

RESONANCE PARAMETERS AND QUANTUM DEFECTS FOR SUPEREXCITED H₂

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The results of R-matrix calculations on electron collisions with H₂⁺ are presented. These calculations include the three lowest states of H₂⁺ (²Σ_g⁺, ²Σ_u⁺ and ²Π_u). Positions and widths of the Feshbach resonances converging to both the ²Σ_u⁺ and ²Π_u states are given, as are autoionization branching ratios for resonances lying above the ²Σ_u⁺ state. Complex quantum defects, calculated by performing scattering calculations above threshold, are presented for all three states considered. Results are tabulated for 12 symmetries (¹Σ_g⁺, ¹Σ_u⁺, ¹Π_u, ¹Π_g, ¹Δ_g, ¹Δ_u, ³Σ_g⁺, ³Σ_u⁺, ³Π_u, ³Π_g, ³Δ_g, ³Δ_u) and 13 internuclear separations from 1 to 4 a₀. © 1996 Academic Press, Inc.

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INTRODUCTION

Scope

Processes involving molecular hydrogen are of great practical and fundamental importance. Superexcited states, or resonances, of H_2 play an important role in a number of these processes including dissociative recombination,¹ photoionization,² and dissociative photoionization.³ There have been many studies of resonance positions and widths for low-lying members of the resonance series which converge to the first excited, ${}^2\Sigma_u^+$ state of H_2^+ (see Refs. 4–7 and references therein).

Despite the importance of this system, only Tennyson and Noble⁴ have systematically studied the resonances of all low-lying symmetries as a function of H–H internuclear separation. These workers used a two-state R-matrix model, which has been superseded by more recent calculations, and did not consider internuclear separations larger than $2.6 a_0$, which is inadequate for modeling dissociative processes.

A number of recent experiments^{1,8,9} have presented challenges to the available theoretical data for this system. It would therefore appear timely to present a complete and systematic evaluation of the low-lying resonances of superexcited molecular hydrogen, H_2^{*+} . This has been done in two ways: by explicitly fitting the eigenphase sums for low-lying resonances in a series and by calculating quantum defects for resonances series by considering above threshold scattering. For resonances converging to the ${}^2\Pi_u$ state of H_2^+ and lying above the ${}^2\Sigma_u^+$ state, branching ratios for autoionization have also been calculated. These resonances, although observed experimentally,¹⁰ have not previously been considered.

The present calculations have been performed using the R-matrix method for the ${}^1\Sigma_g^+$, ${}^1\Sigma_u^+$, ${}^1\Pi_u$, ${}^1\Pi_g$, ${}^1\Delta_g$, ${}^1\Delta_u$, ${}^3\Sigma_g^+$, ${}^3\Sigma_u^+$, ${}^3\Pi_u$, ${}^3\Pi_g$, ${}^3\Delta_g$, and ${}^3\Delta_u$ total symmetries.

The results are tabulated for 13 internuclear separations between 1 and $4 a_0$.

Calculations

Calculations on electron collisions with H_2^+ were performed using the R-matrix method. The wavefunctions used were developed and tested by Branchett and Tennyson¹¹ for studying transitions to Rydberg states of H_2 and by Sarpal and Tennyson¹² for calculating vibrational excitation cross sections.

The present calculations improve on previous R-matrix calculations of H_2^{*+} resonance widths^{4,6,7} in that the wavefunction expansion includes the lowest three states of the target H_2^+ ion with ${}^2\Sigma_g^+$, ${}^2\Sigma_u^+$, and ${}^2\Pi_u$ symmetry. Furthermore, a more flexible representation of the target π orbitals is used to represent not only the ${}^2\Pi_u$ target state but also the Π polarization effects. Further details of the calculations can be found in Refs. 11 and 12.

A new feature of the present calculations is the presence of resonance series converging to the ${}^2\Pi_u$ state of H_2^+ . When such resonances lie above the ${}^2\Sigma_u^+$ state, they can autoionize to either the ground ${}^2\Sigma_g^+$ or excited ${}^2\Sigma_u^+$ of H_2^+ . Branching ratios for this were calculated using the time-delay matrix method of Smith.^{13,14}

Resonances were located and fitted to a Breit–Wigner form using an automated search procedure.¹⁵ For all resonances the time-delay matrix was constructed and diagonalized at the fitted resonance position, E_r . The largest eigenvalue of this matrix yielded an alternative estimate of the resonance width, Γ , and, where appropriate, the corresponding eigenvector gives the branching ratio.¹³ In most cases the two methods of estimating the resonance widths gave excellent agreement. Significant disagreements resulted only from poor initial fits. These cases were refitted. Parameters obtained from these resonance

fits are tabulated in Tables I and II for resonances which converge to the $^2\Sigma_u^+$ and $^2\Pi_u$ state of H_2^+ , respectively.

Complex quantum defects were obtained from the resonances using the formulae

$$E_r = E_t - \frac{1}{\nu^2}, \quad \Gamma = \frac{4B}{\nu^3}, \quad (1)$$

where energies are in rydberg (Ry). E_t is the energy of the threshold with which the particular (resonance) state can be associated. The effective quantum number, ν , is related to the real part of the quantum defect by

$$\nu = n - A, \quad (2)$$

where n is an integer. For bound states, such as the Rydberg states of H_2 detailed in Table III, $B = 0$. For resonances, the complex quantum defect, μ , is given by

$$\mu = A + 2iB. \quad (3)$$

Estimates of A and B , which are assumed to vary smoothly and usually slowly with n , can be obtained by performing scattering calculations above threshold.^{16,17} Such calculations were performed at 0.0008 Ry above each threshold. Table III presents estimates of the quantum defects of the high n Rydberg states of H_2 . Tables IV and V present complex quantum defects for the high n resonances converging to the $^2\Sigma_u^+$ and $^2\Pi_u$ states of H_2^+ respectively. It is possible to correlate the threshold resonance parameters with those presented for the low n members of the same series presented in Tables I and II. As parameters for only a few resonances are presented in Tables I and II, these generally correlate with the lowest partial waves, (l, m) values, given in Tables IV and V.

Accuracy

There are two aspects which need to be considered when attempting to assess the accuracy of the data presented here: the accuracy of the model employed and any errors in the methods used to extract the parameters.

It is difficult to give a definitive estimate of the accuracy of the underlying calculations. However there are many calculations of H_2^{+*} resonance positions and widths, and the present results are in very good agreement with those obtained in recent calculations.^{6,7} Indeed, no evidence could be found for errors or omissions in previous calculations which had been suggested by analysis of some recent experiments.^{8,9}

In estimating resonance parameters, the positions and the widths behave somewhat differently. It is easy to obtain reliable resonance energies in a calculation: even poor fits yield good estimates. Conversely resonance widths can be very sensitive to the fitting procedure used. Usually poor fits were found to significantly overestimate the resonance width. In this work resonances were refitted

until agreement was obtained between estimates obtained from the fitting to the Breit–Wigner form and the time-delay method. In case of minor disagreements the narrower estimate was selected.

It proved difficult to obtain reliable fits to resonances which approached the H_2^+ ground state, such as the lowest $^1\Sigma_g^+$ resonance at internuclear separation $R \sim 2.6 a_0$. This problem has been well studied elsewhere,⁶ and no special effort was made to obtain resonance parameters in the crossing region.

For the quantum defect parameters, the crucial parameter is the energy, ϵ , above threshold at which the S-matrix is computed. A number of tests were performed before it was decided that $\epsilon = 0.0008$ Ry constituted a reliable value. Again it was found that the real part of the complex defect, A , which corresponds to the position was much more stable than the imaginary part, B , from which resonance widths can be estimated. A few B values were found to vary quite strongly as a function of ϵ .

The tables of quantum defects label each column with partial wave quantum numbers. Of course these quantum numbers are only approximate and were obtained by ordering the quantum defects according to their dominant eigenvectors. In most cases the (l, m) values presented do indeed reflect the dominant characteristic of the quantum defects. However in some cases, particularly near (avoided) crossings, this is not so. These instances are characterized by A values which either approach each other and move apart again or cross as a function of internuclear separation, R .

The tabular material presented below may also be obtained in electronic form by anonymous ftp from jonny.phys.ucl.ac.uk or via the author's world wide web home page at <http://jonny.phys.ucl.ac.uk/home.html>. The files have been placed in directory pub/astrodata/H2***, where the tables are given in both L^AT_EX and simple text form.

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References

1. C. Strömholm *et al.*, Phys. Rev. A **52**, R4320 (1995)
2. G. Raseev, J. Phys. B: At. Mol. Phys. **18**, 423 (1985)

3. K. Kirby, T. Uzer, A. C. Allison, and A. Dalgarno, *J. Chem. Phys.* **75**, 2820 (1981); K. P. Kirby, *AIP Conference Proceedings* **347**, 43 (1995)
4. J. Tennyson and C. J. Noble, *J. Phys. B: At. Mol. Phys.* **18**, 155 (1985)
5. L. A. Collins, B. I. Schneider, C. J. Noble, C. W. McCurdy, and S. Yabushita, *Phys. Rev. Lett.* **57**, 980 (1986)
6. I. Shimamura, C. J. Noble, and P. G. Burke, *Phys. Rev. A* **41**, 3545 (1990)
7. L. A. Collins, B. I. Schneider, and C. J. Noble, *Phys. Rev. A* **45**, 4610 (1992); L. A. Collins, B. I. Schneider, D. L. Lynch, and C. J. Noble, *Phys. Rev. A* **52**, 1310 (1995)
8. C. J. Latimer, K. F. Dunn, N. Kouchi, M. A. McDonald, V. Srigengan, and J. Geddes, *J. Phys. B: At. Mol. Opt. Phys.* **26**, L595 (1993) and **27**, 2961 (1994)
9. T. Odagiri, N. Uemura, K. Koyama, M. Ukai, M. Kouchi, and Y. Hatano, *J. Phys. B: At. Mol. Opt. Phys.* **28**, L465 (1995)
10. Z. X. He, J. N. Cutler, S. H. Southworth, L. R. Hughey, and J. A. R. Samson, *J. Chem. Phys.* **103**, 3912 (1995)
11. S. E. Branchett and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.* **25**, 2017 (1992)
12. B. K. Sarpal and J. Tennyson, *Mon. Not. R. Astr. Soc.* **263**, 909 (1993)
13. F. T. Smith, *Phys. Rev.* **114**, 349 (1960)
14. D. Stibbe and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.* **29**, 4267 (1996)
15. J. Tennyson and C. J. Noble, *Comput. Phys. Comm.* **33**, 421 (1984)
16. M. J. Seaton, *Rep. Prog. Phys.* **46**, 167 (1983)
17. J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.* **21**, 805 (1988)

EXPLANATION OF TABLES

- TABLE I.** Resonances Converging to the $^2\Sigma_u^+$ State of H_2^+
TABLE II. Resonances Converging to the $^2\Pi_u$ State of H_2^+
TABLE III. Quantum Defects for Rydberg States of H_2
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TABLE V. Complex Quantum Defects at the $^2\Pi_u$ Threshold

The tables are subdivided according to the total symmetry of the H_2 system. The columns of quantum defect in Tables III–V are labeled by partial wave parameters (l, m). As discussed in the introductory text, these designations are only approximate. Other parameters are defined as:

- R Internuclear separation in a_0 , the Bohr radius
 E_r Resonance position in Ry; Eq. (1)
 Γ Resonance width in Ry; Eq. (1)
 ν Effective quantum number; Eq. (2)
 A Real part of the (complex) quantum defect; Eq. (3)
 B Half the imaginary part of the complex quantum defect; Eq. (3)
 β_0 Branching ratio for autoionization to $\text{H}_2^+ \ ^2\Sigma_g^+$
 β_1 Branching ratio for autoionization to $\text{H}_2^+ \ ^2\Sigma_u^+$

TABLE I. Resonances Converging to the ${}^2\Sigma_u^+$ State of H_2^+
See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | R | E_r | Γ | ν | B |
|----------------------------------|--------|----------|--------|--------|----------------------------------|--------|----------|--------|--------|
| ${}^1\Sigma_g^+$: first series | | | | | ${}^1\Sigma_u^+$: first series | | | | |
| 1.0 | 1.3962 | 0.02818 | 1.6299 | 0.0305 | 1.0 | 1.4711 | 0.01810 | 1.8209 | 0.0273 |
| 1.2 | 1.1567 | 0.03962 | 1.6026 | 0.0408 | 1.2 | 1.2572 | 0.02463 | 1.8608 | 0.0397 |
| 1.4 | 0.9377 | 0.05345 | 1.5709 | 0.0518 | 1.4 | 1.0657 | 0.03138 | 1.8992 | 0.0537 |
| 1.6 | 0.7395 | 0.06892 | 1.5363 | 0.0625 | 1.6 | 0.8968 | 0.03788 | 1.9377 | 0.0689 |
| 1.8 | 0.5619 | 0.08453 | 1.5012 | 0.0715 | 1.8 | 0.7497 | 0.04398 | 1.9766 | 0.0849 |
| 2.0 | 0.4043 | 0.10063 | 1.4674 | 0.0795 | 2.0 | 0.6226 | 0.04929 | 2.0159 | 0.1009 |
| 2.2 | 0.2640 | 0.11617 | 1.4343 | 0.0857 | 2.2 | 0.5138 | 0.05406 | 2.0572 | 0.1177 |
| 2.4 | 0.1398 | 0.12804 | 1.4031 | 0.0884 | 2.4 | 0.4209 | 0.05790 | 2.0996 | 0.1340 |
| 2.6 | | | | | 2.6 | 0.3418 | 0.06126 | 2.1436 | 0.1509 |
| 2.8 | | | | | 2.8 | 0.2755 | 0.06353 | 2.1939 | 0.1677 |
| 3.0 | | | | | 3.0 | 0.2197 | 0.06457 | 2.2489 | 0.1836 |
| 3.5 | | | | | 3.5 | 0.1195 | 0.06031 | 2.4276 | 0.2157 |
| 4.0 | | | | | 4.0 | 0.0554 | 0.04001 | 2.6339 | 0.1828 |
| ${}^1\Sigma_g^+$: second series | | | | | ${}^1\Sigma_u^+$: second series | | | | |
| 1.0 | 1.6471 | 0.00574 | 2.8213 | 0.0322 | 1.0 | 1.6457 | 0.00404 | 2.8068 | 0.0223 |
| 1.2 | 1.4164 | 0.00563 | 2.7771 | 0.0302 | 1.2 | 1.4231 | 0.00571 | 2.8523 | 0.0331 |
| 1.4 | 1.2110 | 0.00697 | 2.7527 | 0.0364 | 1.4 | 1.2236 | 0.00768 | 2.8949 | 0.0466 |
| 1.6 | 1.0286 | 0.00849 | 2.7267 | 0.0430 | 1.6 | 1.0476 | 0.00952 | 2.9421 | 0.0606 |
| 1.8 | 0.8686 | 0.00966 | 2.7016 | 0.0476 | 1.8 | 0.8976 | 0.01185 | 3.0426 | 0.0130 |
| 2.0 | 0.7295 | 0.01024 | 2.6806 | 0.0493 | 2.0 | 0.7599 | 0.01248 | 3.0324 | 0.0173 |
| 2.2 | 0.6094 | 0.01050 | 2.6659 | 0.0497 | 2.2 | 0.6407 | 0.01238 | 3.0226 | 0.0164 |
| 2.4 | 0.5061 | 0.01093 | 2.6573 | 0.0513 | 2.4 | 0.5381 | 0.01218 | 3.0202 | 0.0150 |
| 2.6 | 0.4173 | 0.01169 | 2.6525 | 0.0546 | 2.6 | 0.4498 | 0.01236 | 3.0195 | 0.0163 |
| 2.8 | 0.3409 | 0.01267 | 2.6501 | 0.0589 | 2.8 | 0.3737 | 0.01289 | 3.0203 | 0.0199 |
| 3.0 | 0.2750 | 0.01353 | 2.6492 | 0.0629 | 3.0 | 0.3078 | 0.01386 | 3.0205 | 0.0266 |
| 3.5 | 0.1480 | 0.01433 | 2.6614 | 0.0675 | 3.5 | 0.1805 | 0.01098 | 3.0335 | 0.0634 |
| 4.0 | 0.0629 | 0.01494 | 2.7050 | 0.0739 | 4.0 | 0.0935 | 0.02420 | 3.0700 | 0.1750 |
| ${}^1\Sigma_g^+$: third series | | | | | ${}^1\Pi_u$: first series | | | | |
| 1.0 | 1.7041 | 0.00178 | 3.8173 | 0.0248 | 1.0 | 1.6749 | 0.00243 | 3.1978 | 0.0199 |
| 1.2 | 1.4765 | 0.00317 | 3.7920 | 0.0432 | 1.2 | 1.4299 | 0.00071 | 2.9350 | 0.0045 |
| 1.4 | 1.2724 | 0.00292 | 3.7655 | 0.0390 | 1.4 | 1.2294 | 0.00039 | 2.9683 | 0.0026 |
| 1.6 | 1.0917 | 0.00327 | 3.7400 | 0.0428 | 1.6 | 1.0534 | 0.00051 | 3.0192 | 0.0035 |
| 1.8 | 0.9333 | 0.00348 | 3.7185 | 0.0448 | 1.8 | 0.8979 | 0.00070 | 3.0468 | 0.0050 |
| 2.0 | 0.7957 | 0.00379 | 3.7025 | 0.0469 | 2.0 | 0.7610 | 0.00091 | 3.0482 | 0.0064 |
| 2.2 | 0.6767 | 0.00400 | 3.6909 | 0.0503 | 2.2 | 0.6413 | 0.00130 | 3.0321 | 0.0091 |
| 2.4 | 0.5740 | 0.00439 | 3.6827 | 0.0548 | 2.4 | 0.5381 | 0.00178 | 3.0200 | 0.0123 |
| 2.6 | 0.4855 | 0.00475 | 3.6765 | 0.0590 | 2.6 | 0.4488 | 0.00246 | 3.0062 | 0.0167 |
| 2.8 | 0.4092 | 0.00502 | 3.6730 | 0.0622 | 2.8 | 0.3725 | 0.00274 | 3.0046 | 0.0186 |
| 3.0 | 0.3433 | 0.00516 | 3.6721 | 0.0638 | 3.0 | 0.3074 | 0.00333 | 3.0144 | 0.0228 |
| 3.5 | 0.2159 | 0.00531 | 3.6937 | 0.0669 | 3.5 | 0.1807 | 0.00686 | 3.0364 | 0.0480 |
| 4.0 | 0.1277 | 0.00670 | 3.7310 | 0.0870 | 4.0 | 0.0935 | 0.01258 | 3.0703 | 0.0910 |

TABLE I. Resonances Converging to the ${}^2\Sigma_u^+$ State of H_2^+

See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | R | E_r | Γ | ν | B |
|-----------------------------|--------|----------|--------|--------|-------------------------------|--------|----------|--------|---------|
| ${}^1\Pi_u$: second series | | | | | ${}^1\Pi_g$: third series | | | | |
| 1.0 | 1.7130 | 0.00023 | 4.0950 | 0.0040 | 1.0 | 1.7029 | 0.00116 | 3.7851 | 0.0157 |
| 1.2 | 1.4794 | 0.00144 | 3.8749 | 0.0209 | 1.2 | 1.4783 | 0.00197 | 3.8410 | 0.0279 |
| 1.4 | 1.2798 | 0.00028 | 3.9790 | 0.0044 | 1.4 | 1.2767 | 0.00268 | 3.8850 | 0.0392 |
| 1.6 | 1.0996 | 0.00034 | 3.9662 | 0.0053 | 1.6 | 1.0981 | 0.00342 | 3.9217 | 0.0515 |
| 1.8 | 0.9412 | 0.00054 | 3.9391 | 0.0083 | 1.8 | 0.9429 | 6.3(-5) | 3.9935 | 0.0010 |
| 2.0 | 0.8043 | 0.00060 | 3.9404 | 0.0092 | 2.0 | 0.8062 | 3.9(-5) | 4.0024 | 6.2(-4) |
| 2.2 | 0.6865 | 0.00068 | 3.9645 | 0.0106 | 2.2 | 0.6876 | 9.5(-5) | 4.0000 | 0.0015 |
| 2.4 | 0.5844 | 0.00087 | 3.9734 | 0.0137 | 2.4 | 0.5853 | 9.3(-5) | 4.0007 | 0.0015 |
| 2.6 | 0.4965 | 0.00125 | 3.9854 | 0.0198 | 2.6 | 0.4970 | 8.0(-5) | 4.0009 | 0.0013 |
| 2.8 | 0.4201 | 0.00153 | 3.9788 | 0.0241 | 2.8 | 0.4209 | 5.2(-5) | 4.0028 | 8.4(-4) |
| 3.0 | 0.3549 | 0.00189 | 3.9987 | 0.0302 | 3.0 | 0.3551 | 9.6(-5) | 4.0044 | 0.0015 |
| 3.5 | 0.2269 | 0.00358 | 4.0067 | 0.0576 | 3.5 | 0.2271 | 0.00060 | 4.0124 | 0.0097 |
| 4.0 | 0.1380 | 0.00577 | 4.0297 | 0.0944 | 4.0 | 0.1376 | 0.00094 | 4.0167 | 0.0151 |
| ${}^1\Pi_g$: first series | | | | | ${}^1\Delta_g$: first series | | | | |
| 1.0 | 1.4659 | 0.02049 | 1.8056 | 0.0301 | 1.0 | 1.7102 | 0.4(-5) | 3.9995 | 6.8(-5) |
| 1.2 | 1.2543 | 0.02467 | 1.8513 | 0.0391 | 1.2 | 1.4836 | 3.8(-5) | 4.0011 | 6.1(-4) |
| 1.4 | 1.0646 | 0.02931 | 1.8954 | 0.0499 | 1.4 | 1.2804 | 0.5(-5) | 3.9988 | 7.9(-5) |
| 1.6 | 0.8956 | 0.03412 | 1.9334 | 0.0616 | 1.6 | 1.1006 | 0.8(-5) | 3.9998 | 1.3(-4) |
| 1.8 | 0.7467 | 0.03996 | 1.9650 | 0.0758 | 1.8 | 0.9431 | 2.3(-5) | 4.0002 | 3.7(-4) |
| 2.0 | 0.6151 | 0.04431 | 1.9858 | 0.0867 | 2.0 | 0.8062 | 3.3(-5) | 4.0005 | 5.2(-4) |
| 2.2 | 0.5028 | 0.04488 | 2.0110 | 0.0912 | 2.2 | 0.6876 | 2.9(-5) | 4.0011 | 4.6(-4) |
| 2.4 | 0.4089 | 0.04876 | 2.0463 | 0.1044 | 2.4 | 0.5853 | 2.3(-5) | 4.0019 | 3.8(-5) |
| 2.6 | 0.3278 | 0.05884 | 2.0778 | 0.1319 | 2.6 | 0.4971 | 2.8(-5) | 4.0031 | 4.5(-5) |
| 2.8 | 0.2556 | 0.06916 | 2.0957 | 0.1591 | 2.8 | 0.4209 | 4.4(-5) | 4.0047 | 7.0(-5) |
| 3.0 | 0.1972 | 0.07514 | 2.1308 | 0.1817 | 3.0 | 0.3552 | 8.1(-5) | 4.0070 | 0.0013 |
| 3.5 | 0.1169 | | 2.4094 | | 3.5 | 0.2271 | 0.00047 | 4.0151 | 0.0076 |
| 4.0 | | | | | 4.0 | 0.1378 | 0.00071 | 4.0246 | 0.0116 |
| ${}^1\Pi_g$: second series | | | | | ${}^1\Delta_u$: first series | | | | |
| 1.0 | 1.6505 | 0.00393 | 2.8607 | 0.0230 | 1.0 | 1.6574 | 9.3(-5) | 2.9456 | 6.0(-4) |
| 1.2 | 1.4205 | 0.00535 | 2.8219 | 0.0300 | 1.2 | 1.4316 | 0.00013 | 2.9567 | 8.3(-4) |
| 1.4 | 1.2217 | 0.00711 | 2.8722 | 0.0421 | 1.4 | 1.2293 | 0.00016 | 2.9660 | 0.0011 |
| 1.6 | 1.0460 | 0.00898 | 2.9220 | 0.0560 | 1.6 | 1.0502 | 0.00024 | 2.9755 | 0.0016 |
| 1.8 | 0.8913 | 0.01082 | 2.9577 | 0.0700 | 1.8 | 0.8933 | 0.00037 | 2.9837 | 0.0024 |
| 2.0 | 0.7560 | 0.01242 | 2.9799 | 0.0822 | 2.0 | 0.7569 | 0.00055 | 2.9914 | 0.0037 |
| 2.2 | 0.6382 | 0.01332 | 2.9886 | 0.0889 | 2.2 | 0.6389 | 0.00075 | 2.9985 | 0.0050 |
| 2.4 | 0.5369 | 0.01279 | 3.0036 | 0.0866 | 2.4 | 0.5370 | 0.00092 | 3.0053 | 0.0063 |
| 2.6 | 0.4512 | 0.01379 | 3.0390 | 0.0967 | 2.6 | 0.4493 | 0.00109 | 3.0126 | 0.0074 |
| 2.8 | 0.3779 | 0.01662 | 3.0810 | 0.1215 | 2.8 | 0.3737 | 0.00130 | 3.0209 | 0.0090 |
| 3.0 | 0.3131 | 0.02113 | 3.0956 | 0.1567 | 3.0 | 0.3085 | 0.00162 | 3.0301 | 0.0113 |
| 3.5 | 0.1870 | 0.03095 | 3.1278 | 0.2368 | 3.5 | 0.1821 | 0.00336 | 3.0563 | 0.0240 |
| 4.0 | 0.0863 | 0.03997 | 2.9711 | 0.2620 | 4.0 | 0.0939 | 0.00609 | 3.0765 | 0.0443 |

TABLE I. Resonances Converging to the ${}^2\Sigma_u^+$ State of H_2^+

See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | R | E_r | Γ | ν | B |
|----------------------------------|--------|----------|--------|---------|----------------------------------|--------|----------|--------|---------|
| ${}^1\Delta_u$: second series | | | | | ${}^3\Sigma_u^+$: first series | | | | |
| 1.0 | 1.7084 | 3.9(-5) | 3.9444 | 5.9(-4) | 1.0 | 1.4181 | 0.00012 | 1.6792 | 1.4(-4) |
| 1.2 | 1.4822 | 6.2(-5) | 3.9565 | 9.7(-4) | 1.2 | 1.2188 | 2.5(-5) | 1.7481 | 3.3(-5) |
| 1.4 | 1.2794 | 9.9(-5) | 3.9659 | 0.0015 | 1.4 | 1.0371 | 0.7(-5) | 1.8082 | 1.0(-5) |
| 1.6 | 1.0999 | 0.00015 | 3.9752 | 0.0023 | 1.6 | 0.8740 | 0.00010 | 1.8598 | 1.6(-4) |
| 1.8 | 0.9426 | 0.00020 | 3.9829 | 0.0032 | 1.8 | 0.7298 | 0.00032 | 1.9042 | 5.5(-4) |
| 2.0 | 0.8059 | 0.00025 | 3.9901 | 0.0040 | 2.0 | 0.6038 | 0.00070 | 1.9429 | 0.0013 |
| 2.2 | 0.6875 | 0.00031 | 3.9973 | 0.0050 | 2.2 | 0.4944 | 0.00124 | 1.9775 | 0.0024 |
| 2.4 | 0.5854 | 0.00040 | 4.0045 | 0.0065 | 2.4 | 0.4000 | 0.00194 | 2.0091 | 0.0039 |
| 2.6 | 0.4973 | 0.00054 | 4.0120 | 0.0086 | 2.6 | 0.3188 | 0.00278 | 2.0383 | 0.0059 |
| 2.8 | 0.4214 | 0.00073 | 4.0199 | 0.0119 | 2.8 | 0.2489 | 0.00381 | 2.0656 | 0.0084 |
| 3.0 | 0.3558 | 0.00099 | 4.0274 | 0.0162 | 3.0 | 0.1885 | 0.00507 | 2.0901 | 0.0116 |
| 3.5 | 0.2280 | 0.00193 | 4.0435 | 0.0319 | 3.5 | 0.0733 | 0.00902 | 2.1525 | 0.0225 |
| 4.0 | 0.1391 | 0.00276 | 4.0656 | 0.0464 | 4.0 | | | | |
| ${}^3\Sigma_g^+$: first series | | | | | ${}^3\Sigma_u^+$: second series | | | | |
| 1.0 | 1.6146 | 1.7(-5) | 2.5149 | 6.7(-5) | 1.0 | 1.6377 | 0.7(-5) | 2.7216 | 3.4(-5) |
| 1.2 | 1.3852 | 1.2(-5) | 2.4937 | 4.7(-5) | 1.2 | 1.4166 | 0.6(-5) | 2.7793 | 3.2(-5) |
| 1.4 | 1.1798 | 1.2(-5) | 2.4759 | 4.5(-5) | 1.4 | 1.2183 | 3.3(-5) | 2.8321 | 1.9(-4) |
| 1.6 | 0.9982 | 1.5(-5) | 2.4624 | 5.4(-5) | 1.6 | 1.0425 | 0.00012 | 2.8791 | 6.9(-4) |
| 1.8 | 0.8395 | 1.2(-5) | 2.4533 | 4.4(-5) | 1.8 | 0.8884 | 0.00024 | 2.9207 | 0.0015 |
| 2.0 | 0.7018 | 0.6(-5) | 2.4484 | 2.0(-5) | 2.0 | 0.7544 | 0.00034 | 2.9578 | 0.0022 |
| 2.2 | 0.5831 | 2.4(-5) | 2.4473 | 8.9(-5) | 2.2 | 0.6359 | 0.00201 | 2.9585 | 0.0131 |
| 2.4 | 0.4811 | 0.00010 | 2.4494 | 3.7(-4) | 2.4 | 0.5329 | 0.00279 | 2.9505 | 0.0179 |
| 2.6 | 0.3934 | 0.00024 | 2.4542 | 8.9(-4) | 2.6 | 0.4439 | 0.00370 | 2.9415 | 0.0236 |
| 2.8 | 0.3182 | 0.00041 | 2.4615 | 0.0015 | 2.8 | 0.3669 | 0.00495 | 2.9310 | 0.0311 |
| 3.0 | 0.2537 | 0.00057 | 2.4709 | 0.0022 | 3.0 | 0.2999 | 0.00685 | 2.9166 | 0.0425 |
| 3.5 | 0.1299 | 0.00095 | 2.5059 | 0.0037 | 3.5 | 0.1684 | 0.01608 | 2.8780 | 0.0959 |
| 4.0 | 0.0465 | 0.00225 | 2.5561 | 0.0094 | 4.0 | 0.0723 | 0.03132 | 2.8033 | 0.1725 |
| ${}^3\Sigma_g^+$: second series | | | | | ${}^3\Sigma_u^+$: third series | | | | |
| 1.0 | 1.6926 | 0.5(-5) | 3.5348 | 5.5(-5) | 1.0 | 1.6590 | 0.00021 | 2.9663 | 0.0014 |
| 1.2 | 1.4651 | 1.2(-5) | 3.5146 | 1.3(-4) | 1.2 | 1.4326 | 0.00028 | 2.9693 | 0.0018 |
| 1.4 | 1.2612 | 1.8(-5) | 3.4979 | 1.9(-4) | 1.4 | 1.2296 | 0.00037 | 2.9703 | 0.0024 |
| 1.6 | 1.0808 | 0.9(-5) | 3.4857 | 9.3(-5) | 1.6 | 1.0498 | 0.00053 | 2.9697 | 0.0035 |
| 1.8 | 0.9230 | 0.1(-5) | 3.4780 | 0.8(-5) | 1.8 | 0.8921 | 0.00085 | 2.9675 | 0.0056 |
| 2.0 | 0.7858 | 1.5(-5) | 3.4741 | 1.6(-4) | 2.0 | | | | |
| 2.2 | 0.6673 | 4.0(-5) | 3.4740 | 4.2(-4) | 2.2 | 0.6383 | 0.00046 | 2.9910 | 0.0030 |
| 2.4 | 0.5650 | 5.6(-5) | 3.4767 | 5.9(-4) | 2.4 | 0.5383 | 0.00057 | 3.0222 | 0.0039 |
| 2.6 | 0.4770 | 6.5(-5) | 3.4820 | 6.8(-4) | 2.6 | 0.4521 | 0.00075 | 3.0523 | 0.0053 |
| 2.8 | 0.4012 | 7.7(-5)7 | 3.4897 | 8.2(-4) | 2.8 | 0.3779 | 0.00107 | 3.0809 | 0.0078 |
| 3.0 | 0.3358 | 0.00010 | 3.4994 | 0.0011 | 3.0 | 0.3139 | 0.00158 | 3.1070 | 0.0118 |
| 3.5 | 0.2091 | 0.00035 | 3.5342 | 0.0039 | 3.5 | 0.1899 | 0.00373 | 3.1733 | 0.0298 |
| 4.0 | 0.1211 | 0.00109 | 3.5708 | 0.0124 | 4.0 | 0.1058 | 0.00777 | 3.2659 | 0.0676 |

TABLE I. Resonances Converging to the ${}^2\Sigma_u^+$ State of H_2^+

See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | R | E_r | Γ | ν | B |
|-----------------------------|--------|----------|--------|---------|-------------------------------|--------|----------|--------|---------|
| ${}^3\Pi_u$: first series | | | | | ${}^3\Pi_g$: second series | | | | |
| 1.0 | 1.6529 | 0.00021 | 2.8900 | 0.0012 | 1.0 | 1.6467 | 6.3(-5) | 2.8176 | 3.5(-4) |
| 1.2 | 1.4306 | 0.00025 | 2.9427 | 0.0016 | 1.2 | 1.4151 | 8.4(-5) | 2.7638 | 4.4(-4) |
| 1.4 | 1.2267 | 0.00029 | 2.9337 | 0.0018 | 1.4 | 1.2155 | 0.00019 | 2.8008 | 0.0010 |
| 1.6 | 1.0507 | 0.00045 | 2.9819 | 0.0030 | 1.6 | 1.0394 | 0.00039 | 2.8422 | 0.0023 |
| 1.8 | 0.8951 | 0.00070 | 3.0084 | 0.0048 | 1.8 | 0.8846 | 0.00070 | 2.8743 | 0.0041 |
| 2.0 | 0.7582 | 0.00102 | 3.0083 | 0.0070 | 2.0 | 0.7498 | 0.00100 | 2.9002 | 0.0061 |
| 2.2 | 0.6383 | 0.00147 | 2.9907 | 0.0099 | 2.2 | 0.6328 | 0.00132 | 2.9199 | 0.0082 |
| 2.4 | 0.5349 | 0.00193 | 2.9766 | 0.0127 | 2.4 | 0.5320 | 0.00150 | 2.9394 | 0.0095 |
| 2.6 | 0.4455 | 0.00252 | 2.9618 | 0.0164 | 2.6 | 0.4455 | 0.00193 | 2.9620 | 0.0125 |
| 2.8 | 0.3690 | 0.00292 | 2.9587 | 0.0189 | 2.8 | 0.3710 | 0.00278 | 2.9841 | 0.0185 |
| 3.0 | 0.3037 | 0.00370 | 2.9646 | 0.0241 | 3.0 | 0.3065 | 0.00410 | 3.0018 | 0.0277 |
| 3.5 | 0.1761 | 0.00813 | 2.9739 | 0.0534 | 3.5 | 0.1809 | 0.00816 | 3.0395 | 0.0573 |
| 4.0 | 0.0874 | 0.01506 | 2.9859 | 0.1003 | 4.0 | 0.0935 | 0.01319 | 3.0710 | 0.0955 |
| ${}^3\Pi_u$: second series | | | | | ${}^3\Delta_g$: first series | | | | |
| 1.0 | 1.7077 | 7.8(-5) | 3.9236 | 0.0012 | 1.0 | | | | |
| 1.2 | 1.4821 | 0.00011 | 3.9547 | 0.0017 | 1.2 | 1.4835 | 0.1(-5) | 3.9990 | 1.4(-5) |
| 1.4 | 1.2779 | 0.00018 | 3.9215 | 0.0027 | 1.4 | 1.2804 | 0.2(-5) | 3.9994 | 2.6(-5) |
| 1.6 | 1.0981 | 0.00032 | 3.9207 | 0.0048 | 1.6 | 1.1006 | 0.7(-5) | 3.9999 | 1.1(-4) |
| 1.8 | 0.9394 | 0.00054 | 3.8843 | 0.0079 | 1.8 | 0.9431 | 2.1(-5) | 4.0002 | 3.4(-4) |
| 2.0 | 0.8024 | 0.00062 | 3.8839 | 0.0091 | 2.0 | 0.8062 | 3.1(-5) | 4.0005 | 5.0(-4) |
| 2.2 | 0.6847 | 0.00068 | 3.9109 | 0.0102 | 2.2 | 0.6876 | 2.8(-5) | 4.0010 | 4.5(-4) |
| 2.4 | 0.5827 | 0.00085 | 3.9202 | 0.0128 | 2.4 | 0.5853 | 2.4(-5) | 4.0018 | 3.8(-4) |
| 2.6 | 0.4948 | 0.00116 | 3.9328 | 0.0176 | 2.6 | 0.4971 | 2.9(-5) | 4.0030 | 4.6(-4) |
| 2.8 | 0.4184 | 0.00150 | 3.9269 | 0.0228 | 2.8 | 0.4209 | 4.4(-5) | 4.0046 | 7.1(-4) |
| 3.0 | 0.3530 | 0.00207 | 3.9393 | 0.0316 | 3.0 | 0.3552 | 8.1(-5) | 4.0069 | 0.0013 |
| 3.5 | 0.2244 | 0.00416 | 3.9288 | 0.0630 | 3.5 | 0.2271 | 0.00047 | 4.0149 | 0.0076 |
| 4.0 | 0.1346 | 0.00603 | 3.9230 | 0.0909 | 4.0 | 0.1378 | 0.00071 | 4.0244 | 0.0115 |
| ${}^3\Pi_g$: first series | | | | | ${}^3\Delta_u$: first series | | | | |
| 1.0 | 1.4289 | 0.00017 | 1.7056 | 2.1(-4) | 1.0 | 1.6575 | 8.5(-5) | 2.9460 | 5.5(-4) |
| 1.2 | 1.2182 | 0.00044 | 1.7464 | 5.8(-4) | 1.2 | 1.4316 | 0.00011 | 2.9562 | 7.2(-4) |
| 1.4 | 1.0297 | 0.00090 | 1.7866 | 0.0013 | 1.4 | 1.2292 | 0.00014 | 2.9654 | 9.4(-4) |
| 1.6 | 0.8621 | 0.00166 | 1.8227 | 0.0025 | 1.6 | 1.0501 | 0.00021 | 2.9741 | 0.0014 |
| 1.8 | 0.7149 | 0.00281 | 1.8546 | 0.0045 | 1.8 | 0.8932 | 0.00032 | 2.9822 | 0.0021 |
| 2.0 | 0.5866 | 0.00419 | 1.8829 | 0.0070 | 2.0 | 0.7568 | 0.00049 | 2.9898 | 0.0033 |
| 2.2 | 0.4758 | 0.00563 | 1.9092 | 0.0098 | 2.2 | 0.6388 | 0.00067 | 2.9970 | 0.0045 |
| 2.4 | 0.3806 | 0.00803 | 1.9347 | 0.0145 | 2.4 | 0.5369 | 0.00085 | 3.0039 | 0.0058 |
| 2.6 | 0.2985 | 0.01170 | 1.9577 | 0.0219 | 2.6 | 0.4492 | 0.00101 | 3.0113 | 0.0069 |
| 2.8 | 0.2277 | 0.01531 | 1.9781 | 0.0296 | 2.8 | 0.3736 | 0.00121 | 3.0196 | 0.0083 |
| 3.0 | 0.1677 | 0.02010 | 2.0010 | 0.0403 | 3.0 | 0.3084 | 0.00151 | 3.0288 | 0.0105 |
| 3.5 | 0.0509 | 0.04278 | 2.0485 | 0.0919 | 3.5 | 0.1820 | 0.00323 | 3.0550 | 0.0230 |
| 4.0 | | | | | 4.0 | 0.0938 | 0.00594 | 3.0755 | 0.0432 |

TABLE I. Resonances Converging to the ${}^2\Sigma_u^+$ State of H_2^+
 See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B |
|--------------------------------|--------|----------|--------|---------|
| ${}^3\Delta_u$: second series | | | | |
| 1.0 | 1.7085 | 3.9(-5) | 3.9463 | 6.0(-4) |
| 1.2 | 1.4822 | 5.8(-5) | 3.9566 | 9.0(-4) |
| 1.4 | 1.2793 | 9.2(-5) | 3.9657 | 0.0014 |
| 1.6 | 1.0998 | 0.00014 | 3.9741 | 0.0021 |
| 1.8 | 0.9426 | 0.00018 | 3.9816 | 0.0028 |
| 2.0 | 0.8058 | 0.00023 | 3.9887 | 0.0036 |
| 2.2 | 0.6875 | 0.00028 | 3.9959 | 0.0045 |
| 2.4 | 0.5854 | 0.00037 | 4.0032 | 0.0059 |
| 2.6 | 0.4973 | 0.00050 | 4.0107 | 0.0081 |
| 2.8 | 0.4214 | 0.00068 | 4.0185 | 0.0111 |
| 3.0 | 0.3557 | 0.00094 | 4.0259 | 0.0153 |
| 3.5 | 0.2280 | 0.00186 | 4.0423 | 0.0306 |
| 4.0 | 0.1390 | 0.00268 | 4.0646 | 0.0450 |

TABLE II. Resonances Converging to the ${}^2\Pi_u$ State of H_2^+
See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | β_0 | β_1 | R | E_r | Γ | ν | B | β_0 | β_1 |
|----------------------------------|--------|----------|--------|--------|-----------|-----------|----------------------------------|--------|----------|--------|--------|-----------|-----------|
| ${}^1\Sigma_g^+$: first series | | | | | | | ${}^1\Sigma_u^+$: second series | | | | | | |
| 1.0 | | | | | | | 1.0 | 1.8944 | 0.00053 | 4.0900 | 0.0090 | 0.181 | 0.819 |
| 1.2 | | | | | | | 1.2 | 1.7328 | 0.00046 | 4.0893 | 0.0078 | 0.223 | 0.777 |
| 1.4 | 1.3497 | 0.01451 | 1.8108 | 0.0215 | 0.941 | 0.059 | 1.4 | 1.5948 | 0.00042 | 4.0871 | 0.0071 | 0.259 | 0.741 |
| 1.6 | 1.2357 | 0.01429 | 1.8235 | 0.0217 | 0.924 | 0.076 | 1.6 | 1.4766 | 0.00038 | 4.0885 | 0.0064 | 0.290 | 0.710 |
| 1.8 | 1.1388 | 0.01369 | 1.8384 | 0.0213 | 0.893 | 0.107 | 1.8 | 1.3748 | 0.00035 | 4.0885 | 0.0060 | 0.317 | 0.683 |
| 2.0 | 1.0555 | 0.01308 | 1.8534 | 0.0208 | 0.854 | 0.146 | 2.0 | 1.2868 | 0.00035 | 4.0895 | 0.0060 | 0.343 | 0.657 |
| 2.2 | 0.9833 | 0.01262 | 1.8676 | 0.0206 | 0.813 | 0.187 | 2.2 | 1.2102 | 0.00037 | 4.0890 | 0.0063 | 0.370 | 0.630 |
| 2.4 | 0.9209 | 0.01233 | 1.8812 | 0.0205 | 0.769 | 0.231 | 2.4 | 1.1434 | 0.00040 | 4.0804 | 0.0067 | 0.395 | 0.605 |
| 2.6 | 0.8666 | 0.01223 | 1.8962 | 0.0209 | 0.723 | 0.277 | 2.6 | 1.0846 | 0.00043 | 4.0791 | 0.0072 | 0.411 | 0.589 |
| 2.8 | 0.8194 | 0.01223 | 1.9108 | 0.0213 | 0.674 | 0.326 | 2.8 | 1.0329 | 0.00046 | 4.0668 | 0.0077 | 0.425 | 0.575 |
| 3.0 | 0.7780 | 0.01238 | 1.9240 | 0.0220 | 0.627 | 0.373 | 3.0 | 0.9882 | 0.00053 | 4.0826 | 0.0090 | 0.430 | 0.570 |
| 3.5 | 0.6964 | 0.01266 | 1.9567 | 0.0237 | 0.522 | 0.478 | 3.5 | 0.8973 | 0.00072 | 4.0714 | 0.0121 | 0.432 | 0.568 |
| 4.0 | 0.6382 | 0.01257 | 1.9861 | 0.0246 | 0.456 | 0.544 | 4.0 | 0.8302 | 0.00088 | 4.0300 | 0.0144 | 0.435 | 0.565 |
| ${}^1\Sigma_g^+$: second series | | | | | | | ${}^1\Pi_u$: first series | | | | | | |
| 1.0 | 1.8395 | 0.00296 | 2.9531 | 0.0190 | 0.904 | 0.096 | 1.0 | 1.6374 | 0.00390 | 1.7767 | 0.0055 | 1.0 | 0.0 |
| 1.2 | 1.6788 | 0.00283 | 2.9645 | 0.0185 | 0.930 | 0.070 | 1.2 | 1.5003 | 0.00241 | 1.8497 | 0.0038 | 1.0 | 0.0 |
| 1.4 | 1.5420 | 0.00262 | 2.9792 | 0.0173 | 0.930 | 0.070 | 1.4 | 1.3825 | 0.03538 | 1.9169 | 0.0623 | 0.252 | 0.748 |
| 1.6 | 1.4250 | 0.00239 | 2.9953 | 0.0160 | 0.912 | 0.088 | 1.6 | 1.2751 | 0.02844 | 1.9561 | 0.0532 | 0.282 | 0.718 |
| 1.8 | 1.3244 | 0.00221 | 3.0121 | 0.0151 | 0.883 | 0.117 | 1.8 | 1.1822 | 0.02356 | 1.9904 | 0.0464 | 0.314 | 0.686 |
| 2.0 | 1.2376 | 0.00209 | 3.0296 | 0.0146 | 0.847 | 0.153 | 2.0 | 1.1021 | 0.01926 | 2.0223 | 0.0398 | 0.409 | 0.591 |
| 2.2 | 1.1622 | 0.00207 | 3.0450 | 0.0146 | 0.807 | 0.193 | 2.2 | 1.0314 | 0.01728 | 2.0469 | 0.0370 | 0.549 | 0.451 |
| 2.4 | 1.0965 | 0.00213 | 3.0573 | 0.0152 | 0.765 | 0.235 | 2.4 | 0.9694 | 0.01741 | 2.0668 | 0.0384 | 0.684 | 0.316 |
| 2.6 | 1.0390 | 0.00216 | 3.0756 | 0.0157 | 0.721 | 0.279 | 2.6 | 0.9133 | 0.01631 | 2.0788 | 0.0367 | 0.738 | 0.262 |
| 2.8 | 0.9885 | 0.00227 | 3.0891 | 0.0167 | 0.677 | 0.323 | 2.8 | 0.8626 | 0.01377 | 2.0820 | 0.0311 | 0.738 | 0.262 |
| 3.0 | 0.9448 | 0.00222 | 3.1101 | 0.0167 | 0.633 | 0.367 | 3.0 | 0.8223 | 0.00998 | 2.1043 | 0.0232 | 0.820 | 0.180 |
| 3.5 | 0.8562 | 0.00230 | 3.1403 | 0.0178 | 0.533 | 0.467 | 3.5 | 0.7365 | 0.00592 | 2.1268 | 0.0142 | 0.914 | 0.086 |
| 4.0 | 0.7890 | 0.00226 | 3.1204 | 0.0171 | 0.492 | 0.508 | 4.0 | 0.6770 | 0.00677 | 2.1580 | 0.0170 | 0.930 | 0.070 |
| ${}^1\Sigma_u^+$: first series | | | | | | | ${}^1\Pi_u$: second series | | | | | | |
| 1.0 | 1.8499 | 0.00100 | 3.0968 | 0.0074 | 0.162 | 0.838 | 1.0 | 1.8234 | 0.01056 | 2.7649 | 0.0558 | 0.118 | 0.882 |
| 1.2 | 1.6883 | 0.00090 | 3.0971 | 0.0066 | 0.212 | 0.788 | 1.2 | 1.6655 | 0.01052 | 2.8048 | 0.0580 | 0.148 | 0.852 |
| 1.4 | 1.5504 | 0.00080 | 3.0978 | 0.0060 | 0.256 | 0.744 | 1.4 | 1.5306 | 0.00966 | 2.8389 | 0.0552 | 0.198 | 0.802 |
| 1.6 | 1.4317 | 0.00073 | 3.0899 | 0.0054 | 0.291 | 0.709 | 1.6 | 1.4141 | 0.00784 | 2.8595 | 0.0458 | 0.236 | 0.764 |
| 1.8 | 1.3290 | 0.00068 | 3.0768 | 0.0050 | 0.314 | 0.686 | 1.8 | 1.3132 | 0.00604 | 2.8691 | 0.0356 | 0.256 | 0.744 |
| 2.0 | 1.2408 | 0.00065 | 3.0743 | 0.0047 | 0.330 | 0.670 | 2.0 | 1.2255 | 0.00476 | 2.8741 | 0.0283 | 0.295 | 0.705 |
| 2.2 | 1.1648 | 0.00062 | 3.0828 | 0.0045 | 0.346 | 0.654 | 2.2 | 1.1490 | 0.00401 | 2.8749 | 0.0238 | 0.380 | 0.620 |
| 2.4 | 1.0988 | 0.00062 | 3.0903 | 0.0046 | 0.357 | 0.643 | 2.4 | 1.0820 | 0.00360 | 2.8687 | 0.0213 | 0.485 | 0.515 |
| 2.6 | 1.0407 | 0.00063 | 3.1002 | 0.0047 | 0.369 | 0.631 | 2.6 | 1.0229 | 0.00373 | 2.8651 | 0.0219 | 0.610 | 0.390 |
| 2.8 | 0.9895 | 0.00067 | 3.1037 | 0.0050 | 0.376 | 0.624 | 2.8 | 0.9710 | 0.00448 | 2.8585 | 0.0261 | 0.753 | 0.247 |
| 3.0 | 0.9451 | 0.00077 | 3.1152 | 0.0058 | 0.382 | 0.618 | 3.0 | 0.9239 | 0.00438 | 2.8372 | 0.0250 | 0.677 | 0.323 |
| 3.5 | 0.8549 | 0.00104 | 3.1202 | 0.0079 | 0.394 | 0.606 | 3.5 | 0.8282 | 0.00478 | 2.7800 | 0.0257 | 0.648 | 0.352 |
| 4.0 | 0.7891 | 0.00113 | 3.1208 | 0.0086 | 0.386 | 0.614 | 4.0 | 0.7564 | 0.00618 | 2.7180 | 0.0310 | 0.635 | 0.365 |

TABLE II. Resonances Converging to the ${}^2\Pi_u$ State of H_2^+
See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | β_0 | β_1 | R | E_r | Γ | ν | B | β_0 | β_1 |
|-----------------------------|--------|----------|--------|--------|-----------|-----------|--------------------------------|--------|----------|--------|--------|-----------|-----------|
| ${}^1\Pi_u$: third series | | | | | | | ${}^1\Delta_g$: first series | | | | | | |
| 1.0 | 1.8431 | 0.00040 | 3.0005 | 0.0027 | 0.633 | 0.367 | 1.0 | 1.6145 | 0.01160 | 1.7158 | 0.0146 | 1.0 | 0.0 |
| 1.2 | 1.6818 | 0.00073 | 3.0047 | 0.0049 | 0.576 | 0.424 | 1.2 | 1.4578 | 0.01276 | 1.7283 | 0.0165 | 1.0 | 0.0 |
| 1.4 | 1.5444 | 0.00125 | 3.0116 | 0.0085 | 0.564 | 0.436 | 1.4 | | | | | | |
| 1.6 | 1.4269 | 0.00169 | 3.0217 | 0.0117 | 0.557 | 0.443 | 1.6 | 1.2123 | 0.01600 | 1.7566 | 0.0217 | 0.935 | 0.065 |
| 1.8 | 1.3261 | 0.00186 | 3.0360 | 0.0130 | 0.533 | 0.467 | 1.8 | 1.1160 | 0.01709 | 1.7717 | 0.0238 | 0.912 | 0.088 |
| 2.0 | 1.2394 | 0.00185 | 3.0549 | 0.0132 | 0.537 | 0.463 | 2.0 | 1.0334 | 0.01794 | 1.7869 | 0.0256 | 0.895 | 0.105 |
| 2.2 | 1.1643 | 0.00177 | 3.0751 | 0.0129 | 0.620 | 0.380 | 2.2 | 0.9621 | 0.01840 | 1.8021 | 0.0269 | 0.884 | 0.116 |
| 2.4 | 1.0991 | 0.00161 | 3.0945 | 0.0119 | 0.730 | 0.270 | 2.4 | 0.9005 | 0.01857 | 1.8166 | 0.0278 | 0.873 | 0.127 |
| 2.6 | 1.0418 | 0.00183 | 3.1171 | 0.0138 | 0.873 | 0.127 | 2.6 | 0.8469 | 0.01867 | 1.8324 | 0.0287 | 0.860 | 0.140 |
| 2.8 | 0.9922 | 0.00217 | 3.1441 | 0.0168 | 0.968 | 0.032 | 2.8 | 0.8003 | 0.01843 | 1.8474 | 0.0291 | 0.844 | 0.156 |
| 3.0 | 0.9471 | 0.00210 | 3.1453 | 0.0163 | 0.952 | 0.048 | 3.0 | 0.7594 | 0.01811 | 1.8608 | 0.0292 | 0.826 | 0.174 |
| 3.5 | 0.8584 | 0.00114 | 3.1752 | 0.0092 | 0.965 | 0.035 | 3.5 | 0.6787 | 0.01668 | 1.8934 | 0.0283 | 0.776 | 0.224 |
| 4.0 | 0.7943 | 0.00061 | 3.2037 | 0.0050 | 0.960 | 0.040 | 4.0 | 0.6210 | 0.01468 | 1.9219 | 0.0261 | 0.749 | 0.251 |
| ${}^1\Pi_g$: first series | | | | | | | ${}^1\Delta_g$: second series | | | | | | |
| 1.0 | 1.7978 | 0.01888 | 2.5289 | 0.0763 | 0.158 | 0.842 | 1.0 | 1.8341 | 0.00242 | 2.8855 | 0.0145 | 0.995 | 0.005 |
| 1.2 | 1.6319 | 0.01837 | 2.4946 | 0.0713 | 0.208 | 0.792 | 1.2 | 1.6735 | 0.00259 | 2.8974 | 0.0157 | 0.998 | 0.002 |
| 1.4 | 1.4882 | 0.01673 | 2.4512 | 0.0616 | 0.234 | 0.766 | 1.4 | 1.5366 | 0.00279 | 2.9108 | 0.0172 | 0.978 | 0.022 |
| 1.6 | 1.3648 | 0.01516 | 2.4136 | 0.0533 | 0.261 | 0.739 | 1.6 | 1.4196 | 0.00303 | 2.9253 | 0.0190 | 0.952 | 0.048 |
| 1.8 | 1.2586 | 0.01316 | 2.3832 | 0.0445 | 0.289 | 0.711 | 1.8 | 1.3189 | 0.00332 | 2.9400 | 0.0211 | 0.931 | 0.069 |
| 2.0 | 1.1667 | 0.01110 | 2.3578 | 0.0364 | 0.310 | 0.690 | 2.0 | 1.2321 | 0.00358 | 2.9551 | 0.0231 | 0.917 | 0.083 |
| 2.2 | 1.0869 | 0.00949 | 2.3367 | 0.0303 | 0.319 | 0.681 | 2.2 | 1.1566 | 0.00382 | 2.9689 | 0.0250 | 0.905 | 0.095 |
| 2.4 | 1.0173 | 0.00798 | 2.3172 | 0.0248 | 0.299 | 0.701 | 2.4 | 1.0908 | 0.00407 | 2.9796 | 0.0269 | 0.894 | 0.106 |
| 2.6 | 0.9564 | 0.00742 | 2.3045 | 0.0227 | 0.280 | 0.720 | 2.6 | 1.0334 | 0.00416 | 2.9969 | 0.0280 | 0.882 | 0.118 |
| 2.8 | 0.9025 | 0.00719 | 2.2894 | 0.0216 | 0.236 | 0.764 | 2.8 | 0.9829 | 0.00428 | 3.0088 | 0.0292 | 0.868 | 0.132 |
| 3.0 | 0.8567 | 0.00688 | 2.2852 | 0.0205 | 0.351 | 0.649 | 3.0 | 0.9393 | 0.00412 | 3.0302 | 0.0287 | 0.852 | 0.148 |
| 3.5 | 0.7637 | 0.00630 | 2.2710 | 0.0184 | 0.451 | 0.549 | 3.5 | 0.8510 | 0.00384 | 3.0620 | 0.0275 | 0.810 | 0.190 |
| 4.0 | 0.6977 | 0.00480 | 2.2699 | 0.0140 | 0.534 | 0.466 | 4.0 | 0.7877 | 0.00312 | 3.1009 | 0.0233 | 0.751 | 0.249 |
| ${}^1\Pi_g$: second series | | | | | | | ${}^1\Delta_u$: first series | | | | | | |
| 1.0 | 1.8753 | 0.00686 | 3.5595 | 0.0774 | 0.178 | 0.822 | 1.0 | 1.8473 | 0.00138 | 3.0591 | 0.0098 | 0.022 | 0.978 |
| 1.2 | 1.7118 | 0.00589 | 3.5180 | 0.0641 | 0.217 | 0.783 | 1.2 | 1.6854 | 0.00115 | 3.0542 | 0.0082 | 0.039 | 0.961 |
| 1.4 | 1.5719 | 0.00526 | 3.4775 | 0.0553 | 0.247 | 0.753 | 1.4 | 1.5391 | 0.00237 | 2.9418 | 0.0151 | 0.077 | 0.923 |
| 1.6 | 1.4521 | 0.00457 | 3.4432 | 0.0466 | 0.273 | 0.727 | 1.6 | 1.4284 | 0.00086 | 3.0424 | 0.0060 | 0.078 | 0.922 |
| 1.8 | 1.3489 | 0.00380 | 3.4149 | 0.0379 | 0.286 | 0.714 | 1.8 | 1.3269 | 0.00077 | 3.0467 | 0.0054 | 0.097 | 0.903 |
| 2.0 | 1.2597 | 0.00321 | 3.3925 | 0.0314 | 0.297 | 0.703 | 2.0 | 1.2394 | 0.00068 | 3.0538 | 0.0048 | 0.119 | 0.881 |
| 2.2 | 1.1823 | 0.00281 | 3.3760 | 0.0270 | 0.313 | 0.687 | 2.2 | 1.1634 | 0.00063 | 3.0621 | 0.0045 | 0.148 | 0.852 |
| 2.4 | 1.1150 | 0.00256 | 3.3624 | 0.0244 | 0.327 | 0.673 | 2.4 | 1.1080 | 0.00052 | 3.2363 | 0.0044 | 0.227 | 0.773 |
| 2.6 | 1.0560 | 0.00241 | 3.3578 | 0.0228 | 0.375 | 0.625 | 2.6 | 1.0505 | 0.00049 | 3.2580 | 0.0042 | 0.271 | 0.729 |
| 2.8 | 1.0046 | 0.00247 | 3.3572 | 0.0233 | 0.474 | 0.526 | 2.8 | 0.9931 | 0.00072 | 3.1583 | 0.0056 | 0.295 | 0.705 |
| 3.0 | 0.9591 | 0.00170 | 3.3499 | 0.0160 | 0.454 | 0.546 | 3.0 | 0.9457 | 0.00079 | 3.1247 | 0.0060 | 0.343 | 0.657 |
| 3.5 | 0.8685 | 0.00134 | 3.3498 | 0.0126 | 0.568 | 0.432 | 3.5 | 0.8593 | 0.00078 | 3.1898 | 0.0063 | 0.418 | 0.582 |
| 4.0 | 0.8020 | 0.00091 | 3.3384 | 0.0085 | 0.599 | 0.400 | 4.0 | 0.8012 | 0.00043 | 3.3238 | 0.0040 | 0.432 | 0.568 |

TABLE II. Resonances Converging to the ${}^2\Pi_u$ State of H_2^+
See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | β_0 | β_1 | R | E_r | Γ | ν | B | β_0 | β_1 |
|----------------------------------|--------|----------|--------|---------|-----------|-----------|----------------------------------|--------|----------|--------|---------|-----------|-----------|
| ${}^1\Delta_u$: second series | | | | | | | ${}^3\Sigma_u^+$: first series | | | | | | |
| 1.0 | 1.8902 | 0.00063 | 3.9525 | 0.0097 | 0.015 | 0.985 | 1.0 | 1.8385 | 0.00304 | 2.9405 | 0.0193 | 0.030 | 0.970 |
| 1.2 | 1.7281 | 0.00047 | 3.9379 | 0.0072 | 0.026 | 0.974 | 1.2 | 1.6759 | 0.00250 | 2.9281 | 0.0157 | 0.045 | 0.955 |
| 1.4 | 1.5844 | 0.00088 | 3.7746 | 0.0119 | 0.075 | 0.925 | 1.4 | 1.5368 | 0.00209 | 2.9136 | 0.0129 | 0.062 | 0.938 |
| 1.6 | 1.4714 | 0.00030 | 3.9230 | 0.0045 | 0.071 | 0.929 | 1.6 | 1.4165 | 0.00178 | 2.8876 | 0.0108 | 0.079 | 0.921 |
| 1.8 | 1.3704 | 0.00030 | 3.9439 | 0.0046 | 0.105 | 0.895 | 1.8 | 1.3120 | 0.00154 | 2.8559 | 0.0090 | 0.097 | 0.903 |
| 2.0 | 1.2834 | 0.00024 | 3.9780 | 0.0038 | 0.135 | 0.865 | 2.0 | 1.2220 | 0.00137 | 2.8327 | 0.0078 | 0.114 | 0.886 |
| 2.2 | 1.2066 | 0.00022 | 3.9699 | 0.0034 | 0.175 | 0.825 | 2.2 | 1.1437 | 0.00124 | 2.8132 | 0.0069 | 0.133 | 0.867 |
| 2.4 | 1.1508 | 0.00061 | 4.3568 | 0.0125 | 0.294 | 0.706 | 2.4 | 1.0750 | 0.00113 | 2.7902 | 0.0061 | 0.149 | 0.851 |
| 2.6 | 1.0930 | 0.00058 | 4.3970 | 0.0123 | 0.339 | 0.661 | 2.6 | 1.0141 | 0.00101 | 2.7667 | 0.0053 | 0.167 | 0.833 |
| 2.8 | 1.0303 | 0.00024 | 3.9834 | 0.0039 | 0.296 | 0.704 | 2.8 | 0.9598 | 0.00090 | 2.7363 | 0.0046 | 0.189 | 0.811 |
| 3.0 | 0.9851 | 0.00016 | 3.9811 | 0.0025 | 0.369 | 0.631 | 3.0 | 0.9116 | 0.00085 | 2.7061 | 0.0042 | 0.214 | 0.786 |
| 3.5 | 0.8965 | 0.00027 | 4.0442 | 0.0045 | 0.370 | 0.630 | 3.5 | 0.8117 | 0.00069 | 2.6177 | 0.0031 | 0.299 | 0.701 |
| 4.0 | 0.8418 | 0.00045 | 4.4758 | 0.0100 | 0.496 | 0.504 | 4.0 | 0.7358 | 0.00057 | 2.5323 | 0.0023 | 0.356 | 0.644 |
| ${}^3\Sigma_g^+$: first series | | | | | | | ${}^3\Sigma_u^+$: second series | | | | | | |
| 1.0 | 1.8134 | 0.00028 | 2.6653 | 0.0013 | 0.054 | 0.946 | 1.0 | 1.8884 | 0.00134 | 3.8990 | 0.0199 | 0.034 | 0.966 |
| 1.2 | 1.6532 | 0.00017 | 2.6785 | 8.2(-4) | 0.095 | 0.905 | 1.2 | 1.7264 | 0.00108 | 3.8871 | 0.0159 | 0.044 | 0.956 |
| 1.4 | 1.5167 | 0.00011 | 2.6925 | 5.1(-4) | 0.136 | 0.864 | 1.4 | 1.5879 | 0.00088 | 3.8703 | 0.0127 | 0.058 | 0.943 |
| 1.6 | 1.3999 | 6.7(-5) | 2.7067 | 3.3(-4) | 0.189 | 0.811 | 1.6 | 1.4693 | 0.00071 | 3.8597 | 0.0102 | 0.077 | 0.923 |
| 1.8 | 1.2995 | 4.7(-5) | 2.7203 | 2.4(-4) | 0.276 | 0.724 | 1.8 | 1.3671 | 0.00058 | 3.8487 | 0.0083 | 0.104 | 0.896 |
| 2.0 | 1.2128 | 3.9(-5) | 2.7340 | 2.0(-4) | 0.404 | 0.596 | 2.0 | 1.2785 | 0.00050 | 3.8323 | 0.0071 | 0.136 | 0.864 |
| 2.2 | 1.1376 | 3.8(-5) | 2.7479 | 2.0(-4) | 0.589 | 0.411 | 2.2 | 1.2011 | 0.00044 | 3.8081 | 0.0061 | 0.177 | 0.823 |
| 2.4 | 1.0720 | 4.2(-5) | 2.7581 | 2.2(-4) | 0.744 | 0.256 | 2.4 | 1.1334 | 0.00039 | 3.7775 | 0.0052 | 0.220 | 0.780 |
| 2.6 | 1.0149 | 5.2(-5) | 2.7754 | 2.8(-4) | 0.851 | 0.149 | 2.6 | 1.0738 | 0.00033 | 3.7544 | 0.0044 | 0.268 | 0.732 |
| 2.8 | 0.9646 | 6.4(-5) | 2.7866 | 3.5(-4) | 0.908 | 0.092 | 2.8 | 1.0214 | 0.00029 | 3.7284 | 0.0037 | 0.322 | 0.678 |
| 3.0 | 0.9217 | 7.8(-5) | 2.8119 | 4.3(-4) | 0.945 | 0.055 | 3.0 | 0.9757 | 0.00026 | 3.7141 | 0.0033 | 0.371 | 0.629 |
| 3.5 | 0.8341 | 9.8(-5) | 2.8454 | 5.7(-4) | 0.933 | 0.067 | 3.5 | 0.8833 | 0.00019 | 3.6684 | 0.0023 | 0.492 | 0.508 |
| 4.0 | 0.7698 | 0.00016 | 2.8634 | 9.2(-4) | 0.887 | 0.113 | 4.0 | 0.8137 | 0.00017 | 3.5804 | 0.0020 | 0.580 | 0.420 |
| ${}^3\Sigma_g^+$: second series | | | | | | | ${}^3\Pi_u$: first series | | | | | | |
| 1.0 | 1.8799 | 9.5(-5) | 3.6692 | 0.0012 | 0.018 | 0.982 | 1.0 | 1.5511 | 0.00046 | 1.5751 | 4.4(-4) | 1.0 | 0.0 |
| 1.2 | 1.7188 | 6.3(-5) | 3.6815 | 7.9(-4) | 0.045 | 0.955 | 1.2 | 1.4061 | 0.00039 | 1.6086 | 4.0(-4) | 1.0 | 0.0 |
| 1.4 | 1.5813 | 4.4(-5) | 3.6916 | 5.5(-4) | 0.125 | 0.875 | 1.4 | 1.2863 | 0.00033 | 1.6478 | 3.7(-4) | 1.0 | 0.0 |
| 1.6 | 1.4635 | 3.4(-5) | 3.7041 | 4.3(-4) | 0.301 | 0.699 | 1.6 | 1.1814 | 0.00113 | 1.6784 | 0.0013 | 0.279 | 0.721 |
| 1.8 | 1.3621 | 3.1(-5) | 3.7138 | 4.0(-4) | 0.503 | 0.497 | 1.8 | 1.0922 | 0.00062 | 1.7089 | 7.8(-4) | 0.458 | 0.542 |
| 2.0 | 1.2747 | 3.0(-5) | 3.7287 | 4.0(-4) | 0.672 | 0.328 | 2.0 | 1.0153 | 0.00039 | 1.7375 | 5.1(-4) | 0.753 | 0.247 |
| 2.2 | 1.1987 | 3.1(-5) | 3.7438 | 4.0(-4) | 0.784 | 0.216 | 2.2 | 0.9487 | 0.00030 | 1.7642 | 4.1(-4) | 0.989 | 0.011 |
| 2.4 | 1.1324 | 3.0(-5) | 3.7517 | 4.0(-4) | 0.847 | 0.153 | 2.4 | 0.8910 | 0.00033 | 1.7890 | 4.7(-4) | 0.908 | 0.092 |
| 2.6 | 1.0741 | 3.0(-5) | 3.7622 | 4.0(-4) | 0.889 | 0.111 | 2.6 | 0.8408 | 0.00035 | 1.8139 | 5.2(-4) | 0.648 | 0.352 |
| 2.8 | 1.0227 | 2.8(-5) | 3.7624 | 3.8(-4) | 0.901 | 0.099 | 2.8 | 0.7970 | 0.00040 | 1.8369 | 6.1(-4) | 0.382 | 0.618 |
| 3.0 | 0.9786 | 2.9(-5) | 3.7901 | 4.0(-4) | 0.919 | 0.081 | 3.0 | 0.7577 | 0.00043 | 1.8554 | 6.9(-4) | 0.292 | 0.708 |
| 3.5 | 0.8886 | 2.7(-5) | 3.8064 | 3.7(-4) | 0.831 | 0.169 | 3.5 | 0.6812 | 0.00053 | 1.9020 | 9.1(-4) | 0.162 | 0.838 |
| 4.0 | 0.8212 | 2.9(-5) | 3.7658 | 3.9(-4) | 0.520 | 0.480 | 4.0 | 0.6264 | 0.00080 | 1.9414 | 0.0015 | 0.155 | 0.845 |

TABLE II. Resonances Converging to the ${}^2\Pi_u$ State of H_2^+

See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | β_0 | β_1 | R | E_r | Γ | ν | B | β_0 | β_1 |
|-----------------------------|--------|----------|--------|---------|-----------|-----------|--------------------------------|--------|----------|--------|---------|-----------|-----------|
| ${}^3\Pi_u$: second series | | | | | | | ${}^3\Pi_g$: second series | | | | | | |
| 1.0 | 1.8148 | 0.00034 | 2.6789 | 0.0016 | 0.160 | 0.840 | 1.0 | 1.8750 | 0.00221 | 3.5533 | 0.0248 | 0.001 | 0.999 |
| 1.2 | 1.6563 | 0.00015 | 2.7090 | 7.2(-4) | 0.376 | 0.624 | 1.2 | 1.7117 | 0.00186 | 3.5159 | 0.0203 | 0.003 | 0.997 |
| 1.4 | 1.5212 | 7.4(-5) | 2.7374 | 3.8(-4) | 0.779 | 0.221 | 1.4 | 1.5722 | 0.00169 | 3.4827 | 0.0178 | 0.005 | 0.995 |
| 1.6 | 1.4054 | 0.00013 | 2.7627 | 6.6(-4) | 0.450 | 0.550 | 1.6 | 1.4526 | 0.00151 | 3.4548 | 0.0155 | 0.007 | 0.993 |
| 1.8 | 1.3055 | 0.00041 | 2.7824 | 0.0022 | 0.199 | 0.801 | 1.8 | 1.3498 | 0.00136 | 3.4324 | 0.0137 | 0.010 | 0.990 |
| 2.0 | 1.2179 | 0.00106 | 2.7878 | 0.0058 | 0.158 | 0.842 | 2.0 | 1.2609 | 0.00125 | 3.4154 | 0.0125 | 0.015 | 0.985 |
| 2.2 | 1.1401 | 0.00159 | 2.7746 | 0.0085 | 0.156 | 0.844 | 2.2 | 1.1837 | 0.00120 | 3.4031 | 0.0118 | 0.023 | 0.977 |
| 2.4 | 1.0709 | 0.00183 | 2.7465 | 0.0095 | 0.159 | 0.841 | 2.4 | 1.1166 | 0.00127 | 3.3931 | 0.0124 | 0.037 | 0.963 |
| 2.6 | 1.0090 | 0.00199 | 2.7144 | 0.0099 | 0.169 | 0.832 | 2.6 | 1.0577 | 0.00122 | 3.3899 | 0.0118 | 0.055 | 0.945 |
| 2.8 | 0.9532 | 0.00211 | 2.6715 | 0.0101 | 0.178 | 0.822 | 2.8 | 1.0063 | 0.00102 | 3.3890 | 0.0099 | 0.089 | 0.911 |
| 3.0 | 0.9016 | 0.00257 | 2.6123 | 0.0114 | 0.166 | 0.834 | 3.0 | 0.9606 | 0.00078 | 3.3793 | 0.0075 | 0.082 | 0.918 |
| 3.5 | 0.7928 | 0.00305 | 2.4635 | 0.0114 | 0.122 | 0.878 | 3.5 | 0.8698 | 0.00048 | 3.3744 | 0.0046 | 0.131 | 0.869 |
| 4.0 | 0.7040 | 0.00279 | 2.3079 | 0.0086 | 0.111 | 0.889 | 4.0 | 0.8029 | 0.00042 | 3.3554 | 0.0040 | 0.232 | 0.768 |
| ${}^3\Pi_u$: third series | | | | | | | ${}^3\Delta_g$: first series | | | | | | |
| 1.0 | 1.8356 | 0.00145 | 2.9038 | 0.0089 | 0.074 | 0.926 | 1.0 | 1.8052 | 1.3(-5) | 2.5909 | 0.6(-4) | 1.000 | 0.000 |
| 1.2 | 1.6732 | 0.00150 | 2.8945 | 0.0091 | 0.097 | 0.903 | 1.2 | 1.6465 | 0.00028 | 2.6164 | 0.0013 | 0.031 | 0.969 |
| 1.4 | 1.5344 | 0.00152 | 2.8841 | 0.0090 | 0.116 | 0.884 | 1.4 | 1.5101 | 0.00019 | 2.6300 | 8.8(-4) | 0.046 | 0.954 |
| 1.6 | 1.4152 | 0.00145 | 2.8721 | 0.0086 | 0.130 | 0.870 | 1.6 | 1.3933 | 0.00014 | 2.6438 | 6.2(-4) | 0.080 | 0.920 |
| 1.8 | 1.3126 | 0.00118 | 2.8620 | 0.0069 | 0.141 | 0.859 | 1.8 | 1.2930 | 0.00010 | 2.6567 | 4.7(-4) | 0.146 | 0.854 |
| 2.0 | 1.2244 | 0.00062 | 2.8612 | 0.0036 | 0.151 | 0.849 | 2.0 | 1.2063 | 8.2(-5) | 2.6698 | 3.9(-4) | 0.246 | 0.754 |
| 2.2 | 1.1489 | 0.00019 | 2.8736 | 0.0011 | 0.194 | 0.806 | 2.2 | 1.1311 | 7.5(-5) | 2.6833 | 3.6(-4) | 0.387 | 0.613 |
| 2.4 | 1.0838 | 4.6(-5) | 2.8909 | 2.8(-4) | 0.343 | 0.657 | 2.4 | 1.0656 | 7.4(-5) | 2.6930 | 3.6(-4) | 0.524 | 0.476 |
| 2.6 | 1.0270 | 1.5(-5) | 2.9142 | 0.9(-4) | 0.723 | 0.277 | 2.6 | 1.0085 | 7.7(-5) | 2.7097 | 3.8(-4) | 0.644 | 0.356 |
| 2.8 | 0.9773 | 1.7(-5) | 2.9358 | 0.1(-4) | 0.690 | 0.310 | 2.8 | 0.9582 | 8.0(-5) | 2.7205 | 4.0(-4) | 0.736 | 0.264 |
| 3.0 | 0.9337 | 1.9(-5) | 2.9558 | 0.1(-4) | 0.333 | 0.667 | 3.0 | 0.9154 | 8.5(-5) | 2.7449 | 4.4(-4) | 0.815 | 0.185 |
| 3.5 | 0.8467 | 4.2(-5) | 3.0027 | 0.3(-4) | 0.141 | 0.859 | 3.5 | 0.8281 | 8.7(-5) | 2.7790 | 4.6(-4) | 0.923 | 0.077 |
| 4.0 | 0.7841 | 6.3(-5) | 3.0482 | 0.4(-4) | 0.231 | 0.769 | 4.0 | 0.7659 | 5.5(-5) | 2.8185 | 3.1(-4) | 0.978 | 0.022 |
| ${}^3\Pi_g$: first series | | | | | | | ${}^3\Delta_g$: second series | | | | | | |
| 1.0 | 1.7968 | 0.00693 | 2.5209 | 0.0278 | 0.001 | 0.999 | 1.0 | 1.8678 | 0.1(-5) | 3.4018 | 0.8(-5) | 1.000 | 0.000 |
| 1.2 | 1.6308 | 0.00655 | 2.4863 | 0.0252 | 0.003 | 0.997 | 1.2 | 1.7170 | 9.0(-5) | 3.6379 | 0.0011 | 0.047 | 0.953 |
| 1.4 | 1.4881 | 0.00599 | 2.4503 | 0.0220 | 0.006 | 0.994 | 1.4 | 1.5795 | 7.7(-5) | 3.6481 | 9.4(-4) | 0.101 | 0.899 |
| 1.6 | 1.3656 | 0.00537 | 2.4192 | 0.0190 | 0.009 | 0.991 | 1.6 | 1.4618 | 6.4(-5) | 3.6609 | 7.8(-4) | 0.185 | 0.815 |
| 1.8 | 1.2601 | 0.00465 | 2.3933 | 0.0159 | 0.014 | 0.986 | 1.8 | 1.3604 | 5.3(-5) | 3.6711 | 6.5(-4) | 0.277 | 0.723 |
| 2.0 | 1.1689 | 0.00410 | 2.3722 | 0.0137 | 0.018 | 0.982 | 2.0 | 1.2730 | 4.3(-5) | 3.6860 | 5.4(-4) | 0.365 | 0.635 |
| 2.2 | 1.0897 | 0.00373 | 2.3551 | 0.0122 | 0.023 | 0.977 | 2.2 | 1.1970 | 3.7(-5) | 3.7012 | 4.6(-4) | 0.441 | 0.559 |
| 2.4 | 1.0207 | 0.00351 | 2.3387 | 0.0112 | 0.027 | 0.973 | 2.4 | 1.1308 | 3.1(-5) | 3.7098 | 4.0(-4) | 0.501 | 0.499 |
| 2.6 | 0.9603 | 0.00367 | 2.3289 | 0.0116 | 0.035 | 0.965 | 2.6 | 1.0725 | 2.7(-5) | 3.7207 | 3.5(-4) | 0.566 | 0.434 |
| 2.8 | 0.9072 | 0.00448 | 2.3180 | 0.0139 | 0.055 | 0.945 | 2.8 | 1.0212 | 2.4(-5) | 3.7224 | 3.1(-4) | 0.620 | 0.380 |
| 3.0 | 0.8607 | 0.00342 | 2.3098 | 0.0105 | 0.067 | 0.933 | 3.0 | 0.9770 | 2.3(-5) | 3.7484 | 3.1(-4) | 0.710 | 0.290 |
| 3.5 | 0.7679 | 0.00344 | 2.2957 | 0.0104 | 0.144 | 0.856 | 3.5 | 0.8871 | 2.2(-5) | 3.7661 | 2.9(-4) | 0.862 | 0.138 |
| 4.0 | 0.7000 | 0.00252 | 2.2836 | 0.0075 | 0.209 | 0.791 | 4.0 | 0.8229 | 3.7(-5) | 3.8104 | 5.2(-4) | 0.942 | 0.058 |

TABLE II. Resonances Converging to the ${}^2\Pi_u$ State of H_2^+
 See page 257 for Explanation of Tables

| R | E_r | Γ | ν | B | β_0 | β_1 |
|--------------------------------|--------|----------|--------|--------|-----------|-----------|
| ${}^3\Delta_u$: first series | | | | | | |
| 1.0 | 1.8404 | 0.00086 | 2.9643 | 0.0056 | 0.072 | 0.928 |
| 1.2 | 1.6779 | 0.00090 | 2.9525 | 0.0058 | 0.090 | 0.910 |
| 1.4 | 1.5241 | 0.00153 | 2.7678 | 0.0081 | 0.145 | 0.855 |
| 1.6 | 1.4194 | 0.00080 | 2.9231 | 0.0050 | 0.120 | 0.880 |
| 1.8 | 1.3168 | 0.00074 | 2.9129 | 0.0046 | 0.143 | 0.857 |
| 2.0 | 1.2285 | 0.00070 | 2.9100 | 0.0043 | 0.164 | 0.836 |
| 2.2 | 1.1514 | 0.00068 | 2.9030 | 0.0042 | 0.192 | 0.808 |
| 2.4 | 1.0958 | 0.00091 | 3.0478 | 0.0065 | 0.256 | 0.744 |
| 2.6 | 1.0371 | 0.00099 | 3.0486 | 0.0070 | 0.282 | 0.718 |
| 2.8 | 0.9754 | 0.00087 | 2.9118 | 0.0054 | 0.280 | 0.720 |
| 3.0 | 0.9261 | 0.00091 | 2.8623 | 0.0053 | 0.285 | 0.715 |
| 3.5 | 0.8335 | 0.00100 | 2.8379 | 0.0057 | 0.283 | 0.717 |
| 4.0 | 0.7711 | 0.00134 | 2.8792 | 0.0080 | 0.251 | 0.749 |
| ${}^3\Delta_u$: second series | | | | | | |
| 1.0 | 1.8871 | 0.00029 | 3.8614 | 0.0041 | 0.075 | 0.925 |
| 1.2 | 1.7250 | 0.00028 | 3.8475 | 0.0040 | 0.087 | 0.913 |
| 1.4 | 1.5803 | 0.00029 | 3.6682 | 0.0036 | 0.166 | 0.834 |
| 1.6 | 1.4683 | 0.00025 | 3.8320 | 0.0035 | 0.135 | 0.865 |
| 1.8 | 1.3665 | 0.00027 | 3.8317 | 0.0037 | 0.188 | 0.812 |
| 2.0 | 1.2793 | 0.00027 | 3.8566 | 0.0039 | 0.227 | 0.773 |
| 2.2 | 1.2023 | 0.00027 | 3.8430 | 0.0038 | 0.273 | 0.727 |
| 2.4 | 1.1373 | 0.00100 | 3.8862 | 0.0145 | 0.327 | 0.673 |
| 2.6 | 1.0772 | 0.00104 | 3.8499 | 0.0148 | 0.349 | 0.651 |
| 2.8 | 1.0241 | 0.00031 | 3.7999 | 0.0042 | 0.346 | 0.654 |
| 3.0 | 0.9804 | 0.00027 | 3.8412 | 0.0038 | 0.337 | 0.663 |
| 3.5 | 0.8871 | 0.00033 | 3.7653 | 0.0044 | 0.307 | 0.693 |
| 4.0 | 0.8159 | 0.00044 | 3.6307 | 0.0052 | 0.354 | 0.646 |

TABLE III. Quantum Defects for Rydberg States of H₂
See page 257 for Explanation of Tables

| <i>R</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>R</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>A</i> |
|----------------|----------|----------|----------|----------|--------------|----------|----------|----------|----------|
| $^1\Sigma_g^+$ | | | | | $^1\Pi_g$ | | | | |
| | (0,0) | (2,0) | (4,0) | (6,0) | | (2,1) | (4,1) | (6,1) | |
| 1.0 | 0.0052 | 0.0142 | 0.0007 | 0.0001 | 1.0 | 0.0552 | 0.0008 | 1.0000 | |
| 1.2 | 0.9820 | 0.0200 | 0.0014 | 0.9999 | 1.2 | 0.9704 | 0.0011 | 1.0000 | |
| 1.4 | 0.9546 | 0.0272 | 0.0017 | 0.0001 | 1.4 | 0.0599 | 0.0015 | 0.0031 | |
| 1.6 | 0.9321 | 0.0367 | 0.0022 | 0.0000 | 1.6 | 0.0579 | 0.0019 | 0.9999 | |
| 1.8 | 0.9118 | 0.0499 | 0.0029 | 0.0000 | 1.8 | 0.9792 | 0.0024 | 0.0000 | |
| 2.0 | 0.8941 | 0.0690 | 0.0037 | 0.0000 | 2.0 | 0.0619 | 0.0035 | 0.0000 | |
| 2.2 | 0.8825 | 0.1018 | 0.0041 | 0.9997 | 2.2 | 0.0736 | 0.0039 | 0.9999 | |
| 2.4 | 0.8723 | 0.1708 | 0.0049 | 0.9996 | 2.4 | 0.0888 | 0.0045 | 0.9999 | |
| 2.6 | 0.8729 | 0.3985 | 0.0058 | 0.9996 | 2.6 | 0.1057 | 0.0053 | 1.0000 | |
| 2.8 | 0.7237 | 0.9047 | 0.0079 | 0.0000 | 2.8 | 0.0691 | 0.0063 | 1.0000 | |
| 3.0 | 0.7838 | 0.9602 | 0.0095 | 0.0004 | 3.0 | 0.1043 | 0.0074 | 0.0000 | |
| 3.5 | 0.7956 | 0.0348 | 0.0119 | 0.0004 | 3.5 | 0.3740 | 0.0113 | 1.0000 | |
| 4.0 | 0.8217 | 0.0912 | 0.0320 | 0.0062 | 4.0 | 0.7421 | 0.0287 | 0.0059 | |
| $^1\Sigma_u^+$ | | | | | $^1\Delta_g$ | | | | |
| | (1,0) | (3,0) | (5,0) | | | (2,2) | (4,2) | (6,2) | |
| 1.0 | 0.0610 | 0.0038 | 0.0003 | | 1.0 | 0.9370 | 0.0005 | 0.0000 | |
| 1.2 | 0.0152 | 0.0046 | 0.9999 | | 1.2 | 0.9348 | 0.0008 | 0.0000 | |
| 1.4 | 0.0405 | 0.0061 | 0.0001 | | 1.4 | 0.9322 | 0.0010 | 0.0000 | |
| 1.6 | 0.0707 | 0.0079 | 0.0004 | | 1.6 | 0.9294 | 0.0013 | 0.0000 | |
| 1.8 | 0.1046 | 0.0100 | 0.0009 | | 1.8 | 0.0443 | 0.0011 | 0.9999 | |
| 2.0 | 0.1419 | 0.0126 | 0.0014 | | 2.0 | 0.9230 | 0.0021 | 0.0001 | |
| 2.2 | 0.2394 | 0.0187 | 0.9986 | | 2.2 | 0.0379 | 0.0017 | 0.9999 | |
| 2.4 | 0.2233 | 0.0192 | 0.0024 | | 2.4 | 0.9161 | 0.0031 | 0.0001 | |
| 2.6 | 0.3170 | 0.0272 | 0.9981 | | 2.6 | 0.0312 | 0.0024 | 0.9998 | |
| 2.8 | 0.3154 | 0.0289 | 0.0023 | | 2.8 | 0.9089 | 0.0044 | 0.0001 | |
| 3.0 | 0.3705 | 0.0359 | 0.0015 | | 3.0 | 0.0247 | 0.0033 | 0.9998 | |
| 3.5 | 0.5640 | 0.0629 | 0.0006 | | 3.5 | 0.0181 | 0.0041 | 0.9998 | |
| 4.0 | 0.7764 | 0.1297 | 0.0125 | | 4.0 | 0.9458 | 0.0187 | 0.0047 | |
| $^1\Pi_u$ | | | | | $^1\Delta_u$ | | | | |
| | (1,1) | (3,1) | (5,1) | | | (3,2) | (5,2) | | |
| 1.0 | 0.9358 | 0.9982 | 0.0004 | | 1.0 | 0.9432 | 0.0001 | | |
| 1.2 | 0.9582 | 0.0081 | 0.0018 | | 1.2 | 0.9435 | 0.0001 | | |
| 1.4 | 0.9502 | 0.0087 | 0.0015 | | 1.4 | 0.0587 | 0.0001 | | |
| 1.6 | 0.9135 | 0.0040 | 0.9988 | | 1.6 | 0.9443 | 0.0002 | | |
| 1.8 | 0.9093 | 0.0067 | 0.9991 | | 1.8 | 0.9448 | 0.0002 | | |
| 2.0 | 0.9024 | 0.0091 | 0.9992 | | 2.0 | 0.0603 | 0.0003 | | |
| 2.2 | 0.8951 | 0.0118 | 0.9992 | | 2.2 | 0.0612 | 0.0003 | | |
| 2.4 | 0.8957 | 0.0153 | 0.9994 | | 2.4 | 0.0622 | 0.0004 | | |
| 2.6 | 0.8942 | 0.0190 | 0.9995 | | 2.6 | 0.0635 | 0.0005 | | |
| 2.8 | 0.9058 | 0.0236 | 0.9995 | | 2.8 | 0.0651 | 0.0005 | | |
| 3.0 | 0.9060 | 0.0303 | 0.0014 | | 3.0 | 0.0673 | 0.0006 | | |
| 3.5 | 0.8965 | 0.0479 | 0.9998 | | 3.5 | 0.0758 | 0.0008 | | |
| 4.0 | 0.9061 | 0.0928 | 0.0128 | | 4.0 | 0.0379 | 0.0098 | | |

TABLE III. Quantum Defects for Rydberg States of H₂
See page 257 for Explanation of Tables

| <i>R</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>R</i> | <i>A</i> | <i>A</i> | <i>A</i> | <i>A</i> |
|--|----------|----------|----------|----------|-----------------------------|----------|----------|----------|----------|
| ³ Σ _g ⁺ | | | | | ³ Π _g | | | | |
| | (0,0) | (2,0) | (4,0) | (6,0) | | (2,1) | (4,1) | (6,1) | |
| 1.0 | 0.1259 | 0.0164 | 0.9998 | 0.0003 | 1.0 | 0.9686 | 0.0008 | 1.0000 | |
| 1.2 | 0.0987 | 0.0208 | 0.0005 | 0.0002 | 1.2 | 0.9730 | 0.0011 | 1.0000 | |
| 1.4 | 0.1487 | 0.0311 | 0.0026 | 0.9996 | 1.4 | 0.0625 | 0.0015 | 0.0031 | |
| 1.6 | 0.1225 | 0.0403 | 0.0030 | 0.0000 | 1.6 | 0.0605 | 0.0019 | 0.9999 | |
| 1.8 | 0.0985 | 0.0493 | 0.0035 | 0.0000 | 1.8 | 0.0581 | 0.0026 | 0.9999 | |
| 2.0 | 0.9969 | 0.0616 | 0.0030 | 1.0000 | 2.0 | 0.9886 | 0.0040 | 1.0000 | |
| 2.2 | 0.9750 | 0.0766 | 0.0038 | 0.0001 | 2.2 | 0.0728 | 0.0039 | 0.9999 | |
| 2.4 | 0.9539 | 0.0943 | 0.0048 | 0.0001 | 2.4 | 0.0175 | 0.0039 | 0.0000 | |
| 2.6 | 0.0011 | 0.1222 | 0.0068 | 0.9999 | 2.6 | 0.0317 | 0.0052 | 0.0000 | |
| 2.8 | 0.9821 | 0.1459 | 0.0077 | 1.0000 | 2.8 | 0.0495 | 0.0062 | 1.0000 | |
| 3.0 | 0.8967 | 0.1668 | 0.0083 | 0.0001 | 3.0 | 0.0688 | 0.0073 | 0.0000 | |
| 3.5 | 0.8583 | 0.2484 | 0.0126 | 1.0000 | 3.5 | 0.2599 | 0.0113 | 1.0000 | |
| 4.0 | 0.8706 | 0.3467 | 0.0322 | 0.0062 | 4.0 | 0.9203 | 0.0288 | 0.0059 | |
| ³ Σ _u ⁺ | | | | | ³ Δ _g | | | | |
| | (1,0) | (3,0) | (5,0) | | | (2,2) | (4,2) | (6,2) | |
| 1.0 | 0.2377 | 0.0024 | 0.9999 | | 1.0 | 0.0563 | 0.0004 | 1.0000 | |
| 1.2 | 0.3270 | 0.0066 | 0.0002 | | 1.2 | 0.9368 | 0.0007 | 1.0000 | |
| 1.4 | 0.3747 | 0.0086 | 0.0001 | | 1.4 | 0.0521 | 0.0008 | 1.0000 | |
| 1.6 | 0.3942 | 0.0070 | 0.0002 | | 1.6 | 0.0496 | 0.0010 | 1.0000 | |
| 1.8 | 0.4265 | 0.0095 | 0.0004 | | 1.8 | 0.9289 | 0.0016 | 0.0000 | |
| 2.0 | 0.4501 | 0.0124 | 0.0006 | | 2.0 | 0.0438 | 0.0015 | 0.9999 | |
| 2.2 | 0.4770 | 0.0187 | 0.9997 | | 2.2 | 0.9224 | 0.0025 | 0.0000 | |
| 2.4 | 0.4800 | 0.0197 | 0.0010 | | 2.4 | 0.0374 | 0.0022 | 0.9999 | |
| 2.6 | 0.4965 | 0.0266 | 0.9998 | | 2.6 | 0.9154 | 0.0036 | 0.0000 | |
| 2.8 | 0.4976 | 0.0297 | 0.0008 | | 2.8 | 0.9118 | 0.0043 | 0.0000 | |
| 3.0 | 0.5057 | 0.0365 | 0.0006 | | 3.0 | 0.9083 | 0.0051 | 0.0001 | |
| 3.5 | 0.5362 | 0.0627 | 0.0009 | | 3.5 | 0.0204 | 0.0046 | 0.9998 | |
| 4.0 | 0.3428 | 0.0458 | 0.0125 | | 4.0 | 0.9485 | 0.0187 | 0.0047 | |
| ³ Π _u | | | | | ³ Δ _u | | | | |
| | (1,1) | (3,1) | (5,1) | | | (3,2) | (5,2) | | |
| 1.0 | 0.0922 | 0.0065 | 0.0001 | | 1.0 | 0.9433 | 0.0001 | | |
| 1.2 | 0.0902 | 0.0074 | 0.0019 | | 1.2 | 0.0584 | 0.0001 | | |
| 1.4 | 0.0707 | 0.0026 | 0.9985 | | 1.4 | 0.0587 | 0.0001 | | |
| 1.6 | 0.0816 | 0.0093 | 0.0015 | | 1.6 | 0.0592 | 0.0002 | | |
| 1.8 | 0.0759 | 0.0105 | 0.0013 | | 1.8 | 0.0597 | 0.0002 | | |
| 2.0 | 0.0558 | 0.0094 | 0.9990 | | 2.0 | 0.0604 | 0.0003 | | |
| 2.2 | 0.0478 | 0.0121 | 0.9992 | | 2.2 | 0.9463 | 0.0003 | | |
| 2.4 | 0.0544 | 0.0174 | 0.0012 | | 2.4 | 0.9472 | 0.0004 | | |
| 2.6 | 0.0377 | 0.0191 | 0.9994 | | 2.6 | 0.0636 | 0.0005 | | |
| 2.8 | 0.0474 | 0.0245 | 0.0012 | | 2.8 | 0.0653 | 0.0005 | | |
| 3.0 | 0.0325 | 0.0290 | 0.0013 | | 3.0 | 0.9521 | 0.0007 | | |
| 3.5 | 0.0114 | 0.0482 | 1.0000 | | 3.5 | 0.0759 | 0.0009 | | |
| 4.0 | 0.9962 | 0.0947 | 0.0129 | | 4.0 | 0.0378 | 0.0098 | | |

TABLE IV. Complex Quantum Defects at the ${}^2\Sigma_u^+$ Threshold
See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|------------------|--------|-----------|--------|-----------|--------|-----------|--------|-----------|
| ${}^1\Sigma_g^+$ | | | | | | | | |
| | | (1,0) | | (3,0) | | (5,0) | | |
| 1.0 | 0.1707 | 0.259(-1) | 0.9874 | 0.913(-4) | 0.9998 | 0.181(-5) | | |
| 1.2 | 0.1917 | 0.319(-1) | 0.9884 | 0.175(-3) | 0.9998 | 0.103(-4) | | |
| 1.4 | 0.2135 | 0.476(-1) | 0.9953 | 0.518(-2) | 0.9999 | 0.197(-3) | | |
| 1.6 | 0.2446 | 0.438(-1) | 0.9931 | 0.442(-3) | 0.9999 | 0.231(-4) | | |
| 1.8 | 0.2646 | 0.449(-1) | 0.9939 | 0.691(-3) | 0.9999 | 0.325(-5) | | |
| 2.0 | 0.2790 | 0.470(-1) | 0.9947 | 0.101(-2) | 0.9999 | 0.592(-5) | | |
| 2.2 | 0.2893 | 0.509(-1) | 0.9952 | 0.134(-2) | 0.9998 | 0.150(-4) | | |
| 2.4 | 0.2966 | 0.558(-1) | 0.9954 | 0.177(-2) | 0.9998 | 0.105(-4) | | |
| 2.6 | 0.3018 | 0.604(-1) | 0.9951 | 0.254(-2) | 1.0000 | 0.226(-4) | | |
| 2.8 | 0.2783 | 0.637(-1) | 0.9917 | 0.884(-2) | 0.9987 | 0.447(-3) | | |
| 3.0 | 0.3039 | 0.669(-1) | 0.9928 | 0.610(-2) | 0.9997 | 0.284(-3) | | |
| 3.5 | 0.2816 | 0.748(-1) | 0.9888 | 0.172(-1) | 0.0001 | 0.904(-3) | | |
| 4.0 | 0.2486 | 0.102 | 0.9850 | 0.296(-1) | 0.9992 | 0.917(-3) | | |
| ${}^1\Sigma_u^+$ | | | | | | | | |
| | | (0,0) | | (2,0) | | (4,0) | | (6,0) |
| 1.0 | 0.1989 | 0.209(-1) | 0.9206 | 0.296(-2) | 0.9968 | 0.398(-5) | 0.0000 | 0.738(-7) |
| 1.2 | 0.1534 | 0.315(-1) | 0.9267 | 0.486(-2) | 0.9969 | 0.280(-5) | 0.0000 | 0.302(-6) |
| 1.4 | 0.1122 | 0.427(-1) | 0.9333 | 0.840(-2) | 0.9976 | 0.210(-4) | 0.0000 | 0.189(-6) |
| 1.6 | 0.0727 | 0.521(-1) | 0.9393 | 0.144(-1) | 0.9980 | 0.109(-3) | 1.0000 | 0.307(-6) |
| 1.8 | 0.0324 | 0.589(-1) | 0.9469 | 0.231(-1) | 0.9984 | 0.146(-3) | 1.0000 | 0.284(-6) |
| 2.0 | 0.9802 | 0.636(-1) | 0.9660 | 0.343(-1) | 0.9987 | 0.885(-4) | 1.0000 | 0.112(-6) |
| 2.2 | 0.9347 | 0.936(-1) | 0.9780 | 0.211(-1) | 0.9990 | 0.288(-4) | 0.0000 | 0.348(-6) |
| 2.4 | 0.9012 | 0.115 | 0.9751 | 0.194(-1) | 0.9990 | 0.332(-4) | 1.0000 | 0.179(-5) |
| 2.6 | 0.8624 | 0.135 | 0.9768 | 0.240(-1) | 0.9988 | 0.924(-4) | 0.0000 | 0.271(-5) |
| 2.8 | 0.8226 | 0.157 | 0.9857 | 0.406(-1) | 0.9970 | 0.167(-2) | 0.0002 | 0.684(-5) |
| 3.0 | 0.7823 | 0.187 | 0.9817 | 0.464(-1) | 0.9978 | 0.938(-3) | 1.0000 | 0.850(-7) |
| 3.5 | 0.6470 | 0.299 | 0.0083 | 0.102 | 0.9961 | 0.521(-2) | 0.0000 | 0.259(-5) |
| 4.0 | 0.0672 | 0.214 | 0.2761 | 0.193 | 0.0021 | 0.204(-1) | 0.0022 | 0.105(-4) |
| ${}^1\Pi_u$ | | | | | | | | |
| | | (2,1) | | (4,1) | | (6,1) | | |
| 1.0 | 0.9613 | 0.831(-3) | 0.0009 | 0.777(-4) | 1.0000 | 0.312(-5) | | |
| 1.2 | 0.8730 | 0.655(-2) | 0.9977 | 0.406(-5) | 0.0001 | 0.678(-6) | | |
| 1.4 | 0.0758 | 0.172(-1) | 0.9980 | 0.150(-4) | 0.0001 | 0.126(-5) | | |
| 1.6 | 0.0482 | 0.519(-2) | 0.9945 | 0.158(-2) | 0.9999 | 0.659(-5) | | |
| 1.8 | 0.0544 | 0.754(-2) | 0.9981 | 0.149(-3) | 0.9999 | 0.204(-4) | | |
| 2.0 | 0.0498 | 0.800(-2) | 0.9978 | 0.611(-3) | 1.0000 | 0.648(-5) | | |
| 2.2 | 0.0156 | 0.106(-1) | 0.9989 | 0.439(-4) | 0.0000 | 0.255(-5) | | |
| 2.4 | 0.9963 | 0.127(-1) | 0.0004 | 0.116(-2) | 0.0000 | 0.355(-5) | | |
| 2.6 | 0.9787 | 0.205(-1) | 0.9994 | 0.171(-3) | 0.0000 | 0.302(-5) | | |
| 2.8 | 0.9665 | 0.369(-1) | 0.9973 | 0.162(-2) | 0.0006 | 0.368(-4) | | |
| 3.0 | 0.9688 | 0.347(-1) | 0.9987 | 0.132(-2) | 0.0000 | 0.259(-6) | | |
| 3.5 | 0.9581 | 0.633(-1) | 0.9958 | 0.516(-2) | 1.0000 | 0.424(-5) | | |
| 4.0 | 0.9403 | 0.907(-1) | 0.9935 | 0.563(-2) | 0.0019 | 0.101(-4) | | |

TABLE IV. Complex Quantum Defects at the ${}^2\Sigma_u^+$ Threshold
 See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|----------------|--------|-----------|--------|-----------|--------|-----------|-----|-----|
| ${}^1\Pi_g$ | | | | | | | | |
| | (1,1) | | (3,1) | | (5,1) | | | |
| 1.0 | 0.2586 | 0.375(-2) | 0.9941 | 0.229(-3) | 0.9997 | 0.216(-4) | | |
| 1.2 | 0.1932 | 0.218(-1) | 0.9944 | 0.150(-3) | 0.0002 | 0.220(-4) | | |
| 1.4 | 0.1275 | 0.370(-1) | 0.9954 | 0.190(-3) | 0.0003 | 0.383(-4) | | |
| 1.6 | 0.0853 | 0.481(-1) | 0.9966 | 0.359(-3) | 0.0000 | 0.382(-4) | | |
| 1.8 | 0.0583 | 0.571(-1) | 0.9965 | 0.599(-3) | 0.0015 | 0.623(-4) | | |
| 2.0 | 0.0426 | 0.696(-1) | 0.9966 | 0.114(-2) | 0.9999 | 0.482(-5) | | |
| 2.2 | 0.0308 | 0.860(-1) | 0.9973 | 0.185(-2) | 0.0003 | 0.181(-3) | | |
| 2.4 | 0.0355 | 0.956(-1) | 0.9973 | 0.231(-2) | 0.9999 | 0.187(-4) | | |
| 2.6 | 0.0268 | 0.975(-1) | 0.9967 | 0.298(-2) | 0.9999 | 0.421(-4) | | |
| 2.8 | 0.9901 | 0.114 | 0.9944 | 0.821(-2) | 0.9995 | 0.454(-3) | | |
| 3.0 | 0.9779 | 0.138 | 0.9942 | 0.588(-2) | 0.9998 | 0.276(-3) | | |
| 3.5 | 0.0396 | 0.185 | 0.9899 | 0.165(-1) | 0.0000 | 0.895(-3) | | |
| 4.0 | 0.0359 | 0.191 | 0.9882 | 0.288(-1) | 0.9989 | 0.901(-3) | | |
| ${}^1\Delta_g$ | | | | | | | | |
| | (3,2) | | (5,2) | | | | | |
| 1.0 | 0.0027 | 0.907(-4) | 0.9990 | 0.261(-4) | | | | |
| 1.2 | 0.0015 | 0.159(-3) | 0.9988 | 0.638(-4) | | | | |
| 1.4 | 0.9958 | 0.219(-2) | 0.9999 | 0.119(-3) | | | | |
| 1.6 | 0.0028 | 0.539(-3) | 0.9996 | 0.336(-4) | | | | |
| 1.8 | 0.0011 | 0.387(-3) | 0.9996 | 0.158(-3) | | | | |
| 2.0 | 0.9996 | 0.590(-3) | 0.9999 | 0.159(-3) | | | | |
| 2.2 | 0.9987 | 0.963(-3) | 0.0000 | 0.726(-5) | | | | |
| 2.4 | 0.9974 | 0.126(-2) | 0.9997 | 0.160(-4) | | | | |
| 2.6 | 0.9958 | 0.182(-2) | 1.0000 | 0.149(-4) | | | | |
| 2.8 | 0.9933 | 0.620(-2) | 0.9985 | 0.406(-3) | | | | |
| 3.0 | 0.9915 | 0.434(-2) | 0.9999 | 0.264(-3) | | | | |
| 3.5 | 0.9851 | 0.120(-1) | 0.0001 | 0.783(-3) | | | | |
| 4.0 | 0.9772 | 0.207(-1) | 0.9979 | 0.778(-3) | | | | |
| ${}^1\Delta_u$ | | | | | | | | |
| | (2,2) | | (4,2) | | (6,2) | | | |
| 1.0 | 0.0628 | 0.664(-3) | 0.9987 | 0.489(-5) | 0.0000 | 0.209(-6) | | |
| 1.2 | 0.0484 | 0.114(-2) | 0.9987 | 0.358(-5) | 0.0000 | 0.402(-6) | | |
| 1.4 | 0.0372 | 0.186(-2) | 0.9989 | 0.123(-4) | 0.0000 | 0.416(-6) | | |
| 1.6 | 0.0269 | 0.290(-2) | 0.9990 | 0.703(-4) | 1.0000 | 0.631(-6) | | |
| 1.8 | 0.0188 | 0.387(-2) | 0.9991 | 0.853(-4) | 1.0000 | 0.125(-6) | | |
| 2.0 | 0.0114 | 0.468(-2) | 0.9992 | 0.653(-4) | 0.0000 | 0.130(-6) | | |
| 2.2 | 0.0039 | 0.565(-2) | 0.9992 | 0.975(-4) | 0.0000 | 0.408(-6) | | |
| 2.4 | 0.9964 | 0.731(-2) | 0.9990 | 0.760(-5) | 0.0000 | 0.164(-5) | | |
| 2.6 | 0.9888 | 0.965(-2) | 0.9986 | 0.123(-3) | 0.0001 | 0.252(-5) | | |
| 2.8 | 0.9840 | 0.155(-1) | 0.9965 | 0.138(-2) | 0.0001 | 0.219(-4) | | |
| 3.0 | 0.9737 | 0.183(-1) | 0.9972 | 0.724(-3) | 0.0001 | 0.959(-7) | | |
| 3.5 | 0.9615 | 0.353(-1) | 0.9952 | 0.451(-2) | 0.0001 | 0.370(-5) | | |
| 4.0 | 0.9452 | 0.460(-1) | 0.9913 | 0.477(-2) | 0.0013 | 0.489(-5) | | |

TABLE IV. Complex Quantum Defects at the ${}^2\Sigma_u^+$ Threshold
See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|------------------|--------|-----------|--------|-----------|--------|-----------|--------|-----------|
| ${}^3\Sigma_g^+$ | | | | | | | | |
| | (1,0) | | (3,0) | | (5,0) | | | |
| 1.0 | 0.4436 | 0.700(-4) | 0.9923 | 0.608(-4) | 0.0001 | 0.255(-5) | | |
| 1.2 | 0.4618 | 0.127(-3) | 0.9931 | 0.904(-4) | 0.0000 | 0.161(-4) | | |
| 1.4 | 0.4799 | 0.156(-3) | 0.9940 | 0.152(-3) | 0.9999 | 0.316(-4) | | |
| 1.6 | 0.4917 | 0.915(-4) | 0.9948 | 0.336(-3) | 1.0000 | 0.277(-4) | | |
| 1.8 | 0.4988 | 0.357(-4) | 0.9957 | 0.640(-3) | 0.9999 | 0.988(-5) | | |
| 2.0 | 0.5021 | 0.133(-3) | 0.9968 | 0.985(-3) | 0.9999 | 0.706(-5) | | |
| 2.2 | 0.5016 | 0.359(-3) | 0.9974 | 0.132(-2) | 0.9998 | 0.986(-5) | | |
| 2.4 | 0.4982 | 0.618(-3) | 0.9977 | 0.173(-2) | 0.9998 | 0.187(-4) | | |
| 2.6 | 0.4925 | 0.897(-3) | 0.9973 | 0.247(-2) | 0.9998 | 0.428(-4) | | |
| 2.8 | 0.4567 | 0.166(-2) | 0.9974 | 0.877(-2) | 0.9988 | 0.544(-3) | | |
| 3.0 | 0.4748 | 0.185(-2) | 0.9955 | 0.612(-2) | 0.9998 | 0.282(-3) | | |
| 3.5 | 0.4420 | 0.559(-2) | 0.9924 | 0.178(-1) | 0.0001 | 0.901(-3) | | |
| 4.0 | 0.4073 | 0.152(-1) | 0.9917 | 0.317(-1) | 0.9992 | 0.930(-3) | | |
| ${}^3\Sigma_u^+$ | | | | | | | | |
| | (0,0) | | (2,0) | | (4,0) | | (6,0) | |
| 1.0 | 0.2593 | 0.940(-5) | 0.0773 | 0.197(-2) | 0.9968 | 0.115(-4) | 0.0000 | 0.159(-6) |
| 1.2 | 0.2035 | 0.146(-3) | 0.0697 | 0.288(-2) | 0.9970 | 0.826(-5) | 0.0000 | 0.386(-6) |
| 1.4 | 0.1547 | 0.444(-3) | 0.0641 | 0.447(-2) | 0.9976 | 0.137(-4) | 0.0000 | 0.132(-6) |
| 1.6 | 0.1107 | 0.989(-3) | 0.0640 | 0.677(-2) | 0.9980 | 0.852(-4) | 1.0000 | 0.121(-6) |
| 1.8 | 0.0682 | 0.350(-2) | 0.0702 | 0.763(-2) | 0.9984 | 0.107(-3) | 1.0000 | 0.627(-7) |
| 2.0 | 0.0332 | 0.188(-2) | 0.0754 | 0.130(-1) | 0.9987 | 0.597(-4) | 1.0000 | 0.120(-7) |
| 2.2 | 0.9993 | 0.323(-2) | 0.0844 | 0.165(-1) | 0.9989 | 0.742(-4) | 0.0000 | 0.368(-6) |
| 2.4 | 0.9684 | 0.505(-2) | 0.0947 | 0.217(-1) | 0.9990 | 0.114(-3) | 1.0000 | 0.181(-5) |
| 2.6 | 0.9386 | 0.754(-2) | 0.1090 | 0.299(-1) | 0.9989 | 0.102(-3) | 0.0000 | 0.260(-5) |
| 2.8 | 0.9031 | 0.127(-1) | 0.1725 | 0.417(-1) | 0.9971 | 0.166(-2) | 0.0002 | 0.633(-5) |
| 3.0 | 0.8866 | 0.154(-1) | 0.1619 | 0.566(-1) | 0.9976 | 0.886(-3) | 0.0000 | 0.504(-7) |
| 3.5 | 0.8242 | 0.328(-1) | 0.2723 | 0.803(-1) | 0.9963 | 0.558(-2) | 0.0000 | 0.263(-5) |
| 4.0 | 0.7634 | 0.805(-1) | 0.3892 | 0.635(-1) | 0.0064 | 0.199(-1) | 0.0022 | 0.194(-4) |
| ${}^3\Pi_u$ | | | | | | | | |
| | (2,1) | | (4,1) | | (6,1) | | | |
| 1.0 | 0.0980 | 0.161(-2) | 0.9981 | 0.261(-5) | 0.0000 | 0.267(-7) | | |
| 1.2 | 0.0560 | 0.230(-2) | 0.9976 | 0.192(-4) | 0.0001 | 0.119(-5) | | |
| 1.4 | 0.0414 | 0.360(-2) | 0.9978 | 0.139(-4) | 1.0000 | 0.999(-6) | | |
| 1.6 | 0.0852 | 0.471(-2) | 0.0017 | 0.307(-3) | 0.9999 | 0.105(-4) | | |
| 1.8 | 0.0983 | 0.660(-2) | 0.9988 | 0.110(-3) | 0.0000 | 0.729(-5) | | |
| 2.0 | 0.0955 | 0.762(-2) | 0.9994 | 0.157(-3) | 0.0001 | 0.182(-4) | | |
| 2.2 | 0.0690 | 0.974(-2) | 0.9990 | 0.517(-4) | 0.0001 | 0.565(-6) | | |
| 2.4 | 0.0555 | 0.128(-1) | 0.9993 | 0.314(-3) | 0.9999 | 0.213(-5) | | |
| 2.6 | 0.0437 | 0.185(-1) | 0.9995 | 0.223(-3) | 0.0001 | 0.548(-5) | | |
| 2.8 | 0.0741 | 0.317(-1) | 0.9974 | 0.162(-2) | 0.0005 | 0.363(-4) | | |
| 3.0 | 0.0436 | 0.343(-1) | 0.9976 | 0.127(-2) | 1.0000 | 0.291(-6) | | |
| 3.5 | 0.0552 | 0.664(-1) | 0.9963 | 0.514(-2) | 0.0000 | 0.368(-5) | | |
| 4.0 | 0.0676 | 0.850(-1) | 0.9935 | 0.566(-2) | 0.0019 | 0.101(-4) | | |

TABLE IV. Complex Quantum Defects at the ${}^2\Sigma_u^+$ Threshold
See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|----------------|--------|-----------|--------|-----------|--------|-----------|-----|-----|
| ${}^3\Pi_g$ | | | | | | | | |
| | | (1,1) | | (3,1) | | (5,1) | | |
| 1.0 | 0.2293 | 0.245(-3) | 0.9965 | 0.473(-4) | 0.9999 | 0.123(-4) | | |
| 1.2 | 0.2178 | 0.780(-3) | 0.9966 | 0.689(-4) | 0.0006 | 0.338(-4) | | |
| 1.4 | 0.1755 | 0.148(-2) | 0.9971 | 0.123(-3) | 0.0005 | 0.568(-4) | | |
| 1.6 | 0.1413 | 0.220(-2) | 0.9980 | 0.277(-3) | 0.0002 | 0.795(-4) | | |
| 1.8 | 0.1187 | 0.291(-2) | 0.9978 | 0.535(-3) | 0.0015 | 0.806(-4) | | |
| 2.0 | 0.1034 | 0.422(-2) | 0.9981 | 0.933(-3) | 1.0000 | 0.120(-4) | | |
| 2.2 | 0.0914 | 0.646(-2) | 0.9987 | 0.118(-2) | 0.0005 | 0.605(-4) | | |
| 2.4 | 0.0827 | 0.926(-2) | 0.9986 | 0.162(-2) | 0.9999 | 0.897(-5) | | |
| 2.6 | 0.0684 | 0.122(-1) | 0.9978 | 0.225(-2) | 1.0000 | 0.635(-4) | | |
| 2.8 | 0.0258 | 0.174(-1) | 0.9932 | 0.953(-2) | 0.9993 | 0.505(-3) | | |
| 3.0 | 0.0259 | 0.221(-1) | 0.9949 | 0.595(-2) | 0.9998 | 0.271(-3) | | |
| 3.5 | 0.0083 | 0.415(-1) | 0.9923 | 0.168(-1) | 0.0000 | 0.910(-3) | | |
| 4.0 | 0.9761 | 0.573(-1) | 0.9894 | 0.274(-1) | 0.9989 | 0.904(-3) | | |
| ${}^3\Delta_g$ | | | | | | | | |
| | | (3,2) | | (5,2) | | | | |
| 1.0 | 0.1407 | 0.000 | 0.8828 | 0.000 | | | | |
| 1.2 | 0.0034 | 0.782(-4) | 0.9992 | 0.429(-5) | | | | |
| 1.4 | 0.0023 | 0.130(-3) | 0.9994 | 0.125(-4) | | | | |
| 1.6 | 0.0015 | 0.222(-3) | 0.9995 | 0.495(-4) | | | | |
| 1.8 | 0.0007 | 0.326(-3) | 0.9995 | 0.147(-3) | | | | |
| 2.0 | 0.9995 | 0.602(-3) | 0.0002 | 0.113(-3) | | | | |
| 2.2 | 0.9988 | 0.951(-3) | 0.9998 | 0.886(-5) | | | | |
| 2.4 | 0.9976 | 0.127(-2) | 0.0000 | 0.643(-5) | | | | |
| 2.6 | 0.9961 | 0.182(-2) | 0.9997 | 0.210(-4) | | | | |
| 2.8 | 0.9935 | 0.616(-2) | 0.9985 | 0.411(-3) | | | | |
| 3.0 | 0.9918 | 0.434(-2) | 0.9995 | 0.258(-3) | | | | |
| 3.5 | 0.9854 | 0.120(-1) | 0.0001 | 0.784(-3) | | | | |
| 4.0 | 0.9776 | 0.207(-1) | 0.9979 | 0.779(-3) | | | | |
| ${}^3\Delta_u$ | | | | | | | | |
| | | (2,2) | | (4,2) | | (6,2) | | |
| 1.0 | 0.0581 | 0.802(-3) | 0.9988 | 0.656(-5) | 0.0000 | 0.317(-6) | | |
| 1.2 | 0.0468 | 0.118(-2) | 0.9987 | 0.452(-5) | 0.0001 | 0.470(-6) | | |
| 1.4 | 0.0366 | 0.185(-2) | 0.9989 | 0.118(-4) | 0.0000 | 0.412(-6) | | |
| 1.6 | 0.0276 | 0.273(-2) | 0.9990 | 0.704(-4) | 0.0000 | 0.703(-6) | | |
| 1.8 | 0.0198 | 0.360(-2) | 0.9992 | 0.862(-4) | 0.0000 | 0.200(-6) | | |
| 2.0 | 0.0125 | 0.433(-2) | 0.9992 | 0.584(-4) | 0.0000 | 0.980(-7) | | |
| 2.2 | 0.0052 | 0.521(-2) | 0.9992 | 0.828(-4) | 1.0000 | 0.365(-6) | | |
| 2.4 | 0.9977 | 0.677(-2) | 0.9990 | 0.449(-5) | 1.0000 | 0.164(-5) | | |
| 2.6 | 0.9900 | 0.905(-2) | 0.9986 | 0.126(-3) | 0.0001 | 0.252(-5) | | |
| 2.8 | 0.9849 | 0.147(-1) | 0.9965 | 0.139(-2) | 0.0001 | 0.212(-4) | | |
| 3.0 | 0.9750 | 0.175(-1) | 0.9973 | 0.727(-3) | 0.9999 | 0.330(-7) | | |
| 3.5 | 0.9625 | 0.339(-1) | 0.9952 | 0.449(-2) | 0.0001 | 0.369(-5) | | |
| 4.0 | 0.9460 | 0.444(-1) | 0.9913 | 0.477(-2) | 0.0013 | 0.490(-5) | | |

TABLE V. Complex Quantum Defects at the ${}^2\Pi_u$ Threshold
See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|------------------|--------|-----------|--------|-----------|--------|-----------|--------|-----------|
| ${}^1\Sigma_g^+$ | | | | | | | | |
| | | (1,1) | | (3,1) | | (5,1) | | |
| 1.0 | 0.0359 | 0.212(-1) | 0.9800 | 0.786(-3) | 0.9993 | 0.441(-4) | | |
| 1.2 | 0.0237 | 0.210(-1) | 0.9797 | 0.105(-2) | 0.0007 | 0.715(-4) | | |
| 1.4 | 0.0113 | 0.195(-1) | 0.9786 | 0.157(-2) | 0.9995 | 0.197(-3) | | |
| 1.6 | 0.9985 | 0.165(-1) | 0.9767 | 0.361(-2) | 0.9997 | 0.635(-3) | | |
| 1.8 | 0.9726 | 0.880(-2) | 0.9899 | 0.105(-1) | 0.0003 | 0.615(-3) | | |
| 2.0 | 0.9610 | 0.143(-1) | 0.9876 | 0.478(-2) | 0.0010 | 0.640(-3) | | |
| 2.2 | 0.9464 | 0.162(-1) | 0.9882 | 0.275(-2) | 0.0025 | 0.457(-3) | | |
| 2.4 | 0.9390 | 0.161(-1) | 0.9899 | 0.208(-2) | 0.0037 | 0.576(-3) | | |
| 2.6 | 0.9282 | 0.161(-1) | 0.9904 | 0.202(-2) | 0.0042 | 0.704(-3) | | |
| 2.8 | 0.9297 | 0.149(-1) | 0.9901 | 0.171(-2) | 0.0053 | 0.120(-2) | | |
| 3.0 | 0.8982 | 0.167(-1) | 0.9883 | 0.180(-2) | 0.0051 | 0.104(-2) | | |
| 3.5 | 0.8879 | 0.168(-1) | 0.0137 | 0.275(-2) | 0.9926 | 0.132(-2) | | |
| 4.0 | 0.9048 | 0.180(-1) | 0.0687 | 0.354(-2) | 0.0244 | 0.329(-2) | | |
| ${}^1\Sigma_u^+$ | | | | | | | | |
| | | (2,1) | | (4,1) | | (6,1) | | |
| 1.0 | 0.9011 | 0.103(-1) | 0.9945 | 0.708(-4) | 0.9999 | 0.111(-5) | | |
| 1.2 | 0.9021 | 0.899(-2) | 0.9945 | 0.799(-4) | 0.0001 | 0.121(-5) | | |
| 1.4 | 0.9034 | 0.819(-2) | 0.9946 | 0.867(-4) | 0.9999 | 0.159(-5) | | |
| 1.6 | 0.8963 | 0.771(-2) | 0.9950 | 0.953(-4) | 0.0002 | 0.233(-5) | | |
| 1.8 | 0.8893 | 0.756(-2) | 0.9946 | 0.605(-4) | 0.0002 | 0.157(-5) | | |
| 2.0 | 0.8868 | 0.782(-2) | 0.9955 | 0.485(-4) | 0.9998 | 0.235(-5) | | |
| 2.2 | 0.8884 | 0.830(-2) | 0.9959 | 0.666(-4) | 0.0003 | 0.386(-5) | | |
| 2.4 | 0.8963 | 0.871(-2) | 0.9953 | 0.140(-3) | 0.0001 | 0.632(-5) | | |
| 2.6 | 0.8978 | 0.925(-2) | 0.9963 | 0.153(-3) | 0.0006 | 0.140(-4) | | |
| 2.8 | 0.9044 | 0.955(-2) | 0.9957 | 0.206(-3) | 0.0001 | 0.247(-4) | | |
| 3.0 | 0.8989 | 0.115(-1) | 0.9936 | 0.265(-3) | 0.0001 | 0.127(-4) | | |
| 3.5 | 0.9077 | 0.151(-1) | 0.9965 | 0.317(-3) | 0.0014 | 0.477(-4) | | |
| 4.0 | 0.9356 | 0.166(-1) | 0.0453 | 0.932(-3) | 0.0308 | 0.127(-3) | | |
| ${}^1\Pi_u$ | | | | | | | | |
| | | (0,0) | | (2,0) | | (4,0) | | (6,0) |
| 1.0 | 0.2455 | 0.413(-1) | 0.9929 | 0.220(-2) | 0.0038 | 0.117(-3) | 1.0000 | 0.213(-5) |
| 1.2 | 0.2113 | 0.456(-1) | 0.9889 | 0.340(-2) | 0.0042 | 0.119(-3) | 1.0000 | 0.163(-5) |
| 1.4 | 0.1822 | 0.441(-1) | 0.9818 | 0.559(-2) | 0.0046 | 0.118(-3) | 1.0000 | 0.154(-5) |
| 1.6 | 0.1621 | 0.401(-1) | 0.9730 | 0.832(-2) | 0.0050 | 0.113(-3) | 1.0000 | 0.131(-5) |
| 1.8 | 0.1524 | 0.349(-1) | 0.9621 | 0.102(-1) | 0.0056 | 0.967(-4) | 1.0000 | 0.105(-5) |
| 2.0 | 0.9473 | 0.953(-2) | 0.1471 | 0.281(-1) | 0.0062 | 0.807(-4) | 1.0000 | 0.925(-6) |
| 2.2 | 0.9311 | 0.832(-2) | 0.1475 | 0.234(-1) | 0.0069 | 0.756(-4) | 1.0000 | 0.102(-5) |
| 2.4 | 0.9146 | 0.649(-2) | 0.1550 | 0.211(-1) | 0.0089 | 0.757(-4) | 1.0000 | 0.989(-6) |
| 2.6 | 0.8948 | 0.585(-2) | 0.1637 | 0.214(-1) | 0.0085 | 0.818(-4) | 1.0000 | 0.156(-5) |
| 2.8 | 0.8765 | 0.319(-2) | 0.1797 | 0.209(-1) | 0.0095 | 0.817(-4) | 1.0000 | 0.170(-5) |
| 3.0 | 0.8600 | 0.853(-2) | 0.2082 | 0.278(-1) | 0.0093 | 0.982(-4) | 0.9999 | 0.265(-5) |
| 3.5 | 0.8269 | 0.132(-1) | 0.3085 | 0.421(-1) | 0.0130 | 0.125(-3) | 0.9999 | 0.231(-5) |
| 4.0 | 0.5007 | 0.378(-2) | 0.4340 | 0.424(-2) | 0.0269 | 0.107(-3) | 0.0088 | 0.577(-6) |

TABLE V. Complex Quantum Defects at the ${}^2\Pi_u$ Threshold
See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|----------------|--------|-----------|--------|-----------|--------|-----------|-----|-----|
| ${}^1\Pi_g$ | | | | | | | | |
| | | (1,0) | | (5,0) | | (5,0) | | |
| 1.0 | 0.4218 | 0.690(-1) | 0.0142 | 0.684(-3) | 0.0001 | 0.141(-4) | | |
| 1.2 | 0.4681 | 0.593(-1) | 0.0162 | 0.719(-3) | 0.0001 | 0.119(-4) | | |
| 1.4 | 0.5079 | 0.500(-1) | 0.0185 | 0.731(-3) | 0.0002 | 0.108(-4) | | |
| 1.6 | 0.5414 | 0.409(-1) | 0.0212 | 0.725(-3) | 0.0002 | 0.115(-4) | | |
| 1.8 | 0.5677 | 0.337(-1) | 0.0242 | 0.717(-3) | 0.0002 | 0.135(-4) | | |
| 2.0 | 0.5868 | 0.288(-1) | 0.0272 | 0.729(-3) | 0.0002 | 0.158(-4) | | |
| 2.2 | 0.5998 | 0.246(-1) | 0.0306 | 0.762(-3) | 0.0003 | 0.175(-4) | | |
| 2.4 | 0.6090 | 0.214(-1) | 0.0360 | 0.827(-3) | 0.0005 | 0.182(-4) | | |
| 2.6 | 0.6126 | 0.169(-1) | 0.0384 | 0.892(-3) | 0.0003 | 0.216(-4) | | |
| 2.8 | 0.6140 | 0.121(-1) | 0.0429 | 0.965(-3) | 0.0004 | 0.240(-4) | | |
| 3.0 | 0.6209 | 0.930(-2) | 0.0452 | 0.102(-2) | 0.0001 | 0.291(-4) | | |
| 3.5 | 0.6189 | 0.505(-2) | 0.0584 | 0.128(-2) | 0.0005 | 0.385(-4) | | |
| 4.0 | 0.6158 | 0.387(-2) | 0.0809 | 0.184(-2) | 0.0143 | 0.448(-4) | | |
| ${}^1\Delta_g$ | | | | | | | | |
| | | (1,1) | | (3,1) | | (5,1) | | |
| 1.0 | 0.0912 | 0.159(-1) | 0.0111 | 0.468(-3) | 1.0000 | 0.106(-4) | | |
| 1.2 | 0.0798 | 0.179(-1) | 0.0124 | 0.493(-3) | 1.0000 | 0.986(-5) | | |
| 1.4 | 0.0691 | 0.200(-1) | 0.0141 | 0.516(-3) | 1.0000 | 0.955(-5) | | |
| 1.6 | 0.0571 | 0.222(-1) | 0.0158 | 0.637(-3) | 1.0000 | 0.111(-4) | | |
| 1.8 | 0.0464 | 0.239(-1) | 0.0180 | 0.883(-3) | 0.0001 | 0.253(-4) | | |
| 2.0 | 0.0339 | 0.250(-1) | 0.0209 | 0.148(-2) | 1.0000 | 0.242(-4) | | |
| 2.2 | 0.0192 | 0.259(-1) | 0.0247 | 0.190(-2) | 0.0004 | 0.195(-4) | | |
| 2.4 | 0.0103 | 0.264(-1) | 0.0303 | 0.164(-2) | 0.0003 | 0.456(-4) | | |
| 2.6 | 0.0002 | 0.264(-1) | 0.0334 | 0.177(-2) | 0.0004 | 0.841(-4) | | |
| 2.8 | 0.9983 | 0.250(-1) | 0.0382 | 0.186(-2) | 0.0002 | 0.218(-4) | | |
| 3.0 | 0.9738 | 0.272(-1) | 0.0405 | 0.168(-2) | 0.0001 | 0.456(-4) | | |
| 3.5 | 0.9606 | 0.252(-1) | 0.0593 | 0.216(-2) | 0.0005 | 0.576(-4) | | |
| 4.0 | 0.9262 | 0.249(-1) | 0.0894 | 0.315(-2) | 0.0128 | 0.697(-5) | | |
| ${}^1\Delta_u$ | | | | | | | | |
| | | (2,1) | | (4,1) | | (6,1) | | |
| 1.0 | 0.9416 | 0.108(-1) | 0.0039 | 0.769(-4) | 0.0148 | 0.445(-2) | | |
| 1.2 | 0.9418 | 0.881(-2) | 0.0045 | 0.831(-4) | 0.0148 | 0.382(-2) | | |
| 1.4 | 0.9961 | 0.809(-2) | 0.0058 | 0.716(-3) | 0.9991 | 0.468(-5) | | |
| 1.6 | 0.9378 | 0.690(-2) | 0.0059 | 0.151(-3) | 0.0148 | 0.287(-2) | | |
| 1.8 | 0.9328 | 0.705(-2) | 0.0022 | 0.667(-4) | 0.0131 | 0.252(-2) | | |
| 2.0 | 0.9223 | 0.788(-2) | 0.0028 | 0.766(-4) | 0.0131 | 0.254(-2) | | |
| 2.2 | 0.9250 | 0.773(-2) | 0.0023 | 0.841(-4) | 0.0138 | 0.282(-2) | | |
| 2.4 | 0.8484 | 0.362(-1) | 0.0108 | 0.451(-3) | 0.0170 | 0.322(-2) | | |
| 2.6 | 0.8409 | 0.448(-1) | 0.0109 | 0.499(-3) | 0.0180 | 0.369(-2) | | |
| 2.8 | 0.9341 | 0.850(-2) | 0.0090 | 0.179(-3) | 0.0182 | 0.463(-2) | | |
| 3.0 | 0.9039 | 0.124(-1) | 0.0088 | 0.129(-3) | 0.0189 | 0.564(-2) | | |
| 3.5 | 0.9251 | 0.123(-1) | 0.0116 | 0.439(-3) | 0.0225 | 0.705(-2) | | |
| 4.0 | 0.8964 | 0.625(-1) | 0.0189 | 0.908(-4) | 0.0308 | 0.976(-2) | | |

TABLE V. Complex Quantum Defects at the ${}^2\Pi_u$ Threshold
 See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|------------------|--------|-----------|--------|-----------|--------|-----------|--------|-----------|
| ${}^3\Sigma_g^+$ | | | | | | | | |
| | | (1,1) | | (3,1) | | (5,1) | | |
| 1.0 | 0.3045 | 0.116(-2) | 0.9867 | 0.530(-3) | 0.0003 | 0.283(-4) | | |
| 1.2 | 0.2914 | 0.789(-3) | 0.9871 | 0.518(-3) | 0.0005 | 0.351(-4) | | |
| 1.4 | 0.2774 | 0.565(-3) | 0.9877 | 0.482(-3) | 0.0007 | 0.417(-4) | | |
| 1.6 | 0.2630 | 0.474(-3) | 0.9883 | 0.425(-3) | 0.0011 | 0.652(-4) | | |
| 1.8 | 0.2481 | 0.473(-3) | 0.9890 | 0.372(-3) | 0.0016 | 0.958(-4) | | |
| 2.0 | 0.2324 | 0.509(-3) | 0.9893 | 0.338(-3) | 0.0022 | 0.119(-3) | | |
| 2.2 | 0.2173 | 0.558(-3) | 0.9904 | 0.312(-3) | 0.0030 | 0.156(-3) | | |
| 2.4 | 0.2032 | 0.575(-3) | 0.9921 | 0.264(-3) | 0.0050 | 0.228(-3) | | |
| 2.6 | 0.1887 | 0.561(-3) | 0.9920 | 0.262(-3) | 0.0057 | 0.262(-3) | | |
| 2.8 | 0.1760 | 0.520(-3) | 0.0074 | 0.319(-3) | 0.9929 | 0.243(-3) | | |
| 3.0 | 0.1632 | 0.508(-3) | 0.0089 | 0.369(-3) | 0.9924 | 0.255(-3) | | |
| 3.5 | 0.1398 | 0.417(-3) | 0.0175 | 0.555(-3) | 0.9944 | 0.192(-3) | | |
| 4.0 | 0.1602 | 0.397(-3) | 0.0697 | 0.436(-3) | 0.0261 | 0.544(-3) | | |
| ${}^3\Sigma_u^+$ | | | | | | | | |
| | | (2,1) | | (4,1) | | (6,1) | | |
| 1.0 | 0.1089 | 0.173(-1) | 0.9949 | 0.855(-4) | 0.9999 | 0.185(-5) | | |
| 1.2 | 0.1196 | 0.138(-1) | 0.9944 | 0.868(-4) | 0.0001 | 0.103(-5) | | |
| 1.4 | 0.1320 | 0.110(-1) | 0.9944 | 0.844(-4) | 0.0004 | 0.112(-5) | | |
| 1.6 | 0.1414 | 0.902(-2) | 0.9947 | 0.819(-4) | 0.0000 | 0.193(-5) | | |
| 1.8 | 0.1514 | 0.760(-2) | 0.9948 | 0.549(-4) | 0.0000 | 0.176(-5) | | |
| 2.0 | 0.1671 | 0.649(-2) | 0.9958 | 0.479(-4) | 0.0001 | 0.229(-5) | | |
| 2.2 | 0.1848 | 0.546(-2) | 0.9957 | 0.548(-4) | 0.0002 | 0.299(-5) | | |
| 2.4 | 0.2043 | 0.464(-2) | 0.9958 | 0.706(-4) | 0.0004 | 0.407(-5) | | |
| 2.6 | 0.2186 | 0.397(-2) | 0.9957 | 0.832(-4) | 0.0002 | 0.578(-5) | | |
| 2.8 | 0.2347 | 0.348(-2) | 0.9955 | 0.928(-4) | 0.0005 | 0.624(-5) | | |
| 3.0 | 0.2460 | 0.294(-2) | 0.9944 | 0.977(-4) | 0.0005 | 0.471(-5) | | |
| 3.5 | 0.2800 | 0.219(-2) | 0.9966 | 0.812(-4) | 0.0011 | 0.159(-4) | | |
| 4.0 | 0.3279 | 0.178(-2) | 0.0428 | 0.120(-3) | 0.0304 | 0.303(-4) | | |
| ${}^3\Pi_u$ | | | | | | | | |
| | | (0,0) | | (2,0) | | (4,0) | | (6,0) |
| 1.0 | 0.2909 | 0.106(-2) | 0.1112 | 0.906(-2) | 0.0037 | 0.499(-4) | 1.0000 | 0.563(-6) |
| 1.2 | 0.2592 | 0.377(-3) | 0.1215 | 0.930(-2) | 0.0041 | 0.599(-4) | 1.0000 | 0.590(-6) |
| 1.4 | 0.2292 | 0.133(-3) | 0.1336 | 0.891(-2) | 0.0046 | 0.614(-4) | 1.0000 | 0.659(-6) |
| 1.6 | 0.2017 | 0.666(-3) | 0.1471 | 0.823(-2) | 0.0052 | 0.543(-4) | 1.0000 | 0.602(-6) |
| 1.8 | 0.1540 | 0.372(-2) | 0.1842 | 0.504(-2) | 0.0059 | 0.458(-4) | 1.0000 | 0.443(-6) |
| 2.0 | 0.1361 | 0.328(-3) | 0.1966 | 0.803(-2) | 0.0064 | 0.427(-4) | 1.0000 | 0.452(-6) |
| 2.2 | 0.1118 | 0.442(-4) | 0.2202 | 0.815(-2) | 0.0072 | 0.462(-4) | 1.0000 | 0.603(-6) |
| 2.4 | 0.0876 | 0.731(-4) | 0.2502 | 0.820(-2) | 0.0094 | 0.547(-4) | 1.0000 | 0.801(-6) |
| 2.6 | 0.0626 | 0.164(-3) | 0.2804 | 0.850(-2) | 0.0090 | 0.629(-4) | 1.0000 | 0.120(-5) |
| 2.8 | 0.0391 | 0.277(-3) | 0.3168 | 0.901(-2) | 0.0102 | 0.695(-4) | 1.0000 | 0.164(-5) |
| 3.0 | 0.0179 | 0.355(-3) | 0.3573 | 0.808(-2) | 0.0102 | 0.717(-4) | 0.9999 | 0.203(-5) |
| 3.5 | 0.9664 | 0.542(-3) | 0.4493 | 0.657(-2) | 0.0142 | 0.719(-4) | 0.9999 | 0.141(-5) |
| 4.0 | 0.8056 | 0.902(-1) | 0.5383 | 0.403(-2) | 0.0287 | 0.892(-4) | 0.0088 | 0.576(-6) |

TABLE V. Complex Quantum Defects at the ${}^2\Pi_u$ Threshold
 See page 257 for Explanation of Tables

| R | A | B | A | B | A | B | A | B |
|----------------|--------|-----------|--------|-----------|--------|-----------|-----|-----|
| ${}^3\Pi_g$ | | | | | | | | |
| | (1,0) | | (5,0) | | (5,0) | | | |
| 1.0 | 0.4274 | 0.194(-1) | 0.0182 | 0.311(-3) | 0.0002 | 0.405(-5) | | |
| 1.2 | 0.4641 | 0.173(-1) | 0.0208 | 0.354(-3) | 0.0002 | 0.359(-5) | | |
| 1.4 | 0.4955 | 0.153(-1) | 0.0236 | 0.369(-3) | 0.0003 | 0.286(-5) | | |
| 1.6 | 0.5215 | 0.135(-1) | 0.0270 | 0.372(-3) | 0.0003 | 0.329(-5) | | |
| 1.8 | 0.5413 | 0.124(-1) | 0.0308 | 0.381(-3) | 0.0003 | 0.489(-5) | | |
| 2.0 | 0.5560 | 0.112(-1) | 0.0346 | 0.401(-3) | 0.0004 | 0.650(-5) | | |
| 2.2 | 0.5661 | 0.100(-1) | 0.0390 | 0.443(-3) | 0.0004 | 0.744(-5) | | |
| 2.4 | 0.5736 | 0.860(-2) | 0.0457 | 0.505(-3) | 0.0007 | 0.771(-5) | | |
| 2.6 | 0.5774 | 0.652(-2) | 0.0496 | 0.573(-3) | 0.0005 | 0.854(-5) | | |
| 2.8 | 0.5812 | 0.399(-2) | 0.0559 | 0.644(-3) | 0.0006 | 0.964(-5) | | |
| 3.0 | 0.5873 | 0.419(-2) | 0.0613 | 0.725(-3) | 0.0005 | 0.120(-4) | | |
| 3.5 | 0.5909 | 0.239(-2) | 0.0787 | 0.972(-3) | 0.0008 | 0.197(-4) | | |
| 4.0 | 0.5964 | 0.202(-2) | 0.1057 | 0.130(-2) | 0.0144 | 0.442(-4) | | |
| ${}^3\Delta_g$ | | | | | | | | |
| | (1,1) | | (3,1) | | (5,1) | | | |
| 1.0 | 0.1326 | 0.104(-1) | 0.0040 | 0.736(-4) | 0.9878 | 0.609(-3) | | |
| 1.2 | 0.1520 | 0.114(-1) | 0.0047 | 0.789(-4) | 0.9887 | 0.513(-3) | | |
| 1.4 | 0.0962 | 0.423(-2) | 0.0050 | 0.903(-4) | 0.9991 | 0.129(-5) | | |
| 1.6 | 0.2128 | 0.144(-1) | 0.0066 | 0.702(-4) | 0.9901 | 0.359(-3) | | |
| 1.8 | 0.2147 | 0.129(-1) | 0.0026 | 0.577(-4) | 0.9909 | 0.297(-3) | | |
| 2.0 | 0.2973 | 0.158(-1) | 0.0031 | 0.592(-4) | 0.9916 | 0.248(-3) | | |
| 2.2 | 0.3621 | 0.166(-1) | 0.0027 | 0.635(-4) | 0.9921 | 0.190(-3) | | |
| 2.4 | 0.1775 | 0.253(-2) | 0.0122 | 0.763(-4) | 0.9927 | 0.163(-3) | | |
| 2.6 | 0.1761 | 0.197(-2) | 0.0125 | 0.881(-4) | 0.9936 | 0.128(-3) | | |
| 2.8 | 0.5531 | 0.115(-1) | 0.0101 | 0.919(-4) | 0.9941 | 0.882(-4) | | |
| 3.0 | 0.6672 | 0.431(-2) | 0.0099 | 0.946(-4) | 0.9940 | 0.824(-4) | | |
| 3.5 | 0.6405 | 0.560(-2) | 0.0139 | 0.942(-4) | 0.9952 | 0.455(-4) | | |
| 4.0 | 0.1401 | 0.794(-3) | 0.0761 | 0.103(-2) | 0.0129 | 0.586(-5) | | |
| ${}^3\Delta_u$ | | | | | | | | |
| | (2,1) | | (4,1) | | (6,1) | | | |
| 1.0 | 0.1326 | 0.104(-1) | 0.0040 | 0.736(-4) | 0.9878 | 0.609(-3) | | |
| 1.2 | 0.1520 | 0.114(-1) | 0.0047 | 0.789(-4) | 0.9887 | 0.513(-3) | | |
| 1.4 | 0.0962 | 0.423(-2) | 0.0050 | 0.903(-4) | 0.9991 | 0.129(-5) | | |
| 1.6 | 0.2128 | 0.144(-1) | 0.0066 | 0.702(-4) | 0.9901 | 0.359(-3) | | |
| 1.8 | 0.2147 | 0.129(-1) | 0.0026 | 0.577(-4) | 0.9909 | 0.297(-3) | | |
| 2.0 | 0.2973 | 0.158(-1) | 0.0031 | 0.592(-4) | 0.9916 | 0.248(-3) | | |
| 2.2 | 0.3621 | 0.166(-1) | 0.0027 | 0.635(-4) | 0.9921 | 0.190(-3) | | |
| 2.4 | 0.1775 | 0.253(-2) | 0.0122 | 0.763(-4) | 0.9927 | 0.163(-3) | | |
| 2.6 | 0.1761 | 0.197(-2) | 0.0125 | 0.881(-4) | 0.9936 | 0.128(-3) | | |
| 2.8 | 0.5531 | 0.115(-1) | 0.0101 | 0.919(-4) | 0.9941 | 0.882(-4) | | |
| 3.0 | 0.6672 | 0.431(-2) | 0.0099 | 0.946(-4) | 0.9940 | 0.824(-4) | | |
| 3.5 | 0.6405 | 0.560(-2) | 0.0139 | 0.942(-4) | 0.9952 | 0.455(-4) | | |
| 4.0 | 0.1839 | 0.944(-3) | 0.0205 | 0.811(-4) | 0.0039 | 0.282(-4) | | |