



The stretching-bending bands of $^{13}\text{C}_2\text{HD}$

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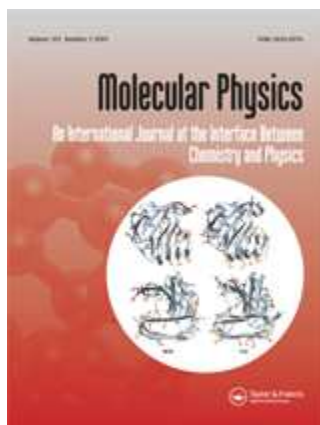
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The stretching-bending bands of $^{13}\text{C}_2\text{HD}$

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Abstract

The infrared spectrum of $^{13}\text{C}_2\text{HD}$ has been investigated by high-resolution Fourier transform infrared spectroscopy. A large number of ro-vibrational transitions in the spectral region 1000–6600 cm^{-1} have been recorded and assigned. This paper is focused only on the vibrational bands involving pure stretching, stretching-bending or stretching-stretching modes. In total, 78 bands have been identified and assigned, 29 related to ν_1 (CH stretch), 27 to ν_2 (CC stretch), and 22 to ν_3 (CD stretch). The data pertaining to each stretching mode have been fitted simultaneously in order to obtain accurate sets of rotational and vibrational parameters for the excited states.

1. Introduction

In our previous paper on $^{13}\text{C}_2\text{HD}$ [1] we pointed out that, among the possible isotopologues of acetylene, this one had been poorly investigated. Indeed, only two experimental works were published on $^{13}\text{C}_2\text{HD}$ [2,3]. The $\nu_5 \leftarrow \text{GS}$ and $\nu_3 \leftarrow \text{GS}$ fundamentals, with band origins at 674.229 and 2547.589 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 2533.281 and 2544.843 cm^{-1} , respectively, were detected [2]. In Ref. [3] only the $\nu_1 \leftarrow \text{GS}$ was analysed. The study of the high-resolution infrared spectra up to 2100 cm^{-1} was reported in Ref. [1]. The analyzed bands involved various combinations of bending states only. From the final fit, a large set of rotational and vibrational parameters was obtained. In this paper, the stretching and stretching-bending transitions up to the overtone region around 6600 cm^{-1} are considered. A few bands involving stretching-stretching modes are also reported. All these data have been analyzed and a number of ro-vibrational parameters characterising the excited states have been determined with great accuracy.

2. Experimental details

The details about the syntheses of the $^{13}\text{C}_2\text{HD}$ isotopically enriched sample were given in Ref. [1].

The spectra were recorded in the region between 900 and 6650 cm^{-1} using a Bomem DA3.002 Fourier transform spectrometer equipped with a Globar source, a KBr beamsplitter, and HgCdTe and InSb detectors. The resolution ranged between 0.006 and 0.010 cm^{-1} . Several hundred scans (up to 1000) were co-added in order to improve the quality of the spectra. The pressures ranged between 1 and 10 Torr and the optical pathlength was either 8 or 10 meters.

The spectra were calibrated by means of CO_2 and H_2O lines as reported in [4]. Occasionally, spectra of $^{13}\text{C}_2\text{H}_2$, present as an impurity, were also used. All the spectra, namely the spectra of this work and of Ref. [1], were recorded within a couple of months from receiving a fresh sample.

The wavenumber precision of the spectra is about $0.3 \times 10^{-3} \text{ cm}^{-1}$, the wavenumber accuracy is about $0.5 \times 10^{-3} \text{ cm}^{-1}$ [4].

3. Results and discussion

3.1 Analysis of the data

The spectrum of $^{13}\text{C}_2\text{HD}$ in the region between 1000 and 6650 cm^{-1} is dominated by the fundamental CH and CD stretching bands around 3300 and 2500 cm^{-1} , respectively, and by their

first overtone and combination transitions. The CC stretching band is centred around 1808 cm^{-1} . A large number of overtone and stretching-bending combination bands associated to these transitions could be detected and a total of 78 bands were analysed. They are collected in Table 1, 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]

In Fig. 1, an overview of the spectral region between 4900 and 6600 cm^{-1} is shown, while in Figs. 2 and 3 some details about the recorded infrared spectrum are illustrated. The intensity pattern shown in fig. 1 is consistent with the intensities measured for $^{12}\text{C}_2\text{HD}$ (see table 2 of Ref. [5]).

[insert Figs. 1 to 3 about here]

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 distortion corrections up to high power in the rotational angular momentum. For the transitions involving doubly degenerate states, the ℓ -doubling energy contributions containing q_v and q'_v coefficients were included in the model.

The ro-vibrational energy term values are given by

$$T^0(v, J) = G_v^0(v) + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3 + \dots \mp \frac{1}{2} \{ q_v [J(J+1)] + q'_v [J(J+1)]^2 \} \quad (1)$$

with the $-$ and $+$ signs related to the e and f levels, respectively, and the centre energy $G_c^0 = G_v^0 - B_v k^2 - D_v k^4$, 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 states.

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.

The analysis described above revealed that some bands are affected by perturbations. They will be described in the next section.

Once this procedure was completed, the wavenumbers relative to a specific stretching mode and to all its overtone, hot, and combination bands were fitted together. In this way, we obtained three independent fits, and therefore three sets of spectroscopic parameters, for the three stretching modes.

The data were fitted to the following expressions, where the vibrational and rotational diagonal contributions are $G^0(\nu, l)$ and $F(\nu, l, J)$, respectively.

$$\begin{aligned}
G^0(v, l) = & \sum_{i=1,5} \omega_i^0 v_i + \sum_{i \leq j} x_{ij}^0 v_i v_j + \sum_{b \leq b'=4,5} g_{l_b l_{b'}}^0 l_b l_{b'} + \sum_{i \leq j \leq m} y_{ijm}^0 v_i v_j v_m + \sum_{i, b \leq b'} y_i^{l_b l_{b'}} v_i l_b l_{b'} \\
& + \sum_{i \leq j \leq m \leq n} z_{ijmn} v_i v_j v_m v_n + \sum_{i \leq j, b \leq b'} z_{ij}^{l_b l_{b'}} v_i v_j l_b l_{b'}
\end{aligned} \quad (3)$$

$$\begin{aligned}
F(v, l, J) = & \left[B_0 - \sum_i \alpha_i^0 v_i + \sum_{i \leq j} \gamma_{ij}^0 v_i v_j + \sum_{b \leq b'=4,5} \gamma^{l_b l_{b'}} l_b l_{b'} + \sum_{i \leq j \leq m} \varepsilon_{ijm} v_i v_j v_m + \sum_{i, b \leq b'=4,5} \varepsilon_i^{l_b l_{b'}} v_i l_b l_{b'} \right] \\
& [M - k^2] - \left[D_0 + \sum_i \beta_i^0 v_i + \sum_{i \leq j} \delta_{ij}^0 v_i v_j + \sum_{b \leq b'} \delta^{l_b l_{b'}} l_b l_{b'} + \sum_{i \leq j \leq m} \theta_{ijm} v_i v_j v_m + \sum_{i, b \leq b'=4,5} \theta_i^{l_b l_{b'}} v_i l_b l_{b'} \right] \\
& [M - k^2]^2 + \left[H_0 + \sum_i h_i v_i \right] [M - k^2]^3
\end{aligned} \quad (4)$$

Vibrational and rotational ℓ -type resonance contributions are expressed by off-diagonal matrix elements containing the following parameters (see Table 1 of Ref. [6]):

$$r_{45} = r_{45}^0 + r_{45}^J M, \quad (5)$$

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

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

and ρ_{45}^0 .

Moreover, the r , q , and ρ parameters for the energy levels involving one quantum of a stretching mode v_s ($s = 1, 2, 3$) in addition to the excitation of the bending modes, are given by the expressions

$$q_{st} = q_{st}^0 + q_{stt}v_t + q_{stt'}v_{t'} + q_{ss't}v_s v_t + q_{st}^J M, \quad (8)$$

$$\rho_{st} = \rho_{st}^0 + \rho_{st}^J M, \quad (9)$$

$$r_{s45} = r_{s45}^0 + r_{s45}^J M, \quad (10)$$

$$\rho_{s45} = \rho_{s45}^0, \quad (11)$$

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

The stretching-stretching combination bands, $\nu_1 + \nu_3 \leftarrow \text{GS}$ and $\nu_2 + \nu_3 \leftarrow \text{GS}$ with associated hot bands, $\nu_2 + \nu_3 + \nu_4 \leftarrow \nu_4$ and $\nu_2 + \nu_3 + \nu_5 \leftarrow \nu_5$, were fitted separately. All the parameters related to the $\nu_s = 1$ ($s = 1, 2, 3$) states in eqs. 3 and 4, i.e. $\omega_s^0, x_{ss}^0, \alpha_s^0, \beta_s^0$, etc., were constrained to the values reported in tables 2 to 4.

Identical unitary weights were assigned to all the transitions, except for lines of very weak bands, which were given a 100 times reduced weight, or overlapped lines, which were given zero weight. In addition, transition wavenumbers that differed from the corresponding calculated values by more than a chosen limit (0.001, 0.002, or 0.01 cm^{-1} , depending on the band) were excluded from the last cycle of the least squares procedure.

In the simultaneous fits the ground state and the pure bending state parameters were held fixed to values obtained from a previous analysis of the bending states up to $\nu_4 + \nu_5 = 3$ [1].

The choice of the refined parameters in each simultaneous fit was dictated by the structure of the data set. Because of the lower number of excited vibrational states analysed, a smaller number of constants of the ν_2 band system could be determined, compared to ν_1 and ν_3 . Particular care has been devoted to the refinement of additional parameters, since they must: a) correspond to lower-order ones previously refined, b) be statistically determined, c) improve the quality of the fit. The adequacy of the Hamiltonian model adopted was tested by comparing the results of the simultaneous analysis to those achieved in the single band fits mentioned above.

The parameters obtained in the simultaneous fits are listed in tables 2 to 5. They are statistically well determined and, in most cases, with low internal correlation.

[insert tables 2 to 5]

For most of the parameters the estimated uncertainties are several orders of magnitude smaller than their values. The least precisely determined ones are some higher order constants, ϵ_3^{55} , β_3^0 , and δ_{13} , whose uncertainties are about 30% of their values.

The ro-vibrational parameters characterizing the stretching modes in tables 2 to 4 can be compared with those of $^{12}\text{C}_2\text{HD}$ (see tables 2 to 4 in Ref. [7]). Since the number of excited states investigated is larger for $^{13}\text{C}_2\text{HD}$ than for $^{12}\text{C}_2\text{HD}$, fewer parameters were determined for $^{12}\text{C}_2\text{HD}$, lacking in particular higher order corrections. In addition, the choice of the refined parameters is slightly different for the two isotopologues. However, most of the corresponding parameters are comparable in magnitude, uncertainty and sign, and follow the expected trend for isotopic substitution. This is particularly true for the lower order constants, x_{st}^0 , α_s^0 , q_{st}^0 , ρ_{st}^0 , r_{s45}^0 , ρ_{s45}^0 , whose values differ in the range 2-20% for the two isotopologues.

The centre term values, G_c^0 , of all the vibrationally excited states involved in the analysed transitions have been collected in table 6. They can be compared with those of $^{12}\text{C}_2\text{HD}$ (see table 5 in Ref. [7]). A comparison between the term values of the first excited state of the

stretching modes, $\nu_s = 1$, evidences that the values for $^{13}\text{C}_2\text{HD}$ are smaller than the corresponding ones of $^{12}\text{C}_2\text{HD}$ by about 18 cm^{-1} (0.5%), 45 cm^{-1} (2.4%), and 36 cm^{-1} (1.4%), for $s = 1, 2, 3$, respectively.

[insert table 6]

Finally, the agreement between the origins of the $\nu_3 \leftarrow \text{GS}$, $\nu_3 + \nu_4 \leftarrow \nu_4$, and $\nu_3 + \nu_5 \leftarrow \nu_5$ bands, the anharmonicity, x_{34}^0 and x_{35}^0 , and the ℓ -doubling, q_{34}^0 and q_{35}^0 , parameters reported in Ref. [2] and those presently obtained is remarkably good.

Tables with the full list of transition wavenumbers, quantum numbers and residuals from the fits associated with ν_1 , ν_2 and ν_3 are deposited with the British Library under the Supplementary Publications scheme. The tables are also available from the authors.

3.2 Perturbations

The rovibrational structure of a few bands shows evidences of the effect of perturbations. The mostly affected bands are $2\nu_3 \leftarrow \text{GS}$ (see fig. 3) and $\nu_2 + \nu_3 \leftarrow \text{GS}$, which show

increasing residuals in the fit, approximately from $J' \geq 10$ and $J' \geq 18$, respectively.

Although both vibrational and ro-vibrational (Coriolis) perturbations can occur, the following discussion is limited to purely vibrational resonances. In such a case, the interacting states must be of the same symmetry, Σ^+ in this case. Therefore, only combinations of pure stretching modes or stretching and bending modes with an even number of bendings are allowed.

The $2\nu_3 \leftarrow$ GS band origin ν_c is about 5049 cm^{-1} . Possible interacting states are $\nu_1 = \nu_2 = 1$ (calculated $G_c = 5120 \text{ cm}^{-1}$) and $\nu_3 = \nu_4 = 1, \nu_5 = 3, \ell_4 = 1, \ell_5 = -1$ (calculated $G_c = 5030 \text{ cm}^{-1}$). The combination of two stretching modes is favourable from the point of view of the interaction Hamiltonian, H_{40} compared to H_{50} of the bending-stretching combination, but less favourable from the point of view of the energy. It is possible to estimate an order of magnitude of the perturbation on the basis of the Nielsen's parameter [8] $\epsilon = (B/\omega)^{1/2}$, where B and ω are mean values of the rotational and vibrational constants, respectively. In the case of $^{13}\text{C}_2\text{HD}$, where $B \approx 0.95 \text{ cm}^{-1}$ and $\omega \approx 5100 \text{ cm}^{-1}$, the ratio H_{40}/H_{50} is proportional to $\epsilon^{-1/2}$, which is about 73. In principle, both perturbation channels can be important but

we believe that an interaction with $\nu_3 = \nu_4 = 1$, $\nu_5 = 3$ (also known as 3/4555) is more effective. Also, the interaction between the $\nu_3 = 2$ and $\nu_1 = \nu_2 = 1$ states resulted to be not relevant in a global analysis of 115 vibrational states up to 25000 cm^{-1} in $^{12}\text{C}_2\text{HD}$ [9]. We calculated the term value differences $\nu_3 = 1 - (\nu_4 = 1, \nu_5 = 3)$ and $\nu_3 = 3 - (\nu_3 = 2, \nu_4 = 1, \nu_5 = 3)$ obtaining 50 and 4 cm^{-1} , respectively. The $\nu_3 \leftarrow$ GS fundamental band is found to be unaffected by the interaction. The $3\nu_3 \leftarrow$ GS band falls in the wavenumber region above 6600 cm^{-1} , which is under investigation and will be reported in a further paper.

For the $\nu_2 + \nu_3 \leftarrow$ GS band, with band origin at about 4338 cm^{-1} , the closest interacting state is $\nu_2 = \nu_4 = 1$, $\nu_5 = 3$, $\ell_4 = 1$, $\ell_5 = -1$ (calculated $G_c = 4299 \text{ cm}^{-1}$), and the interaction term is the same H_{50} mentioned before. Again, this interaction is labelled as 3/4555.

Another evident anomaly in the spectra concerns the $\nu_3 + \nu_4 \leftarrow$ GS, centred around 3042.8 cm^{-1} . The least-squares single band fit shows again increasing discrepancies between observed and calculated values, with the $Q(28)$ transitions that disappears almost completely from the spectrum. The probable interacting state can be identified as $(\nu_4 = 2, \nu_5$

= 3, $^1\Pi$), whose origin can be calculated at 3015.34 cm^{-1} .

Also in this case, the interaction Hamiltonian (3/4555) is of the H_{50} type.

None of the possible interacting state above mentioned has been identified in the spectrum. This is surprising for $\nu_1 + \nu_2$, but not entirely unexpected since this band was not detected also for $^{12}\text{C}_2\text{HD}$ [5].

4. Conclusions

The infrared spectrum of $^{13}\text{C}_2\text{HD}$ has been studied by high-resolution Fourier transform spectroscopy. The spectral region investigated ranged between 1000 and 6600 cm^{-1} . A total of 78 bands, involving the CH, CD, and CC stretching modes, were identified, some of them showing local resonances. The stretching fundamentals and their associated overtones, hot, and combination bands were analysed individually, yielding four sets of parameters. These are the most accurate and complete available data for $^{13}\text{C}_2\text{HD}$ and include all the first order stretching anharmonicity constants, but x_{12} . The spectral region above 6600 cm^{-1} will be the subject of a further paper. Once more information will be available we will attempt a global fit.

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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 (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fit of the ν_1 fundamental and its associated hot bands.

Table 3. Spectroscopic parameters (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fit of the ν_2 fundamental and its associated hot bands.

Table 4. Spectroscopic parameters (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fit of the ν_3 fundamental and its associated hot bands.

Table 5. Spectroscopic parameters (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fits of the $\nu_1 + \nu_3$, $\nu_2 + \nu_3$ and its associated hot bands.

Table 6. Vibrational term values G_c (cm^{-1})^a of the observed levels involving stretching modes in $^{13}\text{C}_2\text{HD}$.

FIGURE LEGENDS

Figure 1

The infrared spectrum of $^{13}\text{C}_2\text{HD}$ between 4900 and 6600 cm^{-1} .
Experimental conditions: pressure 107 Pa, absorption path
length 8 m, resolution 0.01 cm^{-1} , 230 scans.

Figure 2

a) A portion of the infrared spectrum of $^{13}\text{C}_2\text{HD}$ between 3940
and 3980 cm^{-1} . b) an expanded view of a) between 3969 and
3976 cm^{-1} . Experimental conditions: pressure 133 Pa,
absorption path length 10 m, resolution 0.008 cm^{-1} , 250
scans.

Figure 3

A portion of the infrared spectrum of $^{13}\text{C}_2\text{HD}$ between 4372
and 4382 cm^{-1} . Lines marked with an asterisk belong to the
perturber. Experimental conditions: pressure 1.293 kPa,
absorption path length 10 m, resolution 0.008 cm^{-1} , 1000
scans.

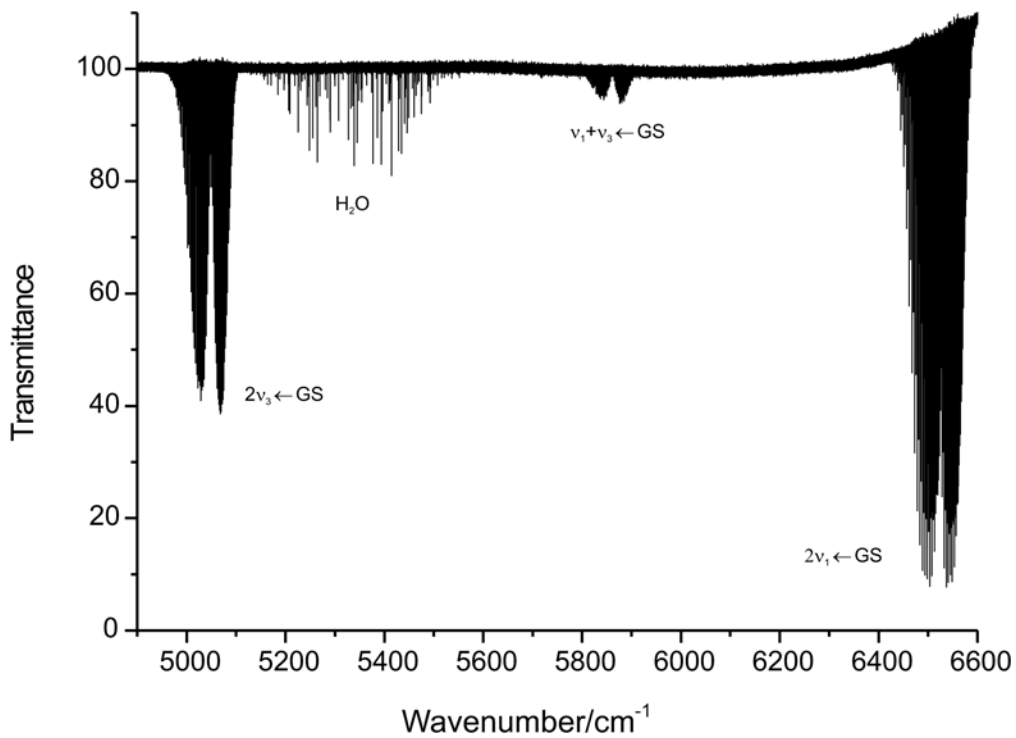
References

- [1] L. Fusina, F. Tamassia, G. Di Lonardo, A. Baldan, *Mol. Phys.*, **107**, 2119 (2009).
- [2] S. Ghersetti, A. Baldacci, S. Giorgianni, R. H. Barnes, K. Narahari Rao, *Gazz. Chim. It.*, **105**, 875 (1975).
- [3] K. A. Mohamed, *Indian J. Pure Appl. Phys.*, **26**, 705 (1998).
- [4] G. Guelachvili, M. Birk, Ch. J. Bordé, J. W. Brault, L. R. Brown, B. Carli, A. R. H. Cole, K. M. Evenson, A. Fayt, D. Hausmann, J. W. C. Johns, J. Kauppinen, Q. Kou, A. G. Maki, K. Narahari Rao, R. A. Toth, W. Urban, A. Valentin, J. Vergès, G. Wagner, M. H. Wappelhorst, J. S. Wells, B. P. Winnewisser, M. Winnewisser, *Pure & Appl. Chem.*, **68**, 193, (1996).
- [5] J. Liévin, M. Abbouti Tamsamani, P. Gaspard, M. Herman, *Chem. Phys.*, **190**, 419 (1995).
- [6] T. R. Huet, M. Herman, J. W. C. Johns, *J. Chem. Phys.*, **94**, 3407 (1991).

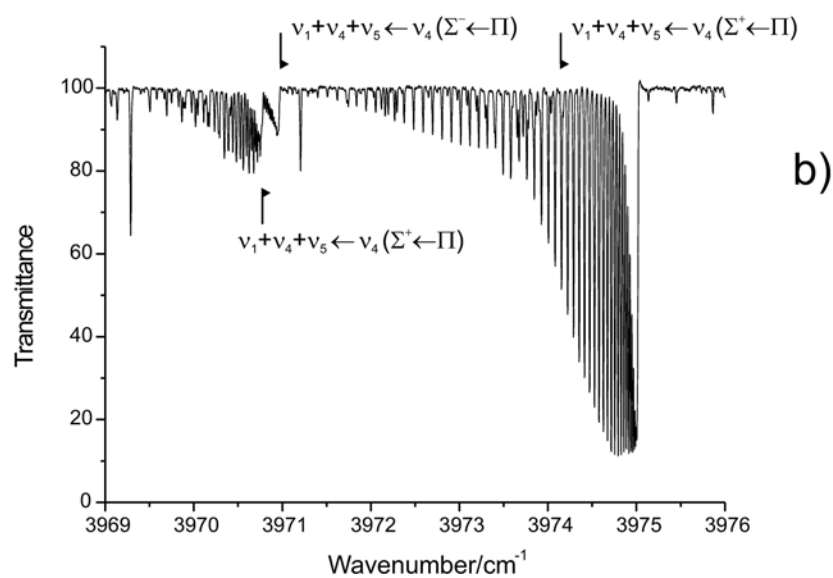
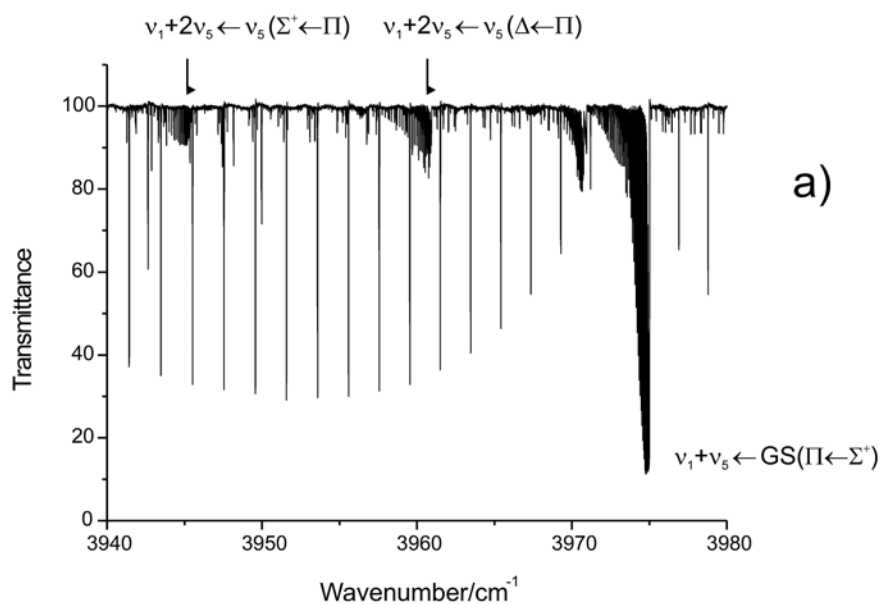
[7] L. Fusina, F. Tamassia, G. Di Lonardo, *Mol. Phys.*, **103**, 2613 (2005).

[8] D. Papoušek, M. R. Aliev, *Molecular vibrational/rotational Spectra* (Academia/Prague 1982).

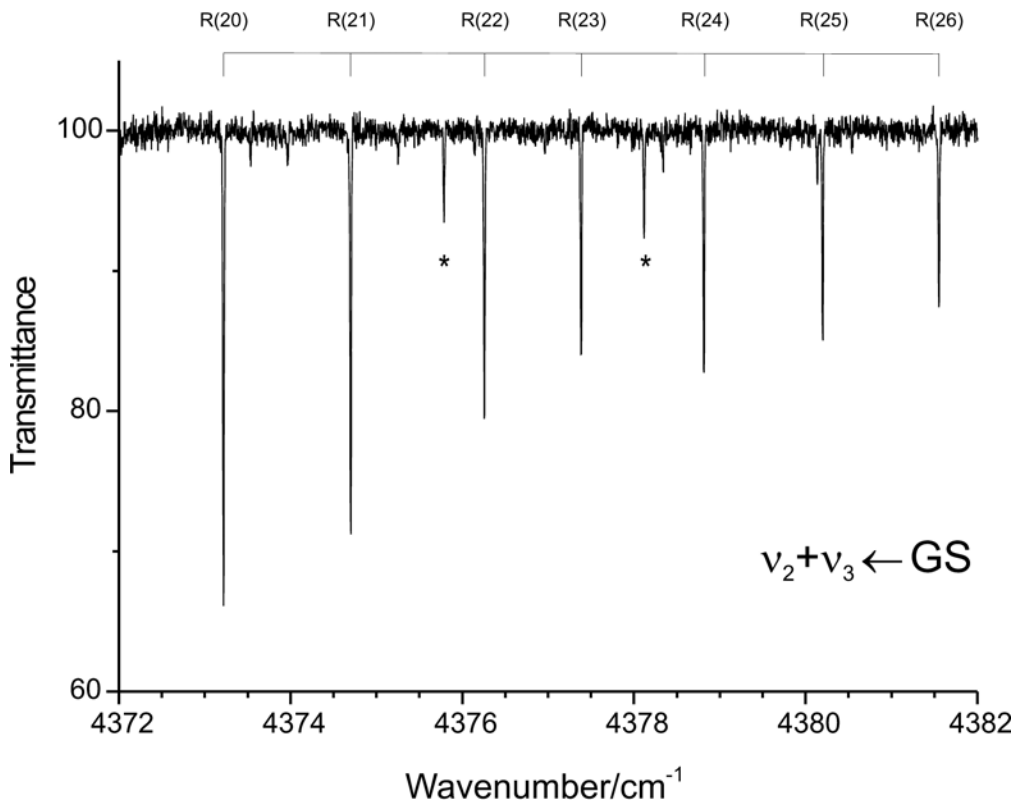
[9] M. Herman, C. Depiesse, G. Di Lonardo, A. Fayt, L. Fusina, D. Hurtmans, S. Kassi, M. Mollabashi, J. Vander Auwera, *J. Mol. Spectrosc.*, **228**, 499 (2004).



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165x228mm (600 x 600 DPI)



219x172mm (600 x 600 DPI)

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

Transition	Symmetry	ν_{C}^a	$P, R, Q \{J_{\min}, J_{\max}\}$	$\sigma (\times 10^4)^b$	n. fitted/ assig. lines
(a) 1100 – 2500 cm^{-1}					
$\nu_2 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	1134.6089	$P_{e-e} (1-32); R_{e-e} (1-29); Q_{e-f} (1-33)$	4.75	90/95
$\nu_2 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	1299.2600	$P_{e-e} (1-34); R_{e-e} (1-32); Q_{e-f} (1-25)$	3.20	79/88
$\nu_2 + \nu_4 + \nu_5 \leftarrow \nu_4 + \nu_5$	$\Sigma^+ \leftarrow \Sigma^+$	1800.7288	$P_{e-e} (2-20); R_{e-e} (0-22)$	4.90	31/44
	$\Sigma^- \leftarrow \Sigma^-$	1801.0709	$P_{f-f} (6-22); R_{f-f} (0-24)$	4.64	35/43
	$\Delta \leftarrow \Delta$	1801.3272	$P_{e-e} (3-22); R_{e-e} (2-22)$ $P_{f-f} (3-22); R_{f-f} (2-22)$	5.11	56/83
$\nu_2 + 2\nu_4 \leftarrow 2\nu_4$	$\Delta \leftarrow \Delta$	1801.1079	$P_{e-e} (3-23); R_{e-e} (2-21)$ $P_{f-f} (3-23); R_{f-f} (2-21)$	4.93	62/83
	$\Sigma^+ \leftarrow \Sigma^+$	1801.9303	$P_{e-e} (1-25); R_{e-e} (0-23)$	4.37	43/50
$\nu_2 + 2\nu_5 \leftarrow 2\nu_5$	$\Delta \leftarrow \Delta$	1801.3353	$P_{e-e} (3-22); R_{e-e} (2-22)$ $P_{f-f} (3-22); R_{f-f} (2-22)$	4.60	60/83
	$\Sigma^+ \leftarrow \Sigma^+$	1801.5178	$P_{e-e} (2-25); R_{e-e} (1-24)$	4.30	41/43
$\nu_2 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	1804.8923	$P_{e-e} (2-37); R_{e-e} (1-36); P_{f-f} (2-32);$ $R_{f-f} (1-34); Q_{f-e} (1-11)$	3.18	144/148
$\nu_2 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	1805.1704	$P_{e-e} (2-34); R_{e-e} (1-33); P_{f-f} (2-35);$ $R_{f-f} (1-34); Q_{f-e} (1-10); Q_{e-f} (8-11)$	3.39	143/148
$\nu_2 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	1808.8453	$P_{e-e} (2-45); R_{e-e} (0-44)$	3.86	86/90
$\nu_3 + \nu_4 \leftarrow 2\nu_4$	$\Pi \leftarrow \Delta$	2021.6128	$P_{e-e} (2-17); R_{e-e} (4-14); P_{f-f} (4-18);$ $R_{f-f} (4-15); Q_{f-e} (2-23); Q_{e-f} (2-23)$	4.47	84/99
	$\Pi \leftarrow \Sigma^+$	2026.0138	$P_{e-e} (3-24); R_{e-e} (0-23); Q_{f-e} (1-20)$	4.57	52/67
$\nu_3 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	2038.0055	$P_{e-e} (1-35); R_{e-e} (1-34); Q_{e-f} (1-36)$	3.41	100/106
$\nu_2 + 2\nu_4 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	2309.1964	$P_{e-e} (2-24); R_{e-e} (1-21); Q_{f-e} (1-20)$	4.33	50/65
	$\Delta \leftarrow \Pi$	2312.7750	$P_{e-e} (3-17); R_{e-e} (1-20); P_{f-f} (5-21);$ $R_{f-f} (1-20); Q_{e-f} (2-27)$	4.42	71/99
$\nu_2 + \nu_4 + \nu_5 \leftarrow \nu_5$	$\Delta \leftarrow \Pi$	2310.5524	$P_{e-e} (9-17); R_{e-e} (3-20); P_{f-f} (5-19);$ $R_{f-f} (3-20); Q_{e-f} (5-15)$	4.81	42/68
$\nu_2 + \nu_4 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	2314.4775	$P_{e-e} (2-32); R_{e-e} (1-34);$	3.65	59/66
$\nu_2 + 2\nu_5 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	2462.5899	$P_{e-e} (4-16); R_{e-e} (4-21); Q_{e-f} (2-15)$	4.83	34/48
	$\Delta \leftarrow \Pi$	2478.9983	$P_{e-e} (7-9); R_{e-e} (2-20);$ $P_{f-f} (8-11); R_{f-f} (2-21)$	5.19	31/48
$\nu_2 + \nu_4 + \nu_5 \leftarrow \nu_4$	$\Sigma^- \leftarrow \Pi$	2475.2300	$P_{f-f} (2-21); R_{f-f} (3-22);$	4.68	28/41
	$\Delta \leftarrow \Pi$	2475.2035	$Q_{f-f} (4-16); Q_{f-e} (4-20)$	4.84	22/30
$\nu_2 + \nu_5 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	2479.4067	$P_{f-f} (2-35); R_{f-f} (1-36); Q_{f-e} (1-30)$	3.73	92/99
(a) 2500 – 3500 cm^{-1}					
$\nu_3 + 2\nu_4 \leftarrow 2\nu_4$	$\Sigma^+ \leftarrow \Sigma^+$	2519.0594	$P_{e-e} (1-26); R_{e-e} (0-24)$	2.85	37/52
	$\Delta \leftarrow \Delta$	2519.0644	$P_{e-e} (3-31); R_{e-e} (2-33); P_{f-f} (3-32);$ $R_{f-f} (2-30); Q_{e-f} (2-13); Q_{f-e} (2-13)$	3.44	110/145
$\nu_3 + \nu_4 + \nu_5 \leftarrow \nu_4 + \nu_5$	$\Sigma^- \leftarrow \Sigma^-$	2530.5179	$P_{f-f} (1-31); R_{f-f} (0-29)$	3.94	51/62
	$\Delta \leftarrow \Delta$	2530.5788	$P_{e-e} (3-30); R_{e-e} (2-29); P_{f-f} (3-30);$ $R_{f-f} (2-29); Q_{e-f} (2-13); Q_{f-e} (2-15)$	4.30	91/140

Table 1. *Continued I*

Transition	Symmetry	ν_c^a	$P, R, Q \{J_{\min}, J_{\max}\}$	$\sigma (\times 10^4)^b$	n. fitted/ assign. lines
	$\Sigma^+ \leftarrow \Sigma^+$	2530.8560	$P_{e-e} (1-28); R_{e-e} (0-28)$	3.36	51/58
$\nu_3 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	2533.2799	$P_{e-e} (2-40); R_{e-e} (1-42); P_{f-f} (2-40);$ $R_{f-f} (1-43); Q_{e-f} (1-20); Q_{f-e} (1-22)$	2.90	127/204
$\nu_3 + 2\nu_5 \leftarrow 2\nu_5$	$\Sigma^+ \leftarrow \Sigma^+$	2542.1325	$P_{e-e} (1-25); R_{e-e} (0-28)$	3.47	48/55
	$\Delta \leftarrow \Delta$	2542.2011	$P_{e-e} (3-24); R_{e-e} (2-27); P_{f-f} (3-25);$ $R_{f-f} (2-28); Q_{f-e} (2-12); Q_{e-f} (2-12)$	3.64	84/121
$\nu_3 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	2544.8538	$P_{e-e} (2-40); R_{e-e} (1-41); P_{f-f} (2-40);$ $R_{f-f} (1-41); Q_{f-e} (1-19); Q_{e-f} (1-20)$	2.78	190/199
$\nu_3 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	2547.5908	$P_{e-e} (1-47); R_{e-e} (0-51)$	3.07	91/99
$\nu_1 + \nu_5 \leftarrow 2\nu_5$	$\Pi \leftarrow \Delta$	2623.1205	$P_{e-e} (6-21); R_{e-e} (10-20); P_{f-f} (6-22);$ $R_{f-f} (5-21); Q_{f-e} (3-20); Q_{e-f} (2-22)$	4.66	60/83
	$\Pi \leftarrow \Sigma^+$	2639.7113	$P_{e-e} (2-25); R_{e-e} (1-22); Q_{f-e} (1-21)$	5.07	43/61
$\nu_1 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	2643.5910	$P_{e-e} (1-34); R_{e-e} (1-36); Q_{f-e} (1-36)$	2.93	103/107
$\nu_1 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	2808.2421	$P_{e-e} (1-23); R_{e-e} (1-19); Q_{f-e} (1-28)$	5.00	61/71
$\nu_2 + 2\nu_4 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	2818.7817	$P_{e-e} (1-24); R_{e-e} (0-21)$	3.93	43/47
$\nu_3 + 2\nu_4 \leftarrow \nu_4$	$\Sigma^+ \leftarrow \Pi$	3026.3255	$P_{e-e} (2-24); R_{e-e} (1-19); Q_{e-f} (1-18)$	4.22	48/61
	$\Delta \leftarrow \Pi$	3030.7315	$P_{e-e} (2-19); R_{e-e} (1-21); P_{f-f} (2-19);$ $R_{f-f} (1-20); Q_{f-e} (2-27); Q_{e-f} (2-27)$	4.39	81/128
$\nu_3 + \nu_4 + \nu_5 \leftarrow \nu_5$	$\Sigma^- \leftarrow \Pi$	3040.0260	$Q_{f-e} (4-16)$	4.87	8/14
	$\Sigma^+ \leftarrow \Pi$	3044.0322	$Q_{e-f} (5-14)$	4.71	5/11
$\nu_3 + \nu_4 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	3042.8652	$P_{e-e} (2-34); R_{e-e} (0-32); Q_{f-e} (2-38)$	4.03	73/104
$\nu_2 + 2\nu_5 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	3136.8263	$P_{e-e} (1-31); R_{e-e} (0-29)$	3.66	58/62
$\nu_1 + 2\nu_5 \leftarrow 2\nu_5$	$\Delta \leftarrow \Delta$	3283.3010	$P_{e-e} (3-26); R_{e-e} (2-23); P_{f-f} (3-25);$ $R_{f-f} (2-24); Q_{f-e} (2-10); Q_{e-f} (2-10)$	4.50	52/111
	$\Sigma^+ \leftarrow \Sigma^+$	3284.3493	$P_{e-e} (1-25); R_{e-e} (0-26)$	3.29	31/53
$\nu_1 + \nu_4 + \nu_5 \leftarrow \nu_4 + \nu_5$	$\Sigma^+ \leftarrow \Sigma^+$	3296.1085	$P_{e-e} (1-28); R_{e-e} (0-26)$	4.08	34/56
	$\Sigma^- \leftarrow \Sigma^-$	3296.8111	$P_{f-f} (1-28); R_{f-f} (0-30)$	4.00	33/60
	$\Delta \leftarrow \Delta$	3296.9083	$P_{e-e} (3-31); R_{e-e} (2-28)$ $P_{f-f} (3-31); R_{f-f} (2-28)$	3.84	60/112
$\nu_1 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	3300.7835	$P_{e-e} (3-41); R_{e-e} (1-39); P_{f-f} (3-36);$ $R_{f-f} (1-39); Q_{f-e} (1-20); Q_{e-f} (1-14)$	4.18	155/179
$\nu_1 + 2\nu_4 \leftarrow 2\nu_4$	$\Delta \leftarrow \Delta$	3310.0087	$P_{e-e} (3-30); R_{e-e} (2-34); P_{f-f} (3-37);$ $R_{f-f} (2-34); Q_{f-e} (2-13); Q_{e-f} (2-12)$	4.32	57/153
	$\Sigma^+ \leftarrow \Sigma^+$	3310.5059	$P_{e-e} (1-35); R_{e-e} (0-34)$	4.17	51/71
$\nu_1 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	3313.8369	$P_{e-e} (2-41); R_{e-e} (1-44); P_{f-f} (2-44);$ $R_{f-f} (1-45); Q_{f-e} (1-20); Q_{e-f} (1-22)$	4.04	173/207
$\nu_1 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	3317.8274	$P_{e-e} (1-49); R_{e-e} (0-51)$	3.56	97/103
<i>(a)</i> 3500 – 6600 cm ⁻¹					
$2\nu_2 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	3607.4016	$P_{e-e} (1-38); R_{e-e} (0-36)$	2.73	69/76
$\nu_3 + \nu_4 + \nu_5 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	3718.2685	$P_{e-e} (1-19); R_{e-e} (0-20)$	4.09	32/41
$\nu_1 + \nu_4 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	3823.4222	$P_{e-e} (2-31); R_{e-e} (1-28)$	5.73	51/59

Table 1. *Continued II*

Transition	Symmetry	ν_c^a	$P, R, Q \{J_{\min}, J_{\max}\}$	$\sigma (\times 10^5)^b$	n. fitted/ assign. lines
$\nu_1 + 2\nu_5 \leftarrow \nu_5$	$\Sigma^+ \leftarrow \Pi$	3945.4215	$P_{e-e} (1-33); R_{e-e} (1-29); Q_{e-f} (1-31)$	2.93	78/94
	$\Delta \leftarrow \Pi$	3960.9640	$P_{e-e} (3-29); R_{e-e} (2-27); P_{f-f} (3-30);$ $R_{f-f} (2-29); Q_{f-e} (2-32); Q_{e-f} (3-29)$	3.44	141/168
$\nu_1 + \nu_4 + \nu_5 \leftarrow \nu_4$	$\Delta \leftarrow \Pi$	3970.7846	$P_{e-e} (3-34); R_{e-e} (1-34); P_{f-f} (3-22);$ $R_{f-f} (1-23); Q_{e-f} (2-26); Q_{f-e} (5-36)$	4.08	112/167
	$\Sigma^- \leftarrow \Pi$	3970.9703	$P_{f-f} (1-35); R_{f-f} (1-32); Q_{f-e} (5-14)$	3.90	62/78
	$\Sigma^+ \leftarrow \Pi$	3973.9358	$P_{e-e} (1-28); R_{e-e} (1-24); Q_{e-f} (1-32)$	4.75	66/85
$\nu_1 + \nu_5 \leftarrow \text{G.S.}$	$\Pi \leftarrow \Sigma^+$	3975.0198	$P_{e-e} (2-40); R_{e-e} (0-39); Q_{e-f} (1-41)$	3.79	108/121
$\nu_1 + 3\nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	4323.7956	$P_{e-e} (4-18); R_{e-e} (2-18);$ $P_{f-f} (4-18); R_{f-f} (2-16);$	52.71	37/63
$\nu_2 + \nu_3 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	4319.7313	$P_{e-e} (2-25); R_{e-e} (1-23);$ $P_{f-f} (2-24); R_{f-f} (1-23);$	9.46	53/94
$\nu_1 + 2\nu_4 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	4327.3573	$P_{e-e} (1-27); R_{e-e} (0-26)$	5.29	45/54
$\nu_2 + \nu_3 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	4331.4759	$P_{e-e} (5-18); R_{e-e} (4-20);$ $P_{f-f} (4-18); R_{f-f} (4-20);$	9.56	52/64
$\nu_2 + \nu_3 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	4337.9791	$P_{e-e} (1-33); R_{e-e} (0-34)$	6.38	35/69
$\nu_1 + \nu_4 + \nu_5 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	4483.5210	$P_{e-e} (2-20); R_{e-e} (1-18)$	5.63	33/38
$\nu_1 + 2\nu_5 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	4619.6578	$P_{e-e} (1-22); R_{e-e} (1-26)$	6.07	38/49
$2\nu_3 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	5020.0835	$P_{e-e} (2-27); R_{e-e} (1-28);$ $P_{f-f} (2-27); R_{f-f} (1-28);$	9.36	80/109
$2\nu_3 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	5043.5550	$P_{e-e} (2-24); R_{e-e} (2-17);$ $P_{f-f} (2-24); R_{f-f} (2-17);$	12.49	71/79
$2\nu_3 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	5049.1851	$P_{e-e} (1-36); R_{e-e} (0-36)$	4.88	37/74
$\nu_1 + \nu_3 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	5861.2378	$P_{e-e} (1-29); R_{e-e} (0-30)$	4.54	57/61
$2\nu_1 + \nu_5 \leftarrow \nu_5$	$\Pi \leftarrow \Pi$	6499.3894	$P_{e-e} (4-16); R_{e-e} (4-15);$ $P_{f-f} (4-16); R_{f-f} (4-14);$	20.75	27/47
$2\nu_1 + \nu_4 \leftarrow \nu_4$	$\Pi \leftarrow \Pi$	6524.3381	$P_{e-e} (2-28); R_{e-e} (1-30);$ $P_{f-f} (2-28); R_{f-f} (1-29);$	4.53	87/114
$2\nu_1 \leftarrow \text{G.S.}$	$\Sigma^+ \leftarrow \Sigma^+$	6532.9423	$P_{e-e} (1-36); R_{e-e} (0-42)$	3.99	71/80

^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.

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Table 2. Spectroscopic parameters (cm⁻¹) of ¹³C₂HD obtained from the fit of the ν₁ fundamental and its associated hot bands.

Parameter		
ω_1^0	3369.183600	(153)
x_{11}^0	-51.3562295	(977)
x_{14}^0	-3.717353	(509)
x_{15}^0	-17.093199	(346)
y_{144}^0	0.141693	(602)
y_{155}^0	0.0429203	(552)
y_{145}^0	-0.108914	(116)
y_{114}^0	-0.311700	(127)
y_{115}^0	0.268325	(285)
z_{1444}^0	0.021236	(194)
y_1^{44}	-0.1287340	(810)
y_1^{55}	-0.2662292	(354)
y_1^{45}	0.2156207	(734)
r_{145}^0	1.4827400	(694)
$r_{145}^J \times 10^4$	-0.20995	(225)
$\alpha_1^0 \times 10^2$	0.4389164	(472)
$\gamma_{11} \times 10^4$	-0.06344	(320)
$\gamma_{14} \times 10^4$	-0.18901	(834)
$\gamma_{15} \times 10^4$	-7.7072	(154)
$\varepsilon_{145} \times 10^4$	-0.03955	(222)
$\varepsilon_{114} \times 10^4$	-0.20489	(269)
$\varepsilon_{115} \times 10^4$	8.8550	(148)
$\varepsilon_1^{44} \times 10^5$	1.1435	(705)
$\varepsilon_1^{55} \times 10^5$	0.1449	(233)
$\varepsilon_1^{45} \times 10^5$	-0.6061	(707)
$\beta_1^0 \times 10^8$	-1.5790	(263)
$\delta_{11} \times 10^8$	0.7444	(198)
$\delta_{14} \times 10^8$	-5.005	(227)
$\delta_{15} \times 10^8$	-0.5749	(483)
$\theta_1^{44} \times 10^8$	4.892	(225)
$\theta_1^{55} \times 10^8$	-0.4293	(502)

$\theta_1^{45} \times 10^8$	2.300 (415)
$q_{14}^0 \times 10^2$	0.406297 (109)
$q_{15}^0 \times 10^2$	0.462848 (308)
$q_{144} \times 10^4$	0.86964 (779)
$q_{145} \times 10^4$	-0.2176 (345)
$q_{155} \times 10^4$	0.1371 (257)
$q_{154} \times 10^4$	0.11640 (572)
$q_{114} \times 10^4$	-0.27650 (442)
$q_{115} \times 10^4$	-13.3010 (159)
$q_{14}^J \times 10^7$	-0.32721 (241)
$q_{15}^J \times 10^7$	-0.19360 (285)
$\rho_{14}^0 \times 10^7$	-1.3899 (581)
$\rho_{15}^0 \times 10^7$	0.1002 (117)
$\rho_{14}^J \times 10^{11}$	-2.668 (309)

N. of fitted / assigned data 1985 / 2624

St. dev. of the fit (cm⁻¹) 0.00100

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Table 3. Spectroscopic parameters (cm⁻¹) of ¹³C₂HD obtained from the fit of the ν₂ fundamental and its associated hot bands.

Parameter		
ω_2^0	1813.9897517	(850)
x_{22}^0	-5.1444661	(522)
x_{24}^0	-4.0371006	(865)
x_{25}^0	-3.5947413	(821)
y_{244}^0	0.2898058	(390)
y_{255}^0	-0.0345110	(359)
y_{245}^0	-0.1039863	(677)
y_2^{44}	-0.2099315	(155)
y_2^{55}	-0.0497456	(161)
y_2^{45}	0.2052422	(507)
r_{245}^0	1.6630448	(844)
$r_{245}^J \times 10^4$	-0.07168	(554)
$\alpha_2^0 \times 10^2$	0.4097933	(185)
$\gamma_{22} \times 10^4$	-0.032688	(853)
$\gamma_{24} \times 10^4$	-1.09983	(148)
$\gamma_{25} \times 10^4$	-0.183696	(813)
$\beta_2^0 \times 10^8$	0.06476	(749)
$\delta_{24} \times 10^8$	-0.0981	(158)
$\theta_{245} \times 10^8$	1.1011	(455)
$q_{24}^0 \times 10^2$	0.4148165	(565)
$q_{25}^0 \times 10^2$	0.3253396	(703)
$q_{244} \times 10^4$	0.29930	(279)
$q_{245} \times 10^4$	-0.13043	(401)
$q_{255} \times 10^4$	-2.3776	(576)
$q_{24}^J \times 10^7$	-0.32077	(377)
$q_{25}^J \times 10^7$	-0.18818	(349)
$\rho_{245} \times 10^7$	-1.3213	(348)
N. of fitted / assigned data 1467 / 1720		
St. dev. of the fit (cm ⁻¹) 0.00041		

Table 4. Spectroscopic parameters (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fit of the ν_3 fundamental and its associated hot bands.

Parameter	
ω_3^0	2570.588997 (121)
x_{33}^0	-22.9982272 (779)
x_{34}^0	-14.118770 (157)
x_{35}^0	-2.701009 (204)
y_{344}^0	0.0465276 (353)
y_{355}^0	0.0249842 (533)
y_{345}^0	0.0900525 (744)
y_{334}^0	-0.2399882 (874)
y_{335}^0	-0.0780680 (994)
y_3^{44}	-0.0045922 (297)
y_3^{55}	0.0109296 (368)
y_3^{45}	-0.0660952 (640)
r_{345}^0	2.0031033 (587)
$r_{345}^J \times 10^4$	-0.18728 (226)
$\alpha_3^0 \times 10^2$	0.6090601 (402)
$\gamma_{33} \times 10^4$	-0.35638 (327)
$\gamma_{34} \times 10^4$	1.32093 (365)
$\gamma_{35} \times 10^4$	-0.52305 (554)
$\epsilon_{334} \times 10^4$	0.09436 (210)
$\epsilon_{335} \times 10^4$	0.16340 (336)
$\epsilon_3^{44} \times 10^5$	-0.1174 (213)
$\epsilon_3^{55} \times 10^5$	-0.0815 (265)
$\epsilon_3^{45} \times 10^5$	0.3175 (581)
$\beta_3^0 \times 10^8$	0.0753 (277)
$\delta_{33} \times 10^8$	-0.6106 (254)
$\delta_{34} \times 10^8$	0.3694 (479)
$\delta_{35} \times 10^8$	-0.3441 (551)
$\theta_{345} \times 10^8$	-0.6639 (237)
$\theta_3^{44} \times 10^8$	-0.3125 (300)
$\theta_3^{55} \times 10^8$	0.2686 (579)

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$\theta_3^{45} \times 10^8$	5.204 (122)
$q_{34}^0 \times 10^2$	0.4116518 (634)
$q_{35}^0 \times 10^2$	0.321814 (338)
$q_{344} \times 10^4$	0.31977 (226)
$q_{345} \times 10^4$	-0.3690 (101)
$q_{355} \times 10^4$	0.5892 (328)
$q_{334} \times 10^4$	0.26427 (326)
$q_{335} \times 10^4$	-0.48767 (606)
$q_{34}^J \times 10^7$	-0.43141 (477)
$q_{35}^J \times 10^7$	-0.20008 (229)
$\rho_{35}^0 \times 10^7$	-0.0849 (143)
N. of fitted / assigned data	1542 / 2005
St. dev. of the fit (cm ⁻¹)	0.00045

Table 5. Spectroscopic parameters (cm^{-1}) of $^{13}\text{C}_2\text{HD}$ obtained from the fit of the $\nu_1 + \nu_3$, $\nu_2 + \nu_3$ and its associated hot bands.

Parameter		
x_{13}^0	-4.180325 (114)	
x_{23}^0	-18.456909 (178)	
y_{234}^0	-0.101742 (314)	
y_{235}^0	-0.217189 (291)	
$\gamma_{13} \times 10^4$	0.17766 (733)	
$\gamma_{23} \times 10^4$	0.62091 (629)	
$\varepsilon_{234} \times 10^4$	2.5920 (284)	
$\varepsilon_{235} \times 10^4$	-0.2202 (124)	
$\delta_{13} \times 10^8$	0.2634 (846)	
$\theta_{234} \times 10^8$	23.850 (514)	
$q_{234}^0 \times 10^2$	0.432507(313)	
$q_{235}^0 \times 10^2$	0.325138(115)	
$q_{234}^J \times 10^7$	-1.3721 (726)	
	$\nu_1 + \nu_3$	$\nu_2 + \nu_3$
N. of fitted/assigned data	57 / 60	138 / 124
St. dev. of the fit (cm^{-1})	0.00047	0.00088

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Table 6. Vibrational term values G_C (cm^{-1})^a of the observed levels involving stretching modes in $^{13}\text{C}_2\text{HD}$.

ν_1	ν_2	ν_3	ν_4	ν_5	ℓ_4	ℓ_5	Sym.	G_C^0
0	1	0	0	0	0	0	Σ^+	1808.8453
0	1	0	1	0	± 1	0	Π	2314.4775
0	1	0	0	1	0	± 1	Π	2479.4067
0	0	1	0	0	0	0	Σ^+	2547.5908
0	1	0	2	0	0	0	Σ^+	2818.7817
0	1	0	2	0	± 2	0	Δ	2822.3602
0	1	0	1	1	± 1	± 1	Δ	2984.7888
0	1	0	1	1	-1	1	Σ^-	2984.8153
0	1	0	1	1	1	-1	Σ^+	2988.1414
0	0	1	1	0	± 1	0	Π	3042.8652
0	1	0	0	2	0	0	Σ^+	3136.8263
0	1	0	0	2	0	± 2	Δ	3153.2346
0	0	1	0	1	0	± 1	Π	3219.0901
1	0	0	0	0	0	0	Σ^+	3317.8274
0	0	1	2	0	0	0	Σ^+	3535.9107
0	0	1	2	0	± 2	0	Δ	3540.3167
0	2	0	0	0	0	0	Σ^+	3607.4016
0	0	1	1	1	± 1	± 1	Δ	3714.0403
0	0	1	1	1	-1	1	Σ^-	3714.2623
0	0	1	1	1	1	-1	Σ^+	3718.2685
1	0	0	1	0	± 1	0	Π	3823.4222
0	0	1	0	2	0	0	Σ^+	3877.4410
0	0	1	0	2	0	± 2	Δ	3894.1004
1	0	0	0	1	0	± 1	Π	3975.0198
1	0	0	2	0	0	0	Σ^+	4327.3573
1	0	0	2	0	± 2	0	Δ	4331.2611
0	1	1	0	0	0	0	Σ^+	4337.9791
1	0	0	1	1	± 1	± 1	Δ	4480.3698
1	0	0	1	1	-1	1	Σ^-	4480.5555
1	0	0	1	1	1	-1	Σ^+	4483.5210
1	0	0	0	2	0	0	Σ^+	4619.6578
1	0	0	0	2	0	± 2	Δ	4635.2003
0	1	1	1	0	± 1	0	Π	4829.3166
1	0	0	3	0	± 1	0	Π	4833.3809
0	1	1	0	1	0	± 1	Π	5005.7122
0	0	2	0	0	0	0	Σ^+	5049.1851
0	0	2	1	0	± 1	0	Π	5529.6687
0	0	2	0	1	0	± 1	Π	5717.7913
1	0	1	0	0	0	0	Σ^+	5861.2378
2	0	0	0	0	0	0	Σ^+	6532.9423
2	0	0	1	0	± 1	0	Π	7033.9233
2	0	0	0	1	0	± 1	Π	7173.6257

^a See text for definition.

Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm⁻¹) for the ν₁ and associated hot bands of ¹³C₂HD ^a (45 pp)

ν₁ (Σ⁺) ← G.S. (Σ⁺)

<i>v</i> ₄ ' <i>l</i> ₄ ' <i>v</i> ₅ ' <i>l</i> ₅ ' <i>J</i>	<i>v</i> ₄ " <i>l</i> ₄ " <i>v</i> ₅ " <i>l</i> ₅ " <i>J</i>	OBS	OBS – CALC	E'	E"
0 0 0 0 0	0 0 0 0 1	3315.92705	0.00034	3315.92671	1.90066
0 0 0 0 1	0 0 0 0 2	3314.01788	0.00059	3314.01729	5.70195
0 0 0 0 2	0 0 0 0 3	3312.09931	0.00018	3312.09913	11.40382
0 0 0 0 3	0 0 0 0 4	3310.17240	0.00015	3310.17225	19.00619
0 0 0 0 4	0 0 0 0 5	3308.23695	0.00027	3308.23668	28.50898
0 0 0 0 5	0 0 0 0 6	3306.29261	0.00016	3306.29245	39.91204
0 0 0 0 6	0 0 0 0 7	3304.33749*	-0.00209	3304.33958	53.21523 †
0 0 0 0 7	0 0 0 0 8	3302.37808	-0.00002	3302.37810	68.41838
0 0 0 0 8	0 0 0 0 9	3300.40846	0.00043	3300.40803	85.52129
0 0 0 0 9	0 0 0 0 10	3298.42925	-0.00016	3298.42941	104.52373
0 0 0 0 10	0 0 0 0 11	3296.44245	0.00020	3296.44225	125.42544
0 0 0 0 11	0 0 0 0 12	3294.44680	0.00021	3294.44659	148.22616
0 0 0 0 12	0 0 0 0 13	3292.44232	-0.00013	3292.44245	172.92558
0 0 0 0 13	0 0 0 0 14	3290.43036	0.00049	3290.42987	199.52337
0 0 0 0 14	0 0 0 0 15	3288.40900	0.00014	3288.40886	228.01920
0 0 0 0 15	0 0 0 0 16	3286.37955	0.00010	3286.37945	258.41268
0 0 0 0 16	0 0 0 0 17	3284.34139	-0.00029	3284.34168	290.70340
0 0 0 0 17	0 0 0 0 18	3282.29581	0.00024	3282.29557	324.89096
0 0 0 0 18	0 0 0 0 19	3280.24127	0.00011	3280.24116	360.97488
0 0 0 0 19	0 0 0 0 20	3278.17870	0.00024	3278.17846	398.95471
0 0 0 0 20	0 0 0 0 21	3276.10772	0.00022	3276.10750	438.82993
0 0 0 0 21	0 0 0 0 22	3274.02841	0.00008	3274.02833	480.60003
0 0 0 0 22	0 0 0 0 23	3271.94118	0.00022	3271.94096	524.26445
0 0 0 0 23	0 0 0 0 24	3269.84529	-0.00014	3269.84543	569.82262
0 0 0 0 24	0 0 0 0 25	3267.74220	0.00044	3267.74176	617.27393
0 0 0 0 25	0 0 0 0 26	3265.63032	0.00034	3265.62998	666.61777
0 0 0 0 26	0 0 0 0 27	3263.51073	0.00060	3263.51013	717.85348
0 0 0 0 27	0 0 0 0 28	3261.38235	0.00012	3261.38223	770.98038
0 0 0 0 28	0 0 0 0 29	3259.24644	0.00012	3259.24632	825.99778
0 0 0 0 29	0 0 0 0 30	3257.10275	0.00033	3257.10242	882.90495
0 0 0 0 30	0 0 0 0 31	3254.95121	0.00064	3254.95057	941.70115
0 0 0 0 31	0 0 0 0 32	3252.79152	0.00072	3252.79080	1002.38559
0 0 0 0 32	0 0 0 0 33	3250.62278	-0.00035	3250.62313	1064.95747
0 0 0 0 33	0 0 0 0 34	3248.44728	-0.00033	3248.44761	1129.41599
0 0 0 0 34	0 0 0 0 35	3246.26393	-0.00032	3246.26425	1195.76027
0 0 0 0 35	0 0 0 0 36	3244.07298	-0.00012	3244.07310	1263.98946
0 0 0 0 36	0 0 0 0 37	3241.87138*	-0.00279	3241.87417	1334.10264 †
0 0 0 0 37	0 0 0 0 38	3239.66835	0.00083	3239.66752	1406.09891
0 0 0 0 38	0 0 0 0 39	3237.45351	0.00035	3237.45316	1479.97730
0 0 0 0 39	0 0 0 0 40	3235.23091	-0.00023	3235.23114	1555.73685
0 0 0 0 40	0 0 0 0 41	3233.00161	0.00014	3233.00147	1633.37656
0 0 0 0 41	0 0 0 0 42	3230.76443	0.00022	3230.76421	1712.89541
0 0 0 0 42	0 0 0 0 43	3228.51962	0.00025	3228.51937	1794.29235
0 0 0 0 43	0 0 0 0 44	3226.26732	0.00033	3226.26699	1877.56630
0 0 0 0 44	0 0 0 0 45	3224.00699	-0.00012	3224.00711	1962.71617
0 0 0 0 45	0 0 0 0 46	3221.73956	-0.00020	3221.73976	2049.74085
0 0 0 0 46	0 0 0 0 47	3219.46477	-0.00020	3219.46497	2138.63917
0 0 0 0 47	0 0 0 0 48	3217.18212	-0.00065	3217.18277	2229.40999
0 0 0 0 48	0 0 0 0 49	3214.89349	0.00028	3214.89321	2322.05209
0 0 0 0 1	0 0 0 0 0	3319.71968	0.00044	3319.71924	0.00000
0 0 0 0 2	0 0 0 0 1	3321.60258	0.00029	3321.60229	1.90066
0 0 0 0 3	0 0 0 0 2	3323.47670	0.00020	3323.47650	5.70195
0 0 0 0 4	0 0 0 0 3	3325.34210	0.00026	3325.34184	11.40382
0 0 0 0 5	0 0 0 0 4	3327.19854	0.00024	3327.19830	19.00619

0	0	0	0	6	0	0	0	0	5	3329.04582	-0.00002	3329.04584	28.50898
0	0	0	0	7	0	0	0	0	6	3330.88502	0.00058	3330.88444	39.91204
0	0	0	0	8	0	0	0	0	7	3332.71437	0.00028	3332.71409	53.21523
0	0	0	0	9	0	0	0	0	8	3334.53477	0.00002	3334.53475	68.41838
0	0	0	0	10	0	0	0	0	9	3336.34669	0.00029	3336.34640	85.52129
0	0	0	0	11	0	0	0	0	10	3338.14884	-0.00018	3338.14902	104.52373
0	0	0	0	12	0	0	0	0	11	3339.94252	-0.00007	3339.94259	125.42544
0	0	0	0	13	0	0	0	0	12	3341.72737	0.00028	3341.72709	148.22616
0	0	0	0	14	0	0	0	0	13	3343.50275	0.00027	3343.50248	172.92558
0	0	0	0	15	0	0	0	0	14	3345.26860	-0.00015	3345.26875	199.52337
0	0	0	0	16	0	0	0	0	15	3347.02593	0.00004	3347.02589	228.01920
0	0	0	0	17	0	0	0	0	16	3348.77435	0.00050	3348.77385	258.41268
0	0	0	0	18	0	0	0	0	17	3350.51269	0.00005	3350.51264	290.70340
0	0	0	0	19	0	0	0	0	18	3352.24237	0.00016	3352.24221	324.89096
0	0	0	0	20	0	0	0	0	19	3353.96222	-0.00034	3353.96256	360.97488
0	0	0	0	21	0	0	0	0	20	3355.67385	0.00020	3355.67365	398.95471
0	0	0	0	22	0	0	0	0	21	3357.37583	0.00035	3357.37548	438.82993
0	0	0	0	23	0	0	0	0	22	3359.06809	0.00008	3359.06801	480.60003
0	0	0	0	24	0	0	0	0	23	3360.75133	0.00009	3360.75124	524.26445
0	0	0	0	25	0	0	0	0	24	3362.42542	0.00029	3362.42513	569.82262
0	0	0	0	26	0	0	0	0	25	3364.08998	0.00031	3364.08967	617.27393
0	0	0	0	27	0	0	0	0	26	3365.74502	0.00018	3365.74484	666.61777
0	0	0	0	28	0	0	0	0	27	3367.39078	0.00016	3367.39062	717.85348
0	0	0	0	29	0	0	0	0	28	3369.02795	0.00095	3369.02700	770.98038
0	0	0	0	30	0	0	0	0	29	3370.65460	0.00066	3370.65394	825.99778
0	0	0	0	31	0	0	0	0	30	3372.27104	-0.00039	3372.27143	882.90495
0	0	0	0	32	0	0	0	0	31	3373.87938	-0.00008	3373.87946	941.70115
0	0	0	0	33	0	0	0	0	32	3375.47745	-0.00056	3375.47801	1002.38559
0	0	0	0	34	0	0	0	0	33	3377.06768	0.00063	3377.06705	1064.95747
0	0	0	0	34	0	0	0	0	33	3377.06768	0.00063	3377.06705	1064.95747
0	0	0	0	35	0	0	0	0	34	3378.64619	-0.00038	3378.64657	1129.41599
0	0	0	0	36	0	0	0	0	35	3380.21599	-0.00056	3380.21655	1195.76027
0	0	0	0	37	0	0	0	0	36	3381.77628	-0.00069	3381.77697	1263.98946
0	0	0	0	38	0	0	0	0	37	3383.32716	-0.00066	3383.32782	1334.10264
0	0	0	0	39	0	0	0	0	38	3384.86901	-0.00007	3384.86908	1406.09891
0	0	0	0	40	0	0	0	0	39	3386.39992	-0.00082	3386.40074	1479.97730
0	0	0	0	41	0	0	0	0	40	3387.92282	0.00006	3387.92276	1555.73685
0	0	0	0	42	0	0	0	0	41	3389.43517	0.00002	3389.43515	1633.37656
0	0	0	0	43	0	0	0	0	42	3390.93797	0.00009	3390.93788	1712.89541
0	0	0	0	44	0	0	0	0	43	3392.43109	0.00015	3392.43094	1794.29235
0	0	0	0	45	0	0	0	0	44	3393.91407	-0.00023	3393.91430	1877.56630
0	0	0	0	46	0	0	0	0	45	3395.38831	0.00034	3395.38797	1962.71617
0	0	0	0	47	0	0	0	0	46	3396.85175	-0.00016	3396.85191	2049.74085
0	0	0	0	48	0	0	0	0	47	3398.30643	0.00031	3398.30612	2138.63917
0	0	0	0	49	0	0	0	0	48	3399.75076	0.00019	3399.75057	2229.40999
0	0	0	0	50	0	0	0	0	49	3401.18391	-0.00135	3401.18526	2322.05209 †
0	0	0	0	51	0	0	0	0	50	3402.60892	-0.00126	3402.61018	2416.56425 †
0	0	0	0	52	0	0	0	0	51	3404.02668	0.00139	3404.02529	2512.94525 †

rms = 0.00036 cm⁻¹

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

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$$v_1(\Sigma^+) \leftarrow v_4(\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	1 1 0 0 1	2806.34215	0.00105	2806.34110	511.48627 †
0 0 0 0 1	1 1 0 0 2	2804.43064	-0.00029	2804.43093	515.28830
0 0 0 0 2	1 1 0 0 3	2802.51203	0.00038	2802.51165	520.99129
0 0 0 0 3	1 1 0 0 4	2800.58346	0.00017	2800.58329	528.59515
0 0 0 0 4	1 1 0 0 5	2798.64710	0.00124	2798.64586	538.09979 †
0 0 0 0 5	1 1 0 0 6	2796.69979	0.00038	2796.69941	549.50508
0 0 0 0 6	1 1 0 0 7	2794.74430	0.00035	2794.74395	562.81086
0 0 0 0 7	1 1 0 0 8	2792.77884	-0.00068	2792.77952	578.01697
0 0 0 0 8	1 1 0 0 9	2790.80556	-0.00058	2790.80614	595.12319
0 0 0 0 9	1 1 0 0 10	2788.82450	0.00066	2788.82384	614.12929
0 0 0 0 10	1 1 0 0 11	2786.83266	0.00000	2786.83266	635.03503
0 0 0 0 11	1 1 0 0 12	2784.83249	-0.00013	2784.83262	657.84012
0 0 0 0 12	1 1 0 0 13	2782.82369	-0.00007	2782.82376	682.54427
0 0 0 0 13	1 1 0 0 14	2780.80531	-0.00080	2780.80611	709.14713
0 0 0 0 14	1 1 0 0 15	2778.78071	0.00101	2778.77970	737.64836 †
0 0 0 0 15	1 1 0 0 16	2776.74444	-0.00012	2776.74456	768.04757
0 0 0 0 16	1 1 0 0 17	2774.70065	-0.00007	2774.70072	800.34436
0 0 0 0 17	1 1 0 0 18	2772.64867	0.00044	2772.64823	834.53830
0 0 0 0 18	1 1 0 0 19	2770.58636*	-0.00075	2770.58711	870.62893
0 0 0 0 19	1 1 0 0 20	2768.51626	-0.00114	2768.51740	908.61577 †
0 0 0 0 20	1 1 0 0 21	2766.43919	0.00006	2766.43913	948.49830
0 0 0 0 21	1 1 0 0 22	2764.35319	0.00084	2764.35235	990.27601
0 0 0 0 22	1 1 0 0 23	2762.25642	-0.00066	2762.25708	1033.94833
0 0 0 0 2	1 1 0 0 1	2812.01681	0.00014	2812.01667	511.48627
0 0 0 0 3	1 1 0 0 2	2813.88929	-0.00085	2813.89014	515.28830
0 0 0 0 4	1 1 0 0 3	2815.75468	0.00031	2815.75437	520.99129
0 0 0 0 5	1 1 0 0 4	2817.60789	-0.00145	2817.60934	528.59515 †
0 0 0 0 6	1 1 0 0 5	2819.45430	-0.00072	2819.45502	538.09979
0 0 0 0 7	1 1 0 0 6	2821.29181	0.00041	2821.29140	549.50508
0 0 0 0 8	1 1 0 0 7	2823.11864	0.00018	2823.11846	562.81086
0 0 0 0 9	1 1 0 0 8	2824.93588	-0.00029	2824.93617	578.01697
0 0 0 0 10	1 1 0 0 9	2826.74368	-0.00083	2826.74451	595.12319
0 0 0 0 11	1 1 0 0 10	2828.54262	-0.00084	2828.54346	614.12929
0 0 0 0 12	1 1 0 0 11	2830.33290	-0.00010	2830.33300	635.03503
0 0 0 0 13	1 1 0 0 12	2832.11386	0.00074	2832.11312	657.84012
0 0 0 0 14	1 1 0 0 13	2833.88416	0.00037	2833.88379	682.54427
0 0 0 0 15	1 1 0 0 14	2835.64422	-0.00078	2835.64500	709.14713
0 0 0 0 16	1 1 0 0 15	2837.39729	0.00056	2837.39673	737.64836
0 0 0 0 17	1 1 0 0 16	2839.13807	-0.00089	2839.13896	768.04757
0 0 0 0 18	1 1 0 0 17	2840.87155	-0.00013	2840.87168	800.34436
0 0 0 0 19	1 1 0 0 18	2842.59483	-0.00004	2842.59487	834.53830
0 0 0 0 20	1 1 0 0 19	2844.30896	0.00045	2844.30851	870.62893
0 0 0 0 1	1 -1 0 0 1	2808.22539	0.00071	2808.22468	511.49456
0 0 0 0 2	1 -1 0 0 2	2808.18971	-0.00007	2808.18978	515.31316
0 0 0 0 3	1 -1 0 0 3	2808.13827	0.00084	2808.13743	521.04101
0 0 0 0 4	1 -1 0 0 4	2808.06769	0.00005	2808.06764	528.67801
0 0 0 0 5	1 -1 0 0 5	2807.98094	0.00052	2807.98042	538.22407
0 0 0 0 6	1 -1 0 0 6	2807.87562	-0.00014	2807.87576	549.67906
0 0 0 0 7	1 -1 0 0 7	2807.75334	-0.00034	2807.75368	563.04281
0 0 0 0 8	1 -1 0 0 8	2807.61395	-0.00023	2807.61418	578.31514
0 0 0 0 9	1 -1 0 0 9	2807.45692	-0.00036	2807.45728	595.49585
0 0 0 0 10	1 -1 0 0 10	2807.28251	-0.00049	2807.28300	614.58469
0 0 0 0 11	1 -1 0 0 11	2807.09138	0.00005	2807.09133	635.58142
0 0 0 0 12	1 -1 0 0 12	2806.88268	0.00038	2806.88230	658.48573
0 0 0 0 13	1 -1 0 0 13	2806.65580	-0.00012	2806.65592	683.29732
0 0 0 0 14	1 -1 0 0 14	2806.41207	-0.00014	2806.41221	710.01584
0 0 0 0 15	1 -1 0 0 15	2806.15153	0.00033	2806.15120	738.64093
0 0 0 0 16	1 -1 0 0 16	2805.87329	0.00040	2805.87289	769.17220
0 0 0 0 17	1 -1 0 0 17	2805.57711	-0.00019	2805.57730	801.60923
0 0 0 0 18	1 -1 0 0 18	2805.26384	-0.00064	2805.26448	835.95156

0	0	0	0	19	1	-1	0	0	19	2804.93367	-0.00075	2804.93442	872.19874
0	0	0	0	20	1	-1	0	0	20	2804.58630	-0.00087	2804.58717	910.35027
0	0	0	0	21	1	-1	0	0	21	2804.22365	0.00090	2804.22275	950.40561
0	0	0	0	22	1	-1	0	0	22	2803.84117	-0.00001	2803.84118	992.36423
0	0	0	0	23	1	-1	0	0	23	2803.44258	0.00008	2803.44250	1036.22555
0	0	0	0	24	1	-1	0	0	24	2803.02628	-0.00045	2803.02673	1081.98896
0	0	0	0	25	1	-1	0	0	25	2802.59466	0.00075	2802.59391	1129.65384
0	0	0	0	26	1	-1	0	0	26	2802.14521	0.00114	2802.14407	1179.21954 †
0	0	0	0	27	1	-1	0	0	27	2801.68199*	0.00475	2801.67724	1230.68537 †
0	0	0	0	28	1	-1	0	0	28	2801.19507	0.00161	2801.19346	1284.05064 †

rms = 0.00050 cm⁻¹

$v_1(\Sigma^+) \leftarrow v_5(\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	0 0 1 1 1	2641.69030	-0.00094	2641.69124	676.13613
0 0 0 0 1	0 0 1 1 2	2639.78357	0.00001	2639.78356	679.93567
0 0 0 0 2	0 0 1 1 3	2637.86819	0.00017	2637.86802	685.63493
0 0 0 0 3	0 0 1 1 4	2635.94377	-0.00085	2635.94462	693.23382
0 0 0 0 4	0 0 1 1 5	2634.01341	-0.00001	2634.01342	702.73224
0 0 0 0 5	0 0 1 1 6	2632.07407	-0.00035	2632.07442	714.13007
0 0 0 0 6	0 0 1 1 7	2630.12781	0.00016	2630.12765	727.42716
0 0 0 0 7	0 0 1 1 8	2628.17314	-0.00001	2628.17315	742.62333
0 0 0 0 8	0 0 1 1 9	2626.21101	0.00007	2626.21094	759.71839
0 0 0 0 9	0 0 1 1 10	2624.24109	0.00005	2624.24104	778.71209
0 0 0 0 10	0 0 1 1 11	2622.26351	0.00002	2622.26349	799.60420
0 0 0 0 11	0 0 1 1 12	2620.27805	-0.00025	2620.27830	822.39444
0 0 0 0 12	0 0 1 1 13	2618.28491	-0.00061	2618.28552	847.08251
0 0 0 0 13	0 0 1 1 14	2616.28475	-0.00041	2616.28516	873.66808
0 0 0 0 14	0 0 1 1 15	2614.27699	-0.00027	2614.27726	902.15079
0 0 0 0 15	0 0 1 1 16	2612.26175	-0.00010	2612.26185	932.53028
0 0 0 0 16	0 0 1 1 17	2610.23894	0.00000	2610.23894	964.80614
0 0 0 0 17	0 0 1 1 18	2608.20842	-0.00016	2608.20858	998.97795
0 0 0 0 18	0 0 1 1 19	2606.17079	-0.00001	2606.17080	1035.04524
0 0 0 0 19	0 0 1 1 20	2604.12578	0.00017	2604.12561	1073.00756
0 0 0 0 20	0 0 1 1 21	2602.07314	0.00009	2602.07305	1112.86438
0 0 0 0 21	0 0 1 1 22	2600.01305	-0.00011	2600.01316	1154.61520
0 0 0 0 22	0 0 1 1 23	2597.94556	-0.00040	2597.94596	1198.25945
0 0 0 0 23	0 0 1 1 24	2595.87148	0.00000	2595.87148	1243.79656
0 0 0 0 24	0 0 1 1 25	2593.78989	0.00013	2593.78976	1291.22593
0 0 0 0 25	0 0 1 1 26	2591.70047	-0.00035	2591.70082	1340.54693
0 0 0 0 26	0 0 1 1 27	2589.60475	0.00005	2589.60470	1391.75891
0 0 0 0 27	0 0 1 1 28	2587.50082	-0.00060	2587.50142	1444.86119
0 0 0 0 28	0 0 1 1 29	2585.39111	0.00008	2585.39103	1499.85307
0 0 0 0 29	0 0 1 1 30	2583.27352	-0.00003	2583.27355	1556.73383
0 0 0 0 30	0 0 1 1 31	2581.14843	-0.00058	2581.14901	1615.50271
0 0 0 0 31	0 0 1 1 32	2579.01626	-0.00119	2579.01745	1676.15894 †
0 0 0 0 32	0 0 1 1 33	2576.87950	0.00060	2576.87890	1738.70171
0 0 0 0 33	0 0 1 1 34	2574.73360	0.00020	2574.73340	1803.13019
0 0 0 0 2	0 0 1 1 1	2647.36631	-0.00051	2647.36682	676.13613
0 0 0 0 3	0 0 1 1 2	2649.24220	-0.00057	2649.24277	679.93567
0 0 0 0 4	0 0 1 1 3	2651.11026	-0.00047	2651.11073	685.63493
0 0 0 0 5	0 0 1 1 4	2652.97054	-0.00013	2652.97067	693.23382
0 0 0 0 6	0 0 1 1 5	2654.82262	0.00005	2654.82257	702.73224
0 0 0 0 7	0 0 1 1 6	2656.66596	-0.00045	2656.66641	714.13007
0 0 0 0 8	0 0 1 1 7	2658.50243	0.00027	2658.50216	727.42716
0 0 0 0 9	0 0 1 1 8	2660.32984	0.00004	2660.32980	742.62333
0 0 0 0 10	0 0 1 1 9	2662.14927	-0.00004	2662.14931	759.71839
0 0 0 0 11	0 0 1 1 10	2663.96062	-0.00003	2663.96065	778.71209
0 0 0 0 12	0 0 1 1 11	2665.76380	-0.00003	2665.76383	799.60420
0 0 0 0 13	0 0 1 1 12	2667.55864	-0.00016	2667.55880	822.39444

1	0	0	0	0	14	0	0	1	1	13	2669.34563	0.00008	2669.34555	847.08251
2	0	0	0	0	15	0	0	1	1	14	2671.12399	-0.00006	2671.12405	873.66808
3	0	0	0	0	16	0	0	1	1	15	2672.89425	-0.00004	2672.89429	902.15079
4	0	0	0	0	17	0	0	1	1	16	2674.65630	0.00005	2674.65625	932.53028
5	0	0	0	0	18	0	0	1	1	17	2676.40986	-0.00004	2676.40990	964.80614
6	0	0	0	0	19	0	0	1	1	18	2678.15529	0.00007	2678.15522	998.97795
7	0	0	0	0	20	0	0	1	1	19	2679.89215	-0.00004	2679.89219	1035.04524
8	0	0	0	0	21	0	0	1	1	20	2681.62075	-0.00005	2681.62080	1073.00756
9	0	0	0	0	22	0	0	1	1	21	2683.34055	-0.00048	2683.34103	1112.86438
10	0	0	0	0	23	0	0	1	1	22	2685.05266	-0.00018	2685.05284	1154.61520
11	0	0	0	0	24	0	0	1	1	23	2686.75607	-0.00017	2686.75624	1198.25945
12	0	0	0	0	25	0	0	1	1	24	2688.45102	-0.00017	2688.45119	1243.79656
13	0	0	0	0	26	0	0	1	1	25	2690.13763	-0.00004	2690.13767	1291.22593
14	0	0	0	0	27	0	0	1	1	26	2691.81523	-0.00045	2691.81568	1340.54693
15	0	0	0	0	28	0	0	1	1	27	2693.48523	0.00004	2693.48519	1391.75891
16	0	0	0	0	29	0	0	1	1	28	2695.14637	0.00019	2695.14618	1444.86119
17	0	0	0	0	30	0	0	1	1	29	2696.79840	-0.00025	2696.79865	1499.85307
18	0	0	0	0	31	0	0	1	1	30	2698.44217	-0.00039	2698.44256	1556.73383
19	0	0	0	0	32	0	0	1	1	31	2700.07759	-0.00031	2700.07790	1615.50271
20	0	0	0	0	33	0	0	1	1	32	2701.70489	0.00023	2701.70466	1676.15894
21	0	0	0	0	34	0	0	1	1	33	2703.32361	0.00080	2703.32281	1738.70171
22	0	0	0	0	35	0	0	1	1	34	2704.93288	0.00052	2704.93236	1803.13019
23	0	0	0	0	36	0	0	1	1	35	2706.53367	0.00040	2706.53327	1869.44355
24	0	0	0	0	37	0	0	1	1	36	2708.12573	0.00020	2708.12553	1937.64090
25	0	0	0	0	1	0	0	1	-1	1	2643.57663	0.00004	2643.57659	676.14265
26	0	0	0	0	2	0	0	1	-1	2	2643.54711	-0.00060	2643.54771	679.95524
27	0	0	0	0	3	0	0	1	-1	3	2643.50439	0.00000	2643.50439	685.67405
28	0	0	0	0	4	0	0	1	-1	4	2643.44665	0.00001	2643.44664	693.29902
29	0	0	0	0	5	0	0	1	-1	5	2643.37452	0.00007	2643.37445	702.83004
30	0	0	0	0	6	0	0	1	-1	6	2643.28789	0.00006	2643.28783	714.26698
31	0	0	0	0	7	0	0	1	-1	7	2643.18680	0.00001	2643.18679	727.60969
32	0	0	0	0	8	0	0	1	-1	8	2643.07124	-0.00009	2643.07133	742.85799
33	0	0	0	0	9	0	0	1	-1	9	2642.94143	-0.00003	2642.94146	760.01168
34	0	0	0	0	10	0	0	1	-1	10	2642.79712	-0.00005	2642.79717	779.07052
35	0	0	0	0	11	0	0	1	-1	11	2642.63845	-0.00004	2642.63849	800.03426
36	0	0	0	0	12	0	0	1	-1	12	2642.46539	-0.00003	2642.46542	822.90261
37	0	0	0	0	13	0	0	1	-1	13	2642.27765	-0.00031	2642.27796	847.67528
38	0	0	0	0	14	0	0	1	-1	14	2642.07614	0.00001	2642.07613	874.35193
39	0	0	0	0	15	0	0	1	-1	15	2641.85955	-0.00038	2641.85993	902.93220
40	0	0	0	0	16	0	0	1	-1	16	2641.62941	0.00003	2641.62938	933.41570
41	0	0	0	0	17	0	0	1	-1	17	2641.38456	0.00007	2641.38449	965.80204
42	0	0	0	0	18	0	0	1	-1	18	2641.12508	-0.00020	2641.12528	1000.09076
43	0	0	0	0	19	0	0	1	-1	19	2640.85192	0.00018	2640.85174	1036.28142
44	0	0	0	0	20	0	0	1	-1	20	2640.56375	-0.00016	2640.56391	1074.37353
45	0	0	0	0	21	0	0	1	-1	21	2640.26192	0.00014	2640.26178	1114.36658
46	0	0	0	0	22	0	0	1	-1	22	2639.94540	0.00001	2639.94539	1156.26002
47	0	0	0	0	23	0	0	1	-1	23	2639.61455	-0.00019	2639.61474	1200.05331
48	0	0	0	0	24	0	0	1	-1	24	2639.27025	0.00040	2639.26985	1245.74584
49	0	0	0	0	25	0	0	1	-1	25	2638.91045	-0.00029	2638.91074	1293.33701
50	0	0	0	0	26	0	0	1	-1	26	2638.53740	-0.00002	2638.53742	1342.82618
51	0	0	0	0	27	0	0	1	-1	27	2638.14983	-0.00010	2638.14993	1394.21269
52	0	0	0	0	28	0	0	1	-1	28	2637.74846	0.00020	2637.74826	1447.49584
53	0	0	0	0	29	0	0	1	-1	29	2637.33221	-0.00024	2637.33245	1502.67492
54	0	0	0	0	30	0	0	1	-1	30	2636.90251	-0.00001	2636.90252	1559.74920
55	0	0	0	0	31	0	0	1	-1	31	2636.45833	-0.00016	2636.45849	1618.71789
56	0	0	0	0	32	0	0	1	-1	32	2636.00024*	-0.00014	2636.00038	1679.58023
57	0	0	0	0	33	0	0	1	-1	33	2635.52637*	-0.00185	2635.52822	1742.33538
58	0	0	0	0	34	0	0	1	-1	34	2635.04208	0.00006	2635.04202	1806.98250
59	0	0	0	0	35	0	0	1	-1	35	2634.54164	-0.00018	2634.54182	1873.52074
60	0	0	0	0	36	0	0	1	-1	36	2634.02689	-0.00074	2634.02763	1941.94919

$$\text{rms} = 0.00029 \text{ cm}^{-1}$$

$$v_1 + v_4 (\Pi) \leftarrow G.S. (\Sigma^+)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 1 0 0 1	0 0 0 0 2	3819.61405	0.00162	3819.61243	5.70195 †
1 1 0 0 2	0 0 0 0 3	3817.69596*	0.00101	3817.69495	11.40382 †
1 1 0 0 3	0 0 0 0 4	3815.76977	0.00069	3815.76908	19.00619
1 1 0 0 4	0 0 0 0 5	3813.83521	0.00035	3813.83486	28.50898
1 1 0 0 5	0 0 0 0 6	3811.89303	0.00072	3811.89231	39.91204
1 1 0 0 6	0 0 0 0 7	3809.94230	0.00084	3809.94146	53.21523
1 1 0 0 7	0 0 0 0 8	3807.98297	0.00064	3807.98233	68.41838
1 1 0 0 8	0 0 0 0 9	3806.01549	0.00055	3806.01494	85.52129
1 1 0 0 9	0 0 0 0 10	3804.04024	0.00092	3804.03932	104.52373
1 1 0 0 10	0 0 0 0 11	3802.05630	0.00081	3802.05549	125.42544
1 1 0 0 11	0 0 0 0 12	3800.06423	0.00075	3800.06348	148.22616
1 1 0 0 12	0 0 0 0 13	3798.06278	-0.00053	3798.06331	172.92558
1 1 0 0 13	0 0 0 0 14	3796.05566	0.00065	3796.05501	199.52337
1 1 0 0 14	0 0 0 0 15	3794.03861	0.00002	3794.03859	228.01920
1 1 0 0 15	0 0 0 0 16	3792.01388	-0.00020	3792.01408	258.41268
1 1 0 0 16	0 0 0 0 17	3789.98247	0.00096	3789.98151	290.70340
1 1 0 0 17	0 0 0 0 18	3787.94142	0.00052	3787.94090	324.89096
1 1 0 0 18	0 0 0 0 19	3785.89268	0.00042	3785.89226	360.97488
1 1 0 0 19	0 0 0 0 20	3783.83616	0.00052	3783.83564	398.95471
1 1 0 0 20	0 0 0 0 21	3781.77145	0.00042	3781.77103	438.82993
1 1 0 0 21	0 0 0 0 22	3779.69888	0.00040	3779.69848	480.60003
1 1 0 0 22	0 0 0 0 23	3777.61806	0.00006	3777.61800	524.26445
1 1 0 0 23	0 0 0 0 24	3775.53026	0.00064	3775.52962	569.82262
1 1 0 0 24	0 0 0 0 25	3773.43382	0.00047	3773.43335	617.27393
1 1 0 0 25	0 0 0 0 26	3771.32829	-0.00093	3771.32922	666.61777
1 1 0 0 26	0 0 0 0 27	3769.21794	0.00068	3769.21726	717.85348
1 1 0 0 27	0 0 0 0 28	3767.09806	0.00058	3767.09748	770.98038
1 1 0 0 28	0 0 0 0 29	3764.96514*	-0.00476	3764.96990	825.99778 †
1 1 0 0 29	0 0 0 0 30	3762.83430	-0.00026	3762.83456	882.90495
1 1 0 0 30	0 0 0 0 31	3760.69104	-0.00042	3760.69146	941.70115
1 1 0 0 2	0 0 0 0 1	3827.19834	0.00024	3827.19810	1.90066
1 1 0 0 3	0 0 0 0 2	3829.07339	0.00006	3829.07333	5.70195
1 1 0 0 4	0 0 0 0 3	3830.94038	0.00036	3830.94002	11.40382
1 1 0 0 5	0 0 0 0 4	3832.79894	0.00078	3832.79816	19.00619
1 1 0 0 6	0 0 0 0 5	3834.64829	0.00057	3834.64772	28.50898
1 1 0 0 7	0 0 0 0 6	3836.48900	0.00033	3836.48867	39.91204
1 1 0 0 8	0 0 0 0 7	3838.32166	0.00066	3838.32100	53.21523
1 1 0 0 9	0 0 0 0 8	3840.14494	0.00028	3840.14466	68.41838
1 1 0 0 10	0 0 0 0 9	3841.96019	0.00055	3841.95964	85.52129
1 1 0 0 11	0 0 0 0 10	3843.76850*	0.00258	3843.76592	104.52373 †
1 1 0 0 12	0 0 0 0 11	3845.56373	0.00028	3845.56345	125.42544
1 1 0 0 13	0 0 0 0 12	3847.35320	0.00097	3847.35223	148.22616
1 1 0 0 14	0 0 0 0 13	3849.13309	0.00088	3849.13221	172.92558
1 1 0 0 15	0 0 0 0 14	3850.90430	0.00091	3850.90339	199.52337
1 1 0 0 16	0 0 0 0 15	3852.66609	0.00037	3852.66572	228.01920
1 1 0 0 17	0 0 0 0 16	3854.41965	0.00047	3854.41918	258.41268
1 1 0 0 18	0 0 0 0 17	3856.16334	-0.00040	3856.16374	290.70340
1 1 0 0 19	0 0 0 0 18	3857.89995	0.00056	3857.89939	324.89096
1 1 0 0 20	0 0 0 0 19	3859.62599	-0.00009	3859.62608	360.97488
1 1 0 0 21	0 0 0 0 20	3861.34469	0.00089	3861.34380	398.95471
1 1 0 0 22	0 0 0 0 21	3863.05257	0.00005	3863.05252	438.82993
1 1 0 0 23	0 0 0 0 22	3864.75021*	-0.00200	3864.75221	480.60003 †
1 1 0 0 24	0 0 0 0 23	3866.44261	-0.00022	3866.44283	524.26445
1 1 0 0 25	0 0 0 0 24	3868.12360*	-0.00077	3868.12437	569.82262
1 1 0 0 26	0 0 0 0 25	3869.79726	0.00046	3869.79680	617.27393
1 1 0 0 27	0 0 0 0 26	3871.46154*	0.00145	3871.46009	666.61777 †
1 1 0 0 28	0 0 0 0 27	3873.11418	-0.00003	3873.11421	717.85348
1 1 0 0 29	0 0 0 0 28	3874.75905	-0.00008	3874.75913	770.98038

rms = 0.00057 cm⁻¹

$$v_1 + v_4 (\Pi) \leftarrow v_4 (\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 1 0 0 1	1 1 0 0 2	3310.02551	-0.00057	3310.02608	515.28830
1 1 0 0 2	1 1 0 0 3	3308.10594*	-0.00153	3308.10747	520.99129 +
1 1 0 0 3	1 1 0 0 4	3306.17959*	-0.00053	3306.18012	528.59515
1 1 0 0 4	1 1 0 0 5	3304.24365	-0.00039	3304.24404	538.09979
1 1 0 0 5	1 1 0 0 6	3302.29856	-0.00071	3302.29927	549.50508
1 1 0 0 6	1 1 0 0 7	3300.34544	-0.00039	3300.34583	562.81086
1 1 0 0 7	1 1 0 0 8	3298.38328	-0.00047	3298.38375	578.01697
1 1 0 0 8	1 1 0 0 9	3296.41260	-0.00045	3296.41305	595.12319
1 1 0 0 11	1 1 0 0 12	3290.44920	-0.00032	3290.44952	657.84012
1 1 0 0 12	1 1 0 0 13	3288.44422	-0.00040	3288.44462	682.54427
1 1 0 0 13	1 1 0 0 14	3286.43077	-0.00048	3286.43125	709.14713
1 1 0 0 14	1 1 0 0 15	3284.40904	-0.00039	3284.40943	737.64836
1 1 0 0 15	1 1 0 0 16	3282.37891	-0.00028	3282.37919	768.04757
1 1 0 0 16	1 1 0 0 17	3280.34012	-0.00043	3280.34055	800.34436
1 1 0 0 17	1 1 0 0 18	3278.29336	-0.00019	3278.29355	834.53830
1 1 0 0 18	1 1 0 0 19	3276.23819	-0.00003	3276.23822	870.62893
1 1 0 0 19	1 1 0 0 20	3274.17438	-0.00020	3274.17458	908.61577
1 1 0 0 20	1 1 0 0 21	3272.10234	-0.00032	3272.10266	948.49830
1 1 0 0 21	1 1 0 0 22	3270.02253	0.00003	3270.02250	990.27601
1 1 0 0 22	1 1 0 0 23	3267.93393	-0.00019	3267.93412	1033.94833
1 1 0 0 23	1 1 0 0 24	3265.83743	-0.00013	3265.83756	1079.51468
1 1 0 0 24	1 1 0 0 25	3263.73259	-0.00024	3263.73283	1126.97445
1 1 0 0 25	1 1 0 0 26	3261.61996	-0.00003	3261.61999	1176.32701
1 1 0 0 26	1 1 0 0 27	3259.49893	-0.00012	3259.49905	1227.57169
1 1 0 0 27	1 1 0 0 28	3257.36956	-0.00048	3257.37004	1280.70782
1 1 0 0 28	1 1 0 0 29	3255.23309	0.00008	3255.23301	1335.73468
1 1 0 0 29	1 1 0 0 30	3253.08753	-0.00044	3253.08797	1392.65154
1 1 0 0 30	1 1 0 0 31	3250.93531	0.00035	3250.93496	1451.45764
1 1 0 0 31	1 1 0 0 32	3248.77171*	-0.00231	3248.77402	1512.15220 +
1 1 0 0 32	1 1 0 0 33	3246.60590	0.00073	3246.60517	1574.73441
1 1 0 0 33	1 1 0 0 34	3244.42878*	0.00033	3244.42845	1639.20342
1 1 0 0 35	1 1 0 0 36	3240.05081	-0.00071	3240.05152	1773.79841
1 1 0 0 36	1 1 0 0 37	3237.85195	0.00058	3237.85137	1843.92260
1 1 0 0 37	1 1 0 0 38	3235.64361	0.00012	3235.64349	1915.93000
1 1 0 0 38	1 1 0 0 39	3233.42820	0.00031	3233.42789	1989.81965
1 1 0 0 39	1 1 0 0 40	3231.20446*	-0.00016	3231.20462	2065.59058
1 1 0 0 40	1 1 0 0 41	3228.97434	0.00063	3228.97371	2143.24177
1 1 0 0 2	1 1 0 0 1	3317.61195	-0.00054	3317.61249	511.48627
1 1 0 0 3	1 1 0 0 2	3319.48644	-0.00053	3319.48697	515.28830
1 1 0 0 4	1 1 0 0 3	3321.35210	-0.00045	3321.35255	520.99129
1 1 0 0 5	1 1 0 0 4	3323.20866	-0.00054	3323.20920	528.59515
1 1 0 0 6	1 1 0 0 5	3325.05644	-0.00046	3325.05690	538.09979
1 1 0 0 7	1 1 0 0 6	3326.89526	-0.00037	3326.89563	549.50508
1 1 0 0 8	1 1 0 0 7	3328.72474	-0.00063	3328.72537	562.81086
1 1 0 0 9	1 1 0 0 8	3330.54551	-0.00057	3330.54608	578.01697
1 1 0 0 10	1 1 0 0 9	3332.35725	-0.00050	3332.35775	595.12319
1 1 0 0 11	1 1 0 0 10	3334.15983	-0.00052	3334.16035	614.12929
1 1 0 0 12	1 1 0 0 11	3335.95296	-0.00090	3335.95386	635.03503
1 1 0 0 14	1 1 0 0 13	3339.51330	-0.00022	3339.51352	682.54427
1 1 0 0 15	1 1 0 0 14	3341.27928	-0.00035	3341.27963	709.14713
1 1 0 0 16	1 1 0 0 15	3343.03617	-0.00039	3343.03656	737.64836
1 1 0 0 17	1 1 0 0 16	3344.78416	-0.00012	3344.78428	768.04757
1 1 0 0 18	1 1 0 0 17	3346.52250	-0.00029	3346.52279	800.34436
1 1 0 0 19	1 1 0 0 18	3348.25181	-0.00024	3348.25205	834.53830
1 1 0 0 20	1 1 0 0 19	3349.97190	-0.00014	3349.97204	870.62893
1 1 0 0 21	1 1 0 0 20	3351.68235	-0.00040	3351.68275	908.61577
1 1 0 0 22	1 1 0 0 21	3353.38420	0.00005	3353.38415	948.49830
1 1 0 0 23	1 1 0 0 22	3355.07616	-0.00006	3355.07622	990.27601
1 1 0 0 24	1 1 0 0 23	3356.75896	0.00001	3356.75895	1033.94833
1 1 0 0 25	1 1 0 0 24	3358.43199	-0.00032	3358.43231	1079.51468

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2	1	-1	0	0	6	1	1	0	0	6	3313.81955*	-0.00514	3313.82469	549.50508 †
3	1	-1	0	0	7	1	1	0	0	7	3313.81955*	-0.00104	3313.82059	562.81086 †
4	1	-1	0	0	8	1	1	0	0	8	3313.81955*	0.00365	3313.81590	578.01697 †
5	1	-1	0	0	9	1	1	0	0	9	3313.81955*	0.00895	3313.81060	595.12319 †
6	1	-1	0	0	10	1	1	0	0	10	3313.81955*	0.01485	3313.80470	614.12929 †
7	1	-1	0	0	11	1	1	0	0	11	3313.78524*	-0.01294	3313.79818	635.03503 †
8	1	-1	0	0	12	1	1	0	0	12	3313.78524*	-0.00581	3313.79105	657.84012 †
9	1	-1	0	0	14	1	1	0	0	14	3313.78524*	0.01034	3313.77490	709.14713 †
10	1	-1	0	0	15	1	1	0	0	15	3313.75835*	-0.00752	3313.76587	737.64836 †
11	1	-1	0	0	16	1	1	0	0	16	3313.75835*	0.00216	3313.75619	768.04757 †
12	1	-1	0	0	17	1	1	0	0	17	3313.75835*	0.01250	3313.74585	800.34436 †
13	1	-1	0	0	18	1	1	0	0	18	3313.73420	-0.00064	3313.73484	834.53830
14	1	-1	0	0	19	1	1	0	0	19	3313.72569*	0.00253	3313.72316	870.62893 †
15	1	-1	0	0	20	1	1	0	0	20	3313.71064	-0.00015	3313.71079	908.61577
16	1	-1	0	0	21	1	1	0	0	21	3313.69858	0.00086	3313.69772	948.49830
17	1	-1	0	0	22	1	1	0	0	22	3313.68112	-0.00282	3313.68394	990.27601 †

rms = 0.00041 cm⁻¹

$v_1 + v_5 (\Pi) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	0 0 0 0 2	3971.20957	0.00053	3971.20904	5.70195
0 0 1 1 2	0 0 0 0 3	3969.28943	-0.00006	3969.28949	11.40382
0 0 1 1 3	0 0 0 0 4	3967.36117	0.00063	3967.36054	19.00619
0 0 1 1 4	0 0 0 0 5	3965.42281	0.00060	3965.42221	28.50898
0 0 1 1 5	0 0 0 0 6	3963.47501	0.00049	3963.47452	39.91204
0 0 1 1 6	0 0 0 0 7	3961.51793	0.00043	3961.51750	53.21523
0 0 1 1 7	0 0 0 0 8	3959.55153	0.00035	3959.55118	68.41838
0 0 1 1 8	0 0 0 0 9	3957.57590	0.00032	3957.57558	85.52129
0 0 1 1 9	0 0 0 0 10	3955.59092	0.00019	3955.59073	104.52373
0 0 1 1 10	0 0 0 0 11	3953.59684	0.00019	3953.59665	125.42544
0 0 1 1 11	0 0 0 0 12	3951.59362	0.00025	3951.59337	148.22616
0 0 1 1 12	0 0 0 0 13	3949.58105	0.00014	3949.58091	172.92558
0 0 1 1 13	0 0 0 0 14	3947.55947	0.00016	3947.55931	199.52337
0 0 1 1 14	0 0 0 0 15	3945.52877	0.00019	3945.52858	228.01920
0 0 1 1 15	0 0 0 0 16	3943.48893	0.00017	3943.48876	258.41268
0 0 1 1 16	0 0 0 0 17	3941.44006	0.00019	3941.43987	290.70340
0 0 1 1 17	0 0 0 0 18	3939.38220	0.00026	3939.38194	324.89096
0 0 1 1 18	0 0 0 0 19	3937.31519	0.00020	3937.31499	360.97488
0 0 1 1 19	0 0 0 0 20	3935.23926	0.00020	3935.23906	398.95471
0 0 1 1 20	0 0 0 0 21	3933.15439	0.00023	3933.15416	438.82993
0 0 1 1 21	0 0 0 0 22	3931.06058	0.00025	3931.06033	480.60003
0 0 1 1 22	0 0 0 0 23	3928.95795	0.00036	3928.95759	524.26445
0 0 1 1 23	0 0 0 0 24	3926.84625	0.00028	3926.84597	569.82262
0 0 1 1 24	0 0 0 0 25	3924.72592	0.00042	3924.72550	617.27393
0 0 1 1 25	0 0 0 0 26	3922.59640	0.00020	3922.59620	666.61777
0 0 1 1 26	0 0 0 0 27	3920.45829	0.00018	3920.45811	717.85348
0 0 1 1 27	0 0 0 0 28	3918.31164	0.00040	3918.31124	770.98038
0 0 1 1 28	0 0 0 0 29	3916.15588	0.00025	3916.15563	825.99778
0 0 1 1 29	0 0 0 0 30	3913.99195	0.00064	3913.99131	882.90495
0 0 1 1 30	0 0 0 0 31	3911.81855	0.00025	3911.81830	941.70115
0 0 1 1 31	0 0 0 0 32	3909.63727	0.00064	3909.63663	1002.38559
0 0 1 1 32	0 0 0 0 33	3907.44715	0.00082	3907.44633	1064.95747
0 0 1 1 33	0 0 0 0 34	3905.24754	0.00011	3905.24743	1129.41599
0 0 1 1 34	0 0 0 0 35	3903.04026	0.00030	3903.03996	1195.76027
0 0 1 1 35	0 0 0 0 36	3900.82414	0.00020	3900.82394	1263.98946
0 0 1 1 36	0 0 0 0 37	3898.59976	0.00036	3898.59940	1334.10264
0 0 1 1 37	0 0 0 0 38	3896.36514*	-0.00123	3896.36637	1406.09891 †
0 0 1 1 38	0 0 0 0 39	3894.12594*	0.00106	3894.12488	1479.97730 †
0 0 1 1 39	0 0 0 0 40	3891.87494	-0.00002	3891.87496	1555.73685
0 0 1 1 1	0 0 0 0 0	3976.91189	0.00091	3976.91098	0.00000
0 0 1 1 2	0 0 0 0 1	3978.79337	0.00072	3978.79265	1.90066

1	0	0	1	1	3	0	0	0	0	2	3980.66553	0.00074	3980.66479	5.70195
2	0	0	1	1	4	0	0	0	0	3	3982.52786	0.00049	3982.52737	11.40382
3	0	0	1	1	5	0	0	0	0	4	3984.38077	0.00040	3984.38037	19.00619
4	0	0	1	1	6	0	0	0	0	5	3986.22417	0.00041	3986.22376	28.50898
5	0	0	1	1	7	0	0	0	0	6	3988.05790	0.00037	3988.05753	39.91204
6	0	0	1	1	8	0	0	0	0	7	3989.88188	0.00024	3989.88164	53.21523
7	0	0	1	1	9	0	0	0	0	8	3991.69631	0.00024	3991.69607	68.41838
8	0	0	1	1	10	0	0	0	0	9	3993.50110	0.00031	3993.50079	85.52129
9	0	0	1	1	11	0	0	0	0	10	3995.29602	0.00022	3995.29580	104.52373
10	0	0	1	1	12	0	0	0	0	11	3997.08108	0.00003	3997.08105	125.42544
11	0	0	1	1	13	0	0	0	0	12	3998.85661	0.00009	3998.85652	148.22616
12	0	0	1	1	14	0	0	0	0	13	4000.62242	0.00022	4000.62220	172.92558
13	0	0	1	1	15	0	0	0	0	14	4002.37852	0.00046	4002.37806	199.52337
14	0	0	1	1	16	0	0	0	0	15	4004.12431	0.00024	4004.12407	228.01920
15	0	0	1	1	17	0	0	0	0	16	4005.86044	0.00022	4005.86022	258.41268
16	0	0	1	1	18	0	0	0	0	17	4007.58650	0.00003	4007.58647	290.70340
17	0	0	1	1	19	0	0	0	0	18	4009.30295	0.00014	4009.30281	324.89096
18	0	0	1	1	20	0	0	0	0	19	4011.00946	0.00025	4011.00921	360.97488
19	0	0	1	1	21	0	0	0	0	20	4012.70584	0.00019	4012.70565	398.95471
20	0	0	1	1	22	0	0	0	0	21	4014.39234	0.00023	4014.39211	438.82993
21	0	0	1	1	23	0	0	0	0	22	4016.06846	-0.00010	4016.06856	480.60003
22	0	0	1	1	24	0	0	0	0	23	4017.73528	0.00030	4017.73498	524.26445
23	0	0	1	1	25	0	0	0	0	24	4019.39171	0.00036	4019.39135	569.82262
24	0	0	1	1	26	0	0	0	0	25	4021.03797	0.00032	4021.03765	617.27393
25	0	0	1	1	27	0	0	0	0	26	4022.67397	0.00012	4022.67385	666.61777
26	0	0	1	1	28	0	0	0	0	27	4024.30029	0.00035	4024.29994	717.85348
27	0	0	1	1	29	0	0	0	0	28	4025.91604	0.00016	4025.91588	770.98038
28	0	0	1	1	30	0	0	0	0	29	4027.52219	0.00052	4027.52167	825.99778
29	0	0	1	1	31	0	0	0	0	30	4029.11761	0.00034	4029.11727	882.90495
30	0	0	1	1	32	0	0	0	0	31	4030.70186	-0.00080	4030.70266	941.70115
31	0	0	1	1	33	0	0	0	0	32	4032.27793	0.00010	4032.27783	1002.38559
32	0	0	1	1	34	0	0	0	0	33	4033.84441*	0.00166	4033.84275	1064.95747 †
33	0	0	1	1	35	0	0	0	0	34	4035.39706	-0.00035	4035.39741	1129.41599
34	0	0	1	1	36	0	0	0	0	35	4036.94231	0.00054	4036.94177	1195.76027
35	0	0	1	1	37	0	0	0	0	36	4038.47650	0.00068	4038.47582	1263.98946
36	0	0	1	1	38	0	0	0	0	37	4039.99994	0.00040	4039.99954	1334.10264
37	0	0	1	1	39	0	0	0	0	38	4041.51255*	-0.00035	4041.51290	1406.09891
38	0	0	1	1	40	0	0	0	0	39	4043.01536	-0.00054	4043.01590	1479.97730
39	0	0	1	-1	1	0	0	0	0	1	3975.00611*	-0.01084	3975.01695	1.90066 †
40	0	0	1	-1	2	0	0	0	0	2	3975.00611*	-0.00513	3975.01124	5.70195 †
41	0	0	1	-1	3	0	0	0	0	3	3975.00611*	0.00345	3975.00266	11.40382 †
42	0	0	1	-1	4	0	0	0	0	4	3974.99340	0.00217	3974.99123	19.00619 †
43	0	0	1	-1	5	0	0	0	0	5	3974.97817	0.00124	3974.97693	28.50898 †
44	0	0	1	-1	6	0	0	0	0	6	3974.96000	0.00023	3974.95977	39.91204
45	0	0	1	-1	7	0	0	0	0	7	3974.93962	-0.00013	3974.93975	53.21523
46	0	0	1	-1	8	0	0	0	0	8	3974.91668	-0.00018	3974.91686	68.41838
47	0	0	1	-1	9	0	0	0	0	9	3974.89069	-0.00040	3974.89109	85.52129
48	0	0	1	-1	10	0	0	0	0	10	3974.86215	-0.00031	3974.86246	104.52373
49	0	0	1	-1	11	0	0	0	0	11	3974.83070	-0.00024	3974.83094	125.42544
50	0	0	1	-1	12	0	0	0	0	12	3974.79635	-0.00020	3974.79655	148.22616
51	0	0	1	-1	13	0	0	0	0	13	3974.75912	-0.00014	3974.75926	172.92558
52	0	0	1	-1	14	0	0	0	0	14	3974.71892	-0.00017	3974.71909	199.52337
53	0	0	1	-1	15	0	0	0	0	15	3974.67599	-0.00003	3974.67602	228.01920
54	0	0	1	-1	16	0	0	0	0	16	3974.62993	-0.00012	3974.63005	258.41268
55	0	0	1	-1	17	0	0	0	0	17	3974.58085	-0.00033	3974.58118	290.70340
56	0	0	1	-1	18	0	0	0	0	18	3974.52929	-0.00010	3974.52939	324.89096
57	0	0	1	-1	19	0	0	0	0	19	3974.47462	-0.00006	3974.47468	360.97488
58	0	0	1	-1	20	0	0	0	0	20	3974.41709	0.00004	3974.41705	398.95471
59	0	0	1	-1	21	0	0	0	0	21	3974.35655	0.00007	3974.35648	438.82993
60	0	0	1	-1	22	0	0	0	0	22	3974.29307	0.00010	3974.29297	480.60003
	0	0	1	-1	23	0	0	0	0	23	3974.22668	0.00017	3974.22651	524.26445
	0	0	1	-1	24	0	0	0	0	24	3974.15726	0.00016	3974.15710	569.82262
	0	0	1	-1	25	0	0	0	0	25	3974.08490	0.00018	3974.08472	617.27393
	0	0	1	-1	26	0	0	0	0	26	3974.00960	0.00024	3974.00936	666.61777
	0	0	1	-1	27	0	0	0	0	27	3973.93090	-0.00012	3973.93102	717.85348

0	0	1	-1	28	0	0	0	0	28	3973.84976	0.00007	3973.84969	770.98038
0	0	1	-1	29	0	0	0	0	29	3973.76576	0.00041	3973.76535	825.99778
0	0	1	-1	30	0	0	0	0	30	3973.67806	0.00007	3973.67799	882.90495
0	0	1	-1	31	0	0	0	0	31	3973.58406*	-0.00356	3973.58762	941.70115 +
0	0	1	-1	32	0	0	0	0	32	3973.49636*	0.00216	3973.49420	1002.38559 +
0	0	1	-1	33	0	0	0	0	33	3973.39966*	0.00192	3973.39774	1064.95747 +
0	0	1	-1	34	0	0	0	0	34	3973.29869	0.00048	3973.29821	1129.41599
0	0	1	-1	35	0	0	0	0	35	3973.19649	0.00087	3973.19562	1195.76027
0	0	1	-1	36	0	0	0	0	36	3973.08953	-0.00041	3973.08994	1263.98946
0	0	1	-1	37	0	0	0	0	37	3972.98189	0.00073	3972.98116	1334.10264
0	0	1	-1	38	0	0	0	0	38	3972.86845	-0.00082	3972.86927	1406.09891
0	0	1	-1	39	0	0	0	0	39	3972.75381	-0.00045	3972.75426	1479.97730
0	0	1	-1	40	0	0	0	0	40	3972.63704	0.00094	3972.63610	1555.73685
0	0	1	-1	41	0	0	0	0	41	3972.51516	0.00036	3972.51480	1633.37656

rms = 0.00038 cm⁻¹

$\nu_1 + \nu_5 (\Pi) \leftarrow \nu_5 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 2	0 0 1 1 3	3295.05852	0.00014	3295.05838	685.63493
0 0 1 1 3	0 0 1 1 4	3293.13297	0.00005	3293.13292	693.23382
0 0 1 1 4	0 0 1 1 5	3291.19878	-0.00017	3291.19895	702.73224
0 0 1 1 5	0 0 1 1 6	3289.25655	0.00006	3289.25649	714.13007
0 0 1 1 6	0 0 1 1 7	3287.30534	-0.00024	3287.30558	727.42716
0 0 1 1 7	0 0 1 1 8	3285.34582	-0.00041	3285.34623	742.62333
0 0 1 1 8	0 0 1 1 9	3283.37825	-0.00024	3283.37849	759.71839
0 0 1 1 9	0 0 1 1 10	3281.40209	-0.00027	3281.40236	778.71209
0 0 1 1 10	0 0 1 1 11	3279.41778	-0.00010	3279.41788	799.60420
0 0 1 1 11	0 0 1 1 12	3277.42518	0.00010	3277.42508	822.39444
0 0 1 1 12	0 0 1 1 13	3275.42344	-0.00054	3275.42398	847.08251
0 0 1 1 13	0 0 1 1 14	3273.41441	-0.00019	3273.41460	873.66808
0 0 1 1 14	0 0 1 1 15	3271.39666	-0.00033	3271.39699	902.15079
0 0 1 1 15	0 0 1 1 16	3269.37064	-0.00051	3269.37115	932.53028
0 0 1 1 16	0 0 1 1 17	3267.33677	-0.00036	3267.33713	964.80614
0 0 1 1 17	0 0 1 1 18	3265.29437	-0.00058	3265.29495	998.97795
0 0 1 1 18	0 0 1 1 19	3263.24406	-0.00057	3263.24463	1035.04524
0 0 1 1 19	0 0 1 1 20	3261.18578	-0.00043	3261.18621	1073.00756
0 0 1 1 20	0 0 1 1 21	3259.11917	-0.00054	3259.11971	1112.86438
0 0 1 1 21	0 0 1 1 22	3257.04433	-0.00083	3257.04516	1154.61520
0 0 1 1 22	0 0 1 1 23	3254.96171	-0.00088	3254.96259	1198.25945
0 0 1 1 23	0 0 1 1 24	3252.87138	-0.00065	3252.87203	1243.79656
0 0 1 1 24	0 0 1 1 25	3250.77276	-0.00074	3250.77350	1291.22593
0 0 1 1 25	0 0 1 1 26	3248.66617	-0.00087	3248.66704	1340.54693
0 0 1 1 26	0 0 1 1 27	3246.55218	-0.00049	3246.55267	1391.75891
0 0 1 1 27	0 0 1 1 28	3244.42969	-0.00074	3244.43043	1444.86119
0 0 1 1 28	0 0 1 1 29	3242.30034	0.00000	3242.30034	1499.85307
0 0 1 1 29	0 0 1 1 30	3240.16288	0.00045	3240.16243	1556.73383
0 0 1 1 30	0 0 1 1 31	3238.01669	-0.00005	3238.01674	1615.50271
0 0 1 1 31	0 0 1 1 32	3235.86253	-0.00075	3235.86328	1676.15894
0 0 1 1 32	0 0 1 1 33	3233.70216	0.00006	3233.70210	1738.70171
0 0 1 1 33	0 0 1 1 34	3231.53350	0.00028	3231.53322	1803.13019
0 0 1 1 34	0 0 1 1 35	3229.35698	0.00030	3229.35668	1869.44355
0 0 1 1 35	0 0 1 1 36	3227.17275	0.00026	3227.17249	1937.64090
0 0 1 1 36	0 0 1 1 37	3224.97978	-0.00092	3224.98070	2007.72134
0 0 1 1 37	0 0 1 1 38	3222.78100	-0.00033	3222.78133	2079.68394
0 0 1 1 38	0 0 1 1 39	3220.57527	0.00085	3220.57442	2153.52776
0 0 1 1 39	0 0 1 1 40	3218.35931	-0.00068	3218.35999	2229.25182
0 0 1 1 40	0 0 1 1 41	3216.13889	0.00081	3216.13808	2306.85512
0 0 1 1 2	0 0 1 1 1	3304.55791*	0.00073	3304.55718	676.13613
0 0 1 1 3	0 0 1 1 2	3306.43130	0.00024	3306.43106	679.93567
0 0 1 1 4	0 0 1 1 3	3308.29714	0.00088	3308.29626	685.63493

1	0	0	1	1	6	0	0	1	1	5	3312.00080	0.00030	3312.00050	702.73224
2	0	0	1	1	7	0	0	1	1	6	3313.84442*	0.00493	3313.83949	714.13007
3	0	0	1	1	8	0	0	1	1	7	3315.66960	-0.00011	3315.66971	727.42716
4	0	0	1	1	9	0	0	1	1	8	3317.49099	-0.00013	3317.49112	742.62333
5	0	0	1	1	10	0	0	1	1	9	3319.30366	-0.00004	3319.30370	759.71839
6	0	0	1	1	11	0	0	1	1	10	3321.10718	-0.00025	3321.10743	778.71209
7	0	0	1	1	12	0	0	1	1	11	3322.90204	-0.00024	3322.90228	799.60420
8	0	0	1	1	13	0	0	1	1	12	3324.68788	-0.00036	3324.68824	822.39444
9	0	0	1	1	14	0	0	1	1	13	3326.46513	-0.00014	3326.46527	847.08251
10	0	0	1	1	15	0	0	1	1	14	3328.23316	-0.00020	3328.23336	873.66808
11	0	0	1	1	16	0	0	1	1	15	3329.99223	-0.00025	3329.99248	902.15079
12	0	0	1	1	17	0	0	1	1	16	3331.74227	-0.00034	3331.74261	932.53028
13	0	0	1	1	18	0	0	1	1	17	3333.48335	-0.00038	3333.48373	964.80614
14	0	0	1	1	19	0	0	1	1	18	3335.21534	-0.00048	3335.21582	998.97795
15	0	0	1	1	20	0	0	1	1	19	3336.93823	-0.00062	3336.93885	1035.04524
16	0	0	1	1	21	0	0	1	1	20	3338.65254	-0.00026	3338.65280	1073.00756
17	0	0	1	1	22	0	0	1	1	21	3340.35745	-0.00021	3340.35766	1112.86438
18	0	0	1	1	23	0	0	1	1	22	3342.05283	-0.00056	3342.05339	1154.61520
19	0	0	1	1	24	0	0	1	1	23	3343.73937	-0.00061	3343.73998	1198.25945
20	0	0	1	1	25	0	0	1	1	24	3345.41644	-0.00097	3345.41741	1243.79656
21	0	0	1	1	26	0	0	1	1	25	3347.08595	0.00030	3347.08565	1291.22593
22	0	0	1	1	27	0	0	1	1	26	3348.74504	0.00035	3348.74469	1340.54693
23	0	0	1	1	28	0	0	1	1	27	3350.39395	-0.00055	3350.39450	1391.75891
24	0	0	1	1	29	0	0	1	1	28	3352.03516	0.00009	3352.03507	1444.86119
25	0	0	1	1	30	0	0	1	1	29	3353.66592	-0.00045	3353.66637	1499.85307
26	0	0	1	1	31	0	0	1	1	30	3355.28808	-0.00031	3355.28839	1556.73383
27	0	0	1	1	32	0	0	1	1	31	3356.90031	-0.00079	3356.90110	1615.50271
28	0	0	1	1	33	0	0	1	1	32	3358.50436	-0.00012	3358.50448	1676.15894
29	0	0	1	1	34	0	0	1	1	33	3360.09701*	-0.00151	3360.09852	1738.70171
30	0	0	1	1	35	0	0	1	1	34	3361.68295	-0.00025	3361.68320	1803.13019
31	0	0	1	1	36	0	0	1	1	35	3363.25796	-0.00053	3363.25849	1869.44355
32	0	0	1	1	37	0	0	1	1	36	3364.82460	0.00022	3364.82438	1937.64090
33	0	0	1	1	38	0	0	1	1	37	3366.38054	-0.00030	3366.38084	2007.72134
34	0	0	1	1	39	0	0	1	1	38	3367.92866	0.00079	3367.92787	2079.68394
35	0	0	1	1	40	0	0	1	1	39	3369.46477	-0.00067	3369.46544	2153.52776
36	0	0	1	-1	2	0	0	1	-1	3	3295.03940	0.00027	3295.03913	685.67405
37	0	0	1	-1	3	0	0	1	-1	4	3293.10745	-0.00001	3293.10746	693.29902
38	0	0	1	-1	4	0	0	1	-1	5	3291.16734	-0.00004	3291.16738	702.83004
39	0	0	1	-1	6	0	0	1	-1	7	3287.26209	-0.00003	3287.26212	727.60969
40	0	0	1	-1	7	0	0	1	-1	8	3285.29688	-0.00011	3285.29699	742.85799
41	0	0	1	-1	8	0	0	1	-1	9	3283.32359	0.00003	3283.32356	760.01168
42	0	0	1	-1	9	0	0	1	-1	10	3281.34164	-0.00023	3281.34187	779.07052
43	0	0	1	-1	10	0	0	1	-1	11	3279.35166	-0.00026	3279.35192	800.03426
44	0	0	1	-1	11	0	0	1	-1	12	3277.35353	-0.00024	3277.35377	822.90261
45	0	0	1	-1	12	0	0	1	-1	13	3275.34736	-0.00006	3275.34742	847.67528
46	0	0	1	-1	13	0	0	1	-1	14	3273.33279	-0.00012	3273.33291	874.35193
47	0	0	1	-1	14	0	0	1	-1	15	3271.31093*	-0.00089	3271.31027	902.93220
48	0	0	1	-1	15	0	0	1	-1	16	3269.27912*	-0.00040	3269.27952	933.41570
49	0	0	1	-1	16	0	0	1	-1	17	3267.24064	-0.00005	3267.24069	965.80204
50	0	0	1	-1	17	0	0	1	-1	18	3265.19363	-0.00019	3265.19382	1000.09076
51	0	0	1	-1	18	0	0	1	-1	19	3263.13878*	-0.00014	3263.13892	1036.28142
52	0	0	1	-1	19	0	0	1	-1	20	3261.07565	-0.00038	3261.07603	1074.37353
53	0	0	1	-1	20	0	0	1	-1	21	3259.00493	-0.00025	3259.00518	1114.36658
54	0	0	1	-1	21	0	0	1	-1	22	3256.92598	-0.00041	3256.92639	1156.26002
55	0	0	1	-1	22	0	0	1	-1	23	3254.83932	-0.00037	3254.83969	1200.05331
56	0	0	1	-1	23	0	0	1	-1	24	3252.74462	-0.00050	3252.74512	1245.74584
57	0	0	1	-1	25	0	0	1	-1	26	3248.53248	0.00001	3248.53247	1342.82618
58	0	0	1	-1	26	0	0	1	-1	27	3246.41446*	0.00002	3246.41444	1394.21269
59	0	0	1	-1	27	0	0	1	-1	28	3244.28814	-0.00052	3244.28866	1447.49584
60	0	0	1	-1	28	0	0	1	-1	29	3242.15472	-0.00042	3242.15514	1502.67492
	0	0	1	-1	29	0	0	1	-1	30	3240.01443*	0.00050	3240.01393	1559.74920
	0	0	1	-1	30	0	0	1	-1	31	3237.86505	0.00000	3237.86505	1618.71789
	0	0	1	-1	31	0	0	1	-1	32	3235.70797	-0.00057	3235.70854	1679.58023
	0	0	1	-1	32	0	0	1	-1	33	3233.54403	-0.00038	3233.54441	1742.33538
	0	0	1	-1	33	0	0	1	-1	34	3231.37249	-0.00022	3231.37271	1806.98250

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1														
2	0	0	1	-1	9	0	0	1	1	9	3300.69342	-0.00058	3300.69400	759.71839
3	0	0	1	-1	10	0	0	1	1	10	3300.67464	0.00055	3300.67409	778.71209
4	0	0	1	-1	11	0	0	1	1	11	3300.66192*	0.00974	3300.65218	799.60420 †
5	0	0	1	-1	13	0	0	1	1	13	3300.60086*	-0.00147	3300.60233	847.08251 †
6	0	0	1	-1	12	0	0	1	1	12	3300.63161*	0.00335	3300.62826	822.39444 †
7	0	0	1	-1	14	0	0	1	1	14	3300.57461	0.00022	3300.57439	873.66808

rms = 0.00041 cm⁻¹

$v_1 + v_5 (\Pi) \leftarrow 2v_5 (\Sigma^+)$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''	
0	0	1	1	1	0	0	2	0	2	2635.87754*	-0.00707	2635.88461	1341.02637	†
0	0	1	1	2	0	0	2	0	3	2633.94270*	-0.00649	2633.94919	1346.74412	†
0	0	1	1	3	0	0	2	0	4	2631.99929	0.00015	2631.99914	1354.36759	
0	0	1	1	4	0	0	2	0	5	2630.03605	0.00148	2630.03457	1363.89662	†
0	0	1	1	5	0	0	2	0	6	2628.05566	0.00009	2628.05557	1375.33100	
0	0	1	1	6	0	0	2	0	7	2626.06227	0.00000	2626.06227	1388.67047	
0	0	1	1	7	0	0	2	0	8	2624.05369	-0.00112	2624.05481	1403.91476	†
0	0	1	1	8	0	0	2	0	9	2622.03291	-0.00044	2622.03335	1421.06352	
0	0	1	1	9	0	0	2	0	10	2619.99816	0.00009	2619.99807	1440.11639	
0	0	1	1	10	0	0	2	0	11	2617.94845	-0.00069	2617.94914	1461.07294	
0	0	1	1	11	0	0	2	0	12	2615.88742	0.00062	2615.88680	1483.93273	
0	0	1	1	12	0	0	2	0	13	2613.81125	0.00001	2613.81124	1508.69525	
0	0	1	1	13	0	0	2	0	14	2611.72364	0.00092	2611.72272	1535.35996	
0	0	1	1	14	0	0	2	0	15	2609.62138	-0.00010	2609.62148	1563.92630	
0	0	1	1	15	0	0	2	0	16	2607.50761	-0.00020	2607.50781	1594.39363	
0	0	1	1	16	0	0	2	0	17	2605.38266	0.00068	2605.38198	1626.76130	
0	0	1	1	18	0	0	2	0	19	2601.09250*	-0.00256	2601.09506	1697.19482	†
0	0	1	1	20	0	0	2	0	21	2596.76467	0.00139	2596.76328	1775.22081	†
0	0	1	1	21	0	0	2	0	22	2594.58081	-0.00061	2594.58142	1817.07894	
0	0	1	1	23	0	0	2	0	24	2590.18692	-0.00061	2590.18753	1906.48106	
0	0	1	1	24	0	0	2	0	25	2587.97585	-0.00039	2587.97624	1954.02319	
0	0	1	1	2	0	0	2	0	1	2643.47967	0.00083	2643.47884	1337.21447	
0	0	1	1	3	0	0	2	0	2	2645.33952	-0.00084	2645.34036	1341.02637	
0	0	1	1	4	0	0	2	0	3	2647.18874	0.00168	2647.18706	1346.74412	†
0	0	1	1	5	0	0	2	0	4	2649.01944	0.00047	2649.01897	1354.36759	
0	0	1	1	6	0	0	2	0	5	2650.83769	0.00157	2650.83612	1363.89662	†
0	0	1	1	7	0	0	2	0	6	2652.63891	0.00034	2652.63857	1375.33100	
0	0	1	1	8	0	0	2	0	7	2654.42625	-0.00015	2654.42640	1388.67047	
0	0	1	1	9	0	0	2	0	8	2656.19995	0.00026	2656.19969	1403.91476	
0	0	1	1	10	0	0	2	0	9	2657.95969	0.00113	2657.95856	1421.06352	†
0	0	1	1	11	0	0	2	0	10	2659.70281	-0.00033	2659.70314	1440.11639	
0	0	1	1	12	0	0	2	0	11	2661.43542*	0.00187	2661.43355	1461.07294	†
0	0	1	1	13	0	0	2	0	12	2663.14999	0.00004	2663.14995	1483.93273	
0	0	1	1	14	0	0	2	0	13	2664.85339	0.00086	2664.85253	1508.69525	
0	0	1	1	15	0	0	2	0	14	2666.54206	0.00059	2666.54147	1535.35996	
0	0	1	1	16	0	0	2	0	15	2668.21676	-0.00022	2668.21698	1563.92630	
0	0	1	1	17	0	0	2	0	16	2669.87872	-0.00055	2669.87927	1594.39363	
0	0	1	1	18	0	0	2	0	17	2671.52677*	-0.00181	2671.52858	1626.76130	†
0	0	1	1	19	0	0	2	0	18	2673.16727	0.00211	2673.16516	1661.02860	†
0	0	1	1	20	0	0	2	0	19	2674.78860	-0.00068	2674.78928	1697.19482	
0	0	1	1	22	0	0	2	0	21	2678.00074	-0.00049	2678.00123	1775.22081	
0	0	1	1	23	0	0	2	0	22	2679.58900	-0.00065	2679.58965	1817.07894	
0	0	1	-1	1	0	0	2	0	1	2639.70215	-0.00099	2639.70314	1337.21447	
0	0	1	-1	2	0	0	2	0	2	2639.68596	-0.00085	2639.68681	1341.02637	
0	0	1	-1	3	0	0	2	0	3	2639.66183	-0.00052	2639.66235	1346.74412	
0	0	1	-1	4	0	0	2	0	4	2639.63129*	0.00146	2639.62983	1354.36759	†
0	0	1	-1	5	0	0	2	0	5	2639.58924	-0.00005	2639.58929	1363.89662	
0	0	1	-1	6	0	0	2	0	6	2639.53980	-0.00102	2639.54082	1375.33100	†
0	0	1	-1	7	0	0	2	0	7	2639.48400*	-0.00051	2639.48451	1388.67047	
0	0	1	-1	8	0	0	2	0	8	2639.42084	0.00036	2639.42048	1403.91476	
0	0	1	-1	9	0	0	2	0	9	2639.34899	0.00013	2639.34886	1421.06352	

0	0	1	-1	10	0	0	2	0	10	2639.27050*	0.00071	2639.26979	1440.11639
0	0	1	-1	11	0	0	2	0	11	2639.18287	-0.00057	2639.18344	1461.07294
0	0	1	-1	12	0	0	2	0	12	2639.09043	0.00045	2639.08998	1483.93273
0	0	1	-1	13	0	0	2	0	13	2638.98837	-0.00122	2638.98959	1508.69525 †
0	0	1	-1	14	0	0	2	0	14	2638.88385*	0.00135	2638.88250	1535.35996 †
0	0	1	-1	15	0	0	2	0	15	2638.76940	0.00047	2638.76893	1563.92630
0	0	1	-1	16	0	0	2	0	16	2638.64904	-0.00006	2638.64910	1594.39363
0	0	1	-1	17	0	0	2	0	17	2638.52295	-0.00034	2638.52329	1626.76130
0	0	1	-1	20	0	0	2	0	20	2638.11303	0.00043	2638.11260	1735.25916
0	0	1	-1	21	0	0	2	0	21	2637.96538	-0.00022	2637.96560	1775.22081

rms = 0.00051 cm⁻¹

$$v_1 + v_5 (\Pi) \leftarrow 2v_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 5	0 0 2 2 6	2611.48212	0.00041	2611.48171	1391.90486
0 0 1 1 6	0 0 2 2 7	2609.49330	0.00029	2609.49301	1405.23972
0 0 1 1 7	0 0 2 2 8	2607.48862	-0.00157	2607.49019	1420.47938 †
0 0 1 1 8	0 0 2 2 9	2605.47343	0.00030	2605.47313	1437.62374
0 0 1 1 9	0 0 2 2 10	2603.44110*	-0.00064	2603.44174	1456.67272
0 0 1 1 10	0 0 2 2 11	2601.39532	-0.00055	2601.39587	1477.62621
0 0 1 1 11	0 0 2 2 12	2599.33559	0.00019	2599.33540	1500.48412
0 0 1 1 14	0 0 2 2 15	2593.06668	0.00200	2593.06468	1580.48310 †
0 0 1 1 15	0 0 2 2 16	2590.94412	0.00006	2590.94406	1610.95737
0 0 1 1 16	0 0 2 2 17	2588.80799	0.00008	2588.80791	1643.33536
0 0 1 1 17	0 0 2 2 18	2586.65694	0.00094	2586.65600	1677.61689
0 0 1 1 18	0 0 2 2 19	2584.48858	0.00049	2584.48809	1713.80178
0 0 1 1 19	0 0 2 2 20	2582.30422	0.00028	2582.30394	1751.88982
0 0 1 1 20	0 0 2 2 21	2580.10373	0.00045	2580.10328	1791.88081
0 0 1 1 11	0 0 2 2 10	2643.14601	-0.00080	2643.14681	1456.67272
0 0 1 1 12	0 0 2 2 11	2644.88135	0.00108	2644.88027	1477.62621 †
0 0 1 1 13	0 0 2 2 12	2646.59858	0.00002	2646.59856	1500.48412
0 0 1 1 14	0 0 2 2 13	2648.30246	0.00101	2648.30145	1525.24633 †
0 0 1 1 15	0 0 2 2 14	2649.99047	0.00173	2649.98874	1551.91270 †
0 0 1 1 16	0 0 2 2 15	2651.66036	0.00018	2651.66018	1580.48310
0 0 1 1 17	0 0 2 2 16	2653.31480	-0.00072	2653.31552	1610.95737
0 0 1 1 19	0 0 2 2 18	2656.57662	-0.00025	2656.57687	1677.61689
0 0 1 1 20	0 0 2 2 19	2658.18216	-0.00015	2658.18231	1713.80178
0 0 1 1 21	0 0 2 2 20	2659.77064	0.00011	2659.77053	1751.88982
0 0 1 -1 5	0 0 2 -2 6	2611.58297	0.00082	2611.58215	1391.90376
0 0 1 -1 6	0 0 2 -2 7	2609.63447	0.00040	2609.63407	1405.23774
0 0 1 -1 8	0 0 2 -2 9	2605.71535	-0.00135	2605.71670	1437.61854 †
0 0 1 -1 9	0 0 2 -2 10	2603.74696*	-0.00050	2603.74746	1456.66492
0 0 1 -1 10	0 0 2 -2 11	2601.77152	0.00029	2601.77123	1477.61496
0 0 1 -1 16	0 0 2 -2 17	2589.76806	-0.00032	2589.76838	1643.27435
0 0 1 -1 17	0 0 2 -2 18	2587.74467	0.00075	2587.74392	1677.54066
0 0 1 -1 18	0 0 2 -2 19	2585.71287	0.00018	2585.71269	1713.70766
0 0 1 -1 19	0 0 2 -2 20	2583.67441	-0.00030	2583.67471	1751.77486
0 0 1 -1 20	0 0 2 -2 21	2581.62999	-0.00001	2581.63000	1791.74175
0 0 1 -1 21	0 0 2 -2 22	2579.57792	-0.00069	2579.57861	1833.60781
0 0 1 -1 6	0 0 2 -2 5	2634.39770	0.00018	2634.39752	1380.47429
0 0 1 -1 7	0 0 2 -2 6	2636.25088	-0.00035	2636.25123	1391.90376
0 0 1 -1 8	0 0 2 -2 7	2638.09497*	-0.00253	2638.09750	1405.23774 †
0 0 1 -1 10	0 0 2 -2 9	2641.76807	0.00043	2641.76764	1437.61854
0 0 1 -1 11	0 0 2 -2 10	2643.59192	0.00046	2643.59146	1456.66492
0 0 1 -1 12	0 0 2 -2 11	2645.40660	-0.00115	2645.40775	1477.61496 †
0 0 1 -1 13	0 0 2 -2 12	2647.21759*	0.00111	2647.21648	1500.46836 †
0 0 1 -1 14	0 0 2 -2 13	2649.01782*	0.00019	2649.01763	1525.22483
0 0 1 -1 15	0 0 2 -2 14	2650.81095*	-0.00023	2650.81118	1551.88404
0 0 1 -1 16	0 0 2 -2 15	2652.59767	0.00056	2652.59711	1580.44562
0 0 1 -1 17	0 0 2 -2 16	2654.37611	0.00072	2654.37539	1610.90919

1														
2	0	0	1	-1	18	0	0	2	-2	17	2656.14568	-0.00031	2656.14599	1643.27435
3	0	0	1	-1	20	0	0	2	-2	19	2659.66519	0.00109	2659.66410	1713.70766 †
4	0	0	1	-1	21	0	0	2	-2	20	2661.41081	-0.00074	2661.41155	1751.77486
5	0	0	1	-1	22	0	0	2	-2	21	2663.15152	0.00027	2663.15125	1791.74175
6	0	0	1	1	2	0	0	2	-2	2	2623.07883	-0.00004	2623.07887	1357.61444
7	0	0	1	1	3	0	0	2	-2	3	2623.03631	-0.00090	2623.03721	1363.32952
8	0	0	1	1	4	0	0	2	-2	4	2622.98189	0.00021	2622.98168	1370.94950
9	0	0	1	1	6	0	0	2	-2	6	2622.83005	0.00107	2622.82898	1391.90376 †
10	0	0	1	1	7	0	0	2	-2	7	2622.73207	0.00025	2622.73182	1405.23774
11	0	0	1	1	8	0	0	2	-2	8	2622.62127	0.00047	2622.62080	1420.47607
12	0	0	1	1	10	0	0	2	-2	10	2622.35739	0.00023	2622.35716	1456.66492
13	0	0	1	1	12	0	0	2	-2	12	2622.03740	-0.00073	2622.03813	1500.46836
14	0	0	1	1	13	0	0	2	-2	13	2621.85895*	0.00110	2621.85785	1525.22483 †
15	0	0	1	1	14	0	0	2	-2	14	2621.66377	0.00003	2621.66374	1551.88404
16	0	0	1	1	15	0	0	2	-2	15	2621.45586	0.00004	2621.45582	1580.44562
17	0	0	1	1	18	0	0	2	-2	18	2620.74852	-0.00069	2620.74921	1677.54066
18	0	0	1	1	19	0	0	2	-2	19	2620.48561	-0.00050	2620.48611	1713.70766
19	0	0	1	1	20	0	0	2	-2	20	2620.20690*	-0.00233	2620.20923	1751.77486 †
20	0	0	1	1	21	0	0	2	-2	21	2619.92061	0.00200	2619.91861	1791.74175 †
21	0	0	1	1	22	0	0	2	-2	22	2619.61368	-0.00055	2619.61423	1833.60781
22	0	0	1	-1	3	0	0	2	2	3	2623.07848*	0.00160	2623.07688	1363.32960 †
23	0	0	1	-1	4	0	0	2	2	4	2623.04992*	0.00224	2623.04768	1370.94974 †
24	0	0	1	-1	5	0	0	2	2	5	2623.01042	-0.00065	2623.01107	1380.47484
25	0	0	1	-1	7	0	0	2	2	7	2622.91340*	-0.00186	2622.91526	1405.23972 †
26	0	0	1	-1	8	0	0	2	2	8	2622.85622	0.00036	2622.85586	1420.47938
27	0	0	1	-1	9	0	0	2	2	9	2622.78918	0.00053	2622.78865	1437.62374
28	0	0	1	-1	10	0	0	2	2	10	2622.71388	0.00041	2622.71347	1456.67272
29	0	0	1	-1	11	0	0	2	2	11	2622.63104	0.00087	2622.63017	1477.62621
30	0	0	1	-1	12	0	0	2	2	12	2622.53853*	-0.00005	2622.53858	1500.48412
31	0	0	1	-1	13	0	0	2	2	13	2622.43818	-0.00033	2622.43851	1525.24633
32	0	0	1	-1	14	0	0	2	2	14	2622.32973*	-0.00004	2622.32977	1551.91270
33	0	0	1	-1	15	0	0	2	2	15	2622.21218	0.00005	2622.21213	1580.48310
34	0	0	1	-1	16	0	0	2	2	16	2622.08563	0.00027	2622.08536	1610.95737
35	0	0	1	-1	17	0	0	2	2	17	2621.94896	-0.00026	2621.94922	1643.33536
36	0	0	1	-1	18	0	0	2	2	18	2621.80384	0.00039	2621.80345	1677.61689
37	0	0	1	-1	19	0	0	2	2	19	2621.64724	-0.00054	2621.64778	1713.80178
38	0	0	1	-1	20	0	0	2	2	20	2621.48226	0.00033	2621.48193	1751.88982

rms = 0.00046 cm⁻¹

$\nu_1 + 2\nu_4 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

45	ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
46	2	0	0	0	0	0	0	0	0	1	4325.45581	-0.00084	4325.45665	1.90066
47	2	0	0	0	1	0	0	0	0	2	4323.55519	-0.00133	4323.55652	5.70195 †
48	2	0	0	0	2	0	0	0	0	3	4321.65603	-0.00081	4321.65684	11.40382
49	2	0	0	0	3	0	0	0	0	4	4319.75806	0.00065	4319.75741	19.00619
50	2	0	0	0	4	0	0	0	0	5	4317.85869	0.00075	4317.85794	28.50898
51	2	0	0	0	5	0	0	0	0	6	4315.95443*	-0.00359	4315.95802	39.91204 †
52	2	0	0	0	6	0	0	0	0	7	4314.05777	0.00063	4314.05714	53.21523
53	2	0	0	0	7	0	0	0	0	8	4312.15503	0.00034	4312.15469	68.41838
54	2	0	0	0	8	0	0	0	0	9	4310.25039	0.00045	4310.24994	85.52129
55	2	0	0	0	9	0	0	0	0	10	4308.34260	0.00048	4308.34212	104.52373
56	2	0	0	0	10	0	0	0	0	11	4306.43109	0.00075	4306.43034	125.42544
57	2	0	0	0	11	0	0	0	0	12	4304.51356	-0.00013	4304.51369	148.22616
58	2	0	0	0	12	0	0	0	0	13	4302.59203	0.00081	4302.59122	172.92558
59	2	0	0	0	13	0	0	0	0	14	4300.66203	0.00005	4300.66198	199.52337
60	2	0	0	0	14	0	0	0	0	15	4298.72497	-0.00007	4298.72504	228.01920
	2	0	0	0	15	0	0	0	0	16	4296.78010	0.00054	4296.77956	258.41268
	2	0	0	0	16	0	0	0	0	17	4294.82505	0.00029	4294.82476	290.70340
	2	0	0	0	17	0	0	0	0	18	4292.86244*	0.00247	4292.85997	324.89096 †
	2	0	0	0	18	0	0	0	0	19	4290.88392	-0.00074	4290.88466	360.97488

1														
2	2	0	0	0	19	0	0	0	0	20	4288.89924	0.00083	4288.89841	398.95471
3	2	0	0	0	20	0	0	0	0	21	4286.90141	0.00046	4286.90095	438.82993
4	2	0	0	0	21	0	0	0	0	22	4284.89187	-0.00022	4284.89209	480.60003
5	2	0	0	0	22	0	0	0	0	23	4282.87137	-0.00040	4282.87177	524.26445
6	2	0	0	0	23	0	0	0	0	24	4280.83927	-0.00071	4280.83998	569.82262
7	2	0	0	0	24	0	0	0	0	25	4278.79721	0.00040	4278.79681	617.27393
8	2	0	0	0	25	0	0	0	0	26	4276.74196	-0.00041	4276.74237	666.61777
9	2	0	0	0	26	0	0	0	0	27	4274.67766	0.00086	4274.67680	717.85348
10	2	0	0	0	1	0	0	0	0	0	4329.25803*	-0.00044	4329.25847	0.00000
11	2	0	0	0	2	0	0	0	0	1	4331.15994*	-0.00006	4331.16000	1.90066
12	2	0	0	0	3	0	0	0	0	2	4333.06141	-0.00025	4333.06166	5.70195
13	2	0	0	0	4	0	0	0	0	3	4334.96297	-0.00013	4334.96310	11.40382
14	2	0	0	0	5	0	0	0	0	4	4336.86301	-0.00086	4336.86387	19.00619
15	2	0	0	0	6	0	0	0	0	5	4338.76375	0.00035	4338.76340	28.50898
16	2	0	0	0	7	0	0	0	0	6	4340.66196	0.00093	4340.66103	39.91204
17	2	0	0	0	8	0	0	0	0	7	4342.55598	-0.00002	4342.55600	53.21523
18	2	0	0	0	9	0	0	0	0	8	4344.44769	0.00023	4344.44746	68.41838
19	2	0	0	0	10	0	0	0	0	9	4346.33387	-0.00062	4346.33449	85.52129
20	2	0	0	0	11	0	0	0	0	10	4348.21586	-0.00026	4348.21612	104.52373
21	2	0	0	0	12	0	0	0	0	11	4350.09158	0.00022	4350.09136	125.42544
22	2	0	0	0	13	0	0	0	0	12	4351.95981	0.00061	4351.95920	148.22616
23	2	0	0	0	14	0	0	0	0	13	4353.81919	0.00052	4353.81867	172.92558
24	2	0	0	0	15	0	0	0	0	14	4355.66810	-0.00076	4355.66886	199.52337
25	2	0	0	0	16	0	0	0	0	15	4357.51036	0.00140	4357.50896	228.01920 +
26	2	0	0	0	17	0	0	0	0	16	4359.33775	-0.00050	4359.33825	258.41268
27	2	0	0	0	18	0	0	0	0	17	4361.15550	-0.00064	4361.15614	290.70340
28	2	0	0	0	19	0	0	0	0	18	4362.96199	-0.00018	4362.96217	324.89096
29	2	0	0	0	20	0	0	0	0	19	4364.75595	-0.00005	4364.75600	360.97488
30	2	0	0	0	21	0	0	0	0	20	4366.53667	-0.00074	4366.53741	398.95471
31	2	0	0	0	22	0	0	0	0	21	4368.30586	-0.00042	4368.30628	438.82993
32	2	0	0	0	23	0	0	0	0	22	4370.06229	-0.00028	4370.06257	480.60003
33	2	0	0	0	24	0	0	0	0	23	4371.80427	-0.00202	4371.80629	524.26445 +
34	2	0	0	0	25	0	0	0	0	24	4373.53894	0.00142	4373.53752	569.82262 +
35	2	0	0	0	26	0	0	0	0	25	4375.25635	0.00001	4375.25634	617.27393

rms = 0.00054 cm⁻¹

$\nu_1 + 2\nu_4 (\Sigma^+) \leftarrow 2\nu_4 (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 0 0 0	2 0 0 0 1	3308.59562	-0.00020	3308.59582	1018.76149
2 0 0 0 1	2 0 0 0 2	3306.67711	0.00023	3306.67688	1022.58159
2 0 0 0 2	2 0 0 0 3	3304.75001	0.00078	3304.74923	1028.31143
2 0 0 0 3	2 0 0 0 4	3302.81276	-0.00020	3302.81296	1035.95064
2 0 0 0 4	2 0 0 0 5	3300.86847	0.00030	3300.86817	1045.49875
2 0 0 0 5	2 0 0 0 6	3298.91534	0.00042	3298.91492	1056.95515
2 0 0 0 6	2 0 0 0 7	3296.95638*	0.00310	3296.95328	1070.31910 †
2 0 0 0 7	2 0 0 0 8	3294.98343	0.00013	3294.98330	1085.58977
2 0 0 0 8	2 0 0 0 9	3293.00460	-0.00042	3293.00502	1102.76621
2 0 0 0 9	2 0 0 0 10	3291.01529*	-0.00317	3291.01846	1121.84738 †
2 0 0 0 10	2 0 0 0 11	3289.02319	-0.00043	3289.02362	1142.83216
2 0 0 0 11	2 0 0 0 12	3287.02031	-0.00018	3287.02049	1165.71936
2 0 0 0 12	2 0 0 0 13	3285.00824	-0.00082	3285.00906	1190.50774
2 0 0 0 13	2 0 0 0 14	3282.98888	-0.00041	3282.98929	1217.19606
2 0 0 0 14	2 0 0 0 15	3280.96079	-0.00037	3280.96116	1245.78308
2 0 0 0 15	2 0 0 0 16	3278.92414	-0.00049	3278.92463	1276.26760
2 0 0 0 16	2 0 0 0 17	3276.87908	-0.00060	3276.87968	1308.64848
2 0 0 0 17	2 0 0 0 18	3274.82570	-0.00057	3274.82627	1342.92466
2 0 0 0 18	2 0 0 0 19	3272.76450	0.00010	3272.76440	1379.09514
2 0 0 0 19	2 0 0 0 20	3270.69368	-0.00039	3270.69407	1417.15906
2 0 0 0 20	2 0 0 0 21	3268.61642	0.00114	3268.61528	1457.11560 †
2 0 0 0 21	2 0 0 0 22	3266.52806	0.00001	3266.52805	1498.96407
2 0 0 0 22	2 0 0 0 23	3264.43289	0.00048	3264.43241	1542.70381

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1														
2	2	0	0	0	23	2	0	0	0	24	3262.32942	0.00106	3262.32836	1588.33424 †
3	2	0	0	0	24	2	0	0	0	25	3260.21638	0.00044	3260.21594	1635.85480
4	2	0	0	0	25	2	0	0	0	26	3258.09576	0.00060	3258.09516	1685.26498
5	2	0	0	0	26	2	0	0	0	27	3255.96710	0.00108	3255.96602	1736.56425 †
6	2	0	0	0	27	2	0	0	0	28	3253.82879	0.00025	3253.82854	1789.75210
7	2	0	0	0	28	2	0	0	0	29	3251.68310	0.00039	3251.68271	1844.82800
8	2	0	0	0	29	2	0	0	0	30	3249.52876	0.00022	3249.52854	1901.79140
9	2	0	0	0	30	2	0	0	0	31	3247.36518	-0.00081	3247.36599	1960.64171
10	2	0	0	0	31	2	0	0	0	32	3245.19185	-0.00321	3245.19506	2021.37834 †
11	2	0	0	0	32	2	0	0	0	33	3243.00885	-0.00686	3243.01571	2084.00064 †
12	2	0	0	0	33	2	0	0	0	34	3240.81358	-0.01433	3240.82791	2148.50794 †
13	2	0	0	0	34	2	0	0	0	35	3238.60591	-0.02572	3238.63163	2214.89954 †
14	2	0	0	0	1	2	0	0	0	0	3312.41024*	0.00316	3312.40708	1016.85139 †
15	2	0	0	0	2	2	0	0	0	1	3314.29883	-0.00033	3314.29916	1018.76149
16	2	0	0	0	3	2	0	0	0	2	3316.18197	-0.00005	3316.18202	1022.58159
17	2	0	0	0	4	2	0	0	0	3	3318.05584	0.00035	3318.05549	1028.31143
18	2	0	0	0	5	2	0	0	0	4	3319.92000	0.00058	3319.91942	1035.95064
19	2	0	0	0	6	2	0	0	0	5	3321.77341	-0.00021	3321.77362	1045.49875
20	2	0	0	0	7	2	0	0	0	6	3323.61857*	0.00065	3323.61792	1056.95515
21	2	0	0	0	8	2	0	0	0	7	3325.45219	0.00005	3325.45214	1070.31910
22	2	0	0	0	9	2	0	0	0	8	3327.27592	-0.00015	3327.27607	1085.58977
23	2	0	0	0	10	2	0	0	0	9	3329.08980	0.00023	3329.08957	1102.76621
24	2	0	0	0	11	2	0	0	0	10	3330.89320	0.00074	3330.89246	1121.84738
25	2	0	0	0	12	2	0	0	0	11	3332.68498	0.00035	3332.68463	1142.83216
26	2	0	0	0	13	2	0	0	0	12	3334.46559	-0.00041	3334.46600	1165.71936
27	2	0	0	0	14	2	0	0	0	13	3336.23606	-0.00045	3336.23651	1190.50774
28	2	0	0	0	15	2	0	0	0	14	3337.99551	-0.00067	3337.99618	1217.19606
29	2	0	0	0	16	2	0	0	0	15	3339.74502	-0.00006	3339.74508	1245.78308
30	2	0	0	0	17	2	0	0	0	16	3341.48277	-0.00055	3341.48332	1276.26760
31	2	0	0	0	18	2	0	0	0	17	3343.21061	-0.00045	3343.21106	1308.64848
32	2	0	0	0	19	2	0	0	0	18	3344.92957	0.00110	3344.92847	1342.92466 †
33	2	0	0	0	20	2	0	0	0	19	3346.63541	-0.00033	3346.63574	1379.09514
34	2	0	0	0	21	2	0	0	0	20	3348.33292	-0.00015	3348.33307	1417.15906
35	2	0	0	0	22	2	0	0	0	21	3350.02051	-0.00011	3350.02062	1457.11560
36	2	0	0	0	23	2	0	0	0	22	3351.69879	0.00026	3351.69853	1498.96407
37	2	0	0	0	24	2	0	0	0	23	3353.36812	0.00118	3353.36694	1542.70381 †
38	2	0	0	0	25	2	0	0	0	24	3355.02649	0.00059	3355.02590	1588.33424
39	2	0	0	0	26	2	0	0	0	25	3356.67627	0.00080	3356.67547	1635.85480
40	2	0	0	0	27	2	0	0	0	26	3358.31625	0.00059	3358.31566	1685.26498
41	2	0	0	0	28	2	0	0	0	27	3359.94695	0.00049	3359.94646	1736.56425
42	2	0	0	0	29	2	0	0	0	28	3361.56796	0.00013	3361.56783	1789.75210
43	2	0	0	0	30	2	0	0	0	29	3363.17880	-0.00090	3363.17970	1844.82800
44	2	0	0	0	31	2	0	0	0	30	3364.77922	-0.00278	3364.78200	1901.79140 †
45	2	0	0	0	32	2	0	0	0	31	3366.36811	-0.00653	3366.37464	1960.64171 †
46	2	0	0	0	33	2	0	0	0	32	3367.94346	-0.01406	3367.95752	2021.37834 †
47	2	0	0	0	34	2	0	0	0	33	3369.50314	-0.02738	3369.53052	2084.00064 †
48	2	0	0	0	35	2	0	0	0	34	3371.06757	-0.02596	3371.09353	2148.50794 †

rms = 0.00045 cm⁻¹

$v_1 + 2v_4 (\Delta) \leftarrow 2v_4 (\Delta)$

54	$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
55	2 2 0 0 2	2 2 0 0 3	3304.24869	-0.00467	3304.25336	1032.70973 †
56	2 2 0 0 3	2 2 0 0 4	3302.32023	0.00332	3302.31691	1040.34843 †
57	2 2 0 0 4	2 2 0 0 5	3300.37500	0.00360	3300.37140	1049.89732 †
58	2 2 0 0 5	2 2 0 0 6	3298.42492	0.00813	3298.41679	1061.35675 †
59	2 2 0 0 6	2 2 0 0 7	3296.45523	0.00217	3296.45306	1074.72712 †
60	2 2 0 0 7	2 2 0 0 8	3294.48430	0.00408	3294.48022	1090.00889 †
	2 2 0 0 8	2 2 0 0 9	3292.50093	0.00266	3292.49827	1107.20259 †
	2 2 0 0 9	2 2 0 0 10	3290.50483*	-0.00241	3290.50724	1126.30879 †
	2 2 0 0 10	2 2 0 0 11	3288.50832	0.00117	3288.50715	1147.32807 †
	2 2 0 0 11	2 2 0 0 12	3286.49876	0.00069	3286.49807	1170.26105

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1											
2	2	-2	0	0	16	2	-2	0	0	17	3276.36270
3	2	-2	0	0	17	2	-2	0	0	18	-0.00039
4	2	-2	0	0	18	2	-2	0	0	19	3276.36309
5	2	-2	0	0	19	2	-2	0	0	20	0.00010
6	2	-2	0	0	20	2	-2	0	0	21	3274.30680
7	2	-2	0	0	21	2	-2	0	0	22	-0.00073
8	2	-2	0	0	22	2	-2	0	0	23	3272.24136
9	2	-2	0	0	23	2	-2	0	0	24	-0.00036
10	2	-2	0	0	24	2	-2	0	0	25	3270.16936
11	2	-2	0	0	25	2	-2	0	0	26	0.00036
12	2	-2	0	0	26	2	-2	0	0	27	3270.16900
13	2	-2	0	0	27	2	-2	0	0	28	-0.00038
14	2	-2	0	0	28	2	-2	0	0	29	3268.08716
15	2	-2	0	0	29	2	-2	0	0	30	-0.00053
16	2	-2	0	0	30	2	-2	0	0	31	3265.99722
17	2	-2	0	0	31	2	-2	0	0	32	-0.00021
18	2	-2	0	0	32	2	-2	0	0	33	3263.89945
19	2	-2	0	0	33	2	-2	0	0	34	-0.00021
20	2	-2	0	0	34	2	-2	0	0	35	3261.79364
21	2	-2	0	0	35	2	-2	0	0	36	0.00034
22	2	-2	0	0	36	2	-2	0	0	37	3261.79330
23	2	-2	0	0	3	2	-2	0	0	38	-0.00094
24	2	-2	0	0	4	2	-2	0	0	39	3259.67777
25	2	-2	0	0	5	2	-2	0	0	40	-0.00010
26	2	-2	0	0	6	2	-2	0	0	41	3257.55583
27	2	-2	0	0	7	2	-2	0	0	42	0.00001
28	2	-2	0	0	8	2	-2	0	0	43	3255.42499
29	2	-2	0	0	9	2	-2	0	0	44	-0.00001
30	2	-2	0	0	10	2	-2	0	0	45	3253.28591*
31	2	-2	0	0	11	2	-2	0	0	46	0.00023
32	2	-2	0	0	12	2	-2	0	0	47	3251.13903
33	2	-2	0	0	13	2	-2	0	0	48	0.00060
34	2	-2	0	0	14	2	-2	0	0	49	3248.98424
35	2	-2	0	0	15	2	-2	0	0	50	0.00085
36	2	-2	0	0	16	2	-2	0	0	51	3246.82137
37	2	-2	0	0	17	2	-2	0	0	52	0.00079
38	2	-2	0	0	18	2	-2	0	0	53	3244.65027
39	2	-2	0	0	19	2	-2	0	0	54	0.00079
40	2	-2	0	0	20	2	-2	0	0	55	-0.00028
41	2	-2	0	0	21	2	-2	0	0	56	3242.47031
42	2	-2	0	0	22	2	-2	0	0	57	0.00012
43	2	-2	0	0	23	2	-2	0	0	58	3240.28401
44	2	-2	0	0	24	2	-2	0	0	59	-0.000509
45	2	-2	0	0	25	2	-2	0	0	60	3238.08439*
46	2	-2	0	0	26	2	-2	0	0	61	0.00000
47	2	-2	0	0	27	2	-2	0	0	62	3235.88741
48	2	-2	0	0	28	2	-2	0	0	63	-0.00043
49	2	-2	0	0	29	2	-2	0	0	64	3233.67733
50	2	-2	0	0	30	2	-2	0	0	65	-0.00043
51	2	-2	0	0	31	2	-2	0	0	66	3233.67733
52	2	-2	0	0	32	2	-2	0	0	67	0.00422
53	2	-2	0	0	33	2	-2	0	0	68	3231.68819
54	2	-2	0	0	34	2	-2	0	0	69	0.00422
55	2	-2	0	0	35	2	-2	0	0	70	3231.68819
56	2	-2	0	0	36	2	-2	0	0	71	-0.00236
57	2	-2	0	0	37	2	-2	0	0	72	3231.68819
58	2	-2	0	0	38	2	-2	0	0	73	-0.00256
59	2	-2	0	0	39	2	-2	0	0	74	3231.68819
60	2	-2	0	0	40	2	-2	0	0	75	0.00374
	2	-2	0	0	41	2	-2	0	0	76	3231.68819
	2	-2	0	0	42	2	-2	0	0	77	0.00377
	2	-2	0	0	43	2	-2	0	0	78	3231.68819
	2	-2	0	0	44	2	-2	0	0	79	0.00341
	2	-2	0	0	45	2	-2	0	0	80	3231.68819
	2	-2	0	0	46	2	-2	0	0	81	0.00177
	2	-2	0	0	47	2	-2	0	0	82	3231.68819
	2	-2	0	0	48	2	-2	0	0	83	0.00133
	2	-2	0	0	49	2	-2	0	0	84	3231.68819
	2	-2	0	0	50	2	-2	0	0	85	0.00043
	2	-2	0	0	51	2	-2	0	0	86	3231.68819
	2	-2	0	0	52	2	-2	0	0	87	-0.00508
	2	-2	0	0	53	2	-2	0	0	88	3231.68819
	2	-2	0	0	54	2	-2	0	0	89	0.00002
	2	-2	0	0	55	2	-2	0	0	90	3231.68819
	2	-2	0	0	56	2	-2	0	0	91	0.00044
	2	-2	0	0	57	2	-2	0	0	92	3231.68819
	2	-2	0	0	58	2	-2	0	0	93	0.00002
	2	-2	0	0	59	2	-2	0	0	94	3231.68819
	2	-2	0	0	60	2	-2	0	0	95	-0.00045
	2	-2	0	0	61	2	-2	0	0	96	3231.68819
	2	-2	0	0	62	2	-2	0	0	97	-0.00047
	2	-2	0	0	63	2	-2	0	0	98	3231.68819
	2	-2	0	0	64	2	-2	0	0	99	-0.00028
	2	-2	0	0	65	2	-2	0	0	100	3231.68819
	2	-2	0	0	66	2	-2	0	0	101	-0.00041
	2	-2	0	0	67	2	-2	0	0	102	3231.68819
	2	-2	0	0	68	2	-2	0	0	103	-0.00038
	2	-2	0	0	69	2	-2	0	0	104	3231.68819
	2	-2	0	0	70	2	-2	0	0	105	-0.00080
	2	-2	0	0	71	2	-2	0	0	106	3231.68819
	2	-2	0	0	72	2	-2	0	0	107	-0.00039
	2	-2	0	0	73	2	-2	0	0	108	3231.68819
	2	-2	0	0	74	2	-2	0	0	109	-0.00052
	2	-2	0	0	75	2	-2	0	0	110	3231.68819
	2	-2	0	0	76	2	-2	0	0	111	-0.00043
	2	-2	0	0	77	2	-2	0	0	112	3231.68819
	2	-2	0	0	78	2	-2	0	0	113	0.000390
	2	-2	0	0	79	2	-2	0	0	114	3231.68819
	2	-2	0	0	80	2	-2	0	0	115	-0.00007
	2	-2	0	0	81	2	-2	0	0	116	3231.68819
	2	-2	0	0	82	2	-2	0	0	117	0.00002
	2	-2	0	0	83	2	-2	0	0	118	3231.68819
	2	-2	0	0	84	2	-2	0	0	119	0.00004
	2	-2	0	0	85	2	-2	0	0	120	3231.68819
	2	-2	0	0	86	2	-2	0	0	121	0.00061
	2	-2	0	0	87	2	-2	0	0	122	3231.68819
	2	-2	0	0	88	2	-2	0	0	123	0.00043
	2	-2	0	0	89	2	-2	0	0	124	3231.68819
	2	-2	0	0	90	2	-2	0	0	125	-0.00003
	2	-2	0	0	91	2	-2	0	0	126	3231.68819
	2	-2	0	0	92	2	-2	0	0	127	0.00042
	2	-2	0	0	93	2	-2	0	0	128	3231.68819
	2	-2	0	0	94	2	-2	0	0	129	0.00016
	2	-2	0	0	95	2	-2	0	0	130	3231.68819
	2	-2	0	0	96	2	-2	0	0	131	-0.00059
	2	-2	0	0	97	2	-2	0	0	132	3231.68819
	2	-2	0	0	98	2	-2	0	0	133	-0.00029
	2	-2	0	0	99	2	-2	0	0	134	3231.68819
	2	-2	0	0	100	2	-2	0	0	135	0.00221
	2	-2	0	0	101	2	-2	0	0	136	3231.68819
	2	-2	0	0	102	2	-2	0	0	137	-0.00244
	2	-2	0	0	103	2	-2	0	0	138	3231.68819
	2	-2	0	0	104	2	-2	0	0	139	0.00399
	2	-2	0	0	105	2	-2	0	0	140	3231.68819
	2	-2	0	0	106	2	-2	0	0	141	0.00716
	2	-2	0	0	107	2	-2	0	0	142	3231.68819
	2	-2	0	0	108	2	-2	0	0	143	0.00229
	2	-2	0	0	109	2	-2	0	0	144	3231.68819
	2	-2	0	0	110	2	-2	0	0	145	0.00168
	2	-2	0	0	111	2	-2	0	0	146	3231.68819
	2	-2	0	0	112	2	-2	0	0	147	0.00204
	2	-2	0	0	113	2	-2	0	0	148	3231.68819
	2	-2	0	0	114	2	-2	0	0	149	-0.00127
	2	-2	0	0	115	2	-2	0	0	150	3231.68819
	2	-2	0	0	116	2	-2	0	0	151	-0.00393
	2	-2	0	0	117	2	-2	0	0	152	3231.68819
	2	-2	0	0	118	2	-2	0	0	153	0.00094
	2	-2	0	0	119	2	-2	0	0	154	3231.68819
	2	-2	0	0	120	2	-2	0	0	155	0.00181

1														
2	2	2	0	0	2	2	-2	0	0	2	3309.98425	0.00201	3309.98224	1026.98084 +
3	2	2	0	0	3	2	-2	0	0	3	3309.95264	-0.00345	3309.95609	1032.70925 +
4	2	2	0	0	4	2	-2	0	0	4	3309.92270	0.00098	3309.92172	1040.34700
5	2	2	0	0	5	2	-2	0	0	5	3309.87968	0.00014	3309.87954	1049.89400
6	2	2	0	0	6	2	-2	0	0	6	3309.83263*	0.00255	3309.83008	1061.35010 +
7	2	2	0	0	7	2	-2	0	0	7	3309.77617*	0.00220	3309.77397	1074.71514 +
8	2	2	0	0	8	2	-2	0	0	8	3309.71060*	-0.00131	3309.71191	1089.98896 +
9	2	2	0	0	9	2	-2	0	0	9	3309.64659*	0.00188	3309.64471	1107.17132 +
10	2	2	0	0	10	2	-2	0	0	10	3309.57748*	0.00425	3309.57323	1126.26199 +
11	2	2	0	0	11	2	-2	0	0	11	3309.49038*	-0.00802	3309.49840	1147.26072 +
12	2	2	0	0	12	2	-2	0	0	12	3309.42181	0.00065	3309.42116	1170.16720
13	2	2	0	0	13	2	-2	0	0	13	3309.33274*	-0.00971	3309.34245	1194.98112 +

rms = 0.00047 cm⁻¹

$v_1 + 2v_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 0	0 0 0 0 1	4617.75749*	0.00034	4617.75715	1.90066
0 0 2 0 1	0 0 0 0 2	4615.85201*	-0.00149	4615.85350	5.70195 †
0 0 2 0 2	0 0 0 0 3	4613.94717	0.00030	4613.94687	11.40382
0 0 2 0 3	0 0 0 0 4	4612.03743	0.00019	4612.03724	19.00619
0 0 2 0 4	0 0 0 0 5	4610.12340*	-0.00118	4610.12458	28.50898 †
0 0 2 0 5	0 0 0 0 6	4608.20848	-0.00038	4608.20886	39.91204
0 0 2 0 6	0 0 0 0 7	4606.29050	0.00050	4606.29000	53.21523
0 0 2 0 7	0 0 0 0 8	4604.36829	0.00037	4604.36792	68.41838
0 0 2 0 8	0 0 0 0 9	4602.44240	-0.00013	4602.44253	85.52129
0 0 2 0 9	0 0 0 0 10	4600.51390*	0.00020	4600.51370	104.52373
0 0 2 0 10	0 0 0 0 11	4598.58109	-0.00021	4598.58130	125.42544
0 0 2 0 11	0 0 0 0 12	4596.64603	0.00086	4596.64517	148.22616
0 0 2 0 12	0 0 0 0 13	4594.70587*	0.00072	4594.70515	172.92558
0 0 2 0 13	0 0 0 0 14	4592.76065	-0.00039	4592.76104	199.52337
0 0 2 0 14	0 0 0 0 15	4590.81207	-0.00057	4590.81264	228.01920
0 0 2 0 15	0 0 0 0 16	4588.86066	0.00093	4588.85973	258.41268
0 0 2 0 16	0 0 0 0 17	4586.90138	-0.00069	4586.90207	290.70340
0 0 2 0 17	0 0 0 0 18	4584.93959	0.00019	4584.93940	324.89096
0 0 2 0 18	0 0 0 0 19	4582.97191	0.00046	4582.97145	360.97488
0 0 2 0 19	0 0 0 0 20	4580.99862	0.00067	4580.99795	398.95471
0 0 2 0 20	0 0 0 0 21	4579.02004	0.00145	4579.01859	438.82993 †
0 0 2 0 21	0 0 0 0 22	4577.03399	0.00093	4577.03306	480.60003
0 0 2 0 22	0 0 0 0 23	4575.04000	-0.00105	4575.04106	524.26445 †
0 0 2 0 23	0 0 0 0 24	4573.04146	-0.00078	4573.04224	569.82262
0 0 2 0 24	0 0 0 0 25	4571.03638	0.00009	4571.03629	617.27393
0 0 2 0 2	0 0 0 0 1	4623.45108	0.00106	4623.45002	1.90066 †
0 0 2 0 3	0 0 0 0 2	4625.34047	-0.00101	4625.34148	5.70195 †
0 0 2 0 4	0 0 0 0 3	4627.22877	-0.00097	4627.22974	11.40382
0 0 2 0 5	0 0 0 0 4	4629.11431	-0.00039	4629.11470	19.00619
0 0 2 0 6	0 0 0 0 5	4630.99560	-0.00066	4630.99626	28.50898
0 0 2 0 7	0 0 0 0 6	4632.87375	-0.00051	4632.87426	39.91204
0 0 2 0 8	0 0 0 0 7	4634.74951	0.00093	4634.74858	53.21523
0 0 2 0 9	0 0 0 0 8	4636.61996	0.00092	4636.61904	68.41838
0 0 2 0 10	0 0 0 0 9	4638.48578	0.00034	4638.48544	85.52129
0 0 2 0 11	0 0 0 0 10	4640.34679	-0.00081	4640.34760	104.52373
0 0 2 0 12	0 0 0 0 11	4642.20549	0.00020	4642.20529	125.42544
0 0 2 0 13	0 0 0 0 12	4644.05887	0.00061	4644.05826	148.22616
0 0 2 0 14	0 0 0 0 13	4645.90669	0.00042	4645.90627	172.92558
0 0 2 0 15	0 0 0 0 14	4647.74962	0.00059	4647.74903	199.52337
0 0 2 0 16	0 0 0 0 15	4649.58691*	0.00064	4649.58627	228.01920
0 0 2 0 17	0 0 0 0 16	4651.41815	0.00047	4651.41768	258.41268
0 0 2 0 18	0 0 0 0 17	4653.24190	-0.00103	4653.24293	290.70340 †
0 0 2 0 19	0 0 0 0 18	4655.06128	-0.00042	4655.06170	324.89096
0 0 2 0 20	0 0 0 0 19	4656.87300	-0.00064	4656.87364	360.97488
0 0 2 0 21	0 0 0 0 20	4658.67781	-0.00057	4658.67838	398.95471

1														
2	0	0	2	0	22	0	0	0	0	21	4660.47618	0.00061	4660.47557	438.82993
3	0	0	2	0	23	0	0	0	0	22	4662.26515	0.00032	4662.26483	480.60003
4	0	0	2	0	24	0	0	0	0	23	4664.04666	0.00089	4664.04577	524.26445
5	0	0	2	0	25	0	0	0	0	24	4665.81818	0.00017	4665.81801	569.82262
6	0	0	2	0	26	0	0	0	0	25	4667.58202	0.00087	4667.58115	617.27393
7	0	0	2	0	27	0	0	0	0	26	4669.33362*	-0.00119	4669.33481	666.61777 +

rms = 0.00060 cm⁻¹

$v_1 + 2v_5 (\Sigma^+) \leftarrow v_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 2 0 0	0 0 1 1 1	3943.52163	-0.00005	3943.52168	676.13613
0 0 2 0 1	0 0 1 1 2	3941.62025*	0.00048	3941.61977	679.93567
0 0 2 0 2	0 0 1 1 3	3939.71555	-0.00020	3939.71575	685.63493
0 0 2 0 3	0 0 1 1 4	3937.80960	-0.00001	3937.80961	693.23382
0 0 2 0 4	0 0 1 1 5	3935.89717*	-0.00415	3935.90132	702.73224 †
0 0 2 0 5	0 0 1 1 6	3933.99064	-0.00018	3933.99082	714.13007
0 0 2 0 6	0 0 1 1 7	3932.07874	0.00067	3932.07807	727.42716
0 0 2 0 7	0 0 1 1 8	3930.16290	-0.00007	3930.16297	742.62333
0 0 2 0 8	0 0 1 1 9	3928.24541	-0.00002	3928.24543	759.71839
0 0 2 0 9	0 0 1 1 10	3926.32496	-0.00037	3926.32533	778.71209
0 0 2 0 10	0 0 1 1 11	3924.40235	-0.00018	3924.40253	799.60420
0 0 2 0 11	0 0 1 1 12	3922.47836*	0.00148	3922.47688	822.39444 †
0 0 2 0 12	0 0 1 1 13	3920.54833	0.00012	3920.54821	847.08251
0 0 2 0 13	0 0 1 1 14	3918.61621	-0.00013	3918.61634	873.66808
0 0 2 0 14	0 0 1 1 15	3916.68101	-0.00004	3916.68105	902.15079
0 0 2 0 15	0 0 1 1 16	3914.74336	0.00123	3914.74213	932.53028 †
0 0 2 0 16	0 0 1 1 17	3912.79978	0.00045	3912.79933	964.80614
0 0 2 0 17	0 0 1 1 18	3910.85211	-0.00030	3910.85241	998.97795
0 0 2 0 18	0 0 1 1 19	3908.90105	-0.00004	3908.90109	1035.04524
0 0 2 0 19	0 0 1 1 20	3906.94542	0.00032	3906.94510	1073.00756
0 0 2 0 20	0 0 1 1 21	3904.98440	0.00026	3904.98414	1112.86438
0 0 2 0 21	0 0 1 1 22	3903.01812	0.00023	3903.01789	1154.61520
0 0 2 0 22	0 0 1 1 23	3901.04688	0.00083	3901.04605	1198.25945
0 0 2 0 23	0 0 1 1 24	3899.06840	0.00010	3899.06830	1243.79656
0 0 2 0 24	0 0 1 1 25	3897.08466	0.00037	3897.08429	1291.22593
0 0 2 0 25	0 0 1 1 26	3895.09337	-0.00032	3895.09369	1340.54693
0 0 2 0 26	0 0 1 1 27	3893.09613	-0.00004	3893.09617	1391.75891
0 0 2 0 27	0 0 1 1 28	3891.09118	-0.00021	3891.09139	1444.86119
0 0 2 0 28	0 0 1 1 29	3889.07883	-0.00017	3889.07900	1499.85307
0 0 2 0 29	0 0 1 1 30	3887.05858	-0.00010	3887.05868	1556.73383
0 0 2 0 30	0 0 1 1 31	3885.02438*	-0.00572	3885.03010	1615.50271 †
0 0 2 0 31	0 0 1 1 32	3882.99290	-0.00005	3882.99295	1676.15894
0 0 2 0 32	0 0 1 1 33	3880.94562	-0.00130	3880.94692	1738.70171 †
0 0 2 0 2	0 0 1 1 1	3949.21451*	-0.00004	3949.21455	676.13613
0 0 2 0 3	0 0 1 1 2	3951.10721	-0.00054	3951.10775	679.93567
0 0 2 0 4	0 0 1 1 3	3952.99832	-0.00031	3952.99863	685.63493
0 0 2 0 5	0 0 1 1 4	3954.88682	-0.00026	3954.88708	693.23382
0 0 2 0 6	0 0 1 1 5	3956.77251	-0.00048	3956.77299	702.73224
0 0 2 0 7	0 0 1 1 6	3958.65626	0.00003	3958.65623	714.13007
0 0 2 0 8	0 0 1 1 7	3960.54031*	0.00366	3960.53665	727.42716 †
0 0 2 0 9	0 0 1 1 8	3962.41403	-0.00006	3962.41409	742.62333
0 0 2 0 10	0 0 1 1 9	3964.28793	-0.00042	3964.28835	759.71839
0 0 2 0 11	0 0 1 1 10	3966.15952	0.00029	3966.15923	778.71209
0 0 2 0 12	0 0 1 1 11	3968.02662	0.00010	3968.02652	799.60420
0 0 2 0 13	0 0 1 1 12	3969.89042	0.00045	3969.88997	822.39444
0 0 2 0 14	0 0 1 1 13	3971.74863	-0.00070	3971.74933	847.08251
0 0 2 0 15	0 0 1 1 14	3973.60566*	0.00133	3973.60433	873.66808 †
0 0 2 0 16	0 0 1 1 15	3975.45493	0.00025	3975.45468	902.15079
0 0 2 0 17	0 0 1 1 16	3977.29996	-0.00011	3977.30007	932.53028
0 0 2 0 18	0 0 1 1 17	3979.14055	0.00036	3979.14019	964.80614
0 0 2 0 19	0 0 1 1 18	3980.97492	0.00021	3980.97471	998.97795

1														
2	0	0	2	0	20	0	0	1	1	19	3982.80347	0.00019	3982.80328	1035.04524
3	0	0	2	0	21	0	0	1	1	20	3984.62549	-0.00005	3984.62554	1073.00756
4	0	0	2	0	22	0	0	1	1	21	3986.44075	-0.00037	3986.44112	1112.86438
5	0	0	2	0	23	0	0	1	1	22	3988.24942	-0.00024	3988.24966	1154.61520
6	0	0	2	0	24	0	0	1	1	23	3990.05072	-0.00005	3990.05077	1198.25945
7	0	0	2	0	25	0	0	1	1	24	3991.84408	0.00002	3991.84406	1243.79656
8	0	0	2	0	26	0	0	1	1	25	3993.61870*	-0.01045	3993.62915	1291.22593 †
9	0	0	2	0	27	0	0	1	1	26	3995.40536	-0.00029	3995.40565	1340.54693
10	0	0	2	0	28	0	0	1	1	27	3997.17341	0.00025	3997.17316	1391.75891
11	0	0	2	0	29	0	0	1	1	28	3998.93107	-0.00025	3998.93132	1444.86119
12	0	0	2	0	30	0	0	1	1	29	4000.67957	-0.00017	4000.67974	1499.85307
13	0	0	2	0	1	0	0	1	-1	1	3945.41306	0.00026	3945.41280	676.14265
14	0	0	2	0	2	0	0	1	-1	2	3945.39538	-0.00006	3945.39544	679.95524
15	0	0	2	0	3	0	0	1	-1	3	3945.36819*	-0.00119	3945.36938	685.67405 †
16	0	0	2	0	4	0	0	1	-1	4	3945.33422	-0.00032	3945.33454	693.29902
17	0	0	2	0	5	0	0	1	-1	5	3945.29092	0.00006	3945.29086	702.83004
18	0	0	2	0	6	0	0	1	-1	6	3945.23836	0.00011	3945.23825	714.26698
19	0	0	2	0	7	0	0	1	-1	7	3945.17673	0.00012	3945.17661	727.60969
20	0	0	2	0	8	0	0	1	-1	8	3945.10565	-0.00017	3945.10582	742.85799
21	0	0	2	0	9	0	0	1	-1	9	3945.02576	0.00002	3945.02574	760.01168
22	0	0	2	0	10	0	0	1	-1	10	3944.93615	-0.00007	3944.93622	779.07052
23	0	0	2	0	11	0	0	1	-1	11	3944.83689	-0.00018	3944.83707	800.03426
24	0	0	2	0	12	0	0	1	-1	12	3944.72814	0.00003	3944.72811	822.90261
25	0	0	2	0	13	0	0	1	-1	13	3944.60917	0.00004	3944.60913	847.67528
26	0	0	2	0	14	0	0	1	-1	14	3944.48013	0.00022	3944.47991	874.35193
27	0	0	2	0	15	0	0	1	-1	15	3944.34009	-0.00012	3944.34021	902.93220
28	0	0	2	0	16	0	0	1	-1	16	3944.19002	0.00025	3944.18977	933.41570
29	0	0	2	0	17	0	0	1	-1	17	3944.02830	-0.00002	3944.02832	965.80204
30	0	0	2	0	18	0	0	1	-1	18	3943.85505	-0.00052	3943.85557	1000.09076
31	0	0	2	0	19	0	0	1	-1	19	3943.67144	0.00021	3943.67123	1036.28142
32	0	0	2	0	20	0	0	1	-1	20	3943.47331*	-0.00168	3943.47499	1074.37353 †
33	0	0	2	0	21	0	0	1	-1	21	3943.26684	0.00033	3943.26651	1114.36658
34	0	0	2	0	22	0	0	1	-1	22	3943.04544	-0.00004	3943.04548	1156.26002
35	0	0	2	0	23	0	0	1	-1	23	3942.81259	0.00104	3942.81155	1200.05331 †
36	0	0	2	0	24	0	0	1	-1	24	3942.56461	0.00023	3942.56438	1245.74584
37	0	0	2	0	25	0	0	1	-1	25	3942.30328	-0.00033	3942.30361	1293.33701
38	0	0	2	0	26	0	0	1	-1	26	3942.02953	0.00063	3942.02890	1342.82618
39	0	0	2	0	27	0	0	1	-1	27	3941.73841	-0.00148	3941.73989	1394.21269 †
40	0	0	2	0	28	0	0	1	-1	28	3941.43745*	0.00122	3941.43623	1447.49584 †
41	0	0	2	0	29	0	0	1	-1	29	3941.11801	0.00042	3941.11759	1502.67492
42	0	0	2	0	30	0	0	1	-1	30	3940.78278	-0.00083	3940.78361	1559.74920
43	0	0	2	0	31	0	0	1	-1	31	3940.43384	-0.00015	3940.43399	1618.71789

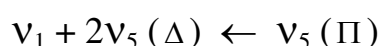
rms = 0.00030 cm⁻¹

$\nu_1 + 2\nu_5 (\Sigma^+) \leftarrow 2\nu_5 (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 0	0 0 2 0 1	3282.44456*	0.00123	3282.44333	1337.21447 †
0 0 2 0 1	0 0 2 0 2	3280.52968	0.00061	3280.52907	1341.02637
0 0 2 0 2	0 0 2 0 3	3278.60623	-0.00033	3278.60656	1346.74412
0 0 2 0 3	0 0 2 0 4	3276.67624	0.00041	3276.67583	1354.36759
0 0 2 0 4	0 0 2 0 5	3274.73640	-0.00054	3274.73694	1363.89662
0 0 2 0 5	0 0 2 0 6	3272.78913	-0.00077	3272.78990	1375.33100
0 0 2 0 6	0 0 2 0 7	3270.83478	0.00002	3270.83476	1388.67047
0 0 2 0 7	0 0 2 0 8	3268.87120	-0.00035	3268.87155	1403.91476
0 0 2 0 8	0 0 2 0 9	3266.90004	-0.00026	3266.90030	1421.06352
0 0 2 0 9	0 0 2 0 10	3264.92264*	0.00160	3264.92104	1440.11639 †
0 0 2 0 10	0 0 2 0 11	3262.93368	-0.00011	3262.93379	1461.07294
0 0 2 0 11	0 0 2 0 12	3260.93849	-0.00011	3260.93860	1483.93273
0 0 2 0 12	0 0 2 0 13	3258.93432*	-0.00116	3258.93548	1508.69525 †
0 0 2 0 13	0 0 2 0 14	3256.92563*	0.00118	3256.92445	1535.35996 †
0 0 2 0 14	0 0 2 0 15	3254.90542	-0.00013	3254.90555	1563.92630

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

1														
2	0	0	2	0	15	0	0	2	0	16	3252.87799*	-0.00079	3252.87878	1594.39363
3	0	0	2	0	16	0	0	2	0	17	3250.84426	0.00008	3250.84418	1626.76130
4	0	0	2	0	17	0	0	2	0	18	3248.80166*	-0.00009	3248.80175	1661.02860
5	0	0	2	0	18	0	0	2	0	19	3246.75130	-0.00022	3246.75152	1697.19482
6	0	0	2	0	19	0	0	2	0	20	3244.69368	0.00018	3244.69350	1735.25916
7	0	0	2	0	20	0	0	2	0	21	3242.62752	-0.00019	3242.62771	1775.22081
8	0	0	2	0	21	0	0	2	0	22	3240.55453	0.00038	3240.55415	1817.07894
9	0	0	2	0	22	0	0	2	0	23	3238.47376*	0.00091	3238.47285	1860.83266
10	0	0	2	0	23	0	0	2	0	24	3236.38341*	-0.00039	3236.38380	1906.48106
11	0	0	2	0	24	0	0	2	0	25	3234.28576	-0.00128	3234.28704	1954.02319 +
12	0	0	2	0	1	0	0	2	0	0	3286.24881	0.00187	3286.24694	1335.30850 +
13	0	0	2	0	2	0	0	2	0	1	3288.13777	0.00156	3288.13621	1337.21447 +
14	0	0	2	0	3	0	0	2	0	2	3290.01694	-0.00011	3290.01705	1341.02637
15	0	0	2	0	4	0	0	2	0	3	3291.88919	-0.00024	3291.88943	1346.74412
16	0	0	2	0	5	0	0	2	0	4	3293.75184*	-0.00146	3293.75330	1354.36759 +
17	0	0	2	0	6	0	0	2	0	5	3295.61231*	0.00370	3295.60861	1363.89662 +
18	0	0	2	0	7	0	0	2	0	6	3297.45494	-0.00037	3297.45531	1375.33100
19	0	0	2	0	8	0	0	2	0	7	3299.29295	-0.00039	3299.29334	1388.67047
20	0	0	2	0	9	0	0	2	0	8	3301.12251	-0.00015	3301.12266	1403.91476
21	0	0	2	0	10	0	0	2	0	9	3302.94326*	0.00005	3302.94321	1421.06352
22	0	0	2	0	11	0	0	2	0	10	3304.75088*	-0.00406	3304.75494	1440.11639 +
23	0	0	2	0	12	0	0	2	0	11	3306.55405*	-0.00374	3306.55779	1461.07294 +
24	0	0	2	0	13	0	0	2	0	12	3308.35147	-0.00022	3308.35169	1483.93273
25	0	0	2	0	14	0	0	2	0	13	3310.13624*	-0.00036	3310.13660	1508.69525
26	0	0	2	0	15	0	0	2	0	14	3311.91227	-0.00018	3311.91245	1535.35996
27	0	0	2	0	16	0	0	2	0	15	3313.68112*	0.00194	3313.67918	1563.92630 +
28	0	0	2	0	17	0	0	2	0	16	3315.43680	0.00007	3315.43673	1594.39363
29	0	0	2	0	18	0	0	2	0	17	3317.18521	0.00017	3317.18504	1626.76130
30	0	0	2	0	19	0	0	2	0	18	3318.92395	-0.00010	3318.92405	1661.02860
31	0	0	2	0	20	0	0	2	0	19	3320.65521	0.00151	3320.65370	1697.19482 +
32	0	0	2	0	21	0	0	2	0	20	3322.36862*	-0.00532	3322.37394	1735.25916 +
33	0	0	2	0	22	0	0	2	0	21	3324.08434	-0.00035	3324.08469	1775.22081
34	0	0	2	0	23	0	0	2	0	22	3325.78658	0.00066	3325.78592	1817.07894
35	0	0	2	0	24	0	0	2	0	23	3327.47757	0.00001	3327.47756	1860.83266
36	0	0	2	0	25	0	0	2	0	24	3329.15948	-0.00009	3329.15957	1906.48106
37	0	0	2	0	26	0	0	2	0	25	3330.83319*	0.00129	3330.83190	1954.02319 +
	0	0	2	0	27	0	0	2	0	26	3332.49390	-0.00060	3332.49450	2003.45808

$$\text{rms} = 0.00033 \text{ cm}^{-1}$$


v_4'	l_4'	v_5'	l_5'	J'	v_4''	l_4''	v_5''	l_5''	J''	OBS	OBS – CALC	E'	E''
0	0	2	2	2	0	0	1	1	3	3955.25544	-0.00016	3955.25560	685.63493
0	0	2	2	3	0	0	1	1	4	3953.34767	0.00077	3953.34690	693.23388
0	0	2	2	4	0	0	1	1	5	3951.43503	-0.00032	3951.43535	702.73224
0	0	2	2	5	0	0	1	1	6	3949.52150	0.00045	3949.52105	714.13007
0	0	2	2	6	0	0	1	1	7	3947.60407	-0.00005	3947.60412	727.42716
0	0	2	2	7	0	0	1	1	8	3945.68463	-0.00004	3945.68467	742.62333
0	0	2	2	8	0	0	1	1	9	3943.76252	-0.00034	3943.76286	759.71839
0	0	2	2	9	0	0	1	1	10	3941.83907	0.00022	3941.83885	778.71209
0	0	2	2	10	0	0	1	1	11	3939.91278	-0.00003	3939.91281	799.60420
0	0	2	2	11	0	0	1	1	12	3937.98504	0.00010	3937.98494	822.39444
0	0	2	2	12	0	0	1	1	13	3936.05585	0.00040	3936.05545	847.08251
0	0	2	2	13	0	0	1	1	14	3934.12441	-0.00017	3934.12458	873.66808
0	0	2	2	14	0	0	1	1	15	3932.19300	0.00043	3932.19257	902.15079
0	0	2	2	15	0	0	1	1	16	3930.25981	0.00013	3930.25968	932.53028
0	0	2	2	16	0	0	1	1	17	3928.32633	0.00014	3928.32619	964.80614
0	0	2	2	17	0	0	1	1	18	3926.39257	0.00018	3926.39239	998.97795
0	0	2	2	18	0	0	1	1	19	3924.45889	0.00030	3924.45859	1035.04524
0	0	2	2	19	0	0	1	1	20	3922.52507	-0.00004	3922.52511	1073.00756
0	0	2	2	20	0	0	1	1	21	3920.59245	0.00018	3920.59227	1112.86438
0	0	2	2	21	0	0	1	1	22	3918.66068	0.00025	3918.66043	1154.61520

1	0	0	2	2	22	0	0	1	1	23	3916.72940	-0.00053	3916.72993	1198.25945
3	0	0	2	2	23	0	0	1	1	24	3914.80139	0.00026	3914.80113	1243.79656
4	0	0	2	2	24	0	0	1	1	25	3912.87487	0.00047	3912.87440	1291.22593
5	0	0	2	2	25	0	0	1	1	26	3910.95028	0.00017	3910.95011	1340.54693
6	0	0	2	2	26	0	0	1	1	27	3909.02880	0.00018	3909.02862	1391.75891
7	0	0	2	2	27	0	0	1	1	28	3907.10956	-0.00075	3907.11031	1444.86119
8	0	0	2	2	28	0	0	1	1	29	3905.19509	-0.00046	3905.19555	1499.85307
9	0	0	2	2	3	0	0	1	1	2	3966.64409	-0.00095	3966.64504	679.93567
10	0	0	2	2	4	0	0	1	1	3	3968.53281	0.00015	3968.53266	685.63493
11	0	0	2	2	5	0	0	1	1	4	3970.41666	-0.00065	3970.41731	693.23382
12	0	0	2	2	6	0	0	1	1	5	3972.29888	-0.00016	3972.29904	702.73224
13	0	0	2	2	7	0	0	1	1	6	3974.17820	0.00027	3974.17793	714.13007
14	0	0	2	2	8	0	0	1	1	7	3976.05415	0.00006	3976.05409	727.42716
15	0	0	2	2	9	0	0	1	1	8	3977.92740	-0.00021	3977.92761	742.62333
16	0	0	2	2	10	0	0	1	1	9	3979.79880	0.00017	3979.79863	759.71839
17	0	0	2	2	11	0	0	1	1	10	3981.66747	0.00018	3981.66729	778.71209
18	0	0	2	2	12	0	0	1	1	11	3983.53415	0.00039	3983.53376	799.60420
19	0	0	2	2	13	0	0	1	1	12	3985.39864	0.00043	3985.39821	822.39444
20	0	0	2	2	14	0	0	1	1	13	3987.26076	-0.00009	3987.26085	847.08251
21	0	0	2	2	15	0	0	1	1	14	3989.12184	-0.00004	3989.12188	873.66808
22	0	0	2	2	16	0	0	1	1	15	3990.98011	-0.00143	3990.98154	902.15079 +
23	0	0	2	2	17	0	0	1	1	16	3992.84009	0.00004	3992.84005	932.53028
24	0	0	2	2	18	0	0	1	1	17	3994.69778	0.00009	3994.69769	964.80614
25	0	0	2	2	19	0	0	1	1	18	3996.55468	-0.00004	3996.55472	998.97795
26	0	0	2	2	20	0	0	1	1	19	3998.41151	0.00010	3998.41141	1035.04524
27	0	0	2	2	21	0	0	1	1	20	4000.26831	0.00024	4000.26807	1073.00756
28	0	0	2	2	22	0	0	1	1	21	4002.12581	0.00081	4002.12500	1112.86438
29	0	0	2	2	23	0	0	1	1	22	4003.98216	-0.00033	4003.98249	1154.61520
30	0	0	2	2	24	0	0	1	1	23	4005.85834*	0.01746	4005.84088	1198.25945 +
31	0	0	2	2	25	0	0	1	1	24	4007.70035	-0.00012	4007.70047	1243.79656
32	0	0	2	2	26	0	0	1	1	25	4009.56053	-0.00107	4009.56160	1291.22593 +
33	0	0	2	2	27	0	0	1	1	26	4011.42446	-0.00011	4011.42457	1340.54693
34	0	0	2	2	28	0	0	1	1	27	4013.28757	-0.00214	4013.28971	1391.75891 +
35	0	0	2	-2	2	0	0	1	-1	3	3955.21715	0.00069	3955.21646	685.67405
36	0	0	2	-2	3	0	0	1	-1	4	3953.28149	-0.00012	3953.28161	693.29902
37	0	0	2	-2	4	0	0	1	-1	5	3951.33740	0.00011	3951.33729	702.83004
38	0	0	2	-2	5	0	0	1	-1	6	3949.38399	0.00045	3949.38354	714.26698
39	0	0	2	-2	6	0	0	1	-1	7	3947.42029	-0.00009	3947.42038	727.60969
40	0	0	2	-2	7	0	0	1	-1	8	3945.44722	-0.00061	3945.44783	742.85799
41	0	0	2	-2	8	0	0	1	-1	9	3943.46567*	-0.00026	3943.46593	760.01168
42	0	0	2	-2	9	0	0	1	-1	10	3941.47428	-0.00042	3941.47470	779.07052
43	0	0	2	-2	10	0	0	1	-1	11	3939.47417	0.00000	3939.47417	800.03426
44	0	0	2	-2	11	0	0	1	-1	12	3937.46433	-0.00004	3937.46437	822.90261
45	0	0	2	-2	12	0	0	1	-1	13	3935.44559	0.00027	3935.44532	847.67528
46	0	0	2	-2	13	0	0	1	-1	14	3933.41744	0.00039	3933.41705	874.35193
47	0	0	2	-2	14	0	0	1	-1	15	3931.37986	0.00027	3931.37959	902.93220
48	0	0	2	-2	15	0	0	1	-1	16	3929.33336	0.00038	3929.33298	933.41570
49	0	0	2	-2	16	0	0	1	-1	17	3927.27741	0.00018	3927.27723	965.80204
50	0	0	2	-2	17	0	0	1	-1	18	3925.21236	-0.00002	3925.21238	1000.09076
51	0	0	2	-2	18	0	0	1	-1	19	3923.13873	0.00027	3923.13846	1036.28142
52	0	0	2	-2	19	0	0	1	-1	20	3921.05579	0.00030	3921.05549	1074.37353
53	0	0	2	-2	20	0	0	1	-1	21	3918.96354	0.00002	3918.96352	1114.36658
54	0	0	2	-2	21	0	0	1	-1	22	3916.86210	-0.00045	3916.86255	1156.26002
55	0	0	2	-2	22	0	0	1	-1	23	3914.75224*	-0.00040	3914.75264	1200.05331
56	0	0	2	-2	23	0	0	1	-1	24	3912.63334	-0.00046	3912.63380	1245.74584
57	0	0	2	-2	24	0	0	1	-1	25	3910.50373	-0.00233	3910.50606	1293.33701 +
58	0	0	2	-2	25	0	0	1	-1	26	3908.36973	0.00026	3908.36947	1342.82618
59	0	0	2	-2	26	0	0	1	-1	27	3906.22392	-0.00012	3906.22404	1394.21269
60	0	0	2	-2	27	0	0	1	-1	28	3904.07047	0.00065	3904.06982	1447.49584
	0	0	2	-2	28	0	0	1	-1	29	3901.90635	-0.00047	3901.90682	1502.67492
	0	0	2	-2	29	0	0	1	-1	30	3899.73486	-0.00023	3899.73509	1559.74920
	0	0	2	-2	3	0	0	1	-1	2	3966.62585	0.00046	3966.62539	679.95524
	0	0	2	-2	4	0	0	1	-1	3	3968.49319	-0.00009	3968.49328	685.67405
	0	0	2	-2	5	0	0	1	-1	4	3970.34803*	-0.00347	3970.35150	693.29902 +
	0	0	2	-2	6	0	0	1	-1	5	3972.19983	-0.00020	3972.20003	702.83004

1	0	0	2	-2	7	0	0	1	-1	6	3974.03879	-0.00005	3974.03884	714.26698
2	0	0	2	-2	8	0	0	1	-1	7	3975.86793	0.00001	3975.86792	727.60969
3	0	0	2	-2	9	0	0	1	-1	8	3977.68719	-0.00004	3977.68723	742.85799
4	0	0	2	-2	10	0	0	1	-1	9	3979.49668	-0.00007	3979.49675	760.01168
5	0	0	2	-2	11	0	0	1	-1	10	3981.29638	-0.00008	3981.29646	779.07052
6	0	0	2	-2	12	0	0	1	-1	11	3983.08683	0.00049	3983.08634	800.03426
7	0	0	2	-2	13	0	0	1	-1	12	3984.86643	0.00007	3984.86636	822.90261
8	0	0	2	-2	14	0	0	1	-1	13	3986.63658	0.00007	3986.63651	847.67528
9	0	0	2	-2	15	0	0	1	-1	14	3988.39686	0.00011	3988.39675	874.35193
10	0	0	2	-2	16	0	0	1	-1	15	3990.14711	0.00004	3990.14707	902.93220
11	0	0	2	-2	17	0	0	1	-1	16	3991.88719	-0.00025	3991.88744	933.41570
12	0	0	2	-2	18	0	0	1	-1	17	3993.61870	0.00085	3993.61785	965.80204
13	0	0	2	-2	19	0	0	1	-1	18	3995.33797	-0.00029	3995.33826	1000.09076
14	0	0	2	-2	20	0	0	1	-1	19	3997.04887	0.00020	3997.04867	1036.28142
15	0	0	2	-2	21	0	0	1	-1	20	3998.75271*	0.00367	3998.74904	1074.37353 +
16	0	0	2	-2	22	0	0	1	-1	21	4000.43870	-0.00066	4000.43936	1114.36658
17	0	0	2	-2	23	0	0	1	-1	22	4002.12185*	0.00224	4002.11961	1156.26002 +
18	0	0	2	-2	24	0	0	1	-1	23	4003.78979	0.00002	4003.78977	1200.05331
19	0	0	2	-2	25	0	0	1	-1	24	4005.44960	-0.00021	4005.44981	1245.74584
20	0	0	2	-2	26	0	0	1	-1	25	4007.10013	0.00041	4007.09972	1293.33701
21	0	0	2	-2	27	0	0	1	-1	26	4008.73776*	-0.00171	4008.73947	1342.82618 +
22	0	0	2	-2	28	0	0	1	-1	27	4010.36960	0.00055	4010.36905	1394.21269
23	0	0	2	-2	29	0	0	1	-1	28	4011.98866	0.00021	4011.98845	1447.49584
24	0	0	2	-2	30	0	0	1	-1	29	4013.59750	-0.00012	4013.59762	1502.67492
25	0	0	2	2	2	0	0	1	-1	2	3960.93496	-0.00033	3960.93529	679.95524
26	0	0	2	2	3	0	0	1	-1	3	3960.90009*	-0.00657	3960.90666	685.67405 +
27	0	0	2	2	4	0	0	1	-1	4	3960.87409*	0.00552	3960.86857	693.29902 +
28	0	0	2	2	5	0	0	1	-1	5	3960.82245*	0.00136	3960.82109	702.83004 +
29	0	0	2	2	6	0	0	1	-1	6	3960.76354*	-0.00076	3960.76430	714.26698
30	0	0	2	2	7	0	0	1	-1	7	3960.69910	0.00078	3960.69832	727.60969
31	0	0	2	2	8	0	0	1	-1	8	3960.62333	0.00007	3960.62326	742.85799
32	0	0	2	2	9	0	0	1	-1	9	3960.53803	-0.00123	3960.53926	760.01168 +
33	0	0	2	2	10	0	0	1	-1	10	3960.44473*	-0.00176	3960.44649	779.07052 +
34	0	0	2	2	11	0	0	1	-1	11	3960.34501	-0.00011	3960.34512	800.03426
35	0	0	2	2	12	0	0	1	-1	12	3960.23493	-0.00042	3960.23535	822.90261
36	0	0	2	2	13	0	0	1	-1	13	3960.11790	0.00052	3960.11738	847.67528
37	0	0	2	2	14	0	0	1	-1	14	3959.99103	-0.00040	3959.99143	874.35193
38	0	0	2	2	15	0	0	1	-1	15	3959.85760	-0.00016	3959.85776	902.93220
39	0	0	2	2	16	0	0	1	-1	16	3959.71727	0.00064	3959.71663	933.41570
40	0	0	2	2	17	0	0	1	-1	17	3959.56719*	-0.00111	3959.56830	965.80204 +
41	0	0	2	2	18	0	0	1	-1	18	3959.41336	0.00029	3959.41307	1000.09076
42	0	0	2	2	19	0	0	1	-1	19	3959.25120	-0.00004	3959.25124	1036.28142
43	0	0	2	2	20	0	0	1	-1	20	3959.08354	0.00042	3959.08312	1074.37353
44	0	0	2	2	21	0	0	1	-1	21	3958.90917	0.00012	3958.90905	1114.36658
45	0	0	2	2	22	0	0	1	-1	22	3958.72935	-0.00001	3958.72936	1156.26002
46	0	0	2	2	23	0	0	1	-1	23	3958.54425	-0.00014	3958.54439	1200.05331
47	0	0	2	2	24	0	0	1	-1	24	3958.35441	-0.00008	3958.35449	1245.74584
48	0	0	2	2	25	0	0	1	-1	25	3958.16019	0.00017	3958.16002	1293.33701
49	0	0	2	2	26	0	0	1	-1	26	3957.96128	-0.00007	3957.96135	1342.82618
50	0	0	2	2	27	0	0	1	-1	27	3957.75905	0.00024	3957.75881	1394.21269
51	0	0	2	2	28	0	0	1	-1	28	3957.54905*	-0.00373	3957.55278	1447.49584 +
52	0	0	2	2	29	0	0	1	-1	29	3957.34374	0.00014	3957.34360	1502.67492
53	0	0	2	2	30	0	0	1	-1	30	3957.13188	0.00027	3957.13161	1559.74920
54	0	0	2	2	31	0	0	1	-1	31	3956.91532	-0.00183	3956.91715	1618.71789 +
55	0	0	2	2	32	0	0	1	-1	32	3956.70034	-0.00020	3956.70054	1679.58023
56	0	0	2	-2	3	0	0	1	1	3	3960.94500	-0.00070	3960.94570	685.63493
57	0	0	2	-2	4	0	0	1	1	4	3960.93310	-0.00041	3960.93351	693.23382
58	0	0	2	-2	5	0	0	1	1	5	3960.91823	-0.00005	3960.91828	702.73224
59	0	0	2	-2	6	0	0	1	1	6	3960.90009	0.00009	3960.90000	714.13007
60	0	0	2	-2	7	0	0	1	1	7	3960.87858	-0.00008	3960.87866	727.42716
	0	0	2	-2	8	0	0	1	1	8	3960.85463	0.00036	3960.85427	742.62333
	0	0	2	-2	9	0	0	1	1	9	3960.82411*	-0.00272	3960.82683	759.71839 +
	0	0	2	-2	10	0	0	1	1	10	3960.79640	0.00007	3960.79633	778.71209
	0	0	2	-2	11	0	0	1	1	11	3960.76288	0.00011	3960.76277	799.60420
	0	0	2	-2	12	0	0	1	1	12	3960.72599	-0.00016	3960.72615	822.39444

0	0	2	-2	13	0	0	1	1	13	3960.68724	0.00077	3960.68647	847.08251
0	0	2	-2	14	0	0	1	1	14	3960.64339	-0.00032	3960.64371	873.66808
0	0	2	-2	15	0	0	1	1	15	3960.59516*	-0.00273	3960.59789	902.15079 +
0	0	2	-2	16	0	0	1	1	16	3960.54996*	0.00097	3960.54899	932.53028
0	0	2	-2	17	0	0	1	1	17	3960.49682	-0.00018	3960.49700	964.80614
0	0	2	-2	18	0	0	1	1	18	3960.44255	0.00061	3960.44194	998.97795
0	0	2	-2	19	0	0	1	1	19	3960.38381	0.00003	3960.38378	1035.04524
0	0	2	-2	20	0	0	1	1	20	3960.32209	-0.00045	3960.32254	1073.00756
0	0	2	-2	21	0	0	1	1	21	3960.25802	-0.00017	3960.25819	1112.86438
0	0	2	-2	22	0	0	1	1	22	3960.19081	0.00007	3960.19074	1154.61520
0	0	2	-2	23	0	0	1	1	23	3960.11805*	-0.00213	3960.12018	1198.25945 +
0	0	2	-2	24	0	0	1	1	24	3960.04686	0.00035	3960.04651	1243.79656
0	0	2	-2	25	0	0	1	1	25	3959.97077	0.00105	3959.96972	1291.22593 +
0	0	2	-2	26	0	0	1	1	26	3959.89032	0.00052	3959.88980	1340.54693
0	0	2	-2	27	0	0	1	1	27	3959.80702	0.00027	3959.80675	1391.75891
0	0	2	-2	28	0	0	1	1	28	3959.71727*	-0.00328	3959.72055	1444.86119 +
0	0	2	-2	29	0	0	1	1	29	3959.63066	-0.00055	3959.63121	1499.85307

rms = 0.00034 cm⁻¹

$$v_1 + 2v_5 (\Delta) \leftarrow 2v_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 2 2	0 0 2 2 3	3277.56030	-0.00063	3277.56093	1363.32960
0 0 2 2 3	0 0 2 2 4	3275.63043	-0.00054	3275.63097	1370.94974
0 0 2 2 4	0 0 2 2 5	3273.69143	-0.00132	3273.69275	1380.47484 †
0 0 2 2 5	0 0 2 2 6	3271.74604	-0.00023	3271.74627	1391.90486
0 0 2 2 6	0 0 2 2 7	3269.78351*	-0.00805	3269.79156	1405.23972 †
0 0 2 2 7	0 0 2 2 8	3267.82864	0.00001	3267.82863	1420.47938
0 0 2 2 8	0 0 2 2 9	3265.85833	0.00082	3265.85751	1437.62374
0 0 2 2 9	0 0 2 2 10	3263.87740	-0.00082	3263.87822	1456.67272
0 0 2 2 10	0 0 2 2 11	3261.89115	0.00035	3261.89080	1477.62621
0 0 2 2 11	0 0 2 2 12	3259.89489	-0.00037	3259.89526	1500.48412
0 0 2 2 12	0 0 2 2 13	3257.89271	0.00108	3257.89163	1525.24633 †
0 0 2 2 13	0 0 2 2 14	3255.88173	0.00177	3255.87996	1551.91270 †
0 0 2 2 14	0 0 2 2 15	3253.86267	0.00240	3253.86027	1580.48310 †
0 0 2 2 15	0 0 2 2 16	3251.83536	0.00277	3251.83259	1610.95737 †
0 0 2 2 16	0 0 2 2 17	3249.79939	0.00242	3249.79697	1643.33536 †
0 0 2 2 17	0 0 2 2 18	3247.75404	0.00060	3247.75344	1677.61689
0 0 2 2 18	0 0 2 2 19	3245.71052	0.00847	3245.70205	1713.80178 †
0 0 2 2 19	0 0 2 2 20	3243.64387	0.00103	3243.64284	1751.88982 †
0 0 2 2 20	0 0 2 2 21	3241.57632	0.00047	3241.57585	1791.88081
0 0 2 2 21	0 0 2 2 22	3239.50631*	0.00519	3239.50112	1833.77451 †
0 0 2 2 22	0 0 2 2 23	3237.41853	-0.00018	3237.41871	1877.57067
0 0 2 2 23	0 0 2 2 24	3235.32850	-0.00017	3235.32867	1923.26903
0 0 2 2 24	0 0 2 2 25	3233.23074	-0.00029	3233.23103	1970.86930
0 0 2 2 25	0 0 2 2 26	3231.12538	-0.00048	3231.12586	2020.37118
0 0 2 2 3	0 0 2 2 2	3288.96502	-0.00123	3288.96625	1357.61446 †
0 0 2 2 4	0 0 2 2 3	3290.83750	-0.00049	3290.83799	1363.32960
0 0 2 2 5	0 0 2 2 4	3292.70140	0.00001	3292.70139	1370.94974
0 0 2 2 6	0 0 2 2 5	3294.55572	-0.00072	3294.55644	1380.47484
0 0 2 2 7	0 0 2 2 6	3296.41125*	0.00810	3296.40315	1391.90486 †
0 0 2 2 8	0 0 2 2 7	3298.23993	-0.00159	3298.24152	1405.23972 †
0 0 2 2 9	0 0 2 2 8	3300.07081	-0.00075	3300.07156	1420.47938
0 0 2 2 10	0 0 2 2 9	3301.89339	0.00012	3301.89327	1437.62374
0 0 2 2 11	0 0 2 2 10	3303.70354	-0.00313	3303.70667	1456.67272 †
0 0 2 2 12	0 0 2 2 11	3305.50445	-0.00730	3305.51175	1477.62621 †
0 0 2 2 13	0 0 2 2 12	3307.30885	0.00032	3307.30853	1500.48412
0 0 2 2 14	0 0 2 2 13	3309.09808	0.00105	3309.09703	1525.24633 †
0 0 2 2 15	0 0 2 2 14	3310.88287*	0.00561	3310.87726	1551.91270 †
0 0 2 2 16	0 0 2 2 15	3312.64905	-0.00018	3312.64923	1580.48310
0 0 2 2 17	0 0 2 2 16	3314.41276	-0.00020	3314.41296	1610.95737
0 0 2 2 18	0 0 2 2 17	3316.17014*	0.00167	3316.16847	1643.33536 †

1	0	0	2	2	19	0	0	2	2	18	3317.91690*	0.00113	3317.91577	1677.61689	+
2	0	0	2	2	20	0	0	2	2	19	3319.65469	-0.00018	3319.65487	1713.80178	
3	0	0	2	2	21	0	0	2	2	20	3321.38301*	-0.00279	3321.38580	1751.88982	+
4	0	0	2	2	22	0	0	2	2	21	3323.10831	-0.00026	3323.10857	1791.88081	
5	0	0	2	2	23	0	0	2	2	22	3324.82348	0.00029	3324.82319	1833.77451	
6	0	0	2	2	24	0	0	2	2	23	3326.53026	0.00060	3326.52966	1877.57067	
7	0	0	2	-2	2	0	0	2	-2	3	3277.56030	-0.00069	3277.56099	1363.32952	
8	0	0	2	-2	3	0	0	2	-2	4	3275.63043	-0.00069	3275.63112	1370.94950	
9	0	0	2	-2	4	0	0	2	-2	5	3273.69143	-0.00161	3273.69304	1380.47429	+
10	0	0	2	-2	5	0	0	2	-2	6	3271.74604	-0.00072	3271.74676	1391.90376	
11	0	0	2	-2	6	0	0	2	-2	7	3269.78351*	-0.00882	3269.79233	1405.23774	
12	0	0	2	-2	7	0	0	2	-2	8	3267.82864	-0.00111	3267.82975	1420.47607	+
13	0	0	2	-2	8	0	0	2	-2	9	3265.85833	-0.00073	3265.85906	1437.61854	
14	0	0	2	-2	9	0	0	2	-2	10	3263.87740	-0.00289	3263.88029	1456.66492	+
15	0	0	2	-2	10	0	0	2	-2	11	3261.89115	-0.00232	3261.89347	1477.61496	+
16	0	0	2	-2	11	0	0	2	-2	12	3259.89489	-0.00373	3259.89862	1500.46836	+
17	0	0	2	-2	12	0	0	2	-2	13	3257.89271	-0.00306	3257.89577	1525.22483	+
18	0	0	2	-2	13	0	0	2	-2	14	3255.88173	-0.00321	3255.88494	1551.88404	+
19	0	0	2	-2	14	0	0	2	-2	15	3253.86267	-0.00350	3253.86617	1580.44562	+
20	0	0	2	-2	15	0	0	2	-2	16	3251.83536	-0.00413	3251.83949	1610.90919	+
21	0	0	2	-2	16	0	0	2	-2	17	3249.79939	-0.00553	3249.80492	1643.27435	+
22	0	0	2	-2	17	0	0	2	-2	18	3247.76367	0.00118	3247.76249	1677.54066	+
23	0	0	2	-2	18	0	0	2	-2	19	3245.71052	-0.00171	3245.71223	1713.70766	+
24	0	0	2	-2	19	0	0	2	-2	20	3243.65291	-0.00126	3243.65417	1751.77486	+
25	0	0	2	-2	20	0	0	2	-2	21	3241.58865	0.00031	3241.58834	1791.74175	
26	0	0	2	-2	21	0	0	2	-2	22	3239.50631*	-0.00846	3239.51477	1833.60781	+
27	0	0	2	-2	22	0	0	2	-2	23	3237.43325	-0.00024	3237.43349	1877.37245	
28	0	0	2	-2	23	0	0	2	-2	24	3235.34378	-0.00075	3235.34453	1923.03511	
29	0	0	2	-2	24	0	0	2	-2	25	3233.24836	0.00045	3233.24791	1970.59516	
30	0	0	2	-2	3	0	0	2	-2	2	3288.96502	-0.00116	3288.96618	1357.61444	+
31	0	0	2	-2	4	0	0	2	-2	3	3290.83750	-0.00031	3290.83781	1363.32952	
32	0	0	2	-2	5	0	0	2	-2	4	3292.70140	0.00038	3292.70102	1370.94950	
33	0	0	2	-2	6	0	0	2	-2	5	3294.55572	-0.00006	3294.55578	1380.47429	
34	0	0	2	-2	7	0	0	2	-2	6	3296.41125	0.00918	3296.40207	1391.90376	+
35	0	0	2	-2	8	0	0	2	-2	7	3298.23993	0.00007	3298.23986	1405.23774	
36	0	0	2	-2	9	0	0	2	-2	8	3300.07081	0.00167	3300.06914	1420.47607	+
37	0	0	2	-2	10	0	0	2	-2	9	3301.89339	0.00351	3301.88988	1437.61854	+
38	0	0	2	-2	11	0	0	2	-2	10	3303.70354	0.00148	3303.70206	1456.66492	+
39	0	0	2	-2	12	0	0	2	-2	11	3305.50445	-0.00119	3305.50564	1477.61496	+
40	0	0	2	-2	13	0	0	2	-2	12	3307.30885	0.00823	3307.30062	1500.46836	+
41	0	0	2	-2	14	0	0	2	-2	13	3309.08801	0.00105	3309.08696	1525.22483	+
42	0	0	2	-2	15	0	0	2	-2	14	3310.86616	0.00152	3310.86464	1551.88404	+
43	0	0	2	-2	16	0	0	2	-2	15	3312.63211	-0.00154	3312.63365	1580.44562	+
44	0	0	2	-2	17	0	0	2	-2	16	3314.39293	-0.00102	3314.39395	1610.90919	+
45	0	0	2	-2	18	0	0	2	-2	17	3316.14545	-0.00008	3316.14553	1643.27435	
46	0	0	2	-2	19	0	0	2	-2	18	3317.88862	0.00025	3317.88837	1677.54066	
47	0	0	2	-2	20	0	0	2	-2	19	3319.62203	-0.00041	3319.62244	1713.70766	
48	0	0	2	-2	21	0	0	2	-2	20	3321.33926*	-0.00846	3321.34772	1751.77486	+
49	0	0	2	-2	22	0	0	2	-2	21	3323.06418	-0.00001	3323.06419	1791.74175	
50	0	0	2	-2	23	0	0	2	-2	22	3324.78037*	0.00854	3324.77183	1833.60781	+
51	0	0	2	-2	24	0	0	2	-2	23	3326.47169	0.00107	3326.47062	1877.37245	+
52	0	0	2	-2	25	0	0	2	-2	24	3328.16006	-0.00048	3328.16054	1923.03511	
53	0	0	2	2	2	0	0	2	-2	2	3283.27737	0.00129	3283.27608	1357.61444	+
54	0	0	2	2	3	0	0	2	-2	3	3283.25088	-0.00031	3283.25119	1363.32952	
55	0	0	2	2	4	0	0	2	-2	4	3283.21746	-0.00063	3283.21809	1370.94950	
56	0	0	2	2	5	0	0	2	-2	5	3283.17575	-0.00108	3283.17683	1380.47429	+
57	0	0	2	2	6	0	0	2	-2	6	3283.12582	-0.00171	3283.12753	1391.90376	+
58	0	0	2	2	7	0	0	2	-2	7	3283.06608	-0.00418	3283.07026	1405.23774	+
59	0	0	2	2	8	0	0	2	-2	8	3283.00566	0.00049	3283.00517	1420.47607	
60	0	0	2	2	9	0	0	2	-2	9	3282.93166*	-0.00074	3282.93240	1437.61854	
	0	0	2	2	10	0	0	2	-2	10	3282.85308	0.00099	3282.85209	1456.66492	
	0	0	2	-2	2	0	0	2	2	2	3283.27737	0.00132	3283.27605	1357.61446	+
	0	0	2	-2	3	0	0	2	2	3	3283.25088	-0.00015	3283.25103	1363.32960	
	0	0	2	-2	4	0	0	2	2	4	3283.21746	-0.00013	3283.21759	1370.94974	
	0	0	2	-2	5	0	0	2	2	5	3283.17575	0.00007	3283.17568	1380.47484	

0	0	2	-2	6	0	0	2	2	6	3283.12582	0.00061	3283.12521	1391.90486
0	0	2	-2	7	0	0	2	2	7	3283.06608	-0.00002	3283.06610	1405.23972
0	0	2	-2	8	0	0	2	2	8	3282.99832	0.00009	3282.99823	1420.47938
0	0	2	-2	9	0	0	2	2	9	3282.91984*	-0.00164	3282.92148	1437.62374 †
0	0	2	-2	10	0	0	2	2	10	3282.83505	-0.00066	3282.83571	1456.67272

rms = 0.00046 cm⁻¹

$V_1 + V_4 + V_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 1	0 0 0 0 2	4479.71843	0.00049	4479.71794	5.70195
1 1 1 -1 2	0 0 0 0 3	4477.81349	-0.00037	4477.81386	11.40382
1 1 1 -1 3	0 0 0 0 4	4475.90670	-0.00167	4475.90837	19.00619 †
1 1 1 -1 4	0 0 0 0 5	4474.00097	-0.00083	4474.00180	28.50898
1 1 1 -1 5	0 0 0 0 6	4472.09501	0.00041	4472.09460	39.91204
1 1 1 -1 6	0 0 0 0 7	4470.18757	0.00027	4470.18730	53.21523
1 1 1 -1 7	0 0 0 0 8	4468.28003	-0.00052	4468.28055	68.41838
1 1 1 -1 8	0 0 0 0 9	4466.37566	0.00059	4466.37507	85.52129
1 1 1 -1 9	0 0 0 0 10	4464.47312	0.00147	4464.47165	104.52373 †
1 1 1 -1 10	0 0 0 0 11	4462.57116	0.00003	4462.57113	125.42544
1 1 1 -1 11	0 0 0 0 12	4460.67380	-0.00061	4460.67441	148.22616
1 1 1 -1 12	0 0 0 0 13	4458.78278	0.00041	4458.78237	172.92558
1 1 1 -1 13	0 0 0 0 14	4456.89568	-0.00018	4456.89586	199.52337
1 1 1 -1 14	0 0 0 0 15	4455.01531	-0.00038	4455.01569	228.01920
1 1 1 -1 15	0 0 0 0 16	4453.14257	-0.00002	4453.14259	258.41268
1 1 1 -1 16	0 0 0 0 17	4451.27686	-0.00029	4451.27715	290.70340
1 1 1 -1 17	0 0 0 0 18	4449.42067	0.00078	4449.41989	324.89096
1 1 1 -1 18	0 0 0 0 19	4447.57237	0.00121	4447.57116	360.97488 †
1 1 1 -1 19	0 0 0 0 20	4445.73009	-0.00114	4445.73123	398.95471 †
1 1 1 -1 2	0 0 0 0 1	4487.31681	-0.00021	4487.31702	1.90066
1 1 1 -1 3	0 0 0 0 2	4489.21196	-0.00065	4489.21261	5.70195
1 1 1 -1 4	0 0 0 0 3	4491.10724	0.00028	4491.10696	11.40382
1 1 1 -1 5	0 0 0 0 4	4493.00045	0.00001	4493.00044	19.00619
1 1 1 -1 6	0 0 0 0 5	4494.89314	-0.00042	4494.89356	28.50898
1 1 1 -1 7	0 0 0 0 6	4496.78641	-0.00049	4496.78690	39.91204
1 1 1 -1 8	0 0 0 0 7	4498.68167	0.00055	4498.68112	53.21523
1 1 1 -1 9	0 0 0 0 8	4500.57658	-0.00041	4500.57699	68.41838
1 1 1 -1 10	0 0 0 0 9	4502.47539	0.00011	4502.47528	85.52129
1 1 1 -1 11	0 0 0 0 10	4504.37622	-0.00062	4504.37684	104.52373
1 1 1 -1 12	0 0 0 0 11	4506.28263	0.00013	4506.28250	125.42544
1 1 1 -1 13	0 0 0 0 12	4508.19259	-0.00049	4508.19308	148.22616
1 1 1 -1 14	0 0 0 0 13	4510.10878	-0.00054	4510.10932	172.92558
1 1 1 -1 15	0 0 0 0 14	4512.03060	-0.00129	4512.03189	199.52337 †
1 1 1 -1 16	0 0 0 0 15	4513.96104	-0.00032	4513.96136	228.01920
1 1 1 -1 17	0 0 0 0 16	4515.89846	0.00029	4515.89817	258.41268
1 1 1 -1 18	0 0 0 0 17	4517.84320	0.00056	4517.84264	290.70340
1 1 1 -1 19	0 0 0 0 18	4519.79574	0.00076	4519.79498	324.89096

rms = 0.00046 cm⁻¹

$V_1 + V_4 + V_5 (\Sigma^+) \leftarrow V_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	1 1 0 0 1	3972.03482	0.00006	3972.03476	511.48627
1 1 1 -1 1	1 1 0 0 2	3970.13191	0.00032	3970.13159	515.28830
1 1 1 -1 2	1 1 0 0 3	3968.22541	-0.00098	3968.22639	520.99129
1 1 1 -1 3	1 1 0 0 4	3966.31936	-0.00005	3966.31941	528.59515
1 1 1 -1 4	1 1 0 0 5	3964.41103	0.00005	3964.41098	538.09979
1 1 1 -1 5	1 1 0 0 6	3962.50206	0.00050	3962.50156	549.50508

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

1	1	1	1	-1	6	1	1	0	0	7	3960.59482*	0.00315	3960.59167	562.81086	†
2	1	1	1	-1	7	1	1	0	0	8	3958.68198	0.00001	3958.68197	578.01697	
3	1	1	1	-1	8	1	1	0	0	9	3956.77283	-0.00034	3956.77317	595.12319	
4	1	1	1	-1	9	1	1	0	0	10	3954.86666	0.00058	3954.86608	614.12929	
5	1	1	1	-1	10	1	1	0	0	11	3952.96169	0.00015	3952.96154	635.03503	
6	1	1	1	-1	11	1	1	0	0	12	3951.06046	0.00002	3951.06044	657.84012	
7	1	1	1	-1	12	1	1	0	0	13	3949.16391	0.00023	3949.16368	682.54427	
8	1	1	1	-1	13	1	1	0	0	14	3947.27264	0.00054	3947.27210	709.14713	
9	1	1	1	-1	14	1	1	0	0	15	3945.38808*	0.00155	3945.38653	737.64836	†
10	1	1	1	-1	15	1	1	0	0	16	3943.50840	0.00071	3943.50769	768.04757	
11	1	1	1	-1	16	1	1	0	0	17	3941.63591	-0.00029	3941.63620	800.34436	
12	1	1	1	-1	17	1	1	0	0	18	3939.77241	-0.00014	3939.77255	834.53830	
13	1	1	1	-1	18	1	1	0	0	19	3937.91699	-0.00013	3937.91712	870.62893	
14	1	1	1	-1	19	1	1	0	0	20	3936.07055	0.00038	3936.07017	908.61577	
15	1	1	1	-1	20	1	1	0	0	21	3934.23171	-0.00014	3934.23185	948.49830	
16	1	1	1	-1	21	1	1	0	0	22	3932.40179	-0.00041	3932.40220	990.27601	
17	1	1	1	-1	22	1	1	0	0	23	3930.58020	-0.00100	3930.58120	1033.94833	
18	1	1	1	-1	23	1	1	0	0	24	3928.76850	-0.00025	3928.76875	1079.51468	
19	1	1	1	-1	24	1	1	0	0	25	3926.96366	-0.00108	3926.96474	1126.97445	†
20	1	1	1	-1	25	1	1	0	0	26	3925.16916*	0.00015	3925.16901	1176.32701	
21	1	1	1	-1	26	1	1	0	0	27	3923.38015	-0.00122	3923.38137	1227.57169	†
22	1	1	1	-1	27	1	1	0	0	28	3921.60240	0.00076	3921.60164	1280.70782	
23	1	1	1	-1	2	1	1	0	0	1	3977.73152	0.00011	3977.73141	511.48627	
24	1	1	1	-1	3	1	1	0	0	2	3979.62493	-0.00133	3979.62626	515.28830	†
25	1	1	1	-1	4	1	1	0	0	3	3981.51964	0.00015	3981.51949	520.99129	
26	1	1	1	-1	5	1	1	0	0	4	3983.41184	0.00036	3983.41148	528.59515	
27	1	1	1	-1	6	1	1	0	0	5	3985.30331	0.00056	3985.30275	538.09979	
28	1	1	1	-1	7	1	1	0	0	6	3987.19413	0.00027	3987.19386	549.50508	
29	1	1	1	-1	8	1	1	0	0	7	3989.08598	0.00048	3989.08550	562.81086	
30	1	1	1	-1	9	1	1	0	0	8	3990.97987	0.00147	3990.97840	578.01697	†
31	1	1	1	-1	10	1	1	0	0	9	3992.87362	0.00023	3992.87339	595.12319	
32	1	1	1	-1	11	1	1	0	0	10	3994.77191	0.00063	3994.77128	614.12929	
33	1	1	1	-1	12	1	1	0	0	11	3996.67331	0.00040	3996.67291	635.03503	
34	1	1	1	-1	13	1	1	0	0	12	3998.57903	-0.00008	3998.57911	657.84012	
35	1	1	1	-1	14	1	1	0	0	13	4000.49079	0.00016	4000.49063	682.54427	
36	1	1	1	-1	15	1	1	0	0	14	4002.40889	0.00076	4002.40813	709.14713	
37	1	1	1	-1	16	1	1	0	0	15	4004.33229	0.00009	4004.33220	737.64836	
38	1	1	1	-1	17	1	1	0	0	16	4006.26324	-0.00003	4006.26327	768.04757	
39	1	1	1	-1	18	1	1	0	0	17	4008.20216	0.00047	4008.20169	800.34436	
40	1	1	1	-1	19	1	1	0	0	18	4010.14795	0.00031	4010.14764	834.53830	
41	1	1	1	-1	20	1	1	0	0	19	4012.10173	0.00051	4012.10122	870.62893	
42	1	1	1	-1	21	1	1	0	0	20	4014.06328	0.00083	4014.06245	908.61577	
43	1	1	1	-1	22	1	1	0	0	21	4016.02951	-0.00171	4016.03122	948.49830	†
44	1	1	1	-1	23	1	1	0	0	22	4017.99967*	-0.00775	4018.00742	990.27601	†
45	1	1	1	-1	24	1	1	0	0	23	4019.98922	-0.00164	4019.99086	1033.94833	†
46	1	1	1	-1	25	1	1	0	0	24	4021.97886*	-0.00247	4021.98133	1079.51468	†
47	1	1	1	-1	1	1	-1	0	0	1	3973.93004*	0.00471	3973.92533	511.49456	†
48	1	1	1	-1	2	1	-1	0	0	2	3973.90556	0.00105	3973.90451	515.31316	†
49	1	1	1	-1	3	1	-1	0	0	3	3973.87311	-0.00044	3973.87355	521.04101	
50	1	1	1	-1	4	1	-1	0	0	4	3973.83271	-0.00005	3973.83276	528.67801	
51	1	1	1	-1	5	1	-1	0	0	5	3973.78164	-0.00092	3973.78256	538.22407	
52	1	1	1	-1	6	1	-1	0	0	6	3973.72366	0.00018	3973.72348	549.67906	
53	1	1	1	-1	7	1	-1	0	0	7	3973.65640	0.00027	3973.65613	563.04281	
54	1	1	1	-1	8	1	-1	0	0	8	3973.58410*	0.00288	3973.58122	578.31514	†
55	1	1	1	-1	9	1	-1	0	0	9	3973.49700*	-0.00252	3973.49952	595.49585	†
56	1	1	1	-1	10	1	-1	0	0	10	3973.41163	-0.00025	3973.41188	614.58469	
57	1	1	1	-1	11	1	-1	0	0	11	3973.31937	0.00022	3973.31915	635.58142	
58	1	1	1	-1	12	1	-1	0	0	12	3973.22256	0.00035	3973.22221	658.48573	
59	1	1	1	-1	13	1	-1	0	0	13	3973.12153	-0.00038	3973.12191	683.29732	
60	1	1	1	-1	14	1	-1	0	0	14	3973.01894	-0.00011	3973.01905	710.01584	
	1	1	1	-1	15	1	-1	0	0	15	3972.91433	0.00000	3972.91433	738.64093	
	1	1	1	-1	16	1	-1	0	0	16	3972.80820	-0.00016	3972.80836	769.17220	
	1	1	1	-1	17	1	-1	0	0	17	3972.70153	-0.00009	3972.70162	801.60923	
	1	1	1	-1	18	1	-1	0	0	18	3972.59463	0.00015	3972.59448	835.95156	
	1	1	1	-1	19	1	-1	0	0	19	3972.48696	-0.00023	3972.48719	872.19874	

1	1	1	-1	20	1	-1	0	0	20	3972.37984	-0.00005	3972.37989	910.35027
1	1	1	-1	21	1	-1	0	0	21	3972.27246	-0.00014	3972.27260	950.40561
1	1	1	-1	22	1	-1	0	0	22	3972.16522	-0.00008	3972.16530	992.36423
1	1	1	-1	23	1	-1	0	0	23	3972.05802	0.00013	3972.05789	1036.22555
1	1	1	-1	24	1	-1	0	0	24	3971.95014	-0.00009	3971.95023	1081.98896
1	1	1	-1	25	1	-1	0	0	25	3971.84196	-0.00021	3971.84217	1129.65384
1	1	1	-1	26	1	-1	0	0	26	3971.73301	-0.00050	3971.73351	1179.21954
1	1	1	-1	27	1	-1	0	0	27	3971.62423	0.00015	3971.62408	1230.68537
1	1	1	-1	28	1	-1	0	0	28	3971.51356	-0.00012	3971.51368	1284.05064
1	1	1	-1	29	1	-1	0	0	29	3971.40173	-0.00040	3971.40213	1339.31460
1	1	1	-1	30	1	-1	0	0	30	3971.29136*	0.00210	3971.28926	1396.47651 +
1	1	1	-1	31	1	-1	0	0	31	3971.17304	-0.00185	3971.17489	1455.53557 +
1	1	1	-1	32	1	-1	0	0	32	3971.05450	-0.00437	3971.05887	1516.49098 +

rms = 0.00039 cm⁻¹

$v_1 + v_4 + v_5 (\Sigma^+) \leftarrow v_4 + v_5 (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	1 1 1 -1 1	3294.20090	-0.00010	3294.20100	1189.32003
1 1 1 -1 1	1 1 1 -1 2	3292.28468	-0.00019	3292.28487	1193.13502
1 1 1 -1 2	1 1 1 -1 3	3290.35811*	-0.00192	3290.36003	1198.85764 †
1 1 1 -1 3	1 1 1 -1 4	3288.42564*	-0.00084	3288.42648	1206.48808
1 1 1 -1 4	1 1 1 -1 5	3286.47722	-0.00701	3286.48423	1216.02655 †
1 1 1 -1 5	1 1 1 -1 6	3284.53325	-0.00005	3284.53330	1227.47333
1 1 1 -1 6	1 1 1 -1 7	3282.57385	0.00009	3282.57376	1240.82878
1 1 1 -1 7	1 1 1 -1 8	3280.60482	-0.00086	3280.60568	1256.09326
1 1 1 -1 8	1 1 1 -1 9	3278.62904	-0.00012	3278.62916	1273.26720
1 1 1 -1 9	1 1 1 -1 10	3276.64422	-0.00009	3276.64431	1292.35106
1 1 1 -1 10	1 1 1 -1 11	3274.65116	-0.00009	3274.65125	1313.34532
1 1 1 -1 11	1 1 1 -1 12	3272.64986	-0.00027	3272.65013	1336.25044
1 1 1 -1 12	1 1 1 -1 13	3270.64161	0.00055	3270.64106	1361.06689
1 1 1 -1 13	1 1 1 -1 14	3268.62479	0.00065	3268.62414	1387.79509
1 1 1 -1 14	1 1 1 -1 15	3266.59933	-0.00016	3266.59949	1416.43541
1 1 1 -1 15	1 1 1 -1 16	3264.56519	-0.00195	3264.56714	1446.98812 †
1 1 1 -1 16	1 1 1 -1 17	3262.52773	0.00059	3262.52714	1479.45342
1 1 1 -1 17	1 1 1 -1 18	3260.47944	-0.00003	3260.47947	1513.83138
1 1 1 -1 18	1 1 1 -1 19	3258.42199	-0.00211	3258.42410	1550.12195 †
1 1 1 -1 19	1 1 1 -1 20	3256.36013	-0.00085	3256.36098	1588.32496
1 1 1 -1 20	1 1 1 -1 21	3254.28590*	-0.00414	3254.29004	1628.44012 †
1 1 1 -1 21	1 1 1 -1 22	3252.21109	-0.00011	3252.21120	1670.46701
1 1 1 -1 22	1 1 1 -1 23	3250.12423	-0.00017	3250.12440	1714.40513
1 1 1 -1 23	1 1 1 -1 24	3248.03140*	0.00183	3248.02957	1760.25386 †
1 1 1 -1 24	1 1 1 -1 25	3245.92636	-0.00031	3245.92667	1808.01252
1 1 1 -1 25	1 1 1 -1 26	3243.81559	-0.00007	3243.81566	1857.68035
1 1 1 -1 26	1 1 1 -1 27	3241.69684*	0.00033	3241.69651	1909.25654
1 1 1 -1 27	1 1 1 -1 28	3239.56889	-0.00034	3239.56923	1962.74023
1 1 1 -1 1	1 1 1 -1 0	3298.00716	-0.00016	3298.00732	1187.41257
1 1 1 -1 2	1 1 1 -1 1	3299.89753	-0.00011	3299.89764	1189.32003
1 1 1 -1 3	1 1 1 -1 2	3301.77980	0.00026	3301.77954	1193.13502
1 1 1 -1 4	1 1 1 -1 3	3303.65263	-0.00050	3303.65313	1198.85764
1 1 1 -1 5	1 1 1 -1 4	3305.51860*	0.00004	3305.51856	1206.48808
1 1 1 -1 6	1 1 1 -1 5	3307.37610	0.00011	3307.37599	1216.02655
1 1 1 -1 7	1 1 1 -1 6	3309.22545	-0.00015	3309.22560	1227.47333
1 1 1 -1 8	1 1 1 -1 7	3311.06756	-0.00002	3311.06758	1240.82878
1 1 1 -1 9	1 1 1 -1 8	3312.89990	-0.00221	3312.90211	1256.09326 †
1 1 1 -1 10	1 1 1 -1 9	3314.72928	-0.00009	3314.72937	1273.26720
1 1 1 -1 11	1 1 1 -1 10	3316.55092*	0.00142	3316.54950	1292.35106 †
1 1 1 -1 12	1 1 1 -1 11	3318.36253	-0.00010	3318.36263	1313.34532
1 1 1 -1 13	1 1 1 -1 12	3320.16886	0.00006	3320.16880	1336.25044
1 1 1 -1 14	1 1 1 -1 13	3321.96852*	0.00052	3321.96800	1361.06689
1 1 1 -1 15	1 1 1 -1 14	3323.76001	-0.00016	3323.76017	1387.79509
1 1 1 -1 16	1 1 1 -1 15	3325.54495	-0.00020	3325.54515	1416.43541

1															
2	1	1	1	-1	17	1	1	1	-1	16	3327.32170	-0.00102	3327.32272	1446.98812	†
3	1	1	1	-1	18	1	1	1	-1	17	3329.08980*	-0.00283	3329.09263	1479.45342	†
4	1	1	1	-1	19	1	1	1	-1	18	3330.85557	0.00101	3330.85456	1513.83138	†
5	1	1	1	-1	20	1	1	1	-1	19	3332.60825	0.00005	3332.60820	1550.12195	
6	1	1	1	-1	21	1	1	1	-1	20	3334.35340	0.00015	3334.35325	1588.32496	
7	1	1	1	-1	22	1	1	1	-1	21	3336.08925	-0.00016	3336.08941	1628.44012	
8	1	1	1	-1	23	1	1	1	-1	22	3337.81676	0.00033	3337.81643	1670.46701	
9	1	1	1	-1	24	1	1	1	-1	23	3339.53449	0.00042	3339.53407	1714.40513	
10	1	1	1	-1	25	1	1	1	-1	24	3341.24226	0.00011	3341.24215	1760.25386	
11	1	1	1	-1	26	1	1	1	-1	25	3342.94900*	0.00847	3342.94053	1808.01252	†
12	1	1	1	-1	27	1	1	1	-1	26	3344.62881	-0.00029	3344.62910	1857.68035	

rms = 0.00032 cm⁻¹

$V_1 + V_4 + V_5 (\Sigma^-) \leftarrow V_4 (\Pi)$

	$v_4' \ell_4' v_5' \ell_5' J'$					$v_4'' \ell_4'' v_5'' \ell_5'' J''$				OBS	OBS – CALC	E'	E''	
19	1	-1	1	1	0	1	-1	0	0	1	3969.06140	0.00040	3969.06100	511.49456
20	1	-1	1	1	1	1	-1	0	0	2	3967.14188	0.00055	3967.14133	515.31316
21	1	-1	1	1	2	1	-1	0	0	3	3965.21194	0.00058	3965.21136	521.04101
22	1	-1	1	1	3	1	-1	0	0	4	3963.27146	0.00032	3963.27114	528.67801
23	1	-1	1	1	4	1	-1	0	0	5	3961.32121	0.00043	3961.32078	538.22407
24	1	-1	1	1	5	1	-1	0	0	6	3959.36080	0.00043	3959.36037	549.67906
25	1	-1	1	1	6	1	-1	0	0	7	3957.39010	0.00007	3957.39003	563.04281
26	1	-1	1	1	7	1	-1	0	0	8	3955.40978	-0.00013	3955.40991	578.31514
27	1	-1	1	1	8	1	-1	0	0	9	3953.42013	-0.00001	3953.42014	595.49585
28	1	-1	1	1	9	1	-1	0	0	10	3951.42136	0.00050	3951.42086	614.58469
29	1	-1	1	1	10	1	-1	0	0	11	3949.41217	-0.00006	3949.41223	635.58142
30	1	-1	1	1	11	1	-1	0	0	12	3947.39420	-0.00018	3947.39438	658.48573
31	1	-1	1	1	12	1	-1	0	0	13	3945.36795	0.00055	3945.36740	683.29732
32	1	-1	1	1	13	1	-1	0	0	14	3943.33127	-0.00013	3943.33140	710.01584
33	1	-1	1	1	14	1	-1	0	0	15	3941.28615	-0.00029	3941.28644	738.64093
34	1	-1	1	1	15	1	-1	0	0	16	3939.23247	-0.00011	3939.23258	769.17220
35	1	-1	1	1	16	1	-1	0	0	17	3937.16976	-0.00009	3937.16985	801.60923
36	1	-1	1	1	17	1	-1	0	0	18	3935.09813	-0.00014	3935.09827	835.95156
37	1	-1	1	1	18	1	-1	0	0	19	3933.01777	-0.00009	3933.01786	872.19874
38	1	-1	1	1	19	1	-1	0	0	20	3930.92864	0.00002	3930.92862	910.35027
39	1	-1	1	1	20	1	-1	0	0	21	3928.83063	0.00008	3928.83055	950.40561
40	1	-1	1	1	21	1	-1	0	0	22	3926.72390	0.00022	3926.72368	992.36423
41	1	-1	1	1	22	1	-1	0	0	23	3924.60800	0.00001	3924.60799	1036.22555
42	1	-1	1	1	23	1	-1	0	0	24	3922.48353	0.00002	3922.48351	1081.98896
43	1	-1	1	1	24	1	-1	0	0	25	3920.35048	0.00023	3920.35025	1129.65384
44	1	-1	1	1	25	1	-1	0	0	26	3918.20824	0.00003	3918.20821	1179.21954
45	1	-1	1	1	26	1	-1	0	0	27	3916.05684	-0.00057	3916.05741	1230.68537
46	1	-1	1	1	27	1	-1	0	0	28	3913.89822	0.00034	3913.89788	1284.05064
47	1	-1	1	1	28	1	-1	0	0	29	3911.72999	0.00037	3911.72962	1339.31460
48	1	-1	1	1	29	1	-1	0	0	30	3909.55538	0.00271	3909.55267	1396.47651 †
49	1	-1	1	1	30	1	-1	0	0	31	3907.36966	0.00262	3907.36704	1455.53557 †
50	1	-1	1	1	31	1	-1	0	0	32	3905.17548	0.00272	3905.17276	1516.49098 †
51	1	-1	1	1	32	1	-1	0	0	33	3902.97285	0.00299	3902.96986	1579.34190 †
52	1	-1	1	1	33	1	-1	0	0	34	3900.75660	-0.00176	3900.75836	1644.08748 †
53	1	-1	1	1	34	1	-1	0	0	35	3898.53845	0.00016	3898.53829	1710.72682
54	1	-1	1	1	2	1	-1	0	0	1	3974.75911*	0.00130	3974.75781	511.49456 †
55	1	-1	1	1	3	1	-1	0	0	2	3976.63667	0.00068	3976.63599	515.31316
56	1	-1	1	1	4	1	-1	0	0	3	3978.50430	0.00046	3978.50384	521.04101
57	1	-1	1	1	5	1	-1	0	0	4	3980.36203	0.00062	3980.36141	528.67801
58	1	-1	1	1	6	1	-1	0	0	5	3982.20894	0.00017	3982.20877	538.22407
59	1	-1	1	1	7	1	-1	0	0	6	3984.04594	-0.00005	3984.04599	549.67906
60	1	-1	1	1	8	1	-1	0	0	7	3985.87378	0.00060	3985.87318	563.04281
	1	-1	1	1	9	1	-1	0	0	8	3987.69014	-0.00028	3987.69042	578.31514
	1	-1	1	1	10	1	-1	0	0	9	3989.49774	-0.00006	3989.49780	595.49585
	1	-1	1	1	11	1	-1	0	0	10	3991.29540	-0.00001	3991.29541	614.58469
	1	-1	1	1	12	1	-1	0	0	11	3993.08316	-0.00014	3993.08330	635.58142

1	-1	1	1	13	1	-1	0	0	12	3994.86147	-0.00004	3994.86151	658.48573
1	-1	1	1	14	1	-1	0	0	13	3996.63052	0.00046	3996.63006	683.29732
1	-1	1	1	15	1	-1	0	0	14	3998.38881	-0.00013	3998.38894	710.01584
1	-1	1	1	16	1	-1	0	0	15	4000.13812	-0.00003	4000.13815	738.64093
1	-1	1	1	17	1	-1	0	0	16	4001.87752	-0.00012	4001.87764	769.17220
1	-1	1	1	18	1	-1	0	0	17	4003.60728	-0.00009	4003.60737	801.60923
1	-1	1	1	19	1	-1	0	0	18	4005.32726	-0.00006	4005.32732	835.95156
1	-1	1	1	20	1	-1	0	0	19	4007.03739	-0.00003	4007.03742	872.19874
1	-1	1	1	21	1	-1	0	0	20	4008.73763	-0.00001	4008.73764	910.35027
1	-1	1	1	22	1	-1	0	0	21	4010.42822	0.00029	4010.42793	950.40561
1	-1	1	1	23	1	-1	0	0	22	4012.10833	0.00009	4012.10824	992.36423
1	-1	1	1	24	1	-1	0	0	23	4013.78422*	0.00568	4013.77854	1036.22555 +
1	-1	1	1	25	1	-1	0	0	24	4015.43916	0.00037	4015.43879	1081.98896
1	-1	1	1	26	1	-1	0	0	25	4017.08936	0.00042	4017.08894	1129.65384
1	-1	1	1	27	1	-1	0	0	26	4018.72794	-0.00103	4018.72897	1179.21954 +
1	-1	1	1	28	1	-1	0	0	27	4020.35904	0.00019	4020.35885	1230.68537
1	-1	1	1	29	1	-1	0	0	28	4021.97943	0.00090	4021.97853	1284.05064
1	-1	1	1	30	1	-1	0	0	29	4023.59024*	0.00224	4023.58800	1339.31460 +
1	-1	1	1	31	1	-1	0	0	30	4025.18716	-0.00007	4025.18723	1396.47651
1	-1	1	1	32	1	-1	0	0	31	4026.77301	-0.00318	4026.77619	1455.53557 +
1	-1	1	1	33	1	-1	0	0	32	4028.35243	-0.00243	4028.35486	1516.49098 +
1	-1	1	1	5	1	1	0	0	5	3970.94280*	0.00317	3970.93963	538.09979 +
1	-1	1	1	6	1	1	0	0	6	3970.92997*	0.00221	3970.92776	549.50508 +
1	-1	1	1	7	1	1	0	0	7	3970.91541*	0.00123	3970.91418	562.81086 +
1	-1	1	1	8	1	1	0	0	8	3970.90063	0.00161	3970.89902	578.01697 +
1	-1	1	1	9	1	1	0	0	9	3970.88279	0.00042	3970.88237	595.12319
1	-1	1	1	10	1	1	0	0	10	3970.86463	0.00027	3970.86436	614.12929
1	-1	1	1	11	1	1	0	0	11	3970.84568	0.00060	3970.84508	635.03503
1	-1	1	1	12	1	1	0	0	12	3970.82463	0.00003	3970.82460	657.84012
1	-1	1	1	13	1	1	0	0	13	3970.80275	-0.00022	3970.80297	682.54427
1	-1	1	1	14	1	1	0	0	14	3970.77810	-0.00215	3970.78025	709.14713 +

rms = 0.00033 cm⁻¹

$$V_1 + V_4 + V_5 (\Sigma^-) \leftarrow V_4 + V_5 (\Sigma^-)$$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	E'	E''
1	-1	1	1	0	1	-1	1	1	1	3294.90354	-0.00004	3294.90358	1185.65198
1	-1	1	1	1	1	-1	1	1	2	3292.98657	-0.00086	3292.98743	1189.46706
1	-1	1	1	2	1	-1	1	1	3	3291.05962*	-0.00307	3291.06269	1195.18967
1	-1	1	1	3	1	-1	1	1	4	3289.12862	-0.00077	3289.12939	1202.81976
1	-1	1	1	4	1	-1	1	1	5	3287.18737	-0.00018	3287.18755	1212.35731
1	-1	1	1	5	1	-1	1	1	6	3285.23718	-0.00001	3285.23719	1223.80224
1	-1	1	1	6	1	-1	1	1	7	3283.27737	-0.00097	3283.27834	1237.15450
1	-1	1	1	7	1	-1	1	1	8	3281.30970	-0.00134	3281.31104	1252.41400
1	-1	1	1	8	1	-1	1	1	9	3279.33604	0.00071	3279.33533	1269.58065
1	-1	1	1	9	1	-1	1	1	10	3277.35175	0.00051	3277.35124	1288.65432
1	-1	1	1	10	1	-1	1	1	11	3275.35913*	0.00034	3275.35879	1309.63487
1	-1	1	1	11	1	-1	1	1	12	3273.35835	0.00034	3273.35801	1332.52210
1	-1	1	1	12	1	-1	1	1	13	3271.34876	-0.00016	3271.34892	1357.31580
1	-1	1	1	13	1	-1	1	1	14	3269.33113	-0.00041	3269.33154	1384.01571
1	-1	1	1	14	1	-1	1	1	15	3267.30518	-0.00068	3267.30586	1412.62152
1	-1	1	1	15	1	-1	1	1	16	3265.27136	-0.00054	3265.27190	1443.13289
1	-1	1	1	16	1	-1	1	1	17	3263.23136*	0.00171	3263.22965	1475.54942
1	-1	1	1	17	1	-1	1	1	18	3261.17852	-0.00062	3261.17914	1509.87069
1	-1	1	1	18	1	-1	1	1	19	3259.11875	-0.00162	3259.12037	1546.09623
1	-1	1	1	19	1	-1	1	1	20	3257.05059*	-0.00278	3257.05337	1584.22551
1	-1	1	1	20	1	-1	1	1	21	3254.97906	0.00091	3254.97815	1624.25802
1	-1	1	1	21	1	-1	1	1	22	3252.89447	-0.00027	3252.89474	1666.19317
1	-1	1	1	22	1	-1	1	1	23	3250.80294	-0.00023	3250.80317	1710.03037
1	-1	1	1	23	1	-1	1	1	24	3248.70446	0.00098	3248.70348	1755.76899
1	-1	1	1	24	1	-1	1	1	25	3246.59670*	0.00100	3246.59570	1803.40839

1														
2	1	-1	1	1	25	1	-1	1	1	26	3244.47948	-0.00039	3244.47987	1852.94788
3	1	-1	1	1	26	1	-1	1	1	27	3242.35768	0.00166	3242.35602	1904.38677 +
4	1	-1	1	1	27	1	-1	1	1	28	3240.22364	-0.00055	3240.22419	1957.72433
5	1	-1	1	1	1	1	-1	1	1	0	3298.71117*	0.00110	3298.71007	1183.74443 +
6	1	-1	1	1	2	1	-1	1	1	1	3300.60086	0.00047	3300.60039	1185.65198
7	1	-1	1	1	3	1	-1	1	1	2	3302.48112	-0.00097	3302.48209	1189.46706
8	1	-1	1	1	4	1	-1	1	1	3	3304.35683*	0.00165	3304.35518	1195.18967 +
9	1	-1	1	1	5	1	-1	1	1	4	3306.21898*	-0.00068	3306.21966	1202.81976
10	1	-1	1	1	6	1	-1	1	1	5	3308.07971*	0.00418	3308.07553	1212.35731 +
11	1	-1	1	1	7	1	-1	1	1	6	3309.92270	-0.00011	3309.92281	1223.80224
12	1	-1	1	1	8	1	-1	1	1	7	3311.76446*	0.00298	3311.76148	1237.15450 +
13	1	-1	1	1	9	1	-1	1	1	8	3313.59124	-0.00032	3313.59156	1252.41400
14	1	-1	1	1	10	1	-1	1	1	9	3315.41193	-0.00107	3315.41300	1269.58065 +
15	1	-1	1	1	11	1	-1	1	1	10	3317.22540	-0.00038	3317.22578	1288.65432
16	1	-1	1	1	12	1	-1	1	1	11	3319.02955	-0.00030	3319.02985	1309.63487
17	1	-1	1	1	13	1	-1	1	1	12	3320.82416	-0.00098	3320.82514	1332.52210
18	1	-1	1	1	14	1	-1	1	1	13	3322.61184	0.00026	3322.61158	1357.31580
19	1	-1	1	1	15	1	-1	1	1	14	3324.38873	-0.00035	3324.38908	1384.01571
20	1	-1	1	1	16	1	-1	1	1	15	3326.15762	0.00006	3326.15756	1412.62152
21	1	-1	1	1	17	1	-1	1	1	16	3327.91639	-0.00056	3327.91695	1443.13289
22	1	-1	1	1	18	1	-1	1	1	17	3329.66691	-0.00027	3329.66718	1475.54942
23	1	-1	1	1	19	1	-1	1	1	18	3331.40789	-0.00030	3331.40819	1509.87069
24	1	-1	1	1	20	1	-1	1	1	19	3333.13969	-0.00025	3333.13994	1546.09623
25	1	-1	1	1	21	1	-1	1	1	20	3334.86186	-0.00054	3334.86240	1584.22551
26	1	-1	1	1	22	1	-1	1	1	21	3336.57529	-0.00023	3336.57552	1624.25802
27	1	-1	1	1	23	1	-1	1	1	22	3338.27849	-0.00082	3338.27931	1666.19317
28	1	-1	1	1	24	1	-1	1	1	23	3339.96706*	-0.00666	3339.97372	1710.03037 +
29	1	-1	1	1	25	1	-1	1	1	24	3341.65891	0.00016	3341.65875	1755.76899
30	1	-1	1	1	26	1	-1	1	1	25	3343.33431	-0.00009	3343.33440	1803.40839
31	1	-1	1	1	27	1	-1	1	1	26	3345.00053	-0.00010	3345.00063	1852.94788
32	1	-1	1	1	28	1	-1	1	1	27	3346.65673*	-0.00072	3346.65745	1904.38677
33	1	-1	1	1	29	1	-1	1	1	28	3348.30451	-0.00034	3348.30485	1957.72433
34	1	-1	1	1	30	1	-1	1	1	29	3349.94308	0.00027	3349.94281	2012.95980
35	1	-1	1	1	31	1	-1	1	1	30	3351.56994	-0.00138	3351.57132	2070.09242 +

rms = 0.00052 cm⁻¹

$V_1 + V_4 + V_5 (\Delta) \leftarrow V_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 2	1 1 0 0 3	3965.07505	-0.00002	3965.07507	520.99129
1 1 1 1 3	1 1 0 0 4	3963.16650	-0.00083	3963.16733	528.59515
1 1 1 1 4	1 1 0 0 5	3961.25665	-0.00026	3961.25691	538.09979
1 1 1 1 5	1 1 0 0 6	3959.34372	0.00031	3959.34341	549.50508
1 1 1 1 6	1 1 0 0 7	3957.42658	0.00024	3957.42634	562.81086
1 1 1 1 7	1 1 0 0 8	3955.50501	-0.00009	3955.50510	578.01697
1 1 1 1 8	1 1 0 0 9	3953.58009*	0.00107	3953.57902	595.12319 †
1 1 1 1 9	1 1 0 0 10	3951.64720	-0.00013	3951.64733	614.12929
1 1 1 1 10	1 1 0 0 11	3949.70945	0.00023	3949.70922	635.03503
1 1 1 1 11	1 1 0 0 12	3947.76396	0.00010	3947.76386	657.84012
1 1 1 1 12	1 1 0 0 13	3945.81049	0.00010	3945.81039	682.54427
1 1 1 1 13	1 1 0 0 14	3943.85021*	0.00222	3943.84799	709.14713 †
1 1 1 1 14	1 1 0 0 15	3941.87635	0.00047	3941.87588	737.64836
1 1 1 1 15	1 1 0 0 16	3939.89381	0.00043	3939.89338	768.04757
1 1 1 1 16	1 1 0 0 17	3937.90011	0.00020	3937.89991	800.34436
1 1 1 1 17	1 1 0 0 18	3935.89717*	0.00218	3935.89499	834.53830 †
1 1 1 1 18	1 1 0 0 19	3933.87850	0.00021	3933.87829	870.62893
1 1 1 1 19	1 1 0 0 20	3931.84968	0.00009	3931.84959	908.61577
1 1 1 1 20	1 1 0 0 21	3929.80913	0.00037	3929.80876	948.49830
1 1 1 1 21	1 1 0 0 22	3927.75636	0.00057	3927.75579	990.27601
1 1 1 1 22	1 1 0 0 23	3925.69062	-0.00013	3925.69075	1033.94833
1 1 1 1 23	1 1 0 0 24	3923.61395	0.00022	3923.61373	1079.51468

1														
2	1	1	1	1	24	1	1	0	0	25	3921.52483	-0.00007	3921.52490	1126.97445
3	1	1	1	1	25	1	1	0	0	26	3919.42455	0.00010	3919.42445	1176.32701
4	1	1	1	1	26	1	1	0	0	27	3917.31201	-0.00056	3917.31257	1227.57169
5	1	1	1	1	27	1	1	0	0	28	3915.18926	-0.00021	3915.18947	1280.70782
6	1	1	1	1	28	1	1	0	0	29	3913.05519	-0.00018	3913.05537	1335.73468
7	1	1	1	1	29	1	1	0	0	30	3910.91118	0.00072	3910.91046	1392.65154
8	1	1	1	1	30	1	1	0	0	31	3908.75512	0.00018	3908.75494	1451.45764
9	1	1	1	1	31	1	1	0	0	32	3906.58611*	-0.00288	3906.58899	1512.15220 †
10	1	1	1	1	32	1	1	0	0	33	3904.41658	0.00379	3904.41279	1574.73441 †
11	1	1	1	1	33	1	1	0	0	34	3902.22862*	0.00212	3902.22650	1639.20342 †
12	1	1	1	1	2	1	1	0	0	1	3974.57282*	-0.00727	3974.58009	511.48627
13	1	1	1	1	3	1	1	0	0	2	3976.47379	-0.00039	3976.47418	515.28830
14	1	1	1	1	4	1	1	0	0	3	3978.36506	-0.00035	3978.36541	520.99129
15	1	1	1	1	5	1	1	0	0	4	3980.25329	-0.00005	3980.25334	528.59515
16	1	1	1	1	6	1	1	0	0	5	3982.13728	-0.00013	3982.13741	538.09979
17	1	1	1	1	7	1	1	0	0	6	3984.01700	0.00001	3984.01699	549.50508
18	1	1	1	1	8	1	1	0	0	7	3985.89240	0.00106	3985.89134	562.81086 †
19	1	1	1	1	9	1	1	0	0	8	3987.75990	0.00025	3987.75965	578.01697
20	1	1	1	1	10	1	1	0	0	9	3989.62105	-0.00002	3989.62107	595.12319
21	1	1	1	1	11	1	1	0	0	10	3991.47468	-0.00002	3991.47470	614.12929
22	1	1	1	1	12	1	1	0	0	11	3993.31970	0.00007	3993.31963	635.03503
23	1	1	1	1	13	1	1	0	0	12	3995.15450	-0.00050	3995.15500	657.84012
24	1	1	1	1	14	1	1	0	0	13	3996.97978	-0.00019	3996.97997	682.54427
25	1	1	1	1	15	1	1	0	0	14	3998.79253*	-0.00129	3998.79382	709.14713 †
26	1	1	1	1	16	1	1	0	0	15	4000.59751	0.00160	4000.59591	737.64836 †
27	1	1	1	1	17	1	1	0	0	16	4002.38105	-0.00467	4002.38572	768.04757 †
28	1	1	1	1	18	1	1	0	0	17	4004.16295	0.00009	4004.16286	800.34436
29	1	1	1	1	19	1	1	0	0	18	4005.92705	0.00000	4005.92705	834.53830
30	1	1	1	1	20	1	1	0	0	19	4007.67853	0.00039	4007.67814	870.62893
31	1	1	1	1	21	1	1	0	0	20	4009.41726*	0.00122	4009.41604	908.61577 †
32	1	1	1	1	22	1	1	0	0	21	4011.14081*	0.00004	4011.14077	948.49830
33	1	1	1	1	23	1	1	0	0	22	4012.85255	0.00015	4012.85240	990.27601
34	1	1	1	1	24	1	1	0	0	23	4014.55125	0.00023	4014.55102	1033.94833
35	1	1	1	1	25	1	1	0	0	24	4016.24863*	0.01186	4016.23677	1079.51468 †
36	1	1	1	1	26	1	1	0	0	25	4017.91005	0.00024	4017.90981	1126.97445
37	1	1	1	1	27	1	1	0	0	26	4019.56913	-0.00115	4019.57028	1176.32701 †
38	1	1	1	1	28	1	1	0	0	27	4021.21996	0.00160	4021.21836	1227.57169 †
39	1	1	1	1	29	1	1	0	0	28	4022.85363	-0.00055	4022.85418	1280.70782
40	1	1	1	1	30	1	1	0	0	29	4024.47672	-0.00118	4024.47790	1335.73468 †
41	1	1	1	1	31	1	1	0	0	30	4026.08990	0.00025	4026.08965	1392.65154
42	1	1	1	1	32	1	1	0	0	31	4027.69107	0.00152	4027.68955	1451.45764 †
43	1	1	1	1	33	1	1	0	0	32	4029.30280*	0.02508	4029.27772	1512.15220 †
44	1	1	1	1	34	1	1	0	0	33	4030.85340	-0.00086	4030.85426	1574.73441
45	1	1	1	1	35	1	1	0	0	34	4032.41960	0.00035	4032.41925	1639.20342
46	1	1	1	1	2	1	-1	0	0	2	3970.75363	0.00044	3970.75319	515.31316
47	1	1	1	1	3	1	-1	0	0	3	3970.72270	0.00123	3970.72147	521.04101 †
48	1	1	1	1	4	1	-1	0	0	4	3970.67991	0.00122	3970.67869	528.67801 †
49	1	1	1	1	5	1	-1	0	0	5	3970.62740	0.00298	3970.62442	538.22407 †
50	1	1	1	1	6	1	-1	0	0	6	3970.56209	0.00394	3970.55815	549.67906 †
51	1	1	1	1	7	1	-1	0	0	7	3970.48534	0.00608	3970.47926	563.04281 †
52	1	1	1	1	8	1	-1	0	0	8	3970.39454	0.00748	3970.38706	578.31514 †
53	1	1	1	1	9	1	-1	0	0	9	3970.28305	0.00228	3970.28077	595.49585 †
54	1	1	1	1	10	1	-1	0	0	10	3970.16081	0.00125	3970.15956	614.58469 †
55	1	1	1	1	11	1	-1	0	0	11	3970.02322	0.00065	3970.02257	635.58142
56	1	1	1	1	12	1	-1	0	0	12	3969.86907	0.00014	3969.86893	658.48573
57	1	1	1	1	13	1	-1	0	0	13	3969.69777	-0.00003	3969.69780	683.29732
58	1	1	1	1	14	1	-1	0	0	14	3969.50783	-0.00057	3969.50840	710.01584
59	1	1	1	1	15	1	-1	0	0	15	3969.28944*	-0.01058	3969.30002	738.64093 †
60	1	1	1	1	16	1	-1	0	0	16	3969.07123	-0.00084	3969.07207	769.17220
	1	1	1	1	17	1	-1	0	0	17	3968.82465	0.00058	3968.82407	801.60923
	1	1	1	1	18	1	-1	0	0	18	3968.55601	0.00035	3968.55566	835.95156
	1	1	1	1	19	1	-1	0	0	19	3968.26711	0.00050	3968.26661	872.19874
	1	1	1	1	20	1	-1	0	0	20	3967.95251	-0.00429	3967.95680	910.35027 †
	1	1	1	1	21	1	-1	0	0	21	3967.62854	0.00235	3967.62619	950.40561 †
	1	1	1	1	22	1	-1	0	0	22	3967.27510	0.00025	3967.27485	992.36423

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1	-1	1	-1	23	1	1	0	0	23	3970.04878	0.000004	3970.04874	1033.94833
1	-1	1	-1	24	1	1	0	0	24	3969.97950*	0.000001	3969.97949	1079.51468
1	-1	1	-1	25	1	1	0	0	25	3969.90701*	-0.000007	3969.90708	1126.97445
1	-1	1	-1	26	1	1	0	0	26	3969.83174	0.000022	3969.83152	1176.32701
1	-1	1	-1	27	1	1	0	0	27	3969.75212	-0.000068	3969.75280	1227.57169
1	-1	1	-1	28	1	1	0	0	28	3969.67098	0.000004	3969.67094	1280.70782
1	-1	1	-1	29	1	1	0	0	29	3969.58565	-0.000028	3969.58593	1335.73468
1	-1	1	-1	30	1	1	0	0	30	3969.49775*	-0.000002	3969.49777	1392.65154
1	-1	1	-1	31	1	1	0	0	31	3969.40685	0.000041	3969.40644	1451.45764
1	-1	1	-1	32	1	1	0	0	32	3969.31168*	-0.000027	3969.31195	1512.15220
1	-1	1	-1	33	1	1	0	0	33	3969.21644	0.000215	3969.21429	1574.73441 +
1	-1	1	-1	34	1	1	0	0	34	3969.11341	-0.000003	3969.11344	1639.20342
1	-1	1	-1	35	1	1	0	0	35	3969.00584	-0.000356	3969.00940	1705.55838 +
1	-1	1	-1	36	1	1	0	0	36	3968.90248	0.000032	3968.90216	1773.79841

rms = 0.00040 cm⁻¹

$$v_1 + v_4 + v_5 (\Delta) \leftarrow v_4 + v_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 2	1 1 1 1 3	3291.16045	0.00018	3291.16027	1194.90609
1 1 1 1 3	1 1 1 1 4	3289.22609	-0.00133	3289.22742	1202.53506 †
1 1 1 1 4	1 1 1 1 5	3287.28522	-0.00102	3287.28624	1212.07046 †
1 1 1 1 5	1 1 1 1 6	3285.33533	-0.00142	3285.33675	1223.51174 †
1 1 1 1 6	1 1 1 1 7	3283.37690	-0.00205	3283.37895	1236.85825 †
1 1 1 1 7	1 1 1 1 8	3281.40869	-0.00413	3281.41282	1252.10924 †
1 1 1 1 8	1 1 1 1 9	3279.43539	-0.00293	3279.43832	1269.26388 †
1 1 1 1 9	1 1 1 1 10	3277.45177	-0.00362	3277.45539	1288.32123 †
1 1 1 1 10	1 1 1 1 11	3275.46234	-0.00161	3275.46395	1309.28031 †
1 1 1 1 11	1 1 1 1 12	3273.45975	-0.00418	3273.46393	1332.14005 †
1 1 1 1 12	1 1 1 1 13	3271.44993	-0.00535	3271.45528	1356.89938 †
1 1 1 1 13	1 1 1 1 14	3269.43354	-0.00438	3269.43792	1383.55720 †
1 1 1 1 14	1 1 1 1 15	3267.40857	-0.00326	3267.41183	1412.11241 †
1 1 1 1 15	1 1 1 1 16	3265.37312	-0.00389	3265.37701	1442.56394 †
1 1 1 1 16	1 1 1 1 17	3263.33206	-0.00143	3263.33349	1474.91078 †
1 1 1 1 17	1 1 1 1 18	3261.28261	0.00129	3261.28132	1509.15197 †
1 1 1 1 18	1 1 1 1 19	3259.22517	0.00456	3259.22061	1545.28661 †
1 1 1 1 19	1 1 1 1 20	3257.15390	0.00243	3257.15147	1583.31388 †
1 1 1 1 20	1 1 1 1 21	3255.07488	0.00086	3255.07402	1623.23305
1 1 1 1 21	1 1 1 1 22	3252.98830	-0.00010	3252.98840	1665.04341
1 1 1 1 22	1 1 1 1 23	3250.89445	-0.00028	3250.89473	1708.74434
1 1 1 1 23	1 1 1 1 24	3248.78871*	-0.00444	3248.79315	1754.33526 †
1 1 1 1 24	1 1 1 1 25	3246.68429	0.00053	3246.68376	1801.81559
1 1 1 1 25	1 1 1 1 26	3244.57582*	0.000916	3244.56666	1851.18480 †
1 1 1 1 26	1 1 1 1 27	3242.44281*	0.00089	3242.44192	1902.44233
1 1 1 1 27	1 1 1 1 28	3240.30944	-0.00019	3240.30963	1955.58766
1 1 1 1 28	1 1 1 1 29	3238.16930	-0.00053	3238.16983	2010.62021
1 1 1 1 29	1 1 1 1 30	3236.01471*	-0.00787	3236.02258	2067.53942 †
1 1 1 1 30	1 1 1 1 31	3233.86605	-0.00185	3233.86790	2126.34468 †
1 1 1 1 3	1 1 1 1 2	3302.57898	0.00048	3302.57850	1189.18398
1 1 1 1 4	1 1 1 1 3	3304.45062	0.000001	3304.45061	1194.90609
1 1 1 1 5	1 1 1 1 4	3306.31488	0.00145	3306.31343	1202.53506 †
1 1 1 1 6	1 1 1 1 5	3308.16810	0.00136	3308.16674	1212.07046 †
1 1 1 1 7	1 1 1 1 6	3310.00804*	-0.00229	3310.01033	1223.51174 †
1 1 1 1 8	1 1 1 1 7	3311.84514	0.00119	3311.84395	1236.85825 †
1 1 1 1 9	1 1 1 1 8	3313.66614*	-0.00123	3313.66737	1252.10924 †
1 1 1 1 10	1 1 1 1 9	3315.47956	-0.00082	3315.48038	1269.26388
1 1 1 1 11	1 1 1 1 10	3317.28257	-0.00018	3317.28275	1288.32123
1 1 1 1 12	1 1 1 1 11	3319.07301	-0.00134	3319.07435	1309.28031 †
1 1 1 1 13	1 1 1 1 12	3320.85436	-0.00071	3320.85507	1332.14005
1 1 1 1 14	1 1 1 1 13	3322.62441	-0.00045	3322.62486	1356.89938
1 1 1 1 15	1 1 1 1 14	3324.38572	0.00197	3324.38375	1383.55720 †

1	1	1	1	1	16	1	1	1	1	15	3326.13127*	-0.00059	3326.13186	1412.11241
2	1	1	1	1	17	1	1	1	1	16	3327.86908	-0.00027	3327.86935	1442.56394
3	1	1	1	1	18	1	1	1	1	17	3329.59659	0.00015	3329.59644	1474.91078
4	1	1	1	1	19	1	1	1	1	18	3331.31342	0.00004	3331.31338	1509.15197
5	1	1	1	1	20	1	1	1	1	19	3333.02007	-0.00039	3333.02046	1545.28661
6	1	1	1	1	21	1	1	1	1	20	3334.71790	-0.00003	3334.71793	1583.31388
7	1	1	1	1	22	1	1	1	1	21	3336.40557	-0.00046	3336.40603	1623.23305
8	1	1	1	1	23	1	1	1	1	22	3338.08438	-0.00062	3338.08500	1665.04341
9	1	1	1	1	24	1	1	1	1	23	3339.74385*	-0.01116	3339.75501	1708.74434 +
10	1	1	1	1	25	1	1	1	1	24	3341.41812*	0.00193	3341.41619	1754.33526 +
11	1	1	1	1	26	1	1	1	1	25	3343.06752	-0.00114	3343.06866	1801.81559
12	1	1	1	1	27	1	1	1	1	26	3344.70924*	-0.00325	3344.71249	1851.18480 +
13	1	1	1	1	29	1	1	1	1	28	3347.97490	0.00056	3347.97434	1955.58766
14	1	-1	1	-1	2	1	-1	1	-1	3	3291.16045	0.00044	3291.16001	1194.90643
15	1	-1	1	-1	3	1	-1	1	-1	4	3289.22609	-0.00074	3289.22683	1202.53608
16	1	-1	1	-1	4	1	-1	1	-1	5	3287.28522	0.00006	3287.28516	1212.07282
17	1	-1	1	-1	5	1	-1	1	-1	6	3285.33533	0.00031	3285.33502	1223.51646
18	1	-1	1	-1	6	1	-1	1	-1	7	3283.37690	0.00046	3283.37644	1236.86675
19	1	-1	1	-1	7	1	-1	1	-1	8	3281.40869	-0.00074	3281.40943	1252.12340
20	1	-1	1	-1	8	1	-1	1	-1	9	3279.43539	0.00136	3279.43403	1269.28609 +
21	1	-1	1	-1	9	1	-1	1	-1	10	3277.45177	0.00152	3277.45025	1288.35448 +
22	1	-1	1	-1	10	1	-1	1	-1	11	3275.46234	0.00423	3275.45811	1309.32820 +
23	1	-1	1	-1	11	1	-1	1	-1	12	3273.45975	0.00209	3273.45766	1332.20685 +
24	1	-1	1	-1	12	1	-1	1	-1	13	3271.44993	0.00101	3271.44892	1356.99004 +
25	1	-1	1	-1	13	1	-1	1	-1	14	3269.43354	0.00161	3269.43193	1383.67734 +
26	1	-1	1	-1	14	1	-1	1	-1	15	3267.40857	0.00181	3267.40676	1412.26833 +
27	1	-1	1	-1	15	1	-1	1	-1	16	3265.37312	-0.00033	3265.37345	1442.76257
28	1	-1	1	-1	16	1	-1	1	-1	17	3263.33206	0.00000	3263.33206	1475.15963
29	1	-1	1	-1	17	1	-1	1	-1	18	3261.28261	-0.00001	3261.28262	1509.45905
30	1	-1	1	-1	18	1	-1	1	-1	19	3259.22380	-0.00139	3259.22519	1545.66036 +
31	1	-1	1	-1	19	1	-1	1	-1	20	3257.15979	-0.00002	3257.15981	1583.76307
32	1	-1	1	-1	20	1	-1	1	-1	21	3255.08629	-0.00022	3255.08651	1623.76670
33	1	-1	1	-1	21	1	-1	1	-1	22	3253.00514	-0.00019	3253.00533	1665.67070
34	1	-1	1	-1	22	1	-1	1	-1	23	3250.91635	0.00006	3250.91629	1709.47454
35	1	-1	1	-1	23	1	-1	1	-1	24	3248.81912	-0.00030	3248.81942	1755.17765
36	1	-1	1	-1	24	1	-1	1	-1	25	3246.71395	-0.00080	3246.71475	1802.77942
37	1	-1	1	-1	25	1	-1	1	-1	26	3244.60256	0.00026	3244.60230	1852.27923
38	1	-1	1	-1	26	1	-1	1	-1	27	3242.48222	0.00012	3242.48210	1903.67642
39	1	-1	1	-1	27	1	-1	1	-1	28	3240.35406	-0.00010	3240.35416	1956.97033
40	1	-1	1	-1	28	1	-1	1	-1	29	3238.21899	0.00047	3238.21852	2012.16024
41	1	-1	1	-1	29	1	-1	1	-1	30	3236.07571	0.00052	3236.07519	2069.24541
42	1	-1	1	-1	30	1	-1	1	-1	31	3233.92773*	0.00352	3233.92421	2128.22510 +
43	1	-1	1	-1	3	1	-1	1	-1	2	3302.57898	0.00012	3302.57886	1189.18404
44	1	-1	1	-1	4	1	-1	1	-1	3	3304.45062	-0.00093	3304.45155	1194.90643
45	1	-1	1	-1	5	1	-1	1	-1	4	3306.31488	-0.00052	3306.31540	1202.53608
46	1	-1	1	-1	6	1	-1	1	-1	5	3308.16810*	-0.00226	3308.17036	1212.07282 +
47	1	-1	1	-1	7	1	-1	1	-1	6	3310.00808*	-0.00829	3310.01637	1223.51646 +
48	1	-1	1	-1	8	1	-1	1	-1	7	3311.85360	0.00023	3311.85337	1236.86675
49	1	-1	1	-1	9	1	-1	1	-1	8	3313.68112	-0.00021	3313.68133	1252.12340
50	1	-1	1	-1	10	1	-1	1	-1	9	3315.50007	-0.00015	3315.50022	1269.28609
51	1	-1	1	-1	11	1	-1	1	-1	10	3317.30971	-0.00032	3317.31003	1288.35448
52	1	-1	1	-1	12	1	-1	1	-1	11	3319.11028	-0.00048	3319.11076	1309.32820
53	1	-1	1	-1	13	1	-1	1	-1	12	3320.90219	-0.00023	3320.90242	1332.20685
54	1	-1	1	-1	14	1	-1	1	-1	13	3322.68472	-0.00033	3322.68505	1356.99004
55	1	-1	1	-1	15	1	-1	1	-1	14	3324.45966	0.00097	3324.45869	1383.67734
56	1	-1	1	-1	16	1	-1	1	-1	15	3326.22307	-0.00029	3326.22336	1412.26833
57	1	-1	1	-1	17	1	-1	1	-1	16	3327.97924	0.00015	3327.97909	1442.76257
58	1	-1	1	-1	18	1	-1	1	-1	17	3329.72574	-0.00018	3329.72592	1475.15963
59	1	-1	1	-1	19	1	-1	1	-1	18	3331.46396	0.00012	3331.46384	1509.45905
60	1	-1	1	-1	20	1	-1	1	-1	19	3333.19279	-0.00006	3333.19285	1545.66036
	1	-1	1	-1	21	1	-1	1	-1	20	3334.91352	0.00056	3334.91296	1583.76307
	1	-1	1	-1	22	1	-1	1	-1	21	3336.62405	-0.00008	3336.62413	1623.76670
	1	-1	1	-1	23	1	-1	1	-1	22	3338.32612	-0.00025	3338.32637	1665.67070
	1	-1	1	-1	24	1	-1	1	-1	23	3340.01934	-0.00028	3340.01962	1709.47454
	1	-1	1	-1	25	1	-1	1	-1	24	3341.70772*	0.00384	3341.70388	1755.17765

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2	1	-1	1	-1	26	1	-1	1	-1	25
3	1	-1	1	-1	27	1	-1	1	-1	26
4	1	-1	1	-1	28	1	-1	1	-1	27
5	1	-1	1	-1	29	1	-1	1	-1	28
6										
7	rms = 0.00042 cm ⁻¹									
8										
9										
10										
11	$\nu_1 + 3\nu_4 (\Pi) \leftarrow \nu_4 (\Pi)$									
12										
13										
14	ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''
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2	3	1	0	0	10	1	1	0	0	9	4342.57724	0.00023	4342.57701	595.12319
3	3	1	0	0	11	1	1	0	0	10	4344.42445	-0.00294	4344.42739	614.12929
4	3	1	0	0	12	1	1	0	0	11	4346.26656	-0.00493	4346.27149	635.03503
5	3	1	0	0	13	1	1	0	0	12	4348.10329	-0.00566	4348.10895	657.84012
6	3	1	0	0	14	1	1	0	0	13	4349.93347	-0.00593	4349.93940	682.54427
7	3	1	0	0	15	1	1	0	0	14	4351.75576	-0.00671	4351.76247	709.14713
8	3	1	0	0	16	1	1	0	0	15	4353.57172	-0.00606	4353.57778	737.64836
9	3	1	0	0	17	1	1	0	0	16	4355.37867	-0.00630	4355.38497	768.04757
10	3	1	0	0	18	1	1	0	0	17	4357.17925	-0.00445	4357.18370	800.34436
11	3	1	0	0	19	1	1	0	0	18	4358.97227	-0.00133	4358.97360	834.53830

rms = 0.00527 cm⁻¹

2ν₁ (Σ⁺) ← 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 ^b	OBS – CALC ^b	E'	E"
0 0 0 0 0	0 0 0 0 1	6531.04141	-0.00022	6531.04163	1.90066
0 0 0 0 1	0 0 0 0 2	6529.12367	0.00028	6529.12339	5.70195
0 0 0 0 2	0 0 0 0 3	6527.18729	-0.00030	6527.18759	11.40382
0 0 0 0 3	0 0 0 0 4	6525.23419	-0.00007	6525.23426	19.00619
0 0 0 0 4	0 0 0 0 5	6523.26338	-0.00005	6523.26343	28.50898
0 0 0 0 5	0 0 0 0 6	6521.27549	0.00038	6521.27511	39.91204
0 0 0 0 6	0 0 0 0 7	6519.26903	-0.00030	6519.26933	53.21523
0 0 0 0 7	0 0 0 0 8	6517.24583	-0.00030	6517.24613	68.41838
0 0 0 0 8	0 0 0 0 9	6515.20544	-0.00008	6515.20552	85.52129
0 0 0 0 9	0 0 0 0 10	6513.14736	-0.00017	6513.14753	104.52373
0 0 0 0 10	0 0 0 0 11	6511.07187	-0.00031	6511.07218	125.42544
0 0 0 0 11	0 0 0 0 12	6508.97942	-0.00009	6508.97951	148.22616
0 0 0 0 12	0 0 0 0 13	6506.86961	0.00008	6506.86953	172.92558
0 0 0 0 13	0 0 0 0 14	6504.74252	0.00025	6504.74227	199.52337
0 0 0 0 14	0 0 0 0 15	6502.59809	0.00033	6502.59776	228.01920
0 0 0 0 15	0 0 0 0 16	6500.43643	0.00041	6500.43602	258.41268
0 0 0 0 16	0 0 0 0 17	6498.25670	-0.00038	6498.25708	290.70340
0 0 0 0 17	0 0 0 0 18	6496.06114	0.00017	6496.06097	324.89096
0 0 0 0 18	0 0 0 0 19	6493.84727	-0.00043	6493.84770	360.97488
0 0 0 0 19	0 0 0 0 20	6491.61777	0.00046	6491.61731	398.95471
0 0 0 0 20	0 0 0 0 21	6489.37006	0.00024	6489.36982	438.82993
0 0 0 0 21	0 0 0 0 22	6487.10585	0.00059	6487.10526	480.60003
0 0 0 0 22	0 0 0 0 23	6484.82458	0.00093	6484.82365	524.26445
0 0 0 0 23	0 0 0 0 24	6482.52556	0.00054	6482.52502	569.82262
0 0 0 0 24	0 0 0 0 25	6480.20977	0.00038	6480.20939	617.27393
0 0 0 0 25	0 0 0 0 26	6477.87712	0.00032	6477.87680	666.61777
0 0 0 0 26	0 0 0 0 27	6475.52723	-0.00003	6475.52726	717.85348
0 0 0 0 27	0 0 0 0 28	6473.16282	0.00201	6473.16081	770.98038 †
0 0 0 0 28	0 0 0 0 29	6470.77798	0.00052	6470.77746	825.99778
0 0 0 0 29	0 0 0 0 30	6468.37686	-0.00039	6468.37725	882.90495
0 0 0 0 30	0 0 0 0 31	6465.95848	-0.00172	6465.96020	941.70115 †
0 0 0 0 31	0 0 0 0 32	6463.52654	0.00020	6463.52634	1002.38559
0 0 0 0 32	0 0 0 0 33	6461.07616	0.00047	6461.07569	1064.95747
0 0 0 0 33	0 0 0 0 34	6458.60752	-0.00077	6458.60829	1129.41599
0 0 0 0 34	0 0 0 0 35	6456.12456	0.00042	6456.12414	1195.76027
0 0 0 0 35	0 0 0 0 36	6453.62291	-0.00038	6453.62329	1263.98946
0 0 0 0 1	0 0 0 0 0	6534.82528	-0.00005	6534.82533	0.00000
0 0 0 0 2	0 0 0 0 1	6536.69043	-0.00032	6536.69075	1.90066
0 0 0 0 3	0 0 0 0 2	6538.53819	-0.00032	6538.53851	5.70195
0 0 0 0 4	0 0 0 0 3	6540.36863	0.00004	6540.36859	11.40382
0 0 0 0 5	0 0 0 0 4	6542.18044	-0.00052	6542.18096	19.00619
0 0 0 0 6	0 0 0 0 5	6543.97569	0.00010	6543.97559	28.50898
0 0 0 0 7	0 0 0 0 6	6545.75293	0.00045	6545.75248	39.91204
0 0 0 0 8	0 0 0 0 7	6547.51184	0.00027	6547.51157	53.21523
0 0 0 0 9	0 0 0 0 8	6549.25263	-0.00024	6549.25287	68.41838
0 0 0 0 10	0 0 0 0 9	6550.97634	0.00001	6550.97633	85.52129

1														
2	0	0	0	0	11	0	0	0	0	10	6552.68174	-0.00020	6552.68194	104.52373
3	0	0	0	0	12	0	0	0	0	11	6554.36983	0.00016	6554.36967	125.42544
4	0	0	0	0	13	0	0	0	0	12	6556.03927	-0.00022	6556.03949	148.22616
5	0	0	0	0	14	0	0	0	0	13	6557.69124	-0.00014	6557.69138	172.92558
6	0	0	0	0	15	0	0	0	0	14	6559.32520	-0.00012	6559.32532	199.52337
7	0	0	0	0	16	0	0	0	0	15	6560.94133	0.00005	6560.94128	228.01920
8	0	0	0	0	17	0	0	0	0	16	6562.53899	-0.00025	6562.53924	258.41268
9	0	0	0	0	18	0	0	0	0	17	6564.11933	0.00015	6564.11918	290.70340
10	0	0	0	0	19	0	0	0	0	18	6565.68110	0.00004	6565.68106	324.89096
11	0	0	0	0	20	0	0	0	0	19	6567.22512	0.00025	6567.22487	360.97488
12	0	0	0	0	21	0	0	0	0	20	6568.75172	0.00114	6568.75058	398.95471 +
13	0	0	0	0	22	0	0	0	0	21	6570.25752	-0.00065	6570.25817	438.82993
14	0	0	0	0	23	0	0	0	0	22	6571.74784	0.00023	6571.74761	480.60003
15	0	0	0	0	24	0	0	0	0	23	6573.21876	-0.00012	6573.21888	524.26445
16	0	0	0	0	25	0	0	0	0	24	6574.67267	0.00072	6574.67195	569.82262
17	0	0	0	0	26	0	0	0	0	25	6576.10677	-0.00004	6576.10681	617.27393
18	0	0	0	0	27	0	0	0	0	26	6577.52402	0.00060	6577.52342	666.61777
19	0	0	0	0	28	0	0	0	0	27	6578.92137	-0.00040	6578.92177	717.85348
20	0	0	0	0	29	0	0	0	0	28	6580.30208	0.00025	6580.30183	770.98038
21	0	0	0	0	30	0	0	0	0	29	6581.66324	-0.00033	6581.66357	825.99778
22	0	0	0	0	31	0	0	0	0	30	6583.00614	-0.00084	6583.00698	882.90495
23	0	0	0	0	32	0	0	0	0	31	6584.33122	-0.00080	6584.33202	941.70115
24	0	0	0	0	33	0	0	0	0	32	6585.63858	-0.00010	6585.63868	1002.38559
25	0	0	0	0	34	0	0	0	0	33	6586.92627	-0.00067	6586.92694	1064.95747
26	0	0	0	0	35	0	0	0	0	34	6588.19500	-0.00176	6588.19676	1129.41599 +
27	0	0	0	0	36	0	0	0	0	35	6589.44772	-0.00041	6589.44813	1195.76027
28	0	0	0	0	37	0	0	0	0	36	6590.68035	-0.00068	6590.68103	1263.98946
29	0	0	0	0	38	0	0	0	0	37	6591.89623	0.00081	6591.89542	1334.10264
30	0	0	0	0	39	0	0	0	0	38	6593.09250	0.00121	6593.09129	1406.09891 +
31	0	0	0	0	40	0	0	0	0	39	6594.27257	0.00396	6594.26861	1479.97730 +
32	0	0	0	0	41	0	0	0	0	40	6595.42977	0.00241	6595.42736	1555.73685 +
33	0	0	0	0	42	0	0	0	0	41	6596.57040	0.00288	6596.56752	1633.37656 +
34	0	0	0	0	43	0	0	0	0	42	6597.68966	0.00059	6597.68907	1712.89541

rms = 0.00040 cm⁻¹

$$2\nu_1 + \nu_4 (\Pi) \leftarrow \nu_4 (\Pi)$$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 0 0 1	1 -1 0 0 2	6520.50235	0.00074	6520.50161	515.31316
1 -1 0 0 2	1 -1 0 0 3	6518.55717	0.00050	6518.55667	521.04101
1 -1 0 0 3	1 -1 0 0 4	6516.59347	-0.00049	6516.59396	528.67801
1 -1 0 0 4	1 -1 0 0 5	6514.61314	-0.00037	6514.61351	538.22407
1 -1 0 0 5	1 -1 0 0 6	6512.61555	0.00022	6512.61533	549.67906
1 -1 0 0 6	1 -1 0 0 7	6510.59931	-0.00016	6510.59947	563.04281
1 -1 0 0 7	1 -1 0 0 8	6508.56610	0.00016	6508.56594	578.31514
1 -1 0 0 8	1 -1 0 0 9	6506.51473	-0.00004	6506.51477	595.49585
1 -1 0 0 9	1 -1 0 0 10	6504.44593	-0.00006	6504.44599	614.58469
1 -1 0 0 10	1 -1 0 0 11	6502.35958	-0.00005	6502.35963	635.58142
1 -1 0 0 11	1 -1 0 0 12	6500.25573	0.00002	6500.25571	658.48573
1 -1 0 0 12	1 -1 0 0 13	6498.13475	0.00049	6498.13426	683.29732
1 -1 0 0 13	1 -1 0 0 14	6495.99475	-0.00056	6495.99531	710.01584
1 -1 0 0 14	1 -1 0 0 15	6493.83980*	0.00091	6493.83889	738.64093
1 -1 0 0 15	1 -1 0 0 16	6491.66460	-0.00042	6491.66502	769.17220
1 -1 0 0 16	1 -1 0 0 17	6489.47255	-0.00117	6489.47372	801.60923 †
1 -1 0 0 17	1 -1 0 0 18	6487.26484	-0.00020	6487.26504	835.95156
1 -1 0 0 18	1 -1 0 0 19	6485.03914	0.00015	6485.03899	872.19874
1 -1 0 0 19	1 -1 0 0 20	6482.79464	-0.00097	6482.79561	910.35027
1 -1 0 0 20	1 -1 0 0 21	6480.53642	0.00150	6480.53492	950.40561 †
1 -1 0 0 21	1 -1 0 0 22	6478.25792	0.00097	6478.25695	992.36423
1 -1 0 0 22	1 -1 0 0 23	6475.96153	-0.00020	6475.96173	1036.22555
1 -1 0 0 23	1 -1 0 0 24	6473.64885*	-0.00044	6473.64929	1081.98896

1											
2	1	-1	0	0	24	1	-1	0	0	25	6471.31874 -0.00091 6471.31965 1129.65384
3	1	-1	0	0	25	1	-1	0	0	26	6468.97270 -0.00014 6468.97284 1179.21954
4	1	-1	0	0	26	1	-1	0	0	27	6466.60915 0.00025 6466.60890 1230.68537
5	1	-1	0	0	27	1	-1	0	0	28	6464.22738 -0.00047 6464.22785 1284.05064
6	1	-1	0	0	2	1	-1	0	0	1	6528.10240 -0.00072 6528.10312 511.49456
7	1	-1	0	0	3	1	-1	0	0	2	6529.95954 0.00073 6529.95881 515.31316
8	1	-1	0	0	4	1	-1	0	0	3	6531.79622 -0.00035 6531.79657 521.04101
9	1	-1	0	0	5	1	-1	0	0	4	6533.61684 0.00046 6533.61638 528.67801
10	1	-1	0	0	6	1	-1	0	0	5	6535.41873 0.00053 6535.41820 538.22407
11	1	-1	0	0	7	1	-1	0	0	6	6537.20205 0.00003 6537.20202 549.67906
12	1	-1	0	0	8	1	-1	0	0	7	6538.96860 0.00079 6538.96781 563.04281
13	1	-1	0	0	9	1	-1	0	0	8	6540.71570 0.00015 6540.71555 578.31514
14	1	-1	0	0	10	1	-1	0	0	9	6542.44564 0.00044 6542.44520 595.49585
15	1	-1	0	0	11	1	-1	0	0	10	6544.15648 -0.00027 6544.15675 614.58469
16	1	-1	0	0	12	1	-1	0	0	11	6545.85025 0.00009 6545.85016 635.58142
17	1	-1	0	0	13	1	-1	0	0	12	6547.52231* -0.00311 6547.52542 658.48573 †
18	1	-1	0	0	14	1	-1	0	0	13	6549.18359 0.00109 6549.18250 683.29732 †
19	1	-1	0	0	15	1	-1	0	0	14	6550.82104 -0.00033 6550.82137 710.01584
20	1	-1	0	0	16	1	-1	0	0	15	6552.44178 -0.00024 6552.44202 738.64093
21	1	-1	0	0	17	1	-1	0	0	16	6554.04435 -0.00005 6554.04440 769.17220
22	1	-1	0	0	18	1	-1	0	0	17	6555.62874 0.00023 6555.62851 801.60923
23	1	-1	0	0	19	1	-1	0	0	18	6557.19526 0.00094 6557.19432 835.95156
24	1	-1	0	0	20	1	-1	0	0	19	6558.74308 0.00129 6558.74179 872.19874 †
25	1	-1	0	0	21	1	-1	0	0	20	6560.27051 -0.00041 6560.27092 910.35027
26	1	-1	0	0	22	1	-1	0	0	21	6561.78210 0.00043 6561.78167 950.40561
27	1	-1	0	0	23	1	-1	0	0	22	6563.27372 -0.00030 6563.27402 992.36423
28	1	-1	0	0	24	1	-1	0	0	23	6564.74888 0.00094 6564.74794 1036.22555
29	1	-1	0	0	25	1	-1	0	0	24	6566.20317 -0.00025 6566.20342 1081.98896
30	1	-1	0	0	26	1	-1	0	0	25	6567.64013 -0.00030 6567.64043 1129.65384
31	1	-1	0	0	27	1	-1	0	0	26	6569.05883 -0.00012 6569.05895 1179.21954
32	1	-1	0	0	28	1	-1	0	0	27	6570.45899 0.00004 6570.45895 1230.68537
33	1	-1	0	0	29	1	-1	0	0	28	6571.84104 0.00064 6571.84040 1284.05064
34	1	-1	0	0	30	1	-1	0	0	29	6573.20269* -0.00061 6573.20330 1339.31460
35	1	1	0	0	1	1	1	0	0	2	6520.51977* 0.00149 6520.51828 515.28830 †
36	1	1	0	0	2	1	1	0	0	3	6518.58143 -0.00039 6518.58182 520.99129
37	1	1	0	0	3	1	1	0	0	4	6516.62741 -0.00028 6516.62769 528.59515
38	1	1	0	0	4	1	1	0	0	5	6514.65581 -0.00010 6514.65591 538.09979
39	1	1	0	0	5	1	1	0	0	6	6512.66649 -0.00001 6512.66650 549.50508
40	1	1	0	0	6	1	1	0	0	7	6510.66009 0.00060 6510.65949 562.81086
41	1	1	0	0	7	1	1	0	0	8	6508.63533 0.00041 6508.63492 578.01697
42	1	1	0	0	8	1	1	0	0	9	6506.59268 -0.00011 6506.59279 595.12319
43	1	1	0	0	9	1	1	0	0	10	6504.53308 -0.00007 6504.53315 614.12929
44	1	1	0	0	10	1	1	0	0	11	6502.45591 -0.00010 6502.45601 635.03503
45	1	1	0	0	11	1	1	0	0	12	6500.36208 0.00068 6500.36140 657.84012
46	1	1	0	0	12	1	1	0	0	13	6498.25519* 0.00584 6498.24935 682.54427 †
47	1	1	0	0	13	1	1	0	0	14	6496.12001 0.00012 6496.11989 709.14713
48	1	1	0	0	14	1	1	0	0	15	6493.97252 -0.00051 6493.97303 737.64836
49	1	1	0	0	15	1	1	0	0	16	6491.80851 -0.00031 6491.80882 768.04757
50	1	1	0	0	16	1	1	0	0	17	6489.62651 -0.00076 6489.62727 800.34436
51	1	1	0	0	17	1	1	0	0	18	6487.42764 -0.00077 6487.42841 834.53830
52	1	1	0	0	18	1	1	0	0	19	6485.21206 -0.00021 6485.21227 870.62893
53	1	1	0	0	19	1	1	0	0	20	6482.97704 -0.00184 6482.97888 908.61577 †
54	1	1	0	0	20	1	1	0	0	21	6480.72830 0.00004 6480.72826 948.49830
55	1	1	0	0	21	1	1	0	0	22	6478.45992 -0.00051 6478.46043 990.27601
56	1	1	0	0	22	1	1	0	0	23	6476.17583 0.00039 6476.17544 1033.94833
57	1	1	0	0	23	1	1	0	0	24	6473.87318 -0.00012 6473.87330 1079.51468
58	1	1	0	0	24	1	1	0	0	25	6471.55498 0.00094 6471.55404 1126.97445
59	1	1	0	0	25	1	1	0	0	26	6469.21840 0.00071 6469.21769 1176.32701
60	1	1	0	0	26	1	1	0	0	27	6466.86414 -0.00014 6466.86428 1227.57169
	1	1	0	0	27	1	1	0	0	28	6464.49456 0.00073 6464.49383 1280.70782
	1	1	0	0	2	1	1	0	0	1	6528.08943* 0.00259 6528.08684 511.48627 †
	1	1	0	0	3	1	1	0	0	2	6529.93472 0.00018 6529.93454 515.28830
	1	1	0	0	4	1	1	0	0	3	6531.76663 0.00222 6531.76441 520.99129 †
	1	1	0	0	5	1	1	0	0	4	6533.57671 0.00028 6533.57643 528.59515
	1	1	0	0	6	1	1	0	0	5	6535.37099 0.00042 6535.37057 538.09979

1	1	0	0	7	1	1	0	0	6	6537.14647	-0.00033	6537.14680	549.50508
1	1	0	0	8	1	1	0	0	7	6538.90478	-0.00033	6538.90511	562.81086
1	1	0	0	9	1	1	0	0	8	6540.64417	-0.00130	6540.64547	578.01697 †
1	1	0	0	10	1	1	0	0	9	6542.36775	-0.00010	6542.36785	595.12319
1	1	0	0	11	1	1	0	0	10	6544.07553	0.00330	6544.07223	614.12929 †
1	1	0	0	12	1	1	0	0	11	6545.74409*	-0.01450	6545.75859	635.03503 †
1	1	0	0	13	1	1	0	0	12	6547.42656	-0.00033	6547.42689	657.84012
1	1	0	0	14	1	1	0	0	13	6549.07692	-0.00020	6549.07712	682.54427
1	1	0	0	15	1	1	0	0	14	6550.70811	-0.00115	6550.70926	709.14713 †
1	1	0	0	16	1	1	0	0	15	6552.32324	-0.00003	6552.32327	737.64836
1	1	0	0	17	1	1	0	0	16	6553.91863	-0.00051	6553.91914	768.04757
1	1	0	0	18	1	1	0	0	17	6555.49520	-0.00164	6555.49684	800.34436 †
1	1	0	0	19	1	1	0	0	18	6557.05663	0.00029	6557.05634	834.53830
1	1	0	0	20	1	1	0	0	19	6558.59751	-0.00012	6558.59763	870.62893
1	1	0	0	21	1	1	0	0	20	6560.11925	-0.00143	6560.12068	908.61577 †
1	1	0	0	22	1	1	0	0	21	6561.62454	-0.00093	6561.62547	948.49830
1	1	0	0	23	1	1	0	0	22	6563.10993	-0.00204	6563.11197	990.27601 †
1	1	0	0	24	1	1	0	0	23	6564.58007	-0.00009	6564.58016	1033.94833
1	1	0	0	25	1	1	0	0	24	6566.02860	-0.00142	6566.03002	1079.51468 †
1	1	0	0	26	1	1	0	0	25	6567.46755	0.00603	6567.46152	1126.97445 †
1	1	0	0	27	1	1	0	0	26	6568.86964	-0.00500	6568.87464	1176.32701 †
1	1	0	0	28	1	1	0	0	27	6570.26554	-0.00382	6570.26936	1227.57169 †
1	1	0	0	29	1	1	0	0	28	6571.64689	0.00123	6571.64566	1280.70782 †
1	1	0	0	30	1	1	0	0	29	6573.00613	0.00262	6573.00351	1335.73468 †
1	1	0	0	31	1	1	0	0	30	6574.34281	-0.00009	6574.34290	1392.65154

rms = 0.00045 cm⁻¹

$2\nu_1 + \nu_5 (\Pi) \leftarrow \nu_5 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS ^b	OBS - CALC ^b	E'	E''
0 0 1 1 3	0 0 1 1 4	6491.60723*	-0.10932	6491.71655	693.23382 †
0 0 1 1 4	0 0 1 1 5	6489.62699*	-0.14073	6489.76772	702.73224 †
0 0 1 1 5	0 0 1 1 6	6487.69697	-0.10973	6487.80670	714.13007 †
0 0 1 1 6	0 0 1 1 7	6485.75467	-0.07884	6485.83351	727.42716 †
0 0 1 1 7	0 0 1 1 8	6483.79317	-0.05501	6483.84818	742.62333 †
0 0 1 1 8	0 0 1 1 9	6481.81357	-0.03715	6481.85072	759.71839 †
0 0 1 1 9	0 0 1 1 10	6479.82060	-0.02056	6479.84116	778.71209 †
0 0 1 1 10	0 0 1 1 11	6477.81106	-0.00847	6477.81953	799.60420
0 0 1 1 11	0 0 1 1 12	6475.78728	0.00142	6475.78586	822.39444
0 0 1 1 12	0 0 1 1 13	6473.74498	0.00482	6473.74016	847.08251
0 0 1 1 13	0 0 1 1 14	6471.68681	0.00435	6471.68246	873.66808
0 0 1 1 14	0 0 1 1 15	6469.61506	0.00227	6469.61279	902.15079
0 0 1 1 15	0 0 1 1 16	6467.52667	-0.00451	6467.53118	932.53028
0 0 1 1 5	0 0 1 1 4	6508.63485	-0.06811	6508.70296	693.23382 †
0 0 1 1 6	0 0 1 1 5	6510.49879*	-0.02965	6510.52844	702.73224 †
0 0 1 1 7	0 0 1 1 6	6512.28486	-0.05658	6512.34144	714.13007 †
0 0 1 1 8	0 0 1 1 7	6514.10634	-0.03560	6514.14194	727.42716 †
0 0 1 1 9	0 0 1 1 8	6515.91051	-0.01941	6515.92992	742.62333 †
0 0 1 1 10	0 0 1 1 9	6517.69673	-0.00862	6517.70535	759.71839
0 0 1 1 11	0 0 1 1 10	6519.46805	-0.00016	6519.46821	778.71209
0 0 1 1 12	0 0 1 1 11	6521.22421	0.00574	6521.21847	799.60420
0 0 1 1 13	0 0 1 1 12	6522.96100	0.00490	6522.95610	822.39444
0 0 1 1 14	0 0 1 1 13	6524.68422	0.00314	6524.68108	847.08251
0 0 1 1 15	0 0 1 1 14	6526.38906	-0.00432	6526.39338	873.66808
0 0 1 1 16	0 0 1 1 15	6528.09067	-0.00231	6528.09298	902.15079
0 0 1 -1 3	0 0 1 -1 4	6491.54225	-0.13287	6491.67512	693.29902 †
0 0 1 -1 4	0 0 1 -1 5	6489.57608	-0.13348	6489.70956	702.83004 †
0 0 1 -1 5	0 0 1 -1 6	6487.62740	-0.10184	6487.72924	714.26698 †
0 0 1 -1 6	0 0 1 -1 7	6485.66287	-0.07132	6485.73419	727.60969 †
0 0 1 -1 7	0 0 1 -1 8	6483.67362	-0.05083	6483.72445	742.85799 †
0 0 1 -1 8	0 0 1 -1 9	6481.66810	-0.03193	6481.70003	760.01168 †

[illegible]
$$\text{rms} = 0.00497 \text{ cm}^{-1}$$

Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm^{-1}) for the ν_2 and associated hot bands of $^{13}\text{C}_2\text{HD}$ ^a (31 pp)

$\nu_2(\Sigma^+) \leftarrow G.S.(\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 1	0 0 0 0 2	1805.03558	-0.00021	1810.73774	5.70195
0 0 0 0 2	0 0 0 0 3	1803.11951	0.00070	1814.52262	11.40382
0 0 0 0 3	0 0 0 0 4	1801.19452	0.00083	1820.19989	19.00619
0 0 0 0 4	0 0 0 0 5	1799.26020	-0.00028	1827.76945	28.50898
0 0 0 0 5	0 0 0 0 6	1797.31917	-0.00001	1837.23122	39.91204
0 0 0 0 6	0 0 0 0 7	1795.37052	0.00068	1848.58507	53.21523
0 0 0 0 7	0 0 0 0 8	1793.41273	0.00026	1861.83085	68.41838
0 0 0 0 8	0 0 0 0 9	1791.44764	0.00055	1876.96838	85.52129
0 0 0 0 9	0 0 0 0 10	1789.47423	0.00049	1893.99746	104.52373
0 0 0 0 10	0 0 0 0 11	1787.49286	0.00043	1912.91787	125.42544
0 0 0 0 11	0 0 0 0 12	1785.50314	-0.00006	1933.72935	148.22616
0 0 0 0 12	0 0 0 0 13	1783.50603	-0.00003	1956.43164	172.92558
0 0 0 0 13	0 0 0 0 14	1781.50161	0.00056	1981.02442	199.52337
0 0 0 0 14	0 0 0 0 15	1779.48864	0.00046	2007.50738	228.01920
0 0 0 0 15	0 0 0 0 16	1777.46791	0.00043	2035.88016	258.41268
0 0 0 0 16	0 0 0 0 17	1775.43943	0.00045	2066.14239	290.70340
0 0 0 0 17	0 0 0 0 18	1773.40285	0.00015	2098.29366	324.89096
0 0 0 0 18	0 0 0 0 19	1771.35843	-0.00024	2132.33355	360.97488
0 0 0 0 19	0 0 0 0 20	1769.30703	0.00012	2168.26162	398.95471
0 0 0 0 20	0 0 0 0 21	1767.24694*	-0.00050	2206.07738	438.82993
0 0 0 0 21	0 0 0 0 22	1765.18108	0.00079	2245.78033	480.60003
0 0 0 0 22	0 0 0 0 23	1763.10508	-0.00041	2287.36994	524.26445
0 0 0 0 23	0 0 0 0 24	1761.02328	0.00022	2330.84568	569.82262
0 0 0 0 24	0 0 0 0 25	1758.93258	-0.00044	2376.20695	617.27393
0 0 0 0 25	0 0 0 0 26	1756.83470	-0.00069	2423.45316	666.61777
0 0 0 0 26	0 0 0 0 27	1754.73027	0.00005	2472.58369	717.85348
0 0 0 0 27	0 0 0 0 28	1752.61748	-0.00002	2523.59788	770.98038
0 0 0 0 28	0 0 0 0 29	1750.49739	0.00011	2576.49506	825.99778
0 0 0 0 29	0 0 0 0 30	1748.36956	-0.00002	2631.27453	882.90495
0 0 0 0 30	0 0 0 0 31	1746.23467	0.00026	2687.93556	941.70115
0 0 0 0 31	0 0 0 0 32	1744.09184	0.00002	2746.47740	1002.38559
0 0 0 0 32	0 0 0 0 33	1741.94215	0.00034	2806.89928	1064.95747
0 0 0 0 33	0 0 0 0 34	1739.78466	0.00025	2869.20040	1129.41599
0 0 0 0 34	0 0 0 0 35	1737.61644*	-0.00321	2933.37992	1195.76027 †
0 0 0 0 35	0 0 0 0 36	1735.44766	0.00010	2999.43701	1263.98946
0 0 0 0 36	0 0 0 0 37	1733.26817	0.00002	3067.37079	1334.10264
0 0 0 0 37	0 0 0 0 38	1731.08153	0.00008	3137.18036	1406.09891
0 0 0 0 38	0 0 0 0 39	1728.88759	0.00010	3208.86479	1479.97730
0 0 0 0 39	0 0 0 0 40	1726.68584	-0.00044	3282.42314	1555.73685
0 0 0 0 40	0 0 0 0 41	1724.47816	0.00030	3357.85443	1633.37656
0 0 0 0 41	0 0 0 0 42	1722.26232	0.00007	3435.15766	1712.89541
0 0 0 0 42	0 0 0 0 43	1720.04060	0.00113	3514.33181	1794.29235 †
0 0 0 0 43	0 0 0 0 44	1717.80881	-0.00073	3595.37584	1877.56630
0 0 0 0 44	0 0 0 0 45	1715.57234	-0.00015	3678.28867	1962.71617
0 0 0 0 1	0 0 0 0 0	1810.73772	-0.00002	1810.73774	0.00000
0 0 0 0 2	0 0 0 0 1	1812.62238	0.00041	1814.52262	1.90066
0 0 0 0 3	0 0 0 0 2	1814.49768	-0.00026	1820.19989	5.70195
0 0 0 0 4	0 0 0 0 3	1816.36567	0.00003	1827.76945	11.40382
0 0 0 0 5	0 0 0 0 4	1818.22541	0.00038	1837.23122	19.00619
0 0 0 0 6	0 0 0 0 5	1820.07653	0.00043	1848.58507	28.50898
0 0 0 0 7	0 0 0 0 6	1821.91938	0.00057	1861.83085	39.91204
0 0 0 0 8	0 0 0 0 7	1823.75337	0.00022	1876.96838	53.21523
0 0 0 0 9	0 0 0 0 8	1825.57893	-0.00015	1893.99746	68.41838
0 0 0 0 10	0 0 0 0 9	1827.39669	0.00011	1912.91787	85.52129

1														
2	0	0	0	0	11	0	0	0	0	10	1829.20575	0.00012	1933.72935	104.52373
3	0	0	0	0	12	0	0	0	0	11	1831.00603	-0.00017	1956.43164	125.42544
4	0	0	0	0	13	0	0	0	0	12	1832.79781	-0.00046	1981.02442	148.22616
5	0	0	0	0	14	0	0	0	0	13	1834.58189	0.00009	2007.50738	172.92558
6	0	0	0	0	15	0	0	0	0	14	1836.35712	0.00034	2035.88016	199.52337
7	0	0	0	0	16	0	0	0	0	15	1838.12293	-0.00026	2066.14239	228.01920
8	0	0	0	0	17	0	0	0	0	16	1839.88040	-0.00058	2098.29366	258.41268
9	0	0	0	0	18	0	0	0	0	17	1841.62951	-0.00064	2132.33355	290.70340
10	0	0	0	0	19	0	0	0	0	18	1843.37160	0.00094	2168.26162	324.89096
11	0	0	0	0	20	0	0	0	0	19	1845.10277	0.00028	2206.07738	360.97488
12	0	0	0	0	21	0	0	0	0	20	1846.82534	-0.00028	2245.78033	398.95471
13	0	0	0	0	22	0	0	0	0	21	1848.54038	0.00037	2287.36994	438.82993
14	0	0	0	0	23	0	0	0	0	22	1850.24520	-0.00045	2330.84568	480.60003
15	0	0	0	0	24	0	0	0	0	23	1851.94218	-0.00032	2376.20695	524.26445
16	0	0	0	0	25	0	0	0	0	24	1853.63028	-0.00027	2423.45316	569.82262
17	0	0	0	0	26	0	0	0	0	25	1855.30920	-0.00056	2472.58369	617.27393
18	0	0	0	0	27	0	0	0	0	26	1856.98009	-0.00002	2523.59788	666.61777
19	0	0	0	0	28	0	0	0	0	27	1858.64169	0.00010	2576.49506	717.85348
20	0	0	0	0	29	0	0	0	0	28	1860.29412	-0.00003	2631.27453	770.98038
21	0	0	0	0	30	0	0	0	0	29	1861.93738	-0.00040	2687.93556	825.99778
22	0	0	0	0	31	0	0	0	0	30	1863.57210	-0.00035	2746.47740	882.90495
23	0	0	0	0	32	0	0	0	0	31	1865.19839	0.00026	2806.89928	941.70115
24	0	0	0	0	33	0	0	0	0	32	1866.81488	0.00007	2869.20040	1002.38559
25	0	0	0	0	34	0	0	0	0	33	1868.42236	-0.00009	2933.37992	1064.95747
26	0	0	0	0	35	0	0	0	0	34	1870.02045	-0.00058	2999.43701	1129.41599
27	0	0	0	0	36	0	0	0	0	35	1871.61071	0.00019	3067.37079	1195.76027
28	0	0	0	0	37	0	0	0	0	36	1873.19101	0.00011	3137.18036	1263.98946
29	0	0	0	0	38	0	0	0	0	37	1874.76208	-0.00007	3208.86479	1334.10264
30	0	0	0	0	39	0	0	0	0	38	1876.32470	0.00047	3282.42314	1406.09891
31	0	0	0	0	40	0	0	0	0	39	1877.87809	0.00097	3357.85443	1479.97730
32	0	0	0	0	41	0	0	0	0	40	1879.42059	-0.00022	3435.15766	1555.73685
33	0	0	0	0	42	0	0	0	0	41	1880.95567	0.00042	3514.33181	1633.37656
34	0	0	0	0	43	0	0	0	0	42	1882.47994	-0.00049	3595.37584	1712.89541
35	0	0	0	0	44	0	0	0	0	43	1883.99668	0.00036	3678.28867	1794.29235
36	0	0	0	0	45	0	0	0	0	44	1885.50295	0.00005	3763.06920	1877.56630

rms = 0.00038 cm⁻¹

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

$v_2(\Sigma^+) \leftarrow v_4(\Pi)$

47														
48	v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	E'	E''
49	0	0	0	0	0	1	1	0	0	1	1297.35939	0.00037	1808.84529	511.48627
50	0	0	0	0	1	1	1	0	0	2	1295.44919	-0.00025	1810.73774	515.28830
51	0	0	0	0	2	1	1	0	0	3	1293.53133	-0.00001	1814.52262	520.99129
52	0	0	0	0	3	1	1	0	0	4	1291.60548*	0.00075	1820.19989	528.59515
53	0	0	0	0	4	1	1	0	0	5	1289.66921	-0.00045	1827.76945	538.09979
54	0	0	0	0	5	1	1	0	0	6	1287.72636	0.00021	1837.23122	549.50508
55	0	0	0	0	6	1	1	0	0	7	1285.77404	-0.00017	1848.58507	562.81086
56	0	0	0	0	7	1	1	0	0	8	1283.81446	0.00058	1861.83085	578.01697
57	0	0	0	0	8	1	1	0	0	9	1281.84552	0.00032	1876.96838	595.12319
58	0	0	0	0	9	1	1	0	0	10	1279.86821	0.00004	1893.99746	614.12929
59	0	0	0	0	10	1	1	0	0	11	1277.88288	0.00004	1912.91787	635.03503
60	0	0	0	0	11	1	1	0	0	12	1275.88915	-0.00008	1933.72935	657.84012
	0	0	0	0	12	1	1	0	0	13	1273.88696	-0.00041	1956.43164	682.54427
	0	0	0	0	13	1	1	0	0	14	1271.87735	0.00006	1981.02442	709.14713
	0	0	0	0	14	1	1	0	0	15	1269.85899	-0.00003	2007.50738	737.64836
	0	0	0	0	15	1	1	0	0	16	1267.83255	-0.00004	2035.88016	768.04757

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1														
2	0	0	0	0	20	1	-1	0	0	20	1295.72751	0.00040	2206.07738	910.35027
3	0	0	0	0	21	1	-1	0	0	21	1295.37790*	0.00319	2245.78033	950.40561 +
4	0	0	0	0	22	1	-1	0	0	22	1295.00556	-0.00015	2287.36994	992.36423
5	0	0	0	0	23	1	-1	0	0	23	1294.62081	0.00068	2330.84568	1036.22555
6	0	0	0	0	24	1	-1	0	0	24	1294.21788	-0.00011	2376.20695	1081.98896
7	0	0	0	0	25	1	-1	0	0	25	1293.80011	0.00079	2423.45316	1129.65384

rms = 0.00032 cm⁻¹

$v_2(\Sigma^+) \leftarrow v_5(\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	0 0 1 1 1	1132.70967	0.00051	1808.84529	676.13613
0 0 0 0 1	0 0 1 1 2	1130.80165	-0.00042	1810.73774	679.93567
0 0 0 0 2	0 0 1 1 3	1128.88673	-0.00097	1814.52262	685.63493
0 0 0 0 3	0 0 1 1 4	1126.96552	-0.00055	1820.19989	693.23382
0 0 0 0 4	0 0 1 1 5	1125.03668	-0.00053	1827.76945	702.73224
0 0 0 0 5	0 0 1 1 6	1123.10153	0.00038	1837.23122	714.13007
0 0 0 0 6	0 0 1 1 7	1121.15781	-0.00010	1848.58507	727.42716
0 0 0 0 7	0 0 1 1 8	1119.20740	-0.00012	1861.83085	742.62333
0 0 0 0 8	0 0 1 1 9	1117.25013	0.00013	1876.96838	759.71839
0 0 0 0 9	0 0 1 1 10	1115.28524	-0.00013	1893.99746	778.71209
0 0 0 0 10	0 0 1 1 11	1113.31358	-0.00009	1912.91787	799.60420
0 0 0 0 11	0 0 1 1 12	1111.33478	-0.00013	1933.72935	822.39444
0 0 0 0 12	0 0 1 1 13	1109.34899	-0.00014	1956.43164	847.08251
0 0 0 0 13	0 0 1 1 14	1107.35546	-0.00088	1981.02442	873.66808
0 0 0 0 14	0 0 1 1 15	1105.35621	-0.00038	2007.50738	902.15079
0 0 0 0 15	0 0 1 1 16	1103.34963	-0.00025	2035.88016	932.53028
0 0 0 0 16	0 0 1 1 17	1101.33711	0.00086	2066.14239	964.80614
0 0 0 0 17	0 0 1 1 18	1099.31641	0.00070	2098.29366	998.97795
0 0 0 0 18	0 0 1 1 19	1097.28787	-0.00044	2132.33355	1035.04524
0 0 0 0 19	0 0 1 1 20	1095.25319	-0.00087	2168.26162	1073.00756
0 0 0 0 20	0 0 1 1 21	1093.21249	-0.00050	2206.07738	1112.86438
0 0 0 0 21	0 0 1 1 22	1091.16605	0.00092	2245.78033	1154.61520
0 0 0 0 22	0 0 1 1 23	1089.10959	-0.00090	2287.36994	1198.25945
0 0 0 0 23	0 0 1 1 24	1087.04966	0.00055	2330.84568	1243.79656
0 0 0 0 24	0 0 1 1 25	1084.98131	0.00029	2376.20695	1291.22593
0 0 0 0 25	0 0 1 1 26	1082.90642	0.00019	2423.45316	1340.54693
0 0 0 0 26	0 0 1 1 27	1080.82379	-0.00099	2472.58369	1391.75891
0 0 0 0 27	0 0 1 1 28	1078.73706	0.00037	2523.59788	1444.86119
0 0 0 0 28	0 0 1 1 29	1076.64208	0.00009	2576.49506	1499.85307
0 0 0 0 29	0 0 1 1 30	1074.53958	-0.00112	2631.27453	1556.73383 †
0 0 0 0 30	0 0 1 1 31	1072.43323	0.00038	2687.93556	1615.50271
0 0 0 0 31	0 0 1 1 32	1070.31925	0.00078	2746.47740	1676.15894
0 0 0 0 2	0 0 1 1 1	1138.38650	0.00000	1814.52262	676.13613
0 0 0 0 3	0 0 1 1 2	1140.26472	0.00051	1820.19989	679.93567
0 0 0 0 4	0 0 1 1 3	1142.13522	0.00069	1827.76945	685.63493
0 0 0 0 5	0 0 1 1 4	1143.99773	0.00032	1837.23122	693.23382
0 0 0 0 6	0 0 1 1 5	1145.85317	0.00034	1848.58507	702.73224
0 0 0 0 7	0 0 1 1 6	1147.70114	0.00036	1861.83085	714.13007
0 0 0 0 8	0 0 1 1 7	1149.54138	0.00016	1876.96838	727.42716
0 0 0 0 9	0 0 1 1 8	1151.37387	-0.00026	1893.99746	742.62333
0 0 0 0 10	0 0 1 1 9	1153.19899	-0.00050	1912.91787	759.71839
0 0 0 0 11	0 0 1 1 10	1155.01730	0.00004	1933.72935	778.71209
0 0 0 0 12	0 0 1 1 11	1156.82683	-0.00060	1956.43164	799.60420
0 0 0 0 13	0 0 1 1 12	1158.63011	0.00013	1981.02442	822.39444
0 0 0 0 14	0 0 1 1 13	1160.42499	0.00012	2007.50738	847.08251
0 0 0 0 15	0 0 1 1 14	1162.21232	0.00024	2035.88016	873.66808
0 0 0 0 16	0 0 1 1 15	1163.99099	-0.00060	2066.14239	902.15079
0 0 0 0 17	0 0 1 1 16	1165.76279	-0.00059	2098.29366	932.53028
0 0 0 0 18	0 0 1 1 17	1167.52743	0.00002	2132.33355	964.80614
0 0 0 0 19	0 0 1 1 18	1169.28355	-0.00012	2168.26162	998.97795

$$\text{rms} = 0.00048 \text{ cm}^{-1}$$
$$\mathbf{v}_2 + \mathbf{v}_4 (\Pi) \leftarrow G.S. (\Sigma^+)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 0 0 1	0 0 0 0 2	2310.66866	0.00052	2316.37008	5.70195
1 1 0 0 2	0 0 0 0 3	2308.75089	-0.00050	2320.15520	11.40382
1 1 0 0 3	0 0 0 0 4	2306.82715	0.00052	2325.83282	19.00619
1 1 0 0 4	0 0 0 0 5	2304.89332	-0.00056	2333.40285	28.50898
1 1 0 0 5	0 0 0 0 6	2302.95272	-0.00045	2342.86521	39.91204
1 1 0 0 6	0 0 0 0 7	2301.00455	0.00003	2354.21976	53.21523
1 1 0 0 7	0 0 0 0 8	2299.04807	0.00011	2367.46634	68.41838
1 1 0 0 8	0 0 0 0 9	2297.08331	-0.00019	2382.60479	85.52129
1 1 0 0 9	0 0 0 0 10	2295.11106	-0.00011	2399.63490	104.52373
1 1 0 0 10	0 0 0 0 11	2293.13057	-0.00043	2418.55644	125.42544
1 1 0 0 11	0 0 0 0 12	2291.14320	0.00021	2439.36915	148.22616
1 1 0 0 12	0 0 0 0 13	2289.14710	-0.00008	2462.07276	172.92558
1 1 0 0 13	0 0 0 0 14	2287.14378	0.00019	2486.66696	199.52337

1	1	1	0	0	14	0	0	0	0	15	2285.13175	-0.00048	2513.15143	228.01920
2	1	1	0	0	15	0	0	0	0	16	2283.11298	-0.00015	2541.52580	258.41268
3	1	1	0	0	16	0	0	0	0	17	2281.08623	-0.00007	2571.78970	290.70340
4	1	1	0	0	17	0	0	0	0	18	2279.05185	0.00008	2603.94273	324.89096
5	1	1	0	0	18	0	0	0	0	19	2277.00990	0.00034	2637.98444	360.97488
6	1	1	0	0	19	0	0	0	0	20	2274.95986	0.00019	2673.91438	398.95471
7	1	1	0	0	20	0	0	0	0	21	2272.90244	0.00030	2711.73208	438.82993
8	1	1	0	0	21	0	0	0	0	22	2270.83699	0.00000	2751.43702	480.60003
9	1	1	0	0	22	0	0	0	0	23	2268.76472	0.00050	2793.02867	524.26445
10	1	1	0	0	23	0	0	0	0	24	2266.68398	0.00013	2836.50647	569.82262
11	1	1	0	0	24	0	0	0	0	25	2264.59570	-0.00021	2881.86985	617.27393
12	1	1	0	0	25	0	0	0	0	26	2262.50072	0.00030	2929.11819	666.61777
13	1	1	0	0	26	0	0	0	0	27	2260.39730	-0.00007	2978.25085	717.85348
14	1	1	0	0	27	0	0	0	0	28	2258.28699	0.00019	3029.26719	770.98038
15	1	1	0	0	28	0	0	0	0	29	2256.16917	0.00045	3082.16651	825.99778
16	1	1	0	0	29	0	0	0	0	30	2254.04378	0.00063	3136.94810	882.90495
17	1	1	0	0	30	0	0	0	0	31	2251.91112	0.00103	3193.61124	941.70115 +
18	1	1	0	0	31	0	0	0	0	32	2249.76932	-0.00025	3252.15516	1002.38559
19	1	1	0	0	2	0	0	0	0	1	2318.25470	0.00015	2320.15520	1.90066
20	1	1	0	0	3	0	0	0	0	2	2320.13038	-0.00049	2325.83282	5.70195
21	1	1	0	0	4	0	0	0	0	3	2321.99857	-0.00047	2333.40285	11.40382
22	1	1	0	0	5	0	0	0	0	4	2323.85933	0.00031	2342.86521	19.00619
23	1	1	0	0	6	0	0	0	0	5	2325.71048	-0.00030	2354.21976	28.50898
24	1	1	0	0	7	0	0	0	0	6	2327.55385	-0.00045	2367.46634	39.91204
25	1	1	0	0	8	0	0	0	0	7	2329.38544*	-0.00412	2382.60479	53.21523 +
26	1	1	0	0	9	0	0	0	0	8	2331.21610	-0.00041	2399.63490	68.41838
27	1	1	0	0	10	0	0	0	0	9	2333.03466	-0.00049	2418.55644	85.52129
28	1	1	0	0	11	0	0	0	0	10	2334.84514	-0.00028	2439.36915	104.52373
29	1	1	0	0	12	0	0	0	0	11	2336.64689	-0.00043	2462.07276	125.42544
30	1	1	0	0	13	0	0	0	0	12	2338.44084	0.00003	2486.66696	148.22616
31	1	1	0	0	14	0	0	0	0	13	2340.22587	0.00002	2513.15143	172.92558
32	1	1	0	0	15	0	0	0	0	14	2342.00241	-0.00002	2541.52580	199.52337
33	1	1	0	0	16	0	0	0	0	15	2343.77003	-0.00047	2571.78970	228.01920
34	1	1	0	0	17	0	0	0	0	16	2345.53078*	0.00073	2603.94273	258.41268
35	1	1	0	0	18	0	0	0	0	17	2347.28105	0.00002	2637.98444	290.70340
36	1	1	0	0	19	0	0	0	0	18	2349.02294	-0.00049	2673.91438	324.89096
37	1	1	0	0	20	0	0	0	0	19	2350.75704	-0.00016	2711.73208	360.97488
38	1	1	0	0	21	0	0	0	0	20	2352.48233	0.00002	2751.43702	398.95471
39	1	1	0	0	22	0	0	0	0	21	2354.19590	-0.00284	2793.02867	438.82993 +
40	1	1	0	0	23	0	0	0	0	22	2355.90925	0.00281	2836.50647	480.60003 +
41	1	1	0	0	24	0	0	0	0	23	2357.60559	0.00019	2881.86985	524.26445
42	1	1	0	0	25	0	0	0	0	24	2359.29561	0.00004	2929.11819	569.82262
43	1	1	0	0	26	0	0	0	0	25	2360.97691	-0.00001	2978.25085	617.27393
44	1	1	0	0	27	0	0	0	0	26	2362.64922	-0.00020	3029.26719	666.61777
45	1	1	0	0	28	0	0	0	0	27	2364.31312	0.00009	3082.16651	717.85348
46	1	1	0	0	29	0	0	0	0	28	2365.96847	0.00075	3136.94810	770.98038
47	1	1	0	0	30	0	0	0	0	29	2367.61354	0.00008	3193.61124	825.99778
48	1	1	0	0	31	0	0	0	0	30	2369.25258*	0.00237	3252.15516	882.90495 +
49	1	1	0	0	32	0	0	0	0	31	2370.87789	-0.00004	3312.57908	941.70115
50	1	1	0	0	33	0	0	0	0	32	2372.49751	0.00092	3374.88218	1002.38559
51	1	1	0	0	34	0	0	0	0	33	2374.10526	-0.00090	3439.06363	1064.95747
52	1	1	0	0	35	0	0	0	0	34	2375.70709	0.00050	3505.12257	1129.41599

53 rms = 0.00036 cm⁻¹

54
55
56
57 $v_2 + v_4 (\Pi) \leftarrow v_4 (\Pi)$

58	59	60	$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
			1 1 0 0 1	1 1 0 0 2	1801.08152	-0.00026	2316.37008	515.28830
			1 1 0 0 2	1 1 0 0 3	1799.16387	-0.00004	2320.15520	520.99129
			1 1 0 0 3	1 1 0 0 4	1797.23762	-0.00005	2325.83282	528.59515
			1 1 0 0 4	1 1 0 0 5	1795.30319	0.00013	2333.40285	538.09979

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1	1	1	0	0	35	1	1	0	0	34	1865.91863	-0.00052	3505.12257	1639.20342
2	1	1	0	0	37	1	1	0	0	36	1869.07036	-0.00059	3642.86936	1773.79841
3	1	-1	0	0	1	1	-1	0	0	2	1801.06490	-0.00038	2316.37844	515.31316
4	1	-1	0	0	2	1	-1	0	0	3	1799.13892	-0.00034	2320.18027	521.04101
5	1	-1	0	0	3	1	-1	0	0	4	1797.20503	0.00009	2325.88295	528.67801
6	1	-1	0	0	4	1	-1	0	0	5	1795.26205	-0.00028	2333.48640	538.22407
7	1	-1	0	0	5	1	-1	0	0	6	1793.31150	0.00003	2342.99052	549.67906
8	1	-1	0	0	6	1	-1	0	0	7	1791.35228	-0.00009	2354.39518	563.04281
9	1	-1	0	0	7	1	-1	0	0	8	1789.38526	0.00018	2367.70022	578.31514
10	1	-1	0	0	8	1	-1	0	0	9	1787.40978	0.00018	2382.90545	595.49585
11	1	-1	0	0	9	1	-1	0	0	10	1785.42590	-0.00007	2400.01067	614.58469
12	1	-1	0	0	10	1	-1	0	0	11	1783.43431	0.00009	2419.01564	635.58142
13	1	-1	0	0	11	1	-1	0	0	12	1781.43448	0.00011	2439.92010	658.48573
14	1	-1	0	0	12	1	-1	0	0	13	1779.42656	0.00012	2462.72376	683.29732
15	1	-1	0	0	13	1	-1	0	0	14	1777.41069	0.00022	2487.42631	710.01584
16	1	-1	0	0	14	1	-1	0	0	15	1775.38676	0.00028	2514.02742	738.64093
17	1	-1	0	0	15	1	-1	0	0	16	1773.35475	0.00025	2542.52670	769.17220
18	1	-1	0	0	16	1	-1	0	0	17	1771.31439	-0.00016	2572.92377	801.60923
19	1	-1	0	0	17	1	-1	0	0	18	1769.26685	0.00019	2605.21822	835.95156
20	1	-1	0	0	18	1	-1	0	0	19	1767.21115	0.00030	2639.40959	872.19874
21	1	-1	0	0	19	1	-1	0	0	20	1765.14719	0.00003	2675.49743	910.35027
22	1	-1	0	0	20	1	-1	0	0	21	1763.07556	-0.00005	2713.48122	950.40561
23	1	-1	0	0	21	1	-1	0	0	22	1760.99634	0.00012	2753.36045	992.36423
24	1	-1	0	0	22	1	-1	0	0	23	1758.90922	0.00020	2795.13457	1036.22555
25	1	-1	0	0	23	1	-1	0	0	24	1756.81420*	0.00015	2838.80301	1081.98896
26	1	-1	0	0	24	1	-1	0	0	25	1754.71139	0.00008	2884.36516	1129.65384
27	1	-1	0	0	25	1	-1	0	0	26	1752.60103	0.00018	2931.82039	1179.21954
28	1	-1	0	0	26	1	-1	0	0	27	1750.48282	0.00013	2981.16807	1230.68537
29	1	-1	0	0	27	1	-1	0	0	28	1748.35612	-0.00073	3032.40749	1284.05064
30	1	-1	0	0	28	1	-1	0	0	29	1746.22327	-0.00010	3085.53797	1339.31460
31	1	-1	0	0	29	1	-1	0	0	30	1744.08306	0.00080	3140.55877	1396.47651
32	1	-1	0	0	30	1	-1	0	0	31	1741.93355	-0.00001	3197.46913	1455.53557
33	1	-1	0	0	31	1	-1	0	0	32	1739.77715*	-0.00013	3256.26826	1516.49098
34	1	-1	0	0	2	1	-1	0	0	1	1808.68572	0.00001	2320.18027	511.49456
35	1	-1	0	0	3	1	-1	0	0	2	1810.56999	0.00020	2325.88295	515.31316
36	1	-1	0	0	4	1	-1	0	0	3	1812.44499	-0.00041	2333.48640	521.04101
37	1	-1	0	0	5	1	-1	0	0	4	1814.31274	0.00023	2342.99052	528.67801
38	1	-1	0	0	6	1	-1	0	0	5	1816.17119	0.00008	2354.39518	538.22407
39	1	-1	0	0	7	1	-1	0	0	6	1818.02132	0.00016	2367.70022	549.67906
40	1	-1	0	0	8	1	-1	0	0	7	1819.86252	-0.00012	2382.90545	563.04281
41	1	-1	0	0	9	1	-1	0	0	8	1821.69544	-0.00009	2400.01067	578.31514
42	1	-1	0	0	10	1	-1	0	0	9	1823.51976	-0.00003	2419.01564	595.49585
43	1	-1	0	0	11	1	-1	0	0	10	1825.33572	0.00032	2439.92010	614.58469
44	1	-1	0	0	12	1	-1	0	0	11	1827.14200	-0.00034	2462.72376	635.58142
45	1	-1	0	0	13	1	-1	0	0	12	1828.94079	0.00021	2487.42631	658.48573
46	1	-1	0	0	14	1	-1	0	0	13	1830.73021	0.00011	2514.02742	683.29732
47	1	-1	0	0	15	1	-1	0	0	14	1832.51066	-0.00020	2542.52670	710.01584
48	1	-1	0	0	16	1	-1	0	0	15	1834.28320	0.00036	2572.92377	738.64093
49	1	-1	0	0	17	1	-1	0	0	16	1836.04600	-0.00002	2605.21822	769.17220
50	1	-1	0	0	18	1	-1	0	0	17	1837.80043	0.00006	2639.40959	801.60923
51	1	-1	0	0	19	1	-1	0	0	18	1839.54608	0.00022	2675.49743	835.95156
52	1	-1	0	0	20	1	-1	0	0	19	1841.28259	0.00011	2713.48122	872.19874
53	1	-1	0	0	21	1	-1	0	0	20	1843.01065	0.00047	2753.36045	910.35027
54	1	-1	0	0	22	1	-1	0	0	21	1844.72918	0.00022	2795.13457	950.40561
55	1	-1	0	0	23	1	-1	0	0	22	1846.43907	0.00029	2838.80301	992.36423
56	1	-1	0	0	24	1	-1	0	0	23	1848.14036	0.00075	2884.36516	1036.22555
57	1	-1	0	0	25	1	-1	0	0	24	1849.83170	0.00027	2931.82039	1081.98896
58	1	-1	0	0	26	1	-1	0	0	25	1851.51418	-0.00004	2981.16807	1129.65384
59	1	-1	0	0	27	1	-1	0	0	26	1853.18762	-0.00033	3032.40749	1179.21954
60	1	-1	0	0	28	1	-1	0	0	27	1854.85259	0.00000	3085.53797	1230.68537
	1	-1	0	0	29	1	-1	0	0	28	1856.50813	0.00000	3140.55877	1284.05064
	1	-1	0	0	30	1	-1	0	0	29	1858.15463	0.00011	3197.46913	1339.31460
	1	-1	0	0	31	1	-1	0	0	30	1859.79116	-0.00060	3256.26826	1396.47651
	1	-1	0	0	32	1	-1	0	0	31	1861.41965	-0.00015	3316.95537	1455.53557
	1	-1	0	0	33	1	-1	0	0	32	1863.03847	-0.00017	3379.52962	1516.49098

1	-1	0	0	34	1	-1	0	0	33	1864.64859	0.00035	3443.99014	1579.34190
1	-1	0	0	35	1	-1	0	0	34	1866.24851	-0.00006	3510.33605	1644.08748
1	1	0	0	1	1	-1	0	0	1	1804.87588	0.00035	2316.37008	511.49456
1	1	0	0	2	1	-1	0	0	2	1804.84202	-0.00002	2320.15520	515.31316
1	1	0	0	3	1	-1	0	0	3	1804.79136	-0.00045	2325.83282	521.04101
1	1	0	0	4	1	-1	0	0	4	1804.72443	-0.00041	2333.40285	528.67801
1	1	0	0	5	1	-1	0	0	5	1804.64169	0.00055	2342.86521	538.22407
1	1	0	0	6	1	-1	0	0	6	1804.54010	-0.00060	2354.21976	549.67906
1	1	0	0	7	1	-1	0	0	7	1804.42293	-0.00061	2367.46634	563.04281
1	1	0	0	8	1	-1	0	0	8	1804.28884	-0.00081	2382.60479	578.31514
1	1	0	0	9	1	-1	0	0	9	1804.13959	0.00054	2399.63490	595.49585
1	1	0	0	10	1	-1	0	0	10	1803.97110	-0.00064	2418.55644	614.58469
1	1	0	0	11	1	-1	0	0	11	1803.78697	-0.00076	2439.36915	635.58142

rms = 0.00032 cm⁻¹

$v_2 + v_5 (\Pi) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	0 0 0 0 2	2475.59642	0.00009	2481.29828	5.70195
0 0 1 1 2	0 0 0 0 3	2473.67733	-0.00017	2485.08131	11.40382
0 0 1 1 3	0 0 0 0 4	2471.75012	0.00051	2490.75580	19.00619
0 0 1 1 4	0 0 0 0 5	2469.81242	-0.00027	2498.32167	28.50898
0 0 1 1 5	0 0 0 0 6	2467.86698	0.00021	2507.77881	39.91204
0 0 1 1 6	0 0 0 0 7	2465.91200	0.00013	2519.12711	53.21523
0 0 1 1 7	0 0 0 0 8	2463.94845	0.00043	2532.36640	68.41838
0 0 1 1 8	0 0 0 0 9	2461.97510	-0.00014	2547.49653	85.52129
0 0 1 1 9	0 0 0 0 10	2459.99277	-0.00078	2564.51727	104.52373
0 0 1 1 10	0 0 0 0 11	2458.00397	0.00099	2583.42842	125.42544
0 0 1 1 11	0 0 0 0 12	2456.00383	0.00027	2604.22971	148.22616
0 0 1 1 12	0 0 0 0 13	2453.99515	-0.00015	2626.92088	172.92558
0 0 1 1 13	0 0 0 0 14	2451.97760	-0.00063	2651.50161	199.52337
0 0 1 1 14	0 0 0 0 15	2449.95268	0.00030	2677.97158	228.01920
0 0 1 1 15	0 0 0 0 16	2447.91830	0.00053	2706.33045	258.41268
0 0 1 1 16	0 0 0 0 17	2445.87426	-0.00017	2736.57783	290.70340
0 0 1 1 17	0 0 0 0 18	2443.82269	0.00032	2768.71332	324.89096
0 0 1 1 18	0 0 0 0 19	2441.76188	0.00027	2802.73650	360.97488
0 0 1 1 19	0 0 0 0 20	2439.69215	-0.00005	2838.64691	398.95471
0 0 1 1 20	0 0 0 0 21	2437.61412	-0.00002	2876.44407	438.82993
0 0 1 1 21	0 0 0 0 22	2435.52757	0.00011	2916.12749	480.60003
0 0 1 1 22	0 0 0 0 23	2433.43149	-0.00069	2957.69664	524.26445
0 0 1 1 23	0 0 0 0 24	2431.32807	-0.00026	3001.15095	569.82262
0 0 1 1 24	0 0 0 0 25	2429.21597	0.00003	3046.48987	617.27393
0 0 1 1 25	0 0 0 0 26	2427.09454	-0.00047	3093.71278	666.61777
0 0 1 1 26	0 0 0 0 27	2424.96547	-0.00011	3142.81906	717.85348
0 0 1 1 27	0 0 0 0 28	2422.82453*	-0.00314	3193.80805	770.98038 †
0 0 1 1 28	0 0 0 0 29	2420.68426*	0.00296	3246.67908	825.99778 †
0 0 1 1 29	0 0 0 0 30	2418.52718	0.00069	3301.43144	882.90495
0 0 1 1 30	0 0 0 0 31	2416.36302	-0.00025	3358.06441	941.70115
0 0 1 1 31	0 0 0 0 32	2414.19224	0.00059	3416.57724	1002.38559
0 0 1 1 32	0 0 0 0 33	2412.01144	-0.00023	3476.96915	1064.95747
0 0 1 1 33	0 0 0 0 34	2409.82393	0.00059	3539.23933	1129.41599
0 0 1 1 34	0 0 0 0 35	2407.62609	-0.00060	3603.38696	1195.76027
0 0 1 1 2	0 0 0 0 1	2483.18111	0.00045	2485.08131	1.90066
0 0 1 1 3	0 0 0 0 2	2485.05376	-0.00010	2490.75580	5.70195
0 0 1 1 4	0 0 0 0 3	2486.91786	0.00001	2498.32167	11.40382
0 0 1 1 5	0 0 0 0 4	2488.77281	0.00019	2507.77881	19.00619
0 0 1 1 6	0 0 0 0 5	2490.61820	0.00007	2519.12711	28.50898
0 0 1 1 7	0 0 0 0 6	2492.45427	-0.00009	2532.36640	39.91204
0 0 1 1 8	0 0 0 0 7	2494.28043*	-0.00086	2547.49653	53.21523
0 0 1 1 9	0 0 0 0 8	2496.09904	0.00015	2564.51727	68.41838
0 0 1 1 10	0 0 0 0 9	2497.90722	0.00009	2583.42842	85.52129

2	0	0	1	1	11	0	0	0	0	10	2499.70576	-0.00023	2604.22971	104.52373
3	0	0	1	1	12	0	0	0	0	11	2501.49506	-0.00038	2626.92088	125.42544
4	0	0	1	1	13	0	0	0	0	12	2503.27545	0.00000	2651.50161	148.22616
5	0	0	1	1	14	0	0	0	0	13	2505.04559	-0.00042	2677.97158	172.92558
6	0	0	1	1	15	0	0	0	0	14	2506.80715	0.00007	2706.33045	199.52337
7	0	0	1	1	16	0	0	0	0	15	2508.55900	0.00037	2736.57783	228.01920
8	0	0	1	1	17	0	0	0	0	16	2510.30062	-0.00002	2768.71332	258.41268
9	0	0	1	1	18	0	0	0	0	17	2512.03305	-0.00004	2802.73650	290.70340
10	0	0	1	1	19	0	0	0	0	18	2513.75533	-0.00062	2838.64691	324.89096
11	0	0	1	1	20	0	0	0	0	19	2515.46895	-0.00024	2876.44407	360.97488
12	0	0	1	1	21	0	0	0	0	20	2517.17292	0.00014	2916.12749	398.95471
13	0	0	1	1	22	0	0	0	0	21	2518.86658	-0.00012	2957.69664	438.82993
14	0	0	1	1	23	0	0	0	0	22	2520.55105	0.00013	3001.15095	480.60003
15	0	0	1	1	24	0	0	0	0	23	2522.22498	-0.00044	3046.48987	524.26445
16	0	0	1	1	25	0	0	0	0	24	2523.89037	0.00021	3093.71278	569.82262
17	0	0	1	1	26	0	0	0	0	25	2525.54545	0.00033	3142.81906	617.27393
18	0	0	1	1	27	0	0	0	0	26	2527.19005	-0.00023	3193.80805	666.61777
19	0	0	1	1	28	0	0	0	0	27	2528.82564	0.00004	3246.67908	717.85348
20	0	0	1	1	29	0	0	0	0	28	2530.45055*	-0.00051	3301.43144	770.98038
21	0	0	1	1	30	0	0	0	0	29	2532.06636	-0.00027	3358.06441	825.99778
22	0	0	1	1	31	0	0	0	0	30	2533.67232	0.00003	3416.57724	882.90495
23	0	0	1	1	32	0	0	0	0	31	2535.26716	-0.00084	3476.96915	941.70115
24	0	0	1	1	33	0	0	0	0	32	2536.85321	-0.00053	3539.23933	1002.38559
25	0	0	1	1	34	0	0	0	0	33	2538.42988	0.00040	3603.38696	1064.95747
26	0	0	1	1	37	0	0	0	0	36	2543.09650	0.00006	3807.08590	1263.98946
27	0	0	1	-1	1	0	0	0	0	1	2479.40426*	0.00008	2481.30483	1.90066
28	0	0	1	-1	2	0	0	0	0	2	2479.39902	-0.00001	2485.10098	5.70195
29	0	0	1	-1	3	0	0	0	0	3	2479.39221	0.00090	2490.79512	11.40382
30	0	0	1	-1	4	0	0	0	0	4	2479.38078	-0.00023	2498.38720	19.00619
31	0	0	1	-1	5	0	0	0	0	5	2479.36815	0.00002	2507.87711	28.50898
32	0	0	1	-1	6	0	0	0	0	6	2479.35288	0.00021	2519.26471	39.91204
33	0	0	1	-1	7	0	0	0	0	7	2479.33449	-0.00014	2532.54987	53.21523
34	0	0	1	-1	8	0	0	0	0	8	2479.31304	-0.00096	2547.73239	68.41838
35	0	0	1	-1	9	0	0	0	0	9	2479.29087	0.00009	2564.81207	85.52129
36	0	0	1	-1	10	0	0	0	0	10	2479.26494	-0.00002	2583.78868	104.52373
37	0	0	1	-1	11	0	0	0	0	11	2479.23648	-0.00005	2604.66197	125.42544
38	0	0	1	-1	12	0	0	0	0	12	2479.20513	-0.00037	2627.43166	148.22616
39	0	0	1	-1	13	0	0	0	0	13	2479.17151	-0.00034	2652.09743	172.92558
40	0	0	1	-1	14	0	0	0	0	14	2479.13509	-0.00050	2678.65896	199.52337
41	0	0	1	-1	15	0	0	0	0	15	2479.09653	-0.00016	2707.11589	228.01920
42	0	0	1	-1	16	0	0	0	0	16	2479.05476	-0.00039	2737.46783	258.41268
43	0	0	1	-1	17	0	0	0	0	17	2479.01084	-0.00013	2769.71437	290.70340
44	0	0	1	-1	18	0	0	0	0	18	2478.96388	-0.00025	2803.85509	324.89096
45	0	0	1	-1	19	0	0	0	0	19	2478.91426	-0.00037	2839.88951	360.97488
46	0	0	1	-1	20	0	0	0	0	20	2478.86204	-0.00042	2877.81716	398.95471
47	0	0	1	-1	21	0	0	0	0	21	2478.80710	-0.00049	2917.63753	438.82993
48	0	0	1	-1	22	0	0	0	0	22	2478.74965	-0.00038	2959.35007	480.60003
49	0	0	1	-1	23	0	0	0	0	23	2478.68908	-0.00069	3002.95422	524.26445
50	0	0	1	-1	24	0	0	0	0	24	2478.62660	-0.00018	3048.44940	569.82262
51	0	0	1	-1	25	0	0	0	0	25	2478.55466*	-0.00640	3095.83499	617.27393 +
52	0	0	1	-1	26	0	0	0	0	26	2478.49243	-0.00016	3145.11036	666.61777
53	0	0	1	-1	27	0	0	0	0	27	2478.42138	0.00002	3196.27484	717.85348
54	0	0	1	-1	28	0	0	0	0	28	2478.34746	0.00011	3249.32773	770.98038
55	0	0	1	-1	29	0	0	0	0	29	2478.27098	0.00042	3304.26834	825.99778
56	0	0	1	-1	30	0	0	0	0	30	2478.19131	0.00036	3361.09591	882.90495

rms = 0.00037 cm⁻¹

$$v_2 + v_5 (\Pi) \leftarrow v_5 (\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	0 0 1 1 2	1801.36239	-0.00022	2481.29828	679.93567
0 0 1 1 2	0 0 1 1 3	1799.44633	-0.00006	2485.08131	685.63493
0 0 1 1 3	0 0 1 1 4	1797.52264	0.00066	2490.75580	693.23382
0 0 1 1 4	0 0 1 1 5	1795.58980	0.00037	2498.32167	702.73224
0 0 1 1 5	0 0 1 1 6	1793.64899	0.00025	2507.77881	714.13007
0 0 1 1 6	0 0 1 1 7	1791.70036	0.00041	2519.12711	727.42716
0 0 1 1 7	0 0 1 1 8	1789.74343	0.00036	2532.36640	742.62333
0 0 1 1 8	0 0 1 1 9	1787.77835	0.00021	2547.49653	759.71839
0 0 1 1 9	0 0 1 1 10	1785.80528	0.00010	2564.51727	778.71209
0 0 1 1 10	0 0 1 1 11	1783.82419	-0.00003	2583.42842	799.60420
0 0 1 1 11	0 0 1 1 12	1781.83534	0.00007	2604.22971	822.39444
0 0 1 1 12	0 0 1 1 13	1779.83842	0.00005	2626.92088	847.08251
0 0 1 1 13	0 0 1 1 14	1777.83370	0.00017	2651.50161	873.66808
0 0 1 1 14	0 0 1 1 15	1775.82075	-0.00004	2677.97158	902.15079
0 0 1 1 15	0 0 1 1 16	1773.80005	-0.00012	2706.33045	932.53028
0 0 1 1 16	0 0 1 1 17	1771.77200	0.00031	2736.57783	964.80614
0 0 1 1 17	0 0 1 1 18	1769.73495	-0.00042	2768.71332	998.97795
0 0 1 1 18	0 0 1 1 19	1767.69095	-0.00030	2802.73650	1035.04524
0 0 1 1 19	0 0 1 1 20	1765.63926	-0.00009	2838.64691	1073.00756
0 0 1 1 20	0 0 1 1 21	1763.57971	0.00002	2876.44407	1112.86438
0 0 1 1 21	0 0 1 1 22	1761.51230	0.00001	2916.12749	1154.61520
0 0 1 1 22	0 0 1 1 23	1759.43700	-0.00018	2957.69664	1198.25945
0 0 1 1 23	0 0 1 1 24	1757.35429	-0.00010	3001.15095	1243.79656
0 0 1 1 24	0 0 1 1 25	1755.26366	-0.00028	3046.48987	1291.22593
0 0 1 1 25	0 0 1 1 26	1753.16592	0.00007	3093.71278	1340.54693
0 0 1 1 26	0 0 1 1 27	1751.06022	0.00007	3142.81906	1391.75891
0 0 1 1 27	0 0 1 1 28	1748.94749	0.00063	3193.80805	1444.86119
0 0 1 1 28	0 0 1 1 29	1746.82595	-0.00005	3246.67908	1499.85307
0 0 1 1 29	0 0 1 1 30	1744.69795	0.00034	3301.43144	1556.73383
0 0 1 1 30	0 0 1 1 31	1742.56113	-0.00057	3358.06441	1615.50271
0 0 1 1 31	0 0 1 1 32	1740.41844	0.00014	3416.57724	1676.15894
0 0 1 1 32	0 0 1 1 33	1738.26786	0.00042	3476.96915	1738.70171
0 0 1 1 33	0 0 1 1 34	1736.10835	-0.00078	3539.23933	1803.13019
0 0 1 1 2	0 0 1 1 1	1808.94593	0.00074	2485.08131	676.13613
0 0 1 1 3	0 0 1 1 2	1810.82029	0.00016	2490.75580	679.93567
0 0 1 1 4	0 0 1 1 3	1812.68700	0.00026	2498.32167	685.63493
0 0 1 1 5	0 0 1 1 4	1814.54518	0.00019	2507.77881	693.23382
0 0 1 1 6	0 0 1 1 5	1816.39481	-0.00006	2519.12711	702.73224
0 0 1 1 7	0 0 1 1 6	1818.23669	0.00036	2532.36640	714.13007
0 0 1 1 8	0 0 1 1 7	1820.06794*	-0.00143	2547.49653	727.42716 †
0 0 1 1 9	0 0 1 1 8	1821.89396	0.00002	2564.51727	742.62333
0 0 1 1 10	0 0 1 1 9	1823.70957	-0.00047	2583.42842	759.71839
0 0 1 1 11	0 0 1 1 10	1825.51746	-0.00016	2604.22971	778.71209
0 0 1 1 12	0 0 1 1 11	1827.31676	0.00009	2626.92088	799.60420
0 0 1 1 13	0 0 1 1 12	1829.10735	0.00018	2651.50161	822.39444
0 0 1 1 14	0 0 1 1 13	1830.88922	0.00015	2677.97158	847.08251
0 0 1 1 15	0 0 1 1 14	1832.66256	0.00019	2706.33045	873.66808
0 0 1 1 16	0 0 1 1 15	1834.42737	0.00033	2736.57783	902.15079
0 0 1 1 17	0 0 1 1 16	1836.18277	-0.00027	2768.71332	932.53028
0 0 1 1 18	0 0 1 1 17	1837.93042	0.00006	2802.73650	964.80614
0 0 1 1 19	0 0 1 1 18	1839.66887	-0.00009	2838.64691	998.97795
0 0 1 1 20	0 0 1 1 19	1841.39891	0.00008	2876.44407	1035.04524
0 0 1 1 21	0 0 1 1 20	1843.11969	-0.00024	2916.12749	1073.00756
0 0 1 1 22	0 0 1 1 21	1844.83217	-0.00008	2957.69664	1112.86438
0 0 1 1 23	0 0 1 1 22	1846.53570	-0.00005	3001.15095	1154.61520
0 0 1 1 24	0 0 1 1 23	1848.23043	0.00001	3046.48987	1198.25945
0 0 1 1 25	0 0 1 1 24	1849.91614	-0.00008	3093.71278	1243.79656
0 0 1 1 26	0 0 1 1 25	1851.59358	0.00046	3142.81906	1291.22593
0 0 1 1 27	0 0 1 1 26	1853.26104	-0.00008	3193.80805	1340.54693

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1											
2	0	0	1	-1	26	0	0	1	-1	25	1851.77338
3	0	0	1	-1	27	0	0	1	-1	26	1853.44913
4	0	0	1	-1	28	0	0	1	-1	27	1855.11483
5	0	0	1	-1	29	0	0	1	-1	28	1856.77305
6	0	0	1	-1	30	0	0	1	-1	29	1858.42036
7	0	0	1	-1	31	0	0	1	-1	30	1860.06099
8	0	0	1	-1	32	0	0	1	-1	31	1861.69099
9	0	0	1	-1	33	0	0	1	-1	32	1863.31208
10	0	0	1	-1	34	0	0	1	-1	33	1864.92384
11	0	0	1	-1	35	0	0	1	-1	34	1866.52730
12	0	0	1	1	1	0	0	1	-1	1	1805.15557
13	0	0	1	1	2	0	0	1	-1	2	1805.12537
14	0	0	1	1	3	0	0	1	-1	3	1805.08095
15	0	0	1	1	4	0	0	1	-1	4	1805.02251
16	0	0	1	1	5	0	0	1	-1	5	1804.94873
17	0	0	1	1	6	0	0	1	-1	6	1804.85931
18	0	0	1	1	7	0	0	1	-1	7	1804.75722
19	0	0	1	1	8	0	0	1	-1	8	1804.63906*
20	0	0	1	1	9	0	0	1	-1	9	1804.50516
21	0	0	1	1	10	0	0	1	-1	10	1804.35893
22	0	0	1	-1	8	0	0	1	1	8	1805.10895
23	0	0	1	-1	9	0	0	1	1	9	1805.09377
24	0	0	1	-1	11	0	0	1	1	11	1805.05788
25	rms = 0.00034 cm ⁻¹										

$\nu_2 + 2\nu_4 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 0 0 0	0 0 0 0 1	2816.88097	-0.00007	2818.78169	1.90066
2 0 0 0 1	0 0 0 0 2	2814.98141	0.00020	2820.68316	5.70195
2 0 0 0 2	0 0 0 0 3	2813.08160	-0.00053	2824.48595	11.40382
2 0 0 0 3	0 0 0 0 4	2811.18365	0.00008	2830.18976	19.00619
2 0 0 0 4	0 0 0 0 5	2809.28493	-0.00027	2837.79417	28.50898
2 0 0 0 5	0 0 0 0 6	2807.38611	-0.00045	2847.29860	39.91204
2 0 0 0 6	0 0 0 0 7	2805.48717	0.00009	2858.70231	53.21523
2 0 0 0 7	0 0 0 0 8	2803.58554	-0.00053	2872.00445	68.41838
2 0 0 0 8	0 0 0 0 9	2801.68191	-0.00083	2887.20403	85.52129
2 0 0 0 9	0 0 0 0 10	2799.77610	-0.00010	2904.29993	104.52373
2 0 0 0 10	0 0 0 0 11	2797.86533	-0.00019	2923.29095	125.42544
2 0 0 0 11	0 0 0 0 12	2795.94916	-0.00051	2944.17582	148.22616
2 0 0 0 12	0 0 0 0 13	2794.02776	0.00011	2966.95322	172.92558
2 0 0 0 13	0 0 0 0 14	2792.09827	-0.00018	2991.62183	199.52337
2 0 0 0 14	0 0 0 0 15	2790.16107	-0.00008	3018.18035	228.01920
2 0 0 0 15	0 0 0 0 16	2788.21441	-0.00049	3046.62757	258.41268
2 0 0 0 16	0 0 0 0 17	2786.25895	-0.00001	3076.96236	290.70340
2 0 0 0 17	0 0 0 0 18	2784.29226	-0.00048	3109.18370	324.89096
2 0 0 0 18	0 0 0 0 19	2782.31638	0.00057	3143.29070	360.97488
2 0 0 0 19	0 0 0 0 20	2780.32804	0.00017	3179.28258	398.95471
2 0 0 0 20	0 0 0 0 21	2778.32845	-0.00029	3217.15868	438.82993
2 0 0 0 21	0 0 0 0 22	2776.31827	-0.00012	3256.91842	480.60003
2 0 0 0 22	0 0 0 0 23	2774.29642	-0.00042	3298.56130	524.26445
2 0 0 0 23	0 0 0 0 24	2772.26427*	0.00004	3342.08685	569.82262
2 0 0 0 1	0 0 0 0 0	2820.68362	0.00046	2820.68316	0.00000
2 0 0 0 2	0 0 0 0 1	2822.58490	-0.00039	2824.48595	1.90066
2 0 0 0 3	0 0 0 0 2	2824.48677	-0.00105	2830.18976	5.70195
2 0 0 0 4	0 0 0 0 3	2826.38991	-0.00045	2837.79417	11.40382
2 0 0 0 5	0 0 0 0 4	2828.29291	0.00050	2847.29860	19.00619
2 0 0 0 6	0 0 0 0 5	2830.19302	-0.00032	2858.70231	28.50898
2 0 0 0 7	0 0 0 0 6	2832.09230	-0.00011	2872.00445	39.91204
2 0 0 0 8	0 0 0 0 7	2833.98877	-0.00002	2887.20403	53.21523
2 0 0 0 9	0 0 0 0 8	2835.88160	0.00006	2904.29993	68.41838
2 0 0 0 10	0 0 0 0 9	2837.76901	-0.00065	2923.29095	85.52129

1														
2	2	0	0	0	11	0	0	0	0	10	2839.65180	-0.00030	2944.17582	104.52373
3	2	0	0	0	12	0	0	0	0	11	2841.52741	-0.00037	2966.95322	125.42544
4	2	0	0	0	13	0	0	0	0	12	2843.39547	-0.00020	2991.62183	148.22616
5	2	0	0	0	14	0	0	0	0	13	2845.25444	-0.00034	3018.18035	172.92558
6	2	0	0	0	15	0	0	0	0	14	2847.10395	-0.00025	3046.62757	199.52337
7	2	0	0	0	16	0	0	0	0	15	2848.94291	-0.00025	3076.96236	228.01920
8	2	0	0	0	17	0	0	0	0	16	2850.77091	-0.00011	3109.18370	258.41268
9	2	0	0	0	18	0	0	0	0	17	2852.58648	-0.00081	3143.29070	290.70340
10	2	0	0	0	19	0	0	0	0	18	2854.39108	-0.00054	3179.28258	324.89096
11	2	0	0	0	20	0	0	0	0	19	2856.18293	-0.00086	3217.15868	360.97488
12	2	0	0	0	21	0	0	0	0	20	2857.96080	-0.00291	3256.91842	398.95471
13	2	0	0	0	22	0	0	0	0	21	2859.73156	0.00020	3298.56130	438.82993

rms = 0.00039 cm⁻¹

$v_2 + 2v_4 (\Sigma^+) \leftarrow v_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 0 0 1	1 1 0 0 2	2305.39565*	0.00079	2820.68316	515.28830
2 0 0 0 2	1 1 0 0 3	2303.49468	0.00002	2824.48595	520.99129
2 0 0 0 3	1 1 0 0 4	2301.59394	-0.00067	2830.18976	528.59515
2 0 0 0 4	1 1 0 0 5	2299.69485	0.00047	2837.79417	538.09979
2 0 0 0 5	1 1 0 0 6	2297.79378	0.00026	2847.29860	549.50508
2 0 0 0 6	1 1 0 0 7	2295.89207	0.00062	2858.70231	562.81086
2 0 0 0 7	1 1 0 0 8	2293.98798	0.00050	2872.00445	578.01697
2 0 0 0 8	1 1 0 0 9	2292.08123	0.00039	2887.20403	595.12319
2 0 0 0 9	1 1 0 0 10	2290.17149	0.00085	2904.29993	614.12929
2 0 0 0 10	1 1 0 0 11	2288.25660	0.00068	2923.29095	635.03503
2 0 0 0 11	1 1 0 0 12	2286.33550	-0.00020	2944.17582	657.84012
2 0 0 0 12	1 1 0 0 13	2284.40979	0.00083	2966.95322	682.54427
2 0 0 0 13	1 1 0 0 14	2282.47595*	0.00125	2991.62183	709.14713
2 0 0 0 14	1 1 0 0 15	2280.53213	0.00013	3018.18035	737.64836
2 0 0 0 15	1 1 0 0 16	2278.58063	0.00063	3046.62757	768.04757
2 0 0 0 16	1 1 0 0 17	2276.61753	-0.00047	3076.96236	800.34436
2 0 0 0 17	1 1 0 0 18	2274.64553	0.00013	3109.18370	834.53830
2 0 0 0 18	1 1 0 0 19	2272.66203	0.00026	3143.29070	870.62893
2 0 0 0 19	1 1 0 0 20	2270.66680	-0.00001	3179.28258	908.61577
2 0 0 0 20	1 1 0 0 21	2268.66138*	0.00101	3217.15868	948.49830
2 0 0 0 21	1 1 0 0 22	2266.64217	-0.00024	3256.91842	990.27601
2 0 0 0 22	1 1 0 0 23	2264.61313	0.00017	3298.56130	1033.94833
2 0 0 0 23	1 1 0 0 24	2262.57269	0.00052	3342.08685	1079.51468
2 0 0 0 2	1 1 0 0 1	2313.00050	0.00082	2824.48595	511.48627
2 0 0 0 3	1 1 0 0 2	2314.90070	-0.00076	2830.18976	515.28830
2 0 0 0 4	1 1 0 0 3	2316.80292	0.00003	2837.79417	520.99129
2 0 0 0 5	1 1 0 0 4	2318.70341	-0.00004	2847.29860	528.59515
2 0 0 0 6	1 1 0 0 5	2320.60240	-0.00012	2858.70231	538.09979
2 0 0 0 7	1 1 0 0 6	2322.49989	0.00052	2872.00445	549.50508
2 0 0 0 8	1 1 0 0 7	2324.39371	0.00055	2887.20403	562.81086
2 0 0 0 9	1 1 0 0 8	2326.28323	0.00027	2904.29993	578.01697
2 0 0 0 10	1 1 0 0 9	2328.16787	0.00010	2923.29095	595.12319
2 0 0 0 11	1 1 0 0 10	2330.04654*	0.00001	2944.17582	614.12929
2 0 0 0 12	1 1 0 0 11	2331.91807	-0.00012	2966.95322	635.03503
2 0 0 0 13	1 1 0 0 12	2333.78212	0.00041	2991.62183	657.84012
2 0 0 0 14	1 1 0 0 13	2335.63575*	-0.00034	3018.18035	682.54427
2 0 0 0 15	1 1 0 0 14	2337.48061	0.00017	3046.62757	709.14713
2 0 0 0 16	1 1 0 0 15	2339.31428*	0.00028	3076.96236	737.64836
2 0 0 0 17	1 1 0 0 16	2341.13477*	-0.00136	3109.18370	768.04757
2 0 0 0 18	1 1 0 0 17	2342.94644	0.00011	3143.29070	800.34436
2 0 0 0 19	1 1 0 0 18	2344.74388	-0.00040	3179.28258	834.53830
2 0 0 0 20	1 1 0 0 19	2346.52852*	-0.00123	3217.15868	870.62893
2 0 0 0 21	1 1 0 0 20	2348.30159*	-0.00106	3256.91842	908.61577
2 0 0 0 22	1 1 0 0 21	2350.06238	-0.00061	3298.56130	948.49830

2	0	0	0	1	1	-1	0	0	1	2309.18849	-0.00011	2820.68316	511.49456
2	0	0	0	2	1	-1	0	0	2	2309.17221	-0.00057	2824.48595	515.31316
2	0	0	0	3	1	-1	0	0	3	2309.14931	0.00055	2830.18976	521.04101
2	0	0	0	4	1	-1	0	0	4	2309.11665	0.00049	2837.79417	528.67801
2	0	0	0	5	1	-1	0	0	5	2309.07483	0.00030	2847.29860	538.22407
2	0	0	0	6	1	-1	0	0	6	2309.02644*	0.00318	2858.70231	549.67906 +
2	0	0	0	7	1	-1	0	0	7	2308.96219	0.00054	2872.00445	563.04281
2	0	0	0	8	1	-1	0	0	8	2308.89206*	0.00317	2887.20403	578.31514 +
2	0	0	0	9	1	-1	0	0	9	2308.80512	0.00104	2904.29993	595.49585 +
2	0	0	0	10	1	-1	0	0	10	2308.70596	-0.00030	2923.29095	614.58469
2	0	0	0	11	1	-1	0	0	11	2308.59413	-0.00028	2944.17582	635.58142
2	0	0	0	12	1	-1	0	0	12	2308.46746	-0.00003	2966.95322	658.48573
2	0	0	0	13	1	-1	0	0	13	2308.32407	-0.00044	2991.62183	683.29732
2	0	0	0	14	1	-1	0	0	14	2308.16413*	-0.00038	3018.18035	710.01584
2	0	0	0	15	1	-1	0	0	15	2307.98946*	0.00282	3046.62757	738.64093 +
2	0	0	0	16	1	-1	0	0	16	2307.79026	0.00010	3076.96236	769.17220
2	0	0	0	17	1	-1	0	0	17	2307.57501	0.00054	3109.18370	801.60923
2	0	0	0	18	1	-1	0	0	18	2307.33923	0.00010	3143.29070	835.95156
2	0	0	0	19	1	-1	0	0	19	2307.08417	0.00034	3179.28258	872.19874
2	0	0	0	20	1	-1	0	0	20	2306.80834	-0.00007	3217.15868	910.35027

rms = 0.00043 cm⁻¹

$v_2 + 2v_4 (\Sigma^+) \leftarrow 2v_4 (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 0 0 0	2 0 0 0 1	1800.02022	0.00002	2818.78169	1018.76149
2 0 0 0 1	2 0 0 0 2	1798.10153	-0.00004	2820.68316	1022.58159
2 0 0 0 2	2 0 0 0 3	1796.17424	-0.00028	2824.48595	1028.31143
2 0 0 0 3	2 0 0 0 4	1794.23984	0.00072	2830.18976	1035.95064
2 0 0 0 4	2 0 0 0 5	1792.29585	0.00043	2837.79417	1045.49875
2 0 0 0 5	2 0 0 0 6	1790.34391	0.00046	2847.29860	1056.95515
2 0 0 0 6	2 0 0 0 7	1788.38390	0.00069	2858.70231	1070.31910
2 0 0 0 7	2 0 0 0 8	1786.41467	-0.00001	2872.00445	1085.58977
2 0 0 0 8	2 0 0 0 9	1784.43794	0.00012	2887.20403	1102.76621
2 0 0 0 9	2 0 0 0 10	1782.45270	0.00016	2904.29993	1121.84738
2 0 0 0 10	2 0 0 0 11	1780.45800	-0.00079	2923.29095	1142.83216
2 0 0 0 11	2 0 0 0 12	1778.45617	-0.00030	2944.17582	1165.71936
2 0 0 0 12	2 0 0 0 13	1776.44535	-0.00013	2966.95322	1190.50774
2 0 0 0 13	2 0 0 0 14	1774.42541	-0.00036	2991.62183	1217.19606
2 0 0 0 14	2 0 0 0 15	1772.39758	0.00031	3018.18035	1245.78308
2 0 0 0 15	2 0 0 0 16	1770.36031	0.00034	3046.62757	1276.26760
2 0 0 0 16	2 0 0 0 17	1768.31143*	-0.00245	3076.96236	1308.64848 †
2 0 0 0 17	2 0 0 0 18	1766.25962	0.00058	3109.18370	1342.92466
2 0 0 0 18	2 0 0 0 19	1764.19638	0.00083	3143.29070	1379.09514
2 0 0 0 19	2 0 0 0 20	1762.12304	-0.00048	3179.28258	1417.15906
2 0 0 0 20	2 0 0 0 21	1760.04292	-0.00016	3217.15868	1457.11560
2 0 0 0 21	2 0 0 0 22	1757.95360	-0.00075	3256.91842	1498.96407
2 0 0 0 22	2 0 0 0 23	1755.85611	-0.00138	3298.56130	1542.70381 †
2 0 0 0 23	2 0 0 0 24	1753.75302	0.00041	3342.08685	1588.33424
2 0 0 0 24	2 0 0 0 25	1751.63949	-0.00035	3387.49464	1635.85480
2 0 0 0 1	2 0 0 0 0	1803.83198	0.00021	2820.68316	1016.85139
2 0 0 0 2	2 0 0 0 1	1805.72430*	-0.00015	2824.48595	1018.76149
2 0 0 0 3	2 0 0 0 2	1807.60865	0.00048	2830.18976	1022.58159
2 0 0 0 4	2 0 0 0 3	1809.48259	-0.00016	2837.79417	1028.31143
2 0 0 0 5	2 0 0 0 4	1811.34735	-0.00060	2847.29860	1035.95064
2 0 0 0 6	2 0 0 0 5	1813.20281	-0.00075	2858.70231	1045.49875
2 0 0 0 7	2 0 0 0 6	1815.04949	0.00018	2872.00445	1056.95515
2 0 0 0 8	2 0 0 0 7	1816.88552	0.00059	2887.20403	1070.31910
2 0 0 0 9	2 0 0 0 8	1818.70952	-0.00064	2904.29993	1085.58977
2 0 0 0 10	2 0 0 0 9	1820.52423	-0.00051	2923.29095	1102.76621
2 0 0 0 11	2 0 0 0 10	1822.32815	-0.00029	2944.17582	1121.84738

1														
2	2	0	0	0	12	2	0	0	0	11	1824.12099	-0.00007	2966.95322	1142.83216
3	2	0	0	0	13	2	0	0	0	12	1825.90234	-0.00013	2991.62183	1165.71936
4	2	0	0	0	14	2	0	0	0	13	1827.67255	-0.00006	3018.18035	1190.50774
5	2	0	0	0	15	2	0	0	0	14	1829.43195	0.00044	3046.62757	1217.19606
6	2	0	0	0	16	2	0	0	0	15	1831.17960	0.00032	3076.96236	1245.78308
7	2	0	0	0	17	2	0	0	0	16	1832.91615	0.00006	3109.18370	1276.26760
8	2	0	0	0	18	2	0	0	0	17	1834.64244	0.00023	3143.29070	1308.64848
9	2	0	0	0	19	2	0	0	0	18	1836.35588*	-0.00204	3179.28258	1342.92466 +
10	2	0	0	0	20	2	0	0	0	19	1838.06302*	-0.00052	3217.15868	1379.09514
11	2	0	0	0	21	2	0	0	0	20	1839.75998	0.00062	3256.91842	1417.15906
12	2	0	0	0	22	2	0	0	0	21	1841.44567	-0.00002	3298.56130	1457.11560
13	2	0	0	0	23	2	0	0	0	22	1843.12000*	-0.00278	3342.08685	1498.96407 +
14	2	0	0	0	24	2	0	0	0	23	1844.79151	0.00068	3387.49464	1542.70381

rms = 0.00044 cm⁻¹

$v_2 + 2v_4 (\Delta) \leftarrow v_4 (\Pi)$

22	$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
23	2 -2 0 0 4	1 -1 0 0 5	2303.14438	0.00001	2841.36845	538.22407
24	2 -2 0 0 5	1 -1 0 0 6	2301.19370	0.00053	2850.87223	549.67906
25	2 -2 0 0 6	1 -1 0 0 7	2299.23378	0.00011	2862.27647	563.04281
26	2 -2 0 0 7	1 -1 0 0 8	2297.26614	0.00026	2875.58102	578.31514
27	2 -2 0 0 8	1 -1 0 0 9	2295.29045	0.00061	2890.78569	595.49585
28	2 -2 0 0 9	1 -1 0 0 10	2293.30332*	-0.00226	2907.89027	614.58469 †
29	2 -2 0 0 10	1 -1 0 0 11	2291.31407	0.00097	2926.89452	635.58142
30	2 -2 0 0 11	1 -1 0 0 12	2289.31169	-0.00075	2947.79817	658.48573
31	2 -2 0 0 12	1 -1 0 0 13	2287.30015*	-0.00347	2970.60094	683.29732 †
32	2 -2 0 0 13	1 -1 0 0 14	2285.28658	-0.00008	2995.30250	710.01584
33	2 -2 0 0 14	1 -1 0 0 15	2283.26182	0.00024	3021.90251	738.64093
34	2 -2 0 0 15	1 -1 0 0 16	2281.22695*	-0.00145	3050.40060	769.17220 †
35	2 -2 0 0 16	1 -1 0 0 17	2279.18737*	0.00022	3080.79638	801.60923
36	2 -2 0 0 17	1 -1 0 0 18	2277.13761*	-0.00024	3113.08941	835.95156
37	2 -2 0 0 18	1 -1 0 0 19	2275.08055	0.00004	3147.27925	872.19874
38	2 -2 0 0 19	1 -1 0 0 20	2273.01517	0.00001	3183.36543	910.35027
39	2 -2 0 0 20	1 -1 0 0 21	2270.94259	0.00077	3221.34743	950.40561
40	2 -2 0 0 2	1 -1 0 0 1	2316.56786	-0.00037	2828.06278	511.49456
41	2 -2 0 0 3	1 -1 0 0 2	2318.45217	0.00007	2833.76526	515.31316
42	2 -2 0 0 4	1 -1 0 0 3	2320.32724	-0.00020	2841.36845	521.04101
43	2 -2 0 0 5	1 -1 0 0 4	2322.19421	0.00000	2850.87223	528.67801
44	2 -2 0 0 6	1 -1 0 0 5	2324.05103	-0.00137	2862.27647	538.22407 †
45	2 -2 0 0 7	1 -1 0 0 6	2325.90175	-0.00022	2875.58102	549.67906
46	2 -2 0 0 8	1 -1 0 0 7	2327.74334	0.00045	2890.78569	563.04281
47	2 -2 0 0 9	1 -1 0 0 8	2329.57533	0.00020	2907.89027	578.31514
48	2 -2 0 0 10	1 -1 0 0 9	2331.39890	0.00023	2926.89452	595.49585
49	2 -2 0 0 11	1 -1 0 0 10	2333.21328	-0.00020	2947.79817	614.58469
50	2 -2 0 0 12	1 -1 0 0 11	2335.01947	-0.00005	2970.60094	635.58142
51	2 -2 0 0 13	1 -1 0 0 12	2336.81726	0.00049	2995.30250	658.48573
52	2 -2 0 0 14	1 -1 0 0 13	2338.60506	-0.00013	3021.90251	683.29732
53	2 -2 0 0 15	1 -1 0 0 14	2340.38531	0.00055	3050.40060	710.01584
54	2 -2 0 0 16	1 -1 0 0 15	2342.15575	0.00031	3080.79638	738.64093
55	2 -2 0 0 17	1 -1 0 0 16	2343.91707	-0.00014	3113.08941	769.17220
56	2 -2 0 0 18	1 -1 0 0 17	2345.67058	0.00055	3147.27925	801.60923
57	2 -2 0 0 19	1 -1 0 0 18	2347.41377	-0.00010	3183.36543	835.95156
58	2 -2 0 0 20	1 -1 0 0 19	2349.14855	-0.00014	3221.34743	872.19874
59	2 -2 0 0 21	1 -1 0 0 20	2350.87377	-0.00070	3261.22474	910.35027
60	2 2 0 0 2	1 1 0 0 3	2307.07228	0.00067	2828.06290	520.99129
	2 2 0 0 3	1 1 0 0 4	2305.16969*	-0.00102	2833.76586	528.59515 †
	2 2 0 0 4	1 1 0 0 5	2303.27084	0.00040	2841.37023	538.09979
	2 2 0 0 5	1 1 0 0 6	2301.37008	-0.00123	2850.87639	549.50508 †
	2 2 0 0 6	1 1 0 0 7	2299.47389	-0.00004	2862.28479	562.81086
	2 2 0 0 7	1 1 0 0 8	2297.57979*	0.00078	2875.59598	578.01697

$$\text{rms} = 0.00044 \text{ cm}^{-1}$$

v_4''	ℓ_4''	v_5''	ℓ_5''	J''	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	E'	E''
2	2	0	0	2	2	2	0	0	3	1795.35327*	0.00009	2828.06290	1032.70973
2	2	0	0	3	2	2	0	0	4	1793.41987*	0.00244	2833.76586	1040.34843
2	2	0	0	4	2	2	0	0	5	1791.47231	-0.00060	2841.37023	1049.89732

1	2	2	0	0	5	2	2	0	0	6	1789.51914	-0.00050	2850.87639	1061.35675
3	2	2	0	0	6	2	2	0	0	7	1787.55772	0.00005	2862.28479	1074.72712
4	2	2	0	0	7	2	2	0	0	8	1785.58628	-0.00081	2875.59598	1090.00889
5	2	2	0	0	8	2	2	0	0	9	1783.60774*	-0.00025	2890.81058	1107.20259
6	2	2	0	0	9	2	2	0	0	10	1781.62036	-0.00013	2907.92928	1126.30879
7	2	2	0	0	10	2	2	0	0	11	1779.62421*	-0.00051	2926.95280	1147.32807
8	2	2	0	0	11	2	2	0	0	12	1777.62023	-0.00060	2947.88189	1170.26105
9	2	2	0	0	12	2	2	0	0	13	1775.61006	0.00110	2970.71728	1195.10832 +
10	2	2	0	0	13	2	2	0	0	14	1773.58977	0.00054	2995.45967	1221.87043
11	2	2	0	0	14	2	2	0	0	15	1771.56088	-0.00088	3022.10964	1250.54788
12	2	2	0	0	15	2	2	0	0	16	1769.52694	0.00032	3050.66770	1281.14108
13	2	2	0	0	16	2	2	0	0	17	1767.48463	0.00079	3081.13416	1313.65031
14	2	2	0	0	17	2	2	0	0	18	1765.43343	-0.00001	3113.50919	1348.07575
15	2	2	0	0	18	2	2	0	0	19	1763.37531	-0.00007	3147.79280	1384.41742
16	2	2	0	0	19	2	2	0	0	20	1761.30943	-0.00018	3183.98480	1422.67519
17	2	2	0	0	20	2	2	0	0	21	1759.23498	-0.00107	3222.08485	1462.84880 +
18	2	2	0	0	21	2	2	0	0	22	1757.15296	-0.00167	3262.09247	1504.93784 +
19	2	2	0	0	22	2	2	0	0	23	1755.06557	0.00032	3304.00706	1548.94181
20	2	2	0	0	3	2	2	0	0	2	1806.78484	-0.00008	2833.76586	1026.98094
21	2	2	0	0	4	2	2	0	0	3	1808.66130	0.00080	2841.37023	1032.70973
22	2	2	0	0	5	2	2	0	0	4	1810.52803	0.00007	2850.87639	1040.34843
23	2	2	0	0	6	2	2	0	0	5	1812.38835	0.00088	2862.28479	1049.89732
24	2	2	0	0	7	2	2	0	0	6	1814.24009	0.00086	2875.59598	1061.35675
25	2	2	0	0	8	2	2	0	0	7	1816.08366	0.00019	2890.81058	1074.72712
26	2	2	0	0	9	2	2	0	0	8	1817.92027	-0.00012	2907.92928	1090.00889
27	2	2	0	0	10	2	2	0	0	9	1819.74997	-0.00024	2926.95280	1107.20259
28	2	2	0	0	11	2	2	0	0	10	1821.57338	0.00028	2947.88189	1126.30879
29	2	2	0	0	12	2	2	0	0	11	1823.38953	0.00032	2970.71728	1147.32807
30	2	2	0	0	13	2	2	0	0	12	1825.19930*	0.00069	2995.45967	1170.26105
31	2	2	0	0	14	2	2	0	0	13	1827.00157	0.00025	3022.10964	1195.10832
32	2	2	0	0	15	2	2	0	0	14	1828.79745	0.00019	3050.66770	1221.87043
33	2	2	0	0	16	2	2	0	0	15	1830.58574	-0.00053	3081.13416	1250.54788
34	2	2	0	0	17	2	2	0	0	16	1832.36798	-0.00013	3113.50919	1281.14108
35	2	2	0	0	18	2	2	0	0	17	1834.14122*	-0.00126	3147.79280	1313.65031 +
36	2	2	0	0	19	2	2	0	0	18	1835.90975	0.00071	3183.98480	1348.07575
37	2	2	0	0	20	2	2	0	0	19	1837.66785	0.00042	3222.08485	1384.41742
38	2	2	0	0	21	2	2	0	0	20	1839.41509	-0.00219	3262.09247	1422.67519 +
39	2	2	0	0	22	2	2	0	0	21	1841.15689	-0.00138	3304.00706	1462.84880 +
40	2	-2	0	0	2	2	-2	0	0	3	1795.35330*	-0.00023	2828.06278	1032.70925
41	2	-2	0	0	3	2	-2	0	0	4	1793.41904*	0.00078	2833.76526	1040.34700
42	2	-2	0	0	4	2	-2	0	0	5	1791.47496	0.00051	2841.36845	1049.89400
43	2	-2	0	0	5	2	-2	0	0	6	1789.52108	-0.00105	2850.87223	1061.35010 +
44	2	-2	0	0	6	2	-2	0	0	7	1787.55986	-0.00147	2862.27647	1074.71514 +
45	2	-2	0	0	7	2	-2	0	0	8	1785.59208	0.00001	2875.58102	1089.98896
46	2	-2	0	0	8	2	-2	0	0	9	1783.61370	-0.00067	2890.78569	1107.17132
47	2	-2	0	0	9	2	-2	0	0	10	1781.62752	-0.00076	2907.89027	1126.26199
48	2	-2	0	0	10	2	-2	0	0	11	1779.63217	-0.00163	2926.89452	1147.26072 +
49	2	-2	0	0	11	2	-2	0	0	12	1777.63102	0.00005	2947.79817	1170.16720
50	2	-2	0	0	12	2	-2	0	0	13	1775.62007	0.00025	2970.60094	1194.98112
51	2	-2	0	0	13	2	-2	0	0	14	1773.60012	-0.00024	2995.30250	1221.70214
52	2	-2	0	0	14	2	-2	0	0	15	1771.57209	-0.00054	3021.90251	1250.32988
53	2	-2	0	0	15	2	-2	0	0	16	1769.53661	-0.00004	3050.40060	1280.86395
54	2	-2	0	0	16	2	-2	0	0	17	1767.49219	-0.00026	3080.79638	1313.30393
55	2	-2	0	0	17	2	-2	0	0	18	1765.44008	0.00003	3113.08941	1347.64936
56	2	-2	0	0	18	2	-2	0	0	19	1763.37869	-0.00080	3147.27925	1383.89977
57	2	-2	0	0	19	2	-2	0	0	20	1761.30955	-0.00122	3183.36543	1422.05465 +
58	2	-2	0	0	20	2	-2	0	0	21	1759.23460	0.00066	3221.34743	1462.11349
59	2	-2	0	0	21	2	-2	0	0	22	1757.15007	0.00105	3261.22474	1504.07572 +
60	2	-2	0	0	22	2	-2	0	0	23	1755.05584	-0.00019	3302.99679	1547.94075
	2	-2	0	0	3	2	-2	0	0	2	1806.78484	0.00042	2833.76526	1026.98084
	2	-2	0	0	4	2	-2	0	0	3	1808.65914*	-0.00006	2841.36845	1032.70925
	2	-2	0	0	5	2	-2	0	0	4	1810.52499	-0.00023	2850.87223	1040.34700
	2	-2	0	0	6	2	-2	0	0	5	1812.38415*	0.00168	2862.27647	1049.89400 +
	2	-2	0	0	7	2	-2	0	0	6	1814.23182	0.00089	2875.58102	1061.35010
	2	-2	0	0	8	2	-2	0	0	7	1816.07023	-0.00032	2890.78569	1074.71514

2	-2	0	0	9	2	-2	0	0	8	1817.90162	0.00031	2907.89027	1089.98896
2	-2	0	0	10	2	-2	0	0	9	1819.72250	-0.00070	2926.89452	1107.17132
2	-2	0	0	11	2	-2	0	0	10	1821.53575	-0.00043	2947.79817	1126.26199
2	-2	0	0	12	2	-2	0	0	11	1823.33909	-0.00113	2970.60094	1147.26072 †
2	-2	0	0	13	2	-2	0	0	12	1825.13573	0.00043	2995.30250	1170.16720
2	-2	0	0	14	2	-2	0	0	13	1826.92131	-0.00008	3021.90251	1194.98112
2	-2	0	0	15	2	-2	0	0	14	1828.69843	-0.00003	3050.40060	1221.70214
2	-2	0	0	16	2	-2	0	0	15	1830.46639	-0.00011	3080.79638	1250.32988
2	-2	0	0	17	2	-2	0	0	16	1832.22516	-0.00030	3113.08941	1280.86395
2	-2	0	0	18	2	-2	0	0	17	1833.97590	0.00057	3147.27925	1313.30393
2	-2	0	0	19	2	-2	0	0	18	1835.71519	-0.00088	3183.36543	1347.64936
2	-2	0	0	20	2	-2	0	0	19	1837.44725	-0.00042	3221.34743	1383.89977
2	-2	0	0	21	2	-2	0	0	20	1839.16981	-0.00027	3261.22474	1422.05465
2	-2	0	0	22	2	-2	0	0	21	1840.88262	-0.00068	3302.99679	1462.11349

rms = 0.00048 cm⁻¹

$v_2 + 2v_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 0 0	0 0 0 0 1	3134.92613	0.00053	3136.82626	1.90066
0 0 2 0 1	0 0 0 0 2	3133.02194	-0.00007	3138.72396	5.70195
0 0 2 0 2	0 0 0 0 3	3131.11484	-0.00065	3142.51931	11.40382
0 0 2 0 3	0 0 0 0 4	3129.20528	-0.00075	3148.21223	19.00619
0 0 2 0 4	0 0 0 0 5	3127.29357	-0.00004	3155.80259	28.50898
0 0 2 0 5	0 0 0 0 6	3125.37769	-0.00050	3165.29023	39.91204
0 0 2 0 6	0 0 0 0 7	3123.45978	0.00007	3176.67495	53.21523
0 0 2 0 7	0 0 0 0 8	3121.53826	0.00016	3189.95648	68.41838
0 0 2 0 8	0 0 0 0 9	3119.61329	0.00004	3205.13454	85.52129
0 0 2 0 9	0 0 0 0 10	3117.68496	-0.00011	3222.20879	104.52373
0 0 2 0 10	0 0 0 0 11	3115.75358	0.00015	3241.17887	125.42544
0 0 2 0 11	0 0 0 0 12	3113.81839	0.00021	3262.04434	148.22616
0 0 2 0 12	0 0 0 0 13	3111.87895	-0.00023	3284.80476	172.92558
0 0 2 0 13	0 0 0 0 14	3109.93563	-0.00061	3309.45961	199.52337
0 0 2 0 14	0 0 0 0 15	3107.98946	0.00029	3336.00837	228.01920
0 0 2 0 15	0 0 0 0 16	3106.03692	-0.00085	3364.45045	258.41268
0 0 2 0 16	0 0 0 0 17	3104.08205	0.00023	3394.78522	290.70340
0 0 2 0 17	0 0 0 0 18	3102.12101	-0.00006	3427.01203	324.89096
0 0 2 0 18	0 0 0 0 19	3100.15569	0.00041	3461.13016	360.97488
0 0 2 0 19	0 0 0 0 20	3098.18388	-0.00030	3497.13889	398.95471
0 0 2 0 20	0 0 0 0 21	3096.20776	0.00026	3535.03743	438.82993
0 0 2 0 21	0 0 0 0 22	3094.22494	0.00000	3574.82497	480.60003
0 0 2 0 22	0 0 0 0 23	3092.23650	0.00029	3616.50066	524.26445
0 0 2 0 23	0 0 0 0 24	3090.24174	0.00074	3660.06361	569.82262
0 0 2 0 24	0 0 0 0 25	3088.23941	0.00043	3705.51291	617.27393
0 0 2 0 25	0 0 0 0 26	3086.22998	0.00014	3752.84761	666.61777
0 0 2 0 26	0 0 0 0 27	3084.21273	-0.00052	3802.06673	717.85348
0 0 2 0 27	0 0 0 0 28	3082.18871	-0.00017	3853.16927	770.98038
0 0 2 0 28	0 0 0 0 29	3080.15781*	0.00140	3906.15419	825.99778 †
0 0 2 0 29	0 0 0 0 30	3078.11491	-0.00058	3961.02045	882.90495
0 0 2 0 30	0 0 0 0 31	3076.06541	-0.00041	4017.76697	941.70115
0 0 2 0 1	0 0 0 0 0	3138.72595	0.00199	3138.72396	0.00000 †
0 0 2 0 2	0 0 0 0 1	3140.61870	0.00005	3142.51931	1.90066
0 0 2 0 3	0 0 0 0 2	3142.51004	-0.00024	3148.21223	5.70195
0 0 2 0 4	0 0 0 0 3	3144.39827	-0.00050	3155.80259	11.40382
0 0 2 0 5	0 0 0 0 4	3146.28411	0.00007	3165.29023	19.00619
0 0 2 0 6	0 0 0 0 5	3148.16571	-0.00026	3176.67495	28.50898
0 0 2 0 7	0 0 0 0 6	3150.04439	-0.00005	3189.95648	39.91204
0 0 2 0 8	0 0 0 0 7	3151.91926	-0.00005	3205.13454	53.21523
0 0 2 0 9	0 0 0 0 8	3153.78981	-0.00060	3222.20879	68.41838
0 0 2 0 10	0 0 0 0 9	3155.65737	-0.00021	3241.17887	85.52129
0 0 2 0 11	0 0 0 0 10	3157.52066	0.00004	3262.04434	104.52373

1														
2	0	0	2	0	12	0	0	0	0	11	3159.37883	-0.00049	3284.80476	125.42544
3	0	0	2	0	13	0	0	0	0	12	3161.23357	0.00011	3309.45961	148.22616
4	0	0	2	0	14	0	0	0	0	13	3163.08329	0.00050	3336.00837	172.92558
5	0	0	2	0	15	0	0	0	0	14	3164.92701	-0.00006	3364.45045	199.52337
6	0	0	2	0	16	0	0	0	0	15	3166.76608	0.00006	3394.78522	228.01920
7	0	0	2	0	17	0	0	0	0	16	3168.59926	-0.00009	3427.01203	258.41268
8	0	0	2	0	18	0	0	0	0	17	3170.42634	-0.00042	3461.13016	290.70340
9	0	0	2	0	19	0	0	0	0	18	3172.24826	0.00032	3497.13889	324.89096
10	0	0	2	0	20	0	0	0	0	19	3174.06305	0.00050	3535.03743	360.97488
11	0	0	2	0	21	0	0	0	0	20	3175.87081	0.00055	3574.82497	398.95471
12	0	0	2	0	22	0	0	0	0	21	3177.67114	0.00041	3616.50066	438.82993
13	0	0	2	0	23	0	0	0	0	22	3179.46395	0.00037	3660.06361	480.60003
14	0	0	2	0	24	0	0	0	0	23	3181.24886	0.00040	3705.51291	524.26445
15	0	0	2	0	25	0	0	0	0	24	3183.02507	0.00008	3752.84761	569.82262
16	0	0	2	0	26	0	0	0	0	25	3184.79272	-0.00008	3802.06673	617.27393
17	0	0	2	0	27	0	0	0	0	26	3186.54837*	-0.00313	3853.16927	666.61777 +
18	0	0	2	0	28	0	0	0	0	27	3188.30044	-0.00027	3906.15419	717.85348
19	0	0	2	0	29	0	0	0	0	28	3190.03986	-0.00021	3961.02045	770.98038
20	0	0	2	0	30	0	0	0	0	29	3191.76944	0.00025	4017.76697	825.99778

rms = 0.00036 cm⁻¹

v₂ + 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	E'	E''
29	0	0	2	0	1	0	0	1	1	2	2458.78788	-0.00040	3138.72396	679.93567
30	0	0	2	0	2	0	0	1	1	3	2456.88504	0.00066	3142.51931	685.63493
31	0	0	2	0	3	0	0	1	1	4	2454.98008*	0.00167	3148.21223	693.23382 †
32	0	0	2	0	4	0	0	1	1	5	2453.07029	-0.00006	3155.80259	702.73224
33	0	0	2	0	5	0	0	1	1	6	2451.16029	0.00013	3165.29023	714.13007
34	0	0	2	0	6	0	0	1	1	7	2449.24746	-0.00033	3176.67495	727.42716
35	0	0	2	0	7	0	0	1	1	8	2447.33585*	0.00270	3189.95648	742.62333 †
36	0	0	2	0	8	0	0	1	1	9	2445.41664	0.00048	3205.13454	759.71839
37	0	0	2	0	9	0	0	1	1	10	2443.49585*	-0.00085	3222.20879	778.71209
38	0	0	2	0	10	0	0	1	1	11	2441.57489*	0.00023	3241.17887	799.60420
39	0	0	2	0	11	0	0	1	1	12	2439.64870*	-0.00120	3262.04434	822.39444 †
40	0	0	2	0	12	0	0	1	1	13	2437.72202	-0.00022	3284.80476	847.08251
41	0	0	2	0	13	0	0	1	1	14	2435.79000	-0.00153	3309.45961	873.66808 †
42	0	0	2	0	14	0	0	1	1	15	2433.85787	0.00029	3336.00837	902.15079
43	0	0	2	0	15	0	0	1	1	16	2431.92043*	0.00027	3364.45045	932.53028
44	0	0	2	0	5	0	0	1	1	4	2472.05700	0.00058	3165.29023	693.23382
45	0	0	2	0	6	0	0	1	1	5	2473.94446*	0.00175	3176.67495	702.73224 †
46	0	0	2	0	7	0	0	1	1	6	2475.82655	0.00014	3189.95648	714.13007
47	0	0	2	0	8	0	0	1	1	7	2477.70752	0.00014	3205.13454	727.42716
48	0	0	2	0	9	0	0	1	1	8	2479.58528	-0.00018	3222.20879	742.62333
49	0	0	2	0	10	0	0	1	1	9	2481.45904	-0.00144	3241.17887	759.71839 †
50	0	0	2	0	11	0	0	1	1	10	2483.33209	-0.00016	3262.04434	778.71209
51	0	0	2	0	12	0	0	1	1	11	2485.19998	-0.00057	3284.80476	799.60420
52	0	0	2	0	13	0	0	1	1	12	2487.06357*	-0.00160	3309.45961	822.39444 †
53	0	0	2	0	14	0	0	1	1	13	2488.92551	-0.00035	3336.00837	847.08251
54	0	0	2	0	15	0	0	1	1	14	2490.78252	0.00015	3364.45045	873.66808
55	0	0	2	0	16	0	0	1	1	15	2492.63433	-0.00010	3394.78522	902.15079
56	0	0	2	0	17	0	0	1	1	16	2494.48236	0.00062	3427.01203	932.53028
57	0	0	2	0	18	0	0	1	1	17	2496.32553*	0.00151	3461.13016	964.80614 †
58	0	0	2	0	19	0	0	1	1	18	2498.16186	0.00091	3497.13889	998.97795
59	0	0	2	0	20	0	0	1	1	19	2499.99138	-0.00081	3535.03743	1035.04524
60	0	0	2	0	21	0	0	1	1	20	2501.81759	0.00017	3574.82497	1073.00756
	0	0	2	0	22	0	0	1	1	21	2503.63640	0.00012	3616.50066	1112.86438
	0	0	2	0	2	0	0	1	-1	2	2462.56320	-0.00087	3142.51931	679.95524
	0	0	2	0	3	0	0	1	-1	3	2462.53790*	-0.00027	3148.21223	685.67405
	0	0	2	0	4	0	0	1	-1	4	2462.50237	-0.00120	3155.80259	693.29902 †
	0	0	2	0	5	0	0	1	-1	5	2462.46076	0.00057	3165.29023	702.83004

0	0	2	0	6	0	0	1	-1	6	2462.40812	0.00015	3176.67495	714.26698
0	0	2	0	7	0	0	1	-1	7	2462.34586	-0.00093	3189.95648	727.60969
0	0	2	0	8	0	0	1	-1	8	2462.27694	0.00039	3205.13454	742.85799
0	0	2	0	9	0	0	1	-1	9	2462.19750	0.00038	3222.20879	760.01168
0	0	2	0	10	0	0	1	-1	10	2462.10737	-0.00098	3241.17887	779.07052
0	0	2	0	11	0	0	1	-1	11	2462.01073	0.00065	3262.04434	800.03426
0	0	2	0	12	0	0	1	-1	12	2461.90202	-0.00012	3284.80476	822.90261
0	0	2	0	13	0	0	1	-1	13	2461.78455	0.00022	3309.45961	847.67528
0	0	2	0	14	0	0	1	-1	14	2461.65641	-0.00003	3336.00837	874.35193
0	0	2	0	15	0	0	1	-1	15	2461.51879	0.00054	3364.45045	902.93220

rms = 0.00048 cm⁻¹

$v_2 + 2v_5 (\Sigma^+) \leftarrow 2v_5 (\Sigma^+)$

$v_4' l_4' v_5' l_5' J'$	$v_4'' l_4'' v_5'' l_5'' J''$	OBS ^b	OBS – CALC ^b	E'	E''
0 0 2 0 1	0 0 2 0 2	1797.69756	-0.00002	3138.72396	1341.02637
0 0 2 0 2	0 0 2 0 3	1795.77519	0.00001	3142.51931	1346.74412
0 0 2 0 3	0 0 2 0 4	1793.84414	-0.00049	3148.21223	1354.36759
0 0 2 0 4	0 0 2 0 5	1791.90655	0.00058	3155.80259	1363.89662
0 0 2 0 5	0 0 2 0 6	1789.95916	-0.00008	3165.29023	1375.33100
0 0 2 0 6	0 0 2 0 7	1788.00412	-0.00035	3176.67495	1388.67047
0 0 2 0 7	0 0 2 0 8	1786.04179	0.00007	3189.95648	1403.91476
0 0 2 0 8	0 0 2 0 9	1784.07085	-0.00017	3205.13454	1421.06352
0 0 2 0 9	0 0 2 0 10	1782.09215	-0.00026	3222.20879	1440.11639
0 0 2 0 10	0 0 2 0 11	1780.10542	-0.00051	3241.17887	1461.07294
0 0 2 0 11	0 0 2 0 12	1778.11232	0.00071	3262.04434	1483.93273
0 0 2 0 12	0 0 2 0 13	1776.10962	0.00011	3284.80476	1508.69525
0 0 2 0 13	0 0 2 0 14	1774.10018	0.00053	3309.45961	1535.35996
0 0 2 0 14	0 0 2 0 15	1772.08236	0.00029	3336.00837	1563.92630
0 0 2 0 15	0 0 2 0 16	1770.05633	-0.00049	3364.45045	1594.39363
0 0 2 0 16	0 0 2 0 17	1768.02395	0.00003	3394.78522	1626.76130
0 0 2 0 17	0 0 2 0 18	1765.98417	0.00075	3427.01203	1661.02860
0 0 2 0 18	0 0 2 0 19	1763.93483	-0.00052	3461.13016	1697.19482
0 0 2 0 19	0 0 2 0 20	1761.88013	0.00039	3497.13889	1735.25916
0 0 2 0 20	0 0 2 0 21	1759.81602	-0.00060	3535.03743	1775.22081
0 0 2 0 21	0 0 2 0 22	1757.74605	0.00002	3574.82497	1817.07894
0 0 2 0 22	0 0 2 0 23	1755.66797	-0.00003	3616.50066	1860.83266
0 0 2 0 23	0 0 2 0 24	1753.58236	-0.00020	3660.06361	1906.48106
0 0 2 0 24	0 0 2 0 25	1751.48919	-0.00054	3705.51291	1954.02319
0 0 2 0 2	0 0 2 0 1	1805.30451	-0.00032	3142.51931	1337.21447
0 0 2 0 3	0 0 2 0 2	1807.18521	-0.00064	3148.21223	1341.02637
0 0 2 0 4	0 0 2 0 3	1809.05791	-0.00056	3155.80259	1346.74412
0 0 2 0 5	0 0 2 0 4	1810.92258	-0.00006	3165.29023	1354.36759
0 0 2 0 6	0 0 2 0 5	1812.77894	0.00061	3176.67495	1363.89662
0 0 2 0 7	0 0 2 0 6	1814.62586	0.00038	3189.95648	1375.33100
0 0 2 0 8	0 0 2 0 7	1816.46381	-0.00026	3205.13454	1388.67047
0 0 2 0 15	0 0 2 0 14	1829.09100	0.00052	3364.45045	1535.35996
0 0 2 0 16	0 0 2 0 15	1830.85891	-0.00001	3394.78522	1563.92630
0 0 2 0 17	0 0 2 0 16	1832.61865	0.00025	3427.01203	1594.39363
0 0 2 0 18	0 0 2 0 17	1834.36955	0.00068	3461.13016	1626.76130
0 0 2 0 19	0 0 2 0 18	1836.11009	-0.00020	3497.13889	1661.02860
0 0 2 0 20	0 0 2 0 19	1837.84276	0.00014	3535.03743	1697.19482
0 0 2 0 21	0 0 2 0 20	1839.56512	-0.00070	3574.82497	1735.25916
0 0 2 0 22	0 0 2 0 21	1841.28258*	0.00273	3616.50066	1775.22081 †
0 0 2 0 23	0 0 2 0 22	1842.98502	0.00035	3660.06361	1817.07894
0 0 2 0 24	0 0 2 0 23	1844.68050	0.00025	3705.51291	1860.83266
0 0 2 0 25	0 0 2 0 24	1846.36742	0.00087	3752.84761	1906.48106

rms = 0.00043 cm⁻¹

$v_2 + 2v_5 (\Delta) \leftarrow v_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 2 6	0 0 1 1 7	2465.63947	0.00023	3193.06640	727.42716
0 0 2 2 7	0 0 1 1 8	2463.72112	0.00110	3206.34335	742.62333 †
0 0 2 2 8	0 0 1 1 9	2461.79862	0.00019	3221.51681	759.71839
0 0 2 2 3	0 0 1 1 2	2484.67626*	-0.00334	3164.61527	679.93567 †
0 0 2 2 4	0 0 1 1 3	2486.56649*	-0.00089	3172.20231	685.63493
0 0 2 2 5	0 0 1 1 4	2488.45229	0.00007	3181.68604	693.23382
0 0 2 2 6	0 0 1 1 5	2490.33548*	0.00132	3193.06640	702.73224 †
0 0 2 2 7	0 0 1 1 6	2492.21330	0.00002	3206.34335	714.13007
0 0 2 2 8	0 0 1 1 7	2494.08953	-0.00012	3221.51681	727.42716
0 0 2 2 9	0 0 1 1 8	2495.96459	0.00121	3238.58671	742.62333 †
0 0 2 2 10	0 0 1 1 9	2497.83433	-0.00025	3257.55296	759.71839
0 0 2 2 11	0 0 1 1 10	2499.70594*	0.00256	3278.41547	778.71209 †
0 0 2 2 12	0 0 1 1 11	2501.57186	0.00194	3301.17412	799.60420 †
0 0 2 2 13	0 0 1 1 12	2503.43354	-0.00083	3325.82881	822.39444
0 0 2 2 14	0 0 1 1 13	2505.29609	-0.00081	3352.37941	847.08251
0 0 2 2 15	0 0 1 1 14	2507.15810	0.00040	3380.82577	873.66808
0 0 2 2 16	0 0 1 1 15	2509.01834*	0.00137	3411.16776	902.15079 †
0 0 2 2 17	0 0 1 1 16	2510.87566	0.00072	3443.40522	932.53028
0 0 2 2 18	0 0 1 1 17	2512.73180	-0.00003	3477.53797	964.80614
0 0 2 2 19	0 0 1 1 18	2514.58726	-0.00063	3513.56583	998.97795
0 0 2 2 20	0 0 1 1 19	2516.44356	0.00019	3551.48861	1035.04524
0 0 2 2 21	0 0 1 1 20	2518.29820	-0.00034	3591.30610	1073.00756
0 0 2 -2 7	0 0 1 -1 8	2463.48390	0.00055	3206.34134	742.85799
0 0 2 -2 8	0 0 1 -1 9	2461.50121	-0.00058	3221.51346	760.01168
0 0 2 -2 9	0 0 1 -1 10	2459.51060	-0.00033	3238.58145	779.07052
0 0 2 -2 10	0 0 1 -1 11	2457.51178	0.00097	3257.54506	800.03426
0 0 2 -2 3	0 0 1 -1 2	2484.66094	0.00098	3164.61519	679.95524
0 0 2 -2 4	0 0 1 -1 3	2486.52905	0.00103	3172.20207	685.67405 †
0 0 2 -2 5	0 0 1 -1 4	2488.38791	0.00145	3181.68548	693.29902 †
0 0 2 -2 6	0 0 1 -1 5	2490.23559	0.00034	3193.06529	702.83004
0 0 2 -2 7	0 0 1 -1 6	2492.07445*	0.00009	3206.34134	714.26698
0 0 2 -2 8	0 0 1 -1 7	2493.90375*	-0.00002	3221.51346	727.60969
0 0 2 -2 9	0 0 1 -1 8	2495.72396	0.00050	3238.58145	742.85799
0 0 2 -2 10	0 0 1 -1 9	2497.53279	-0.00060	3257.54506	760.01168
0 0 2 -2 11	0 0 1 -1 10	2499.33484*	0.00130	3278.40406	779.07052 †
0 0 2 -2 12	0 0 1 -1 11	2501.12430	0.00041	3301.15815	800.03426
0 0 2 -2 13	0 0 1 -1 12	2502.90416	-0.00025	3325.80702	822.90261
0 0 2 -2 14	0 0 1 -1 13	2504.67577	0.00070	3352.35035	847.67528
0 0 2 -2 15	0 0 1 -1 14	2506.43535	-0.00050	3380.78778	874.35193
0 0 2 -2 16	0 0 1 -1 15	2508.18696	0.00023	3411.11892	902.93220
0 0 2 -2 17	0 0 1 -1 16	2509.92721	-0.00046	3443.34337	933.41570
0 0 2 -2 18	0 0 1 -1 17	2511.65874	0.00009	3477.46069	965.80204
0 0 2 -2 19	0 0 1 -1 18	2513.38072	0.00107	3513.47041	1000.09076 †
0 0 2 -2 20	0 0 1 -1 19	2515.09056*	-0.00008	3551.37206	1036.28142
0 0 2 -2 21	0 0 1 -1 20	2516.79130	-0.00029	3591.16513	1074.37353
0 0 2 -2 22	0 0 1 -1 21	2518.48127	-0.00122	3632.84906	1114.36658 †

rms = 0.00050 cm⁻¹

$v_2 + 2v_5 (\Delta) \leftarrow 2v_5 (\Delta)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 2 2 2	0 0 2 2 3	1795.59590*	0.00054	3158.92496	1363.32960
0 0 2 2 3	0 0 2 2 4	1793.66594	0.00041	3164.61527	1370.94974
0 0 2 2 4	0 0 2 2 5	1791.72675	-0.00072	3172.20231	1380.47484
0 0 2 2 5	0 0 2 2 6	1789.78156	0.00038	3181.68604	1391.90486
0 0 2 2 6	0 0 2 2 7	1787.82729	0.00061	3193.06640	1405.23972

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

1														
2	0	0	2	-2	12	0	0	2	-2	11	1823.54459	0.00140	3301.15815	1477.61496 +
3	0	0	2	-2	13	0	0	2	-2	12	1825.33557*	-0.00309	3325.80702	1500.46836 +
4	0	0	2	-2	14	0	0	2	-2	13	1827.12528	-0.00024	3352.35035	1525.22483
5	0	0	2	-2	15	0	0	2	-2	14	1828.90434	0.00060	3380.78778	1551.88404
6	0	0	2	-2	16	0	0	2	-2	15	1830.67334	0.00004	3411.11892	1580.44562
7	0	0	2	-2	17	0	0	2	-2	16	1832.43465	0.00047	3443.34337	1610.90919
8	0	0	2	-2	18	0	0	2	-2	17	1834.18571	-0.00063	3477.46069	1643.27435
9	0	0	2	-2	19	0	0	2	-2	18	1835.93016	0.00041	3513.47041	1677.54066
10	0	0	2	-2	20	0	0	2	-2	19	1837.66461	0.00020	3551.37206	1713.70766
11	0	0	2	-2	21	0	0	2	-2	20	1839.39066	0.00039	3591.16513	1751.77486
12	0	0	2	-2	22	0	0	2	-2	21	1841.10319*	-0.00412	3632.84906	1791.74175 +
13	0	0	2	-2	23	0	0	2	-2	22	1842.81597*	0.00046	3676.42331	1833.60781

rms = 0.00047 cm⁻¹

$v_2 + v_4 + v_5 (\Sigma^+) \leftarrow v_4 + v_5 (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''	
1 1 1 -1 0	1 1 1 -1 1	1798.82780*	0.00646	2988.14138	1189.32003	†
1 1 1 -1 1	1 1 1 -1 2	1796.90307	-0.00232	2990.04041	1193.13502	†
1 1 1 -1 2	1 1 1 -1 3	1794.97910	-0.00180	2993.83855	1198.85764	†
1 1 1 -1 3	1 1 1 -1 4	1793.04807	0.00021	2999.53594	1206.48808	
1 1 1 -1 4	1 1 1 -1 5	1791.10696	0.00070	3007.13280	1216.02655	
1 1 1 -1 5	1 1 1 -1 6	1789.15559	-0.00050	3016.62942	1227.47333	
1 1 1 -1 6	1 1 1 -1 7	1787.19740	0.00002	3028.02616	1240.82878	
1 1 1 -1 7	1 1 1 -1 8	1785.23037	0.00020	3041.32343	1256.09326	
1 1 1 -1 8	1 1 1 -1 9	1783.25440	-0.00012	3056.52172	1273.26720	
1 1 1 -1 9	1 1 1 -1 10	1781.27089	0.00039	3073.62156	1292.35106	
1 1 1 -1 10	1 1 1 -1 11	1779.27772	-0.00046	3092.62349	1313.34532	
1 1 1 -1 11	1 1 1 -1 12	1777.27756	-0.00010	3113.52809	1336.25044	
1 1 1 -1 12	1 1 1 -1 13	1775.26917	0.00015	3136.33591	1361.06689	
1 1 1 -1 13	1 1 1 -1 14	1773.25166	-0.00071	3161.04746	1387.79509	
1 1 1 -1 14	1 1 1 -1 15	1771.22777	0.00000	3187.66318	1416.43541	
1 1 1 -1 15	1 1 1 -1 16	1769.19470	-0.00060	3216.18342	1446.98812	
1 1 1 -1 16	1 1 1 -1 17	1767.15468	-0.00031	3246.60841	1479.45342	
1 1 1 -1 17	1 1 1 -1 18	1765.10645	-0.00042	3278.93825	1513.83138	
1 1 1 -1 18	1 1 1 -1 19	1763.05192	0.00097	3313.17290	1550.12195	
1 1 1 -1 19	1 1 1 -1 20	1760.98869	0.00149	3349.31216	1588.32496	†
1 1 1 -1 1	1 1 1 -1 0	1802.62618	-0.00166	2990.04041	1187.41257	†
1 1 1 -1 2	1 1 1 -1 1	1804.51961	0.00110	2993.83855	1189.32003	†
1 1 1 -1 3	1 1 1 -1 2	1806.39964	-0.00128	2999.53594	1193.13502	†
1 1 1 -1 4	1 1 1 -1 3	1808.27498	-0.00018	3007.13280	1198.85764	
1 1 1 -1 5	1 1 1 -1 4	1810.14255	0.00121	3016.62942	1206.48808	†
1 1 1 -1 6	1 1 1 -1 5	1812.00010	0.00049	3028.02616	1216.02655	
1 1 1 -1 7	1 1 1 -1 6	1813.85028	0.00018	3041.32343	1227.47333	
1 1 1 -1 8	1 1 1 -1 7	1815.69320	0.00025	3056.52172	1240.82878	
1 1 1 -1 9	1 1 1 -1 8	1817.52912	0.00082	3073.62156	1256.09326	
1 1 1 -1 10	1 1 1 -1 9	1819.35569	-0.00060	3092.62349	1273.26720	
1 1 1 -1 11	1 1 1 -1 10	1821.17625	-0.00078	3113.52809	1292.35106	
1 1 1 -1 12	1 1 1 -1 11	1822.99062	0.00003	3136.33591	1313.34532	
1 1 1 -1 13	1 1 1 -1 12	1824.79666	-0.00036	3161.04746	1336.25044	
1 1 1 -1 14	1 1 1 -1 13	1826.59557	-0.00072	3187.66318	1361.06689	
1 1 1 -1 15	1 1 1 -1 14	1828.38768*	-0.00065	3216.18342	1387.79509	
1 1 1 -1 16	1 1 1 -1 15	1830.17355	0.00054	3246.60841	1416.43541	
1 1 1 -1 17	1 1 1 -1 16	1831.95060	0.00047	3278.93825	1446.98812	
1 1 1 -1 18	1 1 1 -1 17	1833.71937	-0.00011	3313.17290	1479.45342	
1 1 1 -1 19	1 1 1 -1 18	1835.48224	0.00146	3349.31216	1513.83138	†
1 1 1 -1 20	1 1 1 -1 19	1837.23378	0.00002	3387.35571	1550.12195	
1 1 1 -1 21	1 1 1 -1 20	1838.97887	0.00072	3427.30311	1588.32496	
1 1 1 -1 22	1 1 1 -1 21	1840.71538	0.00170	3469.15379	1628.44012	†
1 1 1 -1 23	1 1 1 -1 22	1842.44254	0.00244	3512.90711	1670.46701	†

rms = 0.00048 cm⁻¹

$V_2 + V_4 + V_5 (\Sigma^-) \leftarrow V_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 1 1 1	1 -1 0 0 2	2471.40127*	0.00009	2986.71435	515.31316
1 -1 1 1 2	1 -1 0 0 3	2469.47178	0.00017	2990.51262	521.04101
1 -1 1 1 3	1 -1 0 0 4	2467.53244	0.00006	2996.21039	528.67801
1 -1 1 1 4	1 -1 0 0 5	2465.58395	0.00006	3003.80796	538.22407
1 -1 1 1 5	1 -1 0 0 6	2463.62671	0.00026	3013.30551	549.67906
1 -1 1 1 6	1 -1 0 0 7	2461.66020	0.00002	3024.70299	563.04281
1 -1 1 1 7	1 -1 0 0 8	2459.68469	-0.00038	3038.00021	578.31514
1 -1 1 1 8	1 -1 0 0 9	2457.70191	0.00085	3053.19690	595.49585
1 -1 1 1 9	1 -1 0 0 10	2455.70751*	-0.00058	3070.29279	614.58469
1 -1 1 1 10	1 -1 0 0 11	2453.70591	-0.00024	3089.28757	635.58142
1 -1 1 1 11	1 -1 0 0 12	2451.69453	-0.00070	3110.18096	658.48573
1 -1 1 1 12	1 -1 0 0 13	2449.67465	-0.00067	3132.97264	683.29732
1 -1 1 1 13	1 -1 0 0 14	2447.64675	0.00032	3157.66227	710.01584
1 -1 1 1 14	1 -1 0 0 15	2445.60903	0.00045	3184.24952	738.64093
1 -1 1 1 15	1 -1 0 0 16	2443.56104*	-0.00076	3212.73400	769.17220
1 -1 1 1 16	1 -1 0 0 17	2441.50726*	0.00117	3243.11531	801.60923 †
1 -1 1 1 17	1 -1 0 0 18	2439.44109	-0.00040	3275.39305	835.95156
1 -1 1 1 18	1 -1 0 0 19	2437.36784	-0.00017	3309.56675	872.19874
1 -1 1 1 19	1 -1 0 0 20	2435.28539	-0.00030	3345.63595	910.35027
1 -1 1 1 20	1 -1 0 0 21	2433.19715	0.00261	3383.60015	950.40561 †
1 -1 1 1 4	1 -1 0 0 3	2482.76691	-0.00004	3003.80796	521.04101
1 -1 1 1 5	1 -1 0 0 4	2484.62821	0.00072	3013.30551	528.67801
1 -1 1 1 6	1 -1 0 0 5	2486.47860	-0.00032	3024.70299	538.22407
1 -1 1 1 7	1 -1 0 0 6	2488.32086	-0.00030	3038.00021	549.67906
1 -1 1 1 8	1 -1 0 0 7	2490.15514*	0.00104	3053.19690	563.04281 †
1 -1 1 1 9	1 -1 0 0 8	2491.97705	-0.00060	3070.29279	578.31514
1 -1 1 1 10	1 -1 0 0 9	2493.79170*	-0.00002	3089.28757	595.49585
1 -1 1 1 11	1 -1 0 0 10	2495.59722	0.00096	3110.18096	614.58469
1 -1 1 1 12	1 -1 0 0 11	2497.39221*	0.00099	3132.97264	635.58142
1 -1 1 1 13	1 -1 0 0 12	2499.17682	0.00028	3157.66227	658.48573
1 -1 1 1 14	1 -1 0 0 13	2500.95186*	-0.00034	3184.24952	683.29732
1 -1 1 1 15	1 -1 0 0 14	2502.71954*	0.00138	3212.73400	710.01584 †
1 -1 1 1 16	1 -1 0 0 15	2504.47401	-0.00037	3243.11531	738.64093
1 -1 1 1 17	1 -1 0 0 16	2506.22102	0.00017	3275.39305	769.17220
1 -1 1 1 18	1 -1 0 0 17	2507.95769	0.00016	3309.56675	801.60923
1 -1 1 1 19	1 -1 0 0 18	2509.68504*	0.00065	3345.63595	835.95156
1 -1 1 1 20	1 -1 0 0 19	2511.40197	0.00056	3383.60015	872.19874
1 -1 1 1 21	1 -1 0 0 20	2513.10750	-0.00107	3423.45883	910.35027 †
1 -1 1 1 22	1 -1 0 0 21	2514.80448	-0.00135	3465.21145	950.40561 †
1 -1 1 1 23	1 -1 0 0 22	2516.49285	-0.00033	3508.85741	992.36423

rms = 0.00044 cm⁻¹

$V_2 + V_4 + V_5 (\Sigma^-) \leftarrow V_4 + V_5 (\Sigma^-)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 1 1 5	1 -1 1 1 6	1789.50413*	0.00086	3013.30551	1223.80224
1 -1 1 1 6	1 -1 1 1 7	1787.54875	0.00026	3024.70299	1237.15450
1 -1 1 1 7	1 -1 1 1 8	1785.58651	0.00030	3038.00021	1252.41400
1 -1 1 1 8	1 -1 1 1 9	1783.61673*	0.00048	3053.19690	1269.58065
1 -1 1 1 9	1 -1 1 1 10	1781.63820	-0.00026	3070.29279	1288.65432
1 -1 1 1 10	1 -1 1 1 11	1779.65236	-0.00035	3089.28757	1309.63487

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1											
2	1	-1	1	1	11	1	-1	1	1	12	1777.65822
3	1	-1	1	1	12	1	-1	1	1	13	1775.65674
4	1	-1	1	1	13	1	-1	1	1	14	1773.64698
5	1	-1	1	1	14	1	-1	1	1	15	1771.62797
6	1	-1	1	1	15	1	-1	1	1	16	1769.60148
7	1	-1	1	1	16	1	-1	1	1	17	1767.56641*
8	1	-1	1	1	17	1	-1	1	1	18	1765.52223*
9	1	-1	1	1	18	1	-1	1	1	19	1763.47081
10	1	-1	1	1	19	1	-1	1	1	20	1761.40924
11	1	-1	1	1	20	1	-1	1	1	21	1759.34142
12	1	-1	1	1	21	1	-1	1	1	22	1757.26594
13	1	-1	1	1	1	1	-1	1	1	0	1802.97011
14	1	-1	1	1	2	1	-1	1	1	1	1804.86010
15	1	-1	1	1	3	1	-1	1	1	2	1806.74241
16	1	-1	1	1	4	1	-1	1	1	3	1808.61801
17	1	-1	1	1	5	1	-1	1	1	4	1810.48542
18	1	-1	1	1	6	1	-1	1	1	5	1812.34556
19	1	-1	1	1	7	1	-1	1	1	6	1814.19757
20	1	-1	1	1	8	1	-1	1	1	7	1816.04158
21	1	-1	1	1	9	1	-1	1	1	8	1817.87829
22	1	-1	1	1	10	1	-1	1	1	9	1819.70649
23	1	-1	1	1	11	1	-1	1	1	10	1821.52676
24	1	-1	1	1	12	1	-1	1	1	11	1823.33873
25	1	-1	1	1	13	1	-1	1	1	12	1825.14071
26	1	-1	1	1	14	1	-1	1	1	13	1826.93444
27	1	-1	1	1	15	1	-1	1	1	14	1828.71883
28	1	-1	1	1	16	1	-1	1	1	15	1830.49397
29	1	-1	1	1	17	1	-1	1	1	16	1832.26020
30	1	-1	1	1	18	1	-1	1	1	17	1834.01804
31	1	-1	1	1	19	1	-1	1	1	18	1835.76570
32	1	-1	1	1	20	1	-1	1	1	19	1837.50334
33	1	-1	1	1	21	1	-1	1	1	20	1839.23277
34	1	-1	1	1	22	1	-1	1	1	21	1840.95368
35	1	-1	1	1	23	1	-1	1	1	22	1842.66403
36	1	-1	1	1	24	1	-1	1	1	23	1844.36543
37	1	-1	1	1	25	1	-1	1	1	24	1846.05592

rms = 0.00047 cm⁻¹

V₂ + V₄ + V₅ (Δ) ← V₄ (Π)

<i>v</i> ₄ ' <i>l</i> ₄ ' <i>v</i> ₅ ' <i>l</i> ₅ ' <i>J</i> '	<i>v</i> ₄ '' <i>l</i> ₄ '' <i>v</i> ₅ '' <i>l</i> ₅ '' <i>J</i> ''	OBS	OBS - CALC	E'	E''
1 1 1 1 4	1 -1 0 0 4	2475.09852	-0.00093	3003.77746	528.67801
1 1 1 1 5	1 -1 0 0 5	2475.04823*	0.00207	3013.27023	538.22407 †
1 1 1 1 6	1 -1 0 0 6	2474.98248*	0.00136	3024.66017	549.67906 †
1 1 1 1 7	1 -1 0 0 7	2474.90527*	0.00153	3037.94655	563.04281 †
1 1 1 1 8	1 -1 0 0 8	2474.81367	0.00031	3053.12850	578.31514
1 1 1 1 9	1 -1 0 0 9	2474.70888	-0.00034	3070.20507	595.49585
1 1 1 1 10	1 -1 0 0 10	2474.59075	0.00021	3089.17524	614.58469
1 1 1 1 11	1 -1 0 0 11	2474.45669	0.00022	3110.03789	635.58142
1 1 1 1 12	1 -1 0 0 12	2474.30580	-0.00035	3132.79188	658.48573
1 1 1 1 13	1 -1 0 0 13	2474.13930	0.00055	3157.43607	683.29732
1 1 1 1 16	1 -1 0 0 16	2473.52643	-0.00003	3242.69866	769.17220
1 -1 1 -1 4	1 1 0 0 4	2475.18239	0.00102	3003.77652	528.59515 †
1 -1 1 -1 5	1 1 0 0 5	2475.16725*	-0.00150	3013.26854	538.09979 †
1 -1 1 -1 6	1 1 0 0 6	2475.15322	0.00034	3024.65796	549.50508
1 -1 1 -1 7	1 1 0 0 7	2475.13448	0.00066	3037.94468	562.81086
1 -1 1 -1 8	1 1 0 0 8	2475.11110	-0.00053	3053.12859	578.01697
1 -1 1 -1 9	1 1 0 0 9	2475.08448*	-0.00190	3070.20957	595.12319 †
1 -1 1 -1 10	1 1 0 0 10	2475.05881	0.00067	3089.18743	614.12929
1 -1 1 -1 11	1 1 0 0 11	2475.02651	-0.00042	3110.06196	635.03503
1 -1 1 -1 12	1 1 0 0 12	2474.99348	0.00071	3132.83289	657.84012
1 -1 1 -1 13	1 1 0 0 13	2474.95539	-0.00029	3157.49994	682.54427

1	-1	1	-1	14	1	1	0	0	14	2474.91743*	0.00177	3184.06279	709.14713	†
1	-1	1	-1	15	1	1	0	0	15	2474.87325	0.00054	3212.52107	737.64836	
1	-1	1	-1	16	1	1	0	0	16	2474.82665	-0.00020	3242.87442	768.04757	
1	-1	1	-1	17	1	1	0	0	17	2474.77825	0.00020	3275.12241	800.34436	
1	-1	1	-1	18	1	1	0	0	18	2474.72630	-0.00003	3309.26463	834.53830	
1	-1	1	-1	19	1	1	0	0	19	2474.67178	0.00011	3345.30060	870.62893	
1	-1	1	-1	20	1	1	0	0	20	2474.61368	-0.00039	3383.22984	908.61577	

rms = 0.00044 cm⁻¹

$\nu_2 + \nu_4 + \nu_5 (\Delta) \leftarrow \nu_5 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 1 8	0 0 1 1 9	2293.40955	-0.00056	3053.12850	759.71839
1 1 1 1 9	0 0 1 1 10	2291.49241	-0.00057	3070.20507	778.71209
1 1 1 1 10	0 0 1 1 11	2289.57147	0.00044	3089.17524	799.60420
1 1 1 1 11	0 0 1 1 12	2287.64367*	0.00023	3110.03789	822.39444
1 1 1 1 12	0 0 1 1 13	2285.71005	0.00068	3132.79188	847.08251
1 1 1 1 13	0 0 1 1 14	2283.76781	-0.00019	3157.43607	873.66808
1 1 1 1 14	0 0 1 1 15	2281.82057	0.00204	3183.96932	902.15079 †
1 1 1 1 15	0 0 1 1 16	2279.86037	0.00013	3212.39053	932.53028
1 1 1 1 16	0 0 1 1 17	2277.89211	-0.00041	3242.69866	964.80614
1 1 1 1 4	0 0 1 1 3	2318.14211	-0.00042	3003.77746	685.63493
1 1 1 1 5	0 0 1 1 4	2320.03605	-0.00036	3013.27023	693.23382
1 1 1 1 6	0 0 1 1 5	2321.92775	-0.00018	3024.66017	702.73224
1 1 1 1 7	0 0 1 1 6	2323.81806	0.00159	3037.94655	714.13007 †
1 1 1 1 8	0 0 1 1 7	2325.70295*	0.00161	3053.12850	727.42716 †
1 1 1 1 9	0 0 1 1 8	2327.58257	0.00083	3070.20507	742.62333
1 1 1 1 10	0 0 1 1 9	2329.45448*	-0.00237	3089.17524	759.71839 †
1 1 1 1 11	0 0 1 1 10	2331.32652	0.00073	3110.03789	778.71209
1 1 1 1 12	0 0 1 1 11	2333.18790	0.00022	3132.79188	799.60420
1 1 1 1 13	0 0 1 1 12	2335.04135	-0.00028	3157.43607	822.39444
1 1 1 1 14	0 0 1 1 13	2336.88694	0.00013	3183.96932	847.08251
1 1 1 1 15	0 0 1 1 14	2338.72203	-0.00042	3212.39053	873.66808
1 1 1 1 16	0 0 1 1 15	2340.54714	-0.00072	3242.69866	902.15079
1 1 1 1 17	0 0 1 1 16	2342.36230	-0.00018	3274.89277	932.53028
1 1 1 1 18	0 0 1 1 17	2345.95807*	0.00047	3344.93555	998.97795
1 1 1 1 19	0 0 1 1 18	2347.73657	-0.00094	3382.78275	1035.04524
1 1 1 1 20	0 0 1 1 19	2349.50606	0.00063	3422.51299	1073.00756
1 1 1 1 5	0 0 1 -1 5	2310.44028	0.00009	3013.27023	702.83004
1 1 1 1 6	0 0 1 -1 6	2310.39355*	0.00036	3024.66017	714.26698
1 1 1 1 7	0 0 1 -1 7	2310.33333*	-0.00352	3037.94655	727.60969 †
1 1 1 1 8	0 0 1 -1 8	2310.27229	0.00178	3053.12850	742.85799 †
1 1 1 1 9	0 0 1 -1 9	2310.19323	-0.00017	3070.20507	760.01168
1 1 1 1 10	0 0 1 -1 10	2310.10489	0.00017	3089.17524	779.07052
1 1 1 1 11	0 0 1 -1 11	2310.00274	-0.00089	3110.03789	800.03426
1 1 1 1 12	0 0 1 -1 12	2309.89138	0.00211	3132.79188	822.90261 †
1 1 1 1 13	0 0 1 -1 13	2309.75866	-0.00213	3157.43607	847.67528 †
1 1 1 1 14	0 0 1 -1 14	2309.61735	-0.00004	3183.96932	874.35193
1 1 1 1 15	0 0 1 -1 15	2309.45802	-0.00031	3212.39053	902.93220
1 -1 1 -1 4	0 0 1 -1 5	2300.94708	0.00060	3003.77652	702.83004
1 -1 1 -1 5	0 0 1 -1 6	2299.00349	0.00193	3013.26854	714.26698 †
1 -1 1 -1 6	0 0 1 -1 7	2297.04954*	0.00127	3024.65796	727.60969 †
1 -1 1 -1 7	0 0 1 -1 8	2295.08825	0.00156	3037.94468	742.85799 †
1 -1 1 -1 9	0 0 1 -1 10	2291.13444*	-0.00461	3070.20957	779.07052 †
1 -1 1 -1 10	0 0 1 -1 11	2289.15017*	-0.00300	3089.18743	800.03426 †
1 -1 1 -1 11	0 0 1 -1 12	2287.16003	0.00069	3110.06196	822.90261
1 -1 1 -1 12	0 0 1 -1 13	2285.15774	0.00013	3132.83289	847.67528
1 -1 1 -1 13	0 0 1 -1 14	2283.15022	0.00221	3157.49994	874.35193 †
1 -1 1 -1 14	0 0 1 -1 15	2281.12969	-0.00090	3184.06279	902.93220
1 -1 1 -1 15	0 0 1 -1 16	2279.10352	-0.00185	3212.52107	933.41570 †
1 -1 1 -1 17	0 0 1 -1 18	2275.03174	0.00009	3275.12241	1000.09076
1 -1 1 -1 18	0 0 1 -1 19	2272.98373	0.00053	3309.26463	1036.28142

1														
2	1	-1	1	-1	4	0	0	1	-1	3	2318.10214	-0.00033	3003.77652	685.67405
3	1	-1	1	-1	5	0	0	1	-1	4	2319.96963	0.00011	3013.26854	693.29902
4	1	-1	1	-1	6	0	0	1	-1	5	2321.82875*	0.00083	3024.65796	702.83004
5	1	-1	1	-1	7	0	0	1	-1	6	2323.67891	0.00121	3037.94468	714.26698 +
6	1	-1	1	-1	8	0	0	1	-1	7	2325.51759	-0.00131	3053.12859	727.60969 +
7	1	-1	1	-1	9	0	0	1	-1	8	2327.35204	0.00046	3070.20957	742.85799
8	1	-1	1	-1	10	0	0	1	-1	9	2329.17543	-0.00032	3089.18743	760.01168
9	1	-1	1	-1	11	0	0	1	-1	10	2330.99141	-0.00003	3110.06196	779.07052
10	1	-1	1	-1	12	0	0	1	-1	11	2332.79849	-0.00015	3132.83289	800.03426
11	1	-1	1	-1	13	0	0	1	-1	12	2334.59589	-0.00144	3157.49994	822.90261 +
12	1	-1	1	-1	14	0	0	1	-1	13	2336.38817	0.00067	3184.06279	847.67528
13	1	-1	1	-1	15	0	0	1	-1	14	2338.17586*	0.00672	3212.52107	874.35193 +
14	1	-1	1	-1	16	0	0	1	-1	15	2339.94289	0.00067	3242.87442	902.93220
15	1	-1	1	-1	17	0	0	1	-1	16	2341.70711	0.00040	3275.12241	933.41570
16	1	-1	1	-1	18	0	0	1	-1	17	2343.46385	0.00126	3309.26463	965.80204 +
17	1	-1	1	-1	19	0	0	1	-1	18	2345.21151	0.00167	3345.30060	1000.09076 +
18	1	-1	1	-1	21	0	0	1	-1	20	2348.67822	-0.00008	3423.05183	1074.37353

rms = 0.00048 cm⁻¹

$V_2 + V_4 + V_5 (\Delta) \leftarrow V_4 + V_5 (\Delta)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 1 1 1 2	1 1 1 1 3	1795.57924	-0.00049	2990.48582	1194.90609
1 1 1 1 3	1 1 1 1 4	1793.64869*	0.00127	2996.18249	1202.53506 †
1 1 1 1 4	1 1 1 1 5	1791.69999*	-0.00701	3003.77746	1212.07046 †
1 1 1 1 5	1 1 1 1 6	1789.75868	0.00019	3013.27023	1223.51174
1 1 1 1 6	1 1 1 1 7	1787.80131	-0.00061	3024.66017	1236.85825
1 1 1 1 7	1 1 1 1 8	1785.83729	-0.00001	3037.94655	1252.10924
1 1 1 1 8	1 1 1 1 9	1783.86549	0.00087	3053.12850	1269.26388
1 1 1 1 9	1 1 1 1 10	1781.88403	0.00019	3070.20507	1288.32123
1 1 1 1 10	1 1 1 1 11	1779.89546	0.00053	3089.17524	1309.28031
1 1 1 1 11	1 1 1 1 12	1777.89766	-0.00017	3110.03789	1332.14005
1 1 1 1 12	1 1 1 1 13	1775.89159	-0.00091	3132.79188	1356.89938
1 1 1 1 13	1 1 1 1 14	1773.87768	-0.00119	3157.43607	1383.55720 †
1 1 1 1 14	1 1 1 1 15	1771.85683	-0.00008	3183.96932	1412.11241
1 1 1 1 15	1 1 1 1 16	1769.82561	-0.00097	3212.39053	1442.56394
1 1 1 1 16	1 1 1 1 17	1767.78588	-0.00199	3242.69866	1474.91078 †
1 1 1 1 17	1 1 1 1 18	1765.73957	-0.00123	3274.89277	1509.15197 †
1 1 1 1 18	1 1 1 1 19	1763.68417	-0.00121	3308.97199	1545.28661 †
1 1 1 1 19	1 1 1 1 20	1761.62151	-0.00015	3344.93555	1583.31388
1 1 1 1 20	1 1 1 1 21	1759.54964	-0.00007	3382.78275	1623.23305
1 1 1 1 21	1 1 1 1 22	1757.46920	-0.00038	3422.51299	1665.04341
1 1 1 1 3	1 1 1 1 2	1806.99927*	0.00076	2996.18249	1189.18398
1 1 1 1 4	1 1 1 1 3	1808.87222*	0.00085	3003.77746	1194.90609
1 1 1 1 5	1 1 1 1 4	1810.73677*	0.00161	3013.27023	1202.53506 †
1 1 1 1 6	1 1 1 1 5	1812.58916*	-0.00055	3024.66017	1212.07046
1 1 1 1 7	1 1 1 1 6	1814.43703*	0.00222	3037.94655	1223.51174 †
1 1 1 1 8	1 1 1 1 7	1816.27122	0.00097	3053.12850	1236.85825
1 1 1 1 9	1 1 1 1 8	1818.09574	-0.00009	3070.20507	1252.10924
1 1 1 1 10	1 1 1 1 9	1819.91075	-0.00061	3089.17524	1269.26388
1 1 1 1 11	1 1 1 1 10	1821.71465*	-0.00200	3110.03789	1288.32123 †
1 1 1 1 12	1 1 1 1 11	1823.50754*	-0.00404	3132.79188	1309.28031 †
1 1 1 1 13	1 1 1 1 12	1825.29389*	-0.00213	3157.43607	1332.14005 †
1 1 1 1 14	1 1 1 1 13	1827.07000	0.00006	3183.96932	1356.89938
1 1 1 1 15	1 1 1 1 14	1828.83399	0.00067	3212.39053	1383.55720
1 1 1 1 16	1 1 1 1 15	1830.58545	-0.00080	3242.69866	1412.11241
1 1 1 1 17	1 1 1 1 16	1832.32720	-0.00162	3274.89277	1442.56394 †
1 1 1 1 18	1 1 1 1 17	1834.05971	-0.00149	3308.97199	1474.91078 †
1 1 1 1 19	1 1 1 1 18	1835.78329	-0.00029	3344.93555	1509.15197
1 1 1 1 20	1 1 1 1 19	1837.49664	0.00050	3382.78275	1545.28661
1 1 1 1 21	1 1 1 1 20	1839.19968	0.00058	3422.51299	1583.31388

$$\text{rms} = 0.00051 \text{ cm}^{-1}$$

$$2\nu_2(\Sigma^+) \leftarrow G.S.(\Sigma^+)$$

v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
0	0	0	0	0	0	0	0	0	1	3605.50107	0.00009	3607.40164	1.90066
0	0	0	0	1	0	0	0	0	2	3603.58429	0.00036	3609.28588	5.70195
0	0	0	0	2	0	0	0	0	3	3601.65019	-0.00033	3613.05433	11.40382
0	0	0	0	3	0	0	0	0	4	3599.70214*	0.00139	3618.70695	19.00619
0	0	0	0	4	0	0	0	0	5	3597.73497	0.00029	3626.24365	28.50898
0	0	0	0	5	0	0	0	0	6	3595.75182	-0.00049	3635.66435	39.91204
0	0	0	0	6	0	0	0	0	7	3593.75382	0.00015	3646.96890	53.21523
0	0	0	0	7	0	0	0	0	8	3591.73879	0.00001	3660.15717	68.41838
0	0	0	0	8	0	0	0	0	9	3589.70770	0.00002	3675.22897	85.52129
0	0	0	0	9	0	0	0	0	10	3587.66048	0.00009	3692.18411	104.52373
0	0	0	0	10	0	0	0	0	11	3585.59676	-0.00017	3711.02236	125.42544
0	0	0	0	11	0	0	0	0	12	3583.51718	-0.00014	3731.74348	148.22616
0	0	0	0	12	0	0	0	0	13	3581.42152	-0.00007	3754.34717	172.92558

1	0	0	0	0	13	0	0	0	0	14	3579.30971	-0.00006	3778.83315	199.52337
2	0	0	0	0	14	0	0	0	0	15	3577.18189	0.00001	3805.20108	228.01920
3	0	0	0	0	15	0	0	0	0	16	3575.03816	0.00022	3833.45062	258.41268
4	0	0	0	0	16	0	0	0	0	17	3572.87729	-0.00069	3863.58139	290.70340
5	0	0	0	0	17	0	0	0	0	18	3570.70201	-0.00002	3895.59299	324.89096
6	0	0	0	0	18	0	0	0	0	19	3568.50999	-0.00011	3929.48499	360.97488
7	0	0	0	0	19	0	0	0	0	20	3566.30200	-0.00023	3965.25694	398.95471
8	0	0	0	0	20	0	0	0	0	21	3564.07830	-0.00013	4002.90836	438.82993
9	0	0	0	0	21	0	0	0	0	22	3561.83872	-0.00001	4042.43877	480.60003
10	0	0	0	0	22	0	0	0	0	23	3559.58326	0.00010	4083.84761	524.26445
11	0	0	0	0	23	0	0	0	0	24	3557.31176	0.00002	4127.13436	569.82262
12	0	0	0	0	24	0	0	0	0	25	3555.02490	0.00041	4172.29843	617.27393
13	0	0	0	0	25	0	0	0	0	26	3552.72172	0.00028	4219.33921	666.61777
14	0	0	0	0	26	0	0	0	0	27	3550.40213	-0.00049	4268.25609	717.85348
15	0	0	0	0	27	0	0	0	0	28	3548.06775	-0.00029	4319.04842	770.98038
16	0	0	0	0	28	0	0	0	0	29	3545.71838	0.00066	4371.71551	825.99778
17	0	0	0	0	29	0	0	0	0	30	3543.35135	-0.00036	4426.25666	882.90495
18	0	0	0	0	30	0	0	0	0	31	3540.96966	-0.00035	4482.67116	941.70115
19	0	0	0	0	31	0	0	0	0	32	3538.57322	0.00057	4540.95824	1002.38559
20	0	0	0	0	32	0	0	0	0	33	3536.16000	0.00034	4601.11714	1064.95747
21	0	0	0	0	33	0	0	0	0	34	3533.73116	0.00009	4663.14705	1129.41599
22	0	0	0	0	34	0	0	0	0	35	3531.28876	0.00188	4727.04715	1195.76027 +
23	0	0	0	0	35	0	0	0	0	36	3528.82350	-0.00363	4792.81659	1263.98946 +
24	0	0	0	0	36	0	0	0	0	37	3526.35135	-0.00049	4860.45449	1334.10264
25	0	0	0	0	37	0	0	0	0	38	3523.86035	-0.00069	4929.95995	1406.09891
26	0	0	0	0	1	0	0	0	0	0	3609.28587	-0.00001	3609.28588	0.00000
27	0	0	0	0	2	0	0	0	0	1	3611.15389	0.00022	3613.05433	1.90066
28	0	0	0	0	3	0	0	0	0	2	3613.00502	0.00002	3618.70695	5.70195
29	0	0	0	0	4	0	0	0	0	3	3614.84003	0.00019	3626.24365	11.40382
30	0	0	0	0	5	0	0	0	0	4	3616.65976	0.00161	3635.66435	19.00619 +
31	0	0	0	0	6	0	0	0	0	5	3618.45997	0.00004	3646.96890	28.50898
32	0	0	0	0	7	0	0	0	0	6	3620.24517	0.00004	3660.15717	39.91204
33	0	0	0	0	8	0	0	0	0	7	3622.01380	0.00006	3675.22897	53.21523
34	0	0	0	0	9	0	0	0	0	8	3623.76577	0.00004	3692.18411	68.41838
35	0	0	0	0	10	0	0	0	0	9	3625.50113	0.00006	3711.02236	85.52129
36	0	0	0	0	11	0	0	0	0	10	3627.21983	0.00008	3731.74348	104.52373
37	0	0	0	0	12	0	0	0	0	11	3628.92179	0.00006	3754.34717	125.42544
38	0	0	0	0	13	0	0	0	0	12	3630.60699	0.00000	3778.83315	148.22616
39	0	0	0	0	14	0	0	0	0	13	3632.27553	0.00003	3805.20108	172.92558
40	0	0	0	0	15	0	0	0	0	14	3633.92722	-0.00002	3833.45062	199.52337
41	0	0	0	0	16	0	0	0	0	15	3635.56222	0.00003	3863.58139	228.01920
42	0	0	0	0	17	0	0	0	0	16	3637.17987	-0.00044	3895.59299	258.41268
43	0	0	0	0	18	0	0	0	0	17	3638.78149	-0.00009	3929.48499	290.70340
44	0	0	0	0	19	0	0	0	0	18	3640.36599	0.00001	3965.25694	324.89096
45	0	0	0	0	20	0	0	0	0	19	3641.93320	-0.00028	4002.90836	360.97488
46	0	0	0	0	21	0	0	0	0	20	3643.48399	-0.00007	4042.43877	398.95471
47	0	0	0	0	22	0	0	0	0	21	3645.01773	0.00005	4083.84761	438.82993
48	0	0	0	0	23	0	0	0	0	22	3646.53448	0.00015	4127.13436	480.60003
49	0	0	0	0	24	0	0	0	0	23	3648.03398	0.00000	4172.29843	524.26445
50	0	0	0	0	25	0	0	0	0	24	3649.51673	0.00014	4219.33921	569.82262
51	0	0	0	0	26	0	0	0	0	25	3650.98227	0.00011	4268.25609	617.27393
52	0	0	0	0	27	0	0	0	0	26	3652.43081	0.00016	4319.04842	666.61777
53	0	0	0	0	28	0	0	0	0	27	3653.86164	-0.00039	4371.71551	717.85348
54	0	0	0	0	29	0	0	0	0	28	3655.27619	-0.00009	4426.25666	770.98038
55	0	0	0	0	30	0	0	0	0	29	3656.67395	0.00057	4482.67116	825.99778
56	0	0	0	0	31	0	0	0	0	30	3658.05375	0.00046	4540.95824	882.90495
57	0	0	0	0	32	0	0	0	0	31	3659.41590	-0.00009	4601.11714	941.70115
58	0	0	0	0	33	0	0	0	0	32	3660.76552*	0.00406	4663.14705	1002.38559 +
59	0	0	0	0	34	0	0	0	0	33	3662.08951	-0.00017	4727.04715	1064.95747
60	0	0	0	0	35	0	0	0	0	34	3663.40066	0.00006	4792.81659	1129.41599
	0	0	0	0	36	0	0	0	0	35	3664.69470	0.00048	4860.45449	1195.76027
	0	0	0	0	37	0	0	0	0	36	3665.97180	0.00131	4929.95995	1263.98946 +

rms = 0.00027 cm⁻¹

Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm^{-1}) for the ν_3 and associated hot bands of $^{13}\text{C}_2\text{HD}$ ^a (35 pp)

$\nu_3 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	0 0 0 0 1	2545.69067	0.00056	2547.59077	1.90066
0 0 0 0 1	0 0 0 0 2	2543.77728	0.00005	2549.47917	5.70195
0 0 0 0 2	0 0 0 0 3	2541.85262	0.00048	2553.25596	11.40382
0 0 0 0 3	0 0 0 0 4	2539.91481	-0.00007	2558.92107	19.00619
0 0 0 0 4	0 0 0 0 5	2537.96568	0.00022	2566.47444	28.50898
0 0 0 0 5	0 0 0 0 6	2536.00431	0.00039	2575.91596	39.91204
0 0 0 0 6	0 0 0 0 7	2534.03043	0.00015	2587.24552	53.21523
0 0 0 0 7	0 0 0 0 8	2532.04499	0.00042	2600.46295	68.41838
0 0 0 0 8	0 0 0 0 9	2530.04703	0.00023	2615.56809	85.52129
0 0 0 0 9	0 0 0 0 10	2528.03718	0.00016	2632.56074	104.52373
0 0 0 0 10	0 0 0 0 11	2526.01561	0.00038	2651.44067	125.42544
0 0 0 0 11	0 0 0 0 12	2523.98215	0.00067	2672.20764	148.22616
0 0 0 0 12	0 0 0 0 13	2521.93582	0.00003	2694.86136	172.92558
0 0 0 0 13	0 0 0 0 14	2519.87828	0.00011	2719.40155	199.52337
0 0 0 0 14	0 0 0 0 15	2517.80901	0.00034	2745.82787	228.01920
0 0 0 0 15	0 0 0 0 16	2515.72779	0.00049	2774.13998	258.41268
0 0 0 0 16	0 0 0 0 17	2513.63476	0.00066	2804.33751	290.70340
0 0 0 0 17	0 0 0 0 18	2511.52903	-0.00006	2836.42005	324.89096
0 0 0 0 18	0 0 0 0 19	2509.41231	0.00001	2870.38718	360.97488
0 0 0 0 19	0 0 0 0 20	2507.28377	0.00002	2906.23845	398.95471
0 0 0 0 20	0 0 0 0 21	2505.14353	0.00006	2943.97340	438.82993
0 0 0 0 21	0 0 0 0 22	2502.99181	0.00032	2983.59152	480.60003
0 0 0 0 22	0 0 0 0 23	2500.82812	0.00028	3025.09229	524.26445
0 0 0 0 23	0 0 0 0 24	2498.65279	0.00024	3068.47517	569.82262
0 0 0 0 24	0 0 0 0 25	2496.46585	0.00021	3113.73957	617.27393
0 0 0 0 25	0 0 0 0 26	2494.26738	0.00024	3160.88491	666.61777
0 0 0 0 26	0 0 0 0 27	2492.05732	0.00024	3209.91056	717.85348
0 0 0 0 27	0 0 0 0 28	2489.83533	-0.00016	3260.81587	770.98038
0 0 0 0 28	0 0 0 0 29	2487.60227	-0.00012	3313.60017	825.99778
0 0 0 0 29	0 0 0 0 30	2485.35759	-0.00023	3368.26277	882.90495
0 0 0 0 30	0 0 0 0 31	2483.10164	-0.00016	3424.80295	941.70115
0 0 0 0 31	0 0 0 0 32	2480.83421	-0.00016	3483.21995	1002.38559
0 0 0 0 32	0 0 0 0 33	2478.55578	0.00024	3543.51302	1064.95747
0 0 0 0 33	0 0 0 0 34	2476.26567	0.00031	3605.68134	1129.41599
0 0 0 0 34	0 0 0 0 35	2473.96355	-0.00029	3669.72411	1195.76027
0 0 0 0 35	0 0 0 0 36	2471.65109	0.00007	3735.64048	1263.98946
0 0 0 0 36	0 0 0 0 37	2469.32717	0.00024	3803.42957	1334.10264
0 0 0 0 37	0 0 0 0 38	2466.99180	0.00021	3873.09050	1406.09891
0 0 0 0 38	0 0 0 0 39	2464.64549	0.00044	3944.62235	1479.97730
0 0 0 0 39	0 0 0 0 40	2462.28764	0.00033	4018.02417	1555.73685
0 0 0 0 40	0 0 0 0 41	2459.91904	0.00061	4093.29499	1633.37656
0 0 0 0 41	0 0 0 0 42	2457.53875	0.00034	4170.43382	1712.89541
0 0 0 0 42	0 0 0 0 43	2455.14746	0.00015	4249.43965	1794.29235
0 0 0 0 43	0 0 0 0 44	2452.74620	0.00107	4330.31143	1877.56630 †
0 0 0 0 44	0 0 0 0 45	2450.33408	0.00215	4413.04810	1962.71617 †
0 0 0 0 45	0 0 0 0 46	2447.90157	-0.00615	4497.64857	2049.74085 †
0 0 0 0 46	0 0 0 0 47	2445.47124	-0.00129	4584.11171	2138.63917 †
0 0 0 0 1	0 0 0 0 0	2549.47925	0.00008	2549.47917	0.00000
0 0 0 0 2	0 0 0 0 1	2551.35539	0.00009	2553.25596	1.90066
0 0 0 0 3	0 0 0 0 2	2553.21930	0.00017	2558.92107	5.70195
0 0 0 0 4	0 0 0 0 3	2555.07062	0.00000	2566.47444	11.40382
0 0 0 0 5	0 0 0 0 4	2556.90969	-0.00008	2575.91596	19.00619
0 0 0 0 6	0 0 0 0 5	2558.73651	-0.00003	2587.24552	28.50898
0 0 0 0 7	0 0 0 0 6	2560.55086	-0.00005	2600.46295	39.91204

1	0	0	0	0	8	0	0	0	0	7	2562.35276	-0.00010	2615.56809	53.21523
3	0	0	0	0	9	0	0	0	0	8	2564.14237	0.00001	2632.56074	68.41838
4	0	0	0	0	10	0	0	0	0	9	2565.91940	0.00002	2651.44067	85.52129
5	0	0	0	0	11	0	0	0	0	10	2567.68388	-0.00003	2672.20764	104.52373
6	0	0	0	0	12	0	0	0	0	11	2569.43590	-0.00002	2694.86136	125.42544
7	0	0	0	0	13	0	0	0	0	12	2571.17509	-0.00030	2719.40155	148.22616
8	0	0	0	0	14	0	0	0	0	13	2572.90215	-0.00014	2745.82787	172.92558
9	0	0	0	0	15	0	0	0	0	14	2574.61650	-0.00011	2774.13998	199.52337
10	0	0	0	0	16	0	0	0	0	15	2576.31825	-0.00006	2804.33751	228.01920
11	0	0	0	0	17	0	0	0	0	16	2578.00713	-0.00024	2836.42005	258.41268
12	0	0	0	0	18	0	0	0	0	17	2579.68362	-0.00015	2870.38718	290.70340
13	0	0	0	0	19	0	0	0	0	18	2581.34737	-0.00013	2906.23845	324.89096
14	0	0	0	0	20	0	0	0	0	19	2582.99842	-0.00010	2943.97340	360.97488
15	0	0	0	0	21	0	0	0	0	20	2584.63671	-0.00010	2983.59152	398.95471
16	0	0	0	0	22	0	0	0	0	21	2586.26213	-0.00023	3025.09229	438.82993
17	0	0	0	0	23	0	0	0	0	22	2587.87502	-0.00012	3068.47517	480.60003
18	0	0	0	0	24	0	0	0	0	23	2589.47496	-0.00016	3113.73957	524.26445
19	0	0	0	0	25	0	0	0	0	24	2591.06216	-0.00013	3160.88491	569.82262
20	0	0	0	0	26	0	0	0	0	25	2592.63643	-0.00019	3209.91056	617.27393
21	0	0	0	0	27	0	0	0	0	26	2594.19808	-0.00002	3260.81587	666.61777
22	0	0	0	0	28	0	0	0	0	27	2595.74647	-0.00023	3313.60017	717.85348
23	0	0	0	0	29	0	0	0	0	28	2597.28201	-0.00038	3368.26277	770.98038
24	0	0	0	0	30	0	0	0	0	29	2598.80517	0.00000	3424.80295	825.99778
25	0	0	0	0	32	0	0	0	0	31	2601.81176	-0.00011	3543.51302	941.70115
26	0	0	0	0	33	0	0	0	0	32	2603.29557	-0.00019	3605.68134	1002.38559
27	0	0	0	0	34	0	0	0	0	33	2604.76617	-0.00047	3669.72411	1064.95747
28	0	0	0	0	35	0	0	0	0	34	2606.22394	-0.00055	3735.64048	1129.41599
29	0	0	0	0	36	0	0	0	0	35	2607.66918	-0.00012	3803.42957	1195.76027
30	0	0	0	0	37	0	0	0	0	36	2609.10132	0.00027	3873.09050	1263.98946
31	0	0	0	0	38	0	0	0	0	37	2610.52019	0.00048	3944.62235	1334.10264
32	0	0	0	0	39	0	0	0	0	38	2611.92553	0.00027	4018.02417	1406.09891
33	0	0	0	0	40	0	0	0	0	39	2613.31795	0.00026	4093.29499	1479.97730
34	0	0	0	0	41	0	0	0	0	40	2614.69714	0.00017	4170.43382	1555.73685
35	0	0	0	0	42	0	0	0	0	41	2616.06349	0.00040	4249.43965	1633.37656
36	0	0	0	0	43	0	0	0	0	42	2617.41658	0.00056	4330.31143	1712.89541
37	0	0	0	0	44	0	0	0	0	43	2618.75778	0.00202	4413.04810	1794.29235 +
38	0	0	0	0	45	0	0	0	0	44	2620.08404*	0.00177	4497.64857	1877.56630 +
39	0	0	0	0	46	0	0	0	0	45	2621.39481	-0.00073	4584.11171	1962.71617
40	0	0	0	0	47	0	0	0	0	46	2622.69529	-0.00026	4672.43639	2049.74085
41	0	0	0	0	48	0	0	0	0	47	2623.98205	-0.00023	4762.62145	2138.63917
42	0	0	0	0	49	0	0	0	0	48	2625.25543	-0.00029	4854.66570	2229.40999
43	0	0	0	0	50	0	0	0	0	49	2626.51646*	0.00062	4948.56792	2322.05209
44	0	0	0	0	51	0	0	0	0	50	2627.76173	-0.00090	5044.32688	2416.56425
45	0	0	0	0	52	0	0	0	0	51	2628.99693	0.00087	5141.94131	2512.94525

rms = 0.00031 cm⁻¹

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

$v_3(\Sigma^+) \leftarrow v_4(\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	1 1 0 0 1	2036.10388*	-0.00062	2547.59077	511.48627
0 0 0 0 1	1 1 0 0 2	2034.19126	0.00039	2549.47917	515.28830
0 0 0 0 2	1 1 0 0 3	2032.26512	0.00045	2553.25596	520.99129
0 0 0 0 3	1 1 0 0 4	2030.32588	-0.00004	2558.92107	528.59515
0 0 0 0 4	1 1 0 0 5	2028.37495	0.00030	2566.47444	538.09979
0 0 0 0 5	1 1 0 0 6	2026.41098	0.00010	2575.91596	549.50508

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

1														
2	0	0	0	0	3	1	-1	0	0	3	2037.88000	-0.00006	2558.92107	521.04101
3	0	0	0	0	4	1	-1	0	0	4	2037.79644	0.00001	2566.47444	528.67801
4	0	0	0	0	5	1	-1	0	0	5	2037.69141	-0.00048	2575.91596	538.22407
5	0	0	0	0	6	1	-1	0	0	6	2037.56651	0.00005	2587.24552	549.67906
6	0	0	0	0	7	1	-1	0	0	7	2037.41998	-0.00017	2600.46295	563.04281
7	0	0	0	0	8	1	-1	0	0	8	2037.25263	-0.00032	2615.56809	578.31514
8	0	0	0	0	9	1	-1	0	0	9	2037.06436	-0.00053	2632.56074	595.49585
9	0	0	0	0	10	1	-1	0	0	10	2036.85594	-0.00004	2651.44067	614.58469
10	0	0	0	0	11	1	-1	0	0	11	2036.62555	-0.00067	2672.20764	635.58142
11	0	0	0	0	12	1	-1	0	0	12	2036.37492	-0.00071	2694.86136	658.48573
12	0	0	0	0	13	1	-1	0	0	13	2036.10388	-0.00035	2719.40155	683.29732
13	0	0	0	0	14	1	-1	0	0	14	2035.81226	0.00023	2745.82787	710.01584
14	0	0	0	0	15	1	-1	0	0	15	2035.49847	-0.00058	2774.13998	738.64093
15	0	0	0	0	16	1	-1	0	0	16	2035.16481	-0.00049	2804.33751	769.17220
16	0	0	0	0	17	1	-1	0	0	17	2034.81070	-0.00012	2836.42005	801.60923
17	0	0	0	0	18	1	-1	0	0	18	2034.43517	-0.00045	2870.38718	835.95156
18	0	0	0	0	19	1	-1	0	0	19	2034.03957	-0.00014	2906.23845	872.19874
19	0	0	0	0	20	1	-1	0	0	20	2033.62299	-0.00015	2943.97340	910.35027
20	0	0	0	0	21	1	-1	0	0	21	2033.18597	0.00006	2983.59152	950.40561
21	0	0	0	0	22	1	-1	0	0	22	2032.72800	-0.00006	3025.09229	992.36423
22	0	0	0	0	23	1	-1	0	0	23	2032.24960	-0.00002	3068.47517	1036.22555
23	0	0	0	0	24	1	-1	0	0	24	2031.75021	-0.00040	3113.73957	1081.98896
24	0	0	0	0	25	1	-1	0	0	25	2031.23095	-0.00012	3160.88491	1129.65384
25	0	0	0	0	26	1	-1	0	0	26	2030.69093	-0.00009	3209.91056	1179.21954
26	0	0	0	0	27	1	-1	0	0	27	2030.13053	0.00003	3260.81587	1230.68537
27	0	0	0	0	28	1	-1	0	0	28	2029.54988	0.00034	3313.60017	1284.05064
28	0	0	0	0	29	1	-1	0	0	29	2028.94846	0.00029	3368.26277	1339.31460
29	0	0	0	0	30	1	-1	0	0	30	2028.32676	0.00032	3424.80295	1396.47651
30	0	0	0	0	31	1	-1	0	0	31	2027.68411	-0.00028	3483.21995	1455.53557
31	0	0	0	0	32	1	-1	0	0	32	2027.02114	-0.00090	3543.51302	1516.49098
32	0	0	0	0	33	1	-1	0	0	33	2026.34002	0.00058	3605.68134	1579.34190
33	0	0	0	0	34	1	-1	0	0	34	2025.63746	0.00083	3669.72411	1644.08748
34	0	0	0	0	35	1	-1	0	0	35	2024.91335	-0.00031	3735.64048	1710.72682
35	0	0	0	0	36	1	-1	0	0	36	2024.16975	-0.00081	3803.42957	1779.25901

rms = 0.00034 cm⁻¹

$v_3 + v_4 (\Pi) \leftarrow G.S. (\Sigma^+)$

43	v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS - CALC	E'	E''
44														
45	1	1	0	0	1	0	0	0	0	2	3039.05249	0.00024	3044.75420	5.70195
46	1	1	0	0	2	0	0	0	0	3	3037.12800	-0.00041	3048.53223	11.40382
47	1	1	0	0	3	0	0	0	0	4	3035.19246	-0.00055	3054.19920	19.00619
48	1	1	0	0	4	0	0	0	0	5	3033.24517	-0.00091	3061.75506	28.50898
49	1	1	0	0	5	0	0	0	0	6	3031.28764	-0.00001	3071.19969	39.91204
50	1	1	0	0	6	0	0	0	0	7	3029.31803	0.00030	3082.53297	53.21523
51	1	1	0	0	7	0	0	0	0	8	3027.33541	-0.00095	3095.75474	68.41838
52	1	1	0	0	8	0	0	0	0	9	3025.34274	-0.00081	3110.86484	85.52129
53	1	1	0	0	9	0	0	0	0	10	3023.33880	-0.00054	3127.86306	104.52373
54	1	1	0	0	10	0	0	0	0	11	3021.32351	-0.00023	3146.74918	125.42544
55	1	1	0	0	11	0	0	0	0	12	3019.29653	-0.00025	3167.52293	148.22616
56	1	1	0	0	12	0	0	0	0	13	3017.25825	-0.00023	3190.18406	172.92558
57	1	1	0	0	13	0	0	0	0	14	3015.20881	-0.00006	3214.73225	199.52337
58	1	1	0	0	14	0	0	0	0	15	3013.14792	-0.00006	3241.16718	228.01920
59	1	1	0	0	15	0	0	0	0	16	3011.07507	-0.00075	3269.48849	258.41268
60	1	1	0	0	16	0	0	0	0	17	3008.99202	-0.00039	3299.69582	290.70340
	1	1	0	0	17	0	0	0	0	18	3006.89754	-0.00025	3331.78875	324.89096
	1	1	0	0	18	0	0	0	0	19	3004.79180	-0.00018	3365.76686	360.97488
	1	1	0	0	19	0	0	0	0	20	3002.67497	-0.00002	3401.62970	398.95471
	1	1	0	0	20	0	0	0	0	21	3000.54679	-0.00007	3439.37679	438.82993
	1	1	0	0	21	0	0	0	0	22	2998.40742	-0.00018	3479.00763	480.60003

1														
2	1	1	0	0	22	0	0	0	0	23	2996.25702	-0.00021	3520.52169	524.26445
3	1	1	0	0	23	0	0	0	0	24	2994.09539	-0.00040	3563.91841	569.82262
4	1	1	0	0	24	0	0	0	0	25	2991.92358	0.00028	3609.19723	617.27393
5	1	1	0	0	25	0	0	0	0	26	2989.74106	0.00130	3656.35753	666.61777 +
6	1	1	0	0	26	0	0	0	0	27	2987.54560	0.00038	3705.39870	717.85348
7	1	1	0	0	27	0	0	0	0	28	2985.34524	0.00555	3756.32007	770.98038 +
8	1	1	0	0	28	0	0	0	0	29	2983.14596	0.02277	3809.12097	825.99778 +
9	1	1	0	0	29	0	0	0	0	30	2980.86721	-0.02854	3863.80070	882.90495 +
10	1	1	0	0	30	0	0	0	0	31	2978.64305	-0.01433	3920.35853	941.70115 +
11	1	1	0	0	31	0	0	0	0	32	2976.39587	-0.01225	3978.79371	1002.38559 +
12	1	1	0	0	32	0	0	0	0	33	2974.13723	-0.01075	4039.10545	1064.95747 +
13	1	1	0	0	33	0	0	0	0	34	2971.86647	-0.01051	4101.29296	1129.41599 +
14	1	1	0	0	1	0	0	0	0	0	3044.75406	-0.00014	3044.75420	0.00000
15	1	1	0	0	2	0	0	0	0	1	3046.63104	-0.00053	3048.53223	1.90066
16	1	1	0	0	3	0	0	0	0	2	3048.49725	-0.00001	3054.19920	5.70195
17	1	1	0	0	4	0	0	0	0	3	3050.35111	-0.00013	3061.75506	11.40382
18	1	1	0	0	5	0	0	0	0	4	3052.19334	-0.00016	3071.19969	19.00619
19	1	1	0	0	6	0	0	0	0	5	3054.02390	-0.00009	3082.53297	28.50898
20	1	1	0	0	7	0	0	0	0	6	3055.84261	-0.00009	3095.75474	39.91204
21	1	1	0	0	8	0	0	0	0	7	3057.64958	-0.00003	3110.86484	53.21523
22	1	1	0	0	9	0	0	0	0	8	3059.44448	-0.00020	3127.86306	68.41838
23	1	1	0	0	10	0	0	0	0	9	3061.22784	-0.00005	3146.74918	85.52129
24	1	1	0	0	11	0	0	0	0	10	3062.99908	-0.00013	3167.52293	104.52373
25	1	1	0	0	12	0	0	0	0	11	3064.75852	-0.00010	3190.18406	125.42544
26	1	1	0	0	13	0	0	0	0	12	3066.50590	-0.00019	3214.73225	148.22616
27	1	1	0	0	14	0	0	0	0	13	3068.24153	-0.00007	3241.16718	172.92558
28	1	1	0	0	15	0	0	0	0	14	3069.96476	-0.00036	3269.48849	199.52337
29	1	1	0	0	16	0	0	0	0	15	3071.67646	-0.00016	3299.69582	228.01920
30	1	1	0	0	17	0	0	0	0	16	3073.37595	-0.00012	3331.78875	258.41268
31	1	1	0	0	18	0	0	0	0	17	3075.06313	-0.00033	3365.76686	290.70340
32	1	1	0	0	19	0	0	0	0	18	3076.73873	-0.00001	3401.62970	324.89096
33	1	1	0	0	20	0	0	0	0	19	3078.40165	-0.00026	3439.37679	360.97488
34	1	1	0	0	21	0	0	0	0	20	3080.05163	-0.00129	3479.00763	398.95471 +
35	1	1	0	0	22	0	0	0	0	21	3081.69174	-0.00001	3520.52169	438.82993
36	1	1	0	0	23	0	0	0	0	22	3083.31875	0.00037	3563.91841	480.60003
37	1	1	0	0	24	0	0	0	0	23	3084.93301	0.00023	3609.19723	524.26445
38	1	1	0	0	25	0	0	0	0	24	3086.53472	-0.00020	3656.35753	569.82262
39	1	1	0	0	26	0	0	0	0	25	3088.12678	0.00201	3705.39870	617.27393 +
40	1	1	0	0	27	0	0	0	0	26	3089.70760	0.00530	3756.32007	666.61777 +
41	1	1	0	0	28	0	0	0	0	27	3091.29052	0.02302	3809.12097	717.85348 +
42	1	1	0	0	29	0	0	0	0	28	3092.79036	-0.02996	3863.80070	770.98038 +
43	1	1	0	0	30	0	0	0	0	29	3094.34505	-0.01570	3920.35853	825.99778 +
44	1	1	0	0	31	0	0	0	0	30	3095.87728	-0.01147	3978.79371	882.90495 +
45	1	1	0	0	32	0	0	0	0	31	3097.39374	-0.01056	4039.10545	941.70115 +
46	1	1	0	0	33	0	0	0	0	32	3098.89706	-0.01031	4101.29296	1002.38559 +
47	1	-1	0	0	2	0	0	0	0	2	3042.85594	0.00061	3048.55727	5.70195
48	1	-1	0	0	3	0	0	0	0	3	3042.84611	0.00063	3054.24930	11.40382
49	1	-1	0	0	4	0	0	0	0	4	3042.83223	-0.00012	3061.83854	19.00619
50	1	-1	0	0	5	0	0	0	0	5	3042.81551	-0.00041	3071.32490	28.50898
51	1	-1	0	0	6	0	0	0	0	6	3042.79547	-0.00073	3082.70824	39.91204
52	1	-1	0	0	7	0	0	0	0	7	3042.77293	-0.00024	3095.98840	53.21523
53	1	-1	0	0	8	0	0	0	0	8	3042.74626	-0.00057	3111.16521	68.41838
54	1	-1	0	0	9	0	0	0	0	9	3042.71672	-0.00044	3128.23845	85.52129
55	1	-1	0	0	10	0	0	0	0	10	3042.68364	-0.00053	3147.20789	104.52373
56	1	-1	0	0	11	0	0	0	0	11	3042.64733	-0.00050	3168.07327	125.42544
57	1	-1	0	0	12	0	0	0	0	12	3042.60758	-0.00056	3190.83430	148.22616
58	1	-1	0	0	13	0	0	0	0	13	3042.56459	-0.00049	3215.49066	172.92558
59	1	-1	0	0	14	0	0	0	0	14	3042.51790	-0.00073	3242.04201	199.52337
60	1	-1	0	0	15	0	0	0	0	15	3042.46822	-0.00057	3270.48799	228.01920
	1	-1	0	0	16	0	0	0	0	16	3042.41511	-0.00042	3300.82820	258.41268
	1	-1	0	0	17	0	0	0	0	17	3042.35853	-0.00030	3333.06223	290.70340
	1	-1	0	0	18	0	0	0	0	18	3042.29839	-0.00029	3367.18964	324.89096
	1	-1	0	0	19	0	0	0	0	19	3042.23495	-0.00011	3403.20994	360.97488
	1	-1	0	0	20	0	0	0	0	20	3042.16770	-0.00024	3441.12265	398.95471
	1	-1	0	0	21	0	0	0	0	21	3042.09775	0.00045	3480.92723	438.82993

1														
2	1	-1	0	0	22	0	0	0	0	22	3042.02386	0.00074	3522.62315	480.60003
3	1	-1	0	0	23	0	0	0	0	23	3041.94574	0.00037	3566.20982	524.26445
4	1	-1	0	0	24	0	0	0	0	24	3041.86628*	0.00225	3611.68665	569.82262 †
5	1	-1	0	0	25	0	0	0	0	25	3041.78331*	0.00424	3659.05301	617.27393 †
6	1	-1	0	0	26	0	0	0	0	26	3041.69851*	0.00805	3708.30823	666.61777 †
7	1	-1	0	0	27	0	0	0	0	27	3041.62367*	0.02549	3759.45166	717.85348 †
8	1	-1	0	0	28	0	0	0	0	28	3041.46959*	-0.03259	3812.48257	770.98038 †
9	1	-1	0	0	29	0	0	0	0	29	3041.39019*	-0.01226	3867.40023	825.99778 †
10	1	-1	0	0	30	0	0	0	0	30	3041.29037*	-0.00857	3924.20390	882.90495 †
11	1	-1	0	0	31	0	0	0	0	31	3041.18658	-0.00505	3982.89278	941.70115 †
12	1	-1	0	0	32	0	0	0	0	32	3041.07529	-0.00518	4043.46606	1002.38559 †
13	1	-1	0	0	33	0	0	0	0	33	3040.96023	-0.00521	4105.92291	1064.95747 †
14	1	-1	0	0	34	0	0	0	0	34	3040.84355	-0.00294	4170.26248	1129.41599 †
15	1	-1	0	0	35	0	0	0	0	35	3040.72284	-0.00075	4236.48386	1195.76027
16	1	-1	0	0	36	0	0	0	0	36	3040.59186	-0.00483	4304.58615	1263.98946 †
17	1	-1	0	0	37	0	0	0	0	37	3040.46189	-0.00387	4374.56841	1334.10264 †
18	1	-1	0	0	38	0	0	0	0	38	3040.33119	0.00043	4446.42966	1406.09891

rms = 0.00040 cm⁻¹

$V_3 + V_4 (\Pi) \leftarrow V_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 1 0 0 1	1 1 0 0 2	2529.46605	0.00015	3044.75420	515.28830
1 1 0 0 2	1 1 0 0 3	2527.54122	0.00028	3048.53223	520.99129
1 1 0 0 3	1 1 0 0 4	2525.60427	0.00022	3054.19920	528.59515
1 1 0 0 4	1 1 0 0 5	2523.65552	0.00025	3061.75506	538.09979
1 1 0 0 5	1 1 0 0 6	2521.69471	0.00010	3071.19969	549.50508
1 1 0 0 6	1 1 0 0 7	2519.72227	0.00017	3082.53297	562.81086
1 1 0 0 7	1 1 0 0 8	2517.73803	0.00025	3095.75474	578.01697
1 1 0 0 8	1 1 0 0 9	2515.74192	0.00026	3110.86484	595.12319
1 1 0 0 9	1 1 0 0 10	2513.73391	0.00014	3127.86306	614.12929
1 1 0 0 10	1 1 0 0 11	2511.71437	0.00022	3146.74918	635.03503
1 1 0 0 11	1 1 0 0 12	2509.68294	0.00013	3167.52293	657.84012
1 1 0 0 12	1 1 0 0 13	2507.63993	0.00014	3190.18406	682.54427
1 1 0 0 13	1 1 0 0 14	2505.58520	0.00008	3214.73225	709.14713
1 1 0 0 14	1 1 0 0 15	2503.51889	0.00007	3241.16718	737.64836
1 1 0 0 15	1 1 0 0 16	2501.44103	0.00011	3269.48849	768.04757
1 1 0 0 16	1 1 0 0 17	2499.35150	0.00005	3299.69582	800.34436
1 1 0 0 17	1 1 0 0 18	2497.25044	-0.00001	3331.78875	834.53830
1 1 0 0 18	1 1 0 0 19	2495.13785	-0.00008	3365.76686	870.62893
1 1 0 0 19	1 1 0 0 20	2493.01394	0.00001	3401.62970	908.61577
1 1 0 0 20	1 1 0 0 21	2490.87844	-0.00004	3439.37679	948.49830
1 1 0 0 21	1 1 0 0 22	2488.73163	0.00002	3479.00763	990.27601
1 1 0 0 22	1 1 0 0 23	2486.57342	0.00007	3520.52169	1033.94833
1 1 0 0 23	1 1 0 0 24	2484.40397	0.00024	3563.91841	1079.51468
1 1 0 0 24	1 1 0 0 25	2482.22338	0.00060	3609.19723	1126.97445
1 1 0 0 25	1 1 0 0 26	2480.03151	0.00098	3656.35753	1176.32701
1 1 0 0 26	1 1 0 0 27	2477.82933	0.00232	3705.39870	1227.57169 †
1 1 0 0 27	1 1 0 0 28	2475.61796	0.00571	3756.32007	1280.70782 †
1 1 0 0 28	1 1 0 0 29	2473.40873	0.02244	3809.12097	1335.73468 †
1 1 0 0 29	1 1 0 0 30	2471.11966	-0.02950	3863.80070	1392.65154 †
1 1 0 0 30	1 1 0 0 31	2468.88684	-0.01405	3920.35853	1451.45764 †
1 1 0 0 31	1 1 0 0 32	2466.63014	-0.01136	3978.79371	1512.15220 †
1 1 0 0 32	1 1 0 0 33	2464.36126	-0.00978	4039.10545	1574.73441 †
1 1 0 0 33	1 1 0 0 34	2462.07796	-0.01158	4101.29296	1639.20342 †
1 1 0 0 34	1 1 0 0 35	2459.78677	-0.01026	4165.35541	1705.55838 †
1 1 0 0 35	1 1 0 0 36	2457.48501*	-0.00853	4231.29195	1773.79841 †
1 1 0 0 36	1 1 0 0 37	2455.16815	-0.01095	4299.10169	1843.92260 †
1 1 0 0 37	1 1 0 0 38	2452.84197	-0.01178	4368.78375	1915.93000 †
1 1 0 0 38	1 1 0 0 39	2450.49369*	-0.02384	4440.33718	1989.81965 †
1 1 0 0 39	1 1 0 0 40	2448.15737	-0.01309	4513.76104	2065.59058 †

1	1	1	0	0	2	1	1	0	0	1	2537.04631	0.00035	3048.53223	511.48627
3	1	1	0	0	3	1	1	0	0	2	2538.91099	0.00009	3054.19920	515.28830
4	1	1	0	0	4	1	1	0	0	3	2540.76395	0.00018	3061.75506	520.99129
5	1	1	0	0	5	1	1	0	0	4	2542.60473	0.00019	3071.19969	528.59515
6	1	1	0	0	6	1	1	0	0	5	2544.43343	0.00026	3082.53297	538.09979
7	1	1	0	0	7	1	1	0	0	6	2546.24982	0.00016	3095.75474	549.50508
8	1	1	0	0	8	1	1	0	0	7	2548.05417	0.00019	3110.86484	562.81086
9	1	1	0	0	9	1	1	0	0	8	2549.84629	0.00020	3127.86306	578.01697
10	1	1	0	0	10	1	1	0	0	9	2551.62622	0.00023	3146.74918	595.12319
11	1	1	0	0	11	1	1	0	0	10	2553.39385	0.00021	3167.52293	614.12929
12	1	1	0	0	12	1	1	0	0	11	2555.14910	0.00007	3190.18406	635.03503
13	1	1	0	0	13	1	1	0	0	12	2556.89248	0.00036	3214.73225	657.84012
14	1	1	0	0	14	1	1	0	0	13	2558.62301	0.00010	3241.16718	682.54427
15	1	1	0	0	15	1	1	0	0	14	2560.34142	0.00006	3269.48849	709.14713
16	1	1	0	0	16	1	1	0	0	15	2562.04757	0.00011	3299.69582	737.64836
17	1	1	0	0	17	1	1	0	0	16	2563.74130	0.00012	3331.78875	768.04757
18	1	1	0	0	18	1	1	0	0	17	2565.42247	-0.00003	3365.76686	800.34436
19	1	1	0	0	19	1	1	0	0	18	2567.09142	0.00002	3401.62970	834.53830
20	1	1	0	0	20	1	1	0	0	19	2568.74786	0.00000	3439.37679	870.62893
21	1	1	0	0	21	1	1	0	0	20	2570.39165	-0.00021	3479.00763	908.61577
22	1	1	0	0	22	1	1	0	0	21	2572.02335	-0.00003	3520.52169	948.49830
23	1	1	0	0	23	1	1	0	0	22	2573.64253	0.00013	3563.91841	990.27601
24	1	1	0	0	24	1	1	0	0	23	2575.24929*	0.00039	3609.19723	1033.94833
25	1	1	0	0	25	1	1	0	0	24	2576.84373	0.00088	3656.35753	1079.51468
26	1	1	0	0	26	1	1	0	0	25	2578.42651*	0.00226	3705.39870	1126.97445 †
27	1	1	0	0	27	1	1	0	0	26	2579.99857*	0.00550	3756.32007	1176.32701 †
28	1	1	0	0	28	1	1	0	0	27	2581.57183*	0.02255	3809.12097	1227.57169 †
29	1	1	0	0	29	1	1	0	0	28	2583.06388*	-0.02901	3863.80070	1280.70782 †
30	1	1	0	0	30	1	1	0	0	29	2584.60970*	-0.01415	3920.35853	1335.73468 †
31	1	1	0	0	31	1	1	0	0	30	2586.13081*	-0.01136	3978.79371	1392.65154 †
32	1	1	0	0	32	1	1	0	0	31	2587.63745	-0.01036	4039.10545	1451.45764 †
33	1	1	0	0	33	1	1	0	0	32	2589.13053	-0.01023	4101.29296	1512.15220 †
34	1	1	0	0	34	1	1	0	0	33	2590.61727*	-0.00374	4165.35541	1574.73441 †
35	1	1	0	0	35	1	1	0	0	34	2592.07729	-0.01124	4231.29195	1639.20342 †
36	1	1	0	0	36	1	1	0	0	35	2593.53226	-0.01105	4299.10169	1705.55838 †
37	1	1	0	0	37	1	1	0	0	36	2594.97342	-0.01192	4368.78375	1773.79841 †
38	1	1	0	0	38	1	1	0	0	37	2596.39943*	-0.01516	4440.33718	1843.92260 †
39	1	1	0	0	39	1	1	0	0	38	2597.81850	-0.01255	4513.76104	1915.93000 †
40	1	1	0	0	40	1	1	0	0	39	2599.21634	-0.01836	4589.05436	1989.81965 †
41	1	1	0	0	41	1	1	0	0	40	2600.60989	-0.01565	4666.21612	2065.59058 †
42	1	1	0	0	42	1	1	0	0	41	2601.98830	-0.01524	4745.24531	2143.24177 †
43	1	1	0	0	43	1	1	0	0	42	2603.36147	-0.00721	4826.14087	2222.77219 †
44	1	-1	0	0	1	1	-1	0	0	2	2529.44980	0.00041	3044.76255	515.31316
45	1	-1	0	0	2	1	-1	0	0	3	2527.51643	0.00016	3048.55727	521.04101
46	1	-1	0	0	3	1	-1	0	0	4	2525.57144	0.00016	3054.24930	528.67801
47	1	-1	0	0	4	1	-1	0	0	5	2523.61471	0.00024	3061.83854	538.22407
48	1	-1	0	0	5	1	-1	0	0	6	2521.64602	0.00018	3071.32490	549.67906
49	1	-1	0	0	6	1	-1	0	0	7	2519.66545	0.00002	3082.70824	563.04281
50	1	-1	0	0	7	1	-1	0	0	8	2517.67331	0.00005	3095.98840	578.31514
51	1	-1	0	0	8	1	-1	0	0	9	2515.66937	0.00001	3111.16521	595.49585
52	1	-1	0	0	9	1	-1	0	0	10	2513.65376	0.00000	3128.23845	614.58469
53	1	-1	0	0	10	1	-1	0	0	11	2511.62647	-0.00001	3147.20789	635.58142
54	1	-1	0	0	11	1	-1	0	0	12	2509.58750	-0.00004	3168.07327	658.48573
55	1	-1	0	0	12	1	-1	0	0	13	2507.53700	0.00002	3190.83430	683.29732
56	1	-1	0	0	13	1	-1	0	0	14	2505.47469	-0.00012	3215.49066	710.01584
57	1	-1	0	0	14	1	-1	0	0	15	2503.40108	0.00001	3242.04201	738.64093
58	1	-1	0	0	15	1	-1	0	0	16	2501.31580	0.00001	3270.48799	769.17220
59	1	-1	0	0	16	1	-1	0	0	17	2499.21892	-0.00006	3300.82820	801.60923
60	1	-1	0	0	17	1	-1	0	0	18	2497.11075	0.00008	3333.06223	835.95156
	1	-1	0	0	18	1	-1	0	0	19	2494.99115	0.00026	3367.18964	872.19874
	1	-1	0	0	19	1	-1	0	0	20	2492.86003	0.00036	3403.20994	910.35027
	1	-1	0	0	20	1	-1	0	0	21	2490.71755	0.00052	3441.12265	950.40561
	1	-1	0	0	21	1	-1	0	0	22	2488.56382	0.00082	3480.92723	992.36423
	1	-1	0	0	22	1	-1	0	0	23	2486.39885	0.00125	3522.62315	1036.22555 †
	1	-1	0	0	23	1	-1	0	0	24	2484.22271	0.00185	3566.20982	1081.98896 †

1	1	-1	0	0	24	1	-1	0	0	25	2482.03560	0.00279	3611.68665	1129.65384	+
2	1	-1	0	0	25	1	-1	0	0	26	2479.83799	0.00452	3659.05301	1179.21954	+
3	1	-1	0	0	26	1	-1	0	0	27	2477.63130*	0.00844	3708.30823	1230.68537	+
4	1	-1	0	0	27	1	-1	0	0	28	2475.42674*	0.02572	3759.45166	1284.05064	+
5	1	-1	0	0	28	1	-1	0	0	29	2473.13532*	-0.03264	3812.48257	1339.31460	+
6	1	-1	0	0	29	1	-1	0	0	30	2470.91120*	-0.01252	3867.40023	1396.47651	+
7	1	-1	0	0	30	1	-1	0	0	31	2468.66065	-0.00768	3924.20390	1455.53557	+
8	1	-1	0	0	31	1	-1	0	0	32	2466.39595	-0.00584	3982.89278	1516.49098	+
9	1	-1	0	0	32	1	-1	0	0	33	2464.11955	-0.00461	4043.46606	1579.34190	+
10	1	-1	0	0	33	1	-1	0	0	34	2461.83162	-0.00381	4105.92291	1644.08748	+
11	1	-1	0	0	34	1	-1	0	0	35	2459.53243	-0.00323	4170.26248	1710.72682	+
12	1	-1	0	0	35	1	-1	0	0	36	2457.22232	-0.00253	4236.48386	1779.25901	+
13	1	-1	0	0	36	1	-1	0	0	37	2454.90099	-0.00205	4304.58615	1849.68311	+
14	1	-1	0	0	37	1	-1	0	0	38	2452.56835	-0.00190	4374.56841	1921.99816	+
15	1	-1	0	0	38	1	-1	0	0	39	2450.22618	-0.00032	4446.42966	1996.20316	+
16	1	-1	0	0	39	1	-1	0	0	40	2447.87131	-0.00052	4520.16893	2072.29710	+
17	1	-1	0	0	2	1	-1	0	0	1	2537.06296	0.00024	3048.55727	511.49456	
18	1	-1	0	0	3	1	-1	0	0	2	2538.93632	0.00019	3054.24930	515.31316	
19	1	-1	0	0	4	1	-1	0	0	3	2540.79770	0.00017	3061.83854	521.04101	
20	1	-1	0	0	5	1	-1	0	0	4	2542.64711	0.00023	3071.32490	528.67801	
21	1	-1	0	0	6	1	-1	0	0	5	2544.48426	0.00010	3082.70824	538.22407	
22	1	-1	0	0	7	1	-1	0	0	6	2546.30940	0.00005	3095.98840	549.67906	
23	1	-1	0	0	8	1	-1	0	0	7	2548.12246	0.00005	3111.16521	563.04281	
24	1	-1	0	0	9	1	-1	0	0	8	2549.92327	-0.00004	3128.23845	578.31514	
25	1	-1	0	0	10	1	-1	0	0	9	2551.71207	0.00002	3147.20789	595.49585	
26	1	-1	0	0	11	1	-1	0	0	10	2553.48854	-0.00004	3168.07327	614.58469	
27	1	-1	0	0	12	1	-1	0	0	11	2555.25284	-0.00004	3190.83430	635.58142	
28	1	-1	0	0	13	1	-1	0	0	12	2557.00489	-0.00003	3215.49066	658.48573	
29	1	-1	0	0	15	1	-1	0	0	14	2560.47211	-0.00004	3270.48799	710.01584	
30	1	-1	0	0	16	1	-1	0	0	15	2562.18723	-0.00004	3300.82820	738.64093	
31	1	-1	0	0	17	1	-1	0	0	16	2563.89013	0.00010	3333.06223	769.17220	
32	1	-1	0	0	18	1	-1	0	0	17	2565.58057	0.00016	3367.18964	801.60923	
33	1	-1	0	0	19	1	-1	0	0	18	2567.25857	0.00019	3403.20994	835.95156	
34	1	-1	0	0	20	1	-1	0	0	19	2568.92445	0.00055	3441.12265	872.19874	
35	1	-1	0	0	21	1	-1	0	0	20	2570.57767	0.00070	3480.92723	910.35027	
36	1	-1	0	0	22	1	-1	0	0	21	2572.21975	0.00221	3522.62315	950.40561	+
37	1	-1	0	0	23	1	-1	0	0	22	2573.84729	0.00170	3566.20982	992.36423	+
38	1	-1	0	0	24	1	-1	0	0	23	2575.46378	0.00268	3611.68665	1036.22555	+
39	1	-1	0	0	25	1	-1	0	0	24	2577.06846	0.00442	3659.05301	1081.98896	+
40	1	-1	0	0	26	1	-1	0	0	25	2578.66269	0.00830	3708.30823	1129.65384	+
41	1	-1	0	0	27	1	-1	0	0	26	2580.25775	0.02564	3759.45166	1179.21954	+
42	1	-1	0	0	28	1	-1	0	0	27	2581.76469	-0.03250	3812.48257	1230.68537	+
43	1	-1	0	0	29	1	-1	0	0	28	2583.33759	-0.01200	3867.40023	1284.05064	+
44	1	-1	0	0	30	1	-1	0	0	29	2584.88134	-0.00795	3924.20390	1339.31460	+
45	1	-1	0	0	31	1	-1	0	0	30	2586.41032	-0.00595	3982.89278	1396.47651	+
46	1	-1	0	0	32	1	-1	0	0	31	2587.92562	-0.00487	4043.46606	1455.53557	+
47	1	-1	0	0	33	1	-1	0	0	32	2589.42804	-0.00389	4105.92291	1516.49098	+
48	1	-1	0	0	34	1	-1	0	0	33	2590.91707	-0.00350	4170.26248	1579.34190	+
49	1	-1	0	0	35	1	-1	0	0	34	2592.39352	-0.00286	4236.48386	1644.08748	+
50	1	-1	0	0	36	1	-1	0	0	35	2593.85739	-0.00194	4304.58615	1710.72682	+
51	1	-1	0	0	37	1	-1	0	0	36	2595.30801	-0.00139	4374.56841	1779.25901	+
52	1	-1	0	0	38	1	-1	0	0	37	2596.74592	-0.00063	4446.42966	1849.68311	+
53	1	-1	0	0	39	1	-1	0	0	38	2598.17099	0.00021	4520.16893	1921.99816	+
54	1	-1	0	0	40	1	-1	0	0	39	2599.58253	0.00049	4595.78520	1996.20316	+
55	1	-1	0	0	41	1	-1	0	0	40	2600.98814*	0.00783	4673.27741	2072.29710	+
56	1	-1	0	0	42	1	-1	0	0	41	2602.36747	0.00190	4752.64451	2150.27894	+
57	1	-1	0	0	43	1	-1	0	0	42	2603.74389	0.00610	4833.88539	2230.14760	+
58	1	-1	0	0	44	1	-1	0	0	43	2605.10152	0.00458	4916.99894	2311.90200	+
59	1	1	0	0	1	1	-1	0	0	1	2533.26022	0.00058	3044.75420	511.49456	
60	1	1	0	0	2	1	-1	0	0	2	2533.21975	0.00069	3048.53223	515.31316	
	1	1	0	0	3	1	-1	0	0	3	2533.15837	0.00017	3054.19920	521.04101	
	1	1	0	0	4	1	-1	0	0	4	2533.07717	0.00012	3061.75506	528.67801	
	1	1	0	0	5	1	-1	0	0	5	2532.97553	-0.00009	3071.19969	538.22407	
	1	1	0	0	6	1	-1	0	0	6	2532.85384	-0.00007	3082.53297	549.67906	
	1	1	0	0	7	1	-1	0	0	7	2532.71204	0.00010	3095.75474	563.04281	

1															
2	1	1	0	0	8	1	-1	0	0	8	2532.55046	0.00076	3110.86484	578.31514	
3	1	1	0	0	9	1	-1	0	0	9	2532.36738	0.00017	3127.86306	595.49585	
4	1	1	0	0	10	1	-1	0	0	10	2532.16448	0.00000	3146.74918	614.58469	
5	1	1	0	0	11	1	-1	0	0	11	2531.94161	0.00009	3167.52293	635.58142	
6	1	1	0	0	12	1	-1	0	0	12	2531.69834	0.00001	3190.18406	658.48573	
7	1	1	0	0	13	1	-1	0	0	13	2531.43470	-0.00023	3214.73225	683.29732	
8	1	1	0	0	14	1	-1	0	0	14	2531.15116	-0.00017	3241.16718	710.01584	
9	1	1	0	0	15	1	-1	0	0	15	2530.84753	-0.00003	3269.48849	738.64093	
10	1	1	0	0	16	1	-1	0	0	16	2530.52477*	0.00115	3299.69582	769.17220	†
11	1	1	0	0	17	1	-1	0	0	17	2530.17936	-0.00016	3331.78875	801.60923	
12	1	1	0	0	18	1	-1	0	0	18	2529.81526	-0.00004	3365.76686	835.95156	
13	1	1	0	0	19	1	-1	0	0	19	2529.43524*	0.00428	3401.62970	872.19874	†
14	1	1	0	0	20	1	-1	0	0	20	2529.02673	0.00021	3439.37679	910.35027	
15	1	-1	0	0	1	1	1	0	0	1	2533.27172*	-0.00456	3044.76255	511.48627	†
16	1	-1	0	0	2	1	1	0	0	2	2533.27172*	0.00275	3048.55727	515.28830	†
17	1	-1	0	0	3	1	1	0	0	3	2533.26022*	0.00221	3054.24930	520.99129	†
18	1	-1	0	0	4	1	1	0	0	4	2533.24412	0.00073	3061.83854	528.59515	
19	1	-1	0	0	5	1	1	0	0	5	2533.22480	-0.00031	3071.32490	538.09979	
20	1	-1	0	0	6	1	1	0	0	6	2533.20300	-0.00016	3082.70824	549.50508	
21	1	-1	0	0	7	1	1	0	0	7	2533.17745	-0.00009	3095.98840	562.81086	
22	1	-1	0	0	8	1	1	0	0	8	2533.14796	-0.00029	3111.16521	578.01697	
23	1	-1	0	0	9	1	1	0	0	9	2533.11519	-0.00008	3128.23845	595.12319	
24	1	-1	0	0	10	1	1	0	0	10	2533.07717*	-0.00143	3147.20789	614.12929	†
25	1	-1	0	0	11	1	1	0	0	11	2533.03798	-0.00026	3168.07327	635.03503	
26	1	-1	0	0	12	1	1	0	0	12	2532.99383	-0.00034	3190.83430	657.84012	
27	1	-1	0	0	14	1	1	0	0	14	2532.89478	-0.00010	3242.04201	709.14713	
28	1	-1	0	0	15	1	1	0	0	15	2532.83979	0.00016	3270.48799	737.64836	
29	1	-1	0	0	16	1	1	0	0	16	2532.78019	-0.00044	3300.82820	768.04757	
30	1	-1	0	0	17	1	1	0	0	17	2532.71203*	-0.00584	3333.06223	800.34436	†
31	1	-1	0	0	18	1	1	0	0	18	2532.65098	-0.00036	3367.18964	834.53830	
32	1	-1	0	0	19	1	1	0	0	19	2532.58081	-0.00020	3403.20994	870.62893	
33	1	-1	0	0	20	1	1	0	0	20	2532.50761	0.00073	3441.12265	908.61577	
34	1	-1	0	0	21	1	1	0	0	21	2532.42910	0.00017	3480.92723	948.49830	
35	1	-1	0	0	22	1	1	0	0	22	2532.34750	0.00036	3522.62315	990.27601	

rms = 0.00029 cm⁻¹

$$v_3 + v_4 (\Pi) \leftarrow 2v_4 (\Sigma^+)$$

$v_4' \ell_4' V_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 0 0 2	2 0 0 0 3	2020.22353*	0.00273	3048.53223	1028.31143 †
1 1 0 0 3	2 0 0 0 4	2018.24975	0.00119	3054.19920	1035.95064 †
1 1 0 0 4	2 0 0 0 5	2016.25629	-0.00002	3061.75506	1045.49875
1 1 0 0 5	2 0 0 0 6	2014.24624*	0.00170	3071.19969	1056.95515 †
1 1 0 0 6	2 0 0 0 7	2012.21334	-0.00053	3082.53297	1070.31910
1 1 0 0 7	2 0 0 0 8	2010.16464	-0.00033	3095.75474	1085.58977
1 1 0 0 8	2 0 0 0 9	2008.09913	0.00050	3110.86484	1102.76621
1 1 0 0 9	2 0 0 0 10	2006.01364*	-0.00204	3127.86306	1121.84738 †
1 1 0 0 10	2 0 0 0 11	2003.91811	0.00110	3146.74918	1142.83216 †
1 1 0 0 11	2 0 0 0 12	2001.80402	0.00044	3167.52293	1165.71936
1 1 0 0 12	2 0 0 0 13	1999.67639	0.00007	3190.18406	1190.50774
1 1 0 0 13	2 0 0 0 14	1997.53538	-0.00081	3214.73225	1217.19606
1 1 0 0 14	2 0 0 0 15	1995.38372	-0.00038	3241.16718	1245.78308
1 1 0 0 15	2 0 0 0 16	1993.22094	0.00005	3269.48849	1276.26760
1 1 0 0 16	2 0 0 0 17	1991.04694	-0.00039	3299.69582	1308.64848
1 1 0 0 17	2 0 0 0 18	1988.86418	0.00009	3331.78875	1342.92466
1 1 0 0 18	2 0 0 0 19	1986.67183	0.00011	3365.76686	1379.09514
1 1 0 0 19	2 0 0 0 20	1984.46985	-0.00079	3401.62970	1417.15906
1 1 0 0 20	2 0 0 0 21	1982.26067	-0.00052	3439.37679	1457.11560
1 1 0 0 21	2 0 0 0 22	1980.04358	0.00002	3479.00763	1498.96407
1 1 0 0 22	2 0 0 0 23	1977.81813	0.00025	3520.52169	1542.70381
1 1 0 0 23	2 0 0 0 24	1975.58466*	0.00048	3563.91841	1588.33424

1														
2	1	1	0	0	1	2	0	0	0	0	2027.90186	-0.00095	3044.75420	1016.85139
3	1	1	0	0	2	2	0	0	0	1	2029.77225*	0.00152	3048.53223	1018.76149 †
4	1	1	0	0	3	2	0	0	0	2	2031.61712	-0.00050	3054.19920	1022.58159
5	1	1	0	0	4	2	0	0	0	3	2033.44500*	0.00137	3061.75506	1028.31143 †
6	1	1	0	0	5	2	0	0	0	4	2035.24882	-0.00022	3071.19969	1035.95064
7	1	1	0	0	6	2	0	0	0	5	2037.03396	-0.00025	3082.53297	1045.49875
8	1	1	0	0	7	2	0	0	0	6	2038.79903	-0.00057	3095.75474	1056.95515
9	1	1	0	0	8	2	0	0	0	7	2040.54677	0.00103	3110.86484	1070.31910 †
10	1	1	0	0	9	2	0	0	0	8	2042.27357	0.00028	3127.86306	1085.58977
11	1	1	0	0	10	2	0	0	0	9	2043.98298	0.00002	3146.74918	1102.76621
12	1	1	0	0	11	2	0	0	0	10	2045.67570	0.00015	3167.52293	1121.84738
13	1	1	0	0	12	2	0	0	0	11	2047.35168	-0.00022	3190.18406	1142.83216
14	1	1	0	0	13	2	0	0	0	12	2049.01310	0.00021	3214.73225	1165.71936
15	1	1	0	0	14	2	0	0	0	13	2050.66030	0.00086	3241.16718	1190.50774
16	1	1	0	0	15	2	0	0	0	14	2052.29291	0.00048	3269.48849	1217.19606
17	1	1	0	0	16	2	0	0	0	15	2053.91352	0.00078	3299.69582	1245.78308
18	1	1	0	0	17	2	0	0	0	16	2055.52063	-0.00051	3331.78875	1276.26760
19	1	1	0	0	18	2	0	0	0	17	2057.11872	0.00034	3365.76686	1308.64848
20	1	1	0	0	19	2	0	0	0	18	2058.70534	0.00030	3401.62970	1342.92466
21	1	1	0	0	20	2	0	0	0	19	2060.28100	-0.00065	3439.37679	1379.09514
22	1	1	0	0	21	2	0	0	0	20	2061.84786	-0.00071	3479.00763	1417.15906
23	1	1	0	0	22	2	0	0	0	21	2063.40610	0.00002	3520.52169	1457.11560
24	1	1	0	0	23	2	0	0	0	22	2064.95510*	0.00075	3563.91841	1498.96407
25	1	1	0	0	24	2	0	0	0	23	2066.49433*	0.00091	3609.19723	1542.70381
26	1	-1	0	0	1	2	0	0	0	1	2026.00112	0.00007	3044.76255	1018.76149
27	1	-1	0	0	2	2	0	0	0	2	2025.97575	0.00007	3048.55727	1022.58159
28	1	-1	0	0	3	2	0	0	0	3	2025.93725	-0.00062	3054.24930	1028.31143
29	1	-1	0	0	4	2	0	0	0	4	2025.88785	-0.00005	3061.83854	1035.95064
30	1	-1	0	0	5	2	0	0	0	5	2025.82596	-0.00018	3071.32490	1045.49875
31	1	-1	0	0	6	2	0	0	0	6	2025.75251	-0.00058	3082.70824	1056.95515
32	1	-1	0	0	7	2	0	0	0	7	2025.66875	-0.00056	3095.98840	1070.31910
33	1	-1	0	0	8	2	0	0	0	8	2025.57576	0.00032	3111.16521	1085.58977
34	1	-1	0	0	9	2	0	0	0	9	2025.47213	-0.00011	3128.23845	1102.76621
35	1	-1	0	0	10	2	0	0	0	10	2025.36113	0.00062	3147.20789	1121.84738
36	1	-1	0	0	11	2	0	0	0	11	2025.24150	0.00039	3168.07327	1142.83216
37	1	-1	0	0	12	2	0	0	0	12	2025.11430	-0.00064	3190.83430	1165.71936
38	1	-1	0	0	13	2	0	0	0	13	2024.98281	-0.00011	3215.49066	1190.50774
39	1	-1	0	0	14	2	0	0	0	14	2024.84609	0.00014	3242.04201	1217.19606
40	1	-1	0	0	15	2	0	0	0	15	2024.70516	0.00025	3270.48799	1245.78308
41	1	-1	0	0	16	2	0	0	0	16	2024.55870*	-0.00190	3300.82820	1276.26760 †
42	1	-1	0	0	17	2	0	0	0	17	2024.41482*	0.00107	3333.06223	1308.64848 †
43	1	-1	0	0	18	2	0	0	0	18	2024.26567	0.00069	3367.18964	1342.92466
44	1	-1	0	0	19	2	0	0	0	19	2024.11713*	0.00233	3403.20994	1379.09514 †
45	1	-1	0	0	20	2	0	0	0	20	2023.96280	-0.00079	3441.12265	1417.15906

rms = 0.00046 cm⁻¹

$v_3 + v_4 (\Pi) \leftarrow 2v_4 (\Delta)$

53	$v_4' \ell_4' V_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
54	1 1 0 0 1	2 2 0 0 2	2017.77234	-0.00092	3044.75420	1026.98094
55	1 1 0 0 2	2 2 0 0 3	2015.82177	-0.00073	3048.53223	1032.70973
56	1 1 0 0 3	2 2 0 0 4	2013.85060	-0.00017	3054.19920	1040.34843
57	1 1 0 0 4	2 2 0 0 5	2011.85879*	0.00106	3061.75506	1049.89732 †
58	1 1 0 0 5	2 2 0 0 6	2009.84229	-0.00065	3071.19969	1061.35675
59	1 1 0 0 6	2 2 0 0 7	2007.80584	-0.00001	3082.53297	1074.72712
60	1 1 0 0 7	2 2 0 0 8	2005.74647	0.00062	3095.75474	1090.00889
	1 1 0 0 8	2 2 0 0 9	2003.66250	0.00025	3110.86484	1107.20259
	1 1 0 0 9	2 2 0 0 10	2001.55389	-0.00038	3127.86306	1126.30879
	1 1 0 0 10	2 2 0 0 11	1999.42160	0.00050	3146.74918	1147.32807
	1 1 0 0 11	2 2 0 0 12	1997.26242	0.00054	3167.52293	1170.26105

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1														
2	1	1	0	0	2	2	-2	0	0	2	2021.55173	0.00035	3048.53223	1026.98084
3	1	1	0	0	3	2	-2	0	0	3	2021.48981	-0.00014	3054.19920	1032.70925
4	1	1	0	0	4	2	-2	0	0	4	2021.40851	0.00046	3061.75506	1040.34700
5	1	1	0	0	5	2	-2	0	0	5	2021.30507	-0.00062	3071.19969	1049.89400
6	1	1	0	0	6	2	-2	0	0	6	2021.18300	0.00013	3082.53297	1061.35010
7	1	1	0	0	7	2	-2	0	0	7	2021.03714*	-0.00246	3095.75474	1074.71514 +
8	1	1	0	0	8	2	-2	0	0	8	2020.87648	0.00059	3110.86484	1089.98896
9	1	1	0	0	9	2	-2	0	0	9	2020.69161	-0.00013	3127.86306	1107.17132
10	1	1	0	0	10	2	-2	0	0	10	2020.48766	0.00048	3146.74918	1126.26199
11	1	1	0	0	11	2	-2	0	0	11	2020.26250	0.00028	3167.52293	1147.26072
12	1	1	0	0	12	2	-2	0	0	12	2020.01733	0.00047	3190.18406	1170.16720
13	1	1	0	0	13	2	-2	0	0	13	2019.75158	0.00045	3214.73225	1194.98112
14	1	1	0	0	14	2	-2	0	0	14	2019.46514	0.00010	3241.16718	1221.70214
15	1	1	0	0	15	2	-2	0	0	15	2019.15832	-0.00029	3269.48849	1250.32988
16	1	1	0	0	16	2	-2	0	0	16	2018.83248	0.00062	3299.69582	1280.86395
17	1	1	0	0	17	2	-2	0	0	17	2018.48447	-0.00035	3331.78875	1313.30393
18	1	1	0	0	18	2	-2	0	0	18	2018.11786	0.00036	3365.76686	1347.64936
19	1	1	0	0	19	2	-2	0	0	19	2017.72964	-0.00029	3401.62970	1383.89977
20	1	1	0	0	20	2	-2	0	0	20	2017.32216	0.00003	3439.37679	1422.05465
21	1	1	0	0	21	2	-2	0	0	21	2016.89454	0.00040	3479.00763	1462.11349
22	1	1	0	0	22	2	-2	0	0	22	2016.44642	0.00045	3520.52169	1504.07572
23	1	1	0	0	23	2	-2	0	0	23	2015.97773*	0.00007	3563.91841	1547.94075

rms = 0.00045 cm⁻¹

$v_3 + v_5 (\Pi) \leftarrow v_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 1 1	0 0 1 1 2	2541.04230	0.00037	3220.97760	679.93567
0 0 1 1 2	0 0 1 1 3	2539.11759	-0.00004	3224.75256	685.63493
0 0 1 1 3	0 0 1 1 4	2537.18115	0.00003	3230.41494	693.23382
0 0 1 1 4	0 0 1 1 5	2535.23240	-0.00001	3237.96465	702.73224
0 0 1 1 5	0 0 1 1 6	2533.27172	0.00018	3247.40161	714.13007
0 0 1 1 6	0 0 1 1 7	2531.29858	0.00006	3258.72568	727.42716
0 0 1 1 7	0 0 1 1 8	2529.31343	0.00004	3271.93672	742.62333
0 0 1 1 8	0 0 1 1 9	2527.31614	-0.00003	3287.03456	759.71839
0 0 1 1 9	0 0 1 1 10	2525.30694	0.00005	3304.01898	778.71209
0 0 1 1 10	0 0 1 1 11	2523.28559	0.00001	3322.88978	799.60420
0 0 1 1 11	0 0 1 1 12	2521.25223	-0.00002	3343.64669	822.39444
0 0 1 1 12	0 0 1 1 13	2519.20696	0.00002	3366.28945	847.08251
0 0 1 1 13	0 0 1 1 14	2517.14967	-0.00001	3390.81775	873.66808
0 0 1 1 14	0 0 1 1 15	2515.08041	-0.00007	3417.23128	902.15079
0 0 1 1 15	0 0 1 1 16	2512.99949	0.00010	3445.52967	932.53028
0 0 1 1 16	0 0 1 1 17	2510.90618	-0.00024	3475.71256	964.80614
0 0 1 1 17	0 0 1 1 18	2508.80148	-0.00013	3507.77955	998.97795
0 0 1 1 18	0 0 1 1 19	2506.68502	0.00005	3541.73021	1035.04524
0 0 1 1 19	0 0 1 1 20	2504.55663	0.00008	3577.56410	1073.00756
0 0 1 1 20	0 0 1 1 21	2502.41645	0.00009	3615.28074	1112.86438
0 0 1 1 21	0 0 1 1 22	2500.26438	-0.00005	3654.87963	1154.61520
0 0 1 1 22	0 0 1 1 23	2498.10075	-0.00005	3696.36025	1198.25945
0 0 1 1 23	0 0 1 1 24	2495.92577	0.00028	3739.72206	1243.79656
0 0 1 1 24	0 0 1 1 25	2493.73889	0.00036	3784.96447	1291.22593
0 0 1 1 25	0 0 1 1 26	2491.54030	0.00035	3832.08688	1340.54693
0 0 1 1 26	0 0 1 1 27	2489.33008	0.00030	3881.08869	1391.75891
0 0 1 1 27	0 0 1 1 28	2487.10813	0.00009	3931.96923	1444.86119
0 0 1 1 28	0 0 1 1 29	2484.87527	0.00050	3984.72784	1499.85307
0 0 1 1 29	0 0 1 1 30	2482.63045	0.00046	4039.36382	1556.73383
0 0 1 1 30	0 0 1 1 31	2480.37391	0.00018	4095.87644	1615.50271
0 0 1 1 31	0 0 1 1 32	2478.10652	0.00049	4154.26497	1676.15894
0 0 1 1 32	0 0 1 1 33	2475.82656	-0.00035	4214.52862	1738.70171
0 0 1 1 33	0 0 1 1 34	2473.53633	-0.00008	4276.66660	1803.13019
0 0 1 1 34	0 0 1 1 35	2471.23280*	-0.00174	4340.67809	1869.44355 †

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1	0	0	1	-1	20	0	0	1	-1	21	2502.26669	0.00017	3616.63310	1114.36658
2	0	0	1	-1	21	0	0	1	-1	22	2500.10684	0.00003	3656.36683	1156.26002
3	0	0	1	-1	22	0	0	1	-1	23	2497.93543	0.00009	3697.98865	1200.05331
4	0	0	1	-1	23	0	0	1	-1	24	2495.75234	0.00020	3741.49798	1245.74584
5	0	0	1	-1	24	0	0	1	-1	25	2493.55740	0.00017	3786.89424	1293.33701
6	0	0	1	-1	25	0	0	1	-1	26	2491.35069	0.00005	3834.17682	1342.82618
7	0	0	1	-1	26	0	0	1	-1	27	2489.13270	0.00030	3883.34509	1394.21269
8	0	0	1	-1	27	0	0	1	-1	28	2486.90231	-0.00024	3934.39839	1447.49584
9	0	0	1	-1	28	0	0	1	-1	29	2484.66138	0.00028	3987.33602	1502.67492
10	0	0	1	-1	29	0	0	1	-1	30	2482.40851	0.00042	4042.15729	1559.74920
11	0	0	1	-1	30	0	0	1	-1	31	2480.14391	0.00035	4098.86145	1618.71789
12	0	0	1	-1	31	0	0	1	-1	32	2477.86662	-0.00090	4157.44774	1679.58023
13	0	0	1	-1	32	0	0	1	-1	33	2475.57991	-0.00010	4217.91538	1742.33538
14	0	0	1	-1	33	0	0	1	-1	34	2473.28049	-0.00057	4280.26356	1806.98250
15	0	0	1	-1	34	0	0	1	-1	35	2470.97062	-0.00007	4344.49143	1873.52074
16	0	0	1	-1	35	0	0	1	-1	36	2468.64856	-0.00039	4410.59813	1941.94919
17	0	0	1	-1	36	0	0	1	-1	37	2466.31526	-0.00059	4478.58279	2012.26694
18	0	0	1	-1	37	0	0	1	-1	38	2463.97181	0.00038	4548.44447	2084.47304
19	0	0	1	-1	38	0	0	1	-1	39	2461.61549	-0.00023	4620.18226	2158.56653
20	0	0	1	-1	39	0	0	1	-1	40	2459.24833	-0.00043	4693.79518	2234.54642
21	0	0	1	-1	2	0	0	1	-1	1	2548.62934	0.00006	3224.77193	676.14265
22	0	0	1	-1	3	0	0	1	-1	2	2550.49842	-0.00002	3230.45367	679.95524
23	0	0	1	-1	4	0	0	1	-1	3	2552.35526	0.00010	3238.02921	685.67405
24	0	0	1	-1	5	0	0	1	-1	4	2554.19945	0.00003	3247.49844	693.29902
25	0	0	1	-1	6	0	0	1	-1	5	2556.03125	0.00005	3258.86124	702.83004
26	0	0	1	-1	7	0	0	1	-1	6	2557.85041	-0.00006	3272.11745	714.26698
27	0	0	1	-1	8	0	0	1	-1	7	2559.65722	0.00002	3287.26689	727.60969
28	0	0	1	-1	9	0	0	1	-1	8	2561.45135	-0.00003	3304.30937	742.85799
29	0	0	1	-1	10	0	0	1	-1	9	2563.23305	0.00008	3323.24465	760.01168
30	0	0	1	-1	11	0	0	1	-1	10	2565.00199	0.00003	3344.07248	779.07052
31	0	0	1	-1	12	0	0	1	-1	11	2566.75838	0.00006	3366.79258	800.03426
32	0	0	1	-1	13	0	0	1	-1	12	2568.50201	-0.00002	3391.40464	822.90261
33	0	0	1	-1	14	0	0	1	-1	13	2570.23314	0.00009	3417.90834	847.67528
34	0	0	1	-1	15	0	0	1	-1	14	2571.95140	0.00002	3446.30331	874.35193
35	0	0	1	-1	16	0	0	1	-1	15	2573.65707	0.00009	3476.58918	902.93220
36	0	0	1	-1	17	0	0	1	-1	16	2575.34991	0.00008	3508.76554	933.41570
37	0	0	1	-1	18	0	0	1	-1	17	2577.02999	0.00008	3542.83195	965.80204
38	0	0	1	-1	19	0	0	1	-1	18	2578.69720	0.00000	3578.78796	1000.09076
39	0	0	1	-1	20	0	0	1	-1	19	2580.35166	-0.00001	3616.63310	1036.28142
40	0	0	1	-1	21	0	0	1	-1	20	2581.99331	0.00001	3656.36683	1074.37353
41	0	0	1	-1	22	0	0	1	-1	21	2583.62214	0.00007	3697.98865	1114.36658
42	0	0	1	-1	23	0	0	1	-1	22	2585.23806	0.00011	3741.49798	1156.26002
43	0	0	1	-1	24	0	0	1	-1	23	2586.84088	-0.00005	3786.89424	1200.05331
44	0	0	1	-1	25	0	0	1	-1	24	2588.43105	0.00007	3834.17682	1245.74584
45	0	0	1	-1	26	0	0	1	-1	25	2590.00839	0.00031	3883.34509	1293.33701
46	0	0	1	-1	27	0	0	1	-1	26	2591.57245	0.00025	3934.39839	1342.82618
47	0	0	1	-1	28	0	0	1	-1	27	2593.12327	-0.00006	3987.33602	1394.21269
48	0	0	1	-1	29	0	0	1	-1	28	2594.66180	0.00035	4042.15729	1447.49584
49	0	0	1	-1	30	0	0	1	-1	29	2596.18683	0.00030	4098.86145	1502.67492
50	0	0	1	-1	31	0	0	1	-1	30	2597.69827	-0.00028	4157.44774	1559.74920
51	0	0	1	-1	32	0	0	1	-1	31	2599.19704	-0.00045	4217.91538	1618.71789
52	0	0	1	-1	33	0	0	1	-1	32	2600.68321	-0.00012	4280.26356	1679.58023
53	0	0	1	-1	34	0	0	1	-1	33	2602.15592	-0.00013	4344.49143	1742.33538
54	0	0	1	-1	35	0	0	1	-1	34	2603.61551	-0.00012	4410.59813	1806.98250
55	0	0	1	-1	36	0	0	1	-1	35	2605.06203	-0.00002	4478.58279	1873.52074
56	0	0	1	-1	37	0	0	1	-1	36	2606.49554	0.00025	4548.44447	1941.94919
57	0	0	1	-1	38	0	0	1	-1	37	2607.91537	0.00005	4620.18226	2012.26694
58	0	0	1	-1	39	0	0	1	-1	38	2609.32275	0.00061	4693.79518	2084.47304
59	0	0	1	-1	40	0	0	1	-1	39	2610.71597	0.00026	4769.28224	2158.56653
60	0	0	1	-1	41	0	0	1	-1	40	2612.09613	0.00011	4846.64244	2234.54642
	0	0	1	-1	42	0	0	1	-1	41	2613.46307	0.00002	4925.87473	2312.41168
	0	0	1	1	1	0	0	1	-1	1	2544.83497	0.00002	3220.97760	676.14265
	0	0	1	1	2	0	0	1	-1	2	2544.79623*	-0.00110	3224.75256	679.95524
	0	0	1	1	3	0	0	1	-1	3	2544.74107	0.00019	3230.41494	685.67405
	0	0	1	1	4	0	0	1	-1	4	2544.66533	-0.00030	3237.96465	693.29902

1														
2	0	0	1	1	5	0	0	1	-1	5	2544.57182	0.00025	3247.40161	702.83004
3	0	0	1	1	6	0	0	1	-1	6	2544.45844	-0.00026	3258.72568	714.26698
4	0	0	1	1	7	0	0	1	-1	7	2544.32624*	-0.00079	3271.93672	727.60969
5	0	0	1	1	8	0	0	1	-1	8	2544.17652	-0.00005	3287.03456	742.85799
6	0	0	1	1	9	0	0	1	-1	9	2544.00708	-0.00023	3304.01898	760.01168
7	0	0	1	1	10	0	0	1	-1	10	2543.81884	-0.00042	3322.88978	779.07052
8	0	0	1	1	11	0	0	1	-1	11	2543.61203	-0.00041	3343.64669	800.03426
9	0	0	1	1	12	0	0	1	-1	12	2543.38653	-0.00031	3366.28945	822.90261
10	0	0	1	1	13	0	0	1	-1	13	2543.14213	-0.00034	3390.81775	847.67528
11	0	0	1	1	14	0	0	1	-1	14	2542.87872	-0.00063	3417.23128	874.35193
12	0	0	1	1	16	0	0	1	-1	16	2542.29687	0.00001	3475.71256	933.41570
13	0	0	1	1	17	0	0	1	-1	17	2541.97750	-0.00001	3507.77955	965.80204
14	0	0	1	1	18	0	0	1	-1	18	2541.63935	-0.00010	3541.73021	1000.09076
15	0	0	1	1	19	0	0	1	-1	19	2541.28292	0.00024	3577.56410	1036.28142
16	0	0	1	1	20	0	0	1	-1	20	2540.90704	-0.00017	3615.28074	1074.37353
17	0	0	1	-1	1	0	0	1	1	1	2544.84756	-0.00037	3220.98406	676.13613
18	0	0	1	-1	2	0	0	1	1	2	2544.83479*	-0.00147	3224.77193	679.93567 †
19	0	0	1	-1	3	0	0	1	1	3	2544.81830	-0.00044	3230.45367	685.63493
20	0	0	1	-1	4	0	0	1	1	4	2544.79623	0.00084	3238.02921	693.23382
21	0	0	1	-1	5	0	0	1	1	5	2544.76562	-0.00058	3247.49844	702.73224
22	0	0	1	-1	6	0	0	1	1	6	2544.73285*	0.00169	3258.86124	714.13007 †
23	0	0	1	-1	7	0	0	1	1	7	2544.69007	-0.00021	3272.11745	727.42716
24	0	0	1	-1	8	0	0	1	1	8	2544.64390*	0.00034	3287.26689	742.62333
25	0	0	1	-1	9	0	0	1	1	9	2544.59002	-0.00096	3304.30937	759.71839
26	0	0	1	-1	10	0	0	1	1	10	2544.53267	0.00011	3323.24465	778.71209
27	0	0	1	-1	11	0	0	1	1	11	2544.45843*	-0.000984	3344.07248	799.60420 †
28	0	0	1	-1	12	0	0	1	1	12	2544.39791	-0.00022	3366.79258	822.39444
29	0	0	1	-1	13	0	0	1	1	13	2544.32252	0.00039	3391.40464	847.08251
30	0	0	1	-1	14	0	0	1	1	14	2544.23971	-0.00055	3417.90834	873.66808
31	0	0	1	-1	15	0	0	1	1	15	2544.15295	0.00043	3446.30331	902.15079
32	0	0	1	-1	16	0	0	1	1	16	2544.05887	-0.00003	3476.58918	932.53028
33	0	0	1	-1	17	0	0	1	1	17	2543.95898	-0.00041	3508.76554	964.80614
34	0	0	1	-1	18	0	0	1	1	18	2543.85405	0.00005	3542.83195	998.97795
35	0	0	1	-1	19	0	0	1	1	19	2543.74345	0.00073	3578.78796	1035.04524

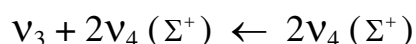
rms = 0.00028 cm⁻¹

$v_3 + 2v_4 (\Sigma^+) \leftarrow v_4 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 0 0 0 1	1 1 0 0 2	3022.51917*	-0.00170	3537.80917	515.28830 †
2 0 0 0 2	1 1 0 0 3	3020.61506	0.00046	3541.60589	520.99129
2 0 0 0 3	1 1 0 0 4	3018.70552	0.00001	3547.30067	528.59515
2 0 0 0 4	1 1 0 0 5	3016.79327	-0.00006	3554.89312	538.09979
2 0 0 0 5	1 1 0 0 6	3014.87738	-0.00032	3564.38277	549.50508
2 0 0 0 6	1 1 0 0 7	3012.95814	0.00000	3575.76900	562.81086
2 0 0 0 7	1 1 0 0 8	3011.03495	0.00084	3589.05108	578.01697
2 0 0 0 8	1 1 0 0 9	3009.10360	-0.00136	3604.22815	595.12319 †
2 0 0 0 9	1 1 0 0 10	3007.17044	0.00047	3621.29926	614.12929
2 0 0 0 10	1 1 0 0 11	3005.22855	0.00022	3640.26336	635.03503
2 0 0 0 11	1 1 0 0 12	3003.27984	0.00064	3661.11932	657.84012
2 0 0 0 12	1 1 0 0 13	3001.32196	0.00028	3683.86594	682.54427
2 0 0 0 13	1 1 0 0 14	2999.35557	0.00071	3708.50199	709.14713
2 0 0 0 14	1 1 0 0 15	2997.37747	-0.00037	3735.02620	737.64836
2 0 0 0 15	1 1 0 0 16	2995.38992	0.00014	3763.43735	768.04757
2 0 0 0 16	1 1 0 0 17	2993.39021	0.00034	3793.73423	800.34436
2 0 0 0 17	1 1 0 0 18	2991.37768	0.00028	3825.91570	834.53830
2 0 0 0 18	1 1 0 0 19	2989.35224	0.00046	3859.98070	870.62893
2 0 0 0 19	1 1 0 0 20	2987.31238	-0.00013	3895.92827	908.61577
2 0 0 0 20	1 1 0 0 21	2985.25883	-0.00040	3933.75753	948.49830
2 0 0 0 21	1 1 0 0 22	2983.19114	-0.00055	3973.46770	990.27601
2 0 0 0 22	1 1 0 0 23	2981.10888	-0.00087	4015.05808	1033.94833

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

1	2	0	0	0	23	1	1	0	0	24	2979.01330	-0.00006	4058.52804	1079.51468
2	2	0	0	0	2	1	1	0	0	1	3030.11997*	0.00035	3541.60589	511.48627
3	2	0	0	0	3	1	1	0	0	2	3032.01163	-0.00073	3547.30067	515.28830
4	2	0	0	0	4	1	1	0	0	3	3033.90159	-0.00025	3554.89312	520.99129
5	2	0	0	0	5	1	1	0	0	4	3035.78870	0.00108	3564.38277	528.59515 +
6	2	0	0	0	6	1	1	0	0	5	3037.66937	0.00016	3575.76900	538.09979
7	2	0	0	0	7	1	1	0	0	6	3039.54756*	0.00156	3589.05108	549.50508 +
8	2	0	0	0	8	1	1	0	0	7	3041.41642	-0.00086	3604.22815	562.81086
9	2	0	0	0	9	1	1	0	0	8	3043.28246	0.00017	3621.29926	578.01697
10	2	0	0	0	10	1	1	0	0	9	3045.13929	-0.00089	3640.26336	595.12319
11	2	0	0	0	11	1	1	0	0	10	3046.99065	0.00062	3661.11932	614.12929
12	2	0	0	0	12	1	1	0	0	11	3048.83199*	0.00108	3683.86594	635.03503 +
13	2	0	0	0	13	1	1	0	0	12	3050.66163	-0.00023	3708.50199	657.84012
14	2	0	0	0	14	1	1	0	0	13	3052.48229	0.00036	3735.02620	682.54427
15	2	0	0	0	15	1	1	0	0	14	3054.29038	0.00016	3763.43735	709.14713
16	2	0	0	0	16	1	1	0	0	15	3056.08529	-0.00058	3793.73423	737.64836
17	2	0	0	0	17	1	1	0	0	16	3057.86861	0.00048	3825.91570	768.04757
18	2	0	0	0	18	1	1	0	0	17	3059.63600*	-0.00034	3859.98070	800.34436
19	2	0	0	0	19	1	1	0	0	18	3061.38990	-0.00007	3895.92827	834.53830
20	2	0	0	0	20	1	1	0	0	19	3063.12857	-0.00004	3933.75753	870.62893
21	2	0	0	0	1	1	-1	0	0	1	3026.31581*	0.00119	3537.80917	511.49456 +
22	2	0	0	0	2	1	-1	0	0	2	3026.29327*	0.00054	3541.60589	515.31316
23	2	0	0	0	3	1	-1	0	0	3	3026.25931	-0.00035	3547.30067	521.04101
24	2	0	0	0	4	1	-1	0	0	4	3026.21526	0.00015	3554.89312	528.67801
25	2	0	0	0	5	1	-1	0	0	5	3026.15922	0.00052	3564.38277	538.22407
26	2	0	0	0	6	1	-1	0	0	6	3026.08982*	-0.00013	3575.76900	549.67906
27	2	0	0	0	7	1	-1	0	0	7	3026.00828	0.00001	3589.05108	563.04281
28	2	0	0	0	8	1	-1	0	0	8	3025.91338	0.00037	3604.22815	578.31514
29	2	0	0	0	9	1	-1	0	0	9	3025.80358	0.00017	3621.29926	595.49585
30	2	0	0	0	10	1	-1	0	0	10	3025.67929*	0.00062	3640.26336	614.58469
31	2	0	0	0	11	1	-1	0	0	11	3025.53761	-0.00030	3661.11932	635.58142
32	2	0	0	0	12	1	-1	0	0	12	3025.38025	0.00004	3683.86594	658.48573
33	2	0	0	0	13	1	-1	0	0	13	3025.20497	0.00030	3708.50199	683.29732
34	2	0	0	0	14	1	-1	0	0	14	3025.01076	0.00040	3735.02620	710.01584
35	2	0	0	0	15	1	-1	0	0	15	3024.79642	0.00001	3763.43735	738.64093
36	2	0	0	0	16	1	-1	0	0	16	3024.56251*	0.00048	3793.73423	769.17220
37	2	0	0	0	17	1	-1	0	0	17	3024.30677	0.00030	3825.91570	801.60923
38	2	0	0	0	18	1	-1	0	0	18	3024.02951	0.00037	3859.98070	835.95156

$$\text{rms} = 0.00042 \text{ cm}^{-1}$$


v_4'	ℓ_4'	v_5'	ℓ_5'	J'	v_4''	ℓ_4''	v_5''	ℓ_5''	J''	OBS	OBS – CALC	E'	E''
2	0	0	0	0	2	0	0	0	1	2517.14875	-0.00051	3535.91075	1018.76149
2	0	0	0	1	2	0	0	0	2	2515.22764	0.00006	3537.80917	1022.58159
2	0	0	0	2	2	0	0	0	3	2513.29674*	0.00228	3541.60589	1028.31143
2	0	0	0	3	2	0	0	0	4	2511.35028	0.00026	3547.30067	1035.95064
2	0	0	0	4	2	0	0	0	5	2509.39541*	0.00104	3554.89312	1045.49875
2	0	0	0	5	2	0	0	0	6	2507.42899	0.00136	3564.38277	1056.95515
2	0	0	0	6	2	0	0	0	7	2505.45012	0.00021	3575.76900	1070.31910
2	0	0	0	7	2	0	0	0	8	2503.45932*	-0.00199	3589.05108	1085.58977
2	0	0	0	8	2	0	0	0	9	2501.46160	-0.00034	3604.22815	1102.76621
2	0	0	0	9	2	0	0	0	10	2499.44928*	-0.00260	3621.29926	1121.84738
2	0	0	0	10	2	0	0	0	11	2497.43179	0.00059	3640.26336	1142.83216
2	0	0	0	11	2	0	0	0	12	2495.40009	0.00012	3661.11932	1165.71936
2	0	0	0	12	2	0	0	0	13	2493.35836	0.00016	3683.86594	1190.50774
2	0	0	0	13	2	0	0	0	14	2491.30576	-0.00017	3708.50199	1217.19606
2	0	0	0	14	2	0	0	0	15	2489.24295	-0.00017	3735.02620	1245.78308
2	0	0	0	15	2	0	0	0	16	2487.16989	0.00015	3763.43735	1276.26760
2	0	0	0	16	2	0	0	0	17	2485.08575	0.00001	3793.73423	1308.64848
2	0	0	0	17	2	0	0	0	18	2482.99111	0.00007	3825.91570	1342.92466

1														
2	2	0	0	0	18	2	0	0	0	19	2480.88513	-0.00043	3859.98070	1379.09514
3	2	0	0	0	19	2	0	0	0	20	2478.76909	-0.00013	3895.92827	1417.15906
4	2	0	0	0	20	2	0	0	0	21	2476.64155	-0.00038	3933.75753	1457.11560
5	2	0	0	0	21	2	0	0	0	22	2474.50343	-0.00021	3973.46770	1498.96407
6	2	0	0	0	22	2	0	0	0	23	2472.35380	-0.00047	4015.05808	1542.70381
7	2	0	0	0	23	2	0	0	0	24	2470.19384	0.00004	4058.52804	1588.33424
8	2	0	0	0	24	2	0	0	0	25	2468.02195	-0.00025	4103.87700	1635.85480
9	2	0	0	0	25	2	0	0	0	26	2465.83911	-0.00035	4151.10444	1685.26498
10	2	0	0	0	1	2	0	0	0	0	2520.95736	-0.00043	3537.80917	1016.85139
11	2	0	0	0	2	2	0	0	0	1	2522.84427	-0.00013	3541.60589	1018.76149
12	2	0	0	0	3	2	0	0	0	2	2524.71790*	-0.00118	3547.30067	1022.58159 †
13	2	0	0	0	4	2	0	0	0	3	2526.58354*	0.00184	3554.89312	1028.31143 †
14	2	0	0	0	5	2	0	0	0	4	2528.43150*	-0.00063	3564.38277	1035.95064
15	2	0	0	0	6	2	0	0	0	5	2530.26959*	-0.00066	3575.76900	1045.49875
16	2	0	0	0	7	2	0	0	0	6	2532.09639*	0.00046	3589.05108	1056.95515
17	2	0	0	0	8	2	0	0	0	7	2533.91187*	0.00282	3604.22815	1070.31910 †
18	2	0	0	0	9	2	0	0	0	8	2535.70965	0.00016	3621.29926	1085.58977
19	2	0	0	0	10	2	0	0	0	9	2537.49723	0.00008	3640.26336	1102.76621
20	2	0	0	0	11	2	0	0	0	10	2539.27198	0.00004	3661.11932	1121.84738
21	2	0	0	0	12	2	0	0	0	11	2541.03521*	0.00143	3683.86594	1142.83216 †
22	2	0	0	0	13	2	0	0	0	12	2542.78280	0.00017	3708.50199	1165.71936
23	2	0	0	0	14	2	0	0	0	13	2544.51856	0.00010	3735.02620	1190.50774
24	2	0	0	0	15	2	0	0	0	14	2546.23981*	-0.00148	3763.43735	1217.19606 †
25	2	0	0	0	16	2	0	0	0	15	2547.95110	-0.00005	3793.73423	1245.78308
26	2	0	0	0	17	2	0	0	0	16	2549.64799	-0.00011	3825.91570	1276.26760
27	2	0	0	0	18	2	0	0	0	17	2551.33231	0.00009	3859.98070	1308.64848
28	2	0	0	0	19	2	0	0	0	18	2553.00311	-0.00051	3895.92827	1342.92466
29	2	0	0	0	20	2	0	0	0	19	2554.66224	-0.00015	3933.75753	1379.09514
30	2	0	0	0	21	2	0	0	0	20	2556.30941	0.00076	3973.46770	1417.15906
31	2	0	0	0	22	2	0	0	0	21	2557.94235	-0.00013	4015.05808	1457.11560
32	2	0	0	0	23	2	0	0	0	22	2559.56369	-0.00028	4058.52804	1498.96407
33	2	0	0	0	24	2	0	0	0	23	2561.17308	-0.00011	4103.87700	1542.70381
34	2	0	0	0	25	2	0	0	0	24	2562.77113*	0.00093	4151.10444	1588.33424

rms = 0.00028 cm⁻¹

$\nu_3 + 2\nu_4 (\Delta) \leftarrow \nu_4 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 0 0 1	1 1 0 0 2	3026.92601*	-0.00024	3542.21455	515.28830
2 2 0 0 2	1 1 0 0 3	3025.01076*	-0.00819	3546.01024	520.99129 †
2 2 0 0 3	1 1 0 0 4	3023.10321*	-0.00558	3551.70395	528.59515 †
2 2 0 0 4	1 1 0 0 5	3021.19599	-0.00010	3559.29588	538.09979
2 2 0 0 5	1 1 0 0 6	3019.28266*	0.00141	3568.78633	549.50508 †
2 2 0 0 6	1 1 0 0 7	3017.36266*	-0.00211	3580.17563	562.81086 †
2 2 0 0 7	1 1 0 0 8	3015.44785	0.00060	3593.46422	578.01697
2 2 0 0 8	1 1 0 0 9	3013.52873	-0.00064	3608.65255	595.12319
2 2 0 0 9	1 1 0 0 10	3011.61379*	0.00190	3625.74118	614.12929 †
2 2 0 0 10	1 1 0 0 11	3009.69071*	-0.00493	3644.73067	635.03503 †
2 2 0 0 11	1 1 0 0 12	3007.78204	0.00054	3665.62162	657.84012
2 2 0 0 12	1 1 0 0 13	3005.87574*	0.00534	3688.41466	682.54427 †
2 2 0 0 13	1 1 0 0 14	3003.96562*	0.00235	3713.11040	709.14713 †
2 2 0 0 14	1 1 0 0 15	3002.06336*	0.00234	3739.70938	737.64836 †
2 2 0 0 15	1 1 0 0 16	3000.16189*	-0.00266	3768.21212	768.04757 †
2 2 0 0 16	1 1 0 0 17	2998.26775*	-0.00691	3798.61902	800.34436 †
2 2 0 0 17	1 1 0 0 18	2996.39160	-0.00048	3830.93038	834.53830
2 2 0 0 18	1 1 0 0 19	2994.51690	-0.00052	3865.14635	870.62893
2 2 0 0 2	1 1 0 0 1	3034.52412	0.00015	3546.01024	511.48627
2 2 0 0 3	1 1 0 0 2	3036.41599	0.00035	3551.70395	515.28830
2 2 0 0 4	1 1 0 0 3	3038.30472	0.00013	3559.29588	520.99129
2 2 0 0 5	1 1 0 0 4	3040.19273	0.00155	3568.78633	528.59515 †
2 2 0 0 6	1 1 0 0 5	3042.07666	0.00082	3580.17563	538.09979

1	2	2	0	0	7	1	1	0	0	6	3043.95943	0.00029	3593.46422	549.50508
2	2	2	0	0	8	1	1	0	0	7	3045.84171	0.00002	3608.65255	562.81086
3	2	2	0	0	9	1	1	0	0	8	3047.72473	0.00052	3625.74118	578.01697
4	2	2	0	0	10	1	1	0	0	9	3049.60699	-0.00049	3644.73067	595.12319
5	2	2	0	0	11	1	1	0	0	10	3051.49227	-0.00006	3665.62162	614.12929
6	2	2	0	0	12	1	1	0	0	11	3053.37946	-0.00017	3688.41466	635.03503
7	2	2	0	0	13	1	1	0	0	12	3055.27029*	0.00002	3713.11040	657.84012
8	2	2	0	0	15	1	1	0	0	14	3059.06470	-0.00029	3768.21212	709.14713
9	2	2	0	0	16	1	1	0	0	15	3060.97192*	0.00126	3798.61902	737.64836 +
10	2	2	0	0	17	1	1	0	0	16	3062.88228	-0.00053	3830.93038	768.04757
11	2	2	0	0	18	1	1	0	0	17	3064.80175	-0.00024	3865.14635	800.34436
12	2	2	0	0	19	1	1	0	0	18	3066.72813	-0.00054	3901.26697	834.53830
13	2	2	0	0	20	1	1	0	0	19	3068.66315*	-0.00001	3939.29209	870.62893
14	2	2	0	0	21	1	1	0	0	20	3070.60501	-0.00068	3979.22145	908.61577
15	2	2	0	0	22	1	1	0	0	21	3072.55480*	-0.00154	4021.05464	948.49830 +
16	2	-2	0	0	1	1	-1	0	0	2	3026.90731*	0.00592	3542.21455	515.31316 +
17	2	-2	0	0	2	1	-1	0	0	3	3024.95272*	-0.01642	3546.01014	521.04101 +
18	2	-2	0	0	3	1	-1	0	0	4	3023.02262*	-0.00283	3551.70346	528.67801 +
19	2	-2	0	0	4	1	-1	0	0	5	3021.06278*	-0.00758	3559.29444	538.22407 +
20	2	-2	0	0	5	1	-1	0	0	6	3019.10499*	0.00109	3568.78295	549.67906 +
21	2	-2	0	0	6	1	-1	0	0	7	3017.12183*	-0.00425	3580.16888	563.04281 +
22	2	-2	0	0	7	1	-1	0	0	8	3015.13846*	0.00153	3593.45207	578.31514 +
23	2	-2	0	0	8	1	-1	0	0	9	3013.13677	0.00029	3608.63233	595.49585
24	2	-2	0	0	9	1	-1	0	0	10	3011.12556	0.00080	3625.70945	614.58469
25	2	-2	0	0	10	1	-1	0	0	11	3009.10360*	0.00182	3644.68320	635.58142 +
26	2	-2	0	0	11	1	-1	0	0	12	3007.06728	-0.00030	3665.55331	658.48573
27	2	-2	0	0	12	1	-1	0	0	13	3005.02244	0.00026	3688.31950	683.29732
28	2	-2	0	0	13	1	-1	0	0	14	3002.96548	-0.00012	3712.98145	710.01584
29	2	-2	0	0	14	1	-1	0	0	15	3000.89749	-0.00039	3739.53881	738.64093
30	2	-2	0	0	15	1	-1	0	0	16	2998.81884	-0.00018	3767.99122	769.17220
31	2	-2	0	0	16	1	-1	0	0	17	2996.73090*	0.00184	3798.33829	801.60923 +
32	2	-2	0	0	17	1	-1	0	0	18	2994.62788	-0.00015	3830.57959	83

1														
2	2	2	0	0	15	1	-1	0	0	15	3029.57158	0.00040	3768.21212	738.64093
3	2	2	0	0	16	1	-1	0	0	16	3029.44652	-0.00030	3798.61902	769.17220
4	2	2	0	0	17	1	-1	0	0	17	3029.31803*	-0.00312	3830.93038	801.60923 +
5	2	2	0	0	18	1	-1	0	0	18	3029.19418	-0.00061	3865.14635	835.95156
6	2	2	0	0	19	1	-1	0	0	19	3029.06760	-0.00063	3901.26697	872.19874
7	2	2	0	0	20	1	-1	0	0	20	3028.94191	0.00008	3939.29209	910.35027
8	2	2	0	0	21	1	-1	0	0	21	3028.81530	-0.00054	3979.22145	950.40561
9	2	2	0	0	22	1	-1	0	0	22	3028.69065	0.00024	4021.05464	992.36423
10	2	2	0	0	23	1	-1	0	0	23	3028.56599	0.00041	4064.79113	1036.22555
11	2	2	0	0	24	1	-1	0	0	24	3028.44137	0.00006	4110.43027	1081.98896
12	2	2	0	0	25	1	-1	0	0	25	3028.31792	0.00043	4157.97134	1129.65384
13	2	2	0	0	26	1	-1	0	0	26	3028.19254	-0.00144	4207.41352	1179.21954 +
14	2	2	0	0	27	1	-1	0	0	27	3028.06862	-0.00197	4258.75596	1230.68537 +
15	2	-2	0	0	2	1	1	0	0	2	3030.72283*	0.00099	3546.01014	515.28830
16	2	-2	0	0	3	1	1	0	0	3	3030.71194	-0.00024	3551.70346	520.99129
17	2	-2	0	0	4	1	1	0	0	4	3030.69876	-0.00052	3559.29444	528.59515
18	2	-2	0	0	5	1	1	0	0	5	3030.68339	0.00023	3568.78295	538.09979
19	2	-2	0	0	6	1	1	0	0	6	3030.66308	-0.00072	3580.16888	549.50508
20	2	-2	0	0	7	1	1	0	0	7	3030.64176	0.00055	3593.45207	562.81086
21	2	-2	0	0	8	1	1	0	0	8	3030.61581	0.00045	3608.63233	578.01697
22	2	-2	0	0	9	1	1	0	0	9	3030.58661	0.00034	3625.70945	595.12319
23	2	-2	0	0	10	1	1	0	0	10	3030.55450	0.00059	3644.68320	614.12929
24	2	-2	0	0	11	1	1	0	0	11	3030.51795	-0.00033	3665.55331	635.03503
25	2	-2	0	0	12	1	1	0	0	12	3030.47971	0.00033	3688.31950	657.84012
26	2	-2	0	0	13	1	1	0	0	13	3030.43780	0.00062	3712.98145	682.54427
27	2	-2	0	0	14	1	1	0	0	14	3030.39199	0.00031	3739.53881	709.14713
28	2	-2	0	0	15	1	1	0	0	15	3030.33916*	-0.00370	3767.99122	737.64836 +
29	2	-2	0	0	16	1	1	0	0	16	3030.29206*	0.00134	3798.33829	768.04757 +
30	2	-2	0	0	17	1	1	0	0	17	3030.23508	-0.00015	3830.57959	800.34436
31	2	-2	0	0	18	1	1	0	0	18	3030.17534*	-0.00104	3864.71468	834.53830 +
32	2	-2	0	0	19	1	1	0	0	19	3030.11451	0.00035	3900.74309	870.62893
33	2	-2	0	0	20	1	1	0	0	20	3030.04849*	-0.00006	3938.66432	908.61577
34	2	-2	0	0	21	1	1	0	0	21	3029.98203*	0.00250	3978.47784	948.49830 +
35	2	-2	0	0	22	1	1	0	0	22	3029.90703	-0.00005	4020.18309	990.27601
36	2	-2	0	0	23	1	1	0	0	23	3029.83107	-0.00011	4063.77952	1033.94833
37	2	-2	0	0	24	1	1	0	0	24	3029.75009*	-0.00173	4109.26650	1079.51468 +
38	2	-2	0	0	25	1	1	0	0	25	3029.66929	0.00033	4156.64341	1126.97445
39	2	-2	0	0	26	1	1	0	0	26	3029.58163*	-0.00096	4205.90960	1176.32701
40	2	-2	0	0	27	1	1	0	0	27	3029.49287	0.00018	4257.06438	1227.57169

rms = 0.00044 cm⁻¹

$$v_3 + 2v_4 (\Delta) \leftarrow 2v_4 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
2 2 0 0 2	2 2 0 0 3	2513.29674*	-0.00377	3546.01024	1032.70973 †
2 2 0 0 3	2 2 0 0 4	2511.35241*	-0.00311	3551.70395	1040.34843 †
2 2 0 0 4	2 2 0 0 5	2509.40811*	0.00955	3559.29588	1049.89732 †
2 2 0 0 5	2 2 0 0 6	2507.42899	-0.00059	3568.78633	1061.35675
2 2 0 0 6	2 2 0 0 7	2505.45009*	0.00157	3580.17563	1074.72712 †
2 2 0 0 7	2 2 0 0 8	2503.45899*	0.00366	3593.46422	1090.00889 †
2 2 0 0 8	2 2 0 0 9	2501.44830*	-0.00166	3608.65255	1107.20259 †
2 2 0 0 9	2 2 0 0 10	2499.43225	-0.00014	3625.74118	1126.30879
2 2 0 0 10	2 2 0 0 11	2497.40254	-0.00005	3644.73067	1147.32807
2 2 0 0 11	2 2 0 0 12	2495.36045	-0.00012	3665.62162	1170.26105
2 2 0 0 12	2 2 0 0 13	2493.30631	-0.00003	3688.41466	1195.10832
2 2 0 0 13	2 2 0 0 14	2491.23999	0.00003	3713.11040	1221.87043
2 2 0 0 14	2 2 0 0 15	2489.16172	0.00022	3739.70938	1250.54788
2 2 0 0 15	2 2 0 0 16	2487.07142	0.00038	3768.21212	1281.14108
2 2 0 0 16	2 2 0 0 17	2484.96917	0.00047	3798.61902	1313.65031
2 2 0 0 17	2 2 0 0 18	2482.85655*	0.00193	3830.93038	1348.07575 †
2 2 0 0 18	2 2 0 0 19	2480.72781	-0.00113	3865.14635	1384.41742 †

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1	2	2	0	0	19	2	2	0	0	20	2478.59108	-0.00070	3901.26697	1422.67519
2	2	2	0	0	20	2	2	0	0	21	2476.44299	-0.00031	3939.29209	1462.84880
3	2	2	0	0	21	2	2	0	0	22	2474.28335	-0.00026	3979.22145	1504.93784
4	2	2	0	0	22	2	2	0	0	23	2472.11252	-0.00031	4021.05464	1548.94181
5	2	2	0	0	23	2	2	0	0	24	2469.93078	-0.00029	4064.79113	1594.86006
6	2	2	0	0	24	2	2	0	0	25	2467.73808	-0.00031	4110.43027	1642.69188
7	2	2	0	0	25	2	2	0	0	26	2465.53464	-0.00024	4157.97134	1692.43646
8	2	2	0	0	26	2	2	0	0	27	2463.32039	-0.00019	4207.41352	1744.09294
9	2	2	0	0	27	2	2	0	0	28	2461.09535	-0.00019	4258.75596	1797.66042
10	2	2	0	0	28	2	2	0	0	29	2458.86000	0.00020	4311.99773	1853.13793
11	2	2	0	0	29	2	2	0	0	30	2456.61332	-0.00005	4367.13787	1910.52450
12	2	2	0	0	30	2	2	0	0	31	2454.35677	0.00049	4424.17539	1969.81911
13	2	2	0	0	3	2	2	0	0	2	2524.72013*	-0.00288	3551.70395	1026.98094 +
14	2	2	0	0	4	2	2	0	0	3	2526.58354*	-0.00262	3559.29588	1032.70973 +
15	2	2	0	0	5	2	2	0	0	4	2528.43458*	-0.00332	3568.78633	1040.34843 +
16	2	2	0	0	6	2	2	0	0	5	2530.27448*	-0.00383	3580.17563	1049.89732 +
17	2	2	0	0	7	2	2	0	0	6	2532.10767*	0.00020	3593.46422	1061.35675
18	2	2	0	0	8	2	2	0	0	7	2533.92453*	-0.00091	3608.65255	1074.72712
19	2	2	0	0	9	2	2	0	0	8	2535.73224	-0.00005	3625.74118	1090.00889
20	2	2	0	0	10	2	2	0	0	9	2537.52799	-0.00008	3644.73067	1107.20259
21	2	2	0	0	11	2	2	0	0	10	2539.31289	0.00006	3665.62162	1126.30879
22	2	2	0	0	12	2	2	0	0	11	2541.08663	0.00004	3688.41466	1147.32807
23	2	2	0	0	13	2	2	0	0	12	2542.84943	0.00009	3713.11040	1170.26105
24	2	2	0	0	14	2	2	0	0	13	2544.60142	0.00036	3739.70938	1195.10832
25	2	2	0	0	15	2	2	0	0	14	2546.34203	0.00035	3768.21212	1221.87043
26	2	2	0	0	16	2	2	0	0	15	2548.07139	0.00026	3798.61902	1250.54788
27	2	2	0	0	17	2	2	0	0	16	2549.79118*	0.00188	3830.93038	1281.14108 +
28	2	2	0	0	18	2	2	0	0	17	2551.49497	-0.00107	3865.14635	1313.65031 +
29	2	2	0	0	19	2	2	0	0	18	2553.19104	-0.00018	3901.26697	1348.07575
30	2	2	0	0	20	2	2	0	0	19	2554.87438	-0.00030	3939.29209	1384.41742
31	2	2	0	0	21	2	2	0	0	20	2556.54608	-0.00019	3979.22145	1422.67519
32	2	2	0	0	22	2	2	0	0	21	2558.20569	-0.00016	4021.05464	1462.84880
33	2	2	0	0	23	2	2	0	0	22	2559.85304	-0.00024	4064.79113	1504.93784
34	2	2	0	0	24	2	2	0	0	23	2561.48856	0.00010	4110.43027	1548.94181
35	2	2	0	0	25	2	2	0	0	24	2563.11108	-0.00020	4157.97134	1594.86006
36	2	2	0	0	26	2	2	0	0	25	2564.72090	-0.00075	4207.41352	1642.69188
37	2	2	0	0	27	2	2	0	0	26	2566.31939	-0.00011	4258.75596	1692.43646
38	2	2	0	0	28	2	2	0	0	27	2567.90477	-0.00002	4311.99773	1744.09294
39	2	2	0	0	29	2	2	0	0	28	2569.47791*	0.00046	4367.13787	1797.66042
40	2	2	0	0	30	2	2	0	0	29	2571.03713	-0.00033	4424.17539	1853.13793
41	2	2	0	0	31	2	2	0	0	30	2572.58481	0.00004	4483.10927	1910.52450
42	2	2	0	0	32	2	2	0	0	31	2574.11970	0.00033	4543.93848	1969.81911
43	2	2	0	0	33	2	2	0	0	32	2575.64136	0.00013	4606.66195	2031.02072
44	2	2	0	0	34	2	2	0	0	33	2577.15082	0.00050	4671.27861	2094.12829
45	2	-2	0	0	2	2	-2	0	0	3	2513.29674*	-0.00415	3546.01014	1032.70925 +
46	2	-2	0	0	3	2	-2	0	0	4	2511.35241*	-0.00405	3551.70346	1040.34700 +
47	2	-2	0	0	4	2	-2	0	0	5	2509.40811*	0.00767	3559.29444	1049.89400 +
48	2	-2	0	0	5	2	-2	0	0	6	2507.42899*	-0.00387	3568.78295	1061.35010 +
49	2	-2	0	0	6	2	-2	0	0	7	2505.45009*	-0.00365	3580.16888	1074.71514 +
50	2	-2	0	0	7	2	-2	0	0	8	2503.45899*	-0.00413	3593.45207	1089.98896 +
51	2	-2	0	0	8	2	-2	0	0	9	2501.46086	-0.00015	3608.63233	1107.17132
52	2	-2	0	0	9	2	-2	0	0	10	2499.44893*	0.00147	3625.70945	1126.26199 +
53	2	-2	0	0	10	2	-2	0	0	11	2497.42272	0.00024	3644.68320	1147.26072
54	2	-2	0	0	11	2	-2	0	0	12	2495.38619	0.00008	3665.55331	1170.16720
55	2	-2	0	0	12	2	-2	0	0	13	2493.33855	0.00017	3688.31950	1194.98112
56	2	-2	0	0	13	2	-2	0	0	14	2491.27961	0.00030	3712.98145	1221.70214
57	2	-2	0	0	14	2	-2	0	0	15	2489.20907	0.00014	3739.53881	1250.32988
58	2	-2	0	0	15	2	-2	0	0	16	2487.12806	0.00079	3767.99122	1280.86395
59	2	-2	0	0	16	2	-2	0	0	17	2485.03581*	0.00145	3798.33829	1313.30393 +
60	2	-2	0	0	17	2	-2	0	0	18	2482.92982	-0.00041	3830.57959	1347.64936
	2	-2	0	0	18	2	-2	0	0	19	2480.81500	0.00008	3864.71468	1383.89977
	2	-2	0	0	19	2	-2	0	0	20	2478.68876	0.00032	3900.74309	1422.05465
	2	-2	0	0	20	2	-2	0	0	21	2476.55119	0.00036	3938.66432	1462.11349
	2	-2	0	0	21	2	-2	0	0	22	2474.40238	0.00026	3978.47784	1504.07572
	2	-2	0	0	22	2	-2	0	0	23	2472.24260	0.00026	4020.18309	1547.94075

1											
2	2	-2	0	0	23	2	-2	0	0	24	2470.07135
3	2	-2	0	0	24	2	-2	0	0	25	-0.00017
4	2	-2	0	0	25	2	-2	0	0	26	4063.77952
5	2	-2	0	0	26	2	-2	0	0	27	0.00006
6	2	-2	0	0	27	2	-2	0	0	28	4109.26650
7	2	-2	0	0	28	2	-2	0	0	29	0.00007
8	2	-2	0	0	29	2	-2	0	0	30	4156.64341
9	2	-2	0	0	30	2	-2	0	0	31	4205.90960
10	2	-2	0	0	31	2	-2	0	0	32	-0.00018
11	2	-2	0	0	3	2	-2	0	0	2	4257.06438
12	2	-2	0	0	4	2	-2	0	0	3	4310.10704
13	2	-2	0	0	5	2	-2	0	0	4	1851.05410
14	2	-2	0	0	6	2	-2	0	0	5	1795.78589
15	2	-2	0	0	7	2	-2	0	0	6	1908.22031
16	2	-2	0	0	8	2	-2	0	0	7	1967.28373
17	2	-2	0	0	9	2	-2	0	0	8	2028.24354
18	2	-2	0	0	10	2	-2	0	0	9	2452.31181
19	2	-2	0	0	11	2	-2	0	0	10	0.00050
20	2	-2	0	0	12	2	-2	0	0	11	4480.55485
21	2	-2	0	0	13	2	-2	0	0	12	3551.70346
22	2	-2	0	0	14	2	-2	0	0	13	-0.00249
23	2	-2	0	0	15	2	-2	0	0	14	3559.29444
24	2	-2	0	0	16	2	-2	0	0	15	-0.00164
25	2	-2	0	0	17	2	-2	0	0	16	3568.78295
26	2	-2	0	0	18	2	-2	0	0	17	1040.34700
27	2	-2	0	0	19	2	-2	0	0	18	1049.89400
28	2	-2	0	0	20	2	-2	0	0	19	1061.35010
29	2	-2	0	0	21	2	-2	0	0	20	1074.71514
30	2	-2	0	0	22	2	-2	0	0	21	1089.98896
31	2	-2	0	0	23	2	-2	0	0	22	1107.17132
32	2	-2	0	0	24	2	-2	0	0	23	1126.26199
33	2	-2	0	0	25	2	-2	0	0	24	1147.26072
34	2	-2	0	0	26	2	-2	0	0	25	1170.16720
35	2	-2	0	0	27	2	-2	0	0	26	1194.98112
36	2	-2	0	0	28	2	-2	0	0	27	1221.70214
37	2	-2	0	0	29	2	-2	0	0	28	1250.32988
38	2	-2	0	0	30	2	-2	0	0	29	1280.86395
39	2	-2	0	0	31	2	-2	0	0	30	1313.30393
40	2	-2	0	0	2	2	2	0	0	2	1347.64936
41	2	-2	0	0	3	2	2	0	0	3	1383.89977
42	2	-2	0	0	4	2	2	0	0	4	1422.05465
43	2	-2	0	0	5	2	2	0	0	5	1462.11349
44	2	-2	0	0	6	2	2	0	0	6	1504.07572
45	2	-2	0	0	7	2	2	0	0	7	1547.94075
46	2	-2	0	0	8	2	2	0	0	8	1593.70799
47	2	-2	0	0	9	2	2	0	0	9	1641.37680
48	2	-2	0	0	10	2	2	0	0	10	1690.94652
49	2	-2	0	0	11	2	2	0	0	11	1742.41645
50	2	-2	0	0	12	2	2	0	0	12	1795.78589
51	2	-2	0	0	13	2	2	0	0	13	1851.05410
52	2	2	0	0	2	2	-2	0	0	2	1908.22031
53	2	2	0	0	3	2	-2	0	0	3	1026.98094
54	2	2	0	0	4	2	-2	0	0	4	1032.70973
55	2	2	0	0	5	2	-2	0	0	5	1040.34843
56	2	2	0	0	6	2	-2	0	0	6	1049.89732
57	2	2	0	0	7	2	-2	0	0	7	1061.35675
58	2	2	0	0	8	2	-2	0	0	8	1074.72712
59	2	2	0	0	9	2	-2	0	0	9	1090.00889
60	2	2	0	0	10	2	-2	0	0	10	1107.20259
	2	2	0	0	11	2	-2	0	0	11	1126.30879
	2	2	0	0	12	2	-2	0	0	12	1147.32807
	2	2	0	0	13	2	-2	0	0	13	1170.26105
	2	2	0	0	2	2	2	0	0	2	1195.10832
	2	2	0	0	3	2	2	0	0	3	1026.98084
	2	2	0	0	4	2	2	0	0	4	1032.70925
	2	2	0	0	5	2	2	0	0	5	1040.34700
	2	2	0	0	6	2	2	0	0	6	1049.89400
	2	2	0	0	7	2	2	0	0	7	1061.35010
	2	2	0	0	8	2	2	0	0	8	1074.71514
	2	2	0	0	9	2	2	0	0	9	1089.98896
	2	2	0	0	10	2	2	0	0	10	1107.17132
	2	2	0	0	11	2	2	0	0	11	1126.26199
	2	2	0	0	12	2	2	0	0	12	1147.26072
	2	2	0	0	13	2	2	0	0	13	1170.16720
	2	2	0	0	13	2	2	0	0	13	1194.98112

rms = 0.00034 cm⁻¹

1
2
3
4 $\nu_3 + 2\nu_5 (\Sigma^+) \leftarrow 2\nu_5 (\Sigma^+)$
5

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS ^b	OBS – CALC ^b	E'	E''
0 0 2 0 0	0 0 2 0 1	2540.22615	-0.00043	3877.44105	1337.21447
0 0 2 0 1	0 0 2 0 2	2538.30844	0.00018	3879.33463	1341.02637
0 0 2 0 2	0 0 2 0 3	2536.37756	-0.00006	3883.12174	1346.74412
0 0 2 0 3	0 0 2 0 4	2534.43421	-0.00050	3888.80230	1354.36759
0 0 2 0 4	0 0 2 0 5	2532.47920	-0.00037	3896.37619	1363.89662
0 0 2 0 5	0 0 2 0 6	2530.50771*	-0.00454	3905.84325	1375.33100 †
0 0 2 0 6	0 0 2 0 7	2528.53318	0.00039	3917.20326	1388.67047
0 0 2 0 7	0 0 2 0 8	2526.54142	0.00019	3930.45599	1403.91476
0 0 2 0 8	0 0 2 0 9	2524.53782	0.00020	3945.60114	1421.06352
0 0 2 0 9	0 0 2 0 10	2522.52219	0.00018	3962.63840	1440.11639
0 0 2 0 10	0 0 2 0 11	2520.49408	-0.00036	3981.56738	1461.07294
0 0 2 0 11	0 0 2 0 12	2518.45498	0.00003	4002.38767	1483.93273
0 0 2 0 12	0 0 2 0 13	2516.40345	-0.00014	4025.09884	1508.69525
0 0 2 0 13	0 0 2 0 14	2514.33992	-0.00050	4049.70038	1535.35996
0 0 2 0 14	0 0 2 0 15	2512.26555	0.00008	4076.19176	1563.92630
0 0 2 0 15	0 0 2 0 16	2510.17897	0.00018	4104.57241	1594.39363
0 0 2 0 16	0 0 2 0 17	2508.07969	-0.00074	4134.84172	1626.76130
0 0 2 0 17	0 0 2 0 18	2505.97019	-0.00024	4166.99904	1661.02860
0 0 2 0 18	0 0 2 0 19	2503.84892	0.00007	4201.04367	1697.19482
0 0 2 0 19	0 0 2 0 20	2501.71581	0.00009	4236.97488	1735.25916
0 0 2 0 20	0 0 2 0 21	2499.57088	-0.00022	4274.79191	1775.22081
0 0 2 0 21	0 0 2 0 22	2497.42334*	0.00832	4314.49396	1817.07894 †
0 0 2 0 22	0 0 2 0 23	2495.24764*	0.00011	4356.08019	1860.83266
0 0 2 0 23	0 0 2 0 24	2493.06928	0.00062	4399.54972	1906.48106
0 0 2 0 24	0 0 2 0 25	2490.87771	-0.00076	4444.90166	1954.02319
0 0 2 0 1	0 0 2 0 0	2544.02659	0.00046	3879.33463	1335.30850
0 0 2 0 2	0 0 2 0 1	2545.90668	-0.00059	3883.12174	1337.21447
0 0 2 0 3	0 0 2 0 2	2547.77636	0.00043	3888.80230	1341.02637
0 0 2 0 4	0 0 2 0 3	2549.62918*	-0.00289	3896.37619	1346.74412 †
0 0 2 0 5	0 0 2 0 4	2551.47588	0.00023	3905.84325	1354.36759
0 0 2 0 6	0 0 2 0 5	2553.30691	0.00027	3917.20326	1363.89662
0 0 2 0 7	0 0 2 0 6	2555.12564	0.00065	3930.45599	1375.33100
0 0 2 0 8	0 0 2 0 7	2556.93118	0.00051	3945.60114	1388.67047
0 0 2 0 9	0 0 2 0 8	2558.72230*	-0.00134	3962.63840	1403.91476 †
0 0 2 0 10	0 0 2 0 9	2560.50394	0.00008	3981.56738	1421.06352
0 0 2 0 11	0 0 2 0 10	2562.27132	0.00003	4002.38767	1440.11639
0 0 2 0 12	0 0 2 0 11	2564.02569	-0.00021	4025.09884	1461.07294
0 0 2 0 13	0 0 2 0 12	2565.76771	0.00006	4049.70038	1483.93273
0 0 2 0 14	0 0 2 0 13	2567.49774*	0.00122	4076.19176	1508.69525 †
0 0 2 0 15	0 0 2 0 14	2569.21247	0.00002	4104.57241	1535.35996
0 0 2 0 16	0 0 2 0 15	2570.91542	-0.00001	4134.84172	1563.92630
0 0 2 0 17	0 0 2 0 16	2572.60520	-0.00021	4166.99904	1594.39363
0 0 2 0 18	0 0 2 0 17	2574.28241	0.00004	4201.04367	1626.76130
0 0 2 0 19	0 0 2 0 18	2575.94636	0.00009	4236.97488	1661.02860
0 0 2 0 20	0 0 2 0 19	2577.59700	-0.00010	4274.79191	1697.19482
0 0 2 0 21	0 0 2 0 20	2579.23483	0.00003	4314.49396	1735.25916
0 0 2 0 22	0 0 2 0 21	2580.85940	0.00003	4356.08019	1775.22081
0 0 2 0 23	0 0 2 0 22	2582.47089	0.00011	4399.54972	1817.07894
0 0 2 0 24	0 0 2 0 23	2584.06892	-0.00007	4444.90166	1860.83266
0 0 2 0 25	0 0 2 0 24	2585.65433	0.00033	4492.13506	1906.48106
0 0 2 0 26	0 0 2 0 25	2587.22570	-0.00007	4541.24896	1954.02319
0 0 2 0 27	0 0 2 0 26	2588.78427	-0.00002	4592.24237	2003.45808
0 0 2 0 28	0 0 2 0 27	2590.32884	-0.00071	4645.11427	2054.78472
0 0 2 0 29	0 0 2 0 28	2591.86226	0.00074	4699.86362	2108.00210

rms = 0.00035 cm⁻¹

$$v_3 + 2v_5 (\Delta) \leftarrow 2v_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 2 2 2	0 0 2 2 3	2536.44884	0.00011	3899.77833	1363.32960
0 0 2 2 3	0 0 2 2 4	2534.50672	0.00020	3905.45626	1370.94974
0 0 2 2 4	0 0 2 2 5	2532.55057*	-0.00137	3913.02678	1380.47484 †
0 0 2 2 5	0 0 2 2 6	2530.58437	-0.00064	3922.48987	1391.90486
0 0 2 2 6	0 0 2 2 7	2528.60638	0.00065	3933.84546	1405.23972
0 0 2 2 7	0 0 2 2 8	2526.61458	0.00047	3947.09349	1420.47938
0 0 2 2 8	0 0 2 2 9	2524.61081	0.00065	3962.23390	1437.62374
0 0 2 2 9	0 0 2 2 10	2522.59524*	0.00135	3979.26661	1456.67272 †
0 0 2 2 10	0 0 2 2 11	2520.56683*	0.00153	3998.19152	1477.62621 †
0 0 2 2 11	0 0 2 2 12	2518.52645*	0.00204	4019.00853	1500.48412 †
0 0 2 2 12	0 0 2 2 13	2516.47345*	0.00224	4041.71754	1525.24633 †
0 0 2 2 13	0 0 2 2 14	2514.40678*	0.00105	4066.31843	1551.91270 †
0 0 2 2 14	0 0 2 2 15	2512.32840	0.00045	4092.81105	1580.48310
0 0 2 2 15	0 0 2 2 16	2510.23787	-0.00003	4121.19528	1610.95737
0 0 2 2 16	0 0 2 2 17	2508.13562	0.00004	4151.47095	1643.33536
0 0 2 2 17	0 0 2 2 18	2506.02085	-0.00016	4183.63790	1677.61689
0 0 2 2 18	0 0 2 2 19	2503.89417	-0.00001	4217.69596	1713.80178
0 0 2 2 19	0 0 2 2 20	2501.75508	-0.00003	4253.64493	1751.88982
0 0 2 2 20	0 0 2 2 21	2499.60360	-0.00020	4291.48461	1791.88081
0 0 2 2 21	0 0 2 2 22	2497.44007	-0.00022	4331.21479	1833.77451
0 0 2 2 22	0 0 2 2 23	2495.26393	-0.00063	4372.83523	1877.57067
0 0 2 2 23	0 0 2 2 24	2493.07822*	0.00157	4416.34568	1923.26903 †
0 0 2 2 3	0 0 2 2 2	2547.84170	-0.00010	3905.45626	1357.61446
0 0 2 2 4	0 0 2 2 3	2549.69715	-0.00004	3913.02678	1363.32960
0 0 2 2 5	0 0 2 2 4	2551.53999	-0.00014	3922.48987	1370.94974
0 0 2 2 6	0 0 2 2 5	2553.37042	-0.00019	3933.84546	1380.47484
0 0 2 2 7	0 0 2 2 6	2555.18776	-0.00087	3947.09349	1391.90486
0 0 2 2 8	0 0 2 2 7	2557.00340*	0.00922	3962.23390	1405.23972 †
0 0 2 2 9	0 0 2 2 8	2558.78631	-0.00092	3979.26661	1420.47938
0 0 2 2 10	0 0 2 2 9	2560.56041*	-0.00737	3998.19152	1437.62374 †
0 0 2 2 11	0 0 2 2 10	2562.33413*	-0.00169	4019.00853	1456.67272 †
0 0 2 2 12	0 0 2 2 11	2564.08823*	-0.00310	4041.71754	1477.62621 †
0 0 2 2 13	0 0 2 2 12	2565.83112*	-0.00318	4066.31843	1500.48412 †
0 0 2 2 14	0 0 2 2 13	2567.56016*	-0.00456	4092.81105	1525.24633 †
0 0 2 2 15	0 0 2 2 14	2569.28357*	0.00099	4121.19528	1551.91270
0 0 2 2 16	0 0 2 2 15	2570.98851	0.00066	4151.47095	1580.48310
0 0 2 2 17	0 0 2 2 16	2572.68050	-0.00003	4183.63790	1610.95737
0 0 2 2 18	0 0 2 2 17	2574.36075	0.00015	4217.69596	1643.33536
0 0 2 2 19	0 0 2 2 18	2576.02769	-0.00035	4253.64493	1677.61689
0 0 2 2 20	0 0 2 2 19	2577.68296	0.00013	4291.48461	1713.80178
0 0 2 2 21	0 0 2 2 20	2579.32528	0.00031	4331.21479	1751.88982
0 0 2 2 22	0 0 2 2 21	2580.95436	-0.00006	4372.83523	1791.88081
0 0 2 2 23	0 0 2 2 22	2582.57190	0.00073	4416.34568	1833.77451
0 0 2 2 24	0 0 2 2 23	2584.17491	-0.00029	4461.74587	1877.57067
0 0 2 2 25	0 0 2 2 24	2585.76633	-0.00015	4509.03551	1923.26903
0 0 2 2 26	0 0 2 2 25	2587.34477	-0.00022	4558.21429	1970.86930
0 0 2 2 27	0 0 2 2 26	2588.91092	0.00022	4609.28188	2020.37118
0 0 2 2 28	0 0 2 2 27	2590.46371	0.00012	4662.23792	2071.77433
0 0 2 -2 2	0 0 2 -2 3	2536.44884	0.00005	3899.77831	1363.32952
0 0 2 -2 3	0 0 2 -2 4	2534.50672	0.00004	3905.45618	1370.94950
0 0 2 -2 4	0 0 2 -2 5	2532.55057*	-0.00169	3913.02655	1380.47429 †
0 0 2 -2 5	0 0 2 -2 6	2530.58437*	-0.00120	3922.48933	1391.90376 †
0 0 2 -2 6	0 0 2 -2 7	2528.60638	-0.00026	3933.84438	1405.23774
0 0 2 -2 7	0 0 2 -2 8	2526.61458	-0.00090	3947.09155	1420.47607
0 0 2 -2 8	0 0 2 -2 9	2524.61081*	-0.00132	3962.23067	1437.61854 †
0 0 2 -2 9	0 0 2 -2 10	2522.59524*	-0.00137	3979.26153	1456.66492 †
0 0 2 -2 10	0 0 2 -2 11	2520.56938	0.00043	3998.18390	1477.61496
0 0 2 -2 11	0 0 2 -2 12	2518.52645*	-0.00272	4018.99753	1500.46836 †
0 0 2 -2 12	0 0 2 -2 13	2516.47345*	-0.00386	4041.70214	1525.22483 †
0 0 2 -2 13	0 0 2 -2 14	2514.41241*	-0.00097	4066.29742	1551.88404

1	0	0	2	-2	14	0	0	2	-2	15	2512.33734	-0.00009	4092.78305	1580.44562
2	0	0	2	-2	15	0	0	2	-2	16	2510.24997	0.00051	4121.15865	1610.90919
3	0	0	2	-2	16	0	0	2	-2	17	2508.14932	-0.00020	4151.42387	1643.27435
4	0	0	2	-2	17	0	0	2	-2	18	2506.03756	-0.00006	4183.57828	1677.54066
5	0	0	2	-2	18	0	0	2	-2	19	2503.91363	-0.00017	4217.62146	1713.70766
6	0	0	2	-2	19	0	0	2	-2	20	2501.77788	-0.00021	4253.55295	1751.77486
7	0	0	2	-2	20	0	0	2	-2	21	2499.63049	-0.00002	4291.37226	1791.74175
8	0	0	2	-2	21	0	0	2	-2	22	2497.47112	0.00003	4331.07889	1833.60781
9	0	0	2	-2	22	0	0	2	-2	23	2495.29948	-0.00037	4372.67231	1877.37245
10	0	0	2	-2	23	0	0	2	-2	24	2493.11680	-0.00004	4416.15195	1923.03511
11	0	0	2	-2	24	0	0	2	-2	25	2490.92258	0.00051	4461.51723	1970.59516
12	0	0	2	-2	3	0	0	2	-2	2	2547.84169	-0.00005	3905.45618	1357.61444
13	0	0	2	-2	4	0	0	2	-2	3	2549.69715	0.00012	3913.02655	1363.32952
14	0	0	2	-2	5	0	0	2	-2	4	2551.53999	0.00016	3922.48933	1370.94950
15	0	0	2	-2	6	0	0	2	-2	5	2553.37042	0.00033	3933.84438	1380.47429
16	0	0	2	-2	7	0	0	2	-2	6	2555.18776	-0.00004	3947.09155	1391.90376
17	0	0	2	-2	8	0	0	2	-2	7	2557.00340*	0.01047	3962.23067	1405.23774 +
18	0	0	2	-2	9	0	0	2	-2	8	2558.78631	0.00085	3979.26153	1420.47607
19	0	0	2	-2	10	0	0	2	-2	9	2560.57725*	0.01189	3998.18390	1437.61854 +
20	0	0	2	-2	11	0	0	2	-2	10	2562.33109*	-0.00152	4018.99753	1456.66492 +
21	0	0	2	-2	12	0	0	2	-2	11	2564.08823*	0.00104	4041.70214	1477.61496 +
22	0	0	2	-2	13	0	0	2	-2	12	2565.83112*	0.00206	4066.29742	1500.46836 +
23	0	0	2	-2	14	0	0	2	-2	13	2567.56016*	0.00195	4092.78305	1525.22483 +
24	0	0	2	-2	16	0	0	2	-2	15	2570.97840	0.00015	4151.42387	1580.44562
25	0	0	2	-2	17	0	0	2	-2	16	2572.66882	-0.00027	4183.57828	1610.90919
26	0	0	2	-2	18	0	0	2	-2	17	2574.34710	-0.00001	4217.62146	1643.27435
27	0	0	2	-2	19	0	0	2	-2	18	2576.01228	-0.00001	4253.55295	1677.54066
28	0	0	2	-2	20	0	0	2	-2	19	2577.66454	-0.00007	4291.37226	1713.70766
29	0	0	2	-2	21	0	0	2	-2	20	2579.31004*	0.00601	4331.07889	1751.77486 +
30	0	0	2	-2	22	0	0	2	-2	21	2580.93057	0.00002	4372.67231	1791.74175
31	0	0	2	-2	23	0	0	2	-2	22	2582.54399	-0.00015	4416.15195	1833.60781
32	0	0	2	-2	24	0	0	2	-2	23	2584.14477	0.00000	4461.51723	1877.37245
33	0	0	2	-2	25	0	0	2	-2	24	2585.73241	-0.00002	4508.76754	1923.03511
34	0	0	2	-2	26	0	0	2	-2	25	2587.30725	0.00017	4557.90225	1970.59516
35	0	0	2	-2	27	0	0	2	-2	26	2588.86815	-0.00057	4608.92069	2020.05197
36	0	0	2	-2	28	0	0	2	-2	27	2590.41762	0.00031	4661.82218	2071.40488
37	0	0	2	-2	29	0	0	2	-2	28	2591.95292	0.00009	4716.60602	2124.65319
38	0	0	2	2	2	0	0	2	-2	2	2542.16412	0.00024	3899.77833	1357.61444
39	0	0	2	2	3	0	0	2	-2	3	2542.12677	0.00003	3905.45626	1363.32952
40	0	0	2	2	4	0	0	2	-2	4	2542.07751	0.00023	3913.02678	1370.94950
41	0	0	2	2	5	0	0	2	-2	5	2542.01511	-0.00047	3922.48987	1380.47429
42	0	0	2	2	6	0	0	2	-2	6	2541.94087	-0.00083	3933.84546	1391.90376
43	0	0	2	2	7	0	0	2	-2	7	2541.84842*	-0.00733	3947.09349	1405.23774 +
44	0	0	2	2	8	0	0	2	-2	8	2541.75766*	-0.00017	3962.23390	1420.47607
45	0	0	2	2	9	0	0	2	-2	9	2541.64830	0.00024	3979.26661	1437.61854
46	0	0	2	2	10	0	0	2	-2	10	2541.52642	-0.00018	3998.19152	1456.66492
47	0	0	2	2	11	0	0	2	-2	11	2541.39344	-0.00014	4019.00853	1477.61496
48	0	0	2	2	12	0	0	2	-2	12	2541.25082*	0.00164	4041.71754	1500.46836 +
49	0	0	2	-2	2	0	0	2	2	2	2542.16412	0.00027	3899.77831	1357.61446
50	0	0	2	-2	3	0	0	2	2	3	2542.12677	0.00019	3905.45618	1363.32960
51	0	0	2	-2	4	0	0	2	2	4	2542.07751	0.00070	3913.02655	1370.94974
52	0	0	2	-2	5	0	0	2	2	5	2542.01511	0.00062	3922.48933	1380.47484
53	0	0	2	-2	6	0	0	2	2	6	2541.94050*	0.00098	3933.84438	1391.90486
54	0	0	2	-2	7	0	0	2	2	7	2541.84842*	-0.00341	3947.09155	1405.23972 +
55	0	0	2	-2	8	0	0	2	2	8	2541.75760*	0.00631	3962.23067	1420.47938 +
56	0	0	2	-2	9	0	0	2	2	9	2541.63980*	0.00201	3979.26153	1437.62374 +
57	0	0	2	-2	10	0	0	2	2	10	2541.51082	-0.00037	3998.18390	1456.67272
58	0	0	2	-2	11	0	0	2	2	11	2541.37087	-0.00045	4018.99753	1477.62621
59	0	0	2	-2	12	0	0	2	2	12	2541.21929*	0.00127	4041.70214	1500.48412 +
60	rms = 0.00037 cm ⁻¹													

$$\mathbf{v}_3 + \mathbf{v}_4 + \mathbf{v}_5 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	0 0 0 0 1	3716.36989*	0.00201	3718.26853	1.90066 †
1 1 1 -1 1	0 0 0 0 2	3714.46367*	0.00167	3720.16395	5.70195 †
1 1 1 -1 2	0 0 0 0 3	3712.54988	-0.00114	3723.95484	11.40382 †
1 1 1 -1 3	0 0 0 0 4	3710.63489	-0.00022	3729.64130	19.00619
1 1 1 -1 4	0 0 0 0 5	3708.71464	0.00012	3737.22350	28.50898
1 1 1 -1 5	0 0 0 0 6	3706.79126*	0.00166	3746.70164	39.91204 †
1 1 1 -1 6	0 0 0 0 7	3704.86218	0.00144	3758.07598	53.21523 †
1 1 1 -1 7	0 0 0 0 8	3702.92816	-0.00028	3771.34682	68.41838
1 1 1 -1 8	0 0 0 0 9	3700.99382	0.00058	3786.51453	85.52129
1 1 1 -1 9	0 0 0 0 10	3699.05573	-0.00003	3803.57948	104.52373
1 1 1 -1 10	0 0 0 0 11	3697.11670	0.00003	3822.54211	125.42544
1 1 1 -1 11	0 0 0 0 12	3695.17666	-0.00003	3843.40285	148.22616
1 1 1 -1 12	0 0 0 0 13	3693.23641	-0.00016	3866.16215	172.92558
1 1 1 -1 13	0 0 0 0 14	3691.29723	0.00016	3890.82045	199.52337
1 1 1 -1 14	0 0 0 0 15	3689.35840	-0.00055	3917.37815	228.01920
1 1 1 -1 15	0 0 0 0 16	3687.42289	-0.00005	3945.83562	258.41268
1 1 1 -1 16	0 0 0 0 17	3685.48992	0.00017	3976.19315	290.70340
1 1 1 -1 17	0 0 0 0 18	3683.55959	-0.00040	4008.45095	324.89096
1 1 1 -1 18	0 0 0 0 19	3681.63425	0.00002	4042.60912	360.97488
1 1 1 -1 1	0 0 0 0 0	3720.16485*	0.00090	3720.16395	0.00000
1 1 1 -1 2	0 0 0 0 1	3722.05266*	-0.00152	3723.95484	1.90066 †
1 1 1 -1 3	0 0 0 0 2	3723.93880	-0.00056	3729.64130	5.70195
1 1 1 -1 4	0 0 0 0 3	3725.81959	-0.00009	3737.22350	11.40382
1 1 1 -1 5	0 0 0 0 4	3727.69540	-0.00005	3746.70164	19.00619
1 1 1 -1 6	0 0 0 0 5	3729.56705	0.00005	3758.07598	28.50898
1 1 1 -1 7	0 0 0 0 6	3731.43516	0.00038	3771.34682	39.91204
1 1 1 -1 8	0 0 0 0 7	3733.29884	-0.00045	3786.51453	53.21523
1 1 1 -1 9	0 0 0 0 8	3735.16045	-0.00065	3803.57948	68.41838
1 1 1 -1 10	0 0 0 0 9	3737.02117	0.00035	3822.54211	85.52129
1 1 1 -1 11	0 0 0 0 10	3738.87923	0.00010	3843.40285	104.52373
1 1 1 -1 12	0 0 0 0 11	3740.73688	0.00017	3866.16215	125.42544
1 1 1 -1 13	0 0 0 0 12	3742.59524	0.00095	3890.82045	148.22616
1 1 1 -1 14	0 0 0 0 13	3744.45251	-0.00006	3917.37815	172.92558
1 1 1 -1 15	0 0 0 0 14	3746.31706*	0.00481	3945.83562	199.52337 †
1 1 1 -1 16	0 0 0 0 15	3748.17486	0.00091	3976.19315	228.01920
1 1 1 -1 17	0 0 0 0 16	3750.03864	0.00037	4008.45095	258.41268
1 1 1 -1 18	0 0 0 0 17	3751.90610	0.00039	4042.60912	290.70340
1 1 1 -1 19	0 0 0 0 18	3753.77693	0.00023	4078.66766	324.89096
1 1 1 -1 20	0 0 0 0 19	3755.65129	-0.00028	4116.62645	360.97488
1 1 1 -1 21	0 0 0 0 20	3757.52959	-0.00096	4156.48526	398.95471

rms = 0.00041 cm⁻¹

$V_3 + V_4 + V_5 (\Sigma^+) \leftarrow V_5 (\Pi)$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 5	0 0 1 -1 5	3043.86958*	-0.00202	3746.70164	702.83004 †
1 1 1 -1 6	0 0 1 -1 6	3043.80854	-0.00046	3758.07598	714.26698
1 1 1 -1 7	0 0 1 -1 7	3043.73853*	0.00140	3771.34682	727.60969 †
1 1 1 -1 8	0 0 1 -1 8	3043.65702	0.00048	3786.51453	742.85799
1 1 1 -1 9	0 0 1 -1 9	3043.56766	-0.00015	3803.57948	760.01168
1 1 1 -1 10	0 0 1 -1 10	3043.47237	0.00078	3822.54211	779.07052
1 1 1 -1 11	0 0 1 -1 11	3043.36757	-0.00102	3843.40285	800.03426 †
1 1 1 -1 12	0 0 1 -1 12	3043.25803*	-0.00151	3866.16215	822.90261 †
1 1 1 -1 13	0 0 1 -1 13	3043.14662	0.00145	3890.82045	847.67528 †
1 1 1 -1 14	0 0 1 -1 14	3043.02643	0.00021	3917.37815	874.35193

rms = 0.00047 cm⁻¹

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$$V_3 + V_4 + V_5 (\Sigma^+) \leftarrow V_4 + V_5 (\Sigma^+)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 1 1 -1 0	1 1 1 -1 1	2528.94851	0.00001	3718.26853	1189.32003
1 1 1 -1 1	1 1 1 -1 2	2527.02846	-0.00047	3720.16395	1193.13502
1 1 1 -1 2	1 1 1 -1 3	2525.09671	-0.00048	3723.95484	1198.85764
1 1 1 -1 3	1 1 1 -1 4	2523.15299	-0.00024	3729.64130	1206.48808
1 1 1 -1 4	1 1 1 -1 5	2521.19689	-0.00006	3737.22350	1216.02655
1 1 1 -1 5	1 1 1 -1 6	2519.22838	0.00008	3746.70164	1227.47333
1 1 1 -1 6	1 1 1 -1 7	2517.24707	-0.00013	3758.07598	1240.82878
1 1 1 -1 7	1 1 1 -1 8	2515.25380	0.00024	3771.34682	1256.09326
1 1 1 -1 8	1 1 1 -1 9	2513.24716	-0.00017	3786.51453	1273.26720
1 1 1 -1 9	1 1 1 -1 10	2511.22829	-0.00013	3803.57948	1292.35106
1 1 1 -1 10	1 1 1 -1 11	2509.19692	0.00013	3822.54211	1313.34532
1 1 1 -1 11	1 1 1 -1 12	2507.15261	0.00020	3843.40285	1336.25044
1 1 1 -1 12	1 1 1 -1 13	2505.09538	0.00012	3866.16215	1361.06689
1 1 1 -1 13	1 1 1 -1 14	2503.02563	0.00027	3890.82045	1387.79509
1 1 1 -1 14	1 1 1 -1 15	2500.94294	0.00019	3917.37815	1416.43541
1 1 1 -1 15	1 1 1 -1 16	2498.84741	-0.00009	3945.83562	1446.98812
1 1 1 -1 16	1 1 1 -1 17	2496.73974	0.00001	3976.19315	1479.45342
1 1 1 -1 17	1 1 1 -1 18	2494.61949	-0.00008	4008.45095	1513.83138
1 1 1 -1 18	1 1 1 -1 19	2492.48704	-0.00013	4042.60912	1550.12195
1 1 1 -1 19	1 1 1 -1 20	2490.34233	-0.00037	4078.66766	1588.32496
1 1 1 -1 20	1 1 1 -1 21	2488.18601	-0.00033	4116.62645	1628.44012
1 1 1 -1 21	1 1 1 -1 22	2486.01898	0.00073	4156.48526	1670.46701
1 1 1 -1 22	1 1 1 -1 23	2483.83793	-0.00067	4198.24373	1714.40513
1 1 1 -1 23	1 1 1 -1 24	2481.64740	-0.00014	4241.90140	1760.25386
1 1 1 -1 24	1 1 1 -1 25	2479.44555	0.00036	4287.45771	1808.01252
1 1 1 -1 25	1 1 1 -1 26	2477.23253	0.00086	4334.91203	1857.68035
1 1 1 -1 26	1 1 1 -1 27	2475.00727	0.00018	4384.26363	1909.25654
1 1 1 -1 27	1 1 1 -1 28	2472.77725	0.000574	4435.51173	1962.74023 †
1 1 1 -1 1	1 1 1 -1 0	2532.75173	0.00035	3720.16395	1187.41257
1 1 1 -1 2	1 1 1 -1 1	2534.63497	0.00016	3723.95484	1189.32003
1 1 1 -1 3	1 1 1 -1 2	2536.50574	-0.00054	3729.64130	1193.13502
1 1 1 -1 4	1 1 1 -1 3	2538.36583	-0.00003	3737.22350	1198.85764
1 1 1 -1 5	1 1 1 -1 4	2540.21354	-0.00002	3746.70164	1206.48808
1 1 1 -1 6	1 1 1 -1 5	2542.04932	-0.00011	3758.07598	1216.02655
1 1 1 -1 7	1 1 1 -1 6	2543.87392	0.00043	3771.34682	1227.47333
1 1 1 -1 8	1 1 1 -1 7	2545.68676*	0.00101	3786.51453	1240.82878 †
1 1 1 -1 9	1 1 1 -1 8	2547.48649	0.00027	3803.57948	1256.09326
1 1 1 -1 10	1 1 1 -1 9	2549.27518	0.00027	3822.54211	1273.26720
1 1 1 -1 11	1 1 1 -1 10	2551.05173	-0.00006	3843.40285	1292.35106
1 1 1 -1 12	1 1 1 -1 11	2552.81695	0.00012	3866.16215	1313.34532
1 1 1 -1 13	1 1 1 -1 12	2554.56987	-0.00014	3890.82045	1336.25044
1 1 1 -1 14	1 1 1 -1 13	2556.30962	-0.00164	3917.37815	1361.06689 †
1 1 1 -1 15	1 1 1 -1 14	2558.04060	0.00007	3945.83562	1387.79509
1 1 1 -1 16	1 1 1 -1 15	2559.75779	0.00005	3976.19315	1416.43541
1 1 1 -1 17	1 1 1 -1 16	2561.46286	0.00003	4008.45095	1446.98812
1 1 1 -1 18	1 1 1 -1 17	2563.15533	-0.00037	4042.60912	1479.45342
1 1 1 -1 19	1 1 1 -1 18	2564.83596	-0.00032	4078.66766	1513.83138
1 1 1 -1 20	1 1 1 -1 19	2566.50403	-0.00047	4116.62645	1550.12195
1 1 1 -1 21	1 1 1 -1 20	2568.15952	-0.00078	4156.48526	1588.32496
1 1 1 -1 22	1 1 1 -1 21	2569.80312	-0.00049	4198.24373	1628.44012
1 1 1 -1 23	1 1 1 -1 22	2571.43417	-0.00022	4241.90140	1670.46701
1 1 1 -1 24	1 1 1 -1 23	2573.05239	-0.00019	4287.45771	1714.40513
1 1 1 -1 25	1 1 1 -1 24	2574.65869	0.00052	4334.91203	1760.25386
1 1 1 -1 26	1 1 1 -1 25	2576.25379	0.00268	4384.26363	1808.01252 †
1 1 1 -1 27	1 1 1 -1 26	2577.83725	0.00587	4435.51173	1857.68035 †
1 1 1 -1 28	1 1 1 -1 27	2579.41004	0.01107	4488.65551	1909.25654 †
1 1 1 -1 29	1 1 1 -1 28	2580.95436	0.00051	4543.69408	1962.74023

rms = 0.00034 cm⁻¹

$$V_3 + V_4 + V_5 (\Sigma^-) \leftarrow V_5 (\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''	
1 -1 1 1 4	0 0 1 1 4	3039.98442	0.00101	3733.21722	693.23382	†
1 -1 1 1 5	0 0 1 1 5	3039.96221	-0.00019	3742.69464	702.73224	
1 -1 1 1 6	0 0 1 1 6	3039.93559*	-0.00185	3754.06751	714.13007	†
1 -1 1 1 7	0 0 1 1 7	3039.90830	-0.00035	3767.33581	727.42716	
1 -1 1 1 8	0 0 1 1 8	3039.87658	0.00042	3782.49949	742.62333	
1 -1 1 1 9	0 0 1 1 9	3039.83986	-0.00025	3799.55849	759.71839	
1 -1 1 1 10	0 0 1 1 10	3039.80163	0.00100	3818.51273	778.71209	
1 -1 1 1 11	0 0 1 1 11	3039.75998*	0.00213	3839.36205	799.60420	†
1 -1 1 1 12	0 0 1 1 12	3039.71201	0.00016	3862.10630	822.39444	
1 -1 1 1 13	0 0 1 1 13	3039.66220	-0.00052	3886.74523	847.08251	
1 -1 1 1 14	0 0 1 1 14	3039.61198	0.00150	3913.27856	873.66808	†
1 -1 1 1 15	0 0 1 1 15	3039.55562	0.00046	3941.70595	902.15079	
1 -1 1 1 16	0 0 1 1 16	3039.49448*	-0.00227	3972.02703	932.53028	†

rms = 0.00049 cm⁻¹

$$V_3 + V_4 + V_5 (\Sigma^-) \leftarrow V_4 + V_5 (\Sigma^-)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''	
1 -1 1 1 0	1 -1 1 1 1	2528.60638*	-0.00397	3714.26233	1185.65198	†
1 -1 1 1 1	1 -1 1 1 2	2526.69000	-0.00076	3716.15782	1189.46706	
1 -1 1 1 2	1 -1 1 1 3	2524.75905	-0.00008	3719.94880	1195.18967	
1 -1 1 1 3	1 -1 1 1 4	2522.81529	-0.00022	3725.63527	1202.81976	
1 -1 1 1 4	1 -1 1 1 5	2520.85937	-0.00055	3733.21722	1212.35731	
1 -1 1 1 5	1 -1 1 1 6	2518.89147	-0.00093	3742.69464	1223.80224	
1 -1 1 1 6	1 -1 1 1 7	2516.91302	0.00001	3754.06751	1237.15450	
1 -1 1 1 7	1 -1 1 1 8	2514.92156	-0.00024	3767.33581	1252.41400	
1 -1 1 1 8	1 -1 1 1 9	2512.91879	-0.00005	3782.49949	1269.58065	
1 -1 1 1 9	1 -1 1 1 10	2510.90519*	0.00102	3799.55849	1288.65432	†
1 -1 1 1 10	1 -1 1 1 11	2508.87793	0.00007	3818.51273	1309.63487	
1 -1 1 1 11	1 -1 1 1 12	2506.84017	0.00021	3839.36205	1332.52210	
1 -1 1 1 12	1 -1 1 1 13	2504.79080	0.00030	3862.10630	1357.31580	
1 -1 1 1 13	1 -1 1 1 14	2502.72969	0.00017	3886.74523	1384.01571	
1 -1 1 1 14	1 -1 1 1 15	2500.65740	0.00036	3913.27856	1412.62152	
1 -1 1 1 15	1 -1 1 1 16	2498.57287	-0.00019	3941.70595	1443.13289	
1 -1 1 1 16	1 -1 1 1 17	2496.47991*	0.00231	3972.02703	1475.54942	†
1 -1 1 1 17	1 -1 1 1 18	2494.37097	0.00030	4004.24137	1509.87069	
1 -1 1 1 18	1 -1 1 1 19	2492.25233	0.00005	4038.34851	1546.09623	
1 -1 1 1 19	1 -1 1 1 20	2490.12258	0.00014	4074.34795	1584.22551	
1 -1 1 1 20	1 -1 1 1 21	2487.98110	-0.00007	4112.33919	1624.25802	
1 -1 1 1 21	1 -1 1 1 22	2485.82853	0.00004	4152.02166	1666.19317	
1 -1 1 1 22	1 -1 1 1 23	2483.66424	-0.00020	4193.69481	1710.03037	
1 -1 1 1 23	1 -1 1 1 24	2481.48888	-0.00015	4237.25802	1755.76899	
1 -1 1 1 24	1 -1 1 1 25	2479.30450*	0.00219	4282.71070	1803.40839	†
1 -1 1 1 25	1 -1 1 1 26	2477.10373	-0.00057	4330.05219	1852.94788	
1 -1 1 1 26	1 -1 1 1 27	2474.89462	-0.00043	4379.28182	1904.38677	
1 -1 1 1 27	1 -1 1 1 28	2472.67381	-0.00079	4430.39893	1957.72433	
1 -1 1 1 28	1 -1 1 1 29	2470.44275	-0.00023	4483.40278	2012.95980	
1 -1 1 1 29	1 -1 1 1 30	2468.20069	0.00045	4538.29266	2070.09242	
1 -1 1 1 30	1 -1 1 1 31	2465.94951	0.00309	4595.06780	2129.12138	†
1 -1 1 1 1	1 -1 1 1 0	2532.41462*	0.00123	3716.15782	1183.74443	†
1 -1 1 1 2	1 -1 1 1 1	2534.29665	-0.00018	3719.94880	1185.65198	
1 -1 1 1 3	1 -1 1 1 2	2536.16813	-0.00008	3725.63527	1189.46706	
1 -1 1 1 4	1 -1 1 1 3	2538.02716	-0.00039	3733.21722	1195.18967	
1 -1 1 1 5	1 -1 1 1 4	2539.87492	0.00004	3742.69464	1202.81976	
1 -1 1 1 6	1 -1 1 1 5	2541.70986	-0.00035	3754.06751	1212.35731	
1 -1 1 1 7	1 -1 1 1 6	2543.53352	-0.00005	3767.33581	1223.80224	

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1														
2	1	-1	1	1	8	1	-1	1	1	7	2545.34522	0.00023	3782.49949	1237.15450
3	1	-1	1	1	9	1	-1	1	1	8	2547.14463	0.00014	3799.55849	1252.41400
4	1	-1	1	1	10	1	-1	1	1	9	2548.93239	0.00032	3818.51273	1269.58065
5	1	-1	1	1	11	1	-1	1	1	10	2550.70804	0.00031	3839.36205	1288.65432
6	1	-1	1	1	12	1	-1	1	1	11	2552.47165	0.00022	3862.10630	1309.63487
7	1	-1	1	1	13	1	-1	1	1	12	2554.22319	0.00006	3886.74523	1332.52210
8	1	-1	1	1	14	1	-1	1	1	13	2555.96315	0.00039	3913.27856	1357.31580
9	1	-1	1	1	15	1	-1	1	1	14	2557.69054	0.00030	3941.70595	1384.01571
10	1	-1	1	1	16	1	-1	1	1	15	2559.40628	0.00077	3972.02703	1412.62152
11	1	-1	1	1	17	1	-1	1	1	16	2561.10941	0.00093	4004.24137	1443.13289
12	1	-1	1	1	18	1	-1	1	1	17	2562.79973	0.00065	4038.34851	1475.54942
13	1	-1	1	1	19	1	-1	1	1	18	2564.47365*	-0.00361	4074.34795	1509.87069 +
14	1	-1	1	1	20	1	-1	1	1	19	2566.14292	-0.00004	4112.23919	1546.09623
15	1	-1	1	1	21	1	-1	1	1	20	2567.79601	-0.00014	4152.02166	1584.22551
16	1	-1	1	1	22	1	-1	1	1	21	2569.43630*	-0.00049	4193.69481	1624.25802
17	1	-1	1	1	23	1	-1	1	1	22	2571.06478	-0.00007	4237.25802	1666.19317
18	1	-1	1	1	24	1	-1	1	1	23	2572.68050	0.00017	4282.71070	1710.03037
19	1	-1	1	1	25	1	-1	1	1	24	2574.28241	-0.00078	4330.05219	1755.76899
20	1	-1	1	1	26	1	-1	1	1	25	2575.87296	-0.00047	4379.28182	1803.40839
21	1	-1	1	1	27	1	-1	1	1	26	2577.44987	-0.00117	4430.39893	1852.94788 +
22	1	-1	1	1	28	1	-1	1	1	27	2579.01626	0.00025	4483.40278	1904.38677
23	1	-1	1	1	29	1	-1	1	1	28	2580.56900	0.00067	4538.29266	1957.72433
24	1	-1	1	1	30	1	-1	1	1	29	2582.11103	0.00303	4595.06780	2012.95980 +

rms = 0.00039 cm⁻¹

$$V_3 + V_4 + V_5 (\Delta) \leftarrow V_4 + V_5 (\Delta)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 1 1 1 2	1 1 1 1 3	2524.82187*	0.00128	3719.72668	1194.90609 †
1 1 1 1 3	1 1 1 1 4	2522.87713	-0.00051	3725.41270	1202.53506
1 1 1 1 4	1 1 1 1 5	2520.92217	-0.00095	3732.99358	1212.07046
1 1 1 1 5	1 1 1 1 6	2518.95585*	-0.00130	3742.46889	1223.51174 †
1 1 1 1 6	1 1 1 1 7	2516.97623*	-0.00365	3753.83813	1236.85825 †
1 1 1 1 7	1 1 1 1 8	2514.99165	0.00022	3767.10068	1252.10924
1 1 1 1 8	1 1 1 1 9	2512.99247*	0.00054	3782.25581	1269.26388
1 1 1 1 9	1 1 1 1 10	2510.98133	-0.00018	3799.30274	1288.32123
1 1 1 1 10	1 1 1 1 11	2508.96002	-0.00025	3818.24057	1309.28031
1 1 1 1 11	1 1 1 1 12	2506.92827	-0.00003	3839.06836	1332.14005
1 1 1 1 12	1 1 1 1 13	2504.88537	-0.00032	3861.78507	1356.89938
1 1 1 1 13	1 1 1 1 14	2502.83234	-0.00013	3886.38967	1383.55720
1 1 1 1 14	1 1 1 1 15	2500.76853	-0.00012	3912.88106	1412.11241
1 1 1 1 15	1 1 1 1 16	2498.69440	0.00017	3941.25817	1442.56394
1 1 1 1 16	1 1 1 1 17	2496.60933	0.00018	3971.51993	1474.91078
1 1 1 1 17	1 1 1 1 18	2494.51366	0.00031	4003.66531	1509.15197
1 1 1 1 18	1 1 1 1 19	2492.40687	0.00015	4037.69333	1545.28661
1 1 1 1 19	1 1 1 1 20	2490.28975	0.00057	4073.60306	1583.31388
1 1 1 1 20	1 1 1 1 21	2488.16123	0.00063	4111.39364	1623.23305
1 1 1 1 21	1 1 1 1 22	2486.01898*	-0.00189	4151.06428	1665.04341 †
1 1 1 1 22	1 1 1 1 23	2483.87291	0.00300	4192.61426	1708.74434 †
1 1 1 1 23	1 1 1 1 24	2481.70538	-0.00225	4236.04289	1754.33526 †
1 1 1 1 24	1 1 1 1 25	2479.53305	-0.00091	4281.34955	1801.81559
1 1 1 1 25	1 1 1 1 26	2477.34829	-0.00056	4328.53365	1851.18480
1 1 1 1 26	1 1 1 1 27	2475.15279	0.00051	4377.59461	1902.44233
1 1 1 1 27	1 1 1 1 28	2472.94416	-0.00007	4428.53189	1955.58766
1 1 1 1 28	1 1 1 1 29	2470.72500	0.00029	4481.34492	2010.62021
1 1 1 1 29	1 1 1 1 30	2468.49080*	-0.00292	4536.03314	2067.53942 †
1 1 1 1 30	1 1 1 1 31	2466.25130	0.00000	4592.59597	2126.34468
1 1 1 1 3	1 1 1 1 2	2536.22877	0.00004	3725.41270	1189.18398
1 1 1 1 4	1 1 1 1 3	2538.08743	-0.00006	3732.99358	1194.90609
1 1 1 1 5	1 1 1 1 4	2539.93441	0.00058	3742.46889	1202.53506

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1														
2	1	-1	1	-1	15	1	-1	1	-1	14	2557.71315	-0.00013	3941.39062	1383.67734
3	1	-1	1	-1	16	1	-1	1	-1	15	2559.42122	-0.00049	3971.69004	1412.26833
4	1	-1	1	-1	17	1	-1	1	-1	16	2561.11834	0.00077	4003.88015	1442.76257
5	1	-1	1	-1	18	1	-1	1	-1	17	2562.79973*	-0.00118	4037.96055	1475.15963 +
6	1	-1	1	-1	19	1	-1	1	-1	18	2564.47365*	0.00190	4073.93079	1509.45905 +
7	1	-1	1	-1	20	1	-1	1	-1	19	2566.12961	-0.00047	4111.79043	1545.66036
8	1	-1	1	-1	21	1	-1	1	-1	20	2567.77541	-0.00050	4151.53898	1583.76307
9	1	-1	1	-1	22	1	-1	1	-1	21	2569.40940	0.00017	4193.17592	1623.76670
10	1	-1	1	-1	23	1	-1	1	-1	22	2571.03008	0.00005	4236.70073	1665.67070
11	1	-1	1	-1	24	1	-1	1	-1	23	2572.63804	-0.00025	4282.11283	1709.47454
12	1	-1	1	-1	25	1	-1	1	-1	24	2574.23396	-0.00002	4329.41163	1755.17765
13	1	-1	1	-1	26	1	-1	1	-1	25	2575.81714	0.00005	4378.59651	1802.77942
14	1	-1	1	-1	27	1	-1	1	-1	26	2577.38897	0.00139	4429.66681	1852.27923 +
15	1	-1	1	-1	28	1	-1	1	-1	27	2578.94706	0.00163	4482.62185	1903.67642 +
16	1	-1	1	-1	29	1	-1	1	-1	28	2580.49527	0.00466	4537.46094	1956.97033 +
17	1	-1	1	-1	30	1	-1	1	-1	29	2582.03327	0.01018	4594.18333	2012.16024 +
18	1	1	1	1	2	1	-1	1	-1	2	2530.54266	0.00002	3719.72668	1189.18404
19	1	1	1	1	3	1	-1	1	-1	3	2530.50771	0.00143	3725.41270	1194.90643 +
20	1	1	1	1	4	1	-1	1	-1	4	2530.45795	0.00045	3732.99358	1202.53608
21	1	1	1	1	5	1	-1	1	-1	5	2530.39800*	0.00193	3742.46889	1212.07282 +
22	1	1	1	1	6	1	-1	1	-1	6	2530.32155	-0.00012	3753.83813	1223.51646
23	1	1	1	1	7	1	-1	1	-1	7	2530.23394	0.00001	3767.10068	1236.86675
24	1	1	1	1	8	1	-1	1	-1	8	2530.13234	-0.00008	3782.25581	1252.12340
25	1	1	1	1	9	1	-1	1	-1	9	2530.04819*	0.03154	3799.30274	1269.28609 +
26	1	1	1	1	10	1	-1	1	-1	10	2529.88570	-0.00040	3818.24057	1288.35448
27	1	1	1	1	11	1	-1	1	-1	11	2529.74166*	0.00150	3839.06836	1309.32820 +
28	1	1	1	1	12	1	-1	1	-1	12	2529.57795	-0.00027	3861.78507	1332.20685
29	1	1	1	1	13	1	-1	1	-1	13	2529.39792*	-0.00171	3886.38967	1356.99004 +
30	1	1	1	1	14	1	-1	1	-1	14	2529.20368	-0.00004	3912.88106	1383.67734
31	1	1	1	1	15	1	-1	1	-1	15	2528.98955	-0.00029	3941.25817	1412.26833
32	1	-1	1	-1	2	1	1	1	1	2	2530.54266	-0.00010	3719.72674	1189.18398
33	1	-1	1	-1	3	1	1	1	1	3	2530.50771	0.00082	3725.41298	1194.90609
34	1	-1	1	-1	4	1	1	1	1	4	2530.45795	-0.00139	3732.99440	1202.53506 +
35	1	-1	1	-1	5	1	1	1	1	5	2530.39800*	-0.00235	3742.47081	1212.07046 +
36	1	-1	1	-1	6	1	1	1	1	6	2530.32991	-0.00031	3753.84196	1223.51174
37	1	-1	1	-1	7	1	1	1	1	7	2530.24927	-0.00006	3767.10758	1236.85825
38	1	-1	1	-1	8	1	1	1	1	8	2530.15790	-0.00020	3782.26734	1252.10924
39	1	-1	1	-1	9	1	1	1	1	9	2530.04819*	-0.00883	3799.32090	1269.26388 +
40	1	-1	1	-1	10	1	1	1	1	10	2529.94659	-0.00005	3818.26787	1288.32123
41	1	-1	1	-1	11	1	1	1	1	11	2529.82738	-0.00020	3839.10789	1309.28031
42	1	-1	1	-1	12	1	1	1	1	12	2529.70103	0.00052	3861.84056	1332.14005
43	1	-1	1	-1	13	1	1	1	1	13	2529.56530	-0.00081	3886.46550	1356.89938

rms = 0.00043 cm⁻¹

45
46
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48
49

$2\nu_3(\Sigma^+) \leftarrow G.S.(\Sigma^+)$

51	ν_4'	ℓ_4'	ν_5'	ℓ_5'	J'	ν_4''	ℓ_4''	ν_5''	ℓ_5''	J''	OBS	OBS – CALC	E'	E''
52	0	0	0	0	0	0	0	0	0	1	5047.28382	-0.00061	5049.18509	1.90066
53	0	0	0	0	1	0	0	0	0	2	5045.35845	-0.00070	5051.06109	5.70195
54	0	0	0	0	2	0	0	0	0	3	5043.40894	-0.00033	5054.81309	11.40382
55	0	0	0	0	3	0	0	0	0	4	5041.43441	-0.00042	5060.44102	19.00619
56	0	0	0	0	4	0	0	0	0	5	5039.43567	-0.00017	5067.94481	28.50898
57	0	0	0	0	5	0	0	0	0	6	5037.41215	-0.00018	5077.32437	39.91204
58	0	0	0	0	6	0	0	0	0	7	5035.36439	0.00006	5088.57957	53.21523
59	0	0	0	0	7	0	0	0	0	8	5033.29219	0.00031	5101.71026	68.41838
60	0	0	0	0	8	0	0	0	0	9	5031.19587	0.00088	5116.71628	85.52129
	0	0	0	0	9	0	0	0	0	10	5029.07492	0.00122	5133.59742	104.52373 †
	0	0	0	0	10	0	0	0	0	11	5026.92962	0.00158	5152.35347	125.42544 †
	0	0	0	0	11	0	0	0	0	12	5024.76009	0.00206	5172.98419	148.22616 †
	0	0	0	0	12	0	0	0	0	13	5022.56631	0.00259	5195.48929	172.92558 †

$$\text{rms} = 0.00048 \text{ cm}^{-1}$$

$2\nu_3 + \nu_4 (\Pi) \leftarrow \nu_4 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
1 -1 0 0 1	1 -1 0 0 2	5016.24056	-0.00033	5531.55405	515.31316
1 -1 0 0 2	1 -1 0 0 3	5014.28319	-0.00048	5535.32468	521.04101
1 -1 0 0 3	1 -1 0 0 4	5012.30204	-0.00050	5540.98055	528.67801
1 -1 0 0 4	1 -1 0 0 5	5010.29626	-0.00127	5548.52160	538.22407
1 -1 0 0 5	1 -1 0 0 6	5008.26886	0.00020	5557.94771	549.67906
1 -1 0 0 6	1 -1 0 0 7	5006.21702	0.00106	5569.25877	563.04281
1 -1 0 0 7	1 -1 0 0 8	5004.14025*	0.00079	5582.45460	578.31514
1 -1 0 0 8	1 -1 0 0 9	5002.04173	0.00253	5597.53505	595.49585 †
1 -1 0 0 9	1 -1 0 0 10	4999.92035	0.00516	5614.49989	614.58469 †
1 -1 0 0 10	1 -1 0 0 11	4997.79805	0.03058	5633.34889	635.58142 †
1 -1 0 0 11	1 -1 0 0 12	4995.58924	-0.00684	5654.08181	658.48573 †
1 -1 0 0 12	1 -1 0 0 13	4993.39767	-0.00336	5676.69835	683.29732 †
1 -1 0 0 13	1 -1 0 0 14	4991.18063	-0.00173	5701.19820	710.01584
1 -1 0 0 14	1 -1 0 0 15	4988.93899	-0.00112	5727.58104	738.64093
1 -1 0 0 15	1 -1 0 0 16	4986.67296	-0.00133	5755.84650	769.17220
1 -1 0 0 16	1 -1 0 0 17	4984.38396	-0.00100	5785.99419	801.60923
1 -1 0 0 17	1 -1 0 0 18	4982.07145	-0.00068	5818.02370	835.95156
1 -1 0 0 18	1 -1 0 0 19	4979.73551	-0.00034	5851.93459	872.19874
1 -1 0 0 19	1 -1 0 0 20	4977.37670	0.00056	5887.72641	910.35027
1 -1 0 0 20	1 -1 0 0 21	4974.99393	0.00089	5925.39865	950.40561
1 -1 0 0 21	1 -1 0 0 22	4972.58786	0.00128	5964.95082	992.36423
1 -1 0 0 22	1 -1 0 0 23	4970.15715	0.00035	6006.38235	1036.22555
1 -1 0 0 23	1 -1 0 0 24	4967.70433	0.00059	6049.69270	1081.98896
1 -1 0 0 24	1 -1 0 0 25	4965.22788	0.00046	6094.88126	1129.65384
1 -1 0 0 25	1 -1 0 0 26	4962.72709	-0.00079	6141.94742	1179.21954
1 -1 0 0 26	1 -1 0 0 27	4960.20498	-0.00018	6190.89054	1230.68537
1 -1 0 0 2	1 -1 0 0 1	5023.83045	0.00033	5535.32468	511.49456
1 -1 0 0 3	1 -1 0 0 2	5025.66784	0.00045	5540.98055	515.31316
1 -1 0 0 4	1 -1 0 0 3	5027.48052	-0.00007	5548.52160	521.04101
1 -1 0 0 5	1 -1 0 0 4	5029.27021	0.00051	5557.94771	528.67801
1 -1 0 0 6	1 -1 0 0 5	5031.03483	0.00014	5569.25877	538.22407
1 -1 0 0 7	1 -1 0 0 6	5032.77671	0.00116	5582.45460	549.67906
1 -1 0 0 8	1 -1 0 0 7	5034.49381	0.00157	5597.53505	563.04281
1 -1 0 0 9	1 -1 0 0 8	5036.18607	0.00132	5614.49989	578.31514
1 -1 0 0 10	1 -1 0 0 9	5037.88354	0.03049	5633.34889	595.49585 †
1 -1 0 0 11	1 -1 0 0 10	5039.49009	-0.00702	5654.08181	614.58469 †
1 -1 0 0 12	1 -1 0 0 11	5041.11348	-0.00345	5676.69835	635.58142 †
1 -1 0 0 13	1 -1 0 0 12	5042.71046*	-0.00201	5701.19820	658.48573 †
1 -1 0 0 14	1 -1 0 0 13	5044.28239	-0.00133	5727.58104	683.29732
1 -1 0 0 15	1 -1 0 0 14	5045.83000	-0.00065	5755.84650	710.01584
1 -1 0 0 16	1 -1 0 0 15	5047.35221	-0.00104	5785.99419	738.64093
1 -1 0 0 17	1 -1 0 0 16	5048.85144	-0.00006	5818.02370	769.17220
1 -1 0 0 18	1 -1 0 0 17	5050.32502	-0.00035	5851.93459	801.60923
1 -1 0 0 19	1 -1 0 0 18	5051.77621	0.00137	5887.72641	835.95156
1 -1 0 0 20	1 -1 0 0 19	5053.20004	0.00013	5925.39865	872.19874
1 -1 0 0 21	1 -1 0 0 20	5054.60119	0.00064	5964.95082	910.35027
1 -1 0 0 22	1 -1 0 0 21	5055.97718	0.00044	6006.38235	950.40561
1 -1 0 0 23	1 -1 0 0 22	5057.32937	0.00090	6049.69270	992.36423
1 -1 0 0 24	1 -1 0 0 23	5058.65826	0.00255	6094.88126	1036.22555 †
1 -1 0 0 25	1 -1 0 0 24	5059.95779	-0.00067	6141.94742	1081.98896
1 -1 0 0 26	1 -1 0 0 25	5061.23428	-0.00241	6190.89054	1129.65384 †
1 -1 0 0 27	1 -1 0 0 26	5062.48975	-0.00065	6241.70994	1179.21954
1 -1 0 0 28	1 -1 0 0 27	5063.70228*	-0.01728	6294.40494	1230.68537 †
1 -1 0 0 29	1 -1 0 0 28	5064.91737*	-0.00680	6348.97481	1284.05064 †
1 1 0 0 1	1 1 0 0 2	5016.25637	-0.00098	5531.54565	515.28830
1 1 0 0 2	1 1 0 0 3	5014.30985	0.00167	5535.29947	520.99129
1 1 0 0 3	1 1 0 0 4	5012.33512	0.00013	5540.93014	528.59515
1 1 0 0 4	1 1 0 0 5	5010.33784	0.00004	5548.43759	538.09979
1 1 0 0 5	1 1 0 0 6	5008.31723	0.00060	5557.82171	549.50508
1 1 0 0 6	1 1 0 0 7	5006.27299	0.00147	5569.08239	562.81086

$$\text{rms} = 0.00094 \text{ cm}^{-1}$$

$$2v_3 + v_5(\Pi) \leftarrow v_5(\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 1 -1 1	0 0 1 -1 2	5039.71861	0.00102	5719.67283	679.95524
0 0 1 -1 2	0 0 1 -1 3	5037.76092	-0.00082	5723.43579	685.67405
0 0 1 -1 3	0 0 1 -1 4	5035.78114	-0.00002	5729.08018	693.29902
0 0 1 -1 4	0 0 1 -1 5	5033.77598	0.00011	5736.60591	702.83004
0 0 1 -1 5	0 0 1 -1 6	5031.74607	0.00016	5746.01289	714.26698
0 0 1 -1 6	0 0 1 -1 7	5029.69304	0.00174	5757.30099	727.60969
0 0 1 -1 7	0 0 1 -1 8	5027.61054	-0.00153	5770.47006	742.85799
0 0 1 -1 8	0 0 1 -1 9	5025.50825	0.00000	5785.51993	760.01168

1	0	0	1	-1	9	0	0	1	-1	10	5023.38166	0.00178	5802.45039	779.07052
2	0	0	1	-1	10	0	0	1	-1	11	5021.22718	0.00021	5821.26123	800.03426
3	0	0	1	-1	11	0	0	1	-1	12	5019.05001	0.00044	5841.95218	822.90261
4	0	0	1	-1	12	0	0	1	-1	13	5016.84925	0.00155	5864.52298	847.67528
5	0	0	1	-1	13	0	0	1	-1	14	5014.62134	-0.00006	5888.97333	874.35193
6	0	0	1	-1	14	0	0	1	-1	15	5012.37107	0.00037	5915.30289	902.93220
7	0	0	1	-1	15	0	0	1	-1	16	5010.09603	0.00040	5943.51133	933.41570
8	0	0	1	-1	16	0	0	1	-1	17	5007.79532	-0.00091	5973.59827	965.80204
9	0	0	1	-1	17	0	0	1	-1	18	5005.47256	0.00002	6005.56330	1000.09076
10	0	0	1	-1	18	0	0	1	-1	19	5003.12416	-0.00042	6039.40601	1036.28142
11	0	0	1	-1	19	0	0	1	-1	20	5000.75225	-0.00015	6075.12593	1074.37353
12	0	0	1	-1	20	0	0	1	-1	21	4998.35623	0.00020	6112.72261	1114.36658
13	0	0	1	-1	21	0	0	1	-1	22	4995.93609	0.00058	6152.19553	1156.26002
14	0	0	1	-1	22	0	0	1	-1	23	4993.49650*	0.00562	6193.54418	1200.05331 +
15	0	0	1	-1	23	0	0	1	-1	24	4991.02966*	0.00749	6236.76801	1245.74584 +
16	0	0	1	-1	3	0	0	1	-1	2	5049.12726	0.00232	5729.08018	679.95524 +
17	0	0	1	-1	4	0	0	1	-1	3	5050.93114	-0.00072	5736.60591	685.67405
18	0	0	1	-1	5	0	0	1	-1	4	5052.71220	-0.00167	5746.01289	693.29902
19	0	0	1	-1	6	0	0	1	-1	5	5054.46960	-0.00135	5757.30099	702.83004
20	0	0	1	-1	7	0	0	1	-1	6	5056.20225	-0.00083	5770.47006	714.26698
21	0	0	1	-1	8	0	0	1	-1	7	5057.90958	-0.00066	5785.51993	727.60969
22	0	0	1	-1	9	0	0	1	-1	8	5059.59256	0.00016	5802.45039	742.85799
23	0	0	1	-1	10	0	0	1	-1	9	5061.24843	-0.00112	5821.26123	760.01168
24	0	0	1	-1	11	0	0	1	-1	10	5062.88134	-0.00032	5841.95218	779.07052
25	0	0	1	-1	12	0	0	1	-1	11	5064.48834	-0.00038	5864.52298	800.03426
26	0	0	1	-1	13	0	0	1	-1	12	5066.07041	-0.00030	5888.97333	822.90261
27	0	0	1	-1	14	0	0	1	-1	13	5067.62813	0.00052	5915.30289	847.67528
28	0	0	1	-1	15	0	0	1	-1	14	5069.16238	0.00298	5943.51133	874.35193 +
29	0	0	1	-1	16	0	0	1	-1	15	5070.66549	-0.00058	5973.59827	902.93220
30	0	0	1	-1	17	0	0	1	-1	16	5072.14755	-0.00005	6005.56330	933.41570
31	0	0	1	-1	18	0	0	1	-1	17	5073.60660*	0.00263	6039.40601	965.80204 +
32	0	0	1	1	1	0	0	1	1	2	5039.72959*	-0.00120	5719.66647	679.93567
33	0	0	1	1	2	0	0	1	1	3	5037.78080	-0.00099	5723.41672	685.63493
34	0	0	1	1	3	0	0	1	1	4	5035.80814	-0.00007	5729.04203	693.23382
35	0	0	1	1	4	0	0	1	1	5	5033.81003	-0.00006	5736.54233	702.73224
36	0	0	1	1	5	0	0	1	1	6	5031.78805	0.00060	5745.91752	714.13007
37	0	0	1	1	6	0	0	1	1	7	5029.74155	0.00122	5757.16749	727.42716
38	0	0	1	1	7	0	0	1	1	8	5027.67014	0.00140	5770.29207	742.62333
39	0	0	1	1	8	0	0	1	1	9	5025.57341	0.00069	5785.29111	759.71839
40	0	0	1	1	9	0	0	1	1	10	5023.45546	0.00316	5802.16440	778.71209 +
41	0	0	1	1	10	0	0	1	1	11	5021.31071	0.00319	5820.91172	799.60420 +
42	0	0	1	1	11	0	0	1	1	12	5019.13878	0.00039	5841.53283	822.39444
43	0	0	1	1	12	0	0	1	1	13	5016.94423	-0.00072	5864.02746	847.08251
44	0	0	1	1	13	0	0	1	1	14	5014.72819	0.00095	5888.39532	873.66808
45	0	0	1	1	14	0	0	1	1	15	5012.48218	-0.00310	5914.63608	902.15079 +
46	0	0	1	1	15	0	0	1	1	16	5010.21980	0.00068	5942.74940	932.53028
47	0	0	1	1	16	0	0	1	1	17	5007.92766	-0.00112	5972.73492	964.80614
48	0	0	1	1	17	0	0	1	1	18	5005.61683	0.00254	6004.59224	998.97795 +
49	0	0	1	1	18	0	0	1	1	19	5003.27522	-0.00049	6038.32095	1035.04524
50	0	0	1	1	19	0	0	1	1	20	5000.91248	-0.00057	6073.92060	1073.00756
51	0	0	1	1	20	0	0	1	1	21	4998.52531	-0.00104	6111.39074	1112.86438
52	0	0	1	1	21	0	0	1	1	22	4996.11579	0.00013	6150.73086	1154.61520
53	0	0	1	1	22	0	0	1	1	23	4993.67921*	-0.00180	6191.94047	1198.25945
54	0	0	1	1	23	0	0	1	1	24	4991.22348*	0.00104	6235.01900	1243.79656
55	0	0	1	1	3	0	0	1	1	2	5049.10543	-0.00093	5729.04203	679.93567
56	0	0	1	1	4	0	0	1	1	3	5050.90790	0.00050	5736.54233	685.63493
57	0	0	1	1	5	0	0	1	1	4	5052.68219	-0.00152	5745.91752	693.23382
58	0	0	1	1	6	0	0	1	1	5	5054.43636	0.00111	5757.16749	702.73224
59	0	0	1	1	7	0	0	1	1	6	5056.15947	-0.00253	5770.29207	714.13007 +
60	0	0	1	1	8	0	0	1	1	7	5057.86718	0.00323	5785.29111	727.42716 +
	0	0	1	1	9	0	0	1	1	8	5059.54236	0.00130	5802.16440	742.62333
	0	0	1	1	10	0	0	1	1	9	5061.19344	0.00011	5820.91172	759.71839
	0	0	1	1	11	0	0	1	1	10	5062.81952	-0.00122	5841.53283	778.71209
	0	0	1	1	12	0	0	1	1	11	5064.42315	-0.00011	5864.02746	799.60420
	0	0	1	1	13	0	0	1	1	12	5066.00038	-0.00049	5888.39532	822.39444

0	0	1	1	14	0	0	1	1	13	5067.55401	0.00044	5914.63608	847.08251
0	0	1	1	15	0	0	1	1	14	5069.08308	0.00176	5942.74940	873.66808
0	0	1	1	16	0	0	1	1	15	5070.58403	-0.00009	5972.73492	902.15079
0	0	1	1	17	0	0	1	1	16	5072.06277	0.00081	6004.59224	932.53028
0	0	1	1	18	0	0	1	1	17	5073.51480*	-0.00001	6038.32095	964.80614

rms = 0.00085 cm⁻¹

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Quantum number assignments, observed wavenumbers, residuals, and upper and lower state term values (in cm⁻¹) for the $\nu_2 + \nu_3$ and associated hot bands of $^{13}\text{C}_2\text{HD}$ ^a (4 pp)

$\nu_2 + \nu_3 (\Sigma^+) \leftarrow G.S. (\Sigma^+)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS – CALC	E'	E''
0 0 0 0 0	0 0 0 0 1	4336.07868	0.00019	4337.97915	1.90066
0 0 0 0 1	0 0 0 0 2	4334.15849	0.00081	4339.85963	5.70195
0 0 0 0 2	0 0 0 0 3	4332.21756	0.00081	4343.62057	11.40382
0 0 0 0 3	0 0 0 0 4	4330.25599	0.00027	4349.26191	19.00619
0 0 0 0 4	0 0 0 0 5	4328.27455	-0.00006	4356.78359	28.50898
0 0 0 0 5	0 0 0 0 6	4326.27339	-0.00007	4366.18550	39.91204
0 0 0 0 6	0 0 0 0 7	4324.25231	0.00003	4377.46752	53.21523
0 0 0 0 7	0 0 0 0 8	4322.21051	-0.00060	4390.62949	68.41838
0 0 0 0 8	0 0 0 0 9	4320.14974	-0.00022	4405.67125	85.52129
0 0 0 0 9	0 0 0 0 10	4318.06840	-0.00047	4422.59260	104.52373
0 0 0 0 10	0 0 0 0 11	4315.96669	-0.00117	4441.39330	125.42544
0 0 0 0 11	0 0 0 0 12	4313.84627	-0.00069	4462.07311	148.22616
0 0 0 0 12	0 0 0 0 13	4311.70556	-0.00062	4484.63176	172.92558
0 0 0 0 13	0 0 0 0 14	4309.54495	-0.00062	4509.06895	199.52337
0 0 0 0 14	0 0 0 0 15	4307.36500	-0.00015	4535.38435	228.01920
0 0 0 0 15	0 0 0 0 16	4305.16557	0.00064	4563.57761	258.41268
0 0 0 0 16	0 0 0 0 17	4302.94662	0.00166	4593.64836	290.70340
0 0 0 0 17	0 0 0 0 18	4300.70830	0.00305	4625.59620	324.89096 †
0 0 0 0 18	0 0 0 0 19	4298.45188	0.00605	4659.42071	360.97488 †
0 0 0 0 19	0 0 0 0 20	4296.17443	0.00769	4695.12144	398.95471 †
0 0 0 0 20	0 0 0 0 21	4293.88219	0.01420	4732.69792	438.82993 †
0 0 0 0 21	0 0 0 0 22	4291.57549	0.02588	4772.14964	480.60003 †
0 0 0 0 22	0 0 0 0 23	4289.26762	0.05598	4813.47609	524.26445 †
0 0 0 0 23	0 0 0 0 24	4287.03802	0.18393	4856.67671	569.82262 †
0 0 0 0 24	0 0 0 0 25	4284.37644	-0.10056	4901.75094	617.27393 †
0 0 0 0 25	0 0 0 0 26	4282.02147	-0.05893	4948.69817	666.61777 †
0 0 0 0 26	0 0 0 0 27	4279.62082	-0.04349	4997.51778	717.85348 †
0 0 0 0 27	0 0 0 0 28	4277.19308	-0.03567	5048.20914	770.98038 †
0 0 0 0 28	0 0 0 0 29	4274.74579	-0.02798	5100.77155	825.99778 †
0 0 0 0 29	0 0 0 0 30	4272.27750	-0.02188	5155.20433	882.90495 †
0 0 0 0 30	0 0 0 0 31	4269.78867	-0.01694	5211.50676	941.70115 †
0 0 0 0 31	0 0 0 0 32	4267.28286	-0.00964	5269.67809	1002.38559 †
0 0 0 0 32	0 0 0 0 33	4264.76064	0.00057	5329.71754	1064.95747
0 0 0 0 1	0 0 0 0 0	4339.85919	-0.00044	4339.85963	0.00000
0 0 0 0 2	0 0 0 0 1	4341.72071	0.00080	4343.62057	1.90066
0 0 0 0 3	0 0 0 0 2	4343.56080	0.00083	4349.26191	5.70195
0 0 0 0 4	0 0 0 0 3	4345.38018	0.00041	4356.78359	11.40382
0 0 0 0 5	0 0 0 0 4	4347.17929	-0.00002	4366.18550	19.00619
0 0 0 0 6	0 0 0 0 5	4348.95870	0.00016	4377.46752	28.50898
0 0 0 0 7	0 0 0 0 6	4350.71741	-0.00004	4390.62949	39.91204
0 0 0 0 8	0 0 0 0 7	4352.45549	-0.00053	4405.67125	53.21523
0 0 0 0 9	0 0 0 0 8	4354.17361	-0.00060	4422.59260	68.41838
0 0 0 0 10	0 0 0 0 9	4355.87173	-0.00028	4441.39330	85.52129
0 0 0 0 11	0 0 0 0 10	4357.54896	-0.00043	4462.07311	104.52373
0 0 0 0 12	0 0 0 0 11	4359.20547	-0.00085	4484.63176	125.42544
0 0 0 0 13	0 0 0 0 12	4360.84220	-0.00059	4509.06895	148.22616
0 0 0 0 14	0 0 0 0 13	4362.45902	0.00025	4535.38435	172.92558
0 0 0 0 15	0 0 0 0 14	4364.05480	0.00057	4563.57761	199.52337
0 0 0 0 16	0 0 0 0 15	4365.63036	0.00120	4593.64836	228.01920
0 0 0 0 17	0 0 0 0 16	4367.18631	0.00278	4625.59620	258.41268 †
0 0 0 0 18	0 0 0 0 17	4368.72305	0.00574	4659.42071	290.70340 †
0 0 0 0 19	0 0 0 0 18	4370.23848	0.00799	4695.12144	324.89096 †
0 0 0 0 20	0 0 0 0 19	4371.73708	0.01404	4732.69792	360.97488 †
0 0 0 0 21	0 0 0 0 20	4373.22060	0.02567	4772.14964	398.95471 †
0 0 0 0 22	0 0 0 0 21	4374.70207	0.05591	4813.47609	438.82993 †

0	0	0	0	23	0	0	0	0	22	4376.26000	0.18332	4856.67671	480.60003 †
0	0	0	0	24	0	0	0	0	23	4377.38782	-0.09867	4901.75094	524.26445 †
0	0	0	0	25	0	0	0	0	24	4378.81680	-0.05875	4948.69817	569.82262 †
0	0	0	0	26	0	0	0	0	25	4380.20152	-0.04233	4997.51778	617.27393 †
0	0	0	0	27	0	0	0	0	26	4381.55553	-0.03584	5048.20914	666.61777 †
0	0	0	0	28	0	0	0	0	27	4382.88923	-0.02884	5100.77155	717.85348 †
0	0	0	0	29	0	0	0	0	28	4384.19956	-0.02439	5155.20433	770.98038 †
0	0	0	0	30	0	0	0	0	29	4385.49218	-0.01680	5211.50676	825.99778 †
0	0	0	0	31	0	0	0	0	30	4386.76268	-0.01045	5269.67809	882.90495 †
0	0	0	0	32	0	0	0	0	31	4388.01565	-0.00075	5329.71754	941.70115
0	0	0	0	33	0	0	0	0	32	4389.25104	0.01230	5391.62433	1002.38559 †
0	0	0	0	34	0	0	0	0	33	4390.46640	0.02625	5455.39763	1064.95747 †
0	0	0	0	35	0	0	0	0	34	4391.67388	0.05327	5521.03659	1129.41599 †

rms = 0.00064 cm⁻¹

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

$\nu_2 + \nu_3 + \nu_4 (\Pi) \leftarrow \nu_4 (\Pi)$

$\nu_4' \ell_4' \nu_5' \ell_5' J'$	$\nu_4'' \ell_4'' \nu_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
1 -1 0 0 1	1 -1 0 0 2	4315.89016	-0.00314	4831.20646	515.31316 †
1 -1 0 0 2	1 -1 0 0 3	4313.94249	-0.00270	4834.98620	521.04101 †
1 -1 0 0 3	1 -1 0 0 4	4311.96876*	-0.00895	4840.65573	528.67801 †
1 -1 0 0 4	1 -1 0 0 5	4309.98868	-0.00218	4848.21494	538.22407 †
1 -1 0 0 5	1 -1 0 0 6	4307.98098	-0.00366	4857.66370	549.67906 †
1 -1 0 0 6	1 -1 0 0 7	4305.95982	0.00077	4869.00185	563.04281
1 -1 0 0 7	1 -1 0 0 8	4303.91465	0.00059	4882.22920	578.31514
1 -1 0 0 8	1 -1 0 0 9	4301.85137	0.00172	4897.34550	595.49585
1 -1 0 0 9	1 -1 0 0 10	4299.76730	0.00150	4914.35049	614.58469
1 -1 0 0 10	1 -1 0 0 11	4297.66500	0.00253	4933.24389	635.58142 †
1 -1 0 0 11	1 -1 0 0 12	4295.53995	0.00034	4954.02534	658.48573
1 -1 0 0 12	1 -1 0 0 13	4293.40021	0.00303	4976.69450	683.29732 †
1 -1 0 0 13	1 -1 0 0 14	4291.23474	-0.00038	5001.25096	710.01584
1 -1 0 0 14	1 -1 0 0 15	4289.05002	-0.00334	5027.69429	738.64093 †
1 -1 0 0 15	1 -1 0 0 16	4286.84856*	-0.00328	5056.02404	769.17220 †
1 -1 0 0 16	1 -1 0 0 17	4284.62772	-0.00275	5086.23970	801.60923 †
1 -1 0 0 17	1 -1 0 0 18	4282.38433	-0.00485	5118.34074	835.95156 †
1 -1 0 0 18	1 -1 0 0 19	4280.12339	-0.00447	5152.32660	872.19874 †
1 -1 0 0 19	1 -1 0 0 20	4277.84089	-0.00554	5188.19669	910.35027 †
1 -1 0 0 20	1 -1 0 0 21	4275.54422	-0.00055	5225.95038	950.40561
1 -1 0 0 21	1 -1 0 0 22	4273.22005	-0.00272	5265.58701	992.36423 †
1 -1 0 0 22	1 -1 0 0 23	4270.88045	0.00013	5307.10587	1036.22555
1 -1 0 0 23	1 -1 0 0 24	4268.51795	0.00066	5350.50625	1081.98896
1 -1 0 0 2	1 -1 0 0 1	4323.49035	-0.00130	4834.98620	511.49456
1 -1 0 0 3	1 -1 0 0 2	4325.34115	-0.00141	4840.65573	515.31316
1 -1 0 0 4	1 -1 0 0 3	4327.17319	-0.00074	4848.21494	521.04101
1 -1 0 0 5	1 -1 0 0 4	4328.98133	-0.00436	4857.66370	528.67801 †
1 -1 0 0 6	1 -1 0 0 5	4330.77819	0.00041	4869.00185	538.22407
1 -1 0 0 7	1 -1 0 0 6	4332.55094	0.00080	4882.22920	549.67906
1 -1 0 0 8	1 -1 0 0 7	4334.30879	0.00610	4897.34550	563.04281 †
1 -1 0 0 9	1 -1 0 0 8	4336.03630	0.00094	4914.35049	578.31514
1 -1 0 0 10	1 -1 0 0 9	4337.75123	0.00319	4933.24389	595.49585 †
1 -1 0 0 11	1 -1 0 0 10	4339.44048	-0.00017	4954.02534	614.58469
1 -1 0 0 12	1 -1 0 0 11	4341.11345	0.00037	4976.69450	635.58142
1 -1 0 0 13	1 -1 0 0 12	4342.76434	-0.00089	5001.25096	658.48573
1 -1 0 0 14	1 -1 0 0 13	4344.39858	0.00161	5027.69429	683.29732
1 -1 0 0 15	1 -1 0 0 14	4346.00689	-0.00131	5056.02404	710.01584
1 -1 0 0 16	1 -1 0 0 15	4347.59688	-0.00188	5086.23970	738.64093

1	1	-1	0	0	17	1	-1	0	0	16	4349.16180	-0.00674	5118.34074	769.17220	+
2	1	-1	0	0	18	1	-1	0	0	17	4350.71741	0.00003	5152.32660	801.60923	
3	1	-1	0	0	19	1	-1	0	0	18	4352.23797	-0.00716	5188.19669	835.95156	+
4	1	-1	0	0	20	1	-1	0	0	19	4353.74546	-0.00618	5225.95038	872.19874	+
5	1	-1	0	0	21	1	-1	0	0	20	4355.23346	-0.00328	5265.58701	910.35027	+
6	1	-1	0	0	22	1	-1	0	0	21	4356.70025	-0.00001	5307.10587	950.40561	
7	1	-1	0	0	23	1	-1	0	0	22	4358.14766	0.00564	5350.50625	992.36423	+
8	1	-1	0	0	24	1	-1	0	0	23	4359.59444*	0.03260	5395.78739	1036.22555	+
9	1	1	0	0	1	1	1	0	0	2	4315.90660	-0.00291	4831.19781	515.28830	
10	1	1	0	0	2	1	1	0	0	3	4313.96884	-0.00013	4834.96026	520.99129	
11	1	1	0	0	3	1	1	0	0	4	4312.00687	-0.00182	4840.60384	528.59515	
12	1	1	0	0	4	1	1	0	0	5	4310.02839	-0.00031	4848.12849	538.09979	
13	1	1	0	0	5	1	1	0	0	6	4308.02550	-0.00349	4857.53407	549.50508	+
14	1	1	0	0	6	1	1	0	0	7	4306.00924	-0.00034	4868.82044	562.81086	
15	1	1	0	0	7	1	1	0	0	8	4303.96875	-0.00171	4881.98742	578.01697	
16	1	1	0	0	8	1	1	0	0	9	4301.91105	-0.00057	4897.03481	595.12319	
17	1	1	0	0	9	1	1	0	0	10	4299.83379	0.00073	4913.96235	614.12929	
18	1	1	0	0	10	1	1	0	0	11	4297.73534	0.00058	4932.76979	635.03503	
19	1	1	0	0	11	1	1	0	0	12	4295.61754	0.00084	4953.45682	657.84012	
20	1	1	0	0	12	1	1	0	0	13	4293.47861	-0.00025	4976.02313	682.54427	
21	1	1	0	0	13	1	1	0	0	14	4291.32220	0.00099	5000.46834	709.14713	
22	1	1	0	0	14	1	1	0	0	15	4289.14467	0.00095	5026.79208	737.64836	
23	1	1	0	0	15	1	1	0	0	16	4286.94440	-0.00195	5054.99392	768.04757	
24	1	1	0	0	16	1	1	0	0	17	4284.72386	-0.00521	5085.07343	800.34436	+
25	1	1	0	0	17	1	1	0	0	18	4282.49169	-0.00013	5117.03011	834.53830	
26	1	1	0	0	18	1	1	0	0	19	4280.23175	-0.00280	5150.86348	870.62893	+
27	1	1	0	0	19	1	1	0	0	20	4277.95658	-0.00063	5186.57298	908.61577	
28	1	1	0	0	20	1	1	0	0	21	4275.65697	-0.00278	5224.15806	948.49830	+
29	1	1	0	0	21	1	1	0	0	22	4273.34760	0.00550	5263.61811	990.27601	+
30	1	1	0	0	22	1	1	0	0	23	4271.00295	-0.00124	5304.95252	1033.94833	
31	1	1	0	0	23	1	1	0	0	24	4268.65132	0.00538	5348.16062	1079.51468	+
32	1	1	0	0	24	1	1	0	0	25	4266.27908*	0.01179	5393.24174	1126.97445	+
33	1	1	0	0	2	1	1	0	0	1	4323.47788	0.00389	4834.96026	511.48627	+
34	1	1	0	0	3	1	1	0	0	2	4325.31662	0.00108	4840.60384	515.28830	
35	1	1	0	0	4	1	1	0	0	3	4327.13318	-0.00402	4848.12849	520.99129	+
36	1	1	0	0	5	1	1	0	0	4	4328.93948	0.00056	4857.53407	528.59515	
37	1	1	0	0	6	1	1	0	0	5	4330.71978	-0.00087	4868.82044	538.09979	
38	1	1	0	0	7	1	1	0	0	6	4332.48472	0.00238	4881.98742	549.50508	+
39	1	1	0	0	8	1	1	0	0	7	4334.22562	0.00168	4897.03481	562.81086	
40	1	1	0	0	9	1	1	0	0	8	4335.94534	-0.00004	4913.96235	578.01697	
41	1	1	0	0	10	1	1	0	0	9	4337.64597	-0.00063	4932.76979	595.12319	
42	1	1	0	0	11	1	1	0	0	10	4339.32654	-0.00099	4953.45682	614.12929	
43	1	1	0	0	12	1	1	0	0	11	4340.98915	0.00105	4976.02313	635.03503	
44	1	1	0	0	13	1	1	0	0	12	4342.62777	-0.00045	5000.46834	657.84012	
45	1	1	0	0	14	1	1	0	0	13	4344.24795	0.00014	5026.79208	682.54427	
46	1	1	0	0	15	1	1	0	0	14	4345.84747	0.00068	5054.99392	709.14713	
47	1	1	0	0	16	1	1	0	0	15	4347.41932	-0.00575	5085.07343	737.64836	+
48	1	1	0	0	17	1	1	0	0	16	4348.97770	-0.00484	5117.03011	768.04757	+
49	1	1	0	0	18	1	1	0	0	17	4350.51280	-0.00632	5150.86348	800.34436	+
50	1	1	0	0	19	1	1	0	0	18	4352.03801	0.00333	5186.57298	834.53830	+
51	1	1	0	0	20	1	1	0	0	19	4353.52906	-0.00007	5224.15806	870.62893	
52	1	1	0	0	21	1	1	0	0	20	4355.00312	0.00077	5263.61811	908.61577	
53	1	1	0	0	22	1	1	0	0	21	4356.45149	-0.00272	5304.95252	948.49830	+
54	1	1	0	0	23	1	1	0	0	22	4357.88544	0.00083	5348.16062	990.27601	
55	1	1	0	0	24	1	1	0	0	23	4359.30455*	0.01114	5393.24174	1033.94833	+

$$\text{rms} = 0.00095 \text{ cm}^{-1}$$

$$\mathbf{v}_2 + \mathbf{v}_3 + \mathbf{v}_5(\Pi) \leftarrow \mathbf{v}_5(\Pi)$$

$v_4' \ell_4' v_5' \ell_5' J'$	$v_4'' \ell_4'' v_5'' \ell_5'' J''$	OBS	OBS - CALC	E'	E''
0 0 1 -1 3	0 0 1 -1 4	4323.72493	-0.00427	5017.02822	693.29902 ± 0.00001

1	0	0	1	-1	4	0	0	1	-1	5	4321.74088	-0.00080	5024.57172	702.83004
3	0	0	1	-1	5	0	0	1	-1	6	4319.73108	-0.00284	5034.00090	714.26698 +
4	0	0	1	-1	6	0	0	1	-1	7	4317.70686	0.00091	5045.31564	727.60969
5	0	0	1	-1	7	0	0	1	-1	8	4315.65629	-0.00150	5058.51578	742.85799
6	0	0	1	-1	8	0	0	1	-1	9	4313.58939	-0.00010	5073.60116	760.01168
7	0	0	1	-1	9	0	0	1	-1	10	4311.50158	0.00052	5090.57157	779.07052
8	0	0	1	-1	10	0	0	1	-1	11	4309.39331	0.00078	5109.42679	800.03426
9	0	0	1	-1	11	0	0	1	-1	12	4307.26240	-0.00154	5130.16656	822.90261
10	0	0	1	-1	12	0	0	1	-1	13	4305.11277	-0.00255	5152.79060	847.67528 +
11	0	0	1	-1	13	0	0	1	-1	14	4302.94662	-0.00007	5177.29862	874.35193
12	0	0	1	-1	14	0	0	1	-1	15	4300.75647	-0.00163	5203.69029	902.93220
13	0	0	1	-1	15	0	0	1	-1	16	4298.54931	-0.00025	5231.96526	933.41570
14	0	0	1	-1	16	0	0	1	-1	17	4296.32042	-0.00069	5262.12314	965.80204
15	0	0	1	-1	17	0	0	1	-1	18	4294.07345	0.00067	5294.16354	1000.09076
16	0	0	1	-1	5	0	0	1	-1	4	4340.70931*	0.00743	5034.00090	693.29902 +
17	0	0	1	-1	6	0	0	1	-1	5	4342.48475	-0.00085	5045.31564	702.83004
18	0	0	1	-1	7	0	0	1	-1	6	4344.24795	-0.00085	5058.51578	714.26698
19	0	0	1	-1	8	0	0	1	-1	7	4345.99360	0.00213	5073.60116	727.60969 +
20	0	0	1	-1	9	0	0	1	-1	8	4347.71483	0.00125	5090.57157	742.85799
21	0	0	1	-1	10	0	0	1	-1	9	4349.41523	0.00012	5109.42679	760.01168
22	0	0	1	-1	11	0	0	1	-1	10	4351.09525	-0.00079	5130.16656	779.07052
23	0	0	1	-1	12	0	0	1	-1	11	4352.75913	0.00278	5152.79060	800.03426 +
24	0	0	1	-1	13	0	0	1	-1	12	4354.39537	-0.00064	5177.29862	822.90261
25	0	0	1	-1	14	0	0	1	-1	13	4356.01652	0.00151	5203.69029	847.67528
26	0	0	1	-1	15	0	0	1	-1	14	4357.61282	-0.00051	5231.96526	874.35193
27	0	0	1	-1	16	0	0	1	-1	15	4359.20547*	0.01453	5262.12314	902.93220 +
28	0	0	1	-1	17	0	0	1	-1	16	4360.74931	0.00147	5294.16354	933.41570
29	0	0	1	-1	18	0	0	1	-1	17	4362.28343	-0.00057	5328.08604	965.80204
30	0	0	1	-1	19	0	0	1	-1	18	4363.79927	-0.00013	5363.89017	1000.09076
31	0	0	1	-1	20	0	0	1	-1	19	4365.29478	0.00075	5401.57545	1036.28142
32	0	0	1	-1	21	0	0	1	-1	20	4366.77072	0.00285	5441.14140	1074.37353 +
33	0	0	1	1	4	0	0	1	1	5	4321.77470	0.00025	5024.50669	702.73224
34	0	0	1	1	5	0	0	1	1	6	4319.77600*	0.00272	5033.90336	714.13007 +
35	0	0	1	1	6	0	0	1	1	7	4317.75265*	0.00073	5045.17908	727.42716
36	0	0	1	1	7	0	0	1	1	8	4315.71047	0.00010	5058.33371	742.62333
37	0	0	1	1	8	0	0	1	1	9	4313.64770	-0.00098	5073.36706	759.71839
38	0	0	1	1	9	0	0	1	1	10	4311.56640	-0.00046	5090.27895	778.71209
39	0	0	1	1	10	0	0	1	1	11	4309.46487	-0.00006	5109.06914	799.60420
40	0	0	1	1	11	0	0	1	1	12	4307.34381*	0.00088	5129.73738	822.39444
41	0	0	1	1	12	0	0	1	1	13	4305.20228	0.00140	5152.28339	847.08251
42	0	0	1	1	13	0	0	1	1	14	4303.03998	0.00118	5176.70687	873.66808
43	0	0	1	1	14	0	0	1	1	15	4300.85641	-0.00030	5203.00750	902.15079
44	0	0	1	1	15	0	0	1	1	16	4298.65425	-0.00039	5231.18493	932.53028
45	0	0	1	1	16	0	0	1	1	17	4296.43230	-0.00033	5261.23877	964.80614
46	0	0	1	1	17	0	0	1	1	18	4294.18962	-0.00106	5293.16862	998.97795
47	0	0	1	1	5	0	0	1	1	4	4340.66232*	-0.00722	5033.90336	693.23382 +
48	0	0	1	1	6	0	0	1	1	5	4342.44699	0.00015	5045.17908	702.73224
49	0	0	1	1	7	0	0	1	1	6	4344.20493	0.00130	5058.33371	714.13007
50	0	0	1	1	8	0	0	1	1	7	4345.94051	0.00061	5073.36706	727.42716
51	0	0	1	1	9	0	0	1	1	8	4347.65532	-0.00030	5090.27895	742.62333
52	0	0	1	1	10	0	0	1	1	9	4349.35173	0.00098	5109.06914	759.71839
53	0	0	1	1	11	0	0	1	1	10	4351.02648	0.00120	5129.73738	778.71209
54	0	0	1	1	12	0	0	1	1	11	4352.67947	0.00029	5152.28339	799.60420
55	0	0	1	1	13	0	0	1	1	12	4354.31261	0.00018	5176.70687	822.39444
56	0	0	1	1	14	0	0	1	1	13	4355.92388	-0.00111	5203.00750	847.08251
57	0	0	1	1	15	0	0	1	1	14	4357.51077*	-0.00608	5231.18493	873.66808 +
58	0	0	1	1	16	0	0	1	1	15	4359.08895	0.00098	5261.23877	902.15079
59	0	0	1	1	17	0	0	1	1	16	4360.63680	-0.00154	5293.16862	932.53028
60	0	0	1	1	18	0	0	1	1	17	4362.16876	0.00084	5326.97406	964.80614
	0	0	1	1	19	0	0	1	1	18	4363.67769	0.00100	5362.65464	998.97795
	0	0	1	1	20	0	0	1	1	19	4365.16389	-0.00074	5400.20988	1035.04524
	0	0	1	1	21	0	0	1	1	20	4366.63147	-0.00024	5439.63926	1073.00756

rms = 0.00087 cm⁻¹