$3d^2$ Configuration in six-times-ionized argon, Ar VII

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The transition array $2p^6 3p 3d - 2p^6 3d^2$ has been identified in the spectrum of magnesium-like Ar VII produced by electrical discharges in the vacuum-ultraviolet region. Twenty-five new transitions have been identified as combinations of levels of this transition array. From these transitions we have determined the levels of the $3d^2$ configuration. It was also possible to determine the $2p^6 3p 3d\,^1D_2^o$ level that was missed in the early research with the Ar VII spectrum. Hartree–Fock calculations with relativistic corrections were used to predict energy levels and transitions. Isoelectronic comparisons along the Mg I sequence are used to support the experimental results. © 2001 Optical Society of America

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1. INTRODUCTION AND EXPERIMENT

Some of the present authors recently presented an analysis of transitions and energy levels in the $n = 3$ complex of Mg-like Ar VII.[1] We reported the levels of the $2p^6 3s^2$, $2p^6 3p^2$, $2p^6 3s 3d$, $2p^6 3s 3p$, $2p^6 3p 3d$, and $2p^6 3s 4p$, configurations; the $2p^6 3d^2$ configuration was not taken into account. Predictions for the levels of the $2p^6 3d^2$ configuration show that P IV is the first spectrum along the Mg I sequence containing bound–bound transitions that connect the levels of the $2p^6 3d^2$ configuration to the lower systems. The first analyses for the $2p^6 3d^2$ configuration in the Mg I sequence were made for P IV and S V ions.[2,3] Following these results, Jupén and Fremberg[4] performed an analysis of this configuration for the Cl VI spectrum. Redfors[5] reported the study of the $2p^6 3d^2$ configuration in Ca IX–Zn XIX. Churilov *et al.*[6] extended the analysis of the $2p^6 3d^2$ configuration to K VIII–Cu XVIII. The present research fills a gap in the study of the $2p^6 3d^2$ configuration for the Mg I sequence in P IV–Zn XX spectra. In recent years the Mg-like ions have been the focus of many theoretical calculations, mainly for the elements P, S, and Cl, in which the high configurations of the $n = 3$ complex plunge through the rest of the system and short-range configuration interaction effects appear.[7–14] These calculations have addressed the experimental assignments for some levels reported as $3d^2$ in Refs. 2–4. For the $3d^2$ configuration in Ar VII and higher elements in the Mg I sequence those effects are not present.

The details of our experimental system for obtaining

spectra of inert gases were described in a previous paper.[15] The light source is a Pyrex tube, 30 cm long, with an inner diameter of 0.3 cm. The tube has inner electrodes and is viewed end on. We produce the excitation of the gas by discharging through the tube a bank of low-inductance capacitors that vary from 2.5 to 100 nF and have been charged up to 19 kV. Ilford Q-2 plates were used to record the spectra. The plate factor in the first order was 2.77 Å/mm. C, N, O, Si, and known lines of Ar provided internal wavelength standards. The radiation was recorded with a 3-m normal-incidence spectrograph with a diffraction grating of 1200 lines/mm. The photographic plates were measured in a Grant comparator. This comparator works semiautomatically and permits determination of asymmetric lines through an oscilloscope display. The accuracy of the wavelength values for unperturbed lines is estimated to be ±0.01 Å, and that for perturbed ones is ±0.03 Å.

2. RESULTS AND DISCUSSION

The Ar VII lines observed in the present study are listed in Table 1. There are 25 new lines that belong to the $2p^6 3p3d - 2p^6 3d^2$ transition array. The intensities of the lines in Table 1 are based on visual estimates of the photographic blackening of the plates and of the amplitude of the electronic signal provided by the comparator.

The energy levels derived from the observed lines are listed in Table 2. There are nine new levels that belong to the $2p^6 3d^2$ configuration and one new level that belongs to the $2p^6 3p3d$ configuration. The energy-level values were optimized from the observed wavelengths by an iterative procedure in which the individual wavelengths are weighted according to their uncertainties.[16]

We obtained the theoretical predictions for the energy levels of the $2p^6 3d^2$ configuration by diagonalizing the energy matrices with appropriate Hartree–Fock relativistic (HFR) values for the energy parameters. The Cowan computer code[17] was used for both the *ab initio* calculation and the least-squares fit of the Slater parameters. The fitted parameters are compared in Table 3 with *ab initio* values that result from the HFR calculations. The

Table 2. Energy Levels of Ar VII Established in This Paper

Configuration	Level	Energy Level (cm^{-1})	Percentage Composition of LS Coupling[a]
$2p^6 3d^2$	$^3F_2$	653 903.9	99
$2p^6 3d^2$	$^3F_3$	654 037.8	99
$2p^6 3d^2$	$^3F_4$	654 123.9	99
$2p^6 3d^2$	$^1D_2$	666 547.4	96
$2p^6 3d^2$	$^1G_4$	668 055.2	$95 + 5(2p^6 3p4f\ ^1G)$
$2p^6 3d^2$	$^3P_0$	669 287.3	99
$2p^6 3d^2$	$^3P_1$	669 366.0	99
$2p^6 3d^2$	$^3P_2$	669 406.0	99
$2p^6 3d^2$	$^1S_0$	707 622.6	$96 + (2p^6 3p^2\ ^1S)$
$2p^6 3p3d$	$^1D_2^0$	450 476.0[b]	

[a] Percentages lower than 3% are omitted.
[b] The value of this level was missed in the early study of Trigueiros *et al.*[1] but is determined here.

Table 1. Observed Spectral Lines in the $3p3d - 3d^2$ Transition Array in Ar VII

Intensity[a]	Wavelength (Å)	Wave Number (cm^{-1})	Transition	J–J
3	425.99	234 747.3	$3p3d\ ^3P^0 - 3d^2\ ^1S$	1–0
3	450.37	222 039.7	$3p3d\ ^3F^0 - 3d^2\ ^1G$	4–4
3	450.93	221 763.9	$3p3d\ ^3F^0 - 3d^2\ ^1D$	3–2
6	462.81	216 071.4	$3p3d\ ^3D^0 - 3d^2\ ^1D$	2–2
3	474.65	210 681.6	$3p3d\ ^3F^0 - 3d^2\ ^3F$	2–3
6	474.96	210 544.0	$3p3d\ ^3F^0 - 3d^2\ ^3F$	2–2
6	477.70	209 336.4	$3p3d\ ^3F^0 - 3d^2\ ^3F$	3–4
6	477.88	209 257.6	$3p3d\ ^3F^0 - 3d^2\ ^3F$	3–3
3	480.49	208 120.9	$3p3d\ ^3F^0 - 3d^2\ ^3F$	4–4
12 u	508.83	196 529.3	$3p3d\ ^3P^0 - 3d^2\ ^3P$	1–2
12 bl	508.90	196 502.3	$3p3d\ ^3P^0 - 3d^2\ ^3P$	1–1
9 bl	509.12	196 417.3	$3p3d\ ^3P^0 - 3d^2\ ^3P$	1–0
3	511.37	195 553.1	$3p3d\ ^3P^0 - 3d^2\ ^3P$	0–1
3	523.64	190 970.9	$3p3d\ ^3D^0 - 3d^2\ ^1D$	2–2
6	524.88	190 519.7	$3p3d\ ^1P^0 - 3d^2\ ^1S$	1–0
6	559.63	178 689.5	$3p3d\ ^3D^0 - 3d^2\ ^3F$	1–2
6	560.38	178 450.3	$3p3d\ ^3D^0 - 3d^2\ ^3F$	2–3
9	560.64	178 367.6	$3p3d\ ^3D^0 - 3d^2\ ^3F$	3–4
3	561.36	178 138.8	$3p3d\ ^3D^0 - 3d^2\ ^3F$	3–2
6	633.73	157 795.9	$3p3d\ ^1F^0 - 3d^2\ ^1G$	3–4
3	639.88	156 279.3	$3p3d\ ^1F^0 - 3d^2\ ^1D$	3–2
3	656.58	152 304.4	$3p3d\ ^1P^0 - 3d^2\ ^3P$	1–2
6	656.77	152 260.3	$3p3d\ ^1P^0 - 3d^2\ ^3P$	1–1
6	657.12	152 179.2	$3p3d\ ^1P^0 - 3d^2\ ^3P$	1–0
6	669.14	149 445.6	$3p3d\ ^1P^0 - 3d^2\ ^1D$	1–2

[a] The abbreviations for line characteristics are bl, blended and u, unsymmetrical.

Table 3. Energy Parameters of the Least-Squares Fit for the $2p^6 3d^2$ Configuration of Ar VII

Configuration	Parameter	HFR Value (cm^{-1})	Fitted Value (cm^{-1})	Ratio (Fitted/HFR)
	E_{av}	654 619	663 329	1.013
$2p^6 3d^2$	$F^2(3d3d)$	78 721	68 345	0.868
	$F^4(3d3d)$	50 617	37 592	0.743
	ζ_{3d}	78[a]		
Configuration-Interaction Integrals[b]				
$2p^6\,3s^2-2p^6 3d^2$	$R^2(3s3s3d3d)$	76 180	68 952	0.905
$2p^6\,3p^2-2p^6 3d^2$	$R^1(3p3p3d3d)$	96 267	87 134	0.905
	$R^3(3p3p3d3d)$	60 781	55 015	0.905
$2p^6\,3s3d-2p^6 3d^2$	$R^2(3s3d3d3d)$	76 082	68 864	0.905
$2p^6\,3p4f-2p^6 3d^2$	$R^1(3p4f3d3d)$	−53 706	−48 041	0.905
	$R^3(3p4f3d3d)$	−30 804	−27 882	0.905

[a] Fixed during the fitting procedure.
[b] Linked parameters. These parameters were linked (i.e., the mutual ratios of their values remained constant during the iteration) during the least-squares calculation (Ref. 17, p. 474)

transition wavelengths and line strengths from these calculations were used for preliminary identifications of the lines of the $2p^6 3p3d-2p^6 3d^2$ array. To take into account most of the configuration interaction we included in the calculation of the $2p^6 3d^2$ configuration the following configurations: $2p^6 3s^2$, $2p^6 3p^2$, $2p^6 3s3d$, $2p^6 3d^2$, and $2p^6 3p4f$. In a preliminary calculation, other configurations that lie below the $3d^2$ configuration were included, but they do not strongly influence the level structure of the $3d^2$ configuration.

When we were performing the analysis of the experimental data to identify unknown lines we were guided by isoelectronic extrapolation by Edlén's method.[18] The experimental wave numbers divided by the net charge of the core permitted us to extrapolate the Ar VII transitions through the elements of the Mg I sequence. The power of the method lies in the slow variation of $\sigma_{obs} - \sigma_{cal}/\xi$ values, where σ_{obs} is the observed wave number, σ_{cal} is the calculated wave number, and ξ is the net charge of the core.

3. CONCLUSIONS

The present study has provided 25 new line identifications for the $2p^6 3p3d-2p^6 3d^2$ transition array in the vacuum-ultraviolet spectrum of Ar VII. We have determined the levels for the $2p^6 3d^2$ configuration, and the level $^1D_2^o$ for the $2p^6 3p3d$ configuration was found. For the Mg I sequence, with the results of the Ar VII spectrum we now know the level structure of the $2p^6 3d^2$ configuration for P IV–Zn XIX.

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REFERENCES

1. A. G. Trigueiros, A. J. Mania, M. Gallardo, and J. G. Reyna Almandos, "Atomic transitions for the Ar VII spectrum in the vacuum ultraviolet," J. Opt. Soc. Am. B **14**, 2463–2468 (1997).
2. P. O. Zetterberg and C. E. Magnusson, "The spectrum and term system of P IV," Phys. Scr. **15**, 189–201 (1977).
3. I. Joelsson, P. O. Zetterberg, and C. E. Magnusson, "The spectrum and term system of S V," Phys. Scr. **23**, 1087–1095 (1981).
4. C. Jupén and J. Fremberg, University of Lund, S-22100 Lund, Sweden (personal communication, 1983).
5. A. Redfors, "The $3d^2$ configuration in Ca IX–Zn XIX," Phys. Scr. **38**, 702–706 (1988).
6. S. S. Churilov, V. E. Levashov, and J. F. Wyart, "Extended analysis of the $3p3d-3d^2$ transitions in the sequence K VIII–Cu XVIII and isoelectronic trends in Mg-like ions through Kr XXV," Phys. Scr. **40**, 625–633 (1989).
7. C. Froese-Fischer and M. Godefroid, "Lifetime trends for the $n = 3$ singlet states in the Mg sequence," Nucl. Instrum. Methods Phys. Res. **202**, 307–322 (1982).
8. C. Froese-Fischer and M. Godefroid, "Short-range interactions involving plunging configurations of the $n = 3$ complex in the Mg sequence," Phys. Scr. **25**, 394–400 (1982).
9. N. Reistad, T. Brage, J. O. Ekberg, and L. Engström, "*J*-dependent $3s4p\ ^3P_j$ Lifetimes in Mg-like sulphur and chlorine," Phys. Scr. **30**, 249–254 (1984).
10. K. L. Baluja and A. Hilbbert, "Energy and oscillator strengths for allowed transitions in S V, Cl VI, and Fe XV," Nucl. Instrum. Methods Phys. Res. B **9**, 477–486 (1985).
11. K. Aashamar, T. M. Luke, and J. D. Talman, "Energy levels in the magnesium sequence, Mg I–Mn XIV, calculated in the multiconfiguration optimized potential model," Phys. Scr. **34**, 386–393 (1986).
12. B. C. Fawcett, "Calculated oscillator strengths and wavelengths for allowed transitions within the third shell for ions in the Mg-like isoelectronic sequence between S V and Ni XVII," At. Data Nucl. Data Tables **28**, 579–596 (1983).

13. B. C. Fawcett, "Calculated oscillator strengths, wavelengths and energy levels for allowed 3–3 and 3–4 transitions for Fe XV with isoelectronic comparisons between Dirac–Fock and Hartree–Fock," Phys. Scr. **34**, 331–336 (1986).
14. T. Brage and A. Hibbert, "Plunging configurations and *J*-dependent lifetimes in Mg-like Ions," J. Phys. B **22**, 713–726 (1989).
15. M. Gallardo, F. Bredice, M. Raineri, and J. G. Reyna Almandos, "Light source for obtaining spectra of highly ionized gases," Appl. Opt. **28**, 4513–4515 (1989).
16. L. J. Radziemski and V. Kaufman, "Wavelengths, energy levels, and analysis of neutral chlorine (Cl I)," J. Opt. Soc. Am. **59**, 424–443 (1969).
17. R. D. Cowan, *The Theory of Atomic Structure and Spectra* (U. California Press, Berkeley, Calif., 1981).
18. B. Edlén, "Atomic spectra," in *Encyclopedia of Physics*, S. Flügge, ed. (Springer-Verlag, Berlin, 1964), Vol. 27, p. 80.