.00015	1920.80648	199.52337
2 0 1 1 16	0 0 0 0 15	1723.33608	-0.00068	1951.35596	228.01920
2 0 1 1 17	0 0 0 0 16	1725.39236	-0.00011	1983.80515	258.41268
2 0 1 1 18	0 0 0 0 17	1727.44806	-0.00079	2018.15225	290.70340
2 0 1 1 19	0 0 0 0 18	1729.50404	-0.00048	2054.39547	324.89096
2 0 1 -1 1	0 0 0 0 1	1691.43158	0.00042	1693.33182	1.90066
2 0 1 -1 2	0 0 0 0 2	1691.45237	-0.00032	1697.15463	5.70195
2 0 1 -1 3	0 0 0 0 3	1691.48456	-0.00028	1702.88865	11.40382
2 0 1 -1 4	0 0 0 0 4	1691.52763	0.00020	1710.53362	19.00619
2 0 1 -1 5	0 0 0 0 5	1691.58015	-0.00010	1720.08923	28.50898
2 0 1 -1 6	0 0 0 0 6	1691.64274	-0.00029	1731.55507	39.91204
2 0 1 -1 7	0 0 0 0 7	1691.71557	0.00012	1744.93068	53.21523
2 0 1 -1 8	0 0 0 0 8	1691.79731	0.00015	1760.21554	68.41838
2 0 1 -1 9	0 0 0 0 9	1691.88767	-0.00011	1777.40907	85.52129
2 0 1 -1 10	0 0 0 0 10	1691.98696	0.00005	1796.51064	104.52373
2 0 1 -1 11	0 0 0 0 11	1692.09394	-0.00021	1817.51959	125.42544
2 0 1 -1 12	0 0 0 0 12	1692.20924	0.00017	1840.43522	148.22616
2 0 1 -1 13	0 0 0 0 13	1692.33134	0.00008	1865.25684	172.92558
2 0 1 -1 14	0 0 0 0 14	1692.46050	0.00017	1891.98370	199.52337
2 0 1 -1 15	0 0 0 0 15	1692.59537	-0.00053	1920.61510	228.01920
2 0 1 -1 16	0 0 0 0 16	1692.73773	0.00010	1951.15030	258.41268
2 0 1 -1 17	0 0 0 0 17	1692.88575	0.00056	1983.58860	290.70340
2 0 1 -1 18	0 0 0 0 18	1693.00000	0.00000	2017.92928	324.89096

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

1	2	0	1	-1	19	0	0	0	0	19	1693.19675	-0.00001	2054.17165	360.97488
2	2	0	1	-1	20	0	0	0	0	20	1693.36093	0.00061	2092.31503	398.95471
3	2	0	1	-1	21	0	0	0	0	21	1693.52936	0.00053	2132.35877	438.82993
4	2	0	1	-1	22	0	0	0	0	22	1693.70107*	-0.00109	2174.30219	480.60003W
5	2	0	1	-1	23	0	0	0	0	23	1693.88006	-0.00014	2218.14465	524.26445
6	2	0	1	-1	24	0	0	0	0	24	1694.06342	0.00053	2263.88551	569.82262
7	2	0	1	-1	25	0	0	0	0	25	1694.25273	0.00256	2311.52410	617.27393W
8	2	0	1	-1	26	0	0	0	0	26	1694.44157	-0.00045	2361.05979	666.61777
9	2	0	1	-1	27	0	0	0	0	27	1694.63724	-0.00118	2412.49189	717.85348W
10	2	0	1	-1	28	0	0	0	0	28	1694.83987	0.00050	2465.81975	770.98038

rms = 0.00039 cm⁻¹

2v₄ + v₅ (¹Π) ← G.S. (Σ⁺)

v ₄ '	ℓ ₄ '	v ₅ '	ℓ ₅ '	J'	v ₄ ''	ℓ ₄ ''	v ₅ ''	ℓ ₅ ''	J''	OBS	OBS - CALC	G'	G''
2	2	1	-1	1	0	0	0	0	2	1696.66836	-0.00007	1702.37037	5.70195
2	2	1	-1	2	0	0	0	0	3	1694.78158	-0.00013	1706.18553	11.40382
2	2	1	-1	3	0	0	0	0	4	1692.90134	-0.00077	1711.90830	19.00619
2	2	1	-1	4	0	0	0	0	5	1691.03006	0.00027	1719.53877	28.50898
2	2	1	-1	5	0	0	0	0	6	1689.16540	0.00044	1729.07700	39.91204
2	2	1	-1	6	0	0	0	0	7	1687.30758	-0.00029	1740.52311	53.21523
2	2	1	-1	7	0	0	0	0	8	1685.45931	0.00049	1753.87721	68.41838
2	2	1	-1	8	0	0	0	0	9	1683.61810	-0.00005	1769.13944	85.52129
2	2	1	-1	9	0	0	0	0	10	1681.78579	-0.00045	1786.30996	104.52373
2	2	1	-1	10	0	0	0	0	11	1679.96310	-0.00042	1805.38896	125.42544
2	2	1	-1	11	0	0	0	0	12	1678.15011	-0.00036	1826.37662	148.22616
2	2	1	-1	12	0	0	0	0	13	1676.34777	0.00019	1849.27315	172.92558
2	2	1	-1	13	0	0	0	0	14	1674.55505	-0.00034	1874.07876	199.52337
2	2	1	-1	14	0	0	0	0	15	1672.77474	0.00027	1900.79367	228.01920
2	2	1	-1	15	0	0	0	0	16	1671.00576	0.00036	1929.41808	258.41268
2	2	1	-1	16	0	0	0	0	17	1669.24922	0.00043	1959.95219	290.70340
2	2	1	-1	17	0	0	0	0	18	1667.50518	-0.00005	1992.39619	324.89096
2	2	1	-1	18	0	0	0	0	19	1665.77580	0.00046	2026.75022	360.97488
2	2	1	-1	19	0	0	0	0	20	1664.06019	0.00051	2063.01439	398.95471
2	2	1	-1	20	0	0	0	0	21	1662.35830	-0.00052	2101.18875	438.82993
2	2	1	-1	21	0	0	0	0	22	1660.67217	-0.00112	2141.27332	480.60003W
2	2	1	-1	22	0	0	0	0	23	1659.00275	-0.00082	2183.26802	524.26445
2	2	1	-1	1	0	0	0	0	0	1702.36987	-0.00050	1702.37037	0.00000
2	2	1	-1	2	0	0	0	0	1	1704.28423	-0.00064	1706.18553	1.90066
2	2	1	-1	3	0	0	0	0	2	1706.20568	-0.00068	1711.90830	5.70195
2	2	1	-1	4	0	0	0	0	3	1708.13434	-0.00061	1719.53877	11.40382
2	2	1	-1	5	0	0	0	0	4	1710.07018	-0.00063	1729.07700	19.00619
2	2	1	-1	6	0	0	0	0	5	1712.01416	0.00003	1740.52311	28.50898
2	2	1	-1	7	0	0	0	0	6	1713.96484	-0.00033	1753.87721	39.91204
2	2	1	-1	8	0	0	0	0	7	1715.92432	0.00012	1769.13944	53.21523
2	2	1	-1	9	0	0	0	0	8	1717.89091	-0.00067	1786.30996	68.41838
2	2	1	-1	10	0	0	0	0	9	1719.86688	-0.00079	1805.38896	85.52129
2	2	1	-1	11	0	0	0	0	10	1721.85287	-0.00003	1826.37662	104.52373
2	2	1	-1	12	0	0	0	0	11	1723.84773	0.00002	1849.27315	125.42544
2	2	1	-1	13	0	0	0	0	12	1725.85267	0.00006	1874.07876	148.22616
2	2	1	-1	14	0	0	0	0	13	1727.86752	-0.00057	1900.79367	172.92558
2	2	1	-1	15	0	0	0	0	14	1729.89473	0.00003	1929.41808	199.52337
2	2	1	-1	16	0	0	0	0	15	1731.93279	-0.00020	1959.95219	228.01920
2	2	1	-1	17	0	0	0	0	16	1733.98371	0.00020	1992.39619	258.41268
2	2	1	-1	18	0	0	0	0	17	1736.04657	-0.00024	2026.75022	290.70340
2	2	1	-1	19	0	0	0	0	18	1738.12315	-0.00028	2063.01439	324.89096
2	2	1	-1	20	0	0	0	0	19	1740.21362	-0.00025	2101.18875	360.97488
2	2	1	-1	21	0	0	0	0	20	1742.31887	0.00026	2141.27332	398.95471
2	-2	1	1	3	0	0	0	0	3	1700.55566	0.00037	1711.95911	11.40382
2	-2	1	1	4	0	0	0	0	4	1700.61699	-0.00027	1719.62345	19.00619
2	-2	1	1	5	0	0	0	0	5	1700.69525	0.00018	1729.20404	28.50898
2	-2	1	1	6	0	0	0	0	6	1700.78918	0.00023	1740.70099	39.91204
2	-2	1	1	7	0	0	0	0	7	1700.89901	-0.00018	1754.11443	53.21523
2	-2	1	1	8	0	0	0	0	8	1701.02641	0.00030	1769.44449	68.41838
2	-2	1	1	9	0	0	0	0	9	1701.16135	0.00036	1786.69135	85.52129

2	-2	1	1	10	0	0	0	0	10	1701.33124	-0.00022	1805.85519	104.52373
2	-2	1	1	11	0	0	0	0	11	1701.51032	-0.00043	1826.93619	125.42544
2	-2	1	1	12	0	0	0	0	12	1701.70827	-0.00014	1849.93456	148.22616
2	-2	1	1	13	0	0	0	0	13	1701.92467	-0.00026	1874.85050	172.92558
2	-2	1	1	14	0	0	0	0	14	1702.16139	0.00055	1901.68422	199.52337
2	-2	1	1	15	0	0	0	0	15	1702.41638	-0.00032	1930.43590	228.01920
2	-2	1	1	16	0	0	0	0	16	1702.69342	0.00038	1961.10572	258.41268
2	-2	1	1	17	0	0	0	0	17	1702.99010	-0.00033	1993.69383	290.70340
2	-2	1	1	18	0	0	0	0	18	1703.31034	0.00096	2028.20034	324.89096
2	-2	1	1	19	0	0	0	0	19	1703.65085	0.00041	2064.62532	360.97488
2	-2	1	1	20	0	0	0	0	20	1704.01471	0.00062	2102.96880	398.95471
2	-2	1	1	21	0	0	0	0	21	1704.40040	-0.00038	2143.23071	438.82993
2	-2	1	1	22	0	0	0	0	22	1704.81068	-0.00025	2185.41096	480.60003
2	-2	1	1	23	0	0	0	0	23	1705.24509	0.00018	2229.50936	524.26445
2	-2	1	1	24	0	0	0	0	24	1705.70301	0.00000	2275.52563	569.82262

rms = 0.00041 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	G'	G''
1 -1 2 2 1	0 0 0 0 2	1861.79748	-0.00060	1867.50003	5.70195
1 -1 2 2 2	0 0 0 0 3	1859.91140	-0.00099	1871.31621	11.40382
1 -1 2 2 3	0 0 0 0 4	1858.03397	-0.00034	1877.04050	19.00619
1 -1 2 2 4	0 0 0 0 5	1856.16301	-0.00094	1884.67293	28.50898
1 -1 2 2 5	0 0 0 0 6	1854.30124	-0.00026	1894.21354	39.91204
1 -1 2 2 6	0 0 0 0 7	1852.44715	0.00002	1905.66237	53.21523
1 -1 2 2 7	0 0 0 0 8	1850.60013	-0.00096	1919.01947	68.41838
1 -1 2 2 8	0 0 0 0 9	1848.76332	-0.00030	1934.28491	85.52129
1 -1 2 2 9	0 0 0 0 10	1846.93487	-0.00015	1951.45875	104.52373
1 -1 2 2 10	0 0 0 0 11	1845.11434	-0.00128	1970.54106	125.42544W
1 -1 2 2 11	0 0 0 0 12	1843.30635	0.00060	1991.53191	148.22616
1 -1 2 2 12	0 0 0 0 13	1841.50601	0.00022	2014.43136	172.92558
1 -1 2 2 13	0 0 0 0 14	1839.71638	0.00026	2039.23950	199.52337
1 -1 2 2 14	0 0 0 0 15	1837.93600*	-0.00116	2065.95636	228.01920W
1 -1 2 2 15	0 0 0 0 16	1836.16864	-0.00069	2094.58201	258.41268
1 -1 2 2 16	0 0 0 0 17	1834.41297	-0.00008	2125.11645	290.70340
1 -1 2 2 17	0 0 0 0 18	1832.66888*	0.00014	2157.55970	324.89096
1 -1 2 2 18	0 0 0 0 19	1830.93597	-0.00087	2191.91172	360.97488
1 -1 2 2 19	0 0 0 0 20	1829.21598*	-0.00177	2228.17246	398.95471W
1 -1 2 2 20	0 0 0 0 21	1827.51049	-0.00137	2266.34179	438.82993W
1 -1 2 2 21	0 0 0 0 22	1825.81904	-0.00050	2306.41957	480.60003
1 -1 2 2 1	0 0 0 0 0	1867.50157	0.00154	1867.50003	0.00000W
1 -1 2 2 2	0 0 0 0 1	1869.41601	0.00046	1871.31621	1.90066
1 -1 2 2 3	0 0 0 0 2	1871.33846	-0.00009	1877.04050	5.70195
1 -1 2 2 4	0 0 0 0 3	1873.26881	-0.00030	1884.67293	11.40382
1 -1 2 2 5	0 0 0 0 4	1875.20780	0.00046	1894.21354	19.00619
1 -1 2 2 6	0 0 0 0 5	1877.15368	0.00029	1905.66237	28.50898
1 -1 2 2 7	0 0 0 0 6	1879.10727	-0.00016	1919.01947	39.91204
1 -1 2 2 8	0 0 0 0 7	1881.06888	-0.00079	1934.28491	53.21523
1 -1 2 2 9	0 0 0 0 8	1883.03990	-0.00046	1951.45875	68.41838
1 -1 2 2 10	0 0 0 0 9	1885.02012	0.00035	1970.54106	85.52129
1 -1 2 2 11	0 0 0 0 10	1887.00802	-0.00016	1991.53191	104.52373
1 -1 2 2 12	0 0 0 0 11	1889.00453	-0.00140	2014.43136	125.42544W
1 -1 2 2 13	0 0 0 0 12	1891.01267	-0.00067	2039.23950	148.22616
1 -1 2 2 14	0 0 0 0 13	1893.02971	-0.00108	2065.95636	172.92558W
1 -1 2 2 15	0 0 0 0 14	1895.05779	-0.00084	2094.58201	199.52337
1 -1 2 2 16	0 0 0 0 15	1897.09776	0.00051	2125.11645	228.01920
1 -1 2 2 17	0 0 0 0 16	1899.14658	-0.00044	2157.55970	258.41268
1 -1 2 2 18	0 0 0 0 17	1901.20897	0.00065	2191.91172	290.70340
1 -1 2 2 19	0 0 0 0 18	1903.28131	-0.00019	2228.17246	324.89096
1 -1 2 2 20	0 0 0 0 19	1905.36588	-0.00103	2266.34179	360.97488W
1 -1 2 2 21	0 0 0 0 20	1907.46460	-0.00026	2306.41957	398.95471
1 -1 2 2 22	0 0 0 0 21	1909.57501	-0.00064	2348.40558	438.82993
1 -1 2 2 23	0 0 0 0 22	1911.69857	-0.00096	2392.29956	480.60003
1 -1 2 2 24	0 0 0 0 23	1913.81016	-0.00116	2438.10116	524.26445

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1	1	2	-2	1	0	0	0	0	1	1865.60166	-0.00044	1867.50275	1.90066
1	1	2	-2	2	0	0	0	0	2	1865.62099	-0.00144	1871.32438	5.70195W
1	1	2	-2	3	0	0	0	0	3	1865.65215	-0.00087	1877.05683	11.40382
2	1	1	2	-2	4	0	0	0	4	1865.69344	-0.00052	1884.70016	19.00619
3	1	1	2	-2	5	0	0	0	5	1865.74552	0.00011	1894.25438	28.50898
4	1	1	2	-2	6	0	0	0	6	1865.80763	0.00011	1905.71956	39.91204
5	1	1	2	-2	7	0	0	0	7	1865.87972	-0.00080	1919.09576	53.21523
6	1	1	2	-2	8	0	0	0	8	1865.96483	0.00018	1934.38303	68.41838
7	1	1	2	-2	9	0	0	0	9	1866.06010	-0.00008	1951.58147	85.52129
8	1	1	2	-2	10	0	0	0	10	1866.16749	0.00005	1970.69116	104.52373
9	1	1	2	-2	11	0	0	0	11	1866.28710	0.00034	1991.71220	125.42544
10	1	1	2	-2	12	0	0	0	12	1866.41848	-0.00006	2014.64470	148.22616
11	1	1	2	-2	13	0	0	0	13	1866.56261	-0.00057	2039.48875	172.92558
12	1	1	2	-2	14	0	0	0	14	1866.72085	-0.00026	2066.24449	199.52337
13	1	1	2	-2	15	0	0	0	15	1866.89300	0.00019	2094.91201	228.01920
14	1	1	2	-2	16	0	0	0	16	1867.07875	0.00000	2125.49143	258.41268
15	1	1	2	-2	17	0	0	0	17	1867.27916	-0.00028	2157.98284	290.70340
16	1	1	2	-2	18	0	0	0	18	1867.49569	0.00031	2192.38633	324.89096
17	1	1	2	-2	19	0	0	0	19	1867.72738	0.00030	2228.70197	360.97488
18	1	1	2	-2	20	0	0	0	20	1867.97493	-0.00014	2266.92978	398.95471
19	1	1	2	-2	21	0	0	0	21	1868.23959	-0.00025	2307.06978	438.82993
20	1	1	2	-2	22	0	0	0	22	1868.52135	-0.00055	2349.12193	480.60003
21	1	1	2	-2	23	0	0	0	23	1868.82097	-0.00074	2393.08616	524.26445
22	1	1	2	-2	24	0	0	0	24	1869.13979	0.00006	2438.96235	569.82262
23	1	1	2	-2	25	0	0	0	25	1869.47553	-0.00086	2486.75032	617.27393
24	1	1	2	-2	26	0	0	0	26	1869.83270	0.00062	2536.44985	666.61777
25	1	1	2	-2	27	0	0	0	27	1870.20812	0.00097	2588.06063	717.85348
26	1	1	2	-2	28	0	0	0	28	1870.60136	-0.00059	2641.58233	770.98038

rms = 0.00052 cm⁻¹

3v₅ (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	G'	G"
0 0 3 1 1	0 0 0 0 2	1996.12775	-0.00096	2001.83066	5.70195
0 0 3 1 2	0 0 0 0 3	1994.23192*	0.00143	2005.63431	11.40382W
0 0 3 1 3	0 0 0 0 4	1992.33313	-0.00038	2011.33970	19.00619
0 0 3 1 4	0 0 0 0 5	1990.43756	-0.00021	2018.94675	28.50898
0 0 3 1 5	0 0 0 0 6	1988.54312	-0.00015	2028.45531	39.91204
0 0 3 1 6	0 0 0 0 7	1986.64958	-0.00043	2039.86525	53.21523
0 0 3 1 7	0 0 0 0 8	1984.75768	-0.00030	2053.17636	68.41838
0 0 3 1 8	0 0 0 0 9	1982.86709	-0.00005	2068.38843	85.52129
0 0 3 1 9	0 0 0 0 10	1980.97694	-0.00054	2085.50121	104.52373
0 0 3 1 10	0 0 0 0 11	1979.08923	0.00026	2104.51441	125.42544
0 0 3 1 11	0 0 0 0 12	1977.20154	-0.00003	2125.42773	148.22616
0 0 3 1 12	0 0 0 0 13	1975.31512	-0.00011	2148.24081	172.92558
0 0 3 1 13	0 0 0 0 14	1973.42969	-0.00022	2172.95328	199.52337
0 0 3 1 14	0 0 0 0 15	1971.54563	0.00009	2199.56474	228.01920
0 0 3 1 15	0 0 0 0 16	1969.66159	-0.00049	2228.07476	258.41268
0 0 3 1 16	0 0 0 0 17	1967.77943	-0.00003	2258.48287	290.70340
0 0 3 1 17	0 0 0 0 18	1965.89733	-0.00028	2290.78857	324.89096
0 0 3 1 18	0 0 0 0 19	1964.01675	0.00029	2324.99134	360.97488
0 0 3 1 19	0 0 0 0 20	1962.13618	0.00025	2361.09064	398.95471
0 0 3 1 20	0 0 0 0 21	1960.25605	0.00012	2399.08587	438.82993
0 0 3 1 21	0 0 0 0 22	1958.37127*	-0.00512	2438.97642	480.60003W
0 0 3 1 22	0 0 0 0 23	1956.49816	0.00094	2480.76167	524.26445
0 0 3 1 23	0 0 0 0 24	1954.61811	-0.00021	2524.44094	569.82262
0 0 3 1 24	0 0 0 0 25	1952.73990	0.00030	2570.01353	617.27393
0 0 3 1 25	0 0 0 0 26	1950.86151	0.00055	2617.47873	666.61777
0 0 3 1 26	0 0 0 0 27	1948.98254	0.00022	2666.83579	717.85348
0 0 3 1 27	0 0 0 0 28	1947.10379	0.00023	2718.08394	770.98038
0 0 3 1 28	0 0 0 0 29	1945.22506	0.00048	2771.22236	825.99778
0 0 3 1 29	0 0 0 0 30	1943.34522	-0.00007	2826.25024	882.90495
0 0 3 1 30	0 0 0 0 31	1941.46430	-0.00128	2883.16673	941.70115W
0 0 3 1 31	0 0 0 0 32	1939.58637	0.00102	2941.97094	1002.38559W
0 0 3 1 1	0 0 0 0 1	1901.83066	0.00000	2001.83066	0.00000W

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1	0	0	3	1	2	0	0	0	0	1	2003.73378	0.00013	2005.63431	1.90066
2	0	0	3	1	3	0	0	0	0	2	2005.63784	0.00008	2011.33970	5.70195
3	0	0	3	1	4	0	0	0	0	3	2007.54300	0.00007	2018.94675	11.40382
4	0	0	3	1	5	0	0	0	0	4	2009.44902	-0.00010	2028.45531	19.00619
5	0	0	3	1	6	0	0	0	0	5	2011.35632	0.00005	2039.86525	28.50898
6	0	0	3	1	7	0	0	0	0	6	2013.26418	-0.00014	2053.17636	39.91204
7	0	0	3	1	8	0	0	0	0	7	2015.17303	-0.00017	2068.38843	53.21523
8	0	0	3	1	9	0	0	0	0	8	2017.08254	-0.00028	2085.50121	68.41838
9	0	0	3	1	10	0	0	0	0	9	2018.99280	-0.00032	2104.51441	85.52129
10	0	0	3	1	11	0	0	0	0	10	2020.90342	-0.00058	2125.42773	104.52373
11	0	0	3	1	12	0	0	0	0	11	2022.81532	-0.00005	2148.24081	125.42544
12	0	0	3	1	13	0	0	0	0	12	2024.72706	-0.00006	2172.95328	148.22616
13	0	0	3	1	14	0	0	0	0	13	2026.63908	-0.00009	2199.56474	172.92558
14	0	0	3	1	15	0	0	0	0	14	2028.55114	-0.00025	2228.07476	199.52337
15	0	0	3	1	16	0	0	0	0	15	2030.46311	-0.00056	2258.48287	228.01920
16	0	0	3	1	17	0	0	0	0	16	2032.37608	0.00019	2290.78857	258.41268
17	0	0	3	1	18	0	0	0	0	17	2034.28797	0.00003	2324.99134	290.70340
18	0	0	3	1	19	0	0	0	0	18	2036.19941	-0.00027	2361.09064	324.89096
19	0	0	3	1	20	0	0	0	0	19	2038.11072	-0.00026	2399.08587	360.97488
20	0	0	3	1	21	0	0	0	0	20	2040.02177	0.00006	2438.97642	398.95471
21	0	0	3	1	22	0	0	0	0	21	2041.93198	0.00025	2480.76167	438.82993
22	0	0	3	1	23	0	0	0	0	22	2043.84067	-0.00023	2524.44094	480.60003
23	0	0	3	1	24	0	0	0	0	23	2045.74903	-0.00005	2570.01353	524.26445
24	0	0	3	1	25	0	0	0	0	24	2047.65637	0.00026	2617.47873	569.82262
25	0	0	3	1	26	0	0	0	0	25	2049.56178	-0.00008	2666.83579	617.27393
26	0	0	3	1	27	0	0	0	0	26	2051.46680	0.00063	2718.08394	666.61777
27	0	0	3	1	28	0	0	0	0	27	2053.36882	-0.00007	2771.22236	717.85348
28	0	0	3	1	29	0	0	0	0	28	2055.26981	-0.00005	2826.25024	770.98038
29	0	0	3	1	30	0	0	0	0	29	2057.16979	0.00084	2883.16673	825.99778
30	0	0	3	1	31	0	0	0	0	30	2059.06522	-0.00076	2941.97094	882.90495
31	0	0	3	-1	1	0	0	0	0	1	1999.94324	-0.00015	2001.84405	1.90066
32	0	0	3	-1	2	0	0	0	0	2	1999.97266	0.00013	2005.67447	5.70195
33	0	0	3	-1	3	0	0	0	0	3	2000.01636	0.00015	2011.42003	11.40382
34	0	0	3	-1	4	0	0	0	0	4	2000.07427	-0.00015	2019.08062	19.00619
35	0	0	3	-1	5	0	0	0	0	5	2000.14684	-0.00029	2028.65611	28.50898
36	0	0	3	-1	6	0	0	0	0	6	2000.23437	0.00007	2040.14634	39.91204
37	0	0	3	-1	7	0	0	0	0	7	2000.33562	-0.00026	2053.55111	53.21523
38	0	0	3	-1	8	0	0	0	0	8	2000.45187	0.00005	2068.87020	68.41838
39	0	0	3	-1	9	0	0	0	0	9	2000.58205	0.00000	2086.10334	85.52129
40	0	0	3	-1	10	0	0	0	0	10	2000.72636	-0.00016	2105.25025	104.52373
41	0	0	3	-1	11	0	0	0	0	11	2000.88465	-0.00049	2126.31058	125.42544
42	0	0	3	-1	12	0	0	0	0	12	2001.05770	-0.00012	2149.28398	148.22616
43	0	0	3	-1	13	0	0	0	0	13	2001.24432	-0.00015	2174.17005	172.92558
44	0	0	3	-1	14	0	0	0	0	14	2001.44505	0.00007	2200.96836	199.52337
45	0	0	3	-1	15	0	0	0	0	15	2001.65924	0.00000	2229.67844	228.01920
46	0	0	3	-1	16	0	0	0	0	16	2001.88342	-0.00371	2260.29981	258.41268W
47	0	0	3	-1	17	0	0	0	0	17	2002.12834	-0.00017	2292.83191	290.70340
48	0	0	3	-1	18	0	0	0	0	18	2002.38335	0.00012	2327.27418	324.89096
49	0	0	3	-1	19	0	0	0	0	19	2002.65115	0.00001	2363.62602	360.97488
50	0	0	3	-1	20	0	0	0	0	20	2002.93208	0.00001	2401.88678	398.95471
51	0	0	3	-1	21	0	0	0	0	21	2003.22572	-0.00013	2442.05578	438.82993
52	0	0	3	-1	22	0	0	0	0	22	2003.53194	-0.00034	2484.13231	480.60003
53	0	0	3	-1	23	0	0	0	0	23	2003.85105	-0.00011	2528.11561	524.26445
54	0	0	3	-1	24	0	0	0	0	24	2004.18190	-0.00037	2574.00488	569.82262
55	0	0	3	-1	25	0	0	0	0	25	2004.52525	-0.00012	2621.79931	617.27393
56	0	0	3	-1	26	0	0	0	0	26	2004.88022	-0.00001	2671.49800	666.61777
57	0	0	3	-1	27	0	0	0	0	27	2005.24649	-0.00010	2723.10006	717.85348
58	0	0	3	-1	28	0	0	0	0	28	2005.62384	-0.00032	2776.60454	770.98038
59	0	0	3	-1	29	0	0	0	0	29	2006.01364	0.00099	2832.01043	825.99778
60	0	0	3	-1	30	0	0	0	0	30	2006.41160	-0.00015	2889.31671	882.90495
	0	0	3	-1	31	0	0	0	0	31	2006.82101	-0.00014	2948.52229	941.70115
	0	0	3	-1	32	0	0	0	0	32	2007.23884	-0.00164	3009.62607	1002.38559W

rms = 0.00032 cm⁻¹

237x181mm (300 x 300 DPI)

227x174mm (300 x 300 DPI)

Table 1. Bands of $^{13}\text{C}_2\text{HD}$ included in the least-squares fitting procedure

Transition	Symmetry	ν_{C}^a	$P, R, Q \{J_{\text{min}}, J_{\text{max}}\}$	$\sigma (\times 10^5)^b$	n. fitted/ assig. lines
(a) 100 – 800 cm^{-1}					
$\nu_4 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	509.5852	$\text{P}_{\text{e-e}} (2-34); \text{R}_{\text{e-e}} (0-38); \text{Q}_{\text{f-e}} (1-38)$	18	104/108
$\nu_5 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	674.2363	$\text{P}_{\text{e-e}} (2-46); \text{R}_{\text{e-e}} (0-43); \text{Q}_{\text{f-e}} (1-39)$	24	122/125
$\nu_5 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	164.6511	$\text{P}_{\text{e-e}} (2-26); \text{R}_{\text{e-e}} (1-18); \text{Q}_{\text{f-e}} (1-2)$ $\text{P}_{\text{f-f}} (2-26); \text{R}_{\text{f-f}} (1-18); \text{Q}_{\text{e-f}} (1-3)$	22	83/88
$2\nu_4 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	507.2661	$\text{P}_{\text{e-e}} (1-28); \text{R}_{\text{e-e}} (1-34); \text{Q}_{\text{e-f}} (8-25)$	28	74/80
	$\Delta \leftarrow \Pi$	511.6671	$\text{P}_{\text{e-e}} (3-20); \text{R}_{\text{e-e}} (1-23); \text{Q}_{\text{e-f}} (2-28)$ $\text{P}_{\text{f-f}} (3-25); \text{R}_{\text{f-f}} (1-32); \text{Q}_{\text{f-e}} (2-33)$	31	142/155
$\nu_4 + \nu_5 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	677.8273	$\text{P}_{\text{e-e}} (1-33); \text{R}_{\text{e-e}} (1-28); \text{Q}_{\text{e-f}} (1-33)$	33	82/93
	$\Sigma^- \leftarrow \Pi$	674.1592	$\text{P}_{\text{f-f}} (1-39); \text{R}_{\text{f-f}} (1-37); \text{Q}_{\text{f-e}} (2-29)$	32	94/101
	$\Delta \leftarrow \Pi$	673.8763	$\text{P}_{\text{e-e}} (3-40); \text{R}_{\text{e-e}} (1-40); \text{Q}_{\text{e-f}} (2-35)$ $\text{P}_{\text{f-f}} (3-25); \text{R}_{\text{f-f}} (1-29); \text{Q}_{\text{f-e}} (2-34)$	34	181/197
$\nu_4 + \nu_5 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	513.1762	$\text{P}_{\text{e-e}} (6-15); \text{R}_{\text{e-e}} (6-22); \text{Q}_{\text{e-f}} (5-24)$	50	36/45
	$\Sigma^- \leftarrow \Pi$	509.5081	$\text{P}_{\text{f-f}} (3-15); \text{R}_{\text{f-f}} (3-15); \text{Q}_{\text{f-e}} (5-20)$	46	35/40
	$\Delta \leftarrow \Pi$	509.2252	$\text{P}_{\text{e-e}} (6-17); \text{R}_{\text{e-e}} (3-26); \text{Q}_{\text{e-f}} (3-20)$ $\text{P}_{\text{f-f}} (5-26); \text{R}_{\text{f-f}} (3-27); \text{Q}_{\text{f-e}} (3-16)$	43	95/113
$2\nu_5 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	661.0722	$\text{P}_{\text{e-e}} (1-38); \text{R}_{\text{e-e}} (1-29); \text{Q}_{\text{e-f}} (4-38)$	28	92/101
	$\Delta \leftarrow \Pi$	677.6629	$\text{P}_{\text{e-e}} (4-35); \text{R}_{\text{e-e}} (1-36); \text{Q}_{\text{e-f}} (3-20)$ $\text{P}_{\text{f-f}} (3-37); \text{R}_{\text{f-f}} (1-40); \text{Q}_{\text{f-e}} (2-35)$	36	178/189
$2\nu_4 + \nu_5 \leftarrow 2\nu_4$	$^{\text{II}}\Pi \leftarrow \Sigma^+$	674.5690	$\text{P}_{\text{e-e}} (2-27); \text{R}_{\text{e-e}} (0-24); \text{Q}_{\text{f-e}} (1-23)$	40	62/71
	$^{\text{I}}\Pi \leftarrow \Sigma^+$	683.6114	$\text{Q}_{\text{f-e}} (3-18)$	36	11/16
	$^{\text{I}}\Pi \leftarrow \Delta$	679.2104	$\text{P}_{\text{e-e}} (4-22); \text{R}_{\text{e-e}} (4-19); \text{Q}_{\text{f-e}} (3-29)$ $\text{P}_{\text{f-f}} (4-21); \text{R}_{\text{f-f}} (4-19)$	42	81/96
	$\Phi \leftarrow \Delta$	673.4708	$\text{P}_{\text{e-e}} (5-29); \text{R}_{\text{e-e}} (2-27); \text{Q}_{\text{e-f}} (3-13)$ $\text{P}_{\text{f-f}} (4-27); \text{R}_{\text{f-f}} (2-26); \text{Q}_{\text{f-e}} (3-8)$	46	99/117
$\nu_4 + 2\nu_5 \leftarrow \nu_4 + \nu_5$	$^{\text{II}}\Pi \leftarrow \Sigma^+$	658.5394	$\text{Q}_{\text{f-e}} (3-19)$	62	12/15
	$^{\text{I}}\Pi \leftarrow \Sigma^+$	678.1794	$\text{P}_{\text{e-e}} (2-21); \text{R}_{\text{e-e}} (0-22); \text{Q}_{\text{f-e}} (3-25)$	40	48/64
	$^{\text{II}}\Pi \leftarrow \Sigma^-$	662.2076	$\text{P}_{\text{f-f}} (2-26); \text{R}_{\text{f-f}} (0-24); \text{Q}_{\text{e-f}} (12-23)$	43	39/58
	$^{\text{I}}\Pi \leftarrow \Sigma^-$	681.8475	$\text{P}_{\text{f-f}} (2-20); \text{R}_{\text{f-f}} (0-19); \text{Q}_{\text{e-f}} (6-24)$	47	46/58
	$^{\text{II}}\Pi \leftarrow \Delta$	662.4905	$\text{P}_{\text{e-e}} (2-26); \text{R}_{\text{e-e}} (3-23); \text{Q}_{\text{f-e}} (5-19)$ $\text{P}_{\text{f-f}} (2-17); \text{R}_{\text{f-f}} (3-14)$	53	57/89
	$\Phi \leftarrow \Delta$	677.3190	$\text{P}_{\text{e-e}} (4-25); \text{R}_{\text{e-e}} (2-23); \text{Q}_{\text{e-f}} (3-13)$ $\text{P}_{\text{f-f}} (4-22); \text{R}_{\text{f-f}} (2-24); \text{Q}_{\text{f-e}} (3-13)$	42	87/107
$3\nu_4 \leftarrow 2\nu_4$	$\Pi \leftarrow \Sigma^+$	509.0649	$\text{P}_{\text{e-e}} (2-17); \text{R}_{\text{e-e}} (0-27); \text{Q}_{\text{f-e}} (1-24)$	54	40/67
	$\Pi \leftarrow \Delta$	504.6639	$\text{Q}_{\text{e-f}} (4-22); \text{Q}_{\text{f-e}} (5-20)$	56	23/32
$3\nu_5 \leftarrow 2\nu_5$	$\Pi \leftarrow \Sigma^+$	664.6203	$\text{P}_{\text{e-e}} (2-27); \text{R}_{\text{e-e}} (0-24); \text{Q}_{\text{f-e}} (1-25)$	42	66/76
	$\Pi \leftarrow \Delta$	648.0295	$\text{P}_{\text{e-e}} (2-18); \text{R}_{\text{e-e}} (6-12); \text{Q}_{\text{e-f}} (2-21)$ $\text{P}_{\text{f-f}} (2-20); \text{R}_{\text{f-f}} (5-11); \text{Q}_{\text{f-e}} (2-21)$	47	61/86
	$\Phi \leftarrow \Delta$	681.3781	$\text{P}_{\text{e-e}} (4-24); \text{R}_{\text{e-e}} (2-22); \text{Q}_{\text{e-f}} (3-20)$ $\text{P}_{\text{f-f}} (4-23); \text{R}_{\text{f-f}} (2-21); \text{Q}_{\text{f-e}} (3-21)$	50	89/119

Table 1. *Continued*

Transition	Symmetry	ν_c^a	$P, R, Q \{J_{\min}, J_{\max}\}$	$\sigma (\times 10^5)^b$	n. fitted/ assign. lines
<i>(b) 800 – 1400 cm⁻¹</i>					
2 $\nu_4 \leftarrow$ G.S.	$\Sigma^+ \leftarrow \Sigma^+$	1016.8514	P _{e-e} (1-46); R _{e-e} (1-45)	29	88/91
	($\Delta \leftarrow \Sigma^+$) ^c	1021.2523	P _{e-e} (5-45); R _{e-e} (5-44)	33	77/81
$\nu_4 + \nu_5 \leftarrow$ G.S.	$\Sigma^+ \leftarrow \Sigma^+$	1187.4126	P _{e-e} (1-45); R _{e-e} (0-43)	30	86/89
	($\Delta \leftarrow \Sigma^+$) ^c	1183.4615	P _{e-e} (7-41); R _{e-e} (6-41)	37	70/70
2 $\nu_5 \leftarrow$ G.S.	$\Sigma^+ \leftarrow \Sigma^+$	1335.3085	P _{e-e} (1-48); R _{e-e} (0-48)	28	93/97
	($\Delta \leftarrow \Sigma^+$) ^c	1351.8993	P _{e-e} (12-40); R _{e-e} (10-43)	43	59/63
3 $\nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	1016.3311	P _{e-e} (2-40); R _{e-e} (1-41); Q _{f-e} (1-17) P _{f-f} (2-39); R _{f-f} (1-40); Q _{e-f} (1-15)	31	182/190
2 $\nu_4 + \nu_5 \leftarrow \nu_4$	$^{\Pi}\Pi \leftarrow \Pi$	1181.8351	P _{e-e} (2-39); R _{e-e} (1-38) P _{f-f} (2-23); R _{f-f} (1-23)	40	107/121
	$^I\Pi \leftarrow \Pi$	1190.8776	P _{e-e} (2-39); R _{e-e} (1-37); Q _{e-f} (1-12) P _{f-f} (2-38); R _{f-f} (1-37); Q _{f-e} (1-15)	34	165/176
2 $\nu_4 + \nu_5 \leftarrow \nu_5$	$^{\Pi}\Pi \leftarrow \Pi$	1017.1840	P _{e-e} (2-33); R _{e-e} (1-35); Q _{e-f} (1-8) P _{f-f} (2-36); R _{f-f} (1-36); Q _{f-e} (1-9)	28	149/155
	$^I\Pi \leftarrow \Pi$	1026.2265	P _{e-e} (2-26); R _{e-e} (3-27) P _{f-f} (2-34); R _{f-f} (1-34)	37	87/114
$\nu_4 + 2\nu_5 \leftarrow \nu_4$	$^{\Pi}\Pi \leftarrow \Pi$	1336.3668	P _{e-e} (2-41); R _{e-e} (1-41); Q _{e-f} (1-20) P _{f-f} (2-41); R _{f-f} (1-41); Q _{f-e} (1-18)	42	184/200
	$^I\Pi \leftarrow \Pi$	1356.0067	P _{e-e} (2-23); R _{e-e} (1-24) P _{f-f} (2-28); R _{f-f} (1-37)	40	93/110
$\nu_4 + 2\nu_5 \leftarrow \nu_5$	$^{\Pi}\Pi \leftarrow \Pi$	1171.7157	P _{e-e} (2-36); R _{e-e} (1-35) P _{f-f} (2-32); R _{f-f} (1-31)	39	120/132
	$^I\Pi \leftarrow \Pi$	1191.3556	P _{e-e} (2-35); R _{e-e} (1-35); Q _{e-f} (1-9) P _{f-f} (2-33); R _{f-f} (1-36); Q _{f-e} (1-9)	27	145/153
3 $\nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	1325.6925	P _{e-e} (2-43); R _{e-e} (1-43); Q _{e-f} (1-18) P _{f-f} (2-41); R _{f-f} (1-42); Q _{f-e} (1-13)	32	184/194
<i>(c) 1400 – 2100 cm⁻¹</i>					
3 $\nu_4 \leftarrow$ G.S.	$\Pi \leftarrow \Sigma^+$	1525.9163	P _{e-e} (4-24); R _{e-e} (3-17); Q _{f-e} (1-19)	44	42/55
2 $\nu_4 + \nu_5 \leftarrow$ G.S.	$^{\Pi}\Pi \leftarrow \Sigma^+$	1691.4204	P _{e-e} (2-19); R _{e-e} (0-18); Q _{f-e} (1-28)	39	58/65
	$^I\Pi \leftarrow \Sigma^+$	1700.4628	P _{e-e} (2-23); R _{e-e} (0-20); Q _{f-e} (3-24)	41	64/65
$\nu_4 + 2\nu_5 \leftarrow$ G.S.	$^I\Pi \leftarrow \Sigma^+$	1865.5919	P _{e-e} (2-22); R _{e-e} (0-23); Q _{f-e} (1-28)	52	63/73
3 $\nu_5 \leftarrow$ G.S.	$\Pi \leftarrow \Sigma^+$	1999.9288	P _{e-e} (2-32); R _{e-e} (0-30); Q _{f-e} (1-32)	32	88/94

^a In cm⁻¹. For the definition of the band centre ν_c see text.

^b σ (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 $^{13}\text{C}_2\text{HD}$ resulting from the simultaneous fit of all subbands involving levels up to $\nu_4 + \nu_5 = 3^a$

Parameter				Parameter		
ω_4^0	508.545428	(349)		y_4^{44}	0.037907	(138)
ω_5^0	672.6186164	(558)		y_4^{45}	-0.1010299	(365)
x_{44}^0	0.010493	(259)		y_4^{55}	0.0229860	(327)
x_{45}^0	0.5569594	(664)		y_5^{44}	0.0373008	(431)
x_{55}^0	-2.5366503	(408)		y_5^{45}	-0.0490666	(312)
y_{444}^0	-0.0351803	(429)		y_5^{55}	0.0215576	(125)
y_{555}^0	0.02723375	(932)		r_{45}^0	1.223264	(356)
y_{455}^0	0.0382234	(218)		$r_{45}^J \times 10^3$	-0.021076	(111)
y_{445}^0	0.0463650	(263)		r_{445}	0.2431947	(797)
g_{44}^0	1.979179	(277)		r_{455}	0.062209	(205)
g_{45}^0	0.9991273	(690)				
g_{55}^0	5.0571095	(349)				
B_0	0.950330505	(483)		$\gamma^{45} \times 10^3$	-0.006903	(271)
$\alpha_4^0 \times 10^3$	-2.304464	(123)		$\gamma^{55} \times 10^3$	-0.111836	(100)
$\alpha_5^0 \times 10^3$	-1.283843	(142)		$\gamma_{445} \times 10^6$	1.6549	(484)
$\gamma_{44} \times 10^3$	0.0292437	(396)		$\gamma_4^{45} \times 10^6$	2.642	(116)
$\gamma_{45} \times 10^3$	-0.0243823	(889)		$\gamma_5^{44} \times 10^6$	-2.1860	(736)
$\gamma_{55} \times 10^3$	0.0224114	(501)		$\gamma_5^{45} \times 10^6$	2.4698	(870)
$\gamma^{44} \times 10^3$	-0.0777129	(670)		$\gamma_5^{55} \times 10^6$	-2.1245	(368)

Table 2 – *continued*

Parameter				Parameter			
D_0	$\times 10^6$	1.043909	(548)	δ_{55}	$\times 10^9$	0.3359	(254)
β_4	$\times 10^6$	0.029857	(114)	δ^{44}	$\times 10^9$	0.4819	(880)
β_5	$\times 10^6$	0.0135458	(750)	δ^{55}	$\times 10^9$	−1.6501	(359)
H_0	$\times 10^{12}$	0.572	(178)				
q_4^0	$\times 10^3$	4.1086440	(941)	q_4^k	$\times 10^6$	−2.5093	(850)
q_5^0	$\times 10^3$	3.217260	(110)	q_5^k	$\times 10^6$	−4.793	(117)
q_4^J	$\times 10^6$	−0.0331339	(575)				
q_5^J	$\times 10^6$	−0.0195987	(757)	ρ_4^0	$\times 10^6$	−0.004861	(195)
q_{44}	$\times 10^3$	0.0350370	(434)	ρ_5^0	$\times 10^6$	−0.010483	(587)
q_{45}	$\times 10^3$	−0.0022161	(869)	ρ_{54}	$\times 10^9$	−1.924	(255)
q_{54}	$\times 10^3$	0.0168754	(983)	ρ_{55}	$\times 10^9$	4.810	(273)
q_{55}	$\times 10^3$	0.0432949	(364)	ρ_{45}^0	$\times 10^9$	−2.089	(339)
Number of fitted data = 4342							
St. dev. of the fit $\times 10^4$ = 3.7							

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

Table 3. Vibrational term values, G_c^0 , (in cm^{-1})
of the observed ℓ -substates in $^{13}\text{C}_2\text{HD}$ ^a

ν_4	ν_5	Symmetry	ℓ_4	ℓ_5	G_c^0 ^b
1	0	Π	± 1	0	509.5852
0	1	Π	0	± 1	674.2363
2	0	Σ^+	0	0	1016.8514
2	0	Δ	± 2	0	1021.2523
1	1	Δ	± 1	± 1	1183.4615
1	1	Σ^-	-1	1	1183.7444
1	1	Σ^+	1	-1	1187.4126
0	2	Σ^+	0	0	1335.3085
0	2	Δ	0	± 2	1351.8993
3	0	Π	± 1	0	1525.9163
3	0	Φ	± 3	0	1535.0056 ^c
2	1	$^{\text{II}}\Pi$	0	± 1	1691.4204
2	1	$^{\text{I}}\Pi$	± 2	∓ 1	1700.4628
2	1	Φ	± 2	± 1	1694.7231
1	2	$^{\text{II}}\Pi$	± 1	0	1845.9520
1	2	$^{\text{I}}\Pi$	∓ 1	± 2	1865.5919
1	2	Φ	± 1	± 2	1860.7806
0	3	Π	0	± 1	1999.9288
0	3	Φ	0	± 3	2033.2774

^a Upper signs of ℓ_4 or ℓ_5 refer to 'e' states; lower signs refer to 'f' states

^b Term values, G_c^0 , are expressed as $G^0; \nu, -B; \nu, k^2 - D; \nu, k^4$

^c Calculated value.