Atomic transitions for the Ar VII spectrum in the vacuum ultraviolet

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Two different spectroscopy light sources are used to observe the spectrum of six-times-ionized argon, Ar VII, in the vacuum ultraviolet range, 300–1100 Å. Fifty-eight transitions are identified as combinations between levels of the $2p^6\,(3s^2 + 3p^2 + 3s3d)$ and $2p^6(3s3p + 3p3d + 3s4p)$ configurations. For 44 of these transitions the classification is new. Twenty-nine levels are determined that belong to these configurations, where 14 of these are new. The energy parameters are obtained with Hartree–Fock relativistic calculations. The energy levels of the configurations are interpreted by fitting the theoretical energy expressions to the experimental levels with the least-squares approach. Isoelectronic comparisons along the Mg I sequence are used to support the experimental results. ©1997 Optical Society of America [S0740-3224(97)03410-3]

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1. INTRODUCTION

Six-times-ionized argon, Ar VII, belongs to the Mg I isoelectronic sequence with a ground state of $3s^2\ ^1S_0$. Phillips and Parker published the first results on the Ar VII spectra.[1] Transitions to the ground state from low-lying levels were presented for the Mg I-like ions Mg I–Co XVI in atomic energy levels.[2] Additional spectral information for Mg I, Al II, P IV, S V, and Cl VI can be found in Refs. 3–7. Apart from the results compiled in Ref. 2, Ekberg *et al.*[8] has analyzed the Mg I-like spectra of Ti XI by means of a vacuum-spark light source. This work also contained some check and extension to the Mg-like ions of K VIII, Ca IX, and Sc X. Churilov *et al.*[9] made a detailed analysis of the $n = 3 - n' = 3$ transitions for Mg-like Fe, Co, and Ni. This work used spectra obtained from laser-produced plasmas. Also using laser-produced plasmas, Litzén and Redfors[10] revised and extended the analysis of transitions and energy levels in the $n = 3$ complex for Mg-like Ca IX–Ge XXI. Sugar and Kaufman[11–13] reported results for Cu XII–XXI and Zn XIX. Redfors[14] reported the study of the $3d^2$ configuration in Ca IX–Zn XIX. Levashov[15] studied the spectra for the $n = 3$ complex in K VIII, Ca IX, and Ti X. Churilov *et al.*[16] extended the analysis of the $3p3d - 3d^2$ transitions in the sequence K VIII–Cu XVIII and studied the isoelectronic trends in Mg I-like ions through Kr XXV. Sugar *et al.*[17] reported resonance transitions in the Mg I sequence from Cu to Mo (omitting Rb and Sr) from laser-produced plasmas and the Texas Experimental Tokamak. These same authors then extended this analysis to include other transitions in Mg-like Cu to Mo in Ref. 18. Buchet–Polizac *et al.*[19] studied Argon spectra excited by the beam–foil technique. Lesteven–Vaïsse *et al.*[20] studied the high-resolution VUV spectroscopy of Ar with recoil ion spectroscopy and reported results for the low configurations of Ar VII. Lèvêque *et al.*[21] reported the emission spectra of argon produced by a discharge in a capillary light source, but classification of the spectral lines was not possible. Fawcett *et al.*[22] used a theta-pinch plasma to analyze the spectrum of Ar IX and extended spectral classification in Ar V to Ar VIII and Ar X. Livingston *et al.*[23] studied the spectra of Ar V–Ar VIII using the beam–foil excitation, and several new transition classifications were made in Ar VII and Ar VIII. Reader[24] studied the transitions $3s^2 - 3s3p$ and $3s3p - 3s3d$ in Mg I-like ions from Sr^{26+} to Rh^{33+}. Ekberg *et al.*[25] analyzed the Mg I-like spectra from Mo XXXI to Cs XIV. Jupén *et al.*[26] reported transitions in Mg I Kr and Mo observed in the Joint European Torus Tokamak.

In recent years the Mg I-like ions have been the center of many theoretical calculations, mainly for the elements phosphorus, sulfur, and chlorine, where the high configurations of the $n = 3$ complex plunge through the rest of the system and short-range configuration interaction effects appear.[27–34] The interest in spectroscopy data for rare gases is due to applications in collision physics, laser physics, photoelectron spectroscopy, and fusion diagnostics.

2. EXPERIMENTS

Two different light sources were used in our experiments. The first is a theta-pinch discharge built at Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas,[35] and specially designed for production of highly charged ions. The discharge tube is made of quartz, has a length of 50 cm, and an outer diameter of 5 cm. The power supply can generate a maximum voltage of 60 kV and 100 mA. The capacitance of the bank of capacitors is 7.2 μF. Preionization is reached by means of a radio-frequency (100 MHz, 150 W) discharge. The spectra was recorded with a 2-m normal-incidence spectrograph in the region 300–1300 Å and exposed on Kodak short-wave-region emulsion plates. The grating has 1080 lines/mm and is blazed for 1000 Å. The plate factor in the first diffraction order is 4.61 Å/mm. To distinguish between different stages of ionization, a number of experimental parameters, i.e., gas pressure and discharge voltage, were varied. A well-developed Ar VII spectrum was obtained with the following parameters: 13 mTorr, 14 kV, and 400 discharges. The unperturbed lines have an uncertainty estimated to ± 0.01 Å.

The second light source, described in Ref. 36, is a Pyrex tube, 30 cm long, and with an inner diameter of 0.3 cm. The tube has inner electrodes and is viewed end on. The excitation of the gas is produced by discharging a bank of low-inductance capacitors varying between 2.5 and 100 nF and charged up to 19 kV through the tube. Ilford *Q*-2 plates were used to record the spectra. C, N, O, Si, and known lines of argon provided internal wavelength standards. The radiation was recorded with a 3-m normal-incidence spectrograph with a diffraction grating of 1200 lines/mm. The plate factor in the first order is 2.77 Å/mm. The accuracy of the wavelength values for unperturbed lines is estimated to be ± 0.01 Å.

3. CALCULATIONS, LINE IDENTIFICATIONS, AND ENERGY-LEVEL DETERMINATIONS

The theoretical predictions for the energy levels of the configurations were obtained by diagonalizing the energy matrices with appropriate Hartree–Fock relativistic values for the energy parameters. For this purpose the computer code developed by Cowan[37] was used. The program allowed us to calculate energy levels, wavelengths, and transition probabilities, with the transition probabilities providing a guide to the expected strong lines. The configuration average energies are shifted with $+9914\ \mathrm{cm}^{-1}$. This was done to bring the $3s^2\ {}^1S_0$ ground-state energy to zero, which of course it must be. This procedure has practical importance because the calculated energy-level values will be closer to the experimental determined ones.

The experimental wave numbers minus the calculated ones, divided by the net charge of the core, permit us to extrapolate the Ar VII transitions through the elements of the Mg I isoelectronic sequence. This method was used as a guide to identify unknown lines. The power of the method lies in the slow variation of $\sigma_{\mathrm{obs}} - \sigma_{\mathrm{cal}}/\zeta$ values. Figure 1 shows this method for identification of the transition $3s3d\ {}^3D_2 – 3p3d\ {}^3D_2$ in Ar VII, making use of the ions Cl VI–Mn XIV. The experimental points for the elements below Cl VI, specifically P IV and S V, were not used because of strong correlation effects for these ions. The point for Ti XI in Fig. 1 lies outside the curve, indicating a possible misidentification for this transition. In this figure the value of the net charge of the core is added to by a constant equal to 1.4 determined by a semiempirical method (Ref. 38).

The radiate decay from the $3s3p\ {}^3P$ term to the ground configuration, $3s^2$, is possible only by the $3s^2\ {}^1S_0 – 3s3p\ {}^3P_1$ transition. In pure LS coupling this transition could not decay by emission of dipole radiation, but relativistic spin mixing causes the intercombination line cited above to become dipole allowed. The transition $3s^2\ {}^1S_0 – 3s3p\ {}^3P_1$ determines the $3s3p\ {}^3P_1$ level for the first excited configuration. This line has a very weak intensity, but it is easily observed in a θ-pinch-like gas discharge. The first published result for the $3s3p\ {}^3P_1$ level ($113\,900.0 + X\ \mathrm{cm}^{-1}$) was given by Moore[2] from a semiempirical extrapolation. Curtis and Ramanujam[39] presented a predicated value for the $3s3p\ {}^3P_1$ level at $113\,952.0\ \mathrm{cm}^{-1}$. Peacock *et al.*[40] found the value $113\,904\ \mathrm{cm}^{-1}$ for this level using the $3s^2\ {}^1S_0 – 3s3p\ {}^3P_1$ transition at 877.93 Å from a Tokamak experiment as light source. Träbert *et al.*,[41] using fast-ion-beam spectroscopy, found the same line found by Peacock *et al.* and established its shapes in second diffraction order. More recently Kelly[42] located the $3s3p\ {}^3P_1$ level at $112\,924.0 + E\ \mathrm{cm}^{-1}$ by the line 885.55 Å. This transition is not present in our experiments. We paid special attention to solving the misunderstanding surrounding this transition through a number of experiments with different energies and pressure. In fact, in our experiments the line 877.93 Å appears as an Ar VII line, which is confirmed by Hutton[43] in an experiment using the electron cyclotron resonance light source. Electron cyclotron resonance as a spectroscopy light source uses the method of collision-based spectroscopy. This kind of light source is very useful for distinguishing the different ionization degrees of the ions.[44–47] Table 1 shows the 58 classified lines in the Ar VII spectrum. For 44 of these lines the classification is new. The intensities of the lines vary from 10 to 100 and are visual estimates of the plate blackening. Optimization of the energy-level values was done from the observed wavelengths by an iterative procedure in which the individual wavelengths are weighted according to their uncertainties.[48,49] Table 2 shows the 29 energy levels determined from the experimental transitions, where 14 of these are new.

Tables 3 and Tables 4 show the theoretical Hartree–Fock values for the energy parameters and the fitted ones. For the even-parity configurations we have the following picture: the $3s2$, $3p2$, and $3s3d$ configurations are the purpose of our analysis. To take into account most of the configuration interaction we include in the calculation of the even-parity levels the following configurations: $3s^2$, $3p^2$, $3s3d$, $3d^2$, $3p4p$, $3d4s$, $3d4d$,

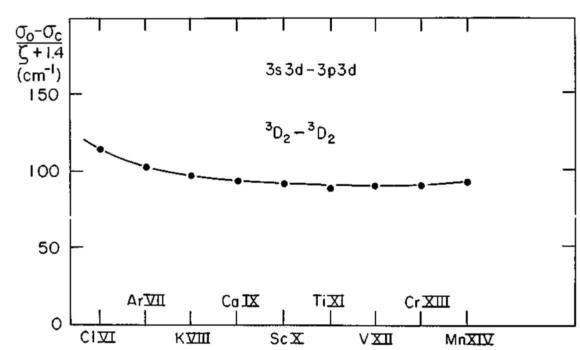

Fig. 1. Observed minus calculated Hartree–Fock wave numbers divided by the net charge of the core plus a constant (1.4) for the transition $3s3d\ {}^2D_2 – 3p3d\ {}^2D_2$.

Table 1. Observed Transitions in the Spectrum of Ar VII

Intensity[a]	Wavelengths (Å)	Wavelengths[b,c] (Å)	Transitions
20bl	326.22	–	$3p^2\ {}^1D_2 - 3s4p\ {}^1P^0_1$
20	396.27	–	$3p^2\ {}^1D_2 - 3p3d\ {}^1P^0_1$
40	404.62	–	$3s3d\ {}^3D_2 - 3s4p\ {}^1P^0_1$
20	407.31	–	$3p^2\ {}^1D_2 - 3p3d\ {}^1F^0_3$
60bl	415.59	–	$3s3d\ {}^3D_1 - 3s4p\ {}^3P^0_2$
60bl	415.66	–	$3s3d\ {}^3D_2 - 3s4p\ {}^3P^0_2$
60bl	415.77	–	$3s3d\ {}^3D_2 - 3s4p\ {}^3P^0_2$
40	416.19	–	$3s3d\ {}^3D_2 - 3s4p\ {}^3P^0_1$
60u	417.06	–	$3s3d\ {}^3D_1 - 3s4p\ {}^3P^0_0$
60	473.93	473.938[b]	$3s3p\ {}^3P^0_0 - 3s3d\ {}^3D_1$
60u	475.66	475.656[b]	$3s3p\ {}^3P^0_1 - 3s3d\ {}^3D_2$
40	475.73	475.73[b]	$3s3p\ {}^3P^0_1 - 3s3d\ {}^3D_1$
60u	479.35	479.379[b]	$3s3p\ {}^3P^0_2 - 3s3d\ {}^3D_3$
60u	479.50	479.49[b]	$3s3p\ {}^3P^0_2 - 3s3d\ {}^3D_2$
40	480.49	–	$3p^2\ {}^1D_2 - 3p3d\ {}^3P^0_1$
40	481.87	–	$3p^2\ {}^1D_2 - 3p3d\ {}^3P^0_2$
40	486.89	–	$3p^2\ {}^3P_0 - 3p3d\ {}^3D^0_1$
40	488.24	–	$3p^2\ {}^3P_1 - 3p3d\ {}^3D^0_2$
40	489.14	–	$3p^2\ {}^3P_1 - 3p3d\ {}^3D^0_2$
60u	492.13	–	$3p^2\ {}^3P_2 - 3p3d\ {}^3D^0_3$
40	492.55	–	$3p^2\ {}^3P_0 - 3p3d\ {}^3P^0_1$
20	493.46	–	$3p^2\ {}^3P_2 - 3p3d\ {}^3D^0_1$
20	494.81	–	$3p^2\ {}^3P_1 - 3p3d\ {}^3P^0_1$
40	496.27	–	$3p^2\ {}^3P_1 - 3p3d\ {}^3P^0_2$
60	499.03	–	$3p^2\ {}^1S_0 - 3p3d\ {}^1P^0_1$
40u	499.23	–	$3p^2\ {}^3P_2 - 3p3d\ {}^3P^0_1$
40	500.69	–	$3p^2\ {}^3P_2 - 3p3d\ {}^3P^0_2$
60u	501.09	501.07[c]	$3s3p\ {}^1P^0_1 - 3s3d\ {}^1D_2$
20	559.86	–	$3p^2\ {}^1D_2 - 3p3d\ {}^3F^0_2$
20	580.69	–	$3p^2\ {}^3P_2 - 3p3d\ {}^3F^0_3$
60u	585.73	585.75[b]	$3s^2\ {}^1S_0 - 3s3p\ {}^1P^0_1$
80u	630.29	630.31[b]	$3s3p\ {}^3P^0_1 - 3p^2\ {}^3P_2$
60bl	634.21	634.21[b]	$3s3p\ {}^3P^0_0 - 3p^2\ {}^3P_1$
80bl	637.10	637.05[b]	$3s3p\ {}^3P^0_2 - 3p^2\ {}^3P_2$
80u	637.47	637.47[b]	$3s3p\ {}^3P^0_1 - 3p^2\ {}^3P_1$
80bl	641.31	641.32[b]	$3s3p\ {}^3P^0_1 - 3p^2\ {}^3P_0$
60u	644.40	644.39[b]	$3s3p\ {}^3P^0_2 - 3p^2\ {}^3P_1$
40	659.54	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3D^0_3$
60	659.83	–	$3s3d\ {}^3D_3 - 3p3d\ {}^3D^0_3$
40	660.13	–	$3s3d\ {}^3D_1 - 3p3d\ {}^3D^0_2$
60	660.31	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3D^0_2$
40	660.61	–	$3s3d\ {}^3D_3 - 3p3d\ {}^3D^0_2$
60bl	661.77	–	$3s3d\ {}^3D_1 - 3p3d\ {}^3D^0_1$
40	661.90	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3D^0_1$
40	667.99	–	$3s3d\ {}^3D_1 - 3p3d\ {}^3P^0_0$
40	672.33	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3P^0_1$
40u	675.01	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3P^0_2$
40	681.14	–	$3s3d\ {}^1D_2 - 3p3d\ {}^1P^0_1$
20	714.43	–	$3s3d\ {}^1D_2 - 3p3d\ {}^1F^0_3$
80	820.99	–	$3s3d\ {}^3D_3 - 3p3d\ {}^3F^0_4$
60	828.91	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3F^0_3$
60	829.41	–	$3s3d\ {}^3D_3 - 3p3d\ {}^3F^0_3$
40	838.80	–	$3s3d\ {}^3D_2 - 3p3d\ {}^3F^0_2$
20	839.18	–	$3s3d\ {}^3D_3 - 3p3\ {}^3F^0_2$
20	953.08	–	$3s3d\ {}^1D_2 - 3p3d\ {}^3D^0_1$
20	974.83	–	$3s3d\ {}^1D_2 - 3p3d\ {}^3P^0_1$
20	1 008.98	–	$3d3p\ {}^1P^0_1 - 3p^2\ {}^3P_0$
40u	1 063.54	1 063.55[c]	$3s3p\ {}^1P^0_1 - 3p^2\ {}^1D_2$

[a] The intensities of the lines are visual estimates of plate blackening. Abbreviations for line characteristics: u, line profile is asymmetric; bl, line is blended.
[b] Ref. 1.
[c] Ref. 8.

$3p4f$, $3p5f$, and $4f^2$. For the odd-parity case we study the $3s3p$, $3s4p$, and $3p3d$ configurations. We include the following configurations in the calculation of the odd-parity states: $3s3p$, $3s4p$, $3p3d$, $3p4d$, $3s4f$, $3s5f$, $3d4p$, $3d4f$, and $3d5f$. Tables 3 and 4 show only the energy parameters for the configurations that are the fo-

Table 2. Experimental Energy-Level Values of Ar VII

Designation	E, Observed (cm^{-1})	E, Calculated[a] (cm^{-1})	Percentage Composition in LS Coupling[b]
$2p^6\,3s^2\ ^1S_0$	0.0	0.0	97
$2p^6\,3s3p\ ^3P_0^0$	113 099.9 ± 6.0	113 098.4	100
$2p^6\,3s3p\ ^3P_1^0$	113 904.5 ± 4.0	113 906.2	100
$2p^6\,3s3p\ ^3P_2^0$	115 594.8 ± 5.5	115 594.6	100
$2p^6\,3s3p\ ^1P_1^0$	170 727.1 ± 3.0	170 727.1	97 ± 3 ($3p3d\ ^1P$)
$2p^6\,3p^2\ ^1D_2$	264 752.2 ± 3.0	264 752.3	77 ± 20 ($3s3d\ ^1D$)
$2p^6\,3p^2\ ^3P_0$	269 837.5 ± 3.0	269 837.5	99
$2p^6\,3p^2\ ^3P_1$	270 775.6 ± 3.0	270 775.6	100
$2p^6\,3p^2\ ^3P_2$	272 562.5 ± 3.0	272 562.5	97
$2p^6\,3p^2\ ^1S_0$	316 716.1 ± 9.0	316 716.1	95
$2p^6\,3s3d\ ^3D_1$	324 102.5 ± 3.5	324 100.2	100
$2p^6\,3s3d\ ^3D_2$	324 138.5 ± 2.0	324 142.2	100
$2p^6\,3s3d\ ^3D_3$	324 206.6 ± 3.0	324 205.1	100
$2p^6\,3s3d\ ^1D_2$	370 292.2 ± 2.0	370 292.2	78 ± 20 ($3p^2\ ^1D$)
$2p^6\,3p3d\ ^3F_2^0$	443 363.3 ± 5.0[c]	443 462.6	98
$2p^6\,3p3d\ ^3F_3^0$	444 776.0 ± 3.0[c]	444 623.4	100
$2p^6\,3p3d\ ^3F_4^0$	446 010.7 ± 4.0[c]	446 063.6	100
$2p^6\,3p3d\ ^1D_2^0$		450 478.5[d]	98
$2p^6\,3p3d\ ^3P_2^0$	472 282.2 ± 4.5[c]	472 198.6	92 ± 7 ($3p3d\ ^3D$)
$2p^6\,3p3d\ ^3P_1^0$	472 873.3 ± 2.0[c]	472 981.5	90 ± 9 ($3p3d\ ^3D$)
$2p^6\,3p3d\ ^3P_0^0$	473 804.0 ± 5.0[c]	473 799.5	99
$2p^6\,3p3d\ ^3D_1^0$	475 216.0 ± 2.0[c]	475 157.6	91 ± 9 ($3p3d\ ^3P$)
$2p^6\,3p3d\ ^3D_2^0$	475 585.1 ± 3.0[c]	475 597.4	93 ± 7 ($3p3d\ ^3P$)
$2p^6\,3p3d\ ^3D_3^0$	475 760.0 ± 4.0[c]	475 787.0	100
$2p^6\,3p3d\ ^1F_3^0$	510 264.1 ± 4.0[c]	510 263.3	97
$2p^6\,3p3d\ ^1P_1^0$	517 104.9 ± 5.0[c]	517 105.4	94 ± 3 ($3s3p\ ^1P$)
$2p^6\,3s4p\ ^3P_0^0$	563 876.2 ± 17.0[c]	564 000.5	99
$2p^6\,3s4p\ ^3P_1^0$	564 413.3 ± 12.0[c]	564 239.0	99
$2p^6\,3s4p\ ^3P_2^0$	564 724.2 ± 12.5[c]	564 773.7	99
$2p^6\,3s4p\ ^1P_1^0$	571 285.6 ± 11.5[c]	571 286.1	99

[a] Energy level values from the least-squares fitting calculation.
[b] Percentages lower than 3% are omitted.
[c] New level determined in this work.
[d] Predicted value from the least-squares fitting calculation.

Table 3. Even-Parity Energy Parameters[a]

Configuration	Parameters	Hartree–Fock Relativistic Value (cm^{-1})	Fitted Value (cm^{-1})	Standard Deviation (cm^{-1})	Ratio (Fitted/Hartree–Fock Relativistic)
$2p^6\,3s^2$	E_{av}	9 914	8 535	3	0.86
$2p^6\,3p^2$	E_{av}	281 589	282 747	1	1.00
$2p^6\,3p^2$	$F^2(2p2p)$	69 691	77 464	6	1.11
	ζ_{2p}	1 513	1 660	2	1.10
$2p^6\,3s3d$	E_{av}	330 969	331 187	1	1.00
	$G^2(3s3d)$	64 805	63 039	10	0.97
	ζ_{3d}	76[b]			
Configuration interaction integrals					
$2p^6\,3s^2$–$2p^6\,3p^2$	$R^1(3s3s3p3p)$	92 979	86 019[c]		0.93
$2p^6\,3p^2$–$2p^6\,3s3d$	$R^2(3p3p3s3d)$	86 181	92 023[c]		1.07

[a] Parameters used in the least-squares fitting calculation for odd-parity configurations. The Hartree–Fock relativistic parameters are compared with the fitting values. The standard deviations for the parameters and the ratio between fitted and the Hartree–Fock values are also shown. The standard deviation for energy adjustment was 3 cm^{-1}.
[b] These parameters were kept fixed under the least-squares fitting calculation.
[c] Blended line.

Table 4. Odd-Parity Energy Parameters

Configuration	Parameter	Hartree–Fock Relativistic Value (cm^{-1})	Fitted Value (cm^{-1})	Standard Deviation (cm^{-1})	Ratio Fitted/Hartree–Fock Relativistic
$2p^6\,3s3p$	E_{av}	130 577	133 675	65	1.02
$2p^6\,3s3p$	$G^1(3s3p)$	93 215	100 208	215	1.08
	ζ_{3p}	1 514	1 679	107	1.11
$2p^6\,3p3d$	E_{av}	468 767	469 767	39	1.00
$2p^6\,3p3d$	$F^2(3p3d)$	67 329	69 015	283	1.03
$2p^6\,3p3d$	$G^1(3p3d)$	81 996	86 240	150	1.05
$2p^6\,3p3d$	ζ_{3p}	1 521	1 951	95	1.28
$2p^6\,3p3d$	ζ_{3d}	77[b]			
$2p^6\,3s4p$	E_{av}	570 343	567 192	64	0.99
$2p^6\,3s4p$	$G^1(3s4p)$	8 822	9 205	219	1.04
$2p^6\,3s4p$	ζ_{4p}	523	523		1.00
Configuration interaction integrals					
$2p^6\,3s3p-2p^6\,3p3d$	$R^1(3s3p3p3d)$	86 290	98 186[b]		1.14
$2p^6\,3s4p-2p^6\,3p3d$	$R^1(3s3p3p3d)$	66 121[b]			
$2p^6\,3s3p-2p^6\,3s4p$	$R^1(3s3p3s4p)$	3 104[b]			
$2p^6\,3s3p-2p^6\,3s4p$	$R^1(3s3p3s4p)$	18 131[b]			

[a] Same as in Table 3, but for odd-parity configurations. Standard deviation is 116 cm^{-1} for the least-squares adjustment.
[b] Parameters were kept fixed in the least-squares fitting calculation.

cus of our analysis. The parameters of the configurations, which are included in the calculation only to take into account the configuration interaction effects, are published elsewhere.[50]

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