Optical transition in the negative magnesium ion

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A search for the Mg^- ion detected via the $2p^6 3p^3\,{}^4S \rightarrow 2p^6 3s 3p^2\,{}^4P$ transition is described. The $Mg^+ \rightarrow Mg^-\ {}^4S$ two-step charge-exchange process is investigated and compared with the recently observed $Be^+ \rightarrow Be^-\ {}^4S$ process. Analysis of the optical spectra shows that the cross section for producing the $Be^-\ {}^4S$ state by beam-foil or beam-gas collisions is much larger, a factor of 30 or more, than for producing $Mg^-\ {}^4S$. The search has been concentrated in the 2860–2950-Å region that covers the two wavelengths 2921 and 2895 Å recently proposed theoretically for the above transition. None of the spectral lines observed within the spectral region studied exhibits the properties of a negative ion. While the possibility of observing the $Mg^-\ {}^4S$-${}^4P$ transition at 2921±4 Å [D. R. Beck, Phys. Rev. A **40**, 2887 (1989)] can be excluded, the 2895±3 Å region [C. Froese Fischer, Phys. Rev. A **41**, 3481 (1990)] is more complicated since it contains a so far unidentified spectral line. We can assign this line to the quintet spectrum of Mg I. This assignment is supported by four lines forming a closed loop, consistent with optical transitions between the $2p^5 3s 3p 4s$ and $2p^5 3s 3p^2$ configurations, and by multiconfiguration Hartree-Fock calculations. The lack of experimental observations of the predicted Mg^- ion is discussed.

I. INTRODUCTION

Beryllium and magnesium are generally assumed to have negative electron affinities in the ${}^1S$ ground state,[1–5] in contrast to calcium;[6–8] whereas metastable negative-ion $nsnp^2\,{}^4P$ states might be bound with respect to the first excited triplet state for all three ions. The $2s2p^2\,{}^4P$ state of Be^- was confirmed some years ago.[9,10] More recently,[11] the $4s4p^2\,{}^4P_{5/2}$ state in Ca^- was reported to have been observed. The search for the $3s3p^2\,{}^4P$ state in Mg^- has so far[12] yielded only negative results. The recent observation of the Be^- ion detected[13] by observing the optical $1s^2 2p^3\,{}^4S \rightarrow 1s^2 2s 2p^2\,{}^4P$ transition between the two lowest-excited states has initiated a new search for the Mg^- ion.

The Mg^- ion was claimed to exist by Bethge, Heinicke, and Baumann[14] more than 20 years ago. The experimental proof was based upon mass spectra of ions emitted from direct-extraction negative-ion sources, but more recent studies,[12,15] using charge exchange of Mg^+ beams in alkali-metal vapor cells, have invalidated the Bethge-Heinicke-Baumann conclusion. The experimental techniques used[12,14,15] all demanded the lifetime of at least one of the ${}^4P_J$ levels to be larger than 10–100 μ s. Calculations performed by Beck[5] in the Hartree-Fock approximation have yielded lifetimes for the ${}^4P_J$ levels to be considerably shorter, i.e., less than 10 ns. The calculated lifetimes could explain the negative results obtained thus far with regard to the $Mg^-\ {}^4P$ levels, but Nicolaides, Aspromallis, and Beck[16] have pointed out that the Hartree-Fock (HF) predictions may be unreliable since the lifetimes are sensitive to a variety of electron correlation and cancellation effects.

An alternative experimental approach for detecting Mg^- would be to search for the excited $3p^3\,{}^4S$ state in Mg^- by observing the $3p^3\,{}^4S \rightarrow 3s3p^2\,{}^4P$ optical transition. The $3p^3\,{}^4S$ state is predicted to decay predominantly by optical emission[2,5,17–19] with a lifetime of 1.4 ns.[17,18] According to Beck's calculations,[17] the $Mg^-\ {}^4S$-${}^4P$ transition wavelength should appear at 2921±4 Å, with fine-structure splittings for the ${}^4P$ state of 19.4 cm^{-1} for the $J=3/2$-$5/2$ splitting and 11.8 cm^{-1} for the $J=1/2$-$3/2$ splitting.

Very recently, Froese Fischer[19] reported a detailed study of variational procedures for predicting energy differences for many-electron systems. Her study included calculations of the transition wavelengths for the optical transition in Li^- and Be^-, the only negative ions thus far proven to possess excited states that decay radiatively, and a prediction for the ${}^4S$-${}^4P$ transition in Mg^-. The predictions[19] of wavelengths for excited ${}^4S$-${}^4P$ transitions in Be^- and Mg^- were based on the observed $np^2\,{}^3P \rightarrow nsnp\,{}^3P^\circ$ transition energies of the neutral atoms and the calculated electron affinities that included only outer correlation and a core-valence correlation. For Be^-, the predicted value agreed with the experimental value[13] within 0.5 Å. For Li^-, the calculated and observed values deviated by only 2 Å. It is therefore reasonable to expect that the ${}^4S$-${}^4P$ transition in Mg^- may occur within a rather narrow wavelength interval (±3 Å) located around 2895 Å, which is the wavelength predicted by Froese Fischer. The two theoretical predictions[17,19] are clearly in disagreement, taking their quoted limits into account. Therefore an experimental search should be conducted over a larger wavelength region. We have selected the 2860–2950-Å region, which con-

tains the two wavelength regions recently proposed theoretically.

Beam-foil spectroscopy has proven to be successful in the search for optical transitions in the Li^- (Ref. 20) and Be^- (Ref. 13) ions. For these two elements, the many spectral lines produced by the beam-foil excitation technique and originating from core-excited states were nearly all identified at the time the search for the negative-ion transitions was performed.[21] For magnesium, the situation is markedly different. Only a very limited part of the core-excited Mg II quartet spectrum has been identified at the present time.[22] On the basis of Froese Fischer's calculations,[23] it is even possible to predict that a number of unidentified spectral lines, belonging to either the Mg II quartet or the Mg I quintet spectrum, will appear in the wavelength region of interest for Mg^- and thus complicate the search for this ion. Beam-gas collision techniques could be applied to reduce the production of core-excited Mg I and Mg II states; but in order to obtain a measurable production of $Mg^-\ ^4S$, it will be necessary to apply gas pressures far outside the single-collision regime, which may invalidate the advantage of changing the target from a foil to a gas target.

Figure 1 illustrates the predicted energy-level diagram for Mg^-, and the relevant levels for Mg I, with the optical transitions indicated.[17,19] Beck[17] calculated the electron affinities (EA) for the two Mg I states to be 321 meV for $3s3p\ ^3P$ and 536 meV for $3p^2\ ^3P$, whereas Froese Fischer's values are slightly larger. Comparison with the Be^- ions shows that the EA values for Mg are 30–100% larger than for Be. The most significant difference between the two systems, however, may be the energy difference between the ionization limit and the energy of the upper neutral atomic state, for magnesium the $3p^2\ ^3P$ state. This energy difference is only 0.47 eV for magnesium, but 1.92 eV for beryllium.

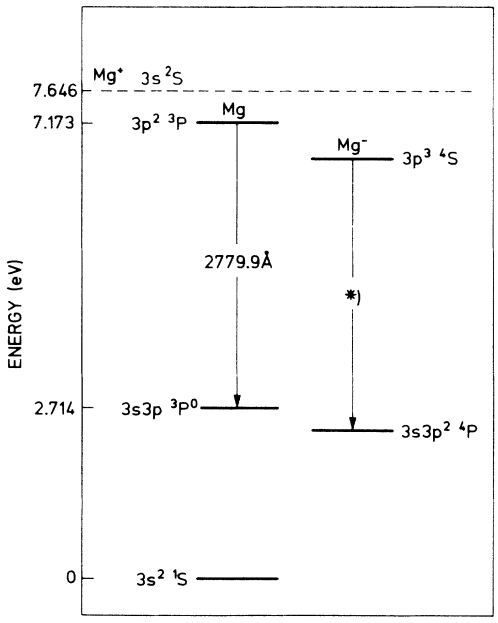

FIG. 1. Energy-level diagram for Mg^- and the relevant levels for neutral Mg, with the optical transitions indicated. (*) For Mg^-, two predictions exist, the wavelength being either 2921 (Ref. 17) or 2895 Å (Ref. 19).

II. EXPERIMENTAL PROCEDURES

The experimental setups used for the beam-foil or beam-gas experiments were similar or identical to the equipment used for the identification of the optical transition in Be^- (Ref. 13) or applied for optical studies of negative-ion–rare-gas collisions.[24] The data-taking and analysis methods used have been described previously.[25] $^{24}Mg^+$ ions with energies ranging from 60 to 300 keV were passed through 2–5-$\mu g/cm^2$ carbon foils or were directed into the gas cell. For some of the beam-gas experiments, the beam was prepared in the $Mg(3s3p\ ^3P^o)$ state by charge exchange in a sodium-metal vapor cell[26] before entering the gas cell. Several different atomic and molecular gases have been used, including gases with rather low ionization potentials such as *N,N* diethylanilin, which has an ionization potential just below 7 eV. Observation of the light in the 2500–3500-Å region was performed with a 1.0-m McPherson model 2051 spectrometer equipped with a 2400-line/mm grating. A circular encoder was mounted on the spectrometer, permitting accumulation of data from several scans into a NORD-12 satellite computer which also controlled the spectrometer.

The assignment of unknown spectral lines was based on a number of criteria described elsewhere,[25] such as charge-state analysis, lifetime measurements to test the assignment of spectral lines assumed to originate from the same upper level, relative line-intensity measurements as compared with line intensities predicted on the basis of theoretical calculations assuming *LS* coupling, and the establishment of closed loops.

III. RESULTS AND DISCUSSION

A. 2900–2950-Å wavelength region

Figure 2 shows the magnesium beam-foil spectrum recorded from ~2900 to ~2950 Å at 60 keV. It contains the region around 2921 Å, the wavelength predicted by Beck[17] for the $Mg^-\ ^4S$-^4P transition. The intense spectral lines at 2928 and 2936 Å belong to the normal Mg II spectrum, whereas the weaker lines at 2899, 2906, 2915, and 2941 Å belong either to the Mg III or to Mg IV, since the intensity ratio between the unknown weaker and the two stronger lines in this spectrum increases at higher energies. Both the lifetime measurements ($\tau \approx 6$–7 ns for the unknown lines) and the Doppler-shift measurements show that none of these lines can be attributed to the negative magnesium ion. By using 2-$\mu g/cm^2$ C foils, it was possible at 100 keV to reduce the full width at half maximum (FWHM) value for the intense 2928-Å line to 1.4 Å, allowing a search for a possible Mg^- line in the entire spectral range 2921±4 Å, but no line could be observed in this region.

The collisional formation of negative beryllium or magnesium ions from positive ions interacting with foils or gases is assumed to involve a two-step electron-capture process ($X^+ \rightarrow X^0 \rightarrow X^-$). We consider it likely that the

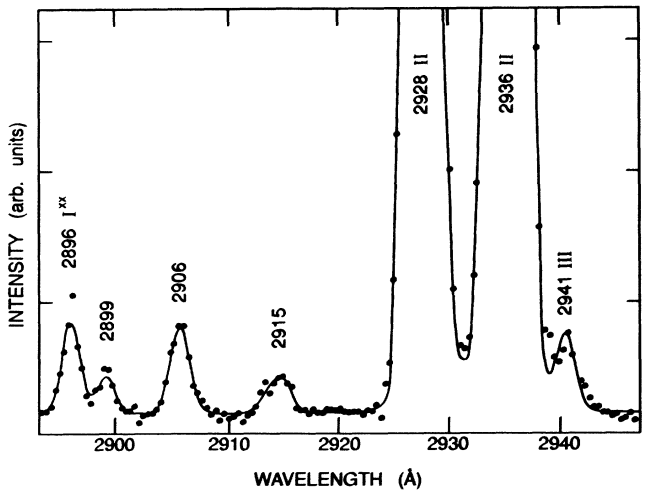

FIG. 2. Beam-foil spectrum of magnesium, recorded at 60 keV, covering the 2900–2950-Å region.

second capture process leading to population of the $np^3\,^4S$ state in the negative ions involves the $np^2\,^3P$ state of the neutral atom, rather than the metastable $nsnp\ ^3P^\circ$ state. If this assumption is correct, the production rate for the ^4S state depends on parameters such as the concentration of the neutral atoms in the $np^2\,^3P$ state, the electron-capture cross section for the $np^2\,^3P \rightarrow np^3\,^4S$ process, and the cross section for destroying the $np^2\,^3P$ atoms due to ionization.

Information about the electron-capture cross section may be gained from a comparison of the line intensities of the ^4S-^4P transition in the negative ion and the $np^2\,^3P \rightarrow nsnp\ ^3P^\circ$ transition in the neutral atom. The experimental observation of the optical transition in Be^- (Ref. 13) showed that the $Be^-\ ^4S$ to Be I ^3P population ratio in beam-foil experiments was approximately 0.01. Taking the electron affinities for magnesium into account, we do not expect the $Mg^-\ ^4S$ to Mg I ^3P population ratio to be significantly different. The spectral intensity of the $np^2\,^3P \rightarrow nsnp\ ^3P^\circ$ transition in the neutral atoms can yield information about the equilibrium concentration of the atoms in the $np^2\,^3P$ state. We have observed that the equilibrium concentration in foil and gas experiments for $Mg(3p^2\,^3P)$ is a factor of 10–20 times lower than for $Be(2p^2\,^3P)$ for the same relative beam velocities. This markedly lower concentration for magnesium may be due to a larger collisionally induced ionization cross section for the $3p^2\,^3P$ state in Mg I than for the $2p^2\,^3P$ state in Be I. It is well established that the collisionally induced ionization cross sections increase rapidly when the energy difference between the ionization limit and the excited state is lowered.[27] For Mg I, experimental data for ionization cross sections for Mg–rare-gas collisions are available[28] for the $3s^2\,^1S$ and $3s3p\ ^3P^\circ$ states, showing that the cross section for the metastable $^3P^\circ$ atoms was a factor of 3–10 times larger at the collision energies used in the present study than for the ^1S ground-state atoms. As pointed out in the Introduction, the two systems compared, Be^- to Be I and Mg^- to Mg I, differ significantly with respect to the location of the $np^2\,^3P$ state, relative to the ionization limit. This difference between the systems may perhaps explain the experimental observations.

On the basis of the beam-foil and beam-gas experiments, we expect the production of the $Mg^-\ ^4S$ state to be a factor of ~ 10 below the production of $Be^-\ ^4S$ for the same beam intensity and relative velocity. For regions free from spectral lines, such as seen at 2921±4 Å, we can estimate that the upper limit for production of $Mg^-\ ^4S$ is at least an additional factor of ~ 10 below the estimate just made, indicating that it is very unlikely that the $Mg^-\ ^4S$-^4P transition lies in the wavelength region suggested by Beck,[17] or in any other region free from spectral lines. We can also estimate an upper limit for the production rate for $Mg^-\ ^4S$, assuming that the Mg^- line was blended by one of the unassigned lines at 2899, 2906, and 2915 Å, respectively, to be a factor of 30 or more below the production rate for $Be^-\ ^4S$. If the Mg^- line were blended by one of the intense Mg II lines (at 2928 and 2936 Å), it would not be possible to detect it even if its production rate were significantly larger than the estimates given above.

B. 2860–2900-Å wavelength region

Figure 3 shows the Mg beam-foil spectrum at 60 keV covering the spectral region between 2800 and 2900 Å, which contains Froese Fischer's predicted region (2895±3 Å). The intense lines belong to the singly excited Mg II and Mg I spectra, whereas the lines at 2817, 2841, 2861, 2881, and 2896 Å all exhibit the same intensity-versus-energy dependence, with a maximum intensity at energies below 100 keV. This behavior indicates that these five lines originate from core-excited states in neutral magnesium. The Doppler-shift technique has been used to prove that the 2896-Å line, or its

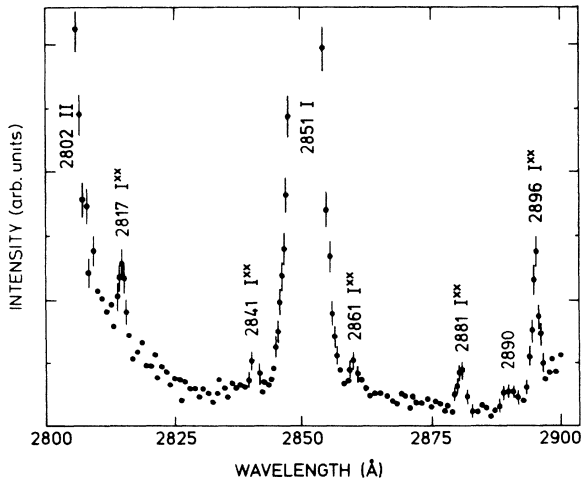

FIG. 3. Beam-foil spectrum of magnesium recorded at 60 keV, covering the 2800–2900-Å region.

dominant component if it consists of two lines, belongs to neutral magnesium. A weak line can be seen at 2890 Å. It belongs either to the Mg II quartet spectrum of Mg III. The 2896-Å line has been carefully studied, since this line coincides with the wavelength proposed by Froese Fischer[19] for the Mg^- ^4S-^4P transition.

The lifetime of the 2896-Å line has been measured to be 2.7±0.3 ns, which is nearly a factor of 2 longer than predicted[17] for the Mg^- transition. The decay analysis showed the existence of only one component. A detailed search in the decay region just after the foil did not reveal a second decay component with a shorter lifetime. Our decay data, however, do not exclude that a minor part of the 2896-Å line, of the order of ~10% of the intensity, could be due to a blended line. If the strongest line of the Mg ^4S-^4P multiplet ($^4S_{3/2} \rightarrow {}^4P_{5/2}$) was indeed blended by a more intense Mg I line, then it should be possible to identify the Mg^- multiplet on the basis of the other fine-structure components. The three $^4S_{3/2} \rightarrow {}^4P_{1/2,3/2,5/2}$ lines should appear at 2893.3, 2894.3, and 2895.9 Å, according to the theoretical predictions.[17,19] The experimental data give no evidence for the presence of the weaker fine-structure components. The intensity of the 2896-Å line is a factor of 2–3 stronger than expected for the Mg^- ^4S-^4P spectral line having an intensity of the order of 1% of the Mg I $3p^2\,{}^3P \rightarrow 3s3p\,{}^3P^\circ$ line. The experimental data in the 2895 region allow us to set an upper limit only for the Mg^- ^4S production to be a factor of ~3–5 smaller than expected. Thus it cannot be excluded that the Mg^- ion can be observed by optical techniques in this wavelength region, but the overlapping line at 2896 Å is a severe disadvantage. Similar studies have been performed for the other lines seen in the region above 2860 Å, such as 2861 and 2881 Å, but without obtaining evidence for a possible blending of a Mg^- line. Thus none of the lines investigated exhibits the properties expected for the Mg^- $^4S \rightarrow {}^4P$ line.

Beck[29] has very recently commented upon the possibility that the 2896-Å line could belong to a $2p^5 3p^3\,{}^5P \rightarrow 2p^5 3s3p^2\,{}^5P$, ^5D, or ^5S transition. The transition energies between $2p^5$ core-excited states in Mg I, however, can be expected to be very similar to transition energies in the Al I atom having a $2p^6$ core.[23] Thus Beck's proposal can be eliminated, since the $3p^3\,{}^4S \rightarrow 3s3p^2\,{}^4P$ transition in Al I appears near 2000 Å. On the other hand, the transitions between the two lowest configurations in the Mg I quintet spectrum, $2p^5 3s3p4s \rightarrow 2p^5 3s3p^2$, can be expected to appear in the wavelength region from ~2600 to ~3400 Å.

C. Identification of the 2896-Å line

A study of the Mg beam-foil spectra at 60, 100, and 300 keV shows a number of unknown spectral lines which belong to the core-excited Mg I quintet spectrum. In the present paper, we will limit the identification to the spectral lines needed to establish an unambiguous identification of the 2896-Å line, which we have more accurately determined to appear at 2895.8±0.2 Å. Figure 4 shows the closed loop we have established on the basis of new $2p^5 3s3p4s\ {}^5P_3$ and $^5D_4$ levels and $2p^5 3s3p^2\,{}^5P_3$ and $^5D_4$ levels. The assignment of the 2895.8-Å line to the $2p^5 3s3p4s\ {}^5D_4 \rightarrow 2p^5 3s3p^2\,{}^5P_3$ transition is based on the following.

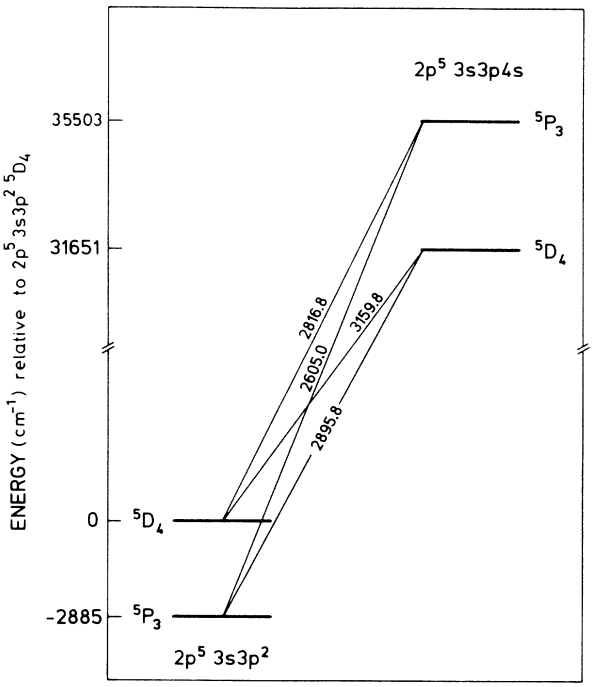

FIG. 4. Partial-energy-level diagram for Mg I quintet spectrum with the observed transitions (in Å) indicated.

(i) The closed loop shown in Fig. 4.

(ii) The lifetimes measured for the different decay channels from the same upper level were identical. For the 2895.8- and 3159.8-Å lines, the lifetime 2.7±0.3 ns was obtained.

TABLE I. Total energies (in a.u.) and the size of CFS expansion for different quintet states of Mg I. NR represents nonrelativistic results, RS represents inclusion of relativistic shifts, and SO represents inclusion of spin orbit.

Levels	No. of CFS's		Total energy (a.u.)
$2p^5 3s3p^2\,{}^5P_3$	259	NR	−197.708 519 1
		RS	−198.002 644 3
		SO	−198.004 280 6
$2p^5 3s3p^2\,{}^5D_4$	333	NR	−197.659 026 0
		RS	−197.989 143 3
		SO	−197.992 417 8
$2p^5 3s3p4s\ {}^5D_4$	335	NR	−197.550 721 4
		RS	−197.845 042 8
		SO	−197.848 110 1
$2p^5 3s3p4s\ {}^5P_3$	259	NR	−197.535 337 3
		RS	−197.829 670 9
		SO	−197.831 305 2

TABLE II. Energies relative to the $2p^5 3s 3p^2\,{}^5D_4$ level. The absolute energy for this level is calculated to be $-197.992\,417\,8$ a.u.

Level	Energies (cm^{-1}) Calculation	Experiment
$2p^5 3s 3p^2\,{}^5P_3$	-2720[a]	-2885
$^5D_4$	(0)	(0)
$2p^5 3s 3p 4s\,{}^5D_4$	31 671	31 651
$^5P_3$	35 359	35 503

[a]Includes an estimate of *LS*-breaking interactions.

TABLE III. Wavelengths (Å) in air for $2p^5 3s 3p 4s \rightarrow 2p^5 3s 3p^2$ quintet transitions in Mg I.

Transition	Experiment	Calculation
$^5D_4 \rightarrow {}^5P_3$	2895.8±0.2	2908[a]
$^5D_4 \rightarrow {}^5D_4$	3159.8±0.2	3157
$^5P_3 \rightarrow {}^5P_3$	2605.0±0.3	2626[a]
$^5P_3 \rightarrow {}^5D_4$	2816.8±0.2	2828

[a]Includes an estimate of *LS*-breaking interactions.

(iii) The charge-state analysis proved that these spectral lines all belong to neutral magnesium.

(iv) The relative intensities for the transitions shown in Fig. 4 were in rather good agreement with values calculated assuming the *LS* coupling. For the ratio I(3159 Å)/I(2896 Å), we observed 1.2±0.2, which compares well with the calculated value of 1.4.

In order to support the identification, theoretical calculations of energies of Mg I quintet levels were performed, using the multiconfiguration Hartree-Fock (MHF) method.[30] Each atomic sate is represented by a linear combination of configuration-state functions (CSF's), Φ_i,

$$\psi(LS) = \sum_i c_i \Phi_i(a_i LS) \ . \tag{1}$$

The CSF's are constructed from one-electron orbitals, the angular momenta of which are coupled as specified by a_i. The radial parts are obtained from self-consistent-field calculations with respect to the state of interest. Details of the method will be reported elsewhere, and here we will outline only the main ideas.

To capture the full correlation between the outer three electrons, we had to use fairly extensive expansions. In earlier studies[31,32] it was found that, to retain numerical stability while performing full variational computations, it is advantageous to apply a technique that could be labeled the "active set–generalized Brillouin's theorem." In this we generate all CSF's from a given active set of orbitals but exclude some with reference to a generalization form of the Brillouin's theorem.[32] In the final stage of our calculations, the active set consisted of

$$\{3s, 4s, 5s, 3p, 4p, 5p, 3d, 4d, 5d, 4f\} \ .$$

The final energies for the four levels are given in Table I, together with the total number of CSF's in (1). After the optimization, we also included relativistic shifts and spin-orbit to obtain the two last energies reported in Table I. The accuracy of the present approach could be expected to be different for the four quintets under consideration. We have only included effects diagonal in the total orbital and spin angular momentum (L and S), and therefore left out *LS*-breaking interactions. For the two $^5D_4$ levels, this is not a severe restriction. For the two $^5P_3$ levels, test calculations with smaller basis sets show that they do interact with other *LS* terms. We have tried to estimate this for the $2p^5 3s 3p^2\,{}^5P_3$ from a limited calculation, including only states of the same complex but with all terms having $J=3$ levels. These estimates are added in Tables II and III.

Tables II and III contain a comparison between the calculated and experimental values. On an absolute scale, the $2p^5 3s 3p^2\,{}^5D_4$ level is predicted ~54 eV above the ground state of neutral magnesium.[33] The data in Tables II and III show that the theoretical model used is well suited to predict the structural properties for the Mg I quintet spectrum, and further studies of this system, experimental as well as theoretical, are in progress and will be reported elsewhere.

IV. CONCLUDING REMARKS

The present experimental data give no evidence for the theoretically predicted Mg^- ion. None of the spectral lines appearing in the 2860–2950-Å region exhibits the properties of an optical transition in a negative ion. The cross section for producing the Mg^- ion in the excited ^4S state by conventional beam-foil or beam-gas experiments is found to be considerably smaller than the equivalent cross section for producing $Be^-\,{}^4S$. If the cross section for producing the $Be^-\,{}^4S$ state had been reduced by a factor of approximately 30, it would have been very difficult to observe the optical transition in this ion.[13] If the mechanisms discussed above represent a reasonable description of the processes involved for transforming Mg^+ to $Mg^-\,{}^4S$, it can be predicted that the search for a ^4S-^4P optical transition in the negative zinc ion[34] will also yield a negative result if based on the techniques used in the present study. The Ca^- ion, however, may still be considered as a possible candidate for further studies.

Winter *et al.*[35] have considered the possibility of describing the beam-foil process in terms of an electron-transfer model, in which the work function for the foil material plays an important role. Experimental studies with foils or surfaces, for which the work function can be varied in a controlled manner, may be of interest for gaining more insight into the formation of negative ions, such as Li^-, Be^-, and perhaps Mg^-, and to the population of excited states in these ions from collisional experiments.

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