In our previous paper [1] we proposed a new method for determination of electronic-vibro-rotational (rovibronic) term values of diatomics from experimental data on the wavenumbers of rovibronic spectral lines. In contrast to existing techniques, this new one is based on the Rydberg—Ritz principle (Bohr frequency rule) only:

\[ \nu_{n^\prime v^\prime J^\prime} = T_{n^\prime v^\prime J^\prime} - T_{n^\prime\prime v^\prime\prime J^\prime\prime}, \]

where \( \nu_{n^\prime v^\prime J^\prime} \) are measured wavenumbers, and \( T_{n v J} \) are corresponding term values, \( n \) indicates electronic state, \( v \) and \( J \) — vibrational and rotational quantum numbers, upper and lower states being marked by single and double primes correspondingly.

It is shown that a link between a set of rovibronic term values and a set of wavenumbers of observed rovibronic spectral lines appears only when three and more different electronic-vibrational (vibronic) states are pairwise-connected by radiative transitions. The method differs from known techniques in several aspects, namely, it:

1) doesn’t need any assumptions concerning an internal structure of a molecule;
2) doesn’t involve any intermediate parameters such as molecular constants in the traditional approach;
3) gives an opportunity to use in one-stage optimization procedure all available experimental data obtained for various band systems, by various authors, and in various works;
4) provides the opportunity of rational selection in an interactive mode of the experimental data, eliminating rough errors, to revise wrong identifications of spectral lines and to compare various sets of experimental data for mutual consistency;
5) allows independent estimation of experimental errors and analysis of the shape of error distribution;
6) allows to obtain not only an optimal set of rovibronic term values, but also the error bars determined only by quantity and quality of existing experimental data.

The method is based on the minimization of the weighted mean-square deviation between observed and calculated (as differences of adjustable term values) values of rovibronic line wavenumbers:

\[ r^2 = \sum_{\nu_{n^\prime v^\prime J^\prime}} \left( \frac{\nu_{n^\prime v^\prime J^\prime} - (T_{n^\prime v^\prime J^\prime} - T_{n^\prime\prime v^\prime\prime J^\prime\prime})}{\sigma_{n^\prime v^\prime J^\prime}} \right)^2, \]

where \( \sigma_{n^\prime v^\prime J^\prime} \) are their standard deviations, and sum is over all existing experimental data. Due to the linearity of the equations used, the optimization problem comes to solving a system of linear algebraic equations.
The goal of present work was a study of applicability and main features of the method within an example of certain molecule, namely $^{11}$B$^3$H isotopomer of boron hydride. This molecule was chosen taking into account following considerations:

1. BH has the developed rotational structure.
2. There are available spectra from far infrared ($2000 \text{ cm}^{-1}$, rotational-vibrational transitions) to far ultraviolet ($70000 \text{ cm}^{-1}$, rovibronic transitions), obtained in many works for many band systems.
3. Non-equilibrium low-pressure plasmas containing boron and hydrogen species are of interest in astrophysics and numerous applications like surface treatment of hard metals, production of semiconductors and thermopolymers, jets of rocket engines and others. Emission bands of BH molecule are known to be an obligatory spectral feature of such plasma.

As sources of experimental data on the wavenumbers of singlet rovibronic spectral lines were taken all know by now to authors works [2–11] on this topic. We restricted ourselves to singlet states and transitions only due to their simplicity and a circumstance that there is only one paper [12] on the experimental study of multiplet transitions ($b^3\Sigma^+, a^3\Pi$ band system) with partially unresolved triplet structure.

Grothrian diagram of vibronic levels and the transitions between them is shown in fig. 1. In tab. 1 are cited volumes of experimental wavenumbers for each vibronic band. One may see that the distribution of investigated lines over vibronic states is highly nonuniform. For example, the information on rotational levels of ground vibronic state $X^1\Sigma^+, v = 0$ contains in wavenumbers of 14 bands belonging to 11 band systems, explored in 9 various works. At the same time some of high vibronic and electronic states have only one band experimentally studied in only one work. The $K^1\Sigma^+$ state was observed in [6] only, and identification for rotational lines cannot be assumed as reliable, thus we did not include this state in present work.

The method under consideration requires mean-square errors of wavenumbers being used in process of term values determination for three purposes. Firstly, weightening of input data in (1) depends on these values. Secondly, selection of input data is based on comparison of deviations between calculated from derivable term values and measured wavenumbers and estimated experimental errors. Thirdly, the estimations of output term values errors are calculated from the input wavenumber errors.

Unfortunately only few original works with experimental data on wavenumbers contain information on accuracy of listed values. And even if error estimations are mentioned, they seem to be doubtful. For example, in [6] is stated following: “The relative accuracy of measurement of the strongest unblended lines is thought to be of the order of $\pm0.05 \text{ cm}^{-1}$.” While there is absolutely incomprehensible which of the lines are strongest, what is the accuracy for other lines, etc. In several works only used spectral resolution is refered.

According to such situation it was necessary to obtain independent estimations of wavenumber errors, fortunately our method provides this opportunity.
Ultimate results of these estimations are listed in tab. 2. During the analysis we detected that data in [2] and [4] contain systematic errors of order 0.05 \ldots 0.10 \text{ cm}^{-1} thus these work were excluded from further analysis, and results for them are not shown in the table. Other work are rather in mutual agreement, except for $G^1\Pi-X^1\Sigma^+$ (0 \textendash 0) and $H^1\Delta-X^1\Sigma^+$ (0 \textendash 0) bands in [6] and [8]. These data are systematically different but we cannot choose one of these works and reject the other because none of them have undoubted advantage and no more information on these bands is available.

From remained 1410 wavenumber 32 were rejected as rough errors according to “3σ-rule”. As a result we found 529 rovibronic term values for 12 electronic states of $^{11}\text{B}\text{H}$ isotopomer of boron hydride molecule. The values with their standard deviations are listed in tab. 3.

References

[1] Lavrov B.P., Ryazanov M.S. // Khimicheskaya Fizika (Soviet Journal of Chemical Physics), in print (2005); e-print: physics/0405132 at http://arXiv.org.
[2] Lochte-Holtgreven W., van der Vleugel E.S. // ZS. f. Phys. 70, 188 (1931).
[3] Thunberg S.F. // ZS. f. Phys. 100, 471 (1936).
[4] Almy G.M., Horsfall R.B., Jr // Phys. Rev. 51, 491 (1937).
[5] Douglas A.E. // Canad. J. Res. 19 A, 27 (1941).
[6] Bauer S.H., Herzberg G., Johns J.W. // J. Mol. Spectr. 13, 256 (1964).
[7] Johns J.W., Grimm F.A., Porter R.F. // J. Mol. Spectr. 22, 435 (1967).
[8] Johns J.W., Lepard D.W. // J. Mol. Spectr. 55, 374 (1975).
[9] Pianalto F.S., O’Brien L.C., Keller P.C., Bernath P.F. // J. Mol. Spectr. 129, 348 (1988).
[10] Fernando W.T.M.L., Bernath P.F. // J. Mol. Spectr. 145, 329 (1991).
[11] Clark J., Konopka M., Zhang L.-M., Grant E.R. // Chem. Phys. Lett. 340, 45 (2001).
[12] Brazier C.R. // J. Mol. Spectr. 177, 90 (1996).
Figure 1. Grotrian diagram of singlet electronic-vibrational states and emission and absorption bands experimentaly studied by now. Symbols of electronic states (in Herzberg notation) are shown on the left-hand side and vibrational quantum numbers on the right-hand side of vibronic levels.
Table 1. Maximum values of rotation quantum number $J''$ of the lower vibronic state for experimentally studied bands. Upper indices denote references to original works.

| $^1\Lambda' - ^1\Lambda''$ | $v''$ | $v' = 0$ | $v' = 1$ | $v' = 2$ | $v' = 3$ |
|----------------------------|-------|----------|----------|----------|----------|
| $X^1\Sigma^+ - X^1\Sigma^+$ | 0     | 9[^9]    |          |          |          |
|                             | 1     |          | 7[^9]    |          |          |
|                             | 2     |          |          | 7[^9]    |          |
| $A^1\Pi - X^1\Sigma^+$     | 0     | 26[^10], 27[^7], 26[^8], 22[^3] | 16[^7]   | 8[^11]   |          |
|                             | 1     |          | 20[^10], 21[^7], 20[^8], 17[^8] | 13[^7]   |          |
|                             | 2     |          |          | 14[^4], 13[^10], 13[^7] | 6[^7]    |
|                             | 3     |          |          |          | 7[^7]    |
| $B^1\Sigma^+ - X^1\Sigma^+$ | 0     | 21[^6]   | 6[^6]    |          |          |
|                             | 1     |          | 8[^6]    |          |          |
|                             | 2     |          |          | 6[^6]    |          |
|                             | 3     |          |          |          | 4[^6]    |
| $C^1\Sigma^+ - X^1\Sigma^+$ | 0     | 5[^6]    |          |          |          |
| $D^1\Pi - X^1\Sigma^+$     | 0     | 7[^6]    |          |          |          |
| $E^1\Sigma^+ - X^1\Sigma^+$ | 0     | 7[^6]    |          |          |          |
| $F^1\Sigma^+ - X^1\Sigma^+$ | 0     | 8[^6], 26[^8] |          |          |          |
|                             | 1     |          |          | 7[^6]    |          |
| $G^1\Pi - X^1\Sigma^+$     | 0     | 7[^6], 14[^8] |          |          |          |
| $H^1\Delta - X^1\Sigma^+$  | 0     | 8[^6], 15[^8] |          |          |          |
| $I^1\Sigma^+ - X^1\Sigma^+$ | 0     | 6[^6]    |          |          |          |
| $J^1\Sigma^+ - X^1\Sigma^+$ | 0     | 3[^6]    |          |          |          |
| $C^1\Delta - A^1\Pi$       | 0     | 22[^7]   |          |          |          |
|                             | 1     |          |          | 21[^7]   |          |
|                             | 2     |          |          | 13[^7]   |          |
| $B^1\Sigma^+ - A^1\Pi$     | 0     | 13[^5]   |          |          |          |
|                             | 1     |          |          | 13[^5]   |          |
| $C^1\Sigma^+ - A^1\Pi$     | 0     | 10[^5], 25[^7] |          |          |          |
|                             | 1     |          |          | 20[^7]   |          |
|                             | 2     |          |          |          | 9[^7]    |
|                             | 3     |          |          |          | 7[^7]    |
| $H^1\Delta - A^1\Pi$       | 0     | 6[^6]    |          |          |          |
Table 2. Characteristic of used data by bands. $\sigma$ — our estimation for standard deviation of wavenumbers, $\sigma_\xi$ and $\delta_\xi$ — obtained standard deviation and bias of $\xi$ variable (see text).

| Source | $^1\Lambda - ^1\Lambda'$ | $v - v'$ | $J'_{\min}$ | $J'_{\max}$ | $\sigma$, cm$^{-1}$ | $\sigma_\xi$ | $\delta_\xi$ |
|--------|----------------|-----------|-------------|-------------|-----------------|-------------|-------------|
| [2]    | $A^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 26          | -               | -           | -           |
|        | 1 - 1               | 0 - 0     | 20          | -           | -               | -           | -           |
| [3]    | $A^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 22          | 0.04           | 1.01        | -0.46       |
|        | 1 - 1               | 1 - 1     | 17          | 0.05        | 1.05            | +0.004      |             |
| [4]    | $A^1\Pi - X^1\Sigma^+$ | 2 - 2     | 0           | 14          | -               | -           | -           |
| [5]    | $B^1\Sigma^+ - A^1\Pi$ | 0 - 0     | 1           | 13          | 0.022          | 1.04        | +0.25       |
|        | 1 - 1               | 1 - 1     | 13          | 0.025       | 0.98            | +0.13       |             |
| [6]    | $C^1\Sigma^+ - A^1\Pi$ | 0 - 0     | 1           | 10          | 0.064          | 1.02        | +0.37       |
|        | 1 - 0               | 0 - 0     | 6           | 0.12        | 0.99            | -0.06       |             |
|        | 1 - 1               | 0 - 0     | 8           | 0.11        | 0.96            | -0.53       |             |
|        | 2 - 2               | 0 - 0     | 6           | 0.12        | 1.02            | -0.39       |             |
|        | 3 - 3               | 1 - 1     | 4           | 0.11        | 1.04            | -0.46       |             |
|        | $C^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 5           | 0.088          | 0.93        | -0.64       |
|        | $D^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 7           | 0.20           | 1.00        | 0           |
|        | $E^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 7           | 0.056          | 0.99        | 0           |
|        | $F^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 8           | 0.14           | 1.05        | -0.33       |
|        | $G^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 7           | 0.13           | 1.00        | -0.91       |
|        | $H^1\Delta - X^1\Sigma^+$ | 0 - 0   | 1           | 8           | 0.11           | 1.01        | -0.77       |
|        | $I^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 6           | 0.21           | 1.02        | 0           |
|        | $J^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 3           | 0.28           | 1.00        | 0           |
|        | $H^1\Delta - A^1\Pi$ | 0 - 0     | 0           | 7           | 0.21           | 1.08        | 0           |
|        | $A^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 27          | 0.023          | 0.98        | -0.36       |
|        | 1 - 0               | 0 - 0     | 16          | 0.011       | 0.90            | -0.32       |             |
|        | 1 - 1               | 0 - 0     | 21          | 0.026       | 1.03            | -0.09       |             |
|        | 2 - 1               | 0 - 0     | 13          | 0.022       | 1.01            | -0.44       |             |
|        | 2 - 2               | 0 - 0     | 13          | 0.014       | 0.97            | +0.37       |             |
|        | 3 - 2               | 0 - 0     | 6           | 0.06        | 1.00            | -0.44       |             |
|        | 3 - 3               | 0 - 0     | 7           | 0.10        | 0.99            | +0.56       |             |
|        | $C^1\Sigma^+ - A^1\Pi$ | 0 - 0    | 1           | 25          | 0.037          | 1.05        | -0.05       |
|        | 1 - 1               | 1 - 1     | 20          | 0.034       | 1.01            | -0.005      |             |
|        | 2 - 2               | 1 - 1     | 9           | 0.026       | 1.06            | +0.002      |             |
|        | 3 - 3               | 1 - 1     | 7           | 0.048       | 1.07            | -0.004      |             |
|        | $C^1\Delta - A^1\Pi$ | 0 - 0     | 1           | 22          | 0.021          | 0.92        | +0.01       |
|        | 1 - 1               | 1 - 1     | 21          | 0.021       | 1.03            | -0.03       |             |
|        | 2 - 2               | 1 - 1     | 13          | 0.027       | 1.06            | -0.03       |             |
| [8]    | $F^1\Sigma^+ - X^1\Sigma^+$ | 0 - 0   | 0           | 26          | 0.10           | 1.07        | +0.17       |
|        | $G^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 14          | 0.07           | 0.98        | +0.87       |
|        | $H^1\Delta - X^1\Sigma^+$ | 0 - 0   | 2           | 15          | 0.067          | 1.05        | +0.87       |
| [9]    | $X^1\Sigma^+ - X^1\Sigma^+$ | 1 - 0   | 0           | 9           | 0.0015         | 1.02        | +0.25       |
|        | 2 - 1               | 0 - 0     | 7           | 0.0015      | 0.93            | +0.20       |             |
|        | 3 - 2               | 2 - 2     | 7           | 0.008       | 1.02            | +0.11       |             |
| [10]   | $A^1\Pi - X^1\Sigma^+$ | 0 - 0     | 0           | 26          | 0.01           | 0.95        | +0.45       |
|        | 1 - 1               | 0 - 0     | 20          | 0.013       | 0.97            | +0.34       |             |
|        | 2 - 2               | 0 - 0     | 13          | 0.011       | 0.98            | -0.02       |             |
| [11]   | $A^1\Pi - X^1\Sigma^+$ | 2 - 0     | 0           | 8           | 0.12           | 1.05        | -0.09       |
Table 3. Energy levels $E_{n,v,J}$ (with standard deviations) of $^{11}$B$^1$H isotopomer of boron hydride in cm$^{-1}$. $N_\nu$ denotes number of used spectral lines.

| $J$ | $v = 0$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|---------|---------|-------------|---------|-------------|---------|-------------|---------|-------------|---------|
| 0   | 0       | 17      | 2269.223(4) | 7       | 4443.035(2) | 5       | 6523.58(11) | 1       |             |         |
| 1   | 23.624(4)| 30      | 2292.0223(15)| 15      | 4465.011(4) | 9       | 6544.72(7)  | 3       |             |         |
| 2   | 70.8479(19)| 41     | 2337.587(3) | 17      | 4508.9455(19)| 13      | 6587.108(9) | 6       |             |         |
| 3   | 141.612(4)| 43     | 2405.863(2) | 20      | 4574.774(4) | 15      | 6650.522(6) | 7       |             |         |
| 4   | 235.824(2)| 40     | 2496.762(3) | 20      | 4662.414(2) | 14      | 6734.946(7) | 6       |             |         |
| 5   | 353.372(3)| 38     | 2610.172(2) | 20      | 4771.752(3) | 15      | 6840.276(6) | 5       |             |         |
| 6   | 494.107(3)| 33     | 2745.949(3) | 19      | 4902.649(3) | 12      | 6966.375(7) | 4       |             |         |
| 7   | 657.863(4)| 30     | 2903.921(3) | 19      | 5054.939(4) | 9       | 7113.077(8) | 2       |             |         |
| 8   | 844.427(3)| 26     | 3083.899(4) | 15      | 5228.421(3) | 7       | 7280.188(9) | 1       |             |         |
| 9   | 1053.583(4)| 20    | 3285.647(3) | 13      | 5422.895(9) | 6       |             |         |             |         |
| 10  | 1285.059(7)| 20    | 3508.920(4) | 13      | 5638.087(9) | 6       |             |         |             |         |
| 11  | 1538.591(9)| 17    | 3753.427(9) | 12      | 5873.751(11)| 6      |             |         |             |         |
| 12  | 1813.840(10)| 18   | 4018.898(10)| 11      | 6129.586(12)| 6      |             |         |             |         |
| 13  | 2110.527(12)| 16   | 4304.990(11)| 11      | 6405.226(14)| 4      |             |         |             |         |
| 14  | 2428.240(13)| 16   | 4611.333(14)| 9       |             |         |             |         |             |         |
| 15  | 2766.659(15)| 14   | 4937.608(15)| 8       |             |         |             |         |             |         |
| 16  | 3125.316(16)| 13   | 5283.316(17)| 8       |             |         |             |         |             |         |
| 17  | 3503.842(19)| 10   | 5648.21(2)  | 8       |             |         |             |         |             |         |
| 18  | 3901.74(2) | 12     | 6031.68(4)  | 6       |             |         |             |         |             |         |
| 19  | 4318.64(2) | 12     | 6433.44(3)  | 4       |             |         |             |         |             |         |
| 20  | 4753.98(2) | 12     | 6852.90(4)  | 3       |             |         |             |         |             |         |
| 21  | 5207.30(3) | 12     | 7289.58(4)  | 1       |             |         |             |         |             |         |
| 22  | 5678.05(3) | 8      |             |         |             |         |             |         |             |         |
| 23  | 6165.75(3) | 7      |             |         |             |         |             |         |             |         |
| 24  | 6669.72(4) | 5      |             |         |             |         |             |         |             |         |
| 25  | 7189.73(3) | 6      |             |         |             |         |             |         |             |         |
| 26  | 7724.80(4) | 4      |             |         |             |         |             |         |             |         |
| 27  | 8274.64(5) | 1      |             |         |             |         |             |         |             |         |
| \( J \) | \( E_{n,v,J} \) | \( N_\nu \) | \( E_{n,v,J} \) | \( N_\nu \) | \( E_{n,v,J} \) | \( N_\nu \) | \( E_{n,v,J} \) | \( N_\nu \) |
|-------|----------------|---------|----------------|---------|----------------|---------|----------------|---------|
| 1     | 23097.810(6)   | 12      | 25183.216(6)   | 10      | 27012.704(7)   | 10      | 28490.98(3)    | 5       |
| 2     | 23145.469(7)   | 13      | 25227.905(6)   | 12      | 27053.620(6)   | 12      | 28526.02(3)    | 6       |
| 3     | 23216.863(6)   | 15      | 25294.849(6)   | 15      | 27114.853(6)   | 13      | 28578.38(3)    | 5       |
| 4     | 23311.884(6)   | 16      | 25383.918(6)   | 14      | 27196.279(6)   | 12      | 28647.61(3)    | 5       |
| 5     | 23430.411(6)   | 14      | 25494.965(6)   | 14      | 27297.696(6)   | 12      | 28733.63(5)    | 3       |
| 6     | 23572.268(6)   | 15      | 25627.796(6)   | 15      | 27418.844(6)   | 12      | 28835.61(7)    | 3       |
| 7     | 23737.235(6)   | 14      | 25782.184(6)   | 14      | 27559.448(7)   | 12      | 28952.84(12)   | 1       |
| 8     | 23925.089(7)   | 13      | 25957.833(6)   | 12      | 27719.129(7)   | 11      |                |         |
| 9     | 24135.526(7)   | 14      | 26154.459(6)   | 12      | 27897.451(7)   | 10      |                |         |
| 10    | 24368.265(8)   | 12      | 26371.677(7)   | 13      | 28093.963(10)  | 8       |                |         |
| 11    | 24622.941(9)   | 11      | 26609.097(8)   | 12      | 28308.053(10)  | 8       |                |         |
| 12    | 24899.204(11)  | 12      | 26866.273(10)  | 13      | 28539.098(12)  | 7       |                |         |
| 13    | 25196.598(12)  | 11      | 27142.700(11)  | 13      | 28786.382(16)  | 3       |                |         |
| 14    | 25514.715(13)  | 11      | 27437.894(13)  | 11      |                |         |                |         |
| 15    | 25853.052(15)  | 11      | 27751.143(16)  | 9       |                |         |                |         |
| 16    | 26211.113(17)  | 10      | 28081.941(19)  | 8       |                |         |                |         |
| 17    | 26588.298(18)  | 9       | 28429.39(3)    | 7       |                |         |                |         |
| 18    | 26984.08(2)    | 8       | 28792.94(2)    | 5       |                |         |                |         |
| 19    | 27397.76(2)    | 9       | 29171.49(4)    | 5       |                |         |                |         |
| 20    | 27828.74(2)    | 8       | 29564.05(4)    | 4       |                |         |                |         |
| 21    | 28276.23(3)    | 8       |                |         |                |         |                |         |
| 22    | 28739.49(3)    | 8       |                |         |                |         |                |         |
| 23    | 29217.67(3)    | 3       |                |         |                |         |                |         |
| 24    | 29709.92(3)    | 4       |                |         |                |         |                |         |
| 25    | 30215.20(4)    | 3       |                |         |                |         |                |         |
| 26    | 30732.46(4)    | 2       |                |         |                |         |                |         |
Table 3. (continued)

| J | \( E_{n,v,J} \) | \( N_v \) | \( E_{n,v,J} \) | \( N_v \) | \( E_{n,v,J} \) | \( N_v \) | \( E_{n,v,J} \) | \( N_v \) |
|---|----------------|---|----------------|---|----------------|---|----------------|---|
| 1 | 23097.736(9)  | 7 | 25183.137(8)  | 7 | 27012.618(10) | 6 | 28490.95(4)  | 3 |
| 2 | 23145.257(8) | 8 | 25227.701(8)  | 8 | 27053.441(8)  | 7 | 28525.90(4)  | 3 |
| 3 | 23216.408(8) | 9 | 25294.427(7)  | 9 | 27114.478(8)  | 8 | 28578.05(4)  | 3 |
| 4 | 23311.139(8) | 8 | 25383.235(7)  | 9 | 27195.678(8)  | 8 | 28647.22(5)  | 3 |
| 5 | 23429.297(8) | 10 | 25493.939(7) | 9 | 27296.790(8)  | 8 | 28732.93(5)  | 3 |
| 6 | 23570.718(8) | 8 | 25626.365(7)  | 9 | 27417.600(8)  | 8 | 28834.62(10) | 3 |
| 7 | 23735.205(8) | 9 | 25780.295(7)  | 8 | 27557.798(8)  | 8 | 28951.8(2)   | 1 |
| 8 | 23922.468(8) | 8 | 25955.424(7)  | 9 | 27717.021(8)  | 8 |            |    |
| 9 | 24132.286(9) | 9 | 26151.498(8)  | 9 | 27894.869(11) | 5 |            |    |
| 10 | 24364.350(10) | 9 | 26368.090(8) | 9 | 28090.832(11) | 5 |            |    |
| 11 | 24618.301(11) | 7 | 26604.866(10) | 9 | 28304.392(13) | 5 |            |    |
| 12 | 24893.772(13) | 7 | 26861.325(11) | 9 | 28534.855(14) | 4 |            |    |
| 13 | 25190.366(14) | 6 | 27137.057(13) | 7 | 28781.445(15) | 3 |            |    |
| 14 | 25507.613(16) | 4 | 27431.438(14) | 8 |            |    |            |    |
| 15 | 25845.069(17) | 4 | 27743.981(16) | 6 |            |    |            |    |
| 16 | 26202.187(18) | 5 | 28073.912(17) | 6 |            |    |            |    |
| 17 | 26578.48(2)   | 4 | 28420.69(2)   | 5 |            |    |            |    |
| 18 | 26973.26(2)   | 5 | 28783.34(4)   | 4 |            |    |            |    |
| 19 | 27386.02(2)   | 5 | 29161.19(3)   | 4 |            |    |            |    |
| 20 | 27816.01(3)   | 5 | 29552.94(5)   | 1 |            |    |            |    |
| 21 | 28262.58(3)   | 5 |            |    |            |    |            |    |
| 22 | 28724.89(3)   | 4 |            |    |            |    |            |    |
| 23 | 29202.16(3)   | 3 |            |    |            |    |            |    |
| 24 | 29693.44(4)   | 3 |            |    |            |    |            |    |
| 25 | 30198.00(3)   | 3 |            |    |            |    |            |    |
| 26 | 30714.41(5)   | 1 |            |    |            |    |            |    |
Table 3. (continued)

$C'\Delta^+$

| $J$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|-------------|---------|-------------|---------|
| 2   | 46178.53(2) | 3       | 48694.490(15)| 3     | 5117.272(19)| 3     |
| 3   | 46253.864(13)| 3      | 48767.452(13)| 3     | 51187.915(16)| 3     |
| 4   | 46354.126(13)| 3      | 48864.583(13)| 3     | 51281.968(19)| 3     |
| 5   | 46479.248(13)| 3      | 48985.794(13)| 3     | 51399.32(2)  | 3     |
| 6   | 46629.091(13)| 3      | 49130.937(13)| 3     | 51539.850(19)| 3     |
| 7   | 46803.465(16)| 3      | 49299.860(13)| 3     | 51703.37(2)  | 3     |
| 8   | 47002.155(16)| 2      | 49492.299(13)| 3     | 51889.695(16)| 3     |
| 9   | 47224.979(16)| 3      | 49708.190(13)| 3     | 52098.64(2)  | 3     |
| 10  | 47471.651(14)| 3      | 49947.110(16)| 2     | 52329.82(2)  | 2     |
| 11  | 47741.906(15)| 3      | 50208.872(16)| 3     | 52583.20(3)  | 1     |
| 12  | 48035.445(15)| 3      | 50493.160(15)| 3     | 52858.30(11)| 1     |
| 13  | 48351.932(17)| 3      | 50799.604(19)| 3     |              |       |
| 14  | 48691.036(19)| 2      | 51127.920(19)| 2     |              |       |
| 15  | 49052.35(2)  | 1       | 51477.81(2)  | 2     |              |       |
| 16  | 49435.44(2)  | 2      | 51847.85(9)  | 1     |              |       |
| 17  | 49840.09(14) | 2      | 52240.35(3)  | 1     |              |       |
| 18  | 50265.25(9)  | 1       | 52652.22(4)  | 1     |              |       |
| 19  | 50711.56(3)  | 1       | 53083.57(9)  | 1     |              |       |
| 20  | 51177.71(3)  | 1       |              |       |              |       |
| 21  | 51663.35(3)  | 1       |              |       |              |       |

$C'\Delta^-$

| $J$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|-------------|---------|-------------|---------|
| 2   | 46178.54(2) | 3       | 48694.484(15)| 3     | 5117.24(3)  | 3     |
| 3   | 46253.846(13)| 3      | 48767.438(15)| 3     | 51187.906(19)| 3     |
| 4   | 46354.121(13)| 3      | 48864.573(13)| 3     | 51281.977(16)| 3     |
| 5   | 46479.247(13)| 3      | 48985.809(13)| 3     | 51399.320(19)| 3     |
| 6   | 46629.096(13)| 3      | 49130.944(13)| 3     | 51539.850(16)| 3     |
| 7   | 46803.450(13)| 3      | 49299.858(13)| 3     | 51703.367(16)| 3     |
| 8   | 47002.24(14) | 2      | 49492.357(16)| 2     | 51889.698(17)| 3     |
| 9   | 47224.978(14)| 3      | 49708.170(16)| 2     | 52098.613(17)| 3     |
| 10  | 47471.668(14)| 3      | 49947.118(14)| 3     | 52329.86(2)  | 2     |
| 11  | 47741.913(17)| 2      | 50208.865(14)| 3     | 52583.21(3)  | 1     |
| 12  | 48035.452(18)| 2      | 50493.146(17)| 2     | 52858.35(3)  | 1     |
| 13  | 48351.924(19)| 2      | 50799.602(16)| 3     | 53153.02(3)  | 1     |
| 14  | 48691.00(2)  | 2       | 51127.981(19)| 2     |              |       |
| 15  | 49052.33(2)  | 2       | 51477.78(2)  | 2     |              |       |
| 16  | 49435.46(2)  | 2       | 51848.71(3)  | 1     |              |       |
| 17  | 49839.98(2)  | 2       | 52240.27(4)  | 1     |              |       |
| 18  | 50265.53(3)  | 1       | 52652.23(3)  | 1     |              |       |
| 19  | 50711.56(3)  | 1       | 53083.99(4)  | 1     |              |       |
| 20  | 51177.67(3)  | 1       | 53535.01(4)  | 1     |              |       |
| 21  | 51663.35(3)  | 1       |              |       |              |       |
| 22  | 52168.12(3)  | 1       |              |       |              |       |
### Table 3. (continued)

TABLE 3: Energies of the $B^1\Sigma^+$ state for $v = 0 \rightarrow 3$

| $J$ | $v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ |
|-----|---------|---------|---------|---------|
|     | $E_{n,v,J}$ | $N_{\nu}$ | $E_{n,v,J}$ | $N_{\nu}$ | $E_{n,v,J}$ | $N_{\nu}$ | $E_{n,v,J}$ | $N_{\nu}$ |
| 0   | 52346.70(2) | 2 | 54594.79(2) | 3 | 56690.26(8) | 2 | 58564.61(11) | 1 |
| 1   | 52370.968(17) | 4 | 54617.846(18) | 5 | 56733.45(8) | 2 | 58605.06(8) | 2 |
| 2   | 52419.279(13) | 5 | 54663.809(15) | 7 | 56798.71(8) | 2 | 58665.55(8) | 2 |
| 3   | 52491.644(13) | 5 | 54732.755(15) | 7 | 56885.20(8) | 2 | 58746.10(11) | 1 |
| 4   | 52587.978(13) | 5 | 54824.470(15) | 7 | 56993.21(8) | 2 |                  |   |
| 5   | 52708.185(13) | 5 | 54938.809(18) | 5 | 57122.25(12) | 1 |                  |   |
| 6   | 52852.061(13) | 5 | 55075.779(18) | 5 |                  |   |                  |   |
| 7   | 53019.456(13) | 5 | 55235.26(2)  | 3 |                  |   |                  |   |
| 8   | 53210.138(13) | 5 | 55416.362(18) | 3 |                  |   |                  |   |
| 9   | 53423.879(13) | 5 | 55619.563(15) | 4 |                  |   |                  |   |
| 10  | 53660.354(14) | 5 | 55844.309(19) | 2 |                  |   |                  |   |
| 11  | 53919.276(15) | 5 | 56090.26(2)  | 2 |                  |   |                  |   |
| 12  | 54200.32(2)   | 2 | 56357.08(2)  | 2 |                  |   |                  |   |
| 13  | 54503.08(2)   | 3 |                  |   |                  |   |                  |   |
| 14  | 54827.17(5)   | 2 |                  |   |                  |   |                  |   |
| 15  | 55172.23(5)   | 2 |                  |   |                  |   |                  |   |
| 16  | 55537.61(6)   | 2 |                  |   |                  |   |                  |   |
| 17  | 55923.46(6)   | 2 |                  |   |                  |   |                  |   |
| 18  | 56328.53(6)   | 2 |                  |   |                  |   |                  |   |
| 19  | 56752.52(6)   | 2 |                  |   |                  |   |                  |   |
| 20  | 57194.86(6)   | 2 |                  |   |                  |   |                  |   |
| 21  | 57655.23(8)   | 1 |                  |   |                  |   |                  |   |
| 22  | 58132.60(8)   | 1 |                  |   |                  |   |                  |   |
Table 3. (continued)

| $C^1 \Sigma^+$ |   |   |   |   |
|----------------|---|---|---|---|
| $J$ | $v = 0$ |   | $v = 1$ |   | $v = 2$ |   | $v = 3$ |   |
| $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
| 0 | 55333.72(3) | 2 | 57700.26(3) | 1 | 59960.28(3) | 1 |   |   |
| 1 | 55358.13(2) | 6 | 57723.90(14) | 2 | 59982.838(19) | 2 | 62139.97(5) | 2 |
| 2 | 55406.872(19) | 7 | 57770.78(2) | 3 | 60028.083(16) | 3 | 62180.69(4) | 3 |
| 3 | 55479.91(2) | 7 | 57841.19(2) | 2 | 60095.791(16) | 3 | 62244.85(4) | 3 |
| 4 | 55577.15(2) | 7 | 57934.98(2) | 3 | 60185.951(16) | 3 | 62331.12(5) | 2 |
| 5 | 55698.467(19) | 6 | 58051.90(2) | 3 | 60298.422(16) | 3 | 62438.86(6) | 2 |
| 6 | 55843.76(2) | 5 | 58191.96(2) | 3 | 60432.992(16) | 3 | 62567.39(11) | 2 |
| 7 | 56012.88(2) | 5 | 58354.92(2) | 3 | 60589.364(16) | 3 |   |   |
| 8 | 56205.38(2) | 5 | 58540.59(2) | 2 | 60766.650(16) | 3 |   |   |
| 9 | 56421.31(2) | 4 | 58748.72(2) |   |   |   |   |   |
| 10 | 56660.33(2) | 4 | 58979.05(2) |   |   |   |   |   |
| 11 | 56922.07(2) | 3 | 59231.32(2) | 3 |   |   |   |   |
| 12 | 57206.34(2) | 3 | 59505.17(2) | 3 |   |   |   |   |
| 13 | 57512.72(2) | 3 | 59800.39(3) | 3 |   |   |   |   |
| 14 | 57840.89(2) | 3 | 60116.47(3) | 3 |   |   |   |   |
| 15 | 58190.45(3) | 3 | 60453.05(3) | 2 |   |   |   |   |
| 16 | 58561.01(3) | 3 | 60809.87(3) | 3 |   |   |   |   |
| 17 | 58952.11(3) | 3 | 61186.39(3) | 3 |   |   |   |   |
| 18 | 59363.27(3) | 3 | 61582.04(4) | 2 |   |   |   |   |
| 19 | 59794.13(3) | 3 | 61996.44(4) | 2 |   |   |   |   |
| 20 | 60244.07(3) | 3 |   |   |   |   |   |   |
| 21 | 60712.65(4) | 2 |   |   |   |   |   |   |
| 22 | 61199.31(4) | 2 |   |   |   |   |   |   |
| 23 | 61703.63(4) | 2 |   |   |   |   |   |   |
| 24 | 62224.77(5) | 1 |   |   |   |   |   |   |
| 25 | 62762.53(5) | 1 |   |   |   |   |   |   |

| $D^1 \Pi^+$ |   |   |   |   |
|-------------|---|---|---|---|
| $J$ | $v = 0$ |   |   |   |
| $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
| 1 | 61128.87(14) | 2 |   |   |
| 2 | 61175.68(14) | 2 |   |   |
| 3 | 61245.93(14) | 2 |   |   |
| 4 | 61339.57(14) | 2 |   |   |
| 5 | 61456.7(2) | 1 |   |   |
| 6 | 61596.6(2) | 1 |   |   |
| 7 | 61760.0(2) | 1 |   |   |

| $D^1 \Pi^-$ |   |   |   |   |
|-------------|---|---|---|---|
| $J$ | $v = 0$ |   |   |   |
| $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
| 1 | 61130.0(2) | 1 |   |   |
| 2 | 61179.3(2) | 1 |   |   |
| 3 | 61253.1(2) | 1 |   |   |
| 4 | 61351.4(2) | 1 |   |   |
| 5 | 61474.0(2) | 1 |   |   |
| 6 | 61620.8(2) | 1 |   |   |
| 7 | 61791.5(2) | 1 |   |   |

| $E^1 \Sigma^+$ |   |   |   |   |
|---------------|---|---|---|---|
| $J$ | $v = 0$ |   |   |   |
| $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ | $E_{n,v,J}$ | $N_\nu$ |
| 0 | 61872.32(6) | 1 |   |   |
| 1 | 61898.53(4) | 2 |   |   |
| 2 | 61950.64(4) | 2 |   |   |
| 3 | 62028.83(4) | 2 |   |   |
| 4 | 62132.63(4) | 2 |   |   |
| 5 | 62262.12(6) | 1 |   |   |
| 6 | 62416.87(6) | 1 |   |   |
Table 3. (continued)

| \( J \) | \( v = 0 \) | \( v = 1 \) |
|---|---|---|
| \( E_{n,v,J} \) | \( N_{\nu} \) | \( E_{n,v,J} \) | \( N_{\nu} \) |
| 0 | 66078.1(14) | 2 | 68268.9(2) | 1 |
| 1 | 66090.37(6) | 4 | 68285.0(4) | 2 |
| 2 | 66119.29(6) | 4 | 68316.4(2) | 2 |
| 3 | 66165.20(7) | 4 | 68366.0(2) | 2 |
| 4 | 66229.99(6) | 4 | 68433.8(2) | 2 |
| 5 | 66315.25(6) | 4 | 68520.9(2) | 2 |
| 6 | 66421.69(7) | 3 | 68628.51(15) | 2 |
| 7 | 66550.20(6) | 4 |  |  |
| 8 | 66700.71(8) | 2 |  |  |
| 9 | 66875.03(7) | 2 |  |  |
| 10 | 67071.30(10) | 1 |  |  |
| 11 | 67290.00(7) | 2 |  |  |
| 12 | 67531.20(7) | 2 |  |  |
| 13 | 67794.50(7) | 2 |  |  |
| 14 | 68079.73(7) | 2 |  |  |
| 15 | 68386.93(7) | 2 |  |  |
| 16 | 68714.95(10) | 1 |  |  |
| 17 | 69063.37(10) | 1 |  |  |
| 18 | 69433.2(2) | 1 |  |  |
| 19 | 69823.84(10) | 1 |  |  |
| 20 | 70232.81(10) | 1 |  |  |
| 21 | 70660.92(10) | 1 |  |  |
| 22 | 71107.50(10) | 1 |  |  |
| 23 | 71571.95(10) | 1 |  |  |
| 24 | 72053.05(10) | 1 |  |  |
| 25 | 72551.57(11) | 1 |  |  |
| 26 | 73064.11(10) | 1 |  |  |
| 27 | 73594.11(11) | 1 |  |  |

\[
\begin{array}{c|c|c}
 J & v = 0 & v = 1 \\
\hline
 E_{n,v,J} & N_{\nu} & E_{n,v,J} & N_{\nu} \\
\hline
\end{array}
\]
Table 3. (continued)

| $J$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|
| 2   | 66548.30(5) | 5       |
| 3   | 66654.40(5) | 4       |
| 4   | 66784.91(5) | 3       |
| 5   | 66946.90(6) | 3       |
| 6   | 67129.62(7) | 1       |
| 7   | 67336.34(7) | 1       |
| 8   | 67566.74(7) | 1       |
| 9   | 67819.91(7) | 1       |
| 10  | 68095.33(7) | 1       |
| 11  | 68392.38(7) | 1       |
| 12  | 68710.50(7) | 1       |
| 13  | 69049.08(7) | 1       |

| $J$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|
| 2   | 66543.04(5) | 4       |
| 3   | 66641.07(6) | 2       |
| 4   | 66763.06(6) | 4       |
| 5   | 66909.05(6) | 2       |
| 6   | 67081.07(6) | 2       |
| 7   | 67273.54(6) | 2       |
| 8   | 67490.70(6) | 2       |
| 9   | 67731.02(7) | 1       |
| 10  | 67994.27(7) | 1       |
| 11  | 68280.04(7) | 1       |
| 12  | 68587.84(7) | 1       |
| 13  | –           |         |
| 14  | 69267.99(7) | 1       |
| 15  | 69637.59(7) | 1       |

| $J$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|
| 0   | 67395.8(2)  | 1       |
| 1   | 67420.43(15)| 2       |
| 2   | 67469.78(15)| 2       |
| 3   | 67543.90(15)| 2       |
| 4   | 67642.24(15)| 2       |
| 5   | 67765.03(15)| 2       |
| 6   | 67912.1(2)  | 1       |

| $J$ | $E_{n,v,J}$ | $N_\nu$ |
|-----|-------------|---------|
| 1   | 70056.8(2)  | 2       |
| 2   | 70092.1(2)  | 2       |