Improved ^{4}He I $1snl$ ionization energy, energy levels, and Lamb shifts for $1sns$ and $1snp$ terms

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The consistencies of calculated term values (ionization energies) for various $1snl$ terms having $n=5-8$, $l=1-5$ are tested by microwave-spectroscopic and other available data. The most accurate $n\,P$, $n\,D$, and $n\,F$ term values obtained from published variational calculations are generally found to be consistent, within the estimated uncertainties, with more accurate $n\,G$ and $n\,H$ energies from core-polarization theory [R. J. Drachman, Phys. Rev. A **26**, 1228 (1982)]. The $n\,^3D$ and $n\,^1D$ term values from variational calculations [A. Kono and S. Hattori, Phys. Rev. A **34**, 1727 (1986)] are confirmed within uncertainties as small as 10^{-4} cm^{-1} ($n=8$), although the ^{1}D values are systematically too large by amounts within the uncertainties. The ionization energy E_I has accordingly been reevaluated by using only the calculated $n\,^3D$ term values ($n=4,5$) and available experimental measurements: The resulting E_I value is 198 310.772 27(40) cm^{-1} with respect to the $2\,^3S$ level at 159 856.077 60 cm^{-1}. The available data and calculated term energies allow determination of the entire $1snl$ excited energy-level system with much improved accuracy for the higher levels. Calculated energies are used instead of experimental results in several cases involving apparently underestimated experimental uncertainties. The levels are given explicitly through $n=8$. Experimental term values based on the new E_I value are combined with calculated term values not including QED contributions to obtain "experimental" Lamb shifts for a number of $n\,S$ and $n\,P$ terms. The experimental Lamb shifts of the $2\,^3S_1-2\,^3P_1$ and $2\,^3P_1-2\,^1P_1$ separations are also reevaluated. Results of comparisons of these experimental shifts with various calculated Lamb shifts vary from agreement within 0.3% experimental uncertainties (for the $2\,^3S$ shift and shift of the $2\,^3S_1-2\,^3P_1$ separation) to relatively large discrepancies for the higher $n\,S$ terms ($\sim$50% for $5\,^3S$). Two-electron QED contributions calculated for $2\,^3S$, $2\,^1S$, and $2\,^1P$ [G. W. F. Drake and A. J. Makowski, J. Phys. B **18**, L103 (1985)] are confirmed within uncertainties of about 35% by the data in each case, the level of confirmation for $2\,^3S$ and $2\,^1P$ being subject to additional uncertainties from as-yet uncalculated contributions.

I. INTRODUCTION

The most accurate calculations of helium $1snl$ term energies (ionization energies) are of two very different types: elaborate variational calculations that include basis functions explicitly dependent on the interelectronic separation[1–10] and, on the other hand, relatively simple core-polarization perturbational calculations.[11] The two methods are complementary in that usefully accurate variational calculations have been made for terms having $l\leq 3$, whereas the core-polarization calculations have high accuracy for $l\geq 4$. The most accurate variationally calculated term values have estimated uncertainties of about 3–10 MHz not including QED contributions, but it is doubtful whether the QED (Lamb) shift for any low $n\,S$ or $n\,P$ term has been calculated with an uncertainty less than 15 MHz. Recent high-accuracy optical measurements of He I term separations involving low $n\,S$ or $n\,P$ levels[12–15] are therefore mainly tests of Lamb-shift calculations rather than of the calculated term energies. In contrast, several higher-l term separations calculated with core-polarization theory have been confirmed by microwave-spectroscopic determinations within uncertainties from about 1 to less than 0.1 MHz.[11]

Kono and Hattori's[8,9] recent extensions of accurate variational calculations up to $1s\,8d$ are of special interest in that the results can be tested for consistency with core-polarization calculations for $1sng$ and $1snh$ terms by use of connecting microwave-spectroscopic data. These comparisons test the $n\,D$ variational energies, since the small Lamb shifts involved contribute negligibly to the uncertainties. Such comparisons, as carried out in Sec. II of this paper, generally confirm the accuracy of the variational $1snd$ and $1snf$ term energies[9,10] ($n=5-8$) within the estimated errors. The agreement extends to the higher $n\,D$ terms having variationally calculated ionization energies with estimated uncertainties at the 3-MHz level.[9]

In addition to their interest for the theory of two-electron atoms, these results have particular significance because the calculated $n\,D$ term energies in helium enter into the most accurate current determinations of the principal ionization energy relative to the $1snl$ excited levels.[16,8,9] In this paper a new value of the ionization energy is derived relative to the $2\,^3S_1$ level, which is involved in the pertinent experimental data.[12,14] This choice of reference level and the avoidance of a systematic error arising from the calculated $n\,^1D$ energies give the ionization energy within an estimated uncertainty of 0.0004 cm^{-1} (12 MHz). The available experimental data and calculated term energies then allow deter-

mination of the entire $1snl$ excited energy-level system with much improved accuracies for the higher levels. The levels of this system are given here explicitly through $n=8$.

Calculations of QED corrections to the helium $1s^2\,{}^1S$ term value were extended some 30 years ago to include contributions of order α^3 a.u. arising from radiative interactions between the electrons.[17] These two-electron contributions to the ground-level Lamb shift have not yet been satisfactorily tested, however, because their sum is comparable to the uncertainty of the 1958 resonance-line measurements[18] (± 0.15 cm^{-1}) on which the experimental value for the $1s^2$ ionization energy is based.[18,19,16] The more satisfactory situation for some of the low excited levels[9] is further improved by results given in this paper. Experimental term values based on the new ionization energy have been combined with available theoretically calculated term values not including QED contributions to obtain improved "experimental" Lamb shifts for a number of $n\,S$ and $n\,P$ terms. These results test calculated two-electron QED contributions for the $n=2$ terms (${}^3S$, ${}^1S$, ${}^3P$, ${}^1P$). The overall results of our comparisons of experimental and calculated Lamb shifts vary from agreement within 0.3% experimental uncertainties (for the $2\,{}^3S$ shift and shift of the $2\,{}^3S-2\,{}^3P$ separation) to relatively large discrepancies ($\sim 50\%$ for $5\,{}^3S$) indicating the need for more accurate calculations.

II. CALCULATED TERM VALUES AND EXPERIMENTAL DATA FOR $1snl$ CONFIGURATIONS ($n=5-8$)

The $n\,G$ and $n\,H$ term values in the second column of Table I are core-polarization theoretical energies,[11] whereas the $n\,F$, $n\,D$, and $n\,P$ terms were obtained from variational calculations.[8–10] Each of these calculated term values was combined with experimental level separations or other pertinent data given under "Additional data" to obtain the $n\,{}^1F$ term value in the fourth column. Comparisons of the different ${}^1F$ term values obtained for a particular n thus test the consistency of the different calculated term values in the second column and the additional data. The choice of the $n\,{}^1F$ levels for this purpose was somewhat arbitrary, but these levels are well represented in the high-accuracy microwave spectroscopic measurements[20–22] of critical importance for these comparisons.

A. Calculated $n\,G$, $n\,H$, and $n\,D$ terms and connecting data

The theoretical $n\,G_{\rm CP}$ and $n\,H_{\rm CP}$ energies in Table I are derived from Drachman's calculations[11] of the core-polarization energy, adiabatic corrections, and some other energies contributing to the $1snl$ term defect. This core-polarization term defect $\Delta_{\rm CP}$ does not include the Coulomb exchange or magnetic-interaction energies. The corresponding $1snl$ core-polarization term energy $T(L_{\rm CP})$ is given by

$$T(L_{\rm CP})=R(^4{\rm He})n^{-2}+\Delta_{\rm CP}+\Delta_r\ . \tag{1}$$

The value of the Rydberg constant for ^{4}He, $R(^4{\rm He})$, and other atomic constants needed in this paper are taken as given in Ref. 16. The approximation for $\Delta_{\rm CP}$ used here,

$$\Delta_{\rm CP}=-[V_4+V_6+\tfrac{1}{2}(V_7+V_8)+\Delta_2]-(-\varepsilon_M)+\varepsilon_{\rm CP}\ , \tag{2}$$

omits the mass-polarization, relativistic-polarizability, and (very small) retardation contributions; the sum of these three contributions is very nearly zero for $l\geq 4$, the first being almost equal in absolute value but of opposite sign to the sum of the latter two contributions.[11] Drachman tabulates the values of V_4, V_6, V_7, V_8, and Δ_2 for the terms of interest here. The mass-polarization contribution $(-\varepsilon_M)$ is subtracted in (2) to compensate for its inclusion in the $-V_4$ contribution. The quantity $\varepsilon_{\rm CP}$ arises from the choice of the core center of mass as the reference point for the outer-electron position; the correction[11] $\varepsilon_{\rm CP}=R(^4{\rm He})(m_e/M_\alpha)n^{-2}$ is equivalent to an increase of 0.002 06 cm^{-1} in the effective Rydberg constant. The relativistic correction Δ_r in (1) is given accurately for high-l configurations by the hydrogenic expression[23]

$$\Delta_r=R\alpha^2 n^{-4}[n(l+\tfrac{1}{2})^{-1}-\tfrac{3}{4}]\ . \tag{3}$$

Drachman's estimate of the uncertainty, $\frac{1}{2}(V_7+V_8)$, is given for the 6,7,8 $G_{\rm CP}$ term values in Table I, but the uncertainty of $5\,G_{\rm CP}$ was increased to include the additional approximation involved in (2) as described above. The small $7\,H_{\rm CP}$ and $8\,H_{\rm CP}$ uncertainties as estimated here are entirely due to the latter approximation.

The $n\,G_{\rm CP}-n\,{}^1G$ and $n\,H_{\rm CP}-n\,{}^1H$ separations were evaluated by using experimental level separations and the theory of $1snl$ structures in an approximation pointed out by Chang[24] and by Lundeen.[24] Details are given in the Appendix.

Kono and Hattori's calculated term values[8,9,25] for $n\,{}^1D$ and $n\,{}^3D_{\rm cg}$ (cg represents center of gravity) include small Lamb shifts Δ_L as estimated by these authors ($n=5,6$) or as extrapolated according to a n^{-3} scaling ($n=7,8$). The term uncertainties were obtained by combining in quadrature the errors given for the nonrelativistic term value $T_{\rm nr}$ and the relativistic correction Δ_r, the errors of the other contributions being negligible according to Kono and Hattori's estimates. The uncertainties of the calculated $n\,{}^1P$ term values[9,25] ($n=6,7,8$) include estimated errors for the Lamb shifts, which have been taken as zero.[26]

No precise confidence levels can be given with the uncertainties of the calculated terms, but the discussions of Kono and Hattori[9] and of Drachman[11] appear to imply at least standard-deviation confidence levels. Farley, MacAdam, and Wing[20] and Farley *et al.*[21] gave standard-deviation errors for their directly measured values of level separations as well as for values derived from series-fitting formulas, but careful analysis by these authors showed that overall the assigned errors were significantly underestimated. The term separations from these data in Table I were mainly obtained by using the direct measurements in preference to, or weighted more heavily than, values from the series-fitting formulas, and the errors have been increased to values believed to correspond at least to the standard-deviation level. The un-

TABLE I. Term values (ionization energies) of $n\,^1F$ levels for $n=5$–8. Each term value under $n\,^1F$ was obtained by combining a calculated term value given in the second column with the additional data. Energies calculated with core-polarization theory are denoted by the subscript CP. The designation $^3D_{cg}$ refers to the ^3D center of gravity. The last column gives the diference between each $n\,^1F$ term value and the adopted $n\,^1F$ term value, designated $n\,^1F$(AV). Units are cm^{-1}.

n	Calculated term value		Additional data		$n\,^1F$	$T(n\,^1F)-T(n\,^1F(\mathrm{AV}))$
5	$5\,G_{CP}$	4389.050 392(50)[a]	$5\,G_{CP}-5\,^1G$	0.003 362(25)[b]	4389.538 08(7)	−0.000 02
			$5\,^1F-5\,^1G$	0.491 054(33)[b]		
	$5\,^1D$	4392.379 30(22)[c]	$5\,^1D-5\,^1F$	2.840 99(17)[d]	4389.538 31(28)	0.000 21
	$5\,^3D_{cg}$	4393.515 43(22)[c]	$5\,^1D-5\,^1F$	2.840 99(17)[d]	4389.538 12(28)	0.000 02
			$5\,^3D_{cg}-5\,^1D$	1.136 32(6)[e]		
	$5\,^1F$	4389.5383(40)[f]	$\Delta_r+\Delta_{s\text{-}t}-\varepsilon_M$	0.0027[g]	4389.5410(40)	0.0029
				$5\,^1F$(AV)	4389.538 10(7)	
6	$6\,G_{CP}$	3047.943 788(40)[a]	$6\,G_{CP}-6\,^1G$	0.001 942(20)[b]	3048.237 18(5)	−0.000 01
			$6\,^1F-6\,^1G$	0.295 336(7)[b]		
	$6\,^1D$	3049.898 57(14)[c]	$6\,^1D-6\,^1F$	1.661 27(1)[h]	3048.237 30(14)	0.000 11
	$6\,^3D_{cg}$	3050.596 29(14)[c]	$6\,^1D-6\,^1F$	1.661 27(1)[h]	3048.237 17(17)	−0.000 02
			$6\,^3D_{cg}-6\,^1D$	0.697 85(9)[i]		
	$6\,^1P$	3035.760 60(33)[c]	$6\,^1F-6\,^1P$	12.4752(5)[j]	3048.2358(6)	−0.0014
	$5\,^1D$	4392.379 30(22)[c]	$5\,^1D-6\,^1F$	1344.1404(10)[k]	3048.2389(10)	0.0017
	$6\,^1F$	3048.238 4(80)[f]	$\Delta_r+\Delta_{s\text{-}t}-\varepsilon_M$	0.0024[g]	3048.241(8)	0.004
				$6\,^1F$(AV)	3048.237 19(5)	
7	$7\,H_{CP}$	2239.253 580(10)[a]	$7\,H_{CP}-7\,^1H$	0.000 816(10)[l]	2239.487 914(18)	0.000 000
			$7\,^1F-7\,^1H$	0.235 150(11)[m]		
	$7\,G_{CP}$	2239.298 910(35)[a]	$7\,G_{CP}-7\,^1G$	0.001 225(10)[h]	2239.487 909(37)	−0.000 005
			$7\,^1F-7\,^1G$	0.190 224(7)[h]		
	$7\,^1D$	2240.540 65(10)[c]	$7\,^1D-7\,^1F$	1.052 67(1)[h]	2239.487 98(10)	0.000 07
	$7\,^3D_{cg}$	2240.995 32(10)[c]	$7\,^1D-7\,^1F$	1.052 67(1)[h]	2239.487 89(10)	−0.000 02
			$7\,^3D_{cg}-7\,^1D$	0.454 76(2)[n]		
	$7\,^1P$	2231.581 41(25)[c]	$7\,^1F-7\,^1P$	7.9060(11)[j]	2239.4874(11)	−0.0005
				$7\,^1F$(AV)	2239.487 914(16)	
8	$8\,H_{CP}$	1714.427 317(7)[a]	$8\,H_{CP}-8\,^1H$	0.000 551(10)[o]	1714.586 860(19)	−0.000 004
			$8\,^1F-8\,^1H$	0.160 094(15)[m]		
	$8\,G_{CP}$	1714.458 429(28)[a]	$8\,G_{CP}-8\,^1G$	0.000 820(5)[p]	1714.586 872(30)	0.000 008
			$8\,^1F-8\,^1G$	0.129 263(7)[q]		
	$8\,^1D$	1715.294 96(10)[c]	$8\,^1D-8\,^1F$	0.708 037(10)[h]	1714.586 92(10)	0.000 06
	$8\,^3D_{cg}$	1715.606 19(10)[c]	$8\,^1D-8\,^1F$	0.708 037(10)[h]	1714.586 85(10)	−0.000 01
			$8\,^3D_{cg}-8\,^1D$	0.311 304(7)[n]		
	$8\,^1P$	1709.268 73(22)[c]	$8\,^1F-8\,^1P$	5.3180(6)[j]	1714.5867(6)	−0.0002
				$8\,^1F$(AV)	1714.586 864(16)	

[a]Term value obtained from calculations of Drachman (Ref. 11).
[b]Measurements by Farley *et al.* (Ref. 21). See Appendix for explanation of $n\,G_{CP}-n\,^1G$ separations.
[c]Value from Kono and Hattori (Refs. 8 and 9) with Lamb shifts as described in text.
[d]Value obtained from formula fitted to experimental frequencies of $n\,^1D-n\,^1F$ transitions for $n=6$–11 (see text).
[e]Measurement by Tepehan *et al.* (Ref. 28).
[f]Sims *et al.* (Ref. 10).
[g]Relativistic and mass-polarization contributions (Δ_r and $-\varepsilon_M$) from Cok and Lundeen (Ref. 31). The singlet-triplet mixing correction $\Delta_{s\text{-}t}$ was evaluated by substituting the experimental $T(^3F_3)-T(^1F_3)$ separation and the value of ζ (Ref. 31) into Eq. (A5) to obtain the exchange energy K. The shift of the ^1F term value due to the magnetic interactions was then obtained as $\Delta_{s\text{-}t}=K-\frac{1}{2}[T(^3F_3)-T(^1F_3)]+\frac{1}{4}\zeta$ [see Eq. (A4)]. The values obtained were $K(5F)=67.1$ MHz, $\Delta_{s\text{-}t}(5\,^1F)=-113.7$ MHz; $K(6F)=47.8$ MHz, $\Delta_{s\text{-}t}(6\,^1F)=-60.7$ MHz.
[h]Measurements by Farley, MacAdam, and Wing (Ref. 20). See Appendix for $7\,G_{CP}-7\,^1G$ separation.
[i]Value obtained from formulas fitted to experimental values of $n\,^3D-n\,^1D$ separations for $n=3$–11 (see text).
[j]Measurement by Le *et al.* (Ref. 32).
[k]Measurement by Nagai *et al.* (Ref. 33).
[l]Based on $7\,^3H_5-7\,^1H_5$ separation obtained from $7F-7H$ measurements (Ref. 22) and $7F$ level separations (Ref. 20). See Appendix.
[m]Measurement by Cok and Lundeen (Ref. 22).
[n]From least-squares fit to experimental data by Farley, MacAdam, and Wing (Ref. 20).
[o]See Appendix.
[p]Based on $8\,^3G_4-8\,^1G_4$ separation obtained by averaging data from Refs. 20 and 22. See Appendix.
[q]Value from averaging of data in Refs. 20 and 22.

certainties given by Cok and Lundeen[22] are apparently standard-deviation errors including allowances for various systematic effects.

The $5\,^1D-5\,^1F$ separation has not been measured with high accuracy. The value in Table I was obtained from a least-squares fit of the $n\,^1D-n\,^1F$ separations for $n=6-11$ to a series formula for small term-value differences, ΔT,

$$\Delta T = An^{-3}+Bn^{-5}+Cn^{-7}\,, \tag{4}$$

where A, B, and C are constants. Since the predicted ΔT value for $n=5$ is an extrapolation, the uncertainty was increased to three times the standard deviation.[27]

The $n\,^3D_{cg}-n\,^1D$ differences are given in Table I as one of two separations connecting each calculated $n\,^3D_{cg}$ term with the $n\,^1F$ value. Accurate experimental values for the $n\,^3D_{cg}-n\,^1D$ separations for $n=3,5,7,8$ are listed in Table II,[15,20,28] along with values from Kono and Hattori's calculations[9] for $n=3-8$. The differences between the experimental and calculated values are within the estimated errors of the calculations. These differences are also very regular, an additive correction of $(0.0047)n^{-2}$ cm^{-1} to the calculated values giving good agreement with experiment. The $6\,^3D_{cg}-6\,^1D$ separation used in Table I and given under Experiment in Table II was not, however, obtained as a corrected theoretical value but was derived by fitting three- and four-term formulas such as (4) to the experimental data for $n=3-11$ (except $n=4$).[15,20,28-30]

B. Consistency tests: core-polarization theoretical $n\,G$ and $n\,H$ term values and variationally calculated $n\,D$ term values

The $n\,^1F$ "adopted value" [$n\,^1F$(AV)] in Table I is an average of the $n\,^1F$ term values obtained from the calculated $n\,G$, $n\,H$, and $n\,D$ terms with weights according to the inverse squares of the uncertainties. The difference between each $n\,^1F$ term value and the adopted term value (last column) can be compared with the estimated uncertainty given in parentheses in the preceding column. Beginning with the most accurate terms, we note that for $n=7$ and 8 the $n\,^1F$ value obtained from the calculated $n\,H$ term is very consistent with the $n\,^1F$ value obtained from the calculated $n\,G$ term. These results could be expected on the basis of Drachman's direct comparisons of his calculated $7G-7H$ and $8G-8H$ separations with the microwave data.[11] The calculated $n\,^3D$ term values[9] for $n=7$ and 8 give $n\,^1F$ values within 0.000 02 cm^{-1} of the values from Drachman's results, and thus the corresponding $n\,^1D$ calculated terms give $n\,^1F$ values too large by additional amounts about equal to the systematic errors of the calculated $n\,^3D_{cg}-n\,^1D$ separations already discussed (Table II). These larger deviations of the $n\,^1F$ values based on the calculated $n\,^1D$ terms are about two-thirds of the corresponding estimated uncertainties. This behavior extends down to $n=5$ and 6; comparing the first three ^1F values in each case, we see that the value from the calculated ^3D term agrees well with the presumably more accurate result from the calculated G term, and the calculated ^1D term gives the ^1F value too large by an amount somewhat smaller than the uncertainty.

It is interesting that the calculated $n\,^1D$ ionization energies[9] are apparently too large, because the variationally determined nonrelativistic main contribution T_{nr} should represent a lower limit for the exact nonrelativistic value. The adopted T_{nr} values[9] are extrapolations of calculated values, but the difference of the extrapolated value and the final calculated value for $T_{nr}(5\,^1D)$, for example, is only 0.0002 cm^{-1}. It seems likely that the apparent small but systematic errors of the calculated $n\,^1D$ term values are at least in part due to corresponding errors in the relativistic contributions Δ_r.

C. Calculated $n\,^1F$ and $n\,^1P$ terms and comments on some experimental data in Table I

Sims *et al.*[10] have made variational calculations of $n\,^1D$ and $n\,^1F$ term energies. Their estimated exact energies for the $5\,^1F$ and $6\,^1F$ terms are listed in the second column of Table I with assumed uncertainties approximately equal to the amounts by which the final calculated term values were increased to obtain the estimated exact values. These increases were probably too large by about 0.0029 cm^{-1} for $5\,^1F$ and 0.004 cm^{-1} for $6\,^1F$ (last

TABLE II. Experimental and calculated values for $n\,^3D_{cg}-n\,^1D$ separations. Units are cm^{-1}. The calculated values are from Kono and Hattori (Ref. 9). No accurate experimental determination has been made for $n=4$. The differences between the experimental and calculated values are approximately equal to the quantities $n^{-2}(0.0047)$ cm^{-1}.

n	$^3D_{cg}-{}^1D$ Experiment	$^3D_{cg}-{}^1D$ Calculation	Difference	$n^{-2}(0.0047)$
3	3.410 13(10)[a]	3.409 57(77)	0.000 56	0.000 52
4		1.970 10(53)		0.000 29
5	1.136 32(6)[b]	1.136 13(32)	0.000 19	0.000 19
6	[0.697 85(9)][c]	0.697 72(20)	0.000 13	0.000 13
7	0.454 759(7)[d]	0.454 67(14)	0.000 09	0.000 10
8	0.311 304(3)[d]	0.311 23(14)	0.000 07	0.000 07

[a]Sansonetti and Martin (Ref. 15).
[b]Tepehan, Beyer, and Kleinpoppen (Ref. 28).
[c]See text.
[d]Farley, MacAdam, and Wing (Ref. 20).

column of Table I), since the small corrections under "Additional data" in Table I should be quite accurate.[31] Comparisons of the calculations of the $n\,^1D$ terms ($n=3,4,5$) by Sims *et al.*[10] with the more highly converged results of Kono and Hattori[9] indicate that the corrections added by Sims *et al.* to the final calculated values were overestimates for all three terms.

The data involving each of the $n\,^1P$ terms ($n=6,7,8$) in Table I test the consistency of the calculated $n\,^1P$ term value[9] and the measured $n\,^1F-n\,^1P$ separation[32] with the adopted $n\,^1F$ term value. The results for $n=7$ and 8 show agreement well within the estimated errors of the separation measurements. The result for $n=6$ indicates that the measured $6\,^1F-6\,^1P$ separation,[32] 373 996(15) MHz, is too small by about 40 MHz. This apparent error associated with the $6\,^1P$ level in the anticrossing measurements also occurs in the $6H-6\,^1P$ and $6\,^1D-6\,^1P$ separations obtained in Ref. 32. The $7H-7\,^1P$ and $n\,^1D-n\,^1P$ ($n=7,8$) anticrossing results[32] agree with the separations obtained by using the calculated $n\,^1P$ term values and other data adopted here (see below).

The $6\,^1F$ term value obtained from the calculated $5\,^1D$ term[9] combined with the experimental $5\,^1D-6\,^1F$ separation[33] is 0.0017 cm^{-1} greater than the adopted $6\,^1F$ value. The comparisons made above indicate that the calculated $5\,^1D$ term value is accurate within about 0.0003 cm^{-1}; the final $5\,^1D$ value adopted here (see below) and the adopted $6\,^1F$ term value give a value of 1344.1420(3) cm^{-1} for the $5\,^1D-6\,^1F$ separation.

III. ENERGY LEVELS AND THE IONIZATION ENERGY

It is of special interest to test the calculated energies of the lower $1snl$ terms because of their relatively large relativistic and QED contributions. The most accurate value for the principal ionization energy relative to the $n=2$ levels, which is needed for these tests, is at present obtained by combining experimental $2\,^3S-n\,D$ separations[12,14] with calculated $n\,D$ term values.[9] It is thus advantageous to adopt the $2\,^3S$ position as the reference for the other $1snl$ experimental levels to avoid inclusion of the $2\,^3S$ uncertainty relative to the $2P$ levels, ±0.0005 cm^{-1}, in the ionization-energy uncertainty. The $2\,^3S$ level is also appropriate because it is the lowest excited level; a more accurate experimental connection with the other low levels can probably be expected in the near future.

A. Experimental levels and the ionization energy

Values for the $1snl$ levels, terms, or configuration centers of gravity are included in Table III through $n=8$. The levels determined more accurately relative to $2\,^3P$ than $2\,^3S$ are listed with the estimated error immediately following the level value.[16] The $3\,^1P$ and $3\,^3P$ levels are derived from measurements of the $3\,^1D_2-3\,^1P_1$ frequency[34] and the $3\,^3P_{2,1,0}-3\,^3D_{3,2,1}$ wave numbers.[35] The $2\,^1S$, $3\,^3S$, $4\,^1S$, and $4\,^1P$ levels are based on older measurements having relatively large uncertainties.[36]

The levels evaluated relative to the $2\,^3S$ level are distinguished by the tabulation of their estimated errors in a final separate column. The experimental level separations used to determine the $4,5,6\,^3S_1$ levels, the $4\,^3P$ levels, the $4,5\,^3D$ and $5\,^1D$ levels were discussed in Ref. 16. The $4\,^1D_2$ level was obtained from the $4\,^3D_{cg}$ position and an assumed value of 1.970 39 cm^{-1} for the $4\,^3D_{cg}-4\,^1D_2$ separation (see Table II). The higher levels given in parentheses are discussed in Sec. III B ($l\geq2$ configurations) or in Sec. V B ($n\,P$ and $n\,S$ levels).

Values of the ionization energy (E_I) obtained by combining experimental $n\,D$ levels with term values calculated by Kono and Hattori[8,9] are given in Table IV. Only those $n\,^3D_{cg}$ and ^1D terms having experimental level uncertainties less than 10^{-3} cm^{-1} are included. While the general agreement of the E_I values within the estimated errors is gratifying, the relative sizes of the errors are such that only the E_I values from the $4\,^3D$, $5\,^3D$, and $5\,^1D$ terms need be considered. In accordance with the $n\,^1D$ and $n\,^3D$ comparisons in Tables I and II, the $5\,^1D$ term value gives a higher E_I value than does the $5\,^3D$ term. The $5\,^1D$ term value can be independently evaluated as 4392.379 07(18) cm^{-1} by combining the $5G_{CP}$ term value with the $5G_{CP}-5\,^1G$, $5\,^1F-5\,^1G$, and $5\,^1D-5\,^1F$ separations, all as given in Table I. The weighted average of this $5\,^1D$ term value and the value 4392.379 30(22) cm^{-1} from Kono and Hattori (Table IV) is 4392.379 16 cm^{-1}; the corresponding E_I value, 198 310.772 29 cm^{-1}, agrees well with the value from the $5\,^3D$ term in Table IV. Both of the $5\,^1D$ term values quoted above are somewhat problematical, the value from Kono and Hattori including an apparent systematic error and the other $5\,^1D$ term value involving an extrapolation for the $5\,^1D-5\,^1F$ separation. Making no direct use of the E_I values from the $5\,^1D$ term, we adopt the weighted average of the E_I value from the $5\,^3D$ and $4\,^3D$ terms: $E_I=198\,310.772\,27(40)$ cm^{-1} relative to the $2\,^3S_1$ level at 159 856.077 60 cm^{-1}. The quoted error should be conservative in view of the apparent relative smallness of any systematic error in the calculated $n\,^3D$ term values.

Kono and Hattori[9] recently combined their calculated $n\,D$ term values with the experimental levels to obtain a value 198 310.7725(5) cm^{-1} for the ionization energy relative to $2\,^1P_1$ at 171 135.0000 cm^{-1}. Although this E_I value agrees with the value derived here within the uncertainties, the value of Kono and Hattori is higher mainly due to the effect of calculated $n\,^1D$ term values omitted here. Chang's recent value[24] of 198 310.7722(5) cm^{-1} for the ionization energy relative to $2\,^1P_1$ also agrees with the E_I value obtained here within the uncertainties.

B. Energy levels derived from calculated term values, $l\geq2$

By combining Drachman's theoretical predictions with the available experimental data, including extrapolations via series formulas, one can now derive usefully accurate term values for all levels of the entire $1snl$ system for $n\geq5$, $l\geq2$. In addition to allowing the inclusion of all configurations having $l\geq4$ in this system, the theory yields accurate connections between

TABLE III. Energy levels of $1snl$ configurations through $n=8$. The estimated error in the last decimal place is given in parentheses. Levels evaluated with respect to the $2\,^3P$ term are listed with errors immediately following the level values. The errors for levels evaluated with respect to the $2\,^3S_1$ level are given separately in the last column. Level values not obtained directly from experimental separations are given in parentheses; these levels are discussed in the text or in the footnotes.

Term	J	Level	Uncertainty (Referred to $2\,^3S$)	Term	J	Level	Uncertainty (Referred to $2\,^3S$)
$1\,^1S$	0	0.00±0.15[a]		$5\,^3S$	1	193 347.094 66	(6)
$2\,^3S$	1	159 856.077 60(50)	Ref.	$5\,^1S$	0	(193 663.614 0)	(16)
$2\,^1S$	0	166 277.542(3)		$5\,^3P$	2	(193 800.810 7)	(6)
$2\,^3P$	2	169 086.869 782 (Ref)			1	(193 800.815 3)	(6)
	1	169 086.946 208 (Ref)			0	(193 800.870 7)	(6)
	0	169 087.934 120 (Ref)		$5\,^3D$	3	193 917.254 57	(8)
$2\,^1P$	1	171 135.000 00(11)			2	193 917.255 23	(8)
$3\,^3S$	1	183 236.892[b]			1	193 917.264 69	(8)
$3\,^1S$	0	184 864.932(2)		$5\,^1D$	2	193 918.393 13	(10)
$3\,^3P$	2	185 564.665 1(10)[c]		$5\,^3F$	3	(193 921.221 54)	(41)
	1	185 564.687 1(10)			4	(193 921.224 63)	(41)
	0	185 564.957 7(10)			2	(193 921.229 03)	(41)
$3\,^3D$	3	186 101.649 50(3)		$5\,^1F$	3	(193 921.234 17)	(41)
	2	186 101.652 04(3)		$5\,^3G$	4	(193 921.718 24)	(41)
	1	186 101.696 22(3)			5	(193 921.720 90)	(41)
$3\,^1D$	2	186 105.069 84(9)			3	(193 921.723 53)	(41)
$3\,^1P$	1	186 209.468 45(14)		$5\,^1G$	4	(193 921.725 22)	(41)
$4\,^3S$	1	190 298.216 51	(8)	$5\,^1P$	1	(193 942.565 6)	(7)
$4\,^1S$	0	190 940.330(4)[d]		$6\,^3S$	1	194 936.223 4	(9)
$4\,^3P$	2	191 217.144 0	(5)	$6\,^1S$	0	(195 114.971 2)	(11)
	1	191 217.153 0	(5)	$6\,^3P$	2	(195 192.846 2)	(5)
	0	191 217.263 3	(5)		1	(195 192.848 8)	(5)
$4\,^3D$	3	191 444.584 27	(6)		0	(195 192.880 5)	(5)
	2	191 444.585 48	(6)	$6\,^3D$	3	(195 260.174 66)[e]	(41)
	1	191 444.603 99	(6)		2	(195 260.175 05)	(41)
$4\,^1D$	2	(191 446.559 01)	(20)		1	(195 260.180 51)	(41)
$4\,^3F$	3	(191 451.977 0)	(7)	$6\,^1D$	2	(195 260.873 81)	(40)
	4	(191 451.984 2)	(7)	$6\,^3F$	3	(195 262.527 52)	(40)
	2	(191 451.992 8)	(7)		4	(195 262.529 12)	(40)
$4\,^1F$	3	(191 452.000 5)	(6)		2	(195 262.531 69)	(40)
$4\,^1P$	1	191 492.816(4)[d]		$6\,^1F$	3	(195 262.535 08)	(40)

configurations of different n and fixes the entire system relative to the ionization limit. The largest estimated uncertainty for any of the core-polarization term values used here (for $5\,G$) is about 2 MHz. The microwave data confirm the accuracy of the theory for $l \geq 4$ (fixed n) and extend the system to include the $n\,F$ ($n \geq 5$) and $n\,D$ ($n \geq 6$) levels within estimated relative errors varying from about 3 MHz to less than 0.1 MHz. Unfortunately, no comparably accurate measurement of any optical transition connecting this system to the $2\,^3S_1$ level has yet been made; the most reliable connection is at present made through the ionization limit and thus involves its estimated uncertainty of 0.000 40 cm^{-1} (12 MHz) relative to $2\,^3S_1$.

All levels or terms of this system up through $n=8$ are included in Table III, and series formulas extending the system to the ionization limit are given for terms up through $l=5$ in Sec. VI. The $n\,^1F$ levels for $n=5$–8 were obtained by subtracting the adopted term values (Table I) from the adopted ionization energy. The $n\,^3D$, ^1D ($n=6$–8), $n\,^3G$, ^1G ($n=5$–8), and $n\,^3H$, ^1H ($n=7,8$) levels were then evaluated by combining the $n\,^1F$ positions with pertinent separations given under "Additional data" in Table I and/or other experimental determinations mentioned previously or noted in Table III. The $n\,^3F$ levels were also obtained by combining the $n\,^1$F levels with microwave data.[20–22] The $6\,H_{CP}$, $7\,I_{CP}$, $8\,I_{CP}$, and $8\,K_{CP}$ positions were derived by subtracting theoretical term values [Eqs. (1), (2), and (3)] from the ionization energy. (The level separations within such configurations can of course be accurately predicted.) In accordance with the above discussion, the uncertainties of all levels of the accurate system are dominated by the ionization-energy uncertainty of 4×10^{-4} cm^{-1}, but most separations within the system should have errors smaller than 10^{-4} cm^{-1}, and the relative positions of most of the higher levels should be accurate within 1 or 2×10^{-5} cm^{-1}.

The $4\,^1F_3$ level was evaluated as the difference between the E_I value and the term value $T_r = 6858.771\,80(36)$ cm^{-1}. This total term value was obtained by adding relativistic (Δ_r), singlet-triplet mixing ($\Delta_{s\text{-}t}$), and mass-polarization ($-\varepsilon_M$) contributions to the T_{nr} value of 6858.771 11(20) cm^{-1} calculated by Sims

TABLE III. (*Continued.*)

Term	J	Level	Uncertainty (Referred to $2\,^3S$)	Term	J	Level	Uncertainty (Referred to $2\,^3S$)
$6\,^3G$	4	(195 262.826 38)	(40)	$7\,^1H$	5	(196 071.519 51)	(40)
	5	(195 262.827 96)	(40)	$7\,I_{CP}$		(196 071.532 82)	(40)
	3	(195 262.829 44)	(40)	$7\,^1P$	1	(196 079.190 9)	(5)
$6\,^1G$	4	(195 262.830 42)	(40)	$8\,^3S$	1	(196 461.465 1)	(7)
$6\,H_{CP}$		(195 262.897 75)	(40)	$8\,^1S$	0	(196 534.666 8)	(7)
$6\,^1P$	1	(195 275.011 7)	(5)	$8\,^3P$	2	(196 566.815 1)	(5)
$7\,^3S$	1	(195 868.340 4)	(9)		1	(196 566.816 2)	(5)
$7\,^1S$	0	(195 978.998 0)	(6)		0	(196 566.829 4)	(5)
$7\,^3P$	2	(196 027.418 4)	(5)	$8\,^3D$	3	(196 595.165 51)	(40)
	1	(196 027.420 0)	(5)		2	(196 595.165 68)	(40)
	0	(196 027.439 8)	(5)		1	(196 595.167 97)	(40)
$7\,^3D$	3	(196 069.776 11)	(40)	$8\,^1D$	2	(196 595.477 37)	(40)
	2	(196 069.776 36)	(40)	$8\,^3F$	3	(196 596.182 07)	(40)
	1	(196 069.779 80)	(40)		4	(196 596.182 69)	(40)
$7\,^1D$	2	(196 070.231 69)	(40)		2	(196 596.183 76)	(40)
$7\,^3F$	3	(196 071.279 47)	(40)	$8\,^1F$	3	(196 596.185 41)	(40)
	4	(196 071.280 42)	(40)	$8\,^3G$	4	(196 596.312 97)	(40)
	2	(196 071.282 02)	(40)		5	(196 596.313 65)	(40)
$7\,^1F$	3	(196 071.284 36)	(40)		3	(196 596.314 25)	(40)
$7\,^3G$	4	(196 071.472 04)	(40)	$8\,^1G$	4	(196 596.314 67)	(40)
	5	(196 071.473 04)	(40)	$8\,^3H_{cg}$		(196 596.344 77)	(40)
	3	(196 071.473 97)	(40)	$8\,^1H$	5	(196 596.345 50)	(40)
$7\,^1G$	4	(196 071.474 58)	(40)	$8\,I_{CP}$		(196 596.354 77)	(40)
$7\,^3H$	5	(196 071.517 83)	(40)	$8\,K_{CP}$		(196 596.358 51)	(40)
	6	(196 071.518 47)	(40)	$8\,^1P$	1	(196 601.503 5)	(5)
	4	(196 071.519 01)	(40)	Limit		198 310.772 27	(40)

[a]This is the experimental position of the ground level. Calculated values for the ionization energy give predicted positions of $+0.071(8)$ to $+0.117(23)$ cm^{-1} for the ground level relative to the other levels in this table (see text).

[b]Value from Ref. 36. Comparisons in Table V indicate the position is accurate within a few digits in the third decimal place. The value given for $3\,^3S_1$ in Ref. 16 was calculated from a series formula. Contrary to an implicit assumption in Ref. 16, the error of such an interpolation for a low (second) series member may exceed the error of the neighboring experimentally determined members by an order of magnitude.

[c]The fine-structure intervals for the $3\,^3P$ term have been determined with high accuracy: $^3P_0$-$^3P_1$, 8113.969(80) MHz; $^3P_1$-$^3P_2$, 658.548(69) MHz; $^3P_0$-$^3P_2$, 8772.517(16) MHz [D. H. Yang, P. McNicholl, and H. Metcalf, Phys. Rev. A **33**, 1725 (1986)].

[d]The $4\,^1S_0$ and $4\,^1P_1$ levels have been adjusted to the measured $4\,^1S_0$–$4\,^1P_1$ separation of 552.4861(10) cm^{-1} (Ref. 35).

[e]The $6\,^3D$ fine-structure intervals are from W. D. Perschmann, G. von Oppen, and D. Szostak, Z. Phys. A **311**, 49 (1983).

TABLE IV. Values of the ionization energy E_I referred to the $2\,^3S_1$ level at 159 856.077 60 cm^{-1}. The experimental positions under Level are from the data in Table III except as noted. The total calculated term values (binding energies) are given as the sums of the relativistic term values T_r and the Lamb shifts Δ_L from Ref. 9. The ionization-energy values E_I are the sums of the level and the total calculated term value. Units are cm^{-1}.

Term	Level	$T_r+\Delta_L$	E_I
$3\,^3D_{cg}$	186 101.659 7(5)[a]	12 209.112 6(6)	198 310.772 3(8)
$4\,^3D_{cg}$	191 444.588 62(6)	6866.183 75(42)	198 310.772 37(42)
$5\,^3D_{cg}$	193 917.256 81(8)	4393.515 43(22)	198 310.772 24(23)
$6\,^3D_{cg}$	195 260.176 6(7)[b]	3050.596 29(14)	198 310.772 9(7)
$3\,^1D_2$	186 105.069 8(5)[a]	12 205.703 0(5)	198 310.772 8(7)
$5\,^1D_2$	193 918.393 13(10)	4392.379 30(22)	198 310.772 43(24)
$6\,^1D_2$	195 260.874 4(7)[b]	3049.898 57(14)	198 310.773 0(7)

[a]The uncertainty of the $3\,^3D_{cg}$ and $3\,^1D_2$ positions is dominated by the uncertainty of the $2\,^3S$-$2\,^3P$ separation.

[b]The $6\,^3D_{cg}$ and $6\,^1D_2$ positions are from Ref. 16, the uncertainty appropriate here being that of the $2\,^3S$-$6\,^3D_3$ wave-number measurement (Ref. 12).

et al.[10,37] The $4\,^3F$ levels were then calculated relative to $4\,^1F$ by using the interaction-parameter values[37] $\zeta=65.2$ MHz and $K=77.5$ MHz. Experimental values for the 4,5,6 $^1F_3$ levels were given previously with estimated uncertainties of 0.005–0.009 cm^{-1}, based on the measured $3\,^1D-n\,^1F$ wave numbers.[38] The experimental value of 191 451.995(5) cm^{-1} for the $4\,^1F$ level agrees with the value in Table III, but the previous $5\,^1F$ and $6\,^1F$ levels are 0.040 and 0.033 cm^{-1} lower than the values given here. The apparent errors of the previous $5\,^1F$ and $6\,^1F$ levels were pointed out by Chang.[24]

IV. LAMB SHIFTS OF *n S* AND *n P* TERMS

A. Explanation of experimental Lamb shifts

The new value for the principal ionization energy is equivalent to a term value of 38 454.694 67(40) cm^{-1} for the $2\,^3S_1$ reference level. We define the experimental term value for any level E_L as the difference $T_{\rm expt}=E_I-E_L$, the uncertainty being taken as the quadratic combination of the two uncertainties relative to $2\,^3S_1$. The difference $T_{\rm expt}-T_r$ is a predicted ("experimental") value for the Lamb shift of a term, since the calculated term value T_r should include all significant contributions except the Lamb shift. Experimental Lamb shifts $T_{\rm expt}-T_r$ for several $n\,S$ and $n\,P$ terms are given in Table V, along with some calculated Lamb shifts Δ_L.[9,39–46] The various contributions to the T_r values for the $n=2$ levels[1–5,44,45] are given in Table VI, and the sources for the other T_r values are noted in Table V.

B. *n S* and *n P* Lamb shifts calculated with hydrogenic approximations

The net Lamb shift Δ_L for the term value (ionization energy) of a He I $1snl$ level is calculated as the difference between the Lamb shift of the He II $1s$ ground level, $E_{L,1}$, and the total Lamb shift of the $1snl$ level, $E_{L,2}$. The net Lamb shifts under the heading Δ_L^0 in the last column of Table V were calculated by using hydrogenic approximations to evaluate the two-electron Bethe logarithm and neglecting some electron-electron interaction corrections and other contributions.[9,41] Comparisons with the $T_{\rm expt}-T_r$ values show that the Δ_L^0 values require positive corrections, i.e., the calculated *level* shifts

TABLE V. Lamb shifts for some $n\,S$ and $n\,P$ terms. The predicted shifts are given as the differences $T_{\rm expt}-T_r$, where $T_{\rm expt}$ is the experimental term value and T_r is the corresponding calculated term value not including the Lamb shift. Quantities entering into the T_r values were adjusted to values of the atomic constants as given in Ref. 16 wherever necessary. Some theoretically calculated Lamb shifts Δ_L and Δ_L^0 are tabulated for comparison. Units are cm^{-1}.

Term	$T_{\rm expt}$	T_r	$T_{\rm expt}-T_r$	Δ_L [a]	Δ_L^0 [a]
$1\,^1S$	198 310.772(150)	198 312.036 5(5)[b]	−1.26(15)	−1.335(8),[c] −1.377[d] −1.381(23),[e] −1.381[f]	
$2\,^1S$	32 033.230 3(30)	32 033.321 75(30)[g]	−0.0914(30)	−0.0906,[h] −0.0912[e]	−0.1025[e]
$3\,^1S$	13 445.840 3(20)	13 445.864 8(10)[i]	−0.0245(22)	−0.0205[e]	−0.0298[e]
$4\,^1S$	7370.442 3(40)	7370.452 40(14)[j]	−0.0101(40)	−0.0061[e]	−0.0121[e]
$2\,^3S$	38 454.694 67(40)	38 454.829 54(10)[g]	−0.134 87(41)	−0.1350,[h] −0.1322[e]	−0.1428[e]
$3\,^3S$	15 073.880	15 073.911 15(14)[j]	−0.031	−0.0290[e]	−0.0374[e]
$4\,^3S$	8012.555 76(41)	8012.568 86(14)[j]	−0.013 10(43)	−0.0091[e]	−0.0149[e]
$5\,^3S$	4963.677 61(41)	4963.684 02(10)[j]	−0.006 41(42)	−0.0033[e]	−0.0076[e]
$6\,^3S$	3374.548 87(99)	3374.552 84(10)[j]	−0.0040(10)		−0.0042[j]
$2\,^3P_1$	29 223.826 06(64)	29 223.783 99(20)[g]	0.0421(7)	0.0427[h]	0.038[j]
$3\,^3P_{\rm cg}$	12 746.067 4(11)	12 746.055 13(14)[j]	0.0123(11)	0.011[f]	0.011[j]
$4\,^3P_{\rm cg}$	7093.612 01(64)	7093.606 50(14)[j]	0.0055(7)		0.0044[j]
$2\,^1P$	27 175.772 27(65)	27 175.772 22(20)[g]	0.0000(7)	0.0001[h]	−0.0047[j]
$3\,^1P$	12 101.303 82(66)	12 101.304 09(14)[j]	−0.0003(7)	−0.0002[k]	−0.0017[j]
$4\,^1P$	6817.9563(40)	6817.956 80(14)[j]	−0.0005(40)		−0.0008[j]

[a]Lamb shifts calculated by using the "hydrogenic" approximation for the two-electron Bethe logarithm are given under Δ_L^0 in the last column. Calculated Lamb shifts including corrections to the hydrogenic approximation are given under the Δ_L heading.

[b]The value of $T_{\rm nr}$ from Freund, Huxtable, and Morgan (Ref. 6) corresponds to 198 317.385 79(20) cm^{-1}, the uncertainty being due to the Rydberg constant. The T_r value was obtained as the sum of $T_{\rm nr}$, the $-\varepsilon_M$ contribution (Refs. 1 and 9), and a Δ_r value of −0.5638 cm^{-1} (average of values from Refs. 1 and 9, which differ by 0.0003 cm^{-1}).

[c]Aashamar and Austvik (Ref. 39).

[d]Hata (Ref. 40).

[e]Ermolaev (Ref. 41).

[f]Drake (Ref. 46).

[g]See Table VI.

[h]Evaluated by Kono and Hattori (Ref. 9) using the two-electron Bethe logarithm given by Goldman and Drake (Ref. 42) and including the Q-term contribution. These shifts are evaluated to three decimal places in Ref. 46.

[i]Value obtained as sum of $T_{\rm nr}$ energy from Ref. 5, 13 445.803 89 cm^{-1}, and Δ_r and $-\varepsilon_M$ contributions from Ref. 9.

[j]Kono and Hattori (Ref. 9).

[k]Value obtained by combining the calculated Lamb shift of 0.0001 cm^{-1} for $2\,^1P$ (see *h* above) and 0.0003 cm^{-1} for the shift of the $2\,^1P-3\,^1P$ separation (Ref. 43).

TABLE VI. Calculated term values for the $2\,^3S_1$, $^1S_0$, $^3P_1$, and $^1P_1$ levels. The tabulated quantities are the nonrelativistic term value T_{nr}, the relativistic correction Δ_r, the singlet-triplet mixing correction $\Delta_{s\text{-}t}$, the mass-polarization energy $-\varepsilon_M$, the electron anomalous-magnetic-moment correction Δ_{eam}, and the resulting total relativistic term value T_r. All quantities were adjusted to values of the atomic constants as given in Ref. 16. Units are cm^{-1}.

Contribution	$2\,^3S_1$	$2\,^1S_0$	$2\,^3P_1$	$2\,^1P_1$
T_{nr}	38 453.131 38(10)[a]	32 033.208 24(4)[b]	29 222.155 40(20)[c]	27 176.689 87(20)[c]
Δ_r	1.922 048[d]	0.399 43(30)[d]	−0.314 809[c]	0.467 725[c]
$\Delta_{s\text{-}t}$			0.000 158[e]	−0.000 158[e]
$-\varepsilon_M$	−0.223 892[d]	−0.285 918[d]	1.942 622[c]	−1.385 221[c]
Δ_{eam}			0.000 62[f]	
T_r	38 454.829 54(10)	32 033.321 75(30)	29 223.783 99(20)	27 175.772 22(20)

[a]Pekeris (Refs. 1 and 2).
[b]Frankowski (Ref. 5).
[c]Schiff *et al.* (Ref. 3).
[d]Pekeris (Ref. 2). Pekeris's extrapolated value of Δ_r for $2\,^1S$, given here, was 0.000 67 cm^{-1} less than the final calculated value.
[e]Schiff *et al.* (Ref. 4).
[f]Drake (Ref. 44) and Drake and Makowski (Ref. 45).

are too large in the upward direction ($n\,^1S$, $n\,^3S$, $n\,^1P$) or too small downward ($n\,^3P$).

C. Lamb shifts of $2\,^1S$, $2\,^3S$, $n\,^1P$, and $n\,^3P$ terms; tests of two-electron QED contributions

The calculated Lamb shifts under the Δ_L heading in Table V include screening corrections and two-body (electron-electron interaction) terms. The experimental data confirm these contributions for all four of the $n=2$ terms. The Kono and Hattori[9] evaluations of Δ_L for these terms are based on the Goldman and Drake[42] values for the Bethe logarithm and include the Q term in the two-electron contributions.[45] Their Δ_L values for $2\,^1S$, $2\,^3S$, $2\,^1P$, and $2\,^3P$ all agree with experiment within the errors. Ermolaev's calculated Δ_L shift[41] for $2\,^1S$ also agrees well with the experimental shift. His Δ_L shift for $2\,^3S$ is 2% smaller (absolute value) than the experimental value.

The Q-term two-electron QED contribution and the total two-electron QED contribution, $E'_{L,2}$, from Ref. 45 are given for each $n=2$ term in Table VII. The Q term is the only nonzero contributor to $E'_{L,2}$ for the triplets. The calculated total shifts Δ_L from Ref. 9 and the $T_{expt}-T_r$ values are also given in Table VII. The $E'_{L,2}$ contributions included in the Δ_L values for $2\,^3S$ and $2\,^3P$ in Ref. 9 agree to four decimal places with the $E'_{L,2}$ contributions calculated in Ref. 45, since the Q-term contributions for all four $n=2$ terms agree to this accuracy in the two references. The values of the $E'_{L,2}$ contributions included in the calculated Δ_L values for $2\,^1S$ and $2\,^1P$ were not given in Ref. 9. The calculated $E'_{L,2}$ contribution for $2\,^1S$ (Ref. 45) is, however, much larger than any reasonably expected difference between the values obtained for this quantity in the two calculations; it will be assumed below that the $E'_{L,2}$ contributions obtained for $2\,^1P$ in Refs. 9 and 45 agree within one or two units in the fourth place.

Comparing the Q-term contribution for $2\,^3S$ in Table VII with the $T_{expt}-T_r$ uncertainty, and noting the good agreement of the $T_{expt}-T_r$ value with the calculated Δ_L total shift,[9] we find that the Q contribution is confirmed within an (experimental) uncertainty of about 35%. This confirmation should be qualified by noting that relativistic-recoil and other small corrections[45] were not included in the Δ_L calculations;[9] these contributions are probably not larger than a few units in the fourth decimal place.[47] The much larger $E'_{L,2}$ contribution for $2\,^1S$ is also confirmed within an uncertainty of about 35%, but the present T_{expt} uncertainty for this term is much larger than the calculated Q-term contribution.

A notable feature of the $n\,P$ Lamb shifts, the relatively large downward shifts of the $n\,^3P$ levels due to decreased electron density at the nucleus,[48] is predicted by the hydrogenic approximations Δ_L^0 calculations[9] (Table V). The corrections included in the more accurate Δ_L shift for $2\,^3P$ quoted[9] in Tables V and VII further increase its value to agreement with experiment. Omission of the Q two-electron contribution for $2\,^3P$ (Table VII) would reduce the calculated Δ_L shift to 0.0412 cm^{-1}, as compared with the $T_{expt}-T_r$ value of 0.0421(7) cm^{-1}; the need for the Q contribution for $2\,^3P$ is indicated, but not well established, by the data now available.

The already relatively small Δ_L^0 value calculated for $2\,^1P$ (upward level shift) is essentially canceled by the corrections included in the more accurate Δ_L value,[9] also in agreement with experiment. The $T_{expt}-T_r$ values for both $2\,^1P$ and $3\,^1P$ indicate Lamb shifts having absolute values $\lesssim 10^{-3}$ cm^{-1}, and the experimental shift for $4\,^1P$ is also consistent with a value of zero within its much larger uncertainty. The calculated total two-electron QED contribution $E'_{L,2}$ for $2\,^1P$ and the included Q contribution (Table VII) (Ref. 45) are confirmed by the data in Table V within fractional uncertainties of about 35 and 55%, respectively. Here again the estimated uncertainties do not take into account any error due to neglect of small additional contributions[45] in the calculated T_r or Δ_L values.[47]

D. Lamb shifts of the $2\,^3S-2\,^3P$ and $2\,^3P-2\,^1P$ separations

These shifts have attracted theoretical interest.[42,43,45,48,49] The differences between the experi-

TABLE VII. Data pertinent to two-electron QED contributions for $n=2$ terms. The calculated Q-term contributions and total two-electron contributions $E'_{L,2}$ are from Ref. 45. The calculated total Lamb shifts Δ_L (Ref. 9) include the two-electron contributions. The experimental Lamb shifts $T_{\text{expt}}-T_r$ are from Table V. Units are cm^{-1}.

	$2\,^3S$	$2\,^1S$	$2\,^3P_1$	$2\,^1P$
Q term	0.001 23	0.002 1	0.001 54	0.001 33
$E'_{L,2}$	0.001 23	0.011 0	0.001 54	0.002 09
Δ_L	−0.013 50	−0.090 6	0.042 7	0.000 1
$T_{\text{expt}}-T_r$	−0.134 87(41)	−0.091 4(30)	0.042 1(7)	0.000 0(7)

mental and calculated wave numbers, $\sigma_{\text{expt}}-\sigma_r$, give experimental Lamb shifts which are compared with calculated shifts Δ_L in Table VIII. The $\Delta_L(2\,^3P_1-2\,^1P_1)$ shift obtained from the most comprehensive calculation[45] agrees well with the $\sigma_{\text{expt}}-\sigma_r$ value, whereas the value 0.0426 cm^{-1} obtained from a less exact calculation[9] is too large by 0.0006(3) cm^{-1}. The latter calculation gave the individual shifts 0.0427 cm^{-1} for $2\,^3P_1$ and 0.0001 cm^{-1} for $2\,^1P_1$ (Table V); a decrease of the $2\,^3P_1$ shift to 0.0421 cm^{-1} would give good agreement with the corresponding $T_{\text{expt}}-T_r$ value in Table V and with the $\sigma_{\text{expt}}-\sigma_r$ value for the $2\,^3S_1-2\,^3P_1$ separation in Table VIII (the calculated value −0.1777 cm^{-1} would be changed to −0.1771 cm^{-1}).

Drake and Makowski's calculation[45] of $\Delta_L(2\,^3P_1-2\,^1P_1)$ as given in Table VIII includes corrections due to screening (−0.000 75 cm^{-1}), the two-electron terms (−0.000 55 cm^{-1}), the finite nuclear size (0.000 11 cm^{-1}), and the relativistic recoil shift (−0.000 49 cm^{-1}). These small contributions give very good agreement with the $\sigma_{\text{expt}}-\sigma_r$ value, but the absolute value of the sum of the last two contributions, for example, is only slightly larger than the estimated σ_r uncertainty of ±0.000 28 cm^{-1}. The uncertainty of ±0.0005 cm^{-1} given for the theoretical Δ_L value represents "further uncalculated contributions arising from second-order cross terms between the Breit interaction and the mass polarization operator."[45] More accurate calculations of σ_r and, eventually, more accurate measurements of σ_{expt}, will be needed to test small but theoretically significant contributions to such term separations.

E. Lamb shifts of $n\,^1S$ and $n\,^3S$ terms, $n \geq 3$

The $T_{\text{expt}}-T_r$ values for $3\,^1S$, $4\,^3S$, and $5\,^3S$ are sufficiently accurate to test the calculated Δ_L shifts in Table V. The absolute values of Ermolaev's Δ_L shifts for these terms[41] are smaller than the $T_{\text{expt}}-T_r$ absolute values by 16%, 30%, and 48%, respectively. The hydrogenic-approximation Δ_L^0 absolute values for the $n\,S$ terms are larger than the $T_{\text{expt}}-T_r$ absolute values by 6% for $2\,^3S$, 12% for $2\,^1S$, and by amounts probably not exceeding 25% for the higher n values. It seems likely that the screening corrections for the shifts of the higher $n\,S$ terms were significantly overestimated in Ref. 41.

F. Ground level

The calculated values of Δ_L for the $1s^2\,^1S$ ground level in Table V agree with the experimental value $[T_{\text{expt}}-T_r=-1.26(15)\ \text{cm}^{-1}]$ within the relatively large uncertainty of the latter. These calculated Δ_L values include two-electron QED contributions, which, as given explicitly in Refs. 40 and 45, amount to $E'_{L,2}=+0.140$ cm^{-1}; the $T_{\text{expt}}-T_r$ result thus supports the total $E'_{L,2}$ two-electron contributions qualitatively in the sense that omission of $E'_{L,2}$ would yield calculated Δ_L values in the range −1.475 to 1.521 cm^{-1}, in disagreement with experiment. The difference between the experimental E_I value and the total calculated $1\,^1S$ term value, $T_r+\Delta_L$, gives a predicted position for the ground level with respect to the excited levels and ionization limit in Table III. The values thus obtained for the ground level by using the calculated values of Δ_L in Table V vary from

TABLE VIII. Lamb shifts of the $2\,^3S_1-2\,^3P_1$ and $2\,^3P_1-2\,^1P_1$ separations. The experimental term separations σ_{expt} are from Table III, and the calculated relativistic separations σ_r are from Table VI. The experimental Lamb shifts, $\sigma_{\text{expt}}-\sigma_r$, are compared with calculated shifts Δ_L. Units are cm^{-1}.

Separation	σ_{expt}	σ_r	$\sigma_{\text{expt}}-\sigma_r$	Δ_L
$2\,^3S_1-2\,^3P_1$	9230.868 61(50)	9231.045 55(22)	−0.176 94(55)	−0.173,[a] −0.1820,[b] −0.1777[c]
$2\,^3P_1-2\,^1P_1$	2048.053 79(11)	2048.011 77(28)	0.042 02(30)	0.042 60,[d] 0.0426,[c] 0.042 15(50)[e]

[a]Ermolaev (Ref. 48).
[b]Hata and Grant (Ref. 49).
[c]Evaluated by Kono and Hattori (Ref. 9) using the Bethe logarithms given by Goldman and Drake (Ref. 42).
[d]Hata (Ref. 43).
[e]Drake and Makowski (Ref. 45). The quoted value of Δ_L is the sum of five contributions beginning with $\Delta E^0_{L,2}+\Delta E^{\text{HO}}_{L,2}$ given in the second column of Table 3 of Ref. 45. The sign of the contribution $\Delta E^0_{L,2}+\Delta E^{\text{HO}}_{L,2}$ in Table 3 should be positive, and the correct value of $\Delta E'_{L,2}$ is −0.000 55 cm^{-1}. The mass-polarization contribution is increased to 3.327 84 cm^{-1} by adjustment to the current values of the atomic constants [G. W. F. Drake (private communication)].

$+0.071(8)$ to $+0.117(23)$ cm^{-1}. An order-of-magnitude increase in the accuracy of the experimental connection between the ground level and the excited levels would quantitatively test the calculated two-electron and higher-order QED contributions to the E_I value and help resolve the discrepancy between the calculated total Lamb shifts in Table V.

V. EVALUATION OF HIGHER $n\,P$ AND $n\,S$ LEVELS

A. Accuracy of the $3\,^3S$, $4\,^1S$, and $4\,^1P$ levels

The data for these levels in Table V allow one to estimate the experimental accuracies by comparisons of the $T_{\text{expt}}-T_r$ values with the calculated Δ_L values. The Δ_L^0 values in the last column, scaled according to comparisons with accurate $T_{\text{expt}}-T_r$ values for other levels, are useful for this purpose. The comparisons indicate that all three of the above levels are accurate within a few units in the third place.

B. Higher $n\,P$ and $n\,S$ levels, including "experimental" Lamb shifts for $7\,^1S$, $8\,^1S$, and $8\,^3S$ terms

The $n\,^3P$ levels for $n=5-8$ in Table III are based on $n\,^3P_{\text{cg}}$ positions obtained as the differences between the adopted ionization energy and term values $T=T_r+\Delta_L$. The calculated T_r values were taken from Ref. 9, and the Δ_L values were obtained by applying the above-noted n^{-3} scaling to the $T_{\text{expt}}-T_r$ value for $2\,^3P_1$. The assumed Δ_L values for $n=5-8$ were 0.002 73(40), 0.001 58(25), 0.001 00(15), and 0.000 67(10) cm^{-1}. The fine-structure intervals are mainly from microwave spectroscopic or level-crossing measurements.[50–52] The $n\,^3P_1-^3P_0$ intervals for $n=7$ and 8 were obtained by extrapolation of regularities of the $n\,^3P$ fine structures[53] for $n=3-6$.

The $n\,^1P$ term values for $n=6-8$ in Table I and the $n\,^1P$ levels for $n=5-8$ in Table III were evaluated by using the calculated T_r values[9] with assumed Δ_L values of zero. The uncertainties of the assumed zero shifts were taken as equal to Δ_L^0 values obtained by extrapolation: 0.0003, 0.0002, and 0.0002 cm^{-1} for $n=6-8$, respectively.

The $7\,^1S$, $8\,^1S$, and $8\,^3S$ levels were evaluated by using corresponding $n\,P$ levels with experimental $n\,S-n\,P$ separations.[54] The data are given under σ_{expt} in Table IX. Some results pertinent to the Lamb shifts of the three $n\,S$ terms are included in this table. The "σ_r'" separations were obtained from the calculated term values[9] with the estimated Δ_L shifts for the $n\,P$ terms, as given above, included. The $\sigma_{\text{expt}}-\sigma_r'$ values are thus experimental Lamb shifts for the $n\,S$ terms involved in the measurements. These Lamb-shift values are consistent with the trends of the values for the corresponding lower $n\,S$ terms in Table V, within the errors.

Calculated term values[9] and estimated Lamb shifts have been used to derive $5\,^1S$, $6\,^1S$, and $7\,^3S$ levels more accurate than the available experimental values and thus to complete Table III through $n=8$. The Δ_L values for $5\,^1S$ as calculated with and without correction for screening are -0.0014 and -0.0056 cm^{-1}, respectively.[41] Based on these values and comparisons of the data and calculated Δ_L values for the $3\,^1S$, $4\,^3S$, and $5\,^3S$ terms in Table V (see above discussion), and on the experimental Δ_L value of $-0.0012(4)$ cm^{-1} for $7\,^1S$ (Table IX), and Δ_L values for $5\,^1S$ and $6\,^1S$ were taken as $-0.0035(15)$ cm^{-1} and $-0.0020(10)$ cm^{-1}, respectively. A value of $-0.0023(8)$ cm^{-1} was estimated for the Lamb shift of the $7\,^3S$ term by using the experimental and calculated $n\,^3S$ shifts in Table V and the experimental $8\,^3S$ shift in Table IX.

VI. SERIES FORMULAS

The energy levels of a $1snl$ configuration for any value of n can be obtained by parametrization of the term value as a function of n (series formula). The series for higher l values can be accurately represented by fitting the term defects Δ (deviations from hydrogenic term values) to expressions such as Eq. (4). Farley *et al.*[20] fitted this expression to the $n\,D$, $n\,F$, and $n\,G$ series taking $n\,^3G_5$ as the reference level; the experimental results represented in their formulas can be transposed to term-defect formulas by using Drachman's values for the $n\,G$ defects. Drachman's results for the $n\,G$ and higher l configurations can also be very accurately reproduced by two-constant core-polarization formulas.[55]

All of the $1snl$ series can be represented by extended Ritz formulas, which give the quantum defects $n-n^*$, instead of the term defects, as a function of n. The effective principal quantum number n^* is defined by the relation $T=R(^4\text{He})/(n^*)^2$, where T is the term value, and the corresponding energy level E_L is obtained as $E_L=E_I-T$. We here use the Ritz formula

$$n-n^*=a+bm^{-2}+cm^{-4}+dm^{-6}\ , \tag{5}$$

TABLE IX. $n\,S-n\,P$ separations, $n=7,8$. The measured separations σ_{expt} are from Ref. 54. The calculated separations σ_r' include estimated Lamb shifts for the $n\,P$ terms involved. The differences $\sigma_{\text{expt}}-\sigma_r'$ are experimental values for the Lamb shifts of the $n\,S$ terms. Units are cm^{-1}.

Separation	σ_{expt}	σ_r' [a]	$\sigma_{\text{expt}}-\sigma_r'$
$7\,^1S_0-7\,^1P_1$	100.192 9(2)	100.194 1(3)	−0.001 2(4)
$8\,^1S_0-8\,^1P_1$	66.836 7(4)	66.837 2(3)	−0.000 5(5)
$8\,^3S_1-8\,^3P_1$	105.351 1(4)	105.352 5(2)	−0.001 4(5)

[a]The values for these term separations obtained from the calculated T_r term values in Ref. 9 are 100.194 12(20), 66.837 23(17), and 105.353 15(14) cm^{-1}, respectively. These calculated separations were combined with estimated Lamb shifts for the $n\,P$ terms involved to obtain the σ_r' values (see text).

where $m=n-a$. The values of the constants a,b,c,d given for the series in Table X thus represent term values for all $1snl$ configurations through $l=5$; the energy-level data for these series in Table III are effectively extended to the series limit.

The constants for the $n\,D$ through $n\,H$ series were evaluated by least-squares fitting of five-place term values through $n=10$. The term values for the higher series members were based on the microwave data and Drachman's $n\,G$ and $n\,H$ term defects [Eqs. (2) and (3)]. The formulas for these series thus represent the relatively accurate system of $1snl$ term values, $n\geq 5$, $l\geq 2$, discussed in Sec. III B. The three $n\,^3D$ levels are represented by the $n\,^3D_3$ series constants in Table X, and the four levels for each $n\,F$, $n\,G$, and $n\,H$ configuration are represented by a single series for each l value ($n\,^1F$, $n\,G_{\rm CP}$, and $n\,H_{\rm CP}$). Term values for the other $n\,^3D$ and $n\,F$ levels can be obtained by combining the series formulas given here with the level-separation formulas of Farley *et al.*[20] The positions of the $n\,G$ and $n\,H$ levels relative to the $n\,G_{\rm CP}$ and $n\,H_{\rm CP}$ positions are given accurately by simplified $1snl$ structure equations (see the Appendix and Ref. 24) and the $n\,G$ level separations can also be obtained from the fitted formulas.[20] Drachman's results[11] can of course be used to obtain series formulas for arbitrarily high l values.

The constants for the $n\,S$ and $n\,P$ series were evaluated by fitting the term values through $n=8$. The estimated uncertainties of the predicted term values near $n=8$ are about 0.0004 and 0.0002 $\rm cm^{-1}$, respectively, but the uncertainties of course decrease for high n values. A gratifying demonstration of the latter point was obtained by comparing the $n\,^1D_2-n\,^1P_1$ separations predicted by the series formulas with experimental determinations for $n=16$, 17, and 18 (22 807 to 16 029 MHz);[56] the largest discrepancy is 1.1(6) MHz.

The $n\,^3P$ fine structures have not been measured for high n values, but the intervals can be approximately predicted by fitting Eq. (4) to the measurements for lower n values.[53] The approximations $6.66/n^3$ and $0.55/n^3$ $\rm cm^{-1}$ for the $n\,^3P_1-{}^3P_0$ and $n\,^3P_2-{}^3P_1$ intervals, respectively, are probably accurate within a few percent for $n\geq 9$.

VII. CONCLUSION

In this paper, experimental data and theoretical calculations for a wide range of energies in helium have been tested for consistency and combined to obtain more accurate levels and ionization energies for the $1snl$ system. As an example of the broad interdependence of these results, it may be noted that the experimental Lamb shifts derived for $2\,S$ and $2\,P$ terms (Tables V and VII) were affected by microwave data for transitions between levels of configurations having $n\geq 5$, $l\geq 2$ and theoretical calculations for $n\,G$ and $n\,H$ terms (Table I). Although it is gratifying that certain combinations of measurements and calculations are now sufficiently accurate to test relatively small two-electron contributions to the $2\,S$ and $2\,P$ Lamb shifts, these results and other basic tests of two-electron atomic theory can be greatly improved by new measurements.

The largest contributions to the uncertainties of the experimental Lamb shifts, $T_{\rm expt}-T_r$, in Tables V and VII are the uncertainties of the experimental ionization energies for the $n\,S$ and $n\,P$ levels involved. Measurements to improve these ionization energies might begin with accurate optical determinations connecting one of the $n=2$ levels (probably $2\,^3S$ or $2\,^1S$) with higher levels having term values accurate to 1 MHz or less. Upper levels connected to the ionization limit via accurate core-polarization theoretical term defects (Sec. III B) would be suitable, and an independent determination of the ionization energy by new measurements and series-formula fitting of one or more $1snl$ series is also desirable. High-accuracy measurements interconnecting the lower $n\,S$ levels and also connecting these levels with the lower $n\,P$ levels would then yield improved experimental term values for the excited levels of most interest for QED calculations.

The need for other new measurements is clear from the fact that most of the levels in Table III were derived at least in part from calculations. It may be useful to recall here in particular some of the level separations incorporated in Table III that disagree with experimental determinations by more than the estimated experimental errors: these include the $3\,^1D-5\,^1F$, $3\,^1D-6\,^1F$,

TABLE X. Ritz-formula constants for $1snl$ series through $l=5$. The effective principal quantum numbers n^* for the members of a particular series are obtained by using the appropriate set of constants a,b,c,d in Eq. (5). The $1s^2\,^1S_0$ ground level was omitted in deriving the constants for the $n\,^1S_0$ series. The value of the ^{4}He Rydberg constant was taken as 109 722.273 09 $\rm cm^{-1}$.

Series	a	b	c	d
$n\,^3S_1$	0.296 654 86	0.038 246 14	0.008 257 4	0.000 359
$n\,^1S_0$	0.139 718 54	0.027 727 93	0.017 488 5	0.002 566
$n\,^3P_2$	0.068 358 86	−0.018 701 11	−0.011 773 0	−0.008 540
$n\,^1P_1$	−0.012 143 07	0.007 440 58	0.014 257 3	0.005 413
$n\,^3D_3$	0.002 890 43	−0.006 469 1	0.001 362	−0.003 25
$n\,^1D_2$	0.002 112 52	−0.003 205 3	0.001 137	−0.005 30
$n\,^1F_3$	0.000 439 24	−0.001 785 0	0.000 465	
$n\,G_{\rm CP}$	0.000 125 68	−0.000 899 2	0.000 70	
$n\,H_{\rm CP}$	0.000 047 56	−0.000 552	0.001 12	

$5\,^3P-7\,^3D$, $5\,^1D-6\,^1F$, $6\,^3P-8\,^3S$, and $6\,^1F-6\,^1P$ transitions and the $7\,^3P_1-{}^3P_0$ fine-structure interval. The $4F$ level positions and separations should also be determined experimentally.

The need for more accurate calculations of a number of $1snl$ term values and Lamb shifts is apparent from the discussions of pertinent data in this paper. Expected improvements in the measurements of this spectrum as outlined above would yield experimental energies for the important lower levels $2S$, $3S$, $2P$, $3P$, etc., with accuracies exceeding the accuracies of any existing calculated ionization energies including QED shifts. It is hoped that the results in this paper will, among other uses, be helpful in planning future experimental and theoretical research on the helium energy-level structure.

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APPENDIX: APPROXIMATE LEVEL STRUCTURE OF HELIUM $1snl$ CONFIGURATIONS FOR HIGH l VALUES

Chang[24] and Lundeen[24] obtained equations for the four $1snl$ energy levels involving a single magnetic-interaction parameter h by using the approximation

$$-h_{\rm SO}=-h_{\rm off}/3=h_{\rm SS}=h\ , \tag{A1}$$

where $h_{\rm SO}$, $h_{\rm off}$, and $h_{\rm SS}$ represent the spin-orbit, the off-diagonal, and the spin-spin magnetic-interaction integrals.[31] The approximation is derived by assuming hydrogenic wave functions, and the magnetic interactions are proportional to $R\alpha^2\langle r^{-3}\rangle_{nl}$. The hydrogenic value of the integral $\langle r^{-3}\rangle_{nl}$ gives the result

$$2h=\zeta_{nl}=R\alpha^2[n^3l(l+\tfrac{1}{2})(l+1)]^{-1}\ , \tag{A2}$$

where we adopt the usual expression of the spin-orbit interaction,[23] ζ_{nl}. The equations[24] connect ζ and the $T(^3L_{l+1})-T(^3L_{l-1})$ interval, the latter being positive as written since the letter T represents the term value,

$$\zeta=2(2l+1)^{-1}[T(^3L_{l+1})-T(^3L_{l-1})]\times[1-6(4l^2+4l+3)^{-1}]\ . \tag{A3}$$

One also finds from these equations[24] an expression for the difference between the term value for the direct Coulomb-interaction configuration energy, $T(L_{\rm CP})$, and the term value of the uppermost level, $T(^1L)$,

$$T(L_{\rm CP})-T(^1L)=\tfrac{1}{2}[T(^3L_l)-T(^1L_l)]-\tfrac{1}{4}\zeta\ . \tag{A4}$$

The ^3L_l-^1L_l separation is of course dependent on the exchange energy K,

$$T(^3L_l)-T(^1L_l)=[(2K+\tfrac{1}{2}\zeta)^2+9l(l+1)\zeta^2]^{1/2}\ , \tag{A5}$$

which simplifies to

$$T(^3L_l)-T(^1L_l)=3\zeta[l(l+1)]^{1/2} \tag{A6}$$

for higher-l configurations, the exchange interaction K then being negligible. The $n\,G_{\rm CP}-n\,^1G$ separations in Table III were obtained from (A4) by using the experimental $^3G_4$-$^1G_4$ separations with ζ values from (A2). The $7H_{\rm CP}-7\,^1H$ separation was evaluated by the same method, and the $8H_{\rm CP}-8\,^1H$ separation was obtained from (A2), (A4), and (A6).

It is interesting to note the even simpler form of the $1snl$ level structures for $l\gg1$. The intervals separating the neighboring levels are then

$$\begin{aligned}&T(^3L_l)-T(^3L_{l+1})=(l+\tfrac{3}{2})\zeta\ ,\\ &T(^3L_{l+1})-T(^3L_{l-1})=(l+\tfrac{1}{2})\zeta\ ,\\ &T(^3L_{l-1})-T(^1L_l)=(l-\tfrac{1}{2})\zeta\ .\end{aligned} \tag{A7}$$

The neighboring intervals differ by ζ, so that the separation of the outer two levels is three times the interval between the inner levels. The separations predicted by (A7) and (A2) agree with the experimental structure[57] for $1s\,10h$ within 5%.

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[26]The Lamb shifts of the $n\,^1P$ levels are discussed in Sec. IV. The uncertainties for the 6,7,8 ^1P term values in Table I include estimated Lamb-shift uncertainties of 0.0003, 0.0002, and 0.0002 cm^{-1}, respectively.

[27]The $n\,^1D-n\,^1F$ data were also fit by including the value 163 148(16) MHz for $n=4$ (see Table III and Sec. III B). The resulting interpolated value for $n=5$ differed from the extrapolated value in Table I by only 0.3 MHz (10^{-5} cm^{-1}).

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