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Comment on Finestructure Data of Three-Electron Quartet States

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Abstract

In recent VUV spectroscopic studies of fast ion beams the $1s2s2p\ ^4P^0 - 1s2p^2\ ^4P$ transitions have been measured and the finestructure intervals and the multiplet separation have been determined for ions of C to Al. Because several of these studies show inconsistencies of the data evaluation, the above entities have been reevaluated from the published wavelengths. A comparison with theory shows an improved agreement with the revised data.

Doubly-excited states of three-electron ions are of interest to experimenters and theoreticians, because they are few-body systems which show a variety of decay modes like in-shell and inter-shell (intercombination) radiative decays and autoionization. There are doubly-excited doublet and quartet states; the quartet states are more amenable to optical studies because the inter-shell decay to singly-excited doublet states and the autoionization decay branch are hindered as a consequence of selection rules. Transitions between the lowest quartet levels, $1s2s2p\ ^4P^0_{1/2,3/2,5/2}$ and $1s2p^2\ ^4P_{1/2,3/2,5/2}$, are the ones for which data are available for the widest range of nuclear charge, namely for ions up to $Z = 13$.

Here we consider only data obtained by employment of fast ion beams. Since the pioneering study of C, N and O by Livingston and Berry [1] observations of the $2\ ^4P^0 - 2\ ^4P$ transitions have been reported for F [2], Ne [3, 4], Mg [5, 6], and Al [7, 8]. Work on Si is in progress at Lyon and at Bochum. Theoretical data on the finestructure intervals of the $2\ ^4P^0$ and $2\ ^4P$ multiplets and on the $2\ ^4P^0 - 2\ ^4P$ multiplet separation have been published by Goldsmith [9], Cheng *et al.* [10], Chen *et al.* [11], Hata and Grant [12], and by Chung [13] or can be derived from a combination of x-ray transition energies [14] with experimental $2\ ^2S - 2\ ^2P^0$ term differences [15].

The relative positions of the 6 levels in the two multiplets can be described by 5 parameters. Here the parameter set defined by Cheng *et al.* [10] is adopted; it consists of the two finestructure (fs) intervals in each multiplet and the term difference (multiplet separation) ΔT_{CG} of the centers of gravity of the multiplets. The term value of the center of gravity of a multiplet is defined as

$$T_{CG} = \frac{\Sigma(2J+1)T_J}{\Sigma(2J+1)}$$

with T_J the term value of an individual level with total angular momentum J. The term separation then is

$$\Delta T_{CG} = T_{CG}(^4P) - T_{CG}(^4P^0)$$

and the mean transition wavelength as used below can be defined as the inverse of the multiplet separation.

$$\bar{\lambda} = 1/\Delta T_{CG}.$$

This choice appears straightforward in terms of the theoretical level structure. A definition of $\bar{\lambda}$ as based on the observed line multiplet would be less reproducible, because the relative line intensities in time-resolved spectroscopy – as is the case for all the above studies – depends on the length of the section of the ion beam observed by the spectrometer and on the lifetime of the upper level of the transition studied; the lifetimes of the $2\ ^4P$ levels (as well as those of the $2\ ^4P^0$ levels) show differential metastability and thus are markedly different. If the section of beam in the field-of-view of the detection system is short compared to the decay length of the transition studied, the observed light intensity is approximately proportional to $N_i \cdot A_{ki}$, with N_i the level population and A_{ki} the probability for the observed transition from level i to level k. If the section is long compared to the decay length, the observed intensity is about proportional to $N_i \cdot A_{ki}/\sum_j A_{ji}$, that is to $N_i \cdot A_{ki} \cdot \tau_i$. Here τ_i is the lifetime of level i, and $\sum_j A_{ji}$ is the total decay probability. $\tau_i \cdot A_{ki}$ is, of course, the branching ratio of the particular decay.

The five parameters wanted are overdetermined if all seven transitions in the $2\ ^4P^0 - 2\ ^4P$ multiplet are observed. In practice a least-squares fit to the observed wavelengths is advisable in order to determine the 5 wanted parameters and to obtain an estimate of the errors. Unresolved or very weak multiplet components enter the fit procedure with large uncertainties and therefore little weight. An inclusion of these lines or even of estimated line positions helps to maintain a formal identity of the fit procedure for all data sets available.

For this study all published experimental wavelength data have been reevaluated using a weighted least squares adjustment of the parameters to the available observations. Each of the seven possible multiplet transitions was expressed as a linear combination of the five parameters (two fine structure splittings each for the lower and upper terms and ΔT_{CG}) which provide the fitting constraint equations. For each observed transition, the squared deviations were weighted by the reciprocal square of the source-quoted uncertainties in the observations (transformed from wavelength to wavenumber space). Since the constraints are linear in the fitting parameters, an analytic solution is possible, but we instead used a standard code [16] utilizing Marquardt's algorithm to accomplish a nonlinear weighted least squares minimization. Similarly the theoretical wavelength

Table 1. $2\,^4P^0$, $2\,^4P$ *multiplet parameters for ions* C^{3+} *to* Al^{10+}. *A published data, B parameters after reevaluation (if necessary), C theoretical data. Experimental errors are not quoted here. Estimates are evident from Figs. 1 and 2.*

		Finestructure interval/cm^{-1}				
		$2\,^4P^0$		$2\,^4P$		
Z	Ref.	1/2–3/2	3/2–5/2	1/2–3/2	3/2–5/2	$(\Delta T_{CG})^{-1} \triangleq \bar{\lambda}$/nm
6	1 A	0	100	83	41	134.42
	B	5.4	94.2	72.0	44.2	134.425
	12 C	8.5	96.8	76.0	32.9	134.250
	13 C	3.8	94.6	76.2	40.1	134.422
7	1 A	35	212	160	115	111.11
	B	40.5	211	162	113.5	111.065
	12 C	40.7	212	158	114	110.943
	13 C	34.5	209	158	113	111.071
8	1 A	102	418	295	252	94.68
	B	111.5	414	291	257	94.596
	12 C	106	409	294	250	94.460
	13 C	98.4	403	294	250	94.561
9	2 A	220	716	523	487	82.247
	12 C	219.5	719	504	475	82.144
	13 C	212	708.5	502	479	82.231
10	3 A	444	1102	746	856	72.651
	4 A	368	1196	816	832	72.671
	B	420	1166	764	860	72.663
	12 C	398	1179	812	821	72.567
12	5 A	1010	2708	1824	1995	58.604
	6 A	1020	2700	1837	1945	58.609
	12 C	1039	2731	1836	2018	58.547
	13 C	1058	2676	1801	1071	58.593
13	7 A	1543	3885	2625	–	53.283
	8 A	1584	3900	2588	2884	53.311
	12 C	1544	3931	2623	2948	53.231

values for $2\,^4P^0$–$2\,^4P$ transitions could be reduced to the 5 basic parameters. This was done to determine missing parameters (like the multiplet separation in [12]), in addition the wavelength data could be checked for consistency. With the exception of 5 wavelength values in [12] where there are deviations by one unit in the last digit, the theoretical data sets [12, 13] could be reproduced in full agreement with the rounded values published.

In Table I the published parameters and the revised ones (if significantly different) are given. The most striking inconsistencies between the published parameter values and the results of this reevaluation based on the published wavelength data are apparent for C, N, O [1] and Ne [4]. In the latter paper the determination of $\bar{\lambda}$ from theoretical data (e.g. of [12]) arrives at values which differ from ours, too. For convenience of the reader, Table I gives the theoretical results published by Hata and Grant [12] and by Chung [13] alongside with the experimental ones.

The notable inconsistencies of the data reduction indicate the need for caution when comparing experimental and theoretical data. On the other hand there are irregularities in theoretical data, too: The data published by Chen et al. [11] for Al seem to suffer either from computational problems or from clerical errors as they do not match the established trends of the other results for other ions in the same isoelectronic sequence computed by those authors. This fact has been noted elsewhere, too [2].

On the basis of the reevaluated parameters it seems worthwhile to compare experimental and theoretical data on a convenient scale. Figure 1 shows that the finestructure results of [12, 13] agree with the experimental data in the full range studied considering the computational uncertainties and the experimental error bars. The other calculations of the finestructure intervals are close to the ones shown in the graph. In one experimental data set [3] the errors appear to have been underestimated or an error in the line identification may be suspected.

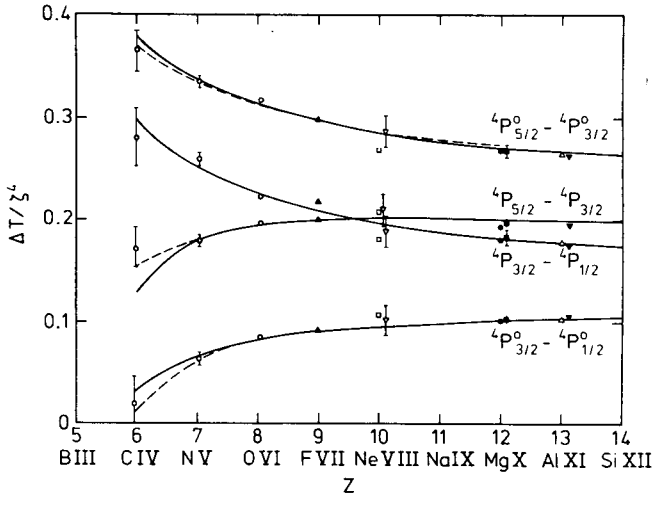

Fig. 1. $2\,^4P^0$ and $2\,^4P$ finestructure intervals for ions C^{3+} to Al^{10+}. The data are scaled with ζ, the net charge of the ionic core. Experimental error bars are indicated if they exceed the symbol size. Identification of the data: ○ [1], ▲ [2], □ [3], ▽ [4], ● [5], ■ [6], △ [7], ▼ [8]. The full lines correspond to theoretical predictions [12], the broken lines to [13].

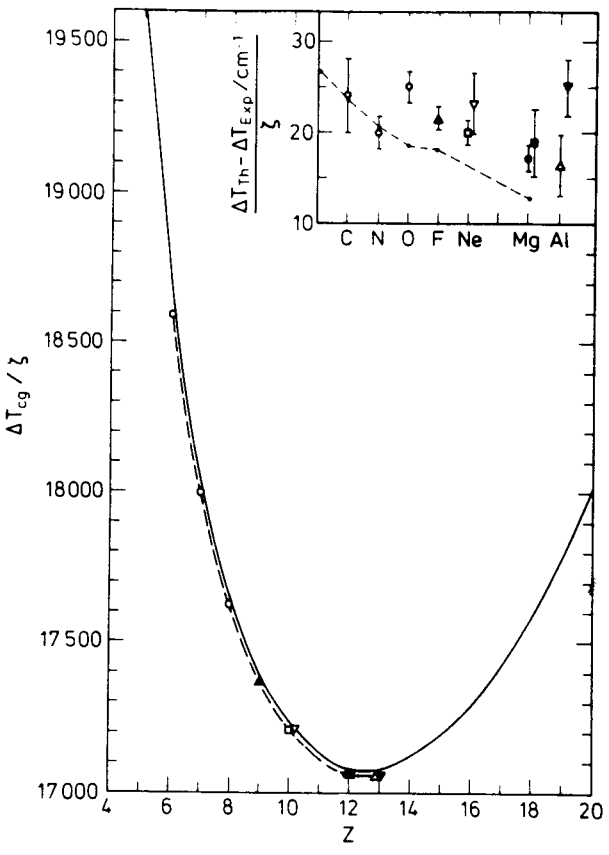

Fig. 2. Comparison of the experimental $2\,^4P^0-2\,^4P$ multiplet separation data (connected by the broken line in the main graph) with theory [12] (full line). The data are scaled with ζ. For identification of data see Fig. 1. The insert shows the deviation of theory [12] from the experimental results. The broken line in the insert indicates the deviation of Chung's results [13] from those of Hata and Grant [12] (ΔT_{CG} [12] − ΔT_{CG} [13]).

For Al XI the published values of the mean transition wavelength [7, 8] do not agree within their mutual errors quoted. Our least-squares analysis suggests that slightly different positions assumed for the blended lines in [8] would shift $\bar{\lambda}$ to a value almost coincident with that given in [7], at the cost of a slightly worse agreement of the finestructure intervals with theory. Unfortunately the low UV fluorescence of the $^4P_{5/2}$ decay did not permit the observation of any of the UV transitions from this level in [7]. The corresponding finestructure interval had to be taken from theory [11], and slight changes of the adopted value would affect the other fit parameters, too.

In Fig. 2 the multiplet separation data – as of this reevaluation – are compared with theory. There is a systematic deviation of theory [12] from the experimental results which seems to be almost proportional to the nuclear charge, suggesting perhaps the neglect of some electron correlation effect. Quantum electrodynamical corrections are already included in [12] (and from there taken for good use in [13], too), they amount only to a fraction of the observed deviation. Chung's calculations [13] reduce the deviation for low Z ions considerably. However, a constant deviation in the insert of Fig. 2, that is a term linear in Z, remains. The deviations of the other theoretical results from the experimental ones are much larger. The reason for the apparent slight irregularity in the difference of the two theoretical data sets [12, 13] in the range N to F is not known.

The reevaluation of some of the published data on the $2\,^4P^0-2\,^4P$ transition array reduces the scatter of the data compared to smooth isoelectronic trends and explains some irregularities noted before [2, 6, 13]. The agreement of experimental data and theoretical predictions is improved noticeably for C, N and O, both for finestructure intervals and for multiplet separations which now almost perfectly coincide with calculated values by Chung [13].

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