# $S$, $P$, and $D$ states of two-electron ions via $Z$-dependent perturbation theory

Frank C. Sanders
*Department of Physics and Astronomy, Southern Illinois University-Carbondale, Carbondale, Illinois 62901*

Robert E. Knight
*Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506*

(Received 26 July 1982)

A perturbation study of singly excited $S$, $P$, and $D$ states of two-electron atoms has been made. Perturbation expansion coefficients for the nonrelativistic energies are computed and estimates of the relativistic corrections to low orders in $Z$ are also obtained. A simple one-electron Lamb-shift correction is then combined with these results to yield theoretical transition energies in excellent agreement with experimental data for He I through Fe XXV.

## I. INTRODUCTION

In a recent application of $Z$-dependent perturbation theory,[1] the authors made use of two-electron, first-order wave functions to obtain accurate transition energies for several $S$, $P$, and $D$ states of three-electron ions. One aspect of the work was a simplified procedure for obtaining relativistic corrections to the energy.[2] The accuracy of these transition energies indicated that this approach to the relativistic corrections might be usefully applied to the corresponding two-electron states. In the latter case, third and higher-order nonrelativistic energy coefficients could be more easily computed, rather than extracted from the experimental data for the first few members of an isoelectronic sequence, as was done in Refs. 1 and 2. Further, very accurate variational calculations for some of these two-electron states are available[3–6]; in particular, relativistic corrections from these calculations[3,4] permit an evaluation of the accuracy to be expected from the simple approach used here.

For the present paper, the accuracy of the two-electron, first-order wave functions has been improved and the computations extended to higher order. In addition to the relativistic corrections, estimates of the Lamb shift are included. These results are then combined to yield theoretical estimates of transition energies for singlet and triplet $NS$, $NP$, and $ND$ states through $N=9$. Finally, these theoretical values are compared with the available experimental data for He I through Fe XXV. The theoretical transition energies obtained form a consistent set of data for all states of the He isoelectronic sequence considered here.

## II. METHOD

### A. The nonrelativistic energy

The Hamiltonian for a nonrelativistic two-electron atom in charge-scaled atomic units is

$$H = H_0 + \frac{1}{Z} H_1 , \tag{1}$$

where

$$H_0 = -\tfrac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{1}{r_1} - \frac{1}{r_2} , \tag{2}$$

$$H_1 = \frac{1}{r_{12}} \tag{3}$$

are the unperturbed Hamiltonian and perturbation, respectively. The wave function and energy are then written as

$$\Psi = \sum_{n=0} Z^{-n} \psi_n , \tag{4}$$

$$E = \sum_{n=0} Z^{2-n} \epsilon_n . \tag{5}$$

The $\psi_n$ are obtained by a variational-perturbation procedure[7] using trial functions of the form

$$\psi_n^{NL} = (1 \pm P_{12})(A + r_{12} B) \times e^{-k_n (r_1 + r_2)/N} P_L(\cos\theta_2) , \tag{6}$$

with $A$ and $B$ both of the form

$$\sum_{abl} C_{abl}^{(n)} r_1^{a+l} r_2^{b+l+L} P_l(\cos\theta_{12}) . \tag{7}$$

For the calculations reported here the expansions for $A$ usually contain about 200 terms, while those

 

for $B$ contain 50 or fewer terms; the expansion for $B$ contains all terms such that $a+b+2l \leq 6$ or 4 while $A$ contains terms with $a+b+2l \leq 12$, but emphasizing those terms with higher powers of $r_2$ (i.e., $b > a$). Note that for $D$ states this form of the trial function includes only $(s-d)$-type terms—no $(p-p)$ terms. Also included in the trial functions for these excited states are the zero-order functions for less excited states of the same symmetry. With the inclusion of these terms the optimized $\psi_n$ yield a rigorous upper bound[8] for $\epsilon_{2n}$ and an estimate of $\epsilon_{2n+1}$.

The nonlinear parameter $k_n$ was optimized for $\psi_1$ only, and then the same basis was used for all the higher-order wave functions. Although less accurate than individually optimizing the $k_n$,[9] this procedure yields higher-order results with very little additional computational effort. Thus the order to which each state was calculated was limited only by the increasing numerical inaccuracy introduced by this simpler approach. It should be noted that this can be a severe limitation, and more accurate results obtained without such restrictions were used where available.[8(c)]

Since the final results are presented in terms of transition energies to the $1^1S$ ground state of the ion, the nonrelativistic contribution to the transition energy is written as

$$T_{\rm nr}=\sum_{n=0}^{n_f} e_n Z^{2-n} , \tag{8}$$

where $e_n=\epsilon_n^{NL}-\epsilon_n^{1^1S}$, and the ground-state expansion coefficients are taken from the work of Aashamar.[10] The truncation point $n_f$, was determined by the accuracy of the excited-state expansion coefficients.

### B. Relativistic corrections

The approach followed here was identical to that of Ref. 1. The relativistic correction is given by the Breit formula[11]

$$E_{\rm rel}=\alpha^2[-\tfrac{1}{4}\langle p_1^4\rangle+\pi Z\langle\delta(\vec{r}_1)\rangle+\pi\langle\delta(\vec{r}_{12})\rangle] , \tag{9}$$

with $\alpha$ the fine-structure constant. Note that no spin-orbit or spin-spin operators are included. The triplet states are thus to be compared to a multiplet average of the experimental fine-structure levels, whenever those are available. The first two terms of Eq. (9) are evaluated to first order in $Z$, the third term to zero order in $Z$, giving the first two terms of the $Z$ expansion of $E_{\rm rel}$,

$$E_{\rm rel}=\alpha^2(Z^4b_0+Z^3b_1) . \tag{10}$$

However the actual expression used is[12]

$$E_{\rm rel}=\alpha^2(Z-\sigma)^4b_0 , \tag{11}$$

which, with $\sigma=-b_1/(4b_0)$, reproduces Eq. (10) through $Z^3$ while providing some contributions of order $Z^2$ and beyond. In the above,

$$b_0=-\frac{1}{8}-\frac{(8N-6L-3)}{8N^4(2L+1)}+\frac{\delta_{L,0}}{2N^3} \tag{12}$$

and the $b_1$ are listed in Table V of Ref. 1. However, since the final results are expressed as transition energies, the contribution of the Breit formula was given by

$$T_{\rm rel}=\alpha^2(Z-\sigma)^4b_0^{NL}-\alpha^2\sum_{n=0} b_n^{1^1S}Z^{4-n} , \tag{13}$$

where the $b_0^{NL}$ in Eq. (13) and in the expression for $\sigma$ differs from that of Eq. (12) by the elimination of the term $-\frac{1}{8}$. Similarly, the $b_0^{1^1S}$ used in Eq. (13) was $-\frac{1}{8}$ rather than the correct value of $-\frac{1}{4}$. This procedure gave a slight improvement in $T_{\rm rel}$. The higher-order $b_n^{1^1S}$ are also taken from the work of Aashamar.[10]

### C. Lamb shift

The Lamb-shift correction is of order $Z^4$ and was neglected in Ref. 1 where the nonrelativistic energy was sufficiently inaccurate to make its inclusion unnecessary. For the present two-electron study, however, inclusion of the Lamb shift is essential, since for many of the excited states the nonrelativistic energies are well converged. In obtaining estimates of the Lamb shift a simple one-electron approximation was used,

$$E_L=E_L(1S,Z)+E_L(NL,Z^*) \tag{14}$$

with

$$E_L(NS,Z)=\frac{Z^4}{N^3}[-2\ln(\alpha Z)-\ln(K_{N,0})+\tfrac{19}{30}] \tag{15}$$

for $S$ states and

$$E_L(NL,Z)=-\frac{Z^4}{N^3}\ln(K_{N,L}) \tag{16}$$

for $P$ and $D$ states. $K_{N,L}$ is the average excitation potential[13] of the one-electron ion and $Z^*=Z-1+(3-L)/N^2$ represents an *ad hoc* screening for the excited electron. No screening was used for the $1S$ electron so that the contribution of $E_L$ to the transition energy would go to the right limit for large $N$. The ground-state Lamb shift necessary for the transition energy was taken from Aashamar.[10]

### D. Mass polarization

In the present calculations, the mass-polarization correction for the excited state is ignored, and only the contribution of the ground state to the transition energy is included. The latter is almost constant with increasing $Z$ with a value of $\sim 7$ cm$^{-1}$ for $Z=6$ through 10 (Ref. 10). In contrast, the mass-polarization correction for $S$ (Ref. 3) and $D$ (Ref. 14) states is quite small and decreases rapidly as $N$ increases. For these states, then, the ground-state correction is sufficient and, indeed, only makes a noticeable contribution for low-$Z$ ions. This is not the case for the $P$ states, however, where the absolute value of the polarization correction for the excited states is increasing with $Z$ although still decreasing rapidly with $N$ (Ref. 3).

## III. RESULTS

The nonrelativistic energy expansion coefficients for the states considered here are listed in Tables I–VI. The higher-order coefficients listed are based on 100-term expansions for the perturbation wave functions using high-precision (28-decimal digit) arithmetic since, given the number of states considered here, calculations with the 200+ terms used for the first-order wave functions would have been prohibitive in terms of computer time. For the $2^3S$ and $2^{1,3}P$ states, the higher-order coefficients listed are taken from the earlier work of Sanders and Scherr,[8(c)] where the $k_n$ for the higher-order wave functions are individually optimized. Values of these coefficients from other theoretical studies of these states are listed for comparison where these are available.

Tables VII and VIII list values of $\alpha^{-2}T_{\rm rel}$ given by Eq. (13) for those $S$ and $P$ states studied by Accad, *et al.*[4] Comparison with the latter authors' accurate calculations permits an evaluation of the accuracy obtained with the approximation used here for the relativistic correction.

Finally, Tables IX–XIV present the transition energies for all $S$, $P$, and $D$ states considered here for all ions from He I through Fe XXV inclusive, together with accurate experimental values for these transition energies. In many cases these experimental values are taken from recent critical compilations of the available data by the National Bureau of Standards Atomic Energy Levels Data Center, and thus include some theoretical values. In the tables, such theoretical values are indicated by parenthesis. For the most highly ionized $S$ and $P$ states, the listed values are almost exclusively theoretical values taken from the work of Ermolaev and Jones.[15]

## IV. DISCUSSION

### A. The nonrelativistic energy

For $Z$-dependent perturbation theory to yield accurate nonrelativistic energies, the $\epsilon_n$ must be known with sufficient accuracy and through a sufficiently high order. In particular, $\epsilon_2$ must be known to high accuracy—indeed, for large $Z$, accurate values of $\epsilon_2$ and $\epsilon_3$ are enough to yield acceptable values of the nonrelativistic energy. Generally, the $\epsilon_n$ computed here and presented in Tables I–VI fulfill these requirements. Note particularly the agreement with the results of Blanchard,[16] where the $\epsilon_n$ for the $S$ and $P$ states are extracted from the accurate variational calculations of Accad *et al.*[4] The agreement is particularly striking for the $\epsilon_2$, but is also remarkably good for the higher-order coefficients, which have been computed here with more limited expansion sets for the $\psi_n$. Also included in the tables are the results of Aashamar *et al.*[17,18] for the $N=2$ and $3S$ and $P$ states and the results of Blanchard and Drake[6] for the $N=3$ for $4D$ states. These results are obtained via variational-perturbation wave functions of a complexity similar to that of the present $\psi_n$. Indeed the 2, $3^3S$ $\epsilon_n$, $n \geq 4$ of Ref. 17 are somewhat superior and the $3D$ $\epsilon_n$ of Ref. 6 clearly superior to those of the present study. The $4D$ results of Ref. 6 appear to be of similar accuracy to those of the present paper. Note that, generally, for the present results the $D$-state calculations are not of as high a quality as the $S$- and $P$-state calculations. Finally, the tables also include some $\epsilon_2$ computed nonvariationally by Ivanova *et al.*[19]

TABLE I. The $\epsilon_n$ in a.u. for the $N^1S$ states.[a]

| $n$ | $2^1S$ | $3^1S$ | $4^1S$ | $5^1S$ | $6^1S$ | $7^1S$ | $8^1S$ | $9^1S$ |
|---|---|---|---|---|---|---|---|---|
| 2 | −0.114 510 11 | −0.049 107 87 | −0.028 163 33 | −0.018 338 00 | −0.012 900 44 | −0.009 569 86 | −0.007 379 95 | −0.005 863 40 |
| | −0.114 510 15[b] | −0.049 061 36[c] | −0.028 156[b] | −0.018 334[b] | | | | |
| | −0.114 487 03[c] | −0.049 16[d] | −0.028 27[d] | −0.018 50[d] | | | | |
| | −0.114 50[d] | | | | | | | |
| 3 | 0.009 327 78 | −0.001 268 78 | −0.000 750 20 | −0.000 394 61 | −0.000 177 94 | −0.000 250 93 | −0.000 259 30 | −0.000 121 82 |
| | 0.009 328 0[b] | −0.000 944 33[c] | −0.000 84[b] | −0.000 47[b] | | | | |
| | 0.009 224 00[c] | | | | | | | |
| 4 | −0.001 283 61 | −0.001 448 29 | −0.000 845 18 | 0.000 229 50 | −0.000 227 54 | −0.000 136 09 | −0.000 164 76 | 0.001 941 98 |
| | −0.001 286[b] | −0.001 5[b] | −0.000 8[b] | −0.000 5[b] | | | | |
| | −0.001 084 86[c] | 0.000 249 81[c] | | | | | | |
| 5 | 0.006 202 11 | 0.005 433 45 | 0.004 443 93 | 0.007 925 95 | 0.001 452 99 | 0.000 368 93 | 0.000 686 80 | |
| | 0.006 2[b] | 0.005[b] | 0.002[b] | 0.001[b] | | | | |
| | 0.005 978 67[c] | 0.010 601 90[c] | | | | | | |
| 6 | −0.001 454 88 | 0.003 330 65 | | | | −0.000 095 19 | | |
| | −0.001 5[b] | 0.013 939 79[c] | | | | | | |
| | −0.001 327 80[c] | | | | | | | |
| 7 | −0.003 485 32 | 0.005 985 52 | | | | | | |
| | −0.005[b] | 0.018 265 91[c] | | | | | | |
| | −0.003 742 10[c] | | | | | | | |
| 8 | −0.000 911 64 | | | | | | | |
| | −0.001 999 19[c] | | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]P. Blanchard, Ref. 16.
[c]K. Aashamar, G. Lyslo, and J. Midtdal, Ref. 18.
[d]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE II. The $\epsilon_n$ in a.u. for the $N^3S$ states.[a]

| $n$ | $2^3S$ | $3^3S$ | $4^3S$ | $5^3S$ | $6^3S$ | $7^3S$ | $8^3S$ | $9^3S$ |
|---|---|---|---|---|---|---|---|---|
| 2 | −0.047 409 30 | −0.032 317 54 | −0.021 301 58 | −0.014 846 95 | −0.010 880 05 | −0.008 296 04 | −0.006 527 12 | −0.005 265 95 |
| | −0.047 409 30[b] | −0.032 317 54[c] | −0.021 301 54[d] | −0.014 846 86[d] | | | | |
| | −0.047 41[e] | −0.032 34[e] | −0.021 37[e] | −0.014 94[e] | | | | |
| 3 | −0.004 872 28 | −0.002 136 84 | −0.001 107 11 | −0.000 639 17 | −0.000 400 21 | −0.000 265 02 | −0.000 191 80 | −0.000 058 12 |
| | −0.004 872 28[b] | −0.002 136 86[c] | | | | | | |
| 4 | −0.003 457 57 | −0.001 517 98 | −0.000 720 11 | −0.000 391 95 | −0.000 233 51 | −0.000 145 90 | −0.000 077 12 | 0.001 718 77 |
| | −0.003 457 80[b] | −0.001 518 85[c] | −0.000 721[d] | −0.000 394[d] | | | | |
| 5 | −0.002 030 06 | −0.000 781 81 | −0.000 368 34 | −0.000 200 55 | −0.000 123 89 | −0.000 084 62 | 0.000 387 06 | |
| | −0.002 029 85[b] | −0.000 786 72[c] | −0.000 37[d] | −0.000 20[d] | | | | |
| 6 | −0.001 287 09 | −0.000 436 20 | −0.000 235 56 | −0.000 105 30 | −0.000 052 67 | 0.000 043 98 | | |
| | −0.001 287 13[b] | −0.000 465 63[c] | −0.000 2[d] | −0.000 1[d] | | | | |
| 7 | −0.000 871 45 | −0.000 129 39 | | −0.000 055 12 | −0.000 021 39 | | | |
| | −0.000 871 42[b] | −0.000 272 07[c] | | | | | | |
| 8 | −0.000 617 90 | 0.000 468 22 | | −0.000 005 18 | 0.000 186 22 | | | |
| | −0.000 618 23[b] | −0.000 175 08[c] | | | | | | |
| 9 | −0.000 454 12 | | | −0.000 335 66 | | | | |
| | −0.000 454 43[b] | | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]K. Aashamar, J. Midtdal, and G. Lyslo, Ref. 17(a).
[c]K. Aashamar, J. Midtdal, and G. Lyslo, Ref. 17(b).
[d]P. Blanchard, Ref. 16.
[e]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE III. The $\epsilon_n$ in a.u. for the $N^1P$ states.[a]

| $n$ | $2^1P$ | $3^1P$ | $4^1P$ | $5^1P$ | $6^1P$ | $7^1P$ | $8^1P$ | $9^1P$ |
|---|---|---|---|---|---|---|---|---|
| 2 | −0.157 028 66 | −0.060 752 36 | −0.032 981 98 | −0.020 788 93 | −0.014 315 01 | −0.010 457 05 | −0.007 970 10 | −0.006 268 64 |
| | −0.157 028 59[b] | −0.060 752 9[b] | −0.032 977[b] | −0.020 787[b] | | | | |
| | −0.157 021 50[c] | −0.060 725 67[c] | | | | | | |
| | −0.157 03[d] | −0.063 91[d] | | | | | | |
| 3 | 0.026 106 28 | −0.000 275 21 | −0.000 654 10 | −0.000 425 04 | −0.000 426 51 | −0.000 491 20 | −0.000 417 51 | −0.000 371 65 |
| | 0.026 059 59[c] | −0.000 257[b] | −0.000 73[b] | −0.000 48[b] | | | | |
| | | −0.000 094 28[c] | | | | | | |
| 4 | 0.005 788 76 | 0.004 219 06 | 0.001 549 06 | 0.004 503 35 | 0.002 887 10 | 0.002 070 01 | 0.000 402 37 | 0.000 142 70 |
| | 0.005 914 90[c] | 0.003 77[b] | 0.001 5[b] | 0.000 7[b] | | | | |
| | | 0.005 003 55[c] | | | | | | |
| 5 | −0.005 041 31 | 0.005 096 54 | 0.005 644 46 | −0.000 382 40 | 0.019 114 53 | 0.014 991 66 | 0.000 857 40 | 0.000 809 83 |
| | −0.005 242 15[c] | 0.006 9[b] | 0.003[b] | 0.002[b] | | | | |
| | | 0.008 791 65[c] | | | | | | |
| 6 | −0.007 066 59 | −0.005 012 94 | | −0.003 698 86 | | | −0.000 742 17 | 0.006 559 50 |
| | −0.006 889 44[c] | −0.010[b] | | | | | | |
| | | 0.004 363 84[c] | | | | | | |
| 7 | −0.001 259 46 | −0.004 680 79 | | −0.001 162 50 | | | −0.000 483 35 | |
| | −0.001 333 82[c] | 0.002[b] | | | | | | |
| | | 0.016 433 51[c] | | | | | | |
| 8 | 0.003 405 12 | | | | | | | |
| | 0.003 424 61[c] | | | | | | | |
| 9 | 0.001 920 93 | | | | | | | |
| | 0.001 953 97[c] | | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]P. Blanchard, Ref. 16.
[c]K. Aashamar, G. Lyslo, and J. Midtdal, Ref. 18.
[d]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE IV. The $\epsilon_n$ in a.u. for the $N^3P$ states.[a]

| $n$ | $2^3P$ | $3^3P$ | $4^3P$ | $5^3P$ | $6^3P$ | $7^3P$ | $8^3P$ | $9^3P$ |
|---|---|---|---|---|---|---|---|---|
| 2 | −0.072 998 98 | −0.041 856 34 | −0.025 644 55 | −0.017 163 25 | −0.012 255 72 | −0.009 177 52 | −0.007 123 63 | −0.005 686 23 |
| | −0.072 998 97[b] | −0.041 856 3[b] | −0.025 644 4[b] | −0.017 163 1[b] | | | | |
| | −0.072 996 75[c] | −0.041 836 63[c] | | | | | | |
| | −0.072 99[d] | −0.044 87[d] | | | | | | |
| 3 | −0.016 585 30 | −0.003 351 17 | −0.001 321 02 | −0.000 667 06 | −0.000 424 41 | −0.000 302 36 | −0.000 239 89 | −0.000 209 86 |
| | −0.016 594 32[c] | −0.003 352[b] | −0.001 323[b] | −0.000 670[b] | | | | |
| | | −0.003 217 65[c] | | | | | | |
| 4 | −0.010 353 09 | −0.002 710 13 | −0.001 010 74 | −0.000 233 99 | 0.000 168 45 | 0.000 806 99 | 0.000 533 94 | 0.000 074 08 |
| | −0.010 339 61[c] | −0.002 72[b] | −0.001 05[b] | −0.000 51[b] | | | | |
| | | −0.002 110 62[c] | | | | | | |
| 5 | −0.005 424 84 | −0.001 497 37 | −0.000 261 71 | 0.001 839 29 | 0.003 090 77 | 0.009 681 05 | 0.005 434 81 | 0.002 882 99 |
| | −0.005 436 13[c] | −0.001 5[b] | −0.000 6[b] | −0.000 3[b] | | | | |
| | | 0.000 550 89[c] | | | | | | |
| 6 | −0.002 020 80 | −0.000 738 41 | 0.001 999 45 | | | | | |
| | −0.002 017 02[c] | −0.000 8[b] | −0.000 4[b] | | | | | |
| | | 0.004 736 45[c] | | | | | | |
| 7 | 0.000 238 27 | −0.000 286 75 | | | | | | |
| | 0.000 236 49[c] | 0.011 852 75[c] | | | | | | |
| 8 | 0.001 610 32 | 0.004 847 30 | | | | | | |
| | 0.001 612 29[c] | 0.021 822 11[c] | | | | | | |
| 9 | 0.002 269 62 | 0.002 946 20 | | | | | | |
| | 0.002 278 54[c] | 0.030 264 80[c] | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]P. Blanchard, Ref. 16.
[c]K. Aashamar, G. Lyslo, and J. Midtdal, Ref. 18.
[d]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE V. The $\epsilon_n$ in a.u. for the $N^1D$ states.[a]

| $n$ | $3^1D$ | $4^1D$ | $5^1D$ | $6^1D$ | $7^1D$ | $8^1D$ | $9^1D$ |
|---|---|---|---|---|---|---|---|
| 2 | −0.057 387 77 | −0.032 110 73 | −0.020 455 82 | −0.014 155 71 | −0.010 371 24 | −0.007 921 53 | −0.006 244 52 |
| | −0.057 482 2[b] | −0.032 121 6[b] | | | | | |
| | −0.057 31[c] | | | | | | |
| 3 | 0.005 538 59 | 0.002 486 95 | 0.001 308 43 | 0.000 852 70 | 0.000 674 28 | 0.000 083 74 | 0.000 032 03 |
| | 0.005 974 4[b] | 0.002 444 71[b] | | | | | |
| 4 | −0.008 121 58[b] | −0.002 882 32 | −0.001 224 59 | 0.000 190 03 | 0.001 559 31 | 0.000 145 14 | 0.000 057 84 |
| | | −0.002 636 34[b] | | | | | |
| 5 | 0.005 564 48[b] | 0.002 445 71 | 0.002 327 04 | 0.006 076 91 | | −0.000 234 54 | −0.000 037 85 |
| | | 0.000 644 30[b] | | | | | |
| 6 | −0.002 318 28[b] | 0.002 134 41 | | | | | |
| | | 0.001 025 81[b] | | | | | |
| 7 | 0.000 816 29[b] | | | | | | |
| 8 | 0.000 145 93[b] | | | | | | |
| 9 | −0.000 664 68[b] | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]P. Blanchard and G. W. F. Drake, Ref. 6.
[c]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE VI. The $\epsilon_n$ in a.u. for the $N^3D$ states.[a]

| $n$ | $3^3D$ | $4^3D$ | $5^3D$ | $6^3D$ | $7^3D$ | $8^3D$ | $9^3D$ |
|---|---|---|---|---|---|---|---|
| 2 | −0.054 615 28 | −0.030 684 33 | −0.019 675 45 | −0.013 691 03 | −0.010 075 30 | −0.007 723 88 | −0.006 108 03 |
| | −0.054 619 3[b] | −0.030 671 37[b] | | | | | |
| | −0.054 59[c] | | | | | | |
| 3 | −0.000 724 88 | −0.000 567 16 | −0.000 337 24 | −0.000 199 89 | −0.000 105 24 | −0.000 173 68 | −0.000 138 33 |
| | −0.000 731 80[b] | −0.000 666 06[b] | | | | | |
| 4 | 0.000 073 74[b] | 0.000 141 74 | 0.000 087 83 | 0.000 090 04 | 0.000 401 74 | 0.000 169 72 | 0.000 155 23 |
| | | 0.000 439 07[b] | | | | | |
| 5 | −0.000 087 86[b] | 0.000 088 86 | 0.000 085 30 | 0.000 340 35 | | 0.000 001 30 | 0.000 178 41 |
| | | −0.000 343 91[b] | | | | | |
| 6 | 0.000 177 09[b] | −0.000 043 03 | 0.000 102 26 | | | | |
| | | −0.000 392 42[b] | | | | | |
| 7 | 0.000 069 71[b] | 0.000 095 09 | | | | | |
| | | 0.001 828 46[b] | | | | | |
| 8 | −0.000 294 96[b] | | | | | | |
| 9 | 0.000 098 88[b] | | | | | | |

[a]The first line in each entry of the table is from the present study. Additional lines are from earlier theoretical studies.
[b]P. Blanchard and G. W. F. Drake, Ref. 6.
[c]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Ref. 19.

TABLE VII. $T_{rel}/\alpha^2$ in a.u. for some $S$ states.[a]

| $Z$ | $2^1S$ | $3^1S$ | $4^1S$ | $5^1S$ | $2^3S$ | $3^3S$ | $4^3S$ | $5^3S$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 1.448 69 | 1.464 65 | 1.470 73 | 1.473 21 | 1.274 31 | 1.422 36 | 1.454 68 | 1.465 52 |
| | 1.441 82 | 1.464 11 | 1.470 68 | 1.473 20 | 1.311 64 | 1.431 02 | 1.457 82 | 1.466 97 |
| 3 | 3.609 75 | 3.933 37 | 4.041 86 | 4.085 20 | 2.590 90 | 3.672 68 | 3.940 04 | 4.035 51 |
| | 3.578 02 | 3.935 58 | 4.044 40 | 4.086 83 | 2.690 42 | 3.697 34 | 3.949 26 | 4.039 83 |
| 4 | 10.364 61 | 12.130 09 | 12.699 34 | 12.925 06 | 7.273 35 | 11.324 71 | 12.381 60 | 12.769 04 |
| | 10.294 30 | 12.142 04 | 12.708 51 | 12.930 45 | 7.463 1 | 11.373 01 | 12.399 88 | 12.777 65 |
| 5 | 27.066 77 | 32.855 03 | 34.686 35 | 35.409 90 | 20.119 91 | 31.028 81 | 33.962 23 | 35.053 18 |
| | 26.945 4 | 32.884 23 | 34.706 30 | 35.421 01 | 20.428 0 | 31.108 39 | 33.992 55 | 35.067 53 |
| 6 | 61.133 09 | 75.575 88 | 80.094 59 | 81.876 03 | 47.992 17 | 72.102 87 | 78.713 31 | 81.194 29 |
| | 60.948 4 | 75.629 92 | 80.129 39 | 81.894 7 | 48.446 6 | 72.221 40 | 78.758 65 | 81.215 81 |
| 7 | 122.043 18 | 152.427 27 | 161.863 65 | 165.578 46 | 99.814 48 | 146.531 69 | 159.514 11 | 164.417 33 |
| | 121.782 9 | 152.513 67 | 161.917 28 | 165.606 3 | 100.443 4 | 146.696 82 | 159.577 46 | 164.447 48 |
| 8 | 221.339 22 | 278.210 59 | 295.780 88 | 302.690 65 | 186.573 78 | 268.966 80 | 292.091 64 | 300.865 77 |
| | 220.991 4 | 278.336 9 | 295.857 3 | 302.729 3 | 187.405 3 | 269.186 23 | 292.176 01 | 300.906 01 |
| 9 | 372.625 95 | 470.393 92 | 500.481 30 | 512.304 51 | 321.319 54 | 456.726 48 | 495.020 63 | 509.601 53 |
| | 372.178 4 | 470.567 5 | 500.584 3 | 512.355 3 | 322.381 7 | 457.007 89 | 495.129 0 | 509.653 32 |
| 10 | 591.570 63 | 749.112 03 | 797.447 62 | 816.430 37 | 519.163 75 | 729.795 65 | 789.723 46 | 812.604 94 |
| | 591.011 2 | 749.340 3 | 797.581 1 | 816.494 6 | 520.484 7 | 730.146 75 | 789.858 9 | 812.669 75 |

[a]For each entry, the first line is the result obtained in the present paper. The second line is from Accad *et al.*, Ref. 4.

### B. The relativistic correction

The relativistic correction as applied here via Eq. (11) is in error by terms of order $Z^2$. Thus, the relative error should decrease as $Z^{-2}$. For low $Z$, the total relativistic correction itself is rather small, $\sim 100$ cm$^{-1}$ for $Z=4$, the error being a few cm$^{-1}$, at most. In contrast, the nonrelativistic transition energy for $Z=4$ is $\sim 10^6$ cm$^{-1}$ with an error of at most a few cm$^{-1}$. For larger values of $Z$, then, the accuracy of the nonrelativistic transition energy will increase and the error in the relativistic correction will determine the overall accuracy of the calculation. The present relativistic correction is compared with the earlier calculations of Accad *et al.*[4] in Tables VII and VIII. Unfortunately, the tables indicate that the relative difference between the present results and those of Ref. 4 decreases roughly as $Z^{-1}$ for the $^3S$ states, or remains roughly constant for the $^1S$ and $^{1,3}P$ states. This holds true for all states ($N=2$ to 5) of a particular symmetry, although the relative difference drops by about a factor of 10 from $N=2$ to $N=5$. It appears that the variational data of Ref. 4 have an error which is growing more rapidly than that of the $Z$-dependent data, i.e., more rapidly than $Z^2$. Thus, the accuracy of the present method is indicated only by a comparison of the $Z=2$ data, for example, where the variational calculations are surely of high accuracy. From that point the relative error must necessarily be decreasing as $Z^{-2}$. It is also not possible to make useful comparisons with the high-$Z$ extrapolations of Ermolaev and Jones,[15] since these are extrapolations based on the calculations of Accad *et al.*,[3] and display similar behavior.

### C. Lamb shift

The Lamb-shift contribution to the transition energies must be included in the present calculations since, even for low values of $Z$, this contribution is of greater magnitude than the error introduced by the approximations leading to Eq. (11) for the rela-

TABLE VIII. $T_{rel}/\alpha^2$ in a.u. for some $P$ states.[a]

| $Z$ | $2^1P$ | $3^1P$ | $4^1P$ | $5^1P$ | $2^3P$ | $3^3P$ | $4^3P$ | $5^3P$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 1.463 84 | 1.470 48 | 1.473 26 | 1.474 49 | 1.450 03 | 1.464 50 | 1.470 62 | 1.473 17 |
| | 1.436 09 | 1.461 27 | 1.469 16 | 1.472 2 | 1.503 04 | 1.480 96 | 1.477 62 | 1.476 79 |
| 3 | 3.895 01 | 4.029 64 | 4.083 10 | 4.106 09 | 3.785 18 | 3.983 25 | 4.062 58 | 4.095 89 |
| | 3.653 19 | 3.955 01 | 4.051 35 | 4.090 33 | 4.005 68 | 4.045 33 | 4.088 07 | 4.108 29 |
| 4 | 11.886 79 | 12.622 01 | 12.909 00 | 13.031 61 | 11.516 52 | 12.466 88 | 12.840 39 | 12.997 51 |
| | 11.079 58 | 12.382 42 | 12.808 98 | 12.983 1 | 11.775 20 | 12.526 64 | 12.863 1 | 13.007 1 |
| 5 | 32.004 56 | 34.416 53 | 35.350 17 | 35.747 84 | 31.127 20 | 34.050 41 | 35.188 29 | 35.667 36 |
| | 30.129 96 | 33.874 20 | 35.125 9 | 35.639 6 | 30.803 71 | 33.910 96 | 35.123 8 | 35.630 1 |
| 6 | 73.377 05 | 79.397 78 | 81.716 86 | 82.702 81 | 71.663 73 | 78.684 54 | 81.401 53 | 82.546 04 |
| | 69.785 34 | 78.377 18 | 81.297 0 | 82.500 | 69.398 27 | 77.926 40 | 81.071 2 | 82.369 |
| 7 | 147.695 73 | 160.365 42 | 165.229 69 | 167.295 20 | 144.735 34 | 159.135 01 | 164.685 78 | 167.024 78 |
| | 141.590 25 | 158.653 3 | 164.528 | 166.957 | 138.178 99 | 157.042 1 | 163.785 5 | 166.552 |
| 8 | 269.214 65 | 292.934 00 | 302.019 53 | 305.874 18 | 264.513 88 | 290.982 49 | 301.156 93 | 305.445 29 |
| | 258.652 14 | 290.279 5 | 300.934 | 305.351 | 250.078 70 | 286.468 0 | 299.226 | 304.439 |
| 9 | 454.750 43 | 495.532 94 | 511.127 46 | 517.739 38 | 447.733 72 | 492.622 49 | 509.841 07 | 517.099 75 |
| | 440.641 1 | 491.647 3 | 509.542 | 516.975 | 420.342 78 | 484.155 0 | 506.681 | 515.227 |
| 10 | 723.682 17 | 789.406 48 | 814.504 73 | 825.140 80 | 713.691 76 | 785.265 35 | 812.674 48 | 824.230 74 |
| | 703.789 9 | 783.963 5 | 812.287 | 824.071 | 666.529 15 | 770.794 5 | 806.517 | 821.045 |

[a]For each entry, the first line is the result obtained in the present paper. The second line is from Accad *et al.*, Ref. 4.

TABLE IX. Transition energies in $cm^{-1}$ for the $N^1S$ states.[a]

| $Z$ | $2^1S$ | $3^1S$ | $4^1S$ | $5^1S$ | $6^1S$ | $7^1S$ | $8^1S$ | $9^1S$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 166 281.0 | 184 882.4 | 191 002.5 | 193 642.1 | 195 142.2 | 195 970.3 | 196 471.8 | 196 822.0 |
| | 166 277.6[b] | 184 864.9[b] | 190 940.3[b] | 193 663.6[b] | 195 115.0[b] | 195 979.0[b] | 196 534.9[b] | 196 913.0[b] |
| 3 | 491 376 | 558 783 | 581 619 | 591 993 | 597 595 | 600 926 | 603 070 | 604 538 |
| | (490 079)[c] | 558 779[c] | 581 590[c] | 591 984[c] | 597 574[c] | 600 925[c] | | |
| 4 | 981 198 | 1 127 721 | 1 177 952 | 1 200 950 | 1 213 367 | 1 220 808 | 1 225 618 | 1 228 912 |
| | 981 177[d] | 1 127 705[d] | 1 177 945[e] | | | | | |
| 5 | 1 635 745 | 1 891 817 | 1 980 125 | 2 020 679 | 2 042 603 | 2 055 769 | 2 064 290 | 2 070 127 |
| | 1 635 714[f] | 1 891 784[f] | | | | | | |
| 6 | 2 455 078 | 2 851 192 | 2 988 265 | 3 051 318 | 3 085 436 | 3 105 946 | 3 119 225 | 3 128 324 |
| | 2 455 024[g] | (2 851 180)[g] | | | | | | |
| 7 | 3 439 311 | 4 006 010 | 4 202 542 | 4 293 043 | 4 342 043 | 4 371 516 | 4 390 602 | 4 403 685 |
| 8 | 4 588 562 | 5 356 432 | 5 623 131 | 5 746 032 | 5 812 603 | 5 852 660 | 5 878 604 | 5 896 391 |
| | 4 587 340[h] | 5 356 420[h] | | | | | | |
| 9 | 5 902 992 | 6 902 671 | 7 250 256 | 7 410 516 | 7 497 351 | 7 549 614 | 7 583 466 | 7 606 679 |
| | | 6 903 580[i] | | | | | | |
| 10 | 7 382 751 | 8 644 927 | 9 084 132 | 9 286 713 | 9 396 507 | 9 462 600 | 9 505 410 | 9 534 772 |

TABLE IX. (*Continued.*)

| $Z$ | $2^1S$ | $3^1S$ | $4^1S$ | $5^1S$ | $6^1S$ | $7^1S$ | $8^1S$ | $9^1S$ |
|---|---|---|---|---|---|---|---|---|
| 11 | 9028074 | 10583499 | 11125077 | 11374953 | 11510402 | 11591951 | 11644772 | 11681006 |
| | (9027981)[j] | (10583431)[j] | (11124986)[j] | (11374868)[j] | (11510320)[j] | (11591874)[j] | (11644747)[j] | (11680966)[j] |
| 12 | 10839156 | 12718647 | 13373369 | 13675516 | 13839323 | 13937954 | 14001839 | 14045668 |
| | (10839030)[k] | (12718550)[k] | (13373240)[k] | (13675400)[k] | | | | |
| 13 | 12816278 | 15050727 | 15829389 | 16188796 | 16383666 | 16501008 | 16577011 | 16629161 |
| | (12816130)[l] | (15050610)[l] | (15829230)[l] | (16188660)[l] | | | | |
| 14 | 14959688 | 17580065 | 18493483 | 18915145 | 19143788 | 19281474 | 19370649 | 19431846 |
| 15 | 17269724 | 20307090 | 21366110 | 21855035 | 22120165 | 22279830 | 22383233 | 22454203 |
| 16 | 19746675 | 23232183 | 24447676 | 25008882 | 25313218 | 25496498 | 25615186 | 25696658 |
| 17 | 22390939 | 26355848 | 27738719 | 28377236 | 28723505 | 28932041 | 29067073 | 29159775 |
| 18 | 25202881 | 29678559 | 31239743 | 31960615 | 32351548 | 32586982 | 32739419 | 32844081 |
| 19 | 28182847 | 33200766 | 34951232 | 35759513 | 36197846 | 36461825 | 36632728 | 36750081 |
| 20 | 31331335 | 36923102 | 38873859 | 39774620 | 40263099 | 40557272 | 40747706 | 40878483 |
| | (31330780)[m] | (36922600)[m] | (38873200)[m] | | | | | |
| 21 | 34648828 | 40846186 | 43008282 | 44006611 | 44547987 | 44874009 | 45085039 | 45229974 |
| 22 | 38135748 | 44970567 | 47355089 | 48456087 | 49053119 | 49412647 | 49645341 | 49805169 |
| | (38135000)[n] | (44969900)[n] | (47354200)[n] | | | | | |
| 23 | 41792626 | 49296925 | 51915005 | 53123791 | 53779246 | 54173943 | 54429370 | 54604829 |
| | (41791780)[o] | (49296140)[o] | (51913970)[o] | | | | | |
| 24 | 45619980 | 53825926 | 56688740 | 58010451 | 58727104 | 59158635 | 59437868 | 59629696 |
| 25 | 49618409 | 58558336 | 61677109 | 63116902 | 63897536 | 64367573 | 64671686 | 64880624 |
| | (49617300)[p] | (58557300)[p] | (61675800)[p] | | | | | |
| 26 | 53788464 | 63494866 | 66880873 | 68443921 | 69291331 | 69801549 | 70131618 | 70358409 |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.

[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).

[c]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stds. (U.S.) Circ. No. 467 (U.S. GPO, Washington D.C., 1949).

[d]B. Löfstrand, Ref. 20.

[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).

[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).

[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3.

[h]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.

[i]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).

[j]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).

[k]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).

[l]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 8, 817 (1979).

[m]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 8, 865 (1979).

[n]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 8, 1 (1979).

[o]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 7, 1191 (1978).

[p]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 6, 1253 (1977).

TABLE X. Transition energies in $cm^{-1}$ for the $N^3S$ states.[a]

| $Z$ | $2^3S$ | $3^3S$ | $4^3S$ | $5^3S$ | $6^3S$ | $7^3S$ | $8^3S$ | $9^3S$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 159 855.8<br>159 856.1[b] | 183 236.5<br>183 236.9[b] | 190 295.3<br>190 298.2[b] | 193 347.0<br>193 347.1[b] | 194 935.5<br>194 936.2[b] | 195 866.4<br>195 868.4[b] | 196 379.2<br>196.461.4[b] | 196 786.7<br>196 862.0[b] |
| 3 | 476 034<br>476 046[c] | 554 754<br>554 761[c] | 579 981<br>579 982[c] | 591 185<br>591 184[c] | 597 122<br>597 122[c] | 600 644<br>600 641[c] | 602 873 | 604 414 |
| 4 | 956 518<br>956 502[d] | 1 121 200<br>1 121 184[d] | 1 175 313<br>1 175 295[d] | 1 199 629<br>1 199 659[e] | 1 212 608 | 1 220 343 | 1 225 304 | 1 228 700 |
| 5 | 1 601 566<br>1 601 540[f] | 1 882 772<br>1 882 746[f] | 1 976 465<br>1 976 436[f] | 2 018 844 | 2 041 552 | 2 055 119 | 2 063 855 | 2 069 827 |
| 6 | 2 411 309<br>2 411 262[g] | 2 839 608<br>2 839 562[g] | 2 983 576<br>(2 983 541)[g] | 3 048 965<br>(3 048 927)[g] | 3 084 089<br>(3 084 048)[g] | 3 105 109<br>(3 105 066)[g] | 3 118 668<br>(3 118 635)[g] | 3 127 938 |
| 7 | 3 385 882<br>3 385 890[h] | 3 991 872 | 4 196 818 | 4 290 170 | 4 340 398 | 4 370 492 | 4 389 922 | 4 403 211 |
| 8 | 4 525 412<br>4 524 640[i] | 5 339 729<br>5 338 820[i] | 5 616 366<br>5 616 100[i] | 5 742 636 | 5 810 660 | 5 851 449 | 5 877 800 | 5 895 830 |
| 9 | 5 830 061<br>5 830 600[j] | 6 883 388<br>6 883 220[k] | 7 242 446<br>7 242 400[k] | 7 406 594 | 7 495 107 | 7 548 214 | 7 582 539 | 7 606 031 |
| 10 | 7 299 976<br>7 300 900[l] | 8 623 048 | 9 075 269 | 9 282 263 | 9 393 959 | 9 461 009 | 9 504 360 | 9 534 037 |
| 11 | 8 935 388<br>(8 935 337)[m] | 10 559 009<br>(10 558 946)[m] | 11 115 156<br>(11 115 065)[m] | 11 369 970<br>(11 369 887)[m] | 11 507 550<br>(11 507 469)[m] | 11 590 169<br>(11 590 091)[m] | 11 643 598<br>(11 643 558)[m] | 11 680 184<br>(11 680 134)[m] |
| 12 | 10 736 488<br>10 730 000[l] | 12 691 526<br>(12 691 440)[n] | 13 362 381<br>(13 362 260)[n] | 13 669 997<br>(13 669 880)[n] | 13 836 164 | 13 935 980 | 14 000 541 | 14 044 760 |
| 13 | 12 703 551<br>(12 703 460)[o] | 15 020 957<br>(15 020 850)[o] | 15 817 327<br>(15 817 170)[o] | 16 182 737<br>(16 182 600)[o] | 16 380 198 | 16 498 841 | 16 575 589 | 16 628 167 |
| 14 | 14 836 821<br>14 840 000[p] | 17 547 624 | 18 480 338 | 18 908 542 | 19 140 009 | 19 279 111 | 19 369 104 | 19 430 764 |
| 15 | 17 136 627 | 20 271 954 | 21 351 873 | 21 847 884 | 22 116 072 | 22 277 270 | 22 381 564 | 22 453 035 |
| 16 | 19 603 255<br>19 210 000[p] | 23 194 327 | 24 432 336 | 25 001 176 | 25 308 808 | 25 493 740 | 25 613 394 | 25 695 403 |
| 17 | 22 237 095 | 26 315 246 | 27 722 266 | 28 368 971 | 28 718 776 | 28 929 082 | 29 065 157 | 29 158 433 |
| 18 | 25 038 507<br>25 030 000[p] | 29 635 182 | 31 222 166 | 31 951 785 | 32 346 495 | 32 583 820 | 32 737 379 | 32 842 652 |
| 19 | 28 007 830 | 33 154 584 | 34 932 518 | 35 750 112 | 36 192 467 | 36 458 459 | 36 630 564 | 36 748 566 |
| 20 | 31 145 557<br>31 180 000[p] | 36 874 084<br>(36 873 600)[q] | 38 853 995<br>(38 853 340)[q] | 39 764 642 | 40 257 390 | 40 553 699 | 40 745 418 | 40 876 880 |
| 21 | 34 452 161 | 40 794 297 | 42 987 255 | 43 996 048 | 44 541 944 | 44 870 227 | 45 082 627 | 45 228 285 |

TABLE X. (*Continued.*)

| Z | $2^3S$ | $3^3S$ | $4^3S$ | $5^3S$ | $6^3S$ | $7^3S$ | $8^3S$ | $9^3S$ |
|---|---|---|---|---|---|---|---|---|
| 22 | 37 928 062<br>(37 927 500)[r] | 44 915 772<br>(44 915 100)[r] | 47 332 885<br>(47 332 000)[r] | 48 444 933 | 49 046 739 | 49 408 654 | 49 642 806 | 49 803 394 |
| 23 | 41 573 783<br>(41 573 150)[s] | 49 239 187<br>(49 238 420)[s] | 51 891 609<br>(51 890 590)[s] | 53 112 039 | 53 772 525 | 54 169 735 | 54 426 711 | 54 602 967 |
| 24 | 45 389 835 | 53 765 207 | 56 664 136 | 57 998 093 | 58 720 037 | 59 154 210 | 59 435 086 | 59 627 748 |
| 25 | 49 376 810<br>(49 376 000)[t] | 58 494 594<br>(58 493 600)[t] | 61 651 281<br>(61 650 000)[t] | 63 103 929 | 63 890 119 | 64 362 928 | 64 668 780 | 64 878 589 |
| 26 | 53 535 254<br>53 604 000[p] | 63 428 060 | 66 853 804 | 68 430 325 | 69 283 558 | 69 796 681 | 70 128 588 | 70 356 286 |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.

[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).

[c]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stds. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1949).

[d]B. Löfstrand, Ref. 20.

[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).

[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).

[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3.

[h]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1971), Vol. 3, Sec. 4.

[i]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data. Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.

[j]N. J. Peacock, M. G. Hobby, and M. Galanti, J. Phys. B 6, L298 (1973).

[k]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).

[l]J. H. Parkinson, Solar Phys. 42, 183 (1975).

[m]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).

[n]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).

[o]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 8, 817 (1979).

[p]W. M. Neupert, Solar Phys. 18, 474 (1971).

[q]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 8, 865 (1979).

[r]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 8, 1 (1979).

[s]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 7, 1191 (1978).

[t]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 6, 1253 (1977).

TABLE XI. Transition energies in $cm^{-1}$ for the $N\,^1P$ states.[a]

| Z | $2^1P$ | $3^1P$ | $4^1P$ | $5^1P$ | $6^1P$ | $7^1P$ | $8^1P$ | $9^1P$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 171 134.4<br>171 135.0[b] | 186 233.5<br>186 209.5[b] | 191 423.4<br>191 492.8[b] | 194 093.4<br>193 942.6[b] | 195 344.8<br>195 275.0[b] | 196 099.9<br>196 079.2[b] | 196 469.5<br>196 601.5[b] | 196 835.0<br>196 959.8[b] |
| 3 | 501 807<br>501 810[c] | 561 759<br>561 730[c] | 582 813<br>582 820[c] | 592 695<br>592 660[c] | 597 979<br>597 940[c] | 601 167<br>601 180[c] | 603 188<br>603 281[c] | 604 625<br>604 704[c] |
| 4 | 997 474<br>997 466[e] | 1 132 411<br>1 132 390[d] | 1 179 890<br>1 179 830[d] | 1 201 986<br>1 201 894[d] | 1 213 954<br>1 213 931[d] | 1 221 176<br>1 221 135[d] | 1 225 840 | 1 229 069 |
| 5 | 1 658 012<br>1 657 975[f] | 1 898 259<br>1 898 230[f] | 1 982 807<br>1 982 761[f] | 2 022 076<br>2 022 044[f] | 2 043 401<br>2 043 360[f] | 2 056 270 | 2 064 610 | 2 070 352 |
| 6 | 2 483 443<br>2 483 371[g] | 2 859 416<br>2 859 375[g] | 2 991 698<br>2 991 710[g] | 3 053 088<br>3 053 044[g] | 3 086 452<br>3 086 439[g] | 3 106 584<br>(3 106 541)[g] | 3 119 643<br>(3 119 619)[g] | 3 128 618 |

TABLE XI. (*Continued.*)

| $Z$ | $2^1P$ | $3^1P$ | $4^1P$ | $5^1P$ | $6^1P$ | $7^1P$ | $8^1P$ | $9^1P$ |
|---|---|---|---|---|---|---|---|---|
| 7 | 3 473 877<br>3 473 790[h] | 4 016 042<br>4 016 390[h] | 4 206 735<br>4 206 810[h] | 4 295 195<br>4 296 100[i] | 4 343 280<br>4 343 300[i] | 4 372 293<br>4 372 500[i] | 4 391 118<br>4 392 700[i] | 4 404 047 |
| 8 | 4 629 450<br>4 629 200[j] | 5 368 306<br>5 368 550[j] | 5 628 097<br>5 628 100[j] | 5 748 574<br>5 748 450[j] | 5 814 067<br>5 813 950[j] | 5 853 580<br>5 852 740[j] | 5 879 220 | 5 896 823 |
| 9 | 5 950 352<br>5 950 900[k] | 6 916 431<br>6 915 600[k] | 7 256 013<br>7 255 800[i] | 7 413 459<br>7 411 800[i] | 7 499 047<br>7 498 500[i] | 7 550 680<br>7 546 000[i] | 7 584 184<br>7 587 200[i] | 7 607 183 |
| 10 | 7 436 768<br>7 437 700[l] | 8 660 626<br>8 660 300[l] | 9 090 701<br>9 071 900[l] | 9 290 070<br>9 313 600[l] | 9 398 441 | 9 463 815 | 9 506 233 | 9 535 350 |
| 11 | 9 088 979<br>9 087 600[m] | 10 601 207<br>10 610 000[m] | 11 132 489<br>(11 132 393)[n] | 11 378 737<br>(11 378 646)[n] | 11 512 584<br>(11 512 505)[n] | 11 593 322<br>(11 593 248)[n] | 11 645 705<br>(11 645 667)[n] | 11 681 661<br>(11 681 612)[n] |
| 12 | 10 907 233<br>10 907 000[m] | 12 738 446<br>12 738 000[m] | 13 381 658<br>13 381 000[m] | 13 679 748<br>13 681 000[m] | 13 841 763<br>13 840 000[m] | 13 939 488<br>(13 939 380)[o] | 14 002 886<br>(14 003 830)[o] | 14 046 404<br>(14 046 330)[o] |
| 13 | 12 891 870<br>12 891 900[m] | 15 072 721<br>15 072 700[m] | 15 838 598<br>15 838 600[m] | 16 193 496<br>16 196 000[m] | 16 386 377<br>16 392 000[m] | 16 502 713<br>16 504 000[m] | 16 578 180<br>16 585 000[m] | 16 629 982<br>16 640 000[m] |
| 14 | 15 043 201<br>15 040 000[m] | 17 604 374<br>17 603 000[m] | 18 503 663<br>18 503 000[m] | 18 920 341<br>18 921 000[m] | 19 146 785 | 19 283 359 | 19 371 947 | 19 432 757 |
| 15 | 17 361 637<br>17 364 000[m] | 20 333 858<br>20 333 000[m] | 21 377 321<br>21 370 000[m] | 21 860 757<br>21 856 000[m] | 22 123 466<br>22 120 000[m] | 22 281 906<br>22 300 000[m] | 22 384 668 | 22 455 211 |
| 16 | 19 847 545<br>19 852 000[m] | 23 261 575<br>23 258 000[m] | 24 459 988<br>24 456 000[m] | 25 015 165<br>25 010 000[m] | 25 316 844<br>25 320 000[m] | 25 498 778 | 25 616 769 | 25 697 770 |
| 17 | 22 501 407<br>22 503 000[m] | 26 388 056<br>26 399 000[m] | 27 752 214 | 28 384 123 | 28 727 480 | 28 934 540 | 29 068 815 | 29 160 998 |
| 18 | 25 323 677<br>25 320 000[p] | 29 713 799<br>29 860 000[p] | 31 254 512 | 31 968 152 | 32 355 898 | 32 589 718 | 32 741 333 | 32 845 425 |
| 19 | 28 314 796<br>28 321 000[m] | 33 239 286 | 34 967 379 | 35 767 753 | 36 202 603 | 36 464 816 | 36 634 828 | 36 751 556 |
| 20 | 31 475 368<br>31 480 000[m] | 36 965 179<br>36 990 000[p] | 38 891 500<br>38 880 000[p] | 39 783 623 | 40 268 297 | 40 560 541 | 40 750 009 | 40 880 100 |
| 21 | 34 805 980<br>34 823 000[m] | 40 892 127 | 43 027 548 | 44 016 444 | 44 553 664 | 44 877 580 | 45 087 562 | 45 231 746 |
| 22 | 38 307 172<br>38 313 000[m] | 45 020 716<br>(45 021 900)[q] | 47 376 125<br>(47 376 200)[q] | 48 466 824 | 49 059 319 | 49 416 547 | 49 648 105 | 49 807 111 |
| 23 | 41 979 595<br>41 976 000[m] | 49 351 661<br>(49 353 420)[r] | 51 937 971<br>(51 938 260)[r] | 53 135 514 | 53 786 016 | 54 178 201 | 54 432 397 | 54 606 955 |
| 24 | 45 823 893<br>45 890 000[s] | 53 885 665 | 56 713 811 | 58 023 250 | 58 734 496 | 59 163 285 | 59 441 182 | 59 632 024 |

TABLE XI. (*Continued.*)

| Z | $2^1P$ | $3^1P$ | $4^1P$ | $5^1P$ | $6^1P$ | $7^1P$ | $8^1P$ | $9^1P$ |
|---|---|---|---|---|---|---|---|---|
| 25 | 49 840 798 | 58 623 534 | 61 704 478 | 63 130 875 | 63 905 607 | 64 372 651 | 64 675 313 | 64 883 171 |
| | (49 853 100)[t] | (58 627 100)[t] | (61 705 400)[t] | | | | | |
| 26 | 54 031 001 | 63 566 021 | 66 910 750 | 68 459 176 | 69 300 142 | 69 807 092 | 70 135 587 | 70 361 195 |
| | 54 039 000[p] | 63 810 000[p] | 66 260 000[p] | | | | | |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.

[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).
[c]A. M. Cantu, W. H. Parkinson, G. Tondello, and G. P. Tozzi, J. Opt. Soc. Am. 67, 1030 (1977).
[d]B. Löfstrand, Ref. 20.
[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).
[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).
[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3.
[h]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1971), Vol. 3, Sec. 4.
[i]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).
[j] C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.
[k]N. J. Peacock, M. G. Hobby, and M. Galanti, J. Phys. B 6, L298 (1973).
[l]J. H. Parkinson, Solar Phys. 42, 183 (1975).
[m]V. A. Boiko, A. Ya. Faenov, and S. A. Pikuz, J. Quant. Spectrosc. Radiat. Transfer 19, 11 (1978).
[n]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).
[o]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).
[p]W. M. Neupert, Solar Phys. 18, 474 (1971).
[q]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 8, 1 (1979).
[r]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 7, 1191 (1978).
[s]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 6, 317 (1977).
[t]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 6, 1253 (1977).

TABLE XII. Transition energies in $cm^{-1}$ for the $N^3P$ states.[a]

| Z | $2^3P$ | $3^3P$ | $4^3P$ | $5^3P$ | $6^3P$ | $7^3P$ | $8^3P$ | $9^3P$ |
|---|---|---|---|---|---|---|---|---|
| 2 | 169 088.6 | 185 564.0 | 191 222.4 | 193 787.2 | 195 180.0 | 196 039.1 | 196 557.2 | 196 843.5 |
| | 169 087.0[b] | 185 564.7[b] | 191 217.1[b] | 193 800.8[b] | 195 192.9[b] | 196 027.4[b] | 196 566.8[b] | 196 935.4[b] |
| 3 | 494 264 | 559 502 | 581 889 | 592 134 | 597 663 | 600 992 | 603 128 | 604 559 |
| | 494 273[c] | 559 501[c] | 581 897[c] | 592 141[c] | 597 666[c] | | | |
| 4 | 983 380 | 1 128 316 | 1 178 193 | 1 201 072 | 1 213 433 | 1 220 864 | 1 225 663 | 1 228 931 |
| | 983 365[d] | 1 128 300[d] | 1 178 174[d] | 1 201 066[e] | | | | |
| 5 | 1 636 965 | 1 892 250 | 1 980 318 | 2 020 780 | 2 042 659 | 2 055 815 | 2 064 327 | 2 070 144 |
| | 1 636 948[f] | 1 892 230[f] | 1 980 295[f] | 2 020 746[f] | | | | |
| 6 | 2 455 248 | 2 851 459 | 2 988 408 | 3 051 398 | 3 085 482 | 3 105 984 | 3 119 257 | 3 128 340 |
| | 2 455 225[g] | 2 851 418[g] | 2 988 359[g] | 3 051 332[g] | (3 085 435)[g] | (3 105 933)[g] | (3 119 212)[g] | |
| 7 | 3 438 424 | 4 006 119 | 4 202 641 | 4 293 104 | 4 342 081 | 4 371 547 | 4 390 631 | 4 403 700 |
| | 3 437 960[h] | 4 006 160[h] | 4 202 620[h] | 4 293 080[h] | 4 342 360[i] | | | |
| 8 | 4 586 668 | 5 356 406 | 5 623 194 | 5 746 080 | 5 812 635 | 5 852 687 | 5 878 632 | 5 896 407 |
| | 4 585 980[j] | 5 355 670[j] | 5 622 600[j] | 5 745 440[j] | 5 811 730[j] | 5 851 890[j] | (5 877 800)[j] | (5 894 500)[j] |
| 9 | 5 900 191 | 6 902 545 | 7 250 300 | 7 410 559 | 7 497 382 | 7 549 640 | 7 583 497 | 7 606 698 |
| | 5 901 100[i] | 6 903 100[i] | 7 250 900[i] | 7 410 800[i] | 7 489 000[k] | | | |

TABLE XII. (*Continued.*)

| $Z$ | $2^3P$ | $3^3P$ | $4^3P$ | $5^3P$ | $6^3P$ | $7^3P$ | $8^3P$ | $9^3P$ |
|---|---|---|---|---|---|---|---|---|
| 10 | 7 379 191<br>7 379 000[l] | 8 644 748 | 9 084 175 | 9 286 762 | 9 396 542 | 9 462 628 | 9 505 448 | 9 534 796 |
| 11 | 9 023 957<br>9 018 800[m] | 10 583 331<br>(10 583 324)[n] | 11 125 148<br>(11 125 103)[n] | 11 375 020<br>(11 374 960)[n] | 11 510 450<br>(11 510 387)[n] | 11 591 987<br>(11 591 920)[n] | 11 644 820<br>(11 644 781)[n] | 11 681 038<br>(11 680 991)[n] |
| 12 | 10 834 741<br>10 836 000[m] | 12 718 567<br>(12 718 550)[o] | 13 373 499<br>(13 373 430)[o] | 13 675 619<br>(13 675 540)[o] | 13 839 393 | 13 938 005 | 14 001 904 | 14 045 712 |
| 13 | 12 811 885<br>12 810 000[m] | 15 050 832<br>(15 050 810)[p] | 15 829 620<br>(15 829 540)[p] | 16 188 955<br>(16 188 850)[p] | 16 383 770 | 16 501 081 | 16 577 099 | 16 629 222 |
| 14 | 14 955 703<br>14 954 000[m] | 17 580 470 | 18 493 863 | 18 915 387 | 19 143 941 | 19 281 578 | 19 370 767 | 19 431 928 |
| 15 | 17 266 605<br>17 265 000[m] | 20 307 933 | 21 366 697 | 21 855 388 | 22 120 384 | 22 279 976 | 22 383 390 | 22 454 313 |
| 16 | 19 744 960<br>19 744 000[m] | 23 233 623 | 24 448 537 | 25 009 380 | 25 313 523 | 25 496 699 | 25 615 393 | 25 696 803 |
| 17 | 22 391 248<br>22 387 000[m] | 26 358 070 | 27 739 933 | 28 377 920 | 28 723 919 | 28 932 310 | 29 067 341 | 29 159 963 |
| 18 | 25 205 926<br>25 195 000[q] | 29 681 773 | 31 241 398 | 31 961 530 | 32 352 097 | 32 587 337 | 32 739 761 | 32 844 321 |
| 19 | 28 189 434<br>28 182 000[m] | 33 205 211 | 34 953 429 | 35 760 711 | 36 198 560 | 36 462 284 | 36 633 158 | 36 750 383 |
| 20 | 31 342 374<br>31 322 000[m] | 36 929 049<br>(36 928 570)[r] | 38 876 712<br>(38 876 210)[r] | 39 776 159 | 40 264 012 | 40 557 857 | 40 748 240 | 40 878 859 |
| 21 | 34 665 334<br>34 664 000[m] | 40 853 935 | 43 011 917 | 44 008 556 | 44 549 136 | 44 874 743 | 45 085 696 | 45 230 436 |
| 22 | 38 158 851<br>38 126 000[m] | 44 980 453<br>(44 979 590)[s] | 47 359 648<br>(47 358 890)[s] | 48 458 510 | 49 054 547 | 49 413 558 | 49 646 141 | 49 805 732 |
| 23 | 41 823 578<br>41 773 000[m] | 49 309 318<br>(49 308 150)[t] | 51 920 644<br>(51 919 670)[t] | 53 126 772 | 53 780 998 | 54 175 058 | 54 430 335 | 54 605 508 |
| 24 | 45 660 157<br>45 540 000[u] | 53 841 235 | 56 695 631 | 58 014 079 | 58 729 232 | 59 159 988 | 59 439 022 | 59 630 508 |
| 25 | 49 669 320<br>(49 666 400)[v] | 58 577 006<br>(58 575 000)[v] | 61 685 440<br>(61 683 900)[v] | 63 121 272 | 63 900 095 | 64 369 198 | 64 673 055 | 64 881 587 |
| 26 | 53 851 756<br>53 894 000[q] | 63 517 386 | 66 890 850 | 68 449 140 | 69 294 382 | 69 803 484 | 70 133 231 | 70 359 542 |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.

[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).

[c]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stds. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1949).

[d]B. Löfstrand, Ref. 20.

TABLE XII. (*Continued.*)

[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).
[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).
[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3.
[h]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1971), Vol. 3, Sec. 4.
[i]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).
[j]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.
[k]N. J. Peacock, M. G. Hobby, and M. Galanti, J. Phys. B 6, L298 (1973).
[l]J. H. Parkinson, Solar Phys. 42, 183 (1975).
[m]V. A. Boiko, A. Ya Faenov, and S. A. Pikuz, J. Quant. Spectrosc. Radiat. Transfer 19, 11 (1978).
[n]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).
[o]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).
[p]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 8, 817 (1979).
[q]W. M. Neupert, Solar Phys. 18, 474 (1971).
[r]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 8, 865 (1979).
[s]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 8, 1 (1979).
[t]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 7, 1191 (1978).
[u]J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 6, 317 (1977).
[v]C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data 6, 1253 (1977).

TABLE XIII. Transition energies in $cm^{-1}$ for the $N\,^1D$ states.[a]

| $Z$ | $3\,^1D$ | $4\,^1D$ | $5\,^1D$ | $6\,^1D$ | $7\,^1D$ | $8\,^1D$ | $9\,^1D$ |
|---|---|---|---|---|---|---|---|
| 2 | 186 075.9<br>186 105.1[b] | 191 470.0<br>191 446.6[b] | 193 877.5<br>193 918.4[b] | 195 279.7<br>195 260.9[b] | 196 027.2<br>196 070.2[b] | 196 497.5<br>196 595.5[b] | 196 858.3<br>196 955.5[b] |
| 3 | 561 260<br>561 276[c] | 582 642<br>582 631[c] | 592 508<br>592 508[c] | 597 903<br>597 877[c] | 601 114<br>601 115[c] | 603 179 | 604 620 |
| 4 | 1 131 474<br>1 131 462[d] | 1 179 523<br>1 179 495[e] | 1 201 747<br>1 201 743[e] | 1 213 837 | 1 221 104 | 1 225 803 | 1 229 044 |
| 5 | 1 896 869<br>1 896 829[f] | 1 982 255<br>1 982 223[f] | 2 021 765 | 2 043 239 | 2 056 173 | 2 064 550 | 2 070 311 |
| 6 | 2 857 577<br>2 857 529[g] | 2 990 969<br>2 990 923[g] | 3 052 702<br>(3 052 656)[g] | 3 086 244<br>(3 086 189)[g] | 3 106 458<br>(3 106 407)[g] | 3 119 562<br>(3 119 630)[g] | 3 128 562 |
| 7 | 4 013 770<br>4 013 770[h] | 4 205 840<br>4 205 830[h] | 4 294 734<br>4 294 670[h] | 4 343 028 | 4 372 141 | 4 391 020 | 4 403 978 |
| 8 | 5 365 626<br>5 365 470[i] | 5 627 048<br>5 626 670[i] | 5 748 043<br>5 748 230[i] | 5 813 774<br>5 813 680[i] | 5 853 402 | 5 879 105 | 5 896 743 |
| 9 | 6 913 377<br>6 913 510[h] | 7 254 826<br>7 254 600[h] | 7 412 865<br>7 412 600[h] | 7 498 717<br>7 498 700[h] | 7 550 480<br>7 548 400[h] | 7 584 057<br>7 584 900[h] | 7 607 094 |
| 10 | 8 657 243 | 9 089 396 | 9 289 421 | 9 398 081 | 9 463 596 | 9 506 096 | 9 535 254 |
| 11 | 10 597 549<br>(10 597 475)[j] | 11 131 088<br>(11 131 017)[j] | 11 378 046<br>(11 377 984)[j] | 11 512 200<br>(11 512 137)[j] | 11 593 088 | 11 645 562 | 11 681 561 |
| 12 | 12 734 584<br>(12 734 480)[k] | 13 380 191<br>(13 380 090)[k] | 13 679 029<br>(13 678 940)[k] | 13 841 364 | 13 939 245 | 14 002 743 | 14 046 303 |
| 13 | 15 068 736 | 15 837 101 | 16 192 767 | 16 385 973 | 16 502 467 | 16 578 040 | 16 629 885 |
| 14 | 17 600 365 | 18 502 177 | 18 919 623 | 19 146 389 | 19 283 118 | 19 371 818 | 19 432 667 |

TABLE XIII. (*Continued.*)

| $Z$ | $3^1D$ | $4^1D$ | $5^1D$ | $6^1D$ | $7^1D$ | $8^1D$ | $9^1D$ |
|---|---|---|---|---|---|---|---|
| 15 | 20 329 940 | 21 375 896 | 21 860 076 | 22 123 093 | 22 281 680 | 22 384 557 | 22 455 133 |
| 16 | 23 257 882 | 24 458 680 | 25 014 549 | 25 316 509 | 25 498 577 | 25 616 684 | 25 697 710 |
| 17 | 26 384 742 | 27 751 087 | 28 383 606 | 28 727 203 | 28 934 376 | 29 068 765 | 29 160 963 |
| 18 | 29 711 039 | 31 253 642 | 31 967 771 | 32 355 702 | 32 589 604 | 32 741 329 | 32 845 423 |
| 19 | 33 237 277 | 34 966 847 | 35 767 551 | 36 202 512 | 36 464 770 | 36 634 882 | 36 751 595 |
| 20 | 36 964 143 | 38 891 402 | 39 783 649 | 40 268 338 | 40 560 579 | 40 750 134 | 40 880 189 |
| 21 | 40 892 312 | 43 027 987 | 44 016 750 | 44 553 870 | 44 877 721 | 45 087 773 | 45 231 895 |
| 22 | 45 022 395 | 47 377 217 | 48 467 470 | 49 059 722 | 49 416 813 | 49 648 418 | 49 807 332 |
| 23 | 49 355 137 | 51 939 842 | 53 136 565 | 53 786 655 | 54 178 616 | 54 432 829 | 54 607 260 |
| 24 | 53 891 270 | 56 716 603 | 58 024 778 | 58 735 413 | 59 163 875 | 59 441 753 | 59 632 426 |
| 25 | 58 631 629 | 61 708 344 | 63 132 958 | 63 906 846 | 64 373 444 | 64 676 044 | 64 883 686 |
| 26 | 63 577 002 | 66 915 855 | 68 461 900 | 69 301 754 | 69 808 121 | 70 136 501 | 70 361 839 |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.
[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).
[c]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stds. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1949).
[d]B. Löfstrand, Ref. 20.
[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).
[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).
[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3.
[h]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).
[i]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data. Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.
[j]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).
[k]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).

TABLE XIV. Transition energies in $cm^{-1}$ for the $N^3D$ states.[a]

| $Z$ | $3^3D$ | $4^3D$ | $5^3D$ | $6^3D$ | $7^3D$ | $8^3D$ | $9^3D$ |
|---|---|---|---|---|---|---|---|
| 2 | 186 099.4 | 191 433.5 | 193 906.5 | 195 259.6 | 196 052.3 | 196 495.6 | 196 857.5 |
| | 186 101.7[b] | 191 444.6[b] | 193 917.2[b] | 195 260.2[b] | 196 069.7[b] | 196 595.2[b] | 196 955.3[b] |
| 3 | 561 244 | 582 612 | 592 503 | 597 878 | 601 116 | 603 178 | 604 620 |
| | 561 245[c] | 582 612[c] | 592 505[c] | 597 876[c] | 601 115[c] | | |
| 4 | 1 131 400 | 1 179 471 | 1 201 721 | 1 213 807 | 1 221 094 | 1 225 798 | 1 229 041 |
| | 1 131 383[d] | 1 179 451[e] | 1 201 702[d] | 1 213 791[e] | | | |
| 5 | 1 896 723 | 1 982 167 | 2 021 717 | 2 043 199 | 2 056 152 | 2 064 540 | 2 070 303 |
| | 1 896 685[f] | 1 982 141[f] | 2 021 696[f] | | | | |
| 6 | 2 857 350 | 2 990 839 | 3 052 629 | 3 086 191 | 3 106 427 | 3 119 545 | 3 128 549 |
| | 2 857 310[g] | 2 990 776[g] | 3 052 589[g] | (3 086 138)[g] | (3 106 374)[g] | (3 119 507)[g] | |
| 7 | 4 013 456 | 4 205 665 | 4 294 635 | 4 342 961 | 4 372 099 | 4 390 995 | 4 403 960 |
| | 4 013 460[h] | 4 205 820[h] | 4 294 570[h] | 4 343 120[i] | | | |

TABLE XIV. (*Continued.*)

| Z | $3^3D$ | $4^3D$ | $5^3D$ | $6^3D$ | $7^3D$ | $8^3D$ | $9^3D$ |
|---|---|---|---|---|---|---|---|
| 8 | 5 365 221 | 5 626 824 | 5 747 917 | 5 813 692 | 5 853 350 | 5 879 074 | 5 896 720 |
| | 5 364 420[j] | 5 626 280[j] | 5 747 420[j] | 5 813 070[j] | 5 853 660[j] | 5 878 400[j] | 5 892 950[j] |
| 9 | 6 912 878 | 7 254 551 | 7 412 710 | 7 498 619 | 7 550 416 | 7 584 017 | 7 607 065 |
| | 6 912 500[i] | 7 254 100[i] | 7 412 100[i] | 7 498 100[i] | 7 549 800[i] | 7 583 300[i] | 7 607 100[i] |
| 10 | 8 656 647 | 9 089 069 | 9 289 237 | 9 397 966 | 9 463 522 | 9 506 049 | 9 535 220 |
| 11 | 10 596 855 | 11 130 709 | 11 377 833 | 11 512 068 | 11 593 002 | 11 645 507 | 11 681 521 |
| | (10 596 783)[k] | (11 130 639)[k] | (11 377 767)[k] | (11 512 003)[k] | | | |
| 12 | 12 733 789 | 13 379 759 | 13 678 786 | 13 841 214 | 13 939 147 | 14 002 679 | 14 046 258 |
| | (12 733 690)[l] | (13 379 660)[l] | (13 678 690)[l] | | | | |
| 13 | 15 067 841 | 15 836 614 | 16 192 494 | 16 385 805 | 16 502 358 | 16 577 969 | 16 629 833 |
| 14 | 17 599 368 | 18 501 636 | 18 919 320 | 19 146 203 | 19 282 997 | 19 371 738 | 19 432 610 |
| 15 | 20 328 841 | 21 375 300 | 21 859 741 | 22 122 888 | 22 281 547 | 22 384 469 | 22 455 070 |
| 16 | 23 256 680 | 24 458 029 | 25 014 184 | 25 316 286 | 25 498 432 | 25 616 588 | 25 697 641 |
| 17 | 26 383 437 | 27 750 381 | 28 383 210 | 28 726 962 | 28 934 219 | 29 068 660 | 29 160 889 |
| 18 | 29 709 631 | 31 252 879 | 31 967 344 | 32 355 442 | 32 589 436 | 32 741 216 | 32 845 342 |
| 19 | 33 235 765 | 34 966 029 | 35 767 093 | 36 202 233 | 36 464 589 | 36 634 769 | 36 751 514 |
| 20 | 36 962 527 | 38 890 528 | 39 783 159 | 40 268 041 | 40 560 385 | 40 750 012 | 40 880 102 |
| 21 | 40 890 592 | 43 027 057 | 44 016 229 | 44 553 553 | 44 877 515 | 45 087 643 | 45 231 802 |
| 22 | 45 020 571 | 47 376 231 | 48 466 918 | 49 059 387 | 49 416 596 | 49 648 280 | 49 807 233 |
| 23 | 49 353 209 | 51 938 800 | 53 135 982 | 53 786 301 | 54 178 387 | 54 432 682 | 54 607 155 |
| 24 | 53 889 237 | 56 715 505 | 58 024 163 | 58 735 039 | 59 163 634 | 59 441 598 | 59 632 316 |
| 25 | 58 629 493 | 61 707 190 | 63 132 311 | 63 906 454 | 64 373 190 | 64 675 880 | 64 883 570 |
| 26 | 63 574 761 | 66 914 645 | 68 461 222 | 69 301 343 | 69 807 855 | 70 136 328 | 70 361 716 |

[a]For each entry, the first line is the result obtained in the present paper, the second line (if present) is from experiment, except where parentheses indicate a theoretical value.

[b]W. C. Martin, J. Phys. Chem. Ref. Data 2, 257 (1973).

[c]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1949).

[d]B. Löfstrand, Ref. 20.

[e]M. Eidelsberg, J. Phys. B 5, 1031 (1972).

[f]M. Eidelsberg, J. Phys. B 7, 1476 (1974).

[g]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1970), Vol. 3, Sec. 3

[h]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1971), Vol. 3, Sec. 4.

[i]A. M. Cantu, E. Jannitti, and G. Tondello, J. Opt. Soc. Am. 64, 699 (1974).

[j]C. E. Moore, *Atomic Energy Levels,* Natl. Stds. Ref. Data Ser. (National Bureau of Standards, Washington, D.C., 1979), Vol. 3, Sec. 8.

[k]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 10, 153 (1981).

[l]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data 9, 1 (1980).

TABLE XV. A comparison of some observed and calculated transitions (in $cm^{-1}$).[a]

| Transition | $Z=4$[b] | $Z=5$[c] | $Z=6$[d] |
|---|---|---|---|
| $2^1S$—$2^1P$ | 16 275.9 | 22 267 | 28 365 |
| | 16 276.8±0.1 | 22 261±1 | 28 347±4 |
| $2^3S$—$2^3P$ | | 35 399 | 43 940 |
| | | 35 408±0.5 | 43 963±1 |
| $4^3P$—$5^3D$ | 23 527.9 | 41 399 | |
| | 23 527.6±0.6 | 41 408±2 | |
| $4^3S$—$5^3P$ | | 44 315 | |
| | | 44 307±2 | |
| $3^3D$—$4^3P$ | | 83 595 | |
| | | 83 608±7 | |
| $3^3P$—$4^3S$ | 46 996.4 | 84 215 | |
| | 46 995.4±0.9 | 84 196±7 | |
| $3^1P$—$4^1D$ | 47 112.6 | 83 996 | |
| | 47 104.5±0.9 | 83 993±7 | |
| $3^3P$—$4^3D$ | 51 154.0 | 89 917 | |
| | 51 151.7±0.8 | 89 912±8 | |
| $3^3S$—$4^3P$ | 56 992.2 | 97 546 | |
| | 56 990.1±1.0 | 97 551±9 | |
| $2^1P$—$3^1S$ | 130 247 | 233 805 | |
| | 130 251±5 | 233 808±27 | |
| $2^1P$—$3^1D$ | 134 000.5 | 238 857 | 374 134 |
| | 134 007.3±1.4 | 238 857±1 | 374 158±7 |
| $2^3P$—$3^3S$ | 137 820.5 | 245 807 | |
| | 137 819.6±2 | 245 797±30 | |
| $2^3P$—$3^3D$ | 148 020.3 | 259 758 | |
| | 148 018.1±2 | 259 740±13 | |
| $2^1S$—$3^1P$ | 151 212.4 | 262 514 | 404 338 |
| | 151 212.3±2 | 262 508±42 | 404 351±33 |
| $2^3S$—$3^3P$ | 171 798.5 | 290 684 | 440 150 |
| | 171 798.3±3 | 290 689±17 | 440 156±10 |
| $2^1P$—$4^1D$ | 182 049 | 324 243 | 507 526 |
| | 182 047±10 | 324 243±52 | 507 552±18 |
| $2^3P$—$4^3D$ | 196 091 | 345 202 | |
| | 196 082±8 | 345 256±58 | |
| $2^3S$—$4^3P$ | | 378 752 | 577 100 |
| | | 378 759±70 | 577 097±17 |

TABLE XV. (*Continued.*)

| Transition | $Z=4$[b] | $Z=5$[c] | $Z=6$[d] |
|---|---|---|---|
| $2^3P$—$5^3D$ | | | 597 381 |
| | | | 597 364±35 |
| $2^3S$—$5^3P$ | | | 640 089 |
| | | | 640 070±41 |

[a]For each entry, the upper line is the result obtained in the present paper. The lower line is the experimental result.

[b]B. Löfstrand, Ref. 20.

[c]M. Eidelsberg, J. Phys. B 7, 1476 (1974).

[d]B. Edlen and B. Löfstrand, J. Phys. B 3, 1380 (1970).

tivistic correction. The simple one-electron screening approximation presented in Eq. (14) appears to be sufficient to assure that the error in the overall transition energy is essentially of the order of the error in the relativistic correction, or less.

### D. Transition energies

The transition energies relative to the ground $1^1S$ state are presented in Tables IX–XIV. For $Z=2$ the accuracy of the present values is determined almost entirely by the convergence of the expansion for the nonrelativistic energy. This rapidly improves with increasing $Z$ so that, as indicated above, for $Z \gtrsim 4$ the accuracy of the tabulated values is determined by the accuracy of the relativistic correction. For increasing $N$ (degree of excitation) the calculated nonrelativistic energies become less reliable because of the lack of accurate, higher-order $\epsilon_n$, while the relativistic, Lamb shift, and mass-polarization corrections increase in accuracy as the contribution of the "excited electron" becomes less reliable because of the lack of accurate, higher-order $\epsilon_n$, while the relativistic, Lamb shift, and mass-polarization corrections increase in accuracy as the contribution of the "excited electron" becomes less significant and these corrections become simply the corresponding corrections to the ground-state ionization energy. Therefore, for $Z \gtrsim 4$, the least reliable results are the $2S$, $2P$, and $3D$ results. That this is not reflected in the comparisons presented in the tables, where any particular row displays a generally constant difference, suggests that the present results are more accurate than the experimental data. In any case the agreement throughout the tables with both experimental and theoretical values is fairly uniform—five significant figures, occasionally four or six figures. However, since the energies in Tables IX through XIV are all relative to the $1^1S$ ground state, the error in the quoted experimental values is in large part due to the difficulty in establishing an accurate value for the energy of the ground state. Thus a more meaningful comparison would make use of the transitions actually observed. Such a comparison is presented in Table XV for $Z=4$, 5, and 6. Whereas differences for those ions in Tables IX through XIV are generally in the range of 20–40 $cm^{-1}$, differences in Table XV are generally less than 10 $cm^{-1}$ for $Z=4$, 5, less than 20 $cm^{-1}$ for $Z=6$, and generally in reasonable agreement with the experimental error limits. Particularly striking is the agreement with the data of Löfstrand[20] for $Z=4$, where the observed wavelengths are given to greater accuracy.

## V. CONCLUSIONS

The results of the present study are based on a uniform set of expansion coefficients for the nonrelativistic energy of two-electron ions. Many of these are presented here for the first time. Relativistic and Lamb-shift corrections for these two-electron ions are computed in a particularly simple manner, and are found to yield reliable results. The accuracy to be expected for the transition energies tabulated here has a predictable behavior with respect to $Z$ and $N$, and the entire set of $S$, $P$, and $D$ state results form a consistent set of data.

[1]R. E. Knight and F. C. Sanders, Phys. Rev. A 22, 1361 (1980).
[2]R. E. Knight, Phys. Rev. A 25, 55 (1982).
[3]Y. Accad, C. L. Pekeris, and B. Schiff, Phys. Rev. A 4, 516 (1971).
[4]Y. Accad, C. L. Pekeris, and B. Schiff, Phys. Rev. A 11, 1479 (1975).
[5]R. T. Brown and J-L. M. Cortez, J. Chem. Phys. 54, 2657 (1971).
[6]P. Blanchard and G. W. F. Drake, J. Phys. B 6, 2495 (1973).
[7]R. E. Knight and C. W. Scherr, Rev. Mod. Phys. 35, 436 (1963).
[8](a) O. Sinanoğlu, Phys. Rev. 122, 49 (1961); (b) W. H. Miller, J. Chem. Phys. 45, 2198 (1966); (c) F. C. Sanders and C. W. Scherr, Phys. Rev. 181, 84 (1969).
[9]F. C. Sanders, Chem. Phys. Lett. 17, 291 (1972).
[10]K. Aashamar, Nucl. Instrum. Methods 90, 263 (1970).
[11]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-electron Atoms* (Academic, New York, 1957).
[12]A. Dalgarno and A. L. Stewart, Proc. R. Soc. London, Ser. A 257, 534 (1960).
[13]J. M. Harriman, Phys. Rev. 101, 594 (1956).
[14]B. F. Davis and K. T. Chung, Phys. Rev. A 25, 1328 (1982).
[15]A. M. Ermolaev and M. Jones, J. Phys. B 7, 199 (1974).
[16]P. Blanchard, Phys. Rev. A 13 1698 (1976).
[17](a) K. Aashamar, J. Midtdal, and G. Lyslo, J. Chem. Phys. 60, 3403 (1974); (b) 61, 1345 (1974).
[18]K. Aashamar, G. Lyslo, and J. Midtdal, J. Chem. Phys. 52, 3324 (1970).
[19]A. N. Ivanova, U. I. Safronova, and V. N. Kharitonova, Opt. Spektrosk. 24, 660 (1968) [Opt. Spectrosc. (USSR) 24, 355 (1968)].
[20]B. Löfstrand, Phys. Scr. 8, 57 (1973).