Correction to the $n\,^3P_1$ Levels of the Helium Isoelectronic Sequence Owing to Mixing with the $n\,^1P_1$ State

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The contribution to the $n\,^3P_1$ ionization energy owing to mixing with the $n\,^1P_1$ state has been computed for the $2\,^3P$ to $5\,^3P$ states of the helium isoelectronic sequence up to $Z = 10$. Corrected values for the fine-structure splittings of these levels are listed. The theoretical and experimental values for the $2\,^3S_1$-$2\,^3P_1$ energy difference are found to be in good agreement provided that the $2\,^1P_1$ mixing correction to the $2\,^3P_1$ level and an estimate of the Lamb-shift correction to the $2\,^3S_1$ energy are included in the calculation.

The high accuracy now obtainable in measurements[1-6] of the spectra of two-electron ions has emphasized the need for more-accurate and extensive calculations of the theoretical ionization energies. In a recent paper[7] (hereafter referred to as APS), the present authors have reported theoretical ionization energies for the low-lying S and P states of the helium isoelectronic sequence up to $Z=10$. The calculations for the P states included the quantum-electrodynamic corrections of order α^3, but not the higher-order corrections. They also did not include the correction to the n^3P_1 level owing to mixing with the $^1P_1$ states. Ermolaev and Jones have recently pointed out[8] that this correction grows in importance with increasing Z. Using approximate wave functions and expansions in powers of Z^{-1}, Ermolaev and Jones computed the correction to the n^3P_1 level due to the mixing with the close-lying n^1P_1 state in the cases of the 2^3P_1 and 3^3P_1 states for various values of Z. Following these authors, we shall denote this correction by E_{st}. It was felt desirable to evaluate E_{st} using more-accurate wave functions, particularly for the lower values of Z, where correlation effects are important. We have used the wave functions described in APS to calculate E_{st} for the $2\,^3P$ to $5\,^3P$ states up to $Z=10$ following the method of Araki *et al.*[9] Wave function expansions containing up to 364 terms were used for He and Li^+, and up to 120 terms for higher values of Z. The results converged satisfactorily as the number of terms in the expansion was increased except for the case of the $5\,^3P$ state, where the values obtained were felt to be reliable to only one significant figure. The values of E_{st} obtained are listed in Table I. The quantity tabulated has to be added to the ionization potential of the $^3P_1$ state. The values for the 2^3P states are in excellent agreement with those previously given by Drake.[10] The n^3P_1 level is also affected by mixing with the other $^1P_1$ states apart from n^1P_1. However, their effect is much smaller, owing to the appearance of the singlet-triplet energy difference in the denominator. A calculation of the contribution from all of the $^1P_1$ states has been carried out by Hambro[11] for the 2^3P_1 level of helium. Hambro's results indicate that the states other than 2^1P_1 contribute as much as 27% to the total correction. The relative magnitude of this effect will probably be similar for the other $^3P_1$ states of helium, but will decrease with increasing Z.

Values for the fine-structure splitting of the ^3P levels were listed in Table XXVI of APS. These values did not include the contribution from the E_{st} term. On including this correction, we obtain the values for the splittings shown in Table II. Measurements exist of the fine-structure splitting of the 2^3P level for various values of Z. On

TABLE I. Values of E_{st} in cm^{-1}. The value listed has to be added to the ionization potential of the $^3P_1$ state.

Z	$2\,^3P$	$3\,^3P$	$4\,^3P$	$5\,^3P$
2	0.000 158 3	0.000 042 1	0.000 017	0.000 01
3	0.004 465	0.001 259	0.000 52	0.0003
4	0.0409	0.0120	0.005	0.003
5	0.2174	0.0651	0.03	0.01
6	0.833	0.254	0.11	0.05
7	2.567	0.790	0.34	0.2
8	6.756	2.10	0.90	0.5
9	15.80	4.94	2.1	1.1
10	33.68	10.59	4.5	2

TABLE II. Fine-structure splitting for the ^3P states, including the correction E_{st}. The quantities $\Delta\nu_{01}$ and $\Delta\nu_{21}$ are to be added to the total ionization energy for the $J=1$ level to obtain the values for the $J=0$ and $J=2$ levels, respectively.

	$2\,^3P$		$3\,^3P$		$4\,^3P$		$5\,^3P$	
Z \ State	$\Delta\nu_{01}$ (cm^{-1})	$\Delta\nu_{21}$ (cm^{-1})	$\Delta\nu_{01}$ (cm^{-1})	$\Delta\nu_{21}$ (cm^{-1})	$\Delta\nu_{01}$ (cm^{-1})	$\Delta\nu_{21}$ (cm^{-1})	$\Delta\nu_{01}$ (cm^{-1})	$\Delta\nu_{21}$ (cm^{-1})
2	−0.988 00	0.076 37	−0.270 67	0.021 95	−0.1103	0.0090	−0.0556	0.0048
3	−5.194 43	−2.089 88	−1.3473	−0.6270	−0.540	−0.265	−0.270	−0.135
4	−11.5586	−14.8829	−2.839	−4.406	−1.12	−1.85	−0.55	−0.94
5	−16.1971	−52.6134	−3.533	−15.523	−1.32	−6.52	−0.64	−3.32
6	−12.504	−135.632	−1.411	−39.982	−0.3	−16.8	−0.1	−8.6
7	8.674	−290.525	6.30	−85.64	3.2	−36.0	1.7	−18.4
8	58.757	−550.394	23.00	−162.30	10.5	−68.3	5.5	−34.9
9	151.04	−955.26	52.67	−281.85	23.3	−118.6	12.1	−60.6
10	300.14	−1552.57	99.60	−458.40	43.5	−192.9	23	−98

adding their values for E_{st} to the fine-structure splittings listed in Table XXVI of APS, Ermolaev and Jones found the agreement between theory and experiment to be satisfactory in all cases. We will not repeat this comparison here, as our values of E_{st} for the 2^3P states agree with those of Ermolaev and Jones to well within the experimental error.

TABLE III. Comparison of theory and experiment for the $2\,^3S_1$-$2\,^3P_1$ lines of O VII, F VIII, and Ne IX. (All quantities in cm^{-1}.)

	O VII	F VIII	Ne IX
		$2\,^3S_1$ (theory)	
Nonrelativistic eigenvalue	1 436 334.7	1 861 450.6	2 341 432.9
Mass polarization and relativistic corrections	1440.1	2378.7	3714.2
Lamb shift estimate	−58	−92	−141
Total ionization potential	1 437 717	1 863 737	2 345 006
		$2\,^3P_1$ (theory)	
Nonrelativistic eigenvalue	1 375 931.9	1 792 710.7	2 264 364.8
Mass polarization and relativistic corrections	737.3	1266.4	2046.6
E_{st}	6.8	15.8	33.7
Total ionization potential	1 376 676.0	1 793 992.9	2 266 445.1
		$\nu(2\,^3S_1 - 2\,^3P_1)$	
Theory	61 041	69 744	78 561
Experiment	61 039 ± 3	69 744 ± 3	78 566 ± 2
Experiment − theory	−2 ± 3	0 ± 3	5 ± 2

Engelhardt and Sommer[6] have recently measured the energy difference between the 2^3S_1 and 2^3P levels for O VII, F VIII, and Ne IX to a particularly high accuracy. Their measured values for the wave number of the 2^3S_1-2^3P_1 transition are compared with our theoretical values in Table III. In order to show the orders of magnitude of the various quantities involved, we have listed the various contributions to the ionization energies separately. Full details of the method of calculation are given in APS. The estimate of the Lamb shift was obtained by scaling up the value for $Z=3$, assuming a Z dependence of Z^4. In view of this rather crude assumption, the degree of agreement between theory and experiment is better than we had a right to expect. The table does, however, verify the need for including E_{st} in order to match the experimental accuracy.

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