Physica Scripta. Vol. 42, 522–529, 1990.

Transitions between Quintet States of Doubly Excited Four-Electron Ions: Experiment and MCDF Theory along the Isoelectronic Sequence

J. H. Blanke, B. Fricke and W.-D. Sepp

Fachbereich Physik, Universität Kassel, D-3500, Kassel, F. R. Germany

and

P. H. Heckmann, G. Möller and C. Wagner

Experimentalphysik III, Ruhr-Universität Bochum, Postfach 10 21 48, D-4630 Bochum 1, F. R. Germany

Received March 1, 1990; accepted April 27, 1990

Abstract

Following an earlier observation in F VI we identified the line pair $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^o$, $^5D^o$ for the elements N, O, Mg, and tentatively for Al and Si in beam-foil spectra. Assignment was established by comparison with Multi-Configuration Dirac–Fock calculations along the isoelectronic sequence. Using this method we also identified some quartet lines of lithium-like ions with $Z > 10$.

1. Introduction

Observation of transitions between doubly excited three – electron quartet states for $Z < 10$ has been nearly completed in agreement with various theoretical approaches [1–4]. In contrast the doubly excited four-electron quintet states still seem to be a challenge for both, theory and experiment [4]. Brage and Froese Fischer [5] reported an elucidating study of the transition between the two lowest lying states $1s2s2p^2\ ^5P$–$1s2p^3\ ^5S^o$ along the isoelectronic sequence of Be-like ions. But no theoretical or experimental result exist on transitions between $n = 2$-states and $n = 3$-states of the general form $1s2s2p3l$ or $1s2p^23l$, except the assignment of B II $1s2p^3\ ^5S^o$–$1s2p^23s\ ^5P$ by Mannervik *et al.* [6], and an earlier observation by Blanke *et al.* in F VI [7]. Also a Grotrian diagram for C III quintet states with calculated energies is presented by Schneider *et al.* [8]. Therefore we attempted to investigate these $n = 2$–$n = 3$ transitions along the isoelectronic sequence. At this point one should mention that the doubly excited quintet states lie above the ionization limit $1s^22s$ of singly excited four-electron states in the continuum. They are stable against E1-dipole transitions to singly excited states because of their maximal spin quantum number $S = 2$. Further, quintet states below the $1s2s2p\ ^4P^o$ limit are also stable against Coulomb autoionization to continuum states. This is the case for all $n = 2$ and $n = 3$ states of the elements considered here. Therefore optical transitions between these quintet states might be observable.

In the theoretical part of this work we used a well defined and well applicable approach, the Multi-Configuration Dirac–Fock program of Desclaux [9]. Its reliability for such low Z systems was tested on doubly excited three-electron ions on which a large amount of experimental data [4] is available. Due to these considerations, some newly observed quartet lines could be identified. Experimentally we relied on the beam-foil facilities in Bochum which allow consistent measurements of the ions of N, O, F, Mg, Al and Si.

After a brief discussion of the theoretical method and the experimental facilities we discuss line identifications for quintet and quartet transitions.

2. Theory

For our calculations the latest version of the Multi-Configuration Dirac–Fock program [9] was used. In a first approach – misleadingly we often call it the "single-configuration" or "SC" approach – we use a basis of jj – coupled states coupled to good total angular momentum J that originates from one single non-relativistic configuration, like e.g., $1s2s2p3d$. In this example of $J = 4$ the multiconfiguration basis set consists of five members:

$$(((1s\ 2s)J = 1,\quad 2p_{1/2})J = 3/2,\quad 3d_{5/2})J = 4,$$
$$(((1s\ 2s)J = 1,\quad 2p_{3/2})J = 3/2,\quad 3d_{5/2})J = 4,$$
$$(((1s\ 2s)J = 1,\quad 2p_{3/2})J = 5/2,\quad 3d_{3/2})J = 4,$$
$$(((1s\ 2s)J = 1,\quad 2p_{3/2})J = 5/2,\quad 3d_{5/2})J = 4,$$
$$(((1s\ 2s)J = 0,\quad 2p_{3/2})J = 3/2,\quad 3d_{5/2})J = 4,$$

The Dirac–Fock equations are then solved separately for all states that arise from this basis in a SCF way. After evaluation of all possible levels for all J, the levels are grouped in certain LS-terms (averaged over the fine structure sublevels statistically in order to obtain LS – term energies), because the fine structure is not resolved in the spectra.

To obtain a better evaluation of the correlation energy improved calculations include the mixing of further non-relativistic configurations. We take those configurations that belong to the same complex and possess the same LS-terms as the term in question; i.e. in order to calculate $1s2s2p3d\ ^5D^o$ the configurations $1s2s2p3d$ and $1s2p^23p$ are taken into account. For $1s2s2p3d\ ^5P^o$ we use $1s2s2p3s$, $1s2s2p3d$ and $1s2p^23p$. Hence for $1s2s2p^2$ we just rely on $1s2s2p^2$.

For all calculations we checked carefully that we did not catch extra energies as described by Huang *et al.* [10]. Setting the inverse velocity of light to zero one performs a non-relativistic calculation. With this procedure one can control

that in a MCDF-calculation all levels for an *LS*-term have the same total non-relativistic energy.

However, the total energy for these self-consistent calculations also includes the contributions of the Breit-interaction, i.e., the magnetic interaction and retardation in pertubation theory. QED-effects are taken into account by using the effective nuclear Z in the formulas of QED, which is calculated from an analogue hydrogenic orbital with the same expectation value of r as the MCDF-orbital in question.

In addition to the existing MCDF-code we formulated an extension to calculate transition probabilities. Upper and lower states of the transition are calculated independly. The consequent non-orthogonality of the orbitals is corrected partly by multiplying the transition matrix elements by the overlaps of the non active orbitals. In the context of this work this extension was used to calculate the lifetimes of the quintet states in question and additionally as a test for some three-electron quartet states. We also evaluated the lifetime of a singly excited boron-like state. The resulting transition led to some difficulties in the identification of the quintet states in F VI.

3. Experiment

The experiments took place in Bochum at the 4 MV Dynamitron Tandem Accelerator Laboratory. Whereas stable ion beam currents of several μA could be used for the elements N, O, F, and Si, only currents of 300 nA were available for Mg- and Al-ions. The ions were excited by being passed through thin carbon foils (about 20 $\mu g\,cm^{-2}$) produced from a glow discharge. Spectra were taken by using a 2.2 m grazing-incidence monochromator (McPherson Md. 247) which viewed the ion beam at right angles. For these experiments we used a ruled grating with 600 l mm^{-1} and a holographic one with 3600 l mm^{-1}. The use of the latter was essential for the resolution of the transition $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^o$ in oxygen. For the elements Mg, Al and Si, where the transitions are expected to have wavelengths around four to six nm, spectra are taken in second order because the lower limit of the grating with 600 l mm^{-1} is 7.5 nm. For these spectra we used foils tilted at a 10° angle to the normal set-up as we wanted a direct view onto the foil's back. This is assumed to be useful as the lifetimes of the upper states of the transitions in question (Mg, Al and Si) are expected to be in the order of one pico-second, i.e. a decay length of 10 μm for energies around 20 MeV used in the experiment. The drawback we suffer is a high background due to bremsstrahlung of secondary electrons; we also observed carbon K-α radiation in second and third order. In general therefore the ratio of signal to background is poor for the spectra of Mg, Al and Si. A normal set-up with a foil at 90° hinders an observation of this background and the desired spectral lines because we observed that the foils bend backwards under ion bombardement. Accordingly the emitted light cannot pass the edge of the foil-mounting to enter the entrance slit. In contrast to [11, 12] we did not observe extra lines due to reflections of the emitted light on the rear surface of the foils. In fact, the resolution we used is not good enough to resolve these possible extra lines. A minor change in the line profile would have also affected the calibration lines.

The linearity of the exit slit disposition is monitored by a 60 mm travel Heidenhain moire fringe length gauge. A detailed description of the apparatus used can be taken from Träbert *et al.* [13].

4. Testing MCDF on quartet states

In order to obtain information on the validity of our theoretical approach we calculated first wavelengths of transitions that belong to doubly excited quartet states of three-electron ions. For comparison [4] a large amount of reliable experimental data, confirmed by elaborate calculations [1–4], exists. We concentrate on $n = 2$ to $n = 3$ transitions and evaluate the difference between experimental and theoretical transition energies for all Z on which data are available. For this first test we performed just a "single configuration"-calculation. Fig. 1 shows these deviations to be linear for all transitions of nuclear charges with $Z > 5$. For the elements Li, Be, B error bars in Fig. 1 are smaller than symbols. For the heavier elements typical error bars are given exemplarily for one transition. To begin with, these linear deviations can of course be used to predict easily and with high accuracy transitions for higher Z, in particular for Mg, Al and Si although relativistic effects may become important for these atomic numbers already. Experiments and results are discussed below. As can be seen in Fig. 1 the $1s2s3s\ ^4S$ difference for oxygen does not follow the linear trend. In order to test this only exception for the elements of interest to us, we reviewed old spectra for the transition O VI $1s2s2p\ ^4P^o$–$1s2s3s\ ^4S$ which was at that time measured with (15.183 ± 0.005) nm [14]. We believe that one cannot exclude that the quartet line in question is in fact blending the transition O V $1s^22s2p\ ^3P^o$–$1s^22s4d\ ^3D$ that was measured by us with (15.151 ± 0.004) nm. This is also a better fit to Laughlin's value of 15.142 nm [15]. In addition we notice that no experi-

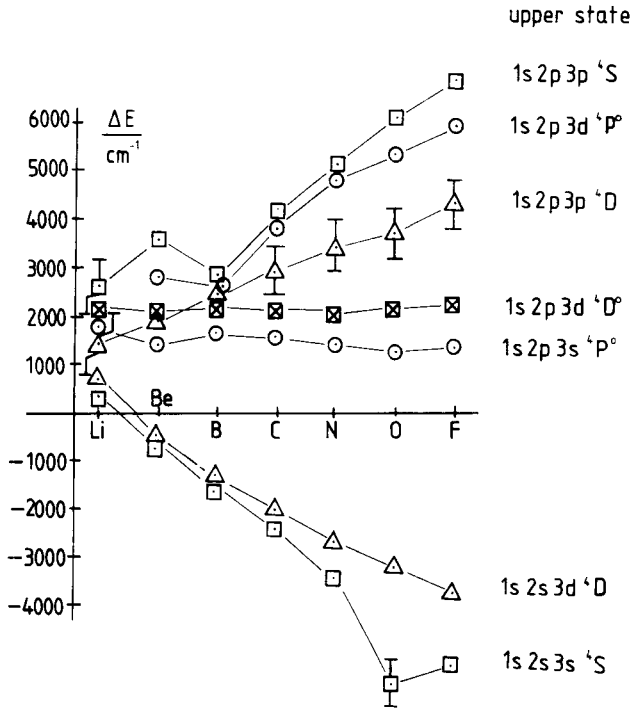

Fig. 1. Deviations between experimental and theoretical transition energies for $n = 2$–$n = 3$ transitions between doubly excited quartet states of three-electron ions. Experimental data are taken for Li from [30, 16], for Be from [3], for B from [31] and for C, N, O and F from [14]. Theoretical values are calculated with MCDF, in a "single-configuration" approach explained in the text.

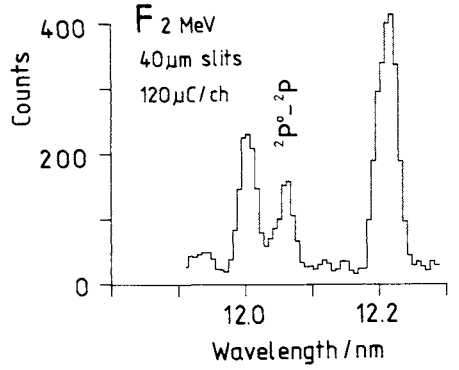

Fig. 2. Beam-foil spectrum of fluorine. At this beam energy of 2 MeV the line at 12.06 nm has to be identified with $1s^22s^22p\ ^2P^o-1s^22s2p(^3P^o)4p\ ^2P$.

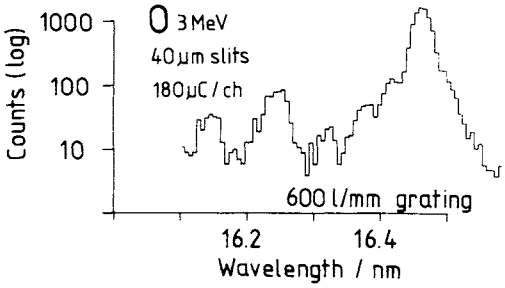

Fig. 4. Spectrum of oxygen using a 600 l mm^{-1} grating. The resolution is not good enough to identify the quintet lines unambiguously. Especially at 16.22 nm, $1s2s2p^2\ ^5P-1s2s2p3d\ ^5P^o$ is not resolved at all from O V $1s^22p^2\ ^1D-1s^22p3d\ ^1F^o$ with a wavelength of 16.2492 nm [26].

mental energy value for Li I $1s2p3d\ ^4P^o$ is available. The values for Li I $1s2p3p\ ^4S$ and $1s2p3p\ ^4D$ in Fig. 1 are from measurements of energies of Auger electrons [16] and thus possess large error bars.

It is known that the correlation effect left out in these first "single configuration" calculations can be handled by adding further configurations to the MC-basis set. Most important are configurations belonging to the same so-called "complex" just as the configuration in question. A complex consists of all configurations that have the same main quantum numbers n in all electrons and the same parity [17]. The contribution to the correlation energy which is included in this extended basis set is known to be linear in first order. Preferably further contributions from outside the complex should be constant in Z [18, 19]. Thus, a calculation that includes all configurations of a complex for both members of the transition should display a constant deviation from experiment, at least in that region of Z we are interested in. But already the "SC"-deviation plot shows an example of constant deviation for one transition. There is just one $^4D^o$ term, namely $1s2p3d\ ^4D^o$, in the complex of the configurations $1s2l3l$. The same holds for the lower $1s2p^2\ ^4P$ term in its complex of $1s2l2l'$ configurations. As a matter of fact, the deviation for the transition $1s2p^2\ ^4P-1s2p3d\ ^4D^o$ is constant already in the "SC"-approach. The deviation for the transition $1s2p^2\ ^4P-1s2p3s\ ^4P^o$ seems also to be linear (Fig. 1). But this is due to the fact that the state $1s2p3s\ ^4P^o$ is shifted by the states $1s2s3p\ ^4P^o$ and $1s2p3d\ ^4P^o$ by approximately the same amount from different directions.

For the quintet transitions we will show the improvement, including contributions from inside the complex, explicitely. To include further contributions from outside the complex is in fact hard to achieve with MCDF because of convergence problems and the rapid growth of the number of configurations. But for our purposes we can actually see that a linear trend in the correlation contribution is enough for identification of lines. One should be aware that actually the simplicity of the quartet system of doubly excited three electron states for $Z > 6$ guarantees the validity of this approach. There are no close perturbers for the $n = 3$ levels, for example, no $1s2snl$ state is near to $1s2p3l$. Such problems are discussed by Froese Fisher for Be II [3], and by Laughlin for the case of mixing $1s2s5p\ ^4P^o$ and $1s2p4d\ ^4P^o$ [20].

5. Quintet transitions

The main question of this work was to find the quintet line pair $1s2s2p^2\ ^5P-1s2s2p3d\ ^5P^o$, $^5D^o$, that we reported for fluorine [7], also for other elements. But we started again with fluorine in order to learn which beam energy should be used for optimum production of photons from quintet transition. With energies of the fluorine ions of 6 and 4 MeV we reproduced first of all the quintet line pair. For comparison see Fig. 1 in [7], where the line pair from our first measurement is displayed. We did, however, run into some problems when we took a spectrum with a lower beam energy of 2 MeV (Fig. 2). There is no line at (12.151 ± 0.002) nm, but the line at (12.058 ± 0.002) nm is still present, and cast some doubt on our identification. However, it is believed now that the line at 12.058 nm at this energy is not due to a quintet transition but to the transition $1s^22s^22p\ ^2P^o-1s^22s2p(^3P^o)4p\ ^2P$, as marked in Fig. 2. This transition has not been observed earlier, but – due to another transition [21] – the level

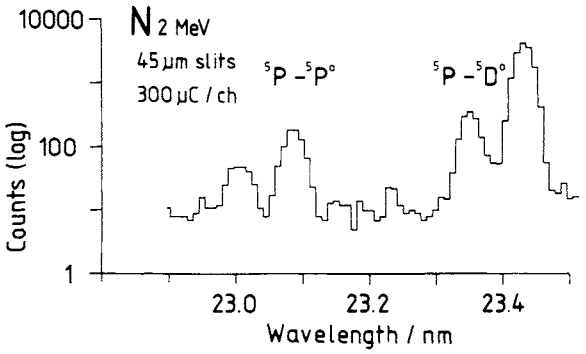

Fig. 3. Beam-foil spectrum of nitrogen recorded at an ion energy of 2 MeV. Two lines at 23.075 nm and at 23.341 nm could be identified with the transitions $1s2s2p^2\ ^5P-1s2s2p3d\ ^5P^o$, $^5D^o$.

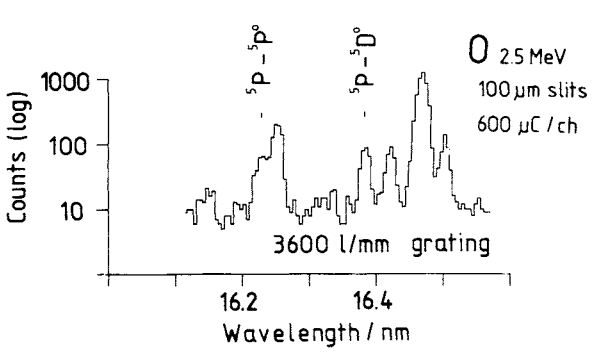

Fig. 5. High resolution spectrum of the region already displayed in Figure 4 recorded with the 3600 l mm^{-1} grating. Now both quintet transitions $1s2s2p^2\ ^5P-1s2s2p3d\ ^5P^o$, $^5D^o$ are well resolved at 16.227 nm and 16.380 nm.

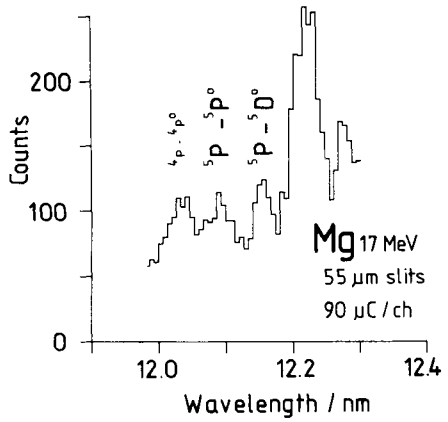

Fig. 6. Qunitet transitions $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^o$, $^5D^o$ as observed for Mg. Beam-foil spectrum shows the transitions in second order using tilted foils. This causes the high background due to bremsstrahlung of secondary electrons in the foil. Also the quartet transtion $1s2s2p\ ^4P$–$1s2p3s\ ^4P$ is displayed.

$1s^22s2p(^3P^o)4p\ ^2P$ is quoted in the table of Moore, and for this $^2P^o$–^2P we calculate a wavelength of 12.0609 nm. A crude MCDF – calculation gives 12.167 nm and this identification is further verified by a lifetime measurement. With the analyzing technique described in [22] we arrived at a lifetime of (67 ± 10) ps for the very dominant main component. And indeed the level $1s^22s2p(^3P^o)4p\ ^2P$ lies just below the ionisation limit of $1s^22s^2\ ^1S$ according to Bashkin *et al.* [23]. No strong feeding cascades are expected for such a level. A calculation with our newly developed extension to the MCDF – code gives us for both fine structure components a lifetime of 78 ps. This calculation takes into account the transitions to all doublet states of the configurations $1s^22s^22p$, $1s^22s2p3s$ and $1s^22s2p3d$. The related transitions $1s^22s^22p\ ^2P^o$–$1s^22s2p(^3P^o)4P\ ^2S$ and $1s^22s^2P\ ^2P^o$–$1s^22s2p(^3P^o)4p\ ^2D$ cannot be identified unambiguously. With the data from Moore [21] one obtains 11.940 nm for the first one and 12.001 nm for the second, respectively. We observed lines at these wavelengths, but F VI transitions are reported at these positions, too: $1s^22p^2\ ^1D$–$1s^22p4d\ ^1P^o$ at 11.9370 nm and $1s^22s2p\ ^1P^o$–$1s^22s4d\ ^1D$ at 12.0117 nm [24, 25]. Blending is assumed. In conclusion we can state that there are no quintet lines at 2 MeV but the observations at 6 MeV are believed to be reliable, because F V lines observed at an energy of 2 MeV with the same intensity as the line at 12.058 nm did not show up in spectra of 6 MeV.

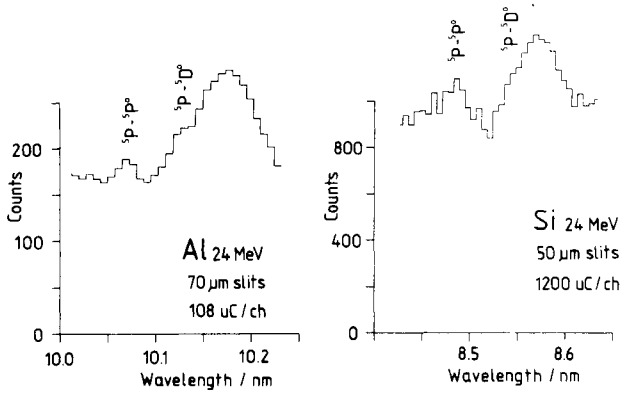

Fig. 7. Beam-foil spectra taken for Al and Si. Here the background problem due to the use of tilted foils is even more severe than for Mg. Therefore results are just tentative.

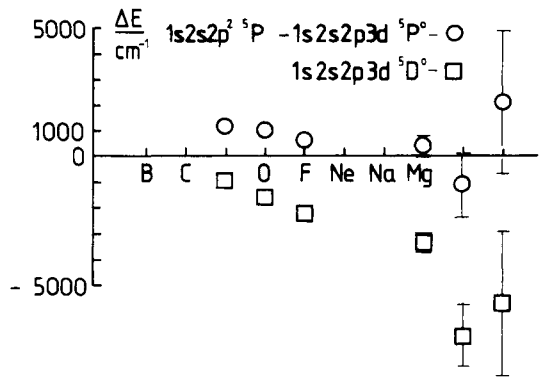

Fig. 8. Deviation between experimental and theoretical transition energies for transitions between doubly excited quintet states. Theoretical values are from MCDF in a "single configuration" approach explained in the text.

For nitrogen, spectra were taken at various beam energies in the region where the quintet line pair was expected. Two lines at (23.075 ± 0.003) nm and at (23.341 ± 0.003) nm were identified as candidates (Fig. 3) posessing approximately the same relative intensity as in the case of fluorine (Fig. 1 in [7]). Both lines are therefore marked as ^5P–$^5P^o$ and ^5P–$^5D^o$, respectively. Again, at higher beam energy the line at 23.34 nm must be preferably identified with N VI $1s2p\ ^3P^o$–$1s5d\ ^3D$ in second order but the observations at 1 and 1.5 MeV are still relevant. With the results for fluorine and nitrogen the deviations between the experimental transition energy and the value from an MCDF-'single configuration' approach were calculated for the quintet line pair. By interpolation and assuming a linear trend, we determined quite exactly the expectations for the spectral position of this line pair in oxygen.

However a spectrum recorded with the 600 l mm^{-1} grating and slits of 35 mm for oxygen was inadequate for this case (Fig. 4). The transition $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^o$ could not be separated at all from the transition $1s^22p^2\ ^1D$–$1s^22p4d\ ^1F^o$, reported by Edlén at 16.2492 nm [26]. Moreover one calculates a value of 16.2405 nm according to Moore [21] for the transition $1s^22p^2\ ^1D$–$1s^22p4d\ ^1P^o$. But this transition is believed to be much weaker. The necessary spectra, taken with a grating with 3600 l mm^{-1}, show the quintet line well resolved with a wavelength of (16.227 ± 0.002) nm at the expected position (Fig. 5), marked as ^5P–$^5P^o$. Also the line for the transition ^5P–$^5D^o$ shows up well exposed. Relative intensity is like that for F and N.

Because Ne and Na beams are not possible to be produced with our tandem machine the next step was an extension to

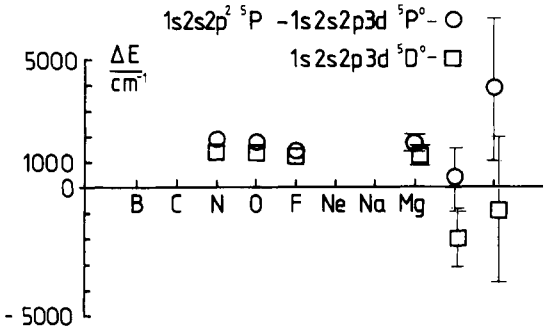

Fig. 9. Deviations as plotted in figure 8. In the MCDF-approach the theoretical values now contain all configurations that belong to the same complex as the states $1s2s2p^2\ ^5P$ and $1s2s2p3d\ ^5P^o$, $^5D^o$.

Mg, Al and Si. As discussed above spectroscopic was tried in second order with tilted foils. Due to this these spectra possess a large background increasing from Mg to Si. For Mg the spectrum is displayed in Fig. 6. Two lines, not reported earlier, show up at the calculated positions and with proper relative intensities. They are marked as ^5P–$^5P^o$ and ^5P–$^5D^o$, respectively. Also the quartet transition $1s2p^2\ ^4P$–$1s2p3s\ ^4P^o$ is identified in this spectrum. The spectra for Al and Si are shown in Fig. 7. The relatively faint features that we identify tentatively with the two quintet transitions are marked again as ^5P–$^5P^o$ and ^5P–$^5D^o$. Other lines present in these spectra are due to transitions from singly-excited four electron systems [24]. The results for Al and Si are tentative, but nevertheless we report them with the error bars in mind.

All experimental data are then compared with the theoretical values of a "single configuration" MCDF-approach and a second improved calculation that includes all members of a complex. Data points for the deviation in transition energy are evaluated and plotted in Figs. 8 and 9, respectively. The "SC"-plot of Fig. 8 demonstrates the linearity of the deviations, whereas the "complex-plot" of Fig. 9 can even show that the the excited basis set turns the deviation to a constant as required by theory. All the data used in these figures are presented as well in Table I. The remaining constant deviation posesses the same sign and order of magnitude as in the case of the quartets.

In Table II and Fig. 10 we quote the relevant data for the term difference between the two quintet terms $1s2s2p3d\ ^5P^o$ and $1s2s2p3d\ ^5D^o$. The values from the "complex-calculations" are quite close to our experimental data and support again our identification. The non-relativistic data deviate from the relativistic ones for Mg and onwards. But experimental values cannot confirm this relativistic effect because of large error bars in the region of interest.

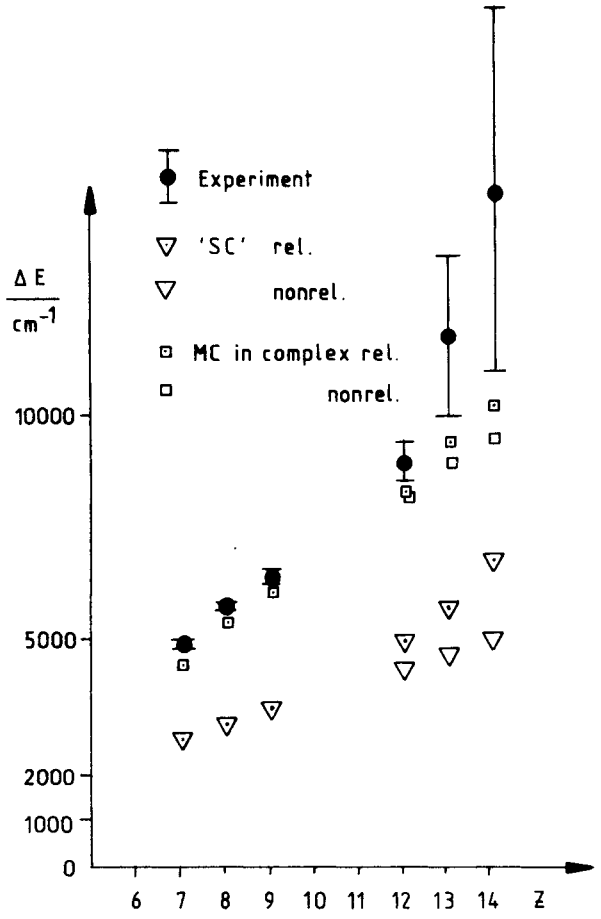

Fig. 10. Term difference of quintet terms $1s2s2p3d\ ^5P^o$ and $1s2s2p3d\ ^5D^o$ arising from doubly excited four electron configurations plotted versus atomic number Z. The mixing inside the complex is essential and sufficient for theoretical confirmation. Relativistic effects cannot be tested due to large error bars in the region of interest.

Extending the experiment to carbon is difficult as the appropriate energy of approximately 0.8 MeV is not well suited to our accelerator. We believe also that the linear trend of deviation might not be stable towards lower Z. In the power series of the remaining correlation energy there is, apart from the constant term, also a term of the form $1/Z$ that becomes important in this region [27]. As of yet no other quintet transitions have been discovered conclusively in our

Table I. *Wavelengths of transitions between doubly excited quintet states, Deviation ΔE between experimental transition energy and theoretical approaches, "SC" means all configurations that belong to one single nonrelativistic configuration, "MC in complex" means all configurations belonging to the complex are taken into account. Results for Al and Si are tentative*

		Theory		Deviation ΔE	
Z	Experiment λ/nm	"SC" λ/nm	MC in complex λ/nm	"SC" $\Delta E/\mathrm{cm}^{-1}$	MC in complex $\Delta E/\mathrm{cm}^{-1}$
$1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^o$					
7	23.075 ± 0.003	23.140	23.177	1219 ± 100	1916 ± 100
8	16.227 ± 0.002	16.254	16.275	1020 ± 100	1813 ± 100
9	12.058 ± 0.002	12.066	12.079	570 ± 140	1442 ± 140
12	6.048 ± 0.001	6.050	6.054	491 ± 300	1720 ± 300
13	5.030 ± 0.003	5.027	5.031	−1067 ± 1200	355 ± 1200
14	4.240 ± 0.005	4.244	4.247	2170 ± 2800	3887 ± 2800
$1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5D^o$					
7	23.341 ± 0.003	23.291	23.420	−927 ± 100	1447 ± 100
8	16.380 ± 0.002	16.339	14.417	−1547 ± 100	1361 ± 100
9	12.151 ± 0.002	12.118	12.168	−2241 ± 150	1177 ± 150
12	6.081 ± 0.001	6.068	6.086	−3333 ± 300	1297 ± 300
13	5.060 ± 0.003	5.042	5.005	−6977 ± 1200	−1997 ± 1200
14	4.257 ± 0.005	4.257	4.265	−5726 ± 2800	−824 ± 2800

Table II. *Energy splitting between the states 1s2s2p3d $^5P^o$ and 1s2s2p3d $^5D^o$, "SC" means all configurations that belong to one single non-relativistic configuration, "MC in complex" means all configurations belonging to the complex are taken into account. Results for Al and Si are tentative*

		Theory			
		"SC"		MC in complex	
Z	Experiment $\Delta E/cm^{-1}$	relativistic $\Delta E/cm^{-1}$	non-relativistic $\Delta E/cm^{-1}$	relativistic $\Delta E/cm^{-1}$	non-relativistic $\Delta E/cm^{-1}$
7	4938 ± 140	2792	2785	4468	4467
8	5756 ± 150	3189	3164	5303	5307
9	6347 ± 210	3556	3500	6084	6082
12	8864 ± 430	5046	4377	8449	8220
13	11787 ± 1700	5891	4652	9400	8901
14	14923 ± 3950	7030	4922	10235	9573

Table III. *Partial lifetimes of doubly excited four electron quintet states due to optical transitions to 1s2s2p^2 ^5P and partial lifetimes of the doubly excited three-electron quartet states 1s2s3d ^4D, 1s2p3d $^4P^o$ and 1s2p3d $^4D^o$ due to optical transitions to 1s2s2p $^4P^o$ or 1s2p^2 ^4P. "SC" means all configurations that belong to one single nonrelativistic configuration. "MC in complex" means of all configurations that belong to the complex are taken into account*

	1s2s2p3d $^5P^o$		1s2s2p3d $^5D^o$	
Z	"SC" τ/ps	MC in complex τ/ps	"SC" τ/ps	MC in complex τ/ps
7	33.4	36.6	19.3	17.1
8	15.1	16.3	8.65	7.68
9	7.85	8.49	4.49	3.98
12	1.75	1.91	1.03	0.91
13	1.17	1.31	0.70	0.62
14	0.84	0.92	0.50	0.44

	1s2s3d ^4D			
Z	Laughlin* τ/ps	"SC" τ/ps	MC in complex τ/ps	Experiment† τ/ps
6	29.7	33.8	27.8	
7	13.2	15.2	12.4	11.9 ± 1.4
8	6.7	7.8	6.3	8.4 ± 0.9
9	3.8	4.4	3.6	2.7 ± 0.9

	1s2p3d $^4P^o$			
Z	Laughlin* τ/ps	"SC" τ/ps	MC in complex τ/ps	Experiment† τ/ps
6	56.0	50.5		55 ± 8
7	24.2	21.6	23.9	19.2 ± 2.3
8	12.1	10.8	11.8	9.2 ± 2.6
9	6.8	5.9	6.6	7.7 ± 0.8

	1s2p3d $^4D^o$			
Z	Laughlin* τ/ps	"SC" τ/ps	MC in complex τ/ps	Experiment† τ/ps
6	29.0	29.2	no other	30.8 ± 3.0
7	12.5	12.5	3*l* $^4D^o$	8.2 ± 2.3
8	6.2	6.2	states	5.7 ± 0.6
9	3.5	3.4		3.6 ± 0.7

* Reference [15, 20, 28].
† Reference [22].

spectra. Further experiments with the highly resolving grating are necessary.

6. Transition probabilities

A crude calculation of transition probabilities for the quintet transitions is presented in Table III. Again the reliability of our calculation was tested for $2p$–$3d$ transitions of three electron quartet states (Table III). Our calculations give values for each substrate J separately, of course. But the values for one LS – term are the same for the transition in question within a few percent. For the elements C, N, O and F the deviation from experimental data [22] and the values of Laughlin [15, 20, 28] is in the region of 10 to 20%. In this context one should mention that the theoretical lifetimes stated in our work are only partial lifetimes of optical transitions inside the doubly excited term system. Auger processes and radiative transitions to singly excited states are not considered. The inclusion of all configurations of a complex does not seem to improve our values significantly. Also, for the two quintet transitions $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^\circ$, $^5D^\circ$ the inclusion of all configurations of a complex does not change the values very much. First experiments on fluorine showed that the quintet lifetimes might be too short for a proper experimental determination. But for O and N experiments should be possible.

7. Quartet transitions for Mg, Al and Si

For completeness sake we also give our experimental data on the wavelengths of quartet transitions for the elements Mg, Al and Si which have been identified when we tried to find quintet transitions. Anyhow, the systematic identification of numerous quartet transitions supports the identification of quintet lines. Again, the deviations determined for the elements C to F were extrapolated to Mg, Al and Si to give an improved theoretical expectation value for the wavelengths according to the "SC"-approach. Data are given in Table IV. Observation was made in second order using tilted foils. The relatively bad ratio of signal to noise forbids identification of some faint features. The lifetimes of the upper states of the transitions are of the order 1 ps or even less [29].

8. Conclusion

We performed MCDF-calculations for $n = 2$–$n = 3$ transitions between doubly excited quintet states of four-electron ions. Using the calculated wavelengths we were able to identify the transitions $1s2s2p^2\ ^5P$–$1s2s2p3d\ ^5P^\circ$, $^5D^\circ$ in the beam-foil spectra for the ions N, O, F and Mg. Identification is verified mainly due to the fact that the deviations between experimental and theoretical transition energies along the isoelectronic sequence is constant if the calculations include all configurations which can be constructed within the complex of both the initial and final states. In the case of quartet transitions between three-electron states we predicted wavelengths for the ions Mg, Al and Si by extrapolating the deviations between experiment and MCDF stated for the ions C to F. Again beam-foil observations confirmed the validity of our approach.

Table IV. *Wavelengths of quartet transitions for the elements Mg, Al, and Si. "SC" means all configuration that belong to one single non-relativistic configuration. "Corrected" means extrapolated correlation energy is added to the transition energy*

Magnesium ($Z = 12$) transition	"SC" λ/nm	Corrected λ/nm	Experiment λ/nm
$1s2s2p\ ^4P^\circ$			
$-1s2s3s\ ^4S$	5.8206	5.847 ± 0.002	5.849 ± 0.003
$-1s2s3d\ ^4D$	5.5466	5.5635 ± 0.001	5.562 ± 0.002
$1s2p\ ^4P$			
$-1s2p3s\ ^4P^\circ$	6.0272	6.023 ± 0.002	6.020 ± 0.003
$-1s2p3d\ ^4P^\circ$	5.7179	5.684 ± 0.001	bl
$-1s2p3d\ ^4D^\circ$	5.7340	5.726 ± 0.001	5.726 ± 0.001
$1s2p3d\ ^4F^\circ$–$1s2p4f\ ^4G$a	17.603	17.560 ± 0.012	17.568 ± 0.005
$1s2s3d\ ^4D$–$1s2s4f\ ^4F^\circ$a	17.886	17.657 ± 0.006	17.652 ± 0.005
Aluminium ($Z = 13$) Transition	"SC" λ/nm	Corrected λ/nm	Experiment λ/nm
$1s2s2p\ ^4P^\circ$			
$-1s2s3s\ ^4S$	4.8597	4.880 ± 0.002	
$-1s2s3d\ ^4D$	4.6477	4.661 ± 0.001	
$1s2p^2\ ^4P$			
$-1s2p3s\ ^4P^\circ$	5.0177	5.015 ± 0.002	
$-1s2p3d\ ^4P^\circ$	4.7776	4.751 ± 0.001	4.745 ± 0.002
$-1s2p3d\ ^4D^\circ$	4.7906	4.785 ± 0.001	4.783 ± 0.001
$1s2p3d\ ^4F^\circ$–$1s2p4f\ ^4G$	14.614	14.593 ± 0.012	14.587 ± 0.015
$1s2s3d\ ^4D$–$1s2s4f\ ^4F^\circ$	14.831	14.657 ± 0.006	14.664 ± 0.010
$1s2p3d\ ^4D^\circ$–$1s2p4f\ ^4F$	15.265	15.251 ± 0.010	15.245 ± 0.010
$1s2p3d\ ^4P^\circ$–$1s2p4f\ ^4D$	15.227	15.325 ± 0.015	15.315 ± 0.010
Silicon ($Z = 14$) transition	"SC" λ/nm	Corrected λ/nm	Experiment λ/nm
$1s2s2p\ ^4P^\circ$			
$-1s2s3s\ ^4S$	4.1204	4.137 ± 0.002	
$-1s2s3d\ ^4D$	3.9562	3.963 ± 0.001	
$1s2p^2\ ^4P$			
$-1s2p3s\ ^4P^\circ$	4.2425	4.241 ± 0.002	
$-1s2p3d\ ^4P^\circ$	4.0514	4.032 ± 0.001	4.029 ± 0.002
$-1s2p3d\ ^4D^\circ$	4.0625	4.058 ± 0.001	4.065 ± 0.002
$1s2p3d\ ^4F^\circ$–$1s2p4f\ ^4G$	12.326	12.311 ± 0.012	12.312 ± 0.005
$1s2s3d\ ^4D$–$1s2s4f\ ^4F^\circ$	12.497	12.362 ± 0.006	12.371 ± 0.003

bl This transition is blended by Mg X $1s^2\ 2p^2\ ^1S$–$1s^2\ 2p4d\ ^1P^\circ$ [24].
[a] already reported in [19].

Acknowledgement

We thank the staff of the Bochum accelerator especially for their effort on the Mg- and Al-beam. The excellent exciter foils were prepared by H. H. Bukow while E. Träbert, B. Sobotka, T. Göbenli and R. Hucke helped with the experiment. The data acquisition system was granted by the Deutsche Forschungsgemeinschaft. Discussions with and help by Tomas Brage (Lund) and E. Träbert are gratefully acknowledged. We would like to thank C. Laughlin for the correspondence and for communicating results prior to publication. Finally we would like to express our thanks to J. P. Desclaux for his continuous support. One of us (J.H.B) is grateful to the Deutsche Forschungsgemeinschaft (DFG) and the Gesellschaft für Schwerionenforschung Darmstadt (GSI) for financial support.

References

1. Laughlin, C., J. Phys. **B16**, 3329 (1983).
2. Chung, K. T., Phys. Rev. **A29**, 682 (1984).
3. Froese Fischer, C., Phys. Rev. **A26**, 2627 (1982).
4. Mannervik, S., Phys. Scr. **40**, 28 (1989).
5. Brage, T. and Froese Fischer, C., J. Phys. **B21**, 2563 (1988).

6. Mannervik, S., Cederquist, H., Martinson, I., Brage, T. and Froese Fischer, C., Phys. Rev. **A35**, 3136 (1987).
7. Blanke, J. H., Heckmann, P. H. and Träbert, E., Z. Phys. **D3**, 375 (1986).
8. Schneider, D., Bruch, R., Butscher, W. and Schwarz, W. H. E., Phys. Rev. **A24**, 1223 (1981).
9. Desclaux, J. P., Comp. Phys. Comm. **9**, 31 (1975).
10. Huang, K. N., Kim, Y. K., Cheng, K. T. and Desclaux, J. P., Phys. Rev. Lett. **48**, 1245 (1982).
11. Mannervik, S., Short, R. T., Sonnek, D., Träbert, E., Möller, G., Lodwig, V., Heckmann, P. H., Blanke, J. H., and Brand, K., Phys. Rev. **A39**, 3964 (1989).
12. Mannervik, S., Short, R. T., Sonnek, D., and Träbert, E., DTL-Jahresbericht **15**, 95 (1988), Ruhr Universität Bochum.
13. Träbert, E., Heckmann, P. H., Schlagheck, W. and Buttlar, H. V., Phys. Scr. **21**, 27 (1980).
14. Blanke, J. H., Heckmann, P. H., Träbert, E. and Hucke, R., Phys. Scr. **35**, 780 (1987).
15. Laughlin, C. and Fairley, N. A., Z. Phys. **D5**, 91 (1987).
16. Bruch, R., Schneider, D., Chung, K. T., Davis, B. F. and Stolterfoht, N., J. Phys. **B20**, L341 (1987).
17. Layzer, D., Ann. Phys. **8**, 271 (1959).
18. Brage, T., Ph.D-Thesis, Lund (1988).
19. Blanke, J. H., Fricke, B., Heinemann, D., Sepp, W.-D., Thies, B., Göbenli, T., Heckmann, P. H., Möller, G. and Träbert, E., Z. Phys. **D13**, 1 (1989).
20. Laughlin, C., (to be published).
21. Moore, C. E., Atomic energy levels NSRDS-NBS-35. Washington D.C., U.S. Gover. Printing Office 1971.
22. Blanke, J. H., Heckmann, P. H. and Träbert, E., Phys. Scr. **32**, 509 (1985).
23. Bashkin's. and Stoner, P., Atomic energy levels and grotrian tables. Amsterdam: North Holland, 1975.
24. Kelly, R. L., Atomic and Ionic Spectrum Lines Below 2000 Å. Hydrogen through Krypton, Oak Ridge National Laboratory Report ORNL-5922 (1982).
25. Engström, L., Phys. Scr. **31**, 379 (1985).
26. Edlen, B., Phys. Scr. **11**, 366 (1975).
27. Rashid, K., Fricke, B., Blanke, J. H. and Desclaux, J. P., Z. Phys. **D11**, 99 (1989).
28. Laughlin, C., Z. Phys. **D9**, 273 (1988).
29. Chen, M. H., Atomic Data and Nuclear Data Tables **34**, 301 (1986).
30. Mannervik, S. and Cederquist, H., Phys. Scr. **27**, 175 (1983).
31. Baudinet-Robinet, Y., Dumont, P. D., Garnir, H. P., Träbert, E. and Heckmann, P. H., Z. Phys. **D7**, 47 (1987).