Experimental investigation of doubly excited states in Be II

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Multiconfiguration Hartree-Fock calculations by Froese Fischer have confirmed nearly all our recent identifications of doubly excited quartet states in Be II and predicted a number of new ones. Experimental data are reported which confirm some of the new theoretical predictions concerning $2p\,4l$ quartet states.

INTRODUCTION

Up to 1980 only a very limited part of the doubly excited quartet spectrum of Be II was identified. Since then it has been possible to establish all the $2s\,3l$, $2p\,3l$, and $2s\,4l$ states due to a close interplay between experimental[1-3] and theoretical[4,5] groups. Of the ten possible $2p\,4l\,^4L$ states, only two have been unambiguously identified ($2p\,4d\,^4D^o$ and $2p\,4f\,^4F$), whereas one ($2p\,4d\,^4F^o$) has been proposed,[3] but not confirmed by calculations.

New theoretical calculations of transition energies, lifetimes, and transition probabilities for the Be II quartet spectrum have now been reported by Froese Fischer[6] in the preceding paper. These calculations are performed by means of the multiconfiguration Hartree-Fock (MCHF) method, which previously has been shown to yield reliable information for two-electron systems.[7] The calculations have confirmed the identifications of all the $2s\,3l$, $2p\,3l$, and $2s\,4l$ states and of the $2p\,4d\,^4D^o$ and $2p\,4f\,^4F$ states, but also predicted a number of other $2p\,4l$ states including the $2p\,4d\,^4F^o$ state, which is proposed to be incorrectly assigned.

The MCHF calculations are generally yielding better agreement with observations than the values calculated by means of the semiempirical model-potential method.[5] In addition, the MCHF method seems better suited to calculate the higher-lying states such as the $2p\,4l$ states. The strong configuration mixing occurring among the higher-lying states prevented Laughlin[5] from calculating the term energy for $2p\,4d\,^4F^o$ at a sufficient level of accuracy to yield unambiguous guidance for assigning[3] the spectral lines for the $2p\,3p\,^4D-2p\,4d\,^4F^o$ and $2s\,4d\,^4D-2p\,4d\,^4F^o$ transitions.

This paper reports new experimental data dealing with $2p\,4l$ quartet states in Be II, which confirm some of the theoretical predictions of Froese Fischer.[6]

EXPERIMENTAL METHODS

The experimental data are obtained by means of the beam-foil method as described in detail before.[2,8] Some of the charge-state determinations are based upon Doppler-shift measurements.[3]

RESULTS AND DISCUSSION

$2p\,4s\,^4P^o$

The MCHF calculations[6] predict for the $2p\,4s\,^4P^o$ state a lifetime of 3.0 ns and decay channels to $2p\,3p\,^4P$ and ^4D at 4611 and 3853 Å, respectively, with a relative intensity ratio for the two decay channels of 2:1. The experimental data contain two spectral lines only shifted 1 Å, with respect to the predicted wavelengths, at 4610 and 3852 Å with the relative intensities being 2:1. Doppler-shift charge-state analysis has been performed for these two spectral lines, both of which exhibit charge + 1. The lifetimes for the upper levels of 3852 and 4610 Å have been measured and found to be the same within the experimental accuracy but slightly larger than the theoretical value for $2p\,4s\,^4P^o$ (Table I). A similar trend for the lifetimes is noticed for the $2p\,3s\,^4P^o$ state.[6] The agreement between the experimental and theoretical data supports Froese Fischer's predictions for the $2p\,4s\,^4P^o$ state.

It has not been possible to identify the two remaining decay channels, at 841.1 Å (to $2p^2\,^4P$) and 3403 Å (to $2s\,4s\,^4S$), since both wavelength regions are dominated by stronger spectral lines

TABLE I. Wavelengths and lifetimes for doubly excited Be II.

	Wavelength (Å)		Lifetime of upper level (ns)	
	This work	Theory[a]	This work	Theory[a]
$2p\,3p\,^4D-2p\,4s\,^4P^o$	3852 ±1	3853	4.4±0.4	3.0
$2p\,3p\,^4P-2p\,4s\,^4P^o$	4610 ±1	4611	3.9±0.8	3.0
$2s\,2p\,^4P^o-2p\,4p\,^4P$	604.1±0.4	604.4		
$2s\,4p\,^4P^o-2p\,4p\,^4P$	3530 ±1	3507	3.9±0.4	4.7
$2p\,3s\,^4P^o-2p\,4p\,^4P$	2775 ±1	2782	3.7±0.4	4.7
$2s\,2p\,^4P^o-2p\,4p\,^4D$	609.6±0.3	609.6		
$2s\,4p\,^4P^o-2p\,4p\,^4D$	3708 ±1	3689	5.5±0.5	5.4
$2p\,3s\,^4P^o-2p\,4p\,^4D$	2895 ±1	2895		
$2p\,3d\,^4F^o(2)-2p\,4f\,^4G$	3995 ±1	4045	3.6±0.3	3.9
$2s\,4f\,^4F^o(1)-2p\,4f\,^4G$	3285 ±1	3318		

[a]Reference 6.

originating from Be II (at 842 Å) or from doubly excited Be II (at 3405 Å, the $2s\,4f\,^4F^o(1)-2p\,4f\,^4F$ transition).

$2p\,4p\,^4P$ and ^4D

The spectral region 600–610 Å (Fig. 1) contains three spectral lines appearing at 601.5, 604.1, and 609.6 Å. It has already been predicted by Ali[9] and Laughlin[10] that the $2s\,2p\,^4P^o-2p\,4p\,^4D$ transition should appear at 608.5 Å (Ref. 9) and that the $2s\,2p\,^4P^o-2p\,4p\,^4P$ transition at 605.8 Å (Ref. 10) with a $2p\,4p\,^4P$ lifetime of 4.3 ns.[5] The MCHF calculations are in good agreement with these previous predictions, but in addition yield the correct splitting between the two spectral lines of interest (predicted 5.2 Å, observed 5.5±0.4 Å) and the transition energies for the decay channels to the $2s\,4p\,^4P^o$ and $2p\,3s\,^4P^o$ states. On the basis of charge-state analysis, lifetime measurements, and

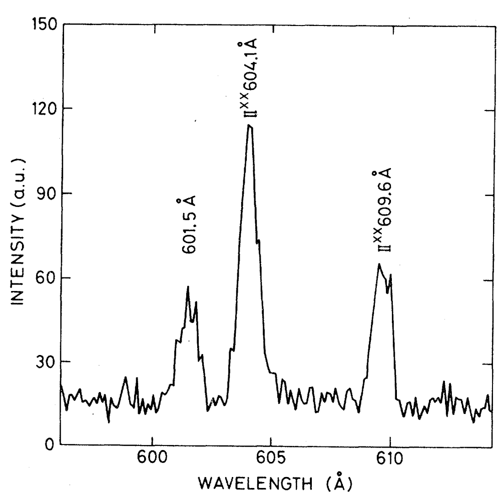

FIG. 1. Partial beam-foil spectrum of Be showing the region 600–610 Å. The three spectral lines are assigned to $2s\,2p\,^4P^o-2p\,4p\,^4S,^4P,^4D$ transitions, respectively. The beam energy was 300 keV.

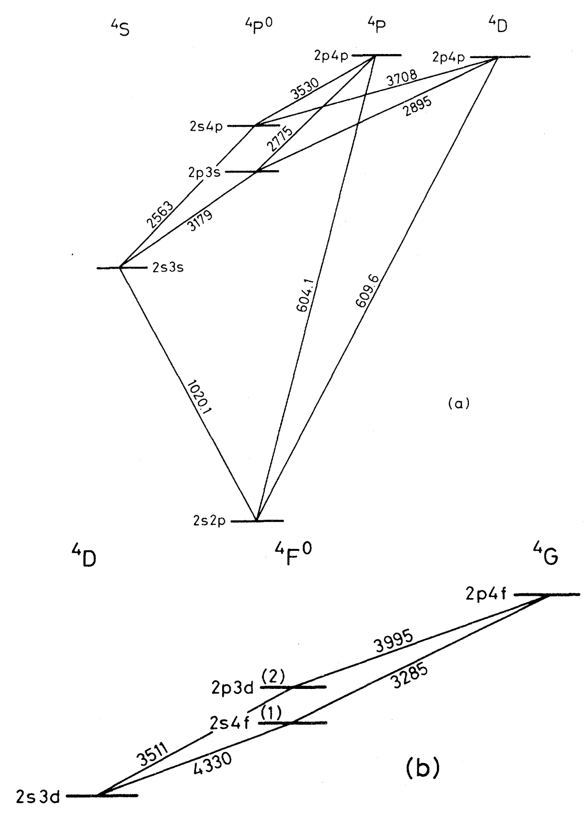

FIG. 2. Term diagrams for doubly excited Be II states discussed in this paper. (a) $2p\,4p\,^4P$ and $2p\,4p\,^4D$, (b) $2p\,4f\,^4G$.

the close-loop principle, it is possible to assign the decay channels from the $2p\,4p\;^4P$ and ^4D states, as shown in Fig. 2(a). The lifetimes for the $2p\,4p\;^4P$ and ^4D states were obtained from the strongest decay components in the visible part of the spectrum. Table I contains a comparison between the experimental and theoretical data.

$2p\,4d\;^4F^o$ and $2p\,4f\;^4G$

The recent proposal[3] for assignment for the 3435- and 3995-Å lines belonging to doubly excited Be II to the $2p\,3d\;^4D-2p\,4d\;^4F^o$ and $2s\,4d\;^4D-2p\,4d\;^4F^o$ transitions has been shown to be incorrect by Froese Fischer,[6] who also has suggested that the 3995-Å line should be assigned to the $2p\,3d\;^4F^o(2)-2p\,4f\;^4G$ transition. The discrepancy between the observed (3995 Å) and the calculated wavelength (4045 Å)[6] is larger than usual, but a plausible explanation exists and is given by Froese Fischer.[6] In order to test the new assignment for the 3995-Å line, the closed loop $2p\,4f\;^4G-2p\,3d\;^4F^o(2)-2s\,3d\;^4D-2s\,4f\;^4F^o(1)-2p\,4f\;^4G$ [Fig. 2(b)] has been considered. If the 3995-Å line were to be attributed to the $2p\,3d\;^4F^o(2)-2p\,4f\;^4G$ transition, there should appear a spectral line at 3287 ± 2 Å, representing the $2s\,4f\;^4F^o(1)-2p\,4f\;^4G$ transition. The theoretical branching ratio between the two lines is predicted to be $\sim$7:1 (Ref. 6), with the 3995-Å line being the stronger component.

The spectral region near 3287 Å contains two so far unidentified singly charged Be lines appearing at 3285 and 3292 Å, respectively. On the basis of the closed-loop prediction and the experimental intensity ratio for the 3995 Å/3285 Å lines of 7:1, we propose the 3285-Å line to be the $2s\,4f\;^4F^o-2p\,4f\;^4G$ transition. Unfortunately, it has not been possible to support the assignment of the 3285-Å line with lifetime measurements for the upper state ($2p\,4f\;^4G$) due to the presence of the rather strong Be II ($3s$-$4p$) spectral line nearby (at 3276 Å). Lifetime measurements for the upper state of the 3292-Å line yielded 9.0 ± 1.5 ns, a value which excludes this line as a possible candidate for the $2s\,4f\;^4F^o-2p\,4f\;^4G$ transition. The present data, however, do not exclude the possibility that the 3995-Å line could belong to the doubly excited Be II doublet spectrum.[6] On the basis of the MCHF calculations,[6] it is proposed that the 3292-Å line should be attributed to the $2p\,3p\;^4D-2p\,4d\;^4F^o$ transition predicted to appear[6] at 3284 Å with an upper-state lifetime of 12 ns.

$2p\,4p\;^4S$, $2p\,4d\;^4P^o$, $2p\,4f\;^4D$

Froese Fischer[6] has calculated the main properties for the $2p\,4d\;^4P$ and $2p\,4f\;^4D$ states, but none of the predicted wavelengths have been observed. In fact, only one medium-strong spectral line with charge state +1 is left unidentified in the wavelength region above 2500 Å and below 5000 Å, the line appearing at 3435 Å which was originally attributed to the $2p\,3p\;^4D-2p\,4d\;^4F^o$ transition.[3] It may be reasonable to consider that the 3435-Å line could be associated with the decay of the $2p\,4p\;^4S$ state, which seems very difficult to calculate with the MCHF method.[6] If the 3435-Å line is due to the $2s\,4p\;^4P^o-2p\,4p\;^4S$ transition, then the lifetime of $2p\,4p\;^4S$ should be approximately 4 ns (experimental value 4.0 ± 0.4 ns),[3] and the $2s\,2p\;^4P^o-2p\,4p\;^4S$ transition should appear at 601.5 ± 0.3 Å. The nonassigned spectral line at this wavelength (see Fig. 1) is a possible candidate. Theoretical calculations dealing with the higher ^4S states in Be II will be needed in order to prove this proposal. The calculations reported by Ali and Samanta[11] for S states are not sufficiently detailed to yield the answer.

Note added in proof. Very recent calculations by Laughlin[12] show that the 3435-Å line should be assigned to the $2s\,4s\;^4S$—$2p\,4s\;^4P^o$ transition.

CONCLUSION

The present data show that calculations performed by means of the MCHF method can be very valuable in order to obtain the correct identifications of quartet states in a three-electron system such as doubly excited Be II, for which all the lower-lying states are now identified. On the basis of MCHF calculations, it should now also be possible to study some of the isoelectronic systems to the same degree of completeness.

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