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Theoretical investigation of energy levels and transition data for S II, Cl III, Ar IV*

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ABSTRACT

Aims. The aim of this work is to present accurate and extensive results of energy spectra and transition data for the S II, Cl III, and Ar IV ions. These data are useful for understanding and probing physical processes and conditions in various types of astrophysical plasmas.
Methods. The multiconfiguration Dirac–Hartree–Fock (MCDHF) and relativistic configuration interaction (RCI) methods, which are implemented in the general-purpose relativistic atomic structure package GRASP2K, are used in the present work. In the RCI calculations the transverse-photon (Breit) interaction, the vacuum polarization, and the self-energy corrections are included.
Results. Energy spectra are presented comprising the 134, 87, and 103 lowest states in S II, Cl III, and Ar IV, respectively. Energy levels are in very good agreement with NIST database recommended values and associated with smaller uncertainties than energies from other theoretical computations. Electric dipole (E1), magnetic dipole (M1), and electric quadrupole (E2) transition data are computed between the above states together with the corresponding lifetimes. Based on internal validation, transition rates for the majority of the stronger transitions are estimated to have uncertainties of less than 3%.

Key words. atomic data

1. Introduction

Atomic data are of importance in the understanding of the physical processes and conditions in various types of astrophysical plasmas, for example in the determination of chemical abundances of the elements and in the estimation of radiative transfer through stellar plasmas. The quality of atomic data have a large impact on the accuracy of chemical abundances (Juan de Dios & Rodríguez 2017; Kisielius et al. 2014). Juan de Dios & Rodríguez (2017) computed the ionic abundances of O II, O III, N II, Cl III, Ar III, Ar IV, Ne III, S II, and S III, and the total abundances of the corresponding elements. They observed that data for some of the studied ions need to be improved in order to derive more reliable values of chemical abundances in high-density nebulae.

The studied elements (S II, Cl III, Ar IV) are in the astrophysically important group of low-ionization ions which belongs to the phosphorous isoelectronic sequence. Fritzsche et al. (1999) used the multiconfiguration Dirac–Fock method to study forbidden transitions in the $3s^23p^3$ configuration for phosphorus-like ions with low nuclear charge Z. Fischer et al. (2006) computed energy levels, lifetimes, and transition data for the sodium-like to argon-like sequences using the multiconfiguration Hartree–Fock (MCHF) and multiconfiguration Dirac–Hartree–Fock (MCDHF) methods.

Tayal & Zatsarinny (2010) used the B-spline Breit-Pauli R-matrix method to compute energy levels of the $3s^23p^3$, $3s3p^4$, $3s^23p^23d$, $3s^23p^24s$, and $3s^23p^24p$ configurations and transitions in S II. Kisielius et al. (2014) presented the energy levels and transition data for S II using HF and quasirelativistic (QR) methods with transformed radial orbitals.

Sossah & Tayal (2012) used the MCHF and B-spline Breit–Pauli R-matrix method to calculate transition probabilities and effective collision strengths for Cl III. Schectman et al. (2005) measured lifetimes and branching fractions with beam-foil techniques and derived oscillator strengths for transitions in Cl II and III.

Bredice et al. (1995) observed the spectra of Ar IV in the 280–5000 Å wavelength range and reanalyzed the $3s^23p^3$, $3s3p^4$, $3s^23p^2(3d + 4s)$ configurations. Djenize & Bukvić (2001) and Burger et al. (2012) studied transition probabilities in Ar III and Ar IV ions. Raineri et al. (2018) used a pulsed discharge light source to study the spectrum of Ar III and Ar IV in the 480–6218 Å region and predicted new levels using the Cowan code (Cowan 1981).

In this work energy spectrum calculations were performed for the 134 (72 even and 62 odd), 87 (52 even and 35 odd), and 103 (44 even and 59 odd) lowest states in the S II, Cl III, and Ar IV ions, respectively. Electric dipole, magnetic dipole, and electric quadrupole transition data were computed along with the corresponding lifetimes of these states. The calculations were done using the general-purpose relativistic atomic structure package GRASP2K (Jönsson et al. 2013) with the modifications that are included in the newest version of the GRASP2018 package (Fischer et al. 2019).

* Tables 5–7 are only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/623/A155

Table 1. Summary of active space construction.

MR set		Active space	N_{CSFs}	
Even	Odd		Even	Odd
		S II		
		RCI		
3s3p^4, 3s^{2}3p^{2}3d, 3s^{2}3p^{2}4s, 3s^{2}3p^{2}4d, 3s^{2}3p^{2}5s	3s^{2}3p^3, 3s^{2}3p^{2}4p, 3s3p^{3}3d, 3s^{2}3p^{2}4f, 3s^{2}3p^{2}5p	{9s, 9p, 9d, 8f, 8g, 8h, 8i}	478 170	873 674
		RCI(CV) additionally included configurations		
3s^{2}3p^{2}5d, 3p^{4}3d, 3s3p^{2}3d^2, 3p^{4}4s, 3p^{4}4d, 3s3p^{2}3d4d, 3s3p^{2}3d4s, 3p^{4}5s, 3s3p^{2}3d5s	3p^5, 3s3p^{2}3d4p, 3s3p^{2}3d5p, 3p^{4}4p, 3p^{4}5p, 3p^{4}4f, 3s3p^{2}3d4f, 3s3p^{3}5d, 3s3p^{3}4d, 3s3p^{3}4s	{9s, 9p, 9d, 8f, 8g, 8h, 8i} {6s, 6p, 5d, 5f} for S from 2p	6 220 422	9 540 812
		Cl III		
		RCI		
3s3p^4, 3s^{2}3p^{2}3d, 3s^{2}3p^{2}4s, 3s^{2}3p^{2}4d	3s^{2}3p^3, 3s^{2}3p^{2}4p, 3s3p^{3}3d, 3p^5	{9s, 9p, 9d, 8f, 8g, 8h, 8i}	492 140	583 117
		RCI(CV) additionally included configurations		
3p^{4}3d, 3s3p^{2}3d^2, 3s3p^{2}3d4s, 3s3p^{2}3d4d	3s^{2}3p3d^2, 3s3p^{3}4s, 3p^{4}4p, 3s3p^{2}3d4p	{9s, 9p, 9d, 8f, 8g, 8h, 8i} {6s, 6p, 6d, 5f} for S from 2p	6 466 816	4 111 005
		Ar IV		
		RCI		
3s3p^4, 3s^{2}3p^{2}3d, 3s^{2}3p^{2}4s	3s^{2}3p^3, 3s^{2}3p^{2}4p, 3s3p^{3}3d, 3p^5	{9s, 8p, 8d, 8f, 8g, 7h, 7i}	224 651	431 584
		RCI(CV) additionally included configurations		
3s^{2}3p^{2}4d, 3p^{4}3d, 3s3p^{2}3d^2, 3s3p^{2}3d4s, 3s3d^{2}4s, 3s^{2}3d^3	3s^{2}3p3d^2, 3s3p^{3}4s, 3p^{4}4p, 3s3p^{2}3d4p, 3p^{3}3d^2, 3s^{2}3p^{2}4f	{9s, 8p, 8d, 8f, 8g, 7h, 7i} {7s, 6p, 6d, 6f, 5g} for S from 2p	4 946 496	7 329 546

Notes. RCI denotes CSF expansions from SD substitutions from the valence electrons of the configurations in the MR. RCI(CV) denotes CSF expansions from SD substitutions from the valence electrons of the configurations in the extended MR along with CSFs obtained by allowing at most one substitution (S) from the 2p shell to a smaller active orbital space. N_{CSFs} is the number of CSFs.

2. Method

2.1. Computational procedure

The GRASP2K package used for the computations is based on the MCDHF and relativistic configuration interaction (RCI) methods. More details about these approaches can be found in Fischer et al. (2016) and Grant (2007).

In the MCDHF approximation atomic state functions (ASFs) are given as linear combinations of symmetry adapted configuration state functions (CSFs)

$$\Psi(\gamma PJM) = \sum_{i=1}^{N_{\mathrm{CSFs}}} c_i \Phi(\gamma_i PJM), \quad (1)$$

where J and M are the angular quantum numbers and P is parity. The CSFs $\Phi(\gamma_i PJM)$ are built from products of one-electron Dirac orbitals. In the relativistic self-consistent field procedure both the radial parts of the Dirac orbitals and the expansion coefficients were optimized to self-consistency.

In RCI computations the wave function is expanded in CSFs and only the expansion coefficients are determined by diagonalizing the Hamiltonian matrix. The RCI method was used to include the transverse-photon (Breit) interaction and quantum electrodynamic (QED) corrections: the vacuum polarization and the self-energy.

In this work ASFs were obtained as expansions over jj-coupled CSFs. To transform these ASFs into an LSJ-coupled CSF basis the method provided by Gaigalas et al. (2003, 2017) was used.

2.2. Computational scheme

For all three ions (S II, Cl III, Ar IV) similar computational schemes were used. As a starting point, MCDHF calculations were performed in the extended optimal level (EOL) scheme (Dyall et al. 1989) for the weighted average of the even and odd parity states. For the construction of the ASFs the multireference-single-double (MR-SD) method (Fischer et al. 2016) was used. In this approach the CSF expansions were obtained by allowing SD substitutions from the configurations in the MR to active orbital sets. Only CSFs that have non-zero matrix elements with the CSFs belonging to the configurations in the MR were retained. No substitutions were allowed from the 1s, 2s, 2p shells, which define an inactive closed core. The MR and the active orbital sets for each of the ions are presented in Table 1. The MCDHF calculations were followed by RCI calculations, including the Breit interaction and leading QED effects. The RCI calculations were done separately for even and odd states.

At the last step, referred to as the RCI(CV) step in the tables, the MR was extended to include additional important configurations, and core-valence (CV) correlation effects were accounted for by allowing at most one substitution also from the 2p shell. The substitutions from the 2p shell increase the number of CSFs dramatically and for this reason these substitutions were restricted to a smaller orbital set.

The large-scale calculations were performed with the MPI version of the GRASP code.

3. Results

The accuracy of the wave functions from the present calculation and some previous calculations was evaluated by comparing calculated energy levels with data from the NIST database (Kramida et al. 2018). In Table 2 a summary of this evaluation is presented: the number of computed energy levels (No. of levels in Ref.) and the average percentage difference between NIST and the different methods for the states covered by these methods (Av. difference).

The inclusion of the CV electron correlations and the extension of the MR set in the calculations improve the results. As is seen from Table 2 the averaged difference of the computed energy spectra (final RCI(CV) results) relative to the energies from the NIST database is 0.22%, 0.18%, and 0.21%, respectively, for the S II, Cl III, and Ar IV ions. Comparing the present results with results from other theoretical computations we obtain a better agreement with values given in the NIST database, except for the S II ion. The averaged uncertainties of energies presented in Tayal & Zatsarinny (2010) is only 0.06%, but they cover fewer energy levels. For the first time, levels of the $3s3p^33d$ configuration are presented for the S II, Cl III, and Ar IV ions.

The mean contribution of the Breit and QED corrections to the final results is 0.05% for the studied ions. For the separate state the contribution of these effects can reach 0.1%.

The uncertainty of electric transition data was evaluated based on the quantity dT (Ekman et al. 2014), which is defined as

$$dT = \frac{|A_l - A_v|}{\max(A_l, A_v)}. \quad (2)$$

Here, A_l and A_v are transition rates in length and velocity forms. The mean dT for all presented E1 transitions is 12.00%, 5.95%, and 6.47%, respectively for the S II, Cl III, and Ar IV ions. The results for the different ions is discussed in more detail below.

3.1. S II

In Table A.1 energy spectra and wave function composition in LS-coupling for 72 even states of the $3s3p^4$, $3s^23p^23d$, $3s^23p^24d$, $3s^23p^24s$, $3s^23p^25s$ configurations and for 62 odd states of the $3s^23p^3$, $3s^23p^24p$, $3s3p^33d$, $3s^23p^24f$, $3s^23p^25p$ configurations for S II are given. The states are given with unique labels (Gaigalas et al. 2017). The contribution was marked in bold for the states in which the labels were not assigned with largest contribution to the composition. In Table A.1 lifetimes in length and velocity gauges are also presented.

In Fig. 1 energy levels computed in this work and other theoretical calculations are compared with data from NIST (Kramida et al. 2018). From the figure we see that the relative uncertainties of energy levels obtained in this work in most cases are about 0.2%. Only for levels of the ground configuration the disagreements are larger, about 1.8%.

Transition data such as wavelengths; weighted oscillator strengths; transition rates of E1, M1, and E2 transitions; and the accuracy indicator dT are given in Table 5, and are available at the CDS. Generally, the uncertainty of transition data is small for the stronger transitions. To display this a scatterplot of dT versus the transition rate A for computed E1 transitions is given in Fig. 2. For most of the transitions, dT is well below 10%, and for the strongest ones dT is well below 3%. The weak transitions are either intercombination transitions, where in relativistic calculations the low rates result from strong cancellation of several large contributions to the transition moment (Ynnerman & Fischer 1995), or two-electron one-photon (TEOP) transitions, where the rate is identically zero in the simplest approximation of the wave function and where the transition results from inclusion of correlation effects (Li et al. 2010). These types of transitions are still extremely challenging for theory and improved methodology is needed to further decrease the uncertainties.

Table 2. Comparison of computed energy levels in the present work and other theoretical results with data from the NIST database for the S II, Cl III, and Ar IV ions.

Av. difference (in %)	No. of levels in Ref.	Ref.
	S II	
0.34	134(126)	RCI
0.22	134(126)	RCI(CV)
0.48	67(67)	1
0.06	70(70)	2
1.12	49(49)	3 a
1.18	49(49)	3 b
	Cl III	
0.38	87(63)	RCI
0.18	87(63)	RCI(CV)
0.55	67(54)	1
1.01	68(51)	4 a
1.81	68(51)	4 b
	Ar IV	
0.47	103(56)	RCI
0.21	103(56)	RCI(CV)
0.60	62(51)	1

Notes. The numbers in parentheses show the number of levels compared with the NIST database.

References. (1) Fischer et al. (2006); (2) Tayal & Zatsarinny (2010); (3) Kisielius et al. (2014) (a – HF data, b – quasirelativistic data); (4) Sossah & Tayal (2012) (a – MCHF calculations with 2893 configurations, b – MCHF calculations with 436 configurations).

3.2. Cl III

In Table A.2 energy spectra, lifetimes, and wave function composition in LS-coupling are presented for 52 even states of the $3s3p^4$, $3s^23p^23d$, $3s^23p^24s$, $3s^23p^24d$ configurations and for 35 odd states of the $3s^23p^3$, $3s^23p^24p$, $3s3p^33d$, $3p^5$ configurations in the Cl III ion. Energy levels are compared with results from NIST (Kramida et al. 2018). In the NIST database some levels of the $3s^23p^24p$, $3s^23p^24d$, and $3p^5$ configurations are flagged with question marks. Comparing these levels with present calculations and other computations there is a good agreement, except for states of the $3p^5$ configuration. Our energies for states of the $3p^5$ configuration are lower by 60 000 cm^{-1}. These levels in NIST are marked as levels that were determined by interpolation or extrapolation of known experimental values or by semiempirical calculations.

The uncertainty of the computed energy levels comparing with NIST data is less than 0.5%, and in most cases about 0.1%. Only for the first excited levels is the disagreement more than 1%. The averaged uncertainty of computed energy spectra

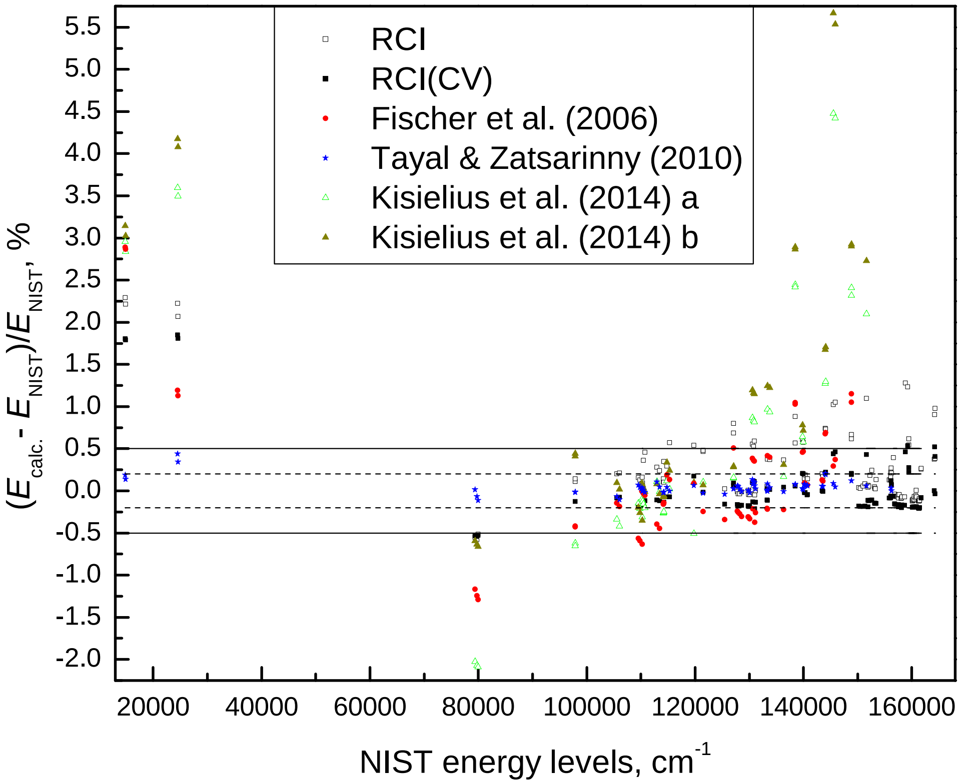

Fig. 1. Comparison of computed energy levels and other theoretical calculations with data from the NIST database for S II. The solid lines indicate 0.5% and the dashed lines 0.2% deviation from the NIST data. (Kisielius et al. 2014) a – HF data. (Kisielius et al. 2014) b – quasirelativistic data.

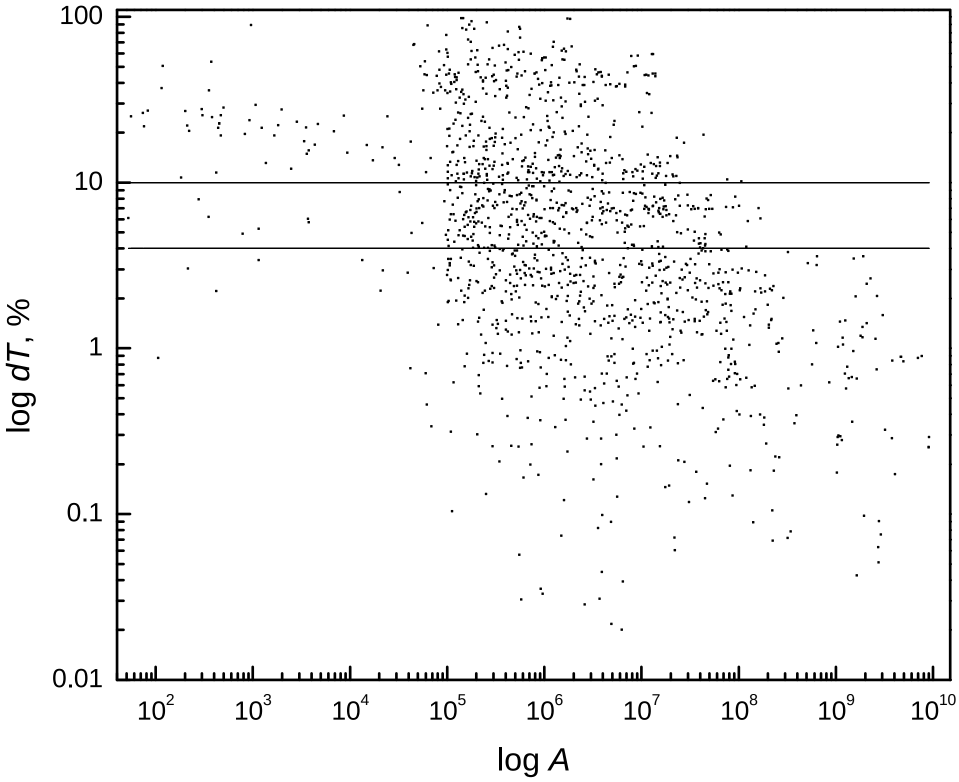

Fig. 2. Scatterplot of dT vs. the transition rate A of E1 transitions for S II. The solid lines indicate the 4% and 10% deviations.

comparing with NIST data is 0.18% (Table 2). The present energies are in better agreement with NIST than energies from previous theoretical computations. In addition, in this work more energy levels were studied, and for the first time levels of the $3s3p^3 3d$ configuration are presented.

Transition data for E1, M1, and E2 transitions are given in Table 6, and are available at the CDS. In Fig. 3 the scatterplot of dT versus the transition rate A is displayed for all presented E1 transitions. The mean dT for the transitions is 5.95%. For most of the strongest transitions, dT is well below 2%. Table 3 gives the comparison of the theoretical and experimental results of wavelengths and oscillator strengths for the $3s^2\,3p^3(^4_3S)\ ^4S^o_{3/2} \rightarrow 3s\,3p^4(^3_2P)\ ^4P_{5/2,3/2,1/2}$ transitions in Cl III. From the table we see a very good agreement of

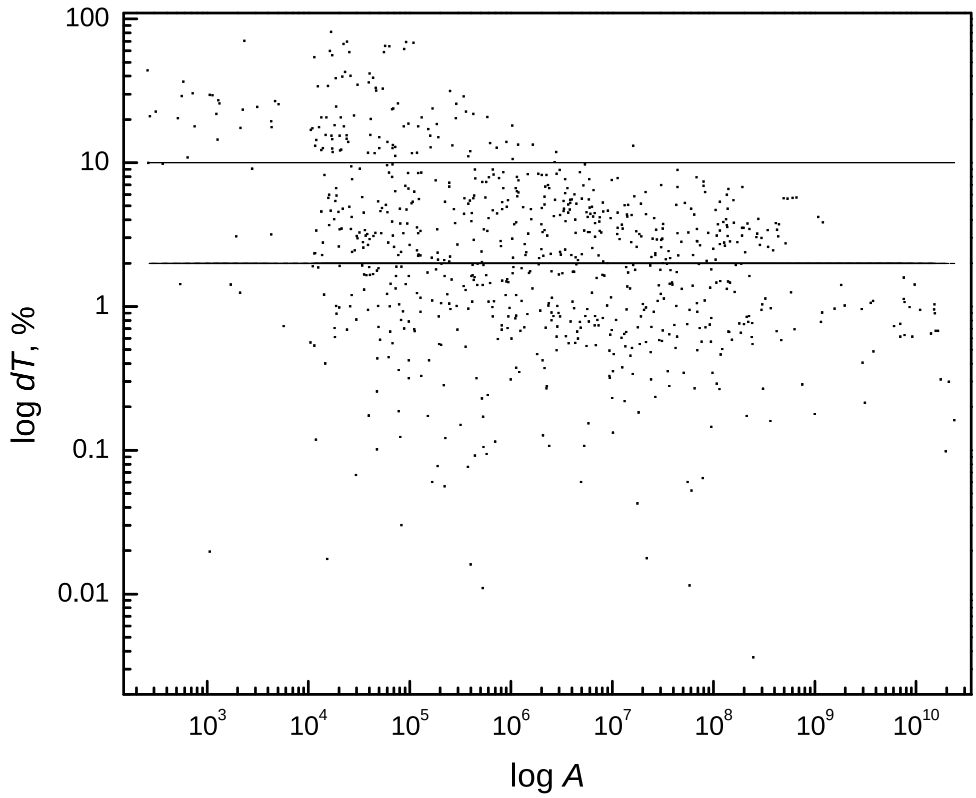

Fig. 3. Scatterplot of dT vs. the transition rate A of E1 transitions for Cl III. The solid lines indicate the 2% and 10% deviations.

Table 3. Comparison of wavelengths and oscillator strengths for the $3s^2\,3p^3(^4_3S)\ ^4S^o_{3/2} \rightarrow 3s\,3p^4(^3_2P)\ ^4P_{5/2,3/2,1/2}$ transitions in Cl III.

$J_i \rightarrow J_f$			Ref.
3/2 → 5/2	3/2 → 3/2	3/2 → 1/2	
	λ (in Å)		
1015.02	1008.78	1005.28	1 (Exp.)
1019.22	1013.05	1009.21	RCI (This work)
1015.14	1008.94	1005.41	RCI(CV) (This work)
1023.21	1017.96	1015.04	2
1024.48	1018.74	1015.46	3
	$f \times 10^{-2}$		
2.85 ± 0.11	1.93 ± 0.08	0.96 ± 0.05	4 (Exp.)
3.14 (2.6)	2.10 (2.9)	1.04 (3.8)	RCI (This work)
3.10 (4.0)	2.07 (3.7)	1.04 (3.6)	RCI(CV) (This work)
3.23	2.15	1.07	2
3.21	2.14	1.07	3

Notes. The oscillator strengths are given in the length gauge. The estimated uncertainty in percentage of the oscillator strengths are given in parentheses.
References. (1) Kramida et al. (2018); (2) Fischer et al. (2006); (3) Sossah & Tayal (2012); (4) Schectman et al. (2005).

wavelengths with the experimental values. Oscillator strengths are a little too large compared with experiment (Schectman et al. 2005).

3.3. Ar IV

Table A.3 displays energy spectra, lifetimes, and wave function composition in LS-coupling for 44 even states of the $3s3p^4$, $3s^23p^23d$, $3s^23p^24s$ configurations and for 59 odd states of the $3s^23p^3$, $3s^23p^24p$, $3s3p^33d$, $3p^5$ configurations in Ar IV. The averaged uncertainty of energy levels obtained in this work compared with the NIST data is 0.21%. The largest disagreement (about 1%) is just for the first few excited levels.

Raineri et al. (2018) presented ten new energy levels of the $3s^23p^23d$ and $3s^23p^24p$ configurations for Ar IV. In Table 4 a comparison of these levels with this work and theoretical results by Fischer et al. (2006) is made. There is very good agreement between the new energy levels and the present calculations, except for the $3s^2\,3p^2(^1_0S)\ ^1S\,3d\ ^2D_{5/2,7/2}$ states for which the relative difference is about 14%. Such a large difference suggests that there is a misidentification and that further experimental analysis is needed.

Transition data for E1, M1, and E2 transitions are given in Table 7, and are available at the CDS. In Fig. 4 a scatterplot of dT versus the transition rate A is displayed for all presented E1 transitions. The mean dT for the transitions is 6.47%. Again, for most of the strongest transitions, dT is well below 2%.

4. Conclusions

Energy spectra and transition data of E1, M1, and E2 transitions are presented for S II, Cl III, and Ar IV using MCDHF and RCI methods. The accuracy of the results is evaluated by comparing energy levels with data from NIST database and by the agreement of transition rates between length and velocity gauges. For the first time levels of the $3s3p^33d$ configuration are presented for the studied elements. The averaged uncertainty of computed energy levels compared with NIST data is 0.22%, 0.18%, and 0.21%, respectively for S II, Cl III, and Ar IV ions. The mean dT for all presented E1 transitions is 12.00%, 5.95%, and 6.47%, respectively, for the S II, Cl III, and Ar IV ions.

Table 4. Comparison of new levels by Raineri et al. (2018) with theoretical computations for Ar IV.

	Raineri et al. (2018)		This work		Fischer et al. (2006)	
Label	Exp.	Cal.	RCI(CV)	Diff. %	Calc.	Diff. %
$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{5/2}$	185 795.6	185 870	187 234	0.77	188 521.63	1.47
$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{7/2}$	186 451.8	186 591	189 057	1.40	189 467.32	1.62
$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P_{1/2}$	245 175.2	245 287	246 701	0.62	248 938.85	1.54
$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{5/2}$	261 761.1	261 946	226 733	−13.38	227 731.72	−13.00
$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{3/2}$	262 626.1	262 735	225 349	−14.19	226 550.48	−13.74
$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2S^\circ_{1/2}$	282 726.0	282 596	280 888	−0.65	280 500.33	−0.79
$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{1/2}$	311 018.3	310 973	312 019	0.32		
$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{3/2}$	311 276.3	311 201	312 497	0.39		
$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{1/2}$	327 113.4	327 126	327 235	0.04		
$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{3/2}$	327 388.9	327 333	327 351	−0.01		

Notes. The Diff. columns give the relative difference of the theoretical results compared with the experimental ones.

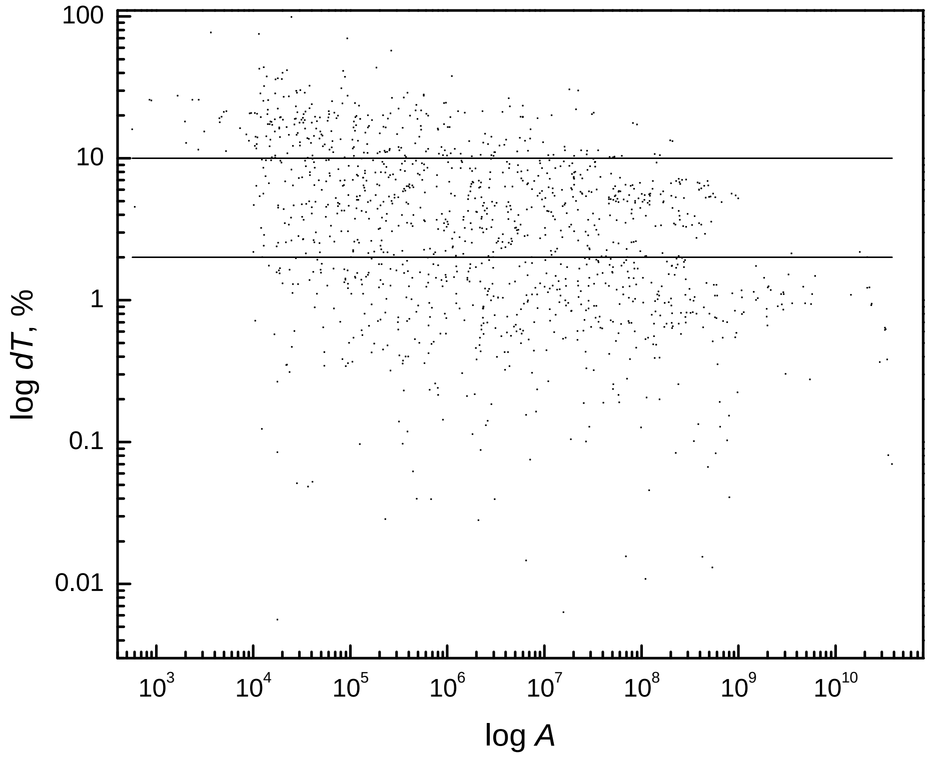

Fig. 4. Scatterplot of dT vs. the transition rate A of E1 transitions for Ar IV. The solid lines indicate the 2% and 10% deviations.

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Appendix A: Wave function composition in *LS*-coupling, energy levels, and lifetimes for the S II, Cl III, and Ar IV ions

Table A.1. Wave function composition (up to three *LS* components with a contribution >0.02 of the total wave function) in *LS*-coupling and energy levels (in cm^{-1}) for S II.

No.	State	*LS*-composition	$E_{RCI(CV)}$	E_{NIST}	τ_l	τ_v
1	$3s^2\,3p^3(^4_3S)\,^4S^\circ_{3/2}$	$0.93 + 0.02\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4S^\circ$	0	0		
2	$3s^2\,3p^3(^2_3D)\,^2D^\circ_{3/2}$	0.92	15 122	14 852.94	1.06e+03	1.06e+03
3	$3s^2\,3p^3(^2_3D)\,^2D^\circ_{5/2}$	0.92	15 152	14 884.73	3.52e+03	3.78e+03
4	$3s^2\,3p^3(^2_1P)\,^2P^\circ_{1/2}$	$0.90 + 0.02\ 3p^5\,^2P^\circ$	24 978	24 524.83	3.01e+00	3.10e+00
5	$3s^2\,3p^3(^2_1P)\,^2P^\circ_{3/2}$	$0.90 + 0.02\ 3p^5\,^2P^\circ$	25 016	24 571.54	1.83e+00	1.86e+00
6	$3s\,^2S\,3p^4(^3_2P)\,^4P_{5/2}$	$0.79 + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	78 971	79 395.39	2.22e−08	2.12e−08
7	$3s\,^2S\,3p^4(^3_2P)\,^4P_{3/2}$	$0.79 + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	79 326	79 756.83	2.21e−08	2.11e−08
8	$3s\,^2S\,3p^4(^3_2P)\,^4P_{1/2}$	$0.79 + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	79 539	79 962.61	2.20e−08	2.11e−08
9	$3s\,^2S\,3p^4(^1_2D)\,^2D_{3/2}$	$0.60 + 0.25\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D + 0.03\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D$	97 765	97 890.74	1.84e−08	1.70e−08
10	$3s\,^2S\,3p^4(^1_2D)\,^2D_{5/2}$	$0.60 + 0.25\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D + 0.03\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D$	97 796	97 918.86	1.91e−08	1.75e−08
11	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P_{3/2}$	$0.66 + 0.16\ 3s\,^2S\,3p^4(^3_2P)\,^2P + 0.08\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P$	105 506	105 599.06	2.05e−08	2.04e−08
12	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P_{1/2}$	$0.66 + 0.17\ 3s\,^2S\,3p^4(^3_2P)\,^2P + 0.07\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P$	105 961	106 044.24	1.98e−08	1.97e−08
13	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{1/2}$	0.92	109 364	109 560.69	9.64e−10	9.62e−10
14	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{3/2}$	0.92	109 627	109 831.59	9.53e−10	9.50e−10
15	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{3/2}$	0.91	110 025	110 177.02	3.73e−06	3.62e−06
16	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{5/2}$	0.92	110 059	110 268.6	9.38e−10	9.35e−10
17	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{5/2}$	0.91	110 161	110 313.4	2.52e−06	2.55e−06
18	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{7/2}$	0.91	110 362	110 508.71	3.47e−06	3.62e−06
19	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{9/2}$	0.91	110 636	110 766.56	1.41e+00	1.34e+00
20	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^2P_{1/2}$	0.91	112 815	112 937.57	4.75e−10	4.72e−10
21	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^2P_{3/2}$	0.90	113 327	113 461.54	4.75e−10	4.72e−10
22	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{1/2}$	0.91	114 002	114 162.3	1.48e−06	1.49e−06
23	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{3/2}$	0.91	114 034	114 200.54	7.91e−07	7.98e−07
24	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{5/2}$	$0.87 + 0.02\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.02\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	114 069	114 231.04	3.30e−07	3.37e−07
25	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{7/2}$	$0.84 + 0.04\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	114 126	114 279.33	5.86e−07	5.97e−07
26	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{5/2}$	$0.44 + 0.42\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F + 0.05\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D$	114 721	114 804.37	2.42e−08	2.48e−08
27	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{7/2}$	$0.43 + 0.40\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F + 0.07\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D$	115 202	115 285.61	2.97e−08	3.03e−08
28	$3s\,^2S\,3p^4(^1_0S)\,^2S_{1/2}$	$0.54 + 0.38\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S$	119 994	119 783.77	6.89e−09	6.32e−09
29	$3s^2\,3p^2(^1_2D)\,^1D\,4s\,^2D_{3/2}$	0.90	121 508	121 528.72	7.15e−10	7.13e−10
30	$3s^2\,3p^2(^1_2D)\,^1D\,4s\,^2D_{5/2}$	0.90	121 511	121 530.02	7.04e−10	7.02e−10
31	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2S^\circ_{1/2}$	0.92	125 286	125 485.29	1.54e−08	1.57e−08
32	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2G_{7/2}$	0.92	127 207	127 127.1	4.73e−07	4.79e−07
33	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2G_{9/2}$	0.92	127 243	127 128.35	4.78e−01	4.87e−01
34	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{1/2}$	0.92	127 613	127 825.08	8.82e−09	8.99e−09
35	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{3/2}$	0.92	127 757	127 976.34	8.78e−09	8.94e−09
36	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{5/2}$	0.92	128 009	128 233.2	8.73e−09	8.89e−09
37	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{7/2}$	0.92	128 374	128 599.16	8.69e−09	8.85e−09
38	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{1/2}$	0.92	129 555	129 787.83	7.14e−09	7.25e−09
39	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{3/2}$	$0.86 + 0.04\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4S^\circ$	129 617	129 858.18	7.01e−09	7.11e−09
40	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{5/2}$	$0.88 + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ$	129 892	130 134.16	7.23e−09	7.33e−09
41	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ_{3/2}$	$0.81 + 0.09\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ$	130 468	130 641.11	1.13e−08	1.13e−08
42	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{5/2}$	$0.76 + 0.10\ 3s\,^2S\,3p^4(^3_2P)\,^4P + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P$	130 728	130 602.21	1.10e−10	1.11e−10
43	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4S^\circ_{3/2}$	$0.86 + 0.05\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ$	130 749	131 028.85	5.04e−09	5.16e−09
44	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{3/2}$	$0.76 + 0.11\ 3s\,^2S\,3p^4(^3_2P)\,^4P + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P$	130 942	130 818.85	1.10e−10	1.10e−10
45	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ_{5/2}$	$0.79 + 0.08\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ + 0.04\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ$	131 005	131 187.19	1.11e−08	1.11e−08
46	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{1/2}$	$0.76 + 0.11\ 3s\,^2S\,3p^4(^3_2P)\,^4P + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P$	131 092	130 948.94	1.09e−10	1.10e−10
47	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ_{1/2}$	$0.83 + 0.06\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ$	133 125	133 268.68	8.01e−09	8.04e−09
48	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ_{3/2}$	$0.82 + 0.08\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ$	133 245	133 399.97	8.00e−09	8.02e−09
49	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D_{3/2}$	$0.72 + 0.11\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.04\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D$	133 387	133 360.86	4.00e−10	4.05e−10
50	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D_{5/2}$	$0.74 + 0.10\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.04\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D$	133 832	133 814.84	3.72e−10	3.76e−10
51	$3s^2\,3p^2(^1_0S)\,^1S\,4s\,^2S_{1/2}$	$0.84 + 0.04\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S + 0.04\ 3p^4(^1_0S)\,^1S\,4s\,^2S$	136 386	136 328.79	3.33e−10	3.33e−10
52	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F_{5/2}$	$0.41 + 0.37\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.11\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2F$	138 586	138 509.17	1.31e−10	1.32e−10
53	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F_{7/2}$	$0.42 + 0.37\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.10\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2F$	138 609	138 527.98	1.29e−10	1.31e−10
54	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P_{1/2}$	$0.79 + 0.07\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P$	140 134	139 844.99	2.24e−10	2.31e−10
55	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2F^\circ_{5/2}$	0.90	140 197	140 230.1	9.05e−09	9.11e−09
56	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2F^\circ_{7/2}$	0.92	140 289	140 319.23	9.01e−09	9.05e−09

Notes. Energy levels are given relative to the ground state. The states 65, 102, and 107 are indicated in bold. The labels for these levels were not assigned with largest contribution to the composition.

Table A.1. continued.

57	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P_{3/2}$	$0.79 + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P$	140 298	140 016.77	2.22e−10	2.29e−10
58	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ_{5/2}$	$0.80 + 0.08\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ$	140 642	140 708.89	6.76e−09	6.90e−09
59	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ_{3/2}$	$0.81 + 0.08\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ$	140 688	140 750.34	6.73e−09	6.88e−09
60	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{1/2}$	$0.83 + 0.05\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ$	143 493	143 488.95	5.79e−09	5.86e−09
61	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{3/2}$	$0.81 + 0.07\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ$	143 613	143 623.56	5.79e−09	5.87e−09
62	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D_{5/2}$	$0.51 + 0.19\;3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.10\;3s\,^2S\,3p^4(^1_2D)\,^2D$	144 308	144 009.42	2.02e−10	2.04e−10
63	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D_{3/2}$	$0.52 + 0.16\;3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.11\;3s\,^2S\,3p^4(^1_2D)\,^2D$	144 459	144 142.16	1.89e−10	1.90e−10
64	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P_{3/2}$	$0.36 + 0.33\;3s\,^2S\,3p^4(^3_2P)\,^2P + 0.13\;3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P$	146 144	145 505.74	1.71e−10	1.70e−10
65	$3s\,^2S\,3p^4(^3_2P)\,^2P_{1/2}$	**0.33** $+ 0.35\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P + 0.13\;3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P$	146 549	145 877.66	1.69e−10	1.69e−10
66	$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{3/2}$	$0.48 + 0.15\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D + 0.10\;3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D$	149 188	148 900.91	1.68e−10	1.69e−10
67	$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{5/2}$	$0.48 + 0.13\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D + 0.11\;3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D$	149 194	148 886.57	1.61e−10	1.62e−10
68	$3s^2\,3p^2(^3_2P)\,^3P\,5s\,^4P_{1/2}$	0.91	149 987	150 258.51	2.36e−09	2.38e−09
69	$3s^2\,3p^2(^3_2P)\,^3P\,5s\,^4P_{3/2}$	0.91	150 251	150 531.31	2.29e−09	2.32e−09
70	$3s^2\,3p^2(^3_2P)\,^3P\,5s\,^4P_{5/2}$	0.92	150 712	150 996.41	2.24e−09	2.26e−09
71	$3s^2\,3p^2(^3_2P)\,^3P\,5s\,^2P_{1/2}$	$0.87 + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P$	151 111	151 383.81	1.16e−09	1.16e−09
72	$3s^2\,3p^2(^3_2P)\,^3P\,5s\,^2P_{3/2}$	$0.87 + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P$	151 623	151 910.83	1.13e−09	1.13e−09
73	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F_{3/2}$	0.89	151 784	151 959.69	4.28e−09	4.38e−09
74	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F_{5/2}$	$0.87 + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D$	151 917	152 094.64	4.27e−09	4.37e−09
75	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F_{7/2}$	$0.87 + 0.04\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D$	152 129	152 305	4.28e−09	4.38e−09
76	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S_{1/2}$	$0.44 + 0.25\;3s\,^2S\,3p^4(^1_0S)\,^2S + 0.13\;3s^2\,3p^2(^1_2D)\,^1D\,4d\,^2S$	152 302	151 651.72	2.11e−10	2.12e−10
77	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F_{9/2}$	0.91	152 446	152 615.46	4.36e−09	4.46e−09
78	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D_{1/2}$	0.91	152 932	153 153.9	4.22e−09	4.27e−09
79	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D_{3/2}$	0.89	152 974	153 201.95	4.09e−09	4.14e−09
80	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D_{5/2}$	$0.87 + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F$	153 054	153 283.07	4.01e−09	4.06e−09
81	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4D_{7/2}$	$0.87 + 0.04\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4F$	153 185	153 413.74	4.53e−09	4.59e−09
82	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P_{5/2}$	0.88	155 684	155 818.71	3.41e−10	3.41e−10
83	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P_{3/2}$	0.88	155 893	156 029.54	3.37e−10	3.37e−10
84	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2F_{5/2}$	$0.72 + 0.12\;3s^2\,3p^2(^1_2D)\,^1D\,4d\,^2F + 0.06\;3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F$	156 019	156 121.7	4.68e−10	4.73e−10
85	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^4P_{1/2}$	0.89	156 022	156 148.48	3.33e−10	3.33e−10
86	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2S^\circ_{1/2}$	$0.78 + 0.08\;3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ$	156 104		1.50e−08	1.89e−08
87	$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{1/2}$	$0.69 + 0.11\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2S^\circ + 0.07\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ$	156 355	156 167.04	8.90e−09	9.27e−09
88	$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{3/2}$	$0.80 + 0.08\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ + 0.04\;3p^4(^1_0S)\,^1S\,4p\,^2P^\circ$	156 391	156 276.83	8.29e−09	8.42e−09
89	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2F_{7/2}$	$0.72 + 0.11\;3s^2\,3p^2(^1_2D)\,^1D\,4d\,^2F + 0.06\;3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F$	156 502	156 604.17	4.77e−10	4.82e−10
90	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ_{1/2}$	0.90	156 588	156 829.75	2.43e−08	3.21e−08
91	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ_{3/2}$	$0.86 + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ$	156 687	156 939.5	2.41e−08	3.23e−08
92	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ_{5/2}$	$0.86 + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ$	156 917	157 173.69	2.42e−08	3.27e−08
93	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ_{3/2}$	$0.47 + 0.39\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4S^\circ + 0.05\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ$	157 274	157 579.68	1.11e−08	1.40e−08
94	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ_{7/2}$	0.93	157 303	157 558.77	2.46e−08	3.33e−08
95	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ_{1/2}$	$0.89 + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2S^\circ$	157 388	157 677.32	1.85e−08	2.46e−08
96	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ_{5/2}$	$0.84 + 0.07\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4D^\circ + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2D^\circ$	157 738	158 038.6	1.89e−08	2.52e−08
97	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4S^\circ_{3/2}$	$0.50 + 0.37\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2D^\circ$	157 801	158 118.75	9.94e−09	1.23e−08
98	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2D^\circ_{3/2}$	$0.85 + 0.04\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ$	157 947	158 215.59	1.91e−08	2.60e−08
99	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2D^\circ_{5/2}$	$0.87 + 0.03\;3s^2\,3p^2(^3_2P)\,^3P\,5p\,^4P^\circ$	158 442	158 715.46	1.89e−08	2.56e−08
100	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ_{1/2}$	$0.79 + 0.09\;3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ$	159 333		1.15e−08	1.51e−08
101	$3s^2\,3p^2(^3_2P)\,^3P\,5p\,^2P^\circ_{3/2}$	$0.80 + 0.08\;3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ + 0.02\;3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ$	159 504		1.18e−08	1.56e−08
102	$3s\,^2S\,3p^4(^3_2P)\,^2P_{3/2}$	**0.18** $+ 0.31\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P + 0.23\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D$	159 564	158 828.31	1.56e−10	1.56e−10
103	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ_{5/2}$	$0.49 + 0.26\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ + 0.08\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ$	159 793	160 104.11	3.24e−09	3.25e−09
104	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ_{7/2}$	$0.50 + 0.19\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ + 0.13\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2G^\circ$	159 818	160 128.9	3.29e−09	3.34e−09
105	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D_{5/2}$	$0.71 + 0.08\;3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.07\;3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D$	159 843	159 492.83	2.90e−10	2.96e−10
106	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2D_{3/2}$	$0.47 + 0.16\;3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P + 0.09\;3s\,^2S\,3p^4(^3_2P)\,^2P$	159 935	159 495.94	2.11e−10	2.12e−10
107	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ_{5/2}$	**0.40** $+ 0.41\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ + 0.12\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ$	159 946	160 258.03	3.24e−09	3.26e−09
108	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ_{7/2}$	$0.40 + 0.36\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ + 0.17\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2G^\circ$	159 975	160 284.24	3.26e−09	3.30e−09
109	$3s^2\,3p^2(^3_2P)\,^3P\,4d\,^2P_{1/2}$	$0.48 + 0.27\;3s\,^2S\,3p^4(^3_2P)\,^2P + 0.05\;3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P$	160 132	159 283.66	1.29e−10	1.28e−10
110	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ_{9/2}$	$0.70 + 0.15\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2G^\circ + 0.08\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4F^\circ$	160 134	160 442.67	3.23e−09	3.21e−09
111	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ_{3/2}$	$0.41 + 0.40\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ + 0.12\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4F^\circ$	160 149	160 462.24	3.30e−09	3.35e−09
112	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ_{5/2}$	$0.62 + 0.20\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ + 0.05\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2F^\circ$	160 155	160 467.51	3.29e−09	3.37e−09
113	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2G^\circ_{7/2}$	$0.58 + 0.28\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2F^\circ$	160 173	160 483.16	3.50e−09	3.58e−09
114	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ_{3/2}$	$0.47 + 0.46\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ$	160 425	160 733.68	3.28e−09	3.36e−09
115	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ_{1/2}$	0.93	160 428	160 733.68	3.22e−09	3.30e−09
116	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ_{11/2}$	0.93	160 522	160 828.69	3.14e−09	3.10e−09
117	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2G^\circ_{9/2}$	$0.75 + 0.18\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4G^\circ$	160 612	160 920.95	3.56e−09	3.67e−09
118	$3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4F^\circ_{3/2}$	$0.81 + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^2D^\circ + 0.06\;3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4D^\circ$	160 888	161 221.05	3.33e−09	3.28e−09

Table A.1. continued.

119	3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}F$^\circ_{5/2}$	0.70 + 0.12 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}F$^\circ$ + 0.10 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}D$^\circ$	160 919	161 253.47	3.40e–09	3.38e–09
120	3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}F$^\circ_{7/2}$	0.82 + 0.06 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}D$^\circ$ + 0.04 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}G$^\circ$	160 992	161 329.65	3.32e–09	3.27e–09
121	3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}F$^\circ_{9/2}$	0.84 + 0.05 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}G$^\circ$ + 0.04 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}G$^\circ$	161 024	161 360.19	3.34e–09	3.29e–09
122	3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}F$^\circ_{5/2}$	0.72 + 0.12 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{4}F$^\circ$ + 0.07 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}D$^\circ$	161 059	161 386.45	3.86e–09	4.03e–09
123	3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}F$^\circ_{7/2}$	0.85 + 0.05 3s^2 3p^2($^3_2$P) ^{3}P 4f ^{2}G$^\circ$	161 127	161 454.96	4.00e–09	4.23e–09
124	3s^2 3p^2($^1_2$D) ^{1}D 5s ^{2}D$_{5/2}$	0.91	161 595	161 733.1	1.52e–09	1.53e–09
125	3s^2 3p^2($^1_2$D) ^{1}D 5s ^{2}D$_{3/2}$	0.91	161 603	161 737.99	1.39e–09	1.40e–09
126	3s ^{2}S 3p^3($^4_3$S) ^{5}S 3d ^{6}D$^\circ_{5/2}$	0.94	164 076		1.43e–05	1.46e–05
127	3s ^{2}S 3p^3($^4_3$S) ^{5}S 3d ^{6}D$^\circ_{3/2}$	0.94	164 077		1.08e–05	1.05e–05
128	3s ^{2}S 3p^3($^4_3$S) ^{5}S 3d ^{6}D$^\circ_{7/2}$	0.94	164 080		2.13e–05	2.26e–05
129	3s ^{2}S 3p^3($^4_3$S) ^{5}S 3d ^{6}D$^\circ_{1/2}$	0.94	164 083		9.17e–06	8.52e–06
130	3s ^{2}S 3p^3($^4_3$S) ^{5}S 3d ^{6}D$^\circ_{9/2}$	0.94	164 088		2.66e–05	2.30e–05
131	3s^2 3p^2($^1_2$D) ^{1}D 4d ^{2}G$_{7/2}$	0.91	164 185	164 181.17	4.17e–09	4.23e–09
132	3s^2 3p^2($^1_2$D) ^{1}D 4d ^{2}G$_{9/2}$	0.92	164 210	164 268.79	4.56e–09	4.62e–09
133	3s^2 3p^2($^1_2$D) ^{1}D 4d ^{2}F$_{7/2}$	0.75 + 0.09 3s^2 3p^2($^3_2$P) ^{3}P 4d ^{2}F + 0.03 3s^2 3p^2($^3_2$P) ^{3}P 5d ^{2}F	165 008	164 337.61	4.36e–10	4.43e–10
134	3s^2 3p^2($^1_2$D) ^{1}D 4d ^{2}F$_{5/2}$	0.76 + 0.10 3s^2 3p^2($^3_2$P) ^{3}P 4d ^{2}F + 0.03 3s^2 3p^2($^3_2$P) ^{3}P 5d ^{2}F	165 084	164 232.36	4.31e–10	4.38e–10

Table A.2. Wave function composition (up to three *LS* components with a contribution >0.02 of the total wave function) in *LS*-coupling and energy levels (in cm^{-1}) for Cl III.

No.	State	*LS*-composition	$E_{RCI(CV)}$	E_{NIST}	τ_l	τ_v
1	3s^2 3p^3($^4_3$S) ^{4}S$^\circ_{3/2}$	0.94 + 0.03 3s ^{2}S 3p^3($^2_3$D) ^{3}D 3d ^{4}S$^\circ$	0	0		
2	3s^2 3p^3($^2_3$D) ^{2}D$^\circ_{3/2}$	0.93	18 286	18 052.46	1.82e+02	1.83e+02
3	3s^2 3p^3($^2_3$D) ^{2}D$^\circ_{5/2}$	0.93	18 345	18 118.43	1.27e+03	1.35e+03
4	3s^2 3p^3($^2_1$P) ^{2}P$^\circ_{1/2}$	0.92 + 0.02 3p^5 ^{2}P$^\circ$	30 117	29 813.92	1.38e+00	1.41e+00
5	3s^2 3p^3($^2_1$P) ^{2}P$^\circ_{3/2}$	0.91 + 0.02 3p^5 ^{2}P$^\circ$	30 200	29 906.45	6.91e–01	6.96e–01
6	3s ^{2}S 3p^4($^3_2$P) ^{4}P$_{5/2}$	0.83 + 0.12 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	98 508	98 520.34	7.47e–09	7.17e–09
7	3s ^{2}S 3p^4($^3_2$P) ^{4}P$_{3/2}$	0.83 + 0.13 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	99 114	99 131.4	7.37e–09	7.10e–09
8	3s ^{2}S 3p^4($^3_2$P) ^{4}P$_{1/2}$	0.83 + 0.13 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	99 462	99 475.22	7.31e–09	7.05e–09
9	3s ^{2}S 3p^4($^1_2$D) ^{2}D$_{3/2}$	0.67 + 0.23 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}D + 0.03 3s^2 3p^2($^1_0$S) ^{1}S 3d ^{2}D	122 392	122 131.66	4.37e–09	4.21e–09
10	3s ^{2}S 3p^4($^1_2$D) ^{2}D$_{5/2}$	0.67 + 0.23 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}D + 0.03 3s^2 3p^2($^1_0$S) ^{1}S 3d ^{2}D	122 443	122 179.8	4.48e–09	4.32e–09
11	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}P$_{3/2}$	0.60 + 0.26 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.07 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P	137 180		2.62e–09	2.55e–09
12	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}P$_{1/2}$	0.60 + 0.26 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.07 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P	137 920		2.52e–09	2.46e–09
13	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}F$_{3/2}$	0.94	146 611	146 521.72	1.12e–06	1.08e–06
14	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}F$_{5/2}$	0.94	146 835	146 746.99	1.28e–06	1.29e–06
15	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}F$_{7/2}$	0.94	147 165	147 069.57	1.94e–06	1.99e–06
16	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}F$_{9/2}$	0.94	147 600	147 494.54	3.10e–01	2.98e–01
17	3s ^{2}S 3p^4($^1_0$S) ^{2}S$_{1/2}$	0.67 + 0.27 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}S	150 041		1.27e–09	1.23e–09
18	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D$_{5/2}$	0.58 + 0.20 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}F + 0.15 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}F	151 972	151 846.4	1.55e–07	1.54e–07
19	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D$_{1/2}$	0.93	151 979	151 944.55	4.10e–07	4.03e–07
20	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D$_{3/2}$	0.93	152 038	151 878.06	2.62e–07	2.59e–07
21	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D$_{7/2}$	0.71 + 0.13 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}F + 0.09 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}F	152 072	151 951.64	1.22e–06	1.16e–06
22	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}F$_{5/2}$	**0.33** + 0.35 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D + 0.25 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}F	152 458		9.59e–08	9.52e–08
23	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}F$_{7/2}$	0.41 + 0.30 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}F + 0.22 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}D	153 210		1.57e–07	1.53e–07
24	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}G$_{7/2}$	0.93	169 142		3.48e–07	3.50e–07
25	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}G$_{9/2}$	0.93	169 202		2.05e–01	2.06e–01
26	3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P$_{1/2}$	0.84 + 0.08 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	173 576	173 735.28	1.42e–10	1.41e–10
27	3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P$_{3/2}$	0.82 + 0.10 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	173 935	174 093.02	1.28e–10	1.28e–10
28	3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P$_{5/2}$	0.78 + 0.13 3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P	174 478	174 611.76	1.08e–10	1.08e–10
29	3s^2 3p^2($^3_2$P) ^{3}P 4s ^{2}P$_{1/2}$	0.87 + 0.02 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.02 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P	178 291	178 369.14	1.14e–10	1.12e–10
30	3s^2 3p^2($^3_2$P) ^{3}P 4s ^{2}P$_{3/2}$	0.84 + 0.04 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.03 3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P	179 006	179 075.2	1.05e–10	1.04e–10
31	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P$_{5/2}$	0.67 + 0.15 3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P + 0.10 3s ^{2}S 3p^4($^3_2$P) ^{4}P	179 918	179 493.96	7.06e–11	7.02e–11
32	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P$_{3/2}$	0.70 + 0.11 3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P + 0.10 3s ^{2}S 3p^4($^3_2$P) ^{4}P	180 105	179 662.15	6.38e–11	6.34e–11
33	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{4}P$_{1/2}$	0.72 + 0.11 3s ^{2}S 3p^4($^3_2$P) ^{4}P + 0.09 3s^2 3p^2($^3_2$P) ^{3}P 4s ^{4}P	180 253	179 780.84	6.05e–11	6.01e–11
34	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}D$_{3/2}$	0.50 + 0.38 3s^2 3p^2($^1_0$S) ^{1}S 3d ^{2}D	182 507	182 075.74	4.32e–10	4.29e–10
35	3s^2 3p^2($^3_2$P) ^{3}P 3d ^{2}D$_{5/2}$	0.51 + 0.38 3s^2 3p^2($^1_0$S) ^{1}S 3d ^{2}D + 0.02 3s ^{2}S 3p^4($^1_2$D) ^{2}D	183 470	183 041.91	3.77e–10	3.73e–10
36	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P$_{3/2}$	0.49 + 0.33 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.07 3s^2 3p^2($^3_2$P) ^{3}P 4s ^{2}P	186 809	185 837.68	1.03e–10	1.01e–10
37	3s^2 3p^2($^1_2$D) ^{1}D 3d ^{2}P$_{1/2}$	0.54 + 0.32 3s ^{2}S 3p^4($^3_2$P) ^{2}P + 0.05 3s^2 3p^2($^3_2$P) ^{3}P 4s ^{2}P	187 208	186 219.67	1.00e–10	9.91e–11

Notes. Energy levels are given relative to the ground state. (Level in NIST column flagged "?" means that level/line may not be real; "[]" means that level was determined by interpolation or extrapolation of known experimental values or by semiempirical calculation.). The states 45 and 46 are indicated in bold. The labels for these levels were not assigned with largest contribution to the composition.

Table A.2. continued.

38	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4s\ ^2D_{5/2}$	$0.83 + 0.07\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D$	188 428	188 389.53	1.25e−10	1.24e−10
39	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4s\ ^2D_{3/2}$	$0.82 + 0.06\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D$	188 490	188 447.52	1.27e−10	1.27e−10
40	$3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D_{5/2}$	$0.49 + 0.13\ 3s\ ^2S\ 3p^4(^1_2D)\ ^2D + 0.09\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4s\ ^2D$	195 683	194 958.79	8.41e−11	8.33e−11
41	$3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D_{3/2}$	$0.54 + 0.15\ 3s\ ^2S\ 3p^4(^1_2D)\ ^2D + 0.09\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4s\ ^2D$	196 011	195 267.76	8.02e−11	7.94e−11
42	$3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2F_{5/2}$	$0.48 + 0.36\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2F + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^2F$	196 688	196 137.22	4.24e−11	4.23e−11
43	$3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2F_{7/2}$	$0.50 + 0.37\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2F + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^2F$	196 724	196 153.36	4.18e−11	4.18e−11
44	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2S^\circ_{1/2}$	0.92	197 580		2.85e−09	2.87e−09
45	$3s\ ^2S\ 3p^4(^3_2P)\ ^2P_{1/2}$	**0.27** $+ 0.30\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2P + 0.27\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2P$	199 748	198 835.25	5.00e−11	4.94e−11
46	$3s\ ^2S\ 3p^4(^3_2P)\ ^2P_{3/2}$	**0.25** $+ 0.31\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2P + 0.30\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2P$	199 855	198 983.79	5.08e−11	5.02e−11
47	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4D^\circ_{1/2}$	0.92	200 890	201 072.41	1.77e−09	1.80e−09
48	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4D^\circ_{3/2}$	0.92	201 139	201 330.92	1.77e−09	1.79e−09
49	$3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2S_{1/2}$	$0.45 + 0.26\ 3s^2\ 3p^2(^1_0S)\ ^1S\ 4s\ ^2S + 0.15\ 3s\ ^2S\ 3p^4(^1_0S)\ ^2S$	201 480		5.29e−11	5.24e−11
50	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4D^\circ_{5/2}$	0.92	201 568	201 763.86	1.76e−09	1.78e−09
51	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4D^\circ_{7/2}$	0.92	202 176	202 366.62	1.75e−09	1.78e−09
52	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ_{1/2}$	0.92	203 807	204 021.26	1.67e−09	1.69e−09
53	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ_{3/2}$	$0.85 + 0.04\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4S^\circ + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ$	203 902	204 124.04	1.68e−09	1.70e−09
54	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ_{5/2}$	$0.84 + 0.06\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ$	204 320	204 540.95	1.72e−09	1.74e−09
55	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ_{3/2}$	$0.76 + 0.14\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2D^\circ + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ$	204 903	205 036.99	2.59e−09	2.59e−09
56	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4S^\circ_{3/2}$	$0.87 + 0.05\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ$	205 705	205 938.06	1.49e−09	1.51e−09
57	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ_{5/2}$	$0.72 + 0.12\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2D^\circ + 0.08\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^4P^\circ$	205 802	205 946.9 ?	2.52e−09	2.53e−09
58	$3s^2\ 3p^2(^1_0S)\ ^1S\ 3d\ ^2D_{5/2}$	$0.40 + 0.28\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2D + 0.09\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D$	206 010		4.67e−11	4.65e−11
59	$3s^2\ 3p^2(^1_0S)\ ^1S\ 3d\ ^2D_{3/2}$	$0.42 + 0.29\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 3d\ ^2D + 0.08\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2D$	206 251		4.73e−11	4.71e−11
60	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2P^\circ_{1/2}$	$0.80 + 0.10\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2P^\circ$	208 929	209 042.8 ?	2.18e−09	2.19e−09
61	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2P^\circ_{3/2}$	$0.78 + 0.12\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2P^\circ$	209 054	209 182.8 ?	2.18e−09	2.19e−09
62	$3s^2\ 3p^2(^1_0S)\ ^1S\ 4s\ ^2S_{1/2}$	$0.65 + 0.17\ 3s^2\ 3p^2(^1_2D)\ ^1D\ 3d\ ^2S + 0.09\ 3s\ ^2S\ 3p^4(^1_0S)\ ^2S$	210 651		1.81e−09	1.75e−09
63	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^6D^\circ_{3/2}$	0.97	212 608		3.79e−06	3.63e−06
64	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^6D^\circ_{5/2}$	0.97	212 608		5.48e−06	5.56e−06
65	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^6D^\circ_{1/2}$	0.97	212 616		3.24e−06	3.06e−06
66	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^6D^\circ_{7/2}$	0.97	212 620		1.07e−05	1.14e−05
67	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^6D^\circ_{9/2}$	0.97	212 654		3.05e−05	2.52e−05
68	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2F^\circ_{5/2}$	$0.91 + 0.02\ 3s\ ^2S\ 3p^2(^3_2P)\ ^2P\ 3d\ ^1D\ 4p\ ^2F^\circ$	216 534	216 524.6 ?	1.96e−09	1.98e−09
69	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2F^\circ_{7/2}$	$0.92 + 0.02\ 3s\ ^2S\ 3p^2(^3_2P)\ ^2P\ 3d\ ^1D\ 4p\ ^2F^\circ$	216 726	216 710.4 ?	1.95e−09	1.96e−09
70	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2D^\circ_{5/2}$	$0.77 + 0.14\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ$	217 852	217 850.2 ?	2.04e−09	2.06e−09
71	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2D^\circ_{3/2}$	$0.77 + 0.14\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2D^\circ$	217 923	217 913.1 ?	2.04e−09	2.06e−09
72	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2P^\circ_{1/2}$	$0.79 + 0.10\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2P^\circ$	221 952	221 862.9 ?	1.86e−09	1.88e−09
73	$3s^2\ 3p^2(^1_2D)\ ^1D\ 4p\ ^2P^\circ_{3/2}$	$0.75 + 0.12\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4p\ ^2P^\circ$	222 175	222 100.7 ?	1.93e−09	1.96e−09
74	$3p^5\ ^2P^\circ_{3/2}$	$0.40 + 0.35\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^2P^\circ + 0.06\ 3s\ ^2S\ 3p^3(^2_1P)\ ^3P\ 3d\ ^2P^\circ$	230 878	292 470 []	1.71e−09	1.66e−09
75	$3p^5\ ^2P^\circ_{1/2}$	$0.39 + 0.35\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^2P^\circ + 0.06\ 3s\ ^2S\ 3p^3(^2_1P)\ ^3P\ 3d\ ^2P^\circ$	231 746	293 540 []	1.86e−09	1.81e−09
76	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^4D^\circ_{7/2}$	$0.45 + 0.40\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^4D^\circ + 0.04\ 3s^2\ 3p\ ^2P\ 3d^2(^3_2F)\ ^4D^\circ$	233 460		8.10e−09	7.93e−09
77	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^4D^\circ_{5/2}$	$0.45 + 0.40\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^4D^\circ + 0.04\ 3s^2\ 3p\ ^2P\ 3d^2(^3_2F)\ ^4D^\circ$	233 478		7.76e−09	7.61e−09
78	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^4D^\circ_{3/2}$	$0.45 + 0.40\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^4D^\circ + 0.04\ 3s^2\ 3p\ ^2P\ 3d^2(^3_2F)\ ^4D^\circ$	233 522		7.57e−09	7.45e−09
79	$3s\ ^2S\ 3p^3(^4_3S)\ ^5S\ 3d\ ^4D^\circ_{1/2}$	$0.45 + 0.40\ 3s\ ^2S\ 3p^3(^2_3D)\ ^3D\ 3d\ ^4D^\circ + 0.04\ 3s^2\ 3p\ ^2P\ 3d^2(^3_2F)\ ^4D^\circ$	233 578		7.45e−09	7.35e−09
80	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F_{3/2}$	0.91	239 418	239 506.3 ?	1.49e−09	1.58e−09
81	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F_{5/2}$	$0.90 + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D$	239 640	239 729.9 ?	1.49e−09	1.58e−09
82	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F_{7/2}$	$0.89 + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D$	239 991	240 075.2 ?	1.50e−09	1.58e−09
83	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F_{9/2}$	0.93	240 490	240 568.4 ?	1.51e−09	1.60e−09
84	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D_{1/2}$	$0.88 + 0.04\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^2P$	241 426	241 559.4 ?	1.33e−09	1.38e−09
85	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D_{3/2}$	$0.80 + 0.06\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^2P + 0.06\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4P$	241 445	241 572.4 ?	1.17e−09	1.21e−09
86	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D_{5/2}$	$0.76 + 0.14\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4P + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F$	241 557	241 685.1 ?	1.13e−09	1.16e−09
87	$3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4D_{7/2}$	$0.88 + 0.03\ 3s^2\ 3p^2(^3_2P)\ ^3P\ 4d\ ^4F$	241 904	242 046.2 ?	1.50e−09	1.57e−09

Table A.3. Wave function composition (up to three *LS* components with a contribution >0.02 of the total wave function) in *LS*-coupling and energy levels (in cm^{-1}) for Ar IV.

No.	State	*LS*-composition	$E_{\mathrm{RCI(CV)}}$	E_{NIST}	τ_{l}	τ_{v}
1	$3s^2\,3p^3(^4_3S)\,^4S^\circ_{3/2}$	$0.95 + 0.03\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4S^\circ$	0	0		
2	$3s^2\,3p^3(^2_3D)\,^2D^\circ_{3/2}$	0.93	21 309	21 090.6	4.27e+01	4.28e+01
3	$3s^2\,3p^3(^2_3D)\,^2D^\circ_{5/2}$	0.94	21 433	21 219.8	5.13e+02	5.30e+02
4	$3s^2\,3p^3(^2_1P)\,^2P^\circ_{1/2}$	0.93	35 210	34 854.6	6.08e−01	6.09e−01
5	$3s^2\,3p^3(^2_1P)\,^2P^\circ_{3/2}$	0.92	35 372	35 032.4	2.73e−01	2.73e−01
6	$3s\,^2S\,3p^4(^3_2P)\,^4P_{5/2}$	$0.85 + 0.12\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	118 023	117 563.4	4.09e−09	3.80e−09
7	$3s\,^2S\,3p^4(^3_2P)\,^4P_{3/2}$	$0.84 + 0.12\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	118 971	118 515.7	4.02e−09	3.75e−09
8	$3s\,^2S\,3p^4(^3_2P)\,^4P_{1/2}$	$0.84 + 0.12\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P$	119 508	119 043.1	3.98e−09	3.71e−09
9	$3s\,^2S\,3p^4(^1_2D)\,^2D_{3/2}$	$0.70 + 0.21\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D + 0.03\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D$	146 525	145 921.2	2.17e−09	2.02e−09
10	$3s\,^2S\,3p^4(^1_2D)\,^2D_{5/2}$	$0.70 + 0.21\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D + 0.03\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D$	146 603	145 999.4	2.23e−09	2.07e−09
11	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P_{3/2}$	$0.55 + 0.32\ 3s\,^2S\,3p^4(^3_2P)\,^2P + 0.07\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P$	166 719	166 356.4	1.01e−09	9.54e−10
12	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P_{1/2}$	$0.55 + 0.32\ 3s\,^2S\,3p^4(^3_2P)\,^2P + 0.06\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P$	167 826	167 444.6	9.85e−10	9.27e−10
13	$3s\,^2S\,3p^4(^1_0S)\,^2S_{1/2}$	$0.72 + 0.23\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S$	178 782	177 832.5	6.65e−10	6.30e−10
14	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{3/2}$	0.95	180 820	180 682.5	4.56e−07	4.37e−07
15	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{5/2}$	0.94	181 169	181 031.8	6.05e−07	6.00e−07
16	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{7/2}$	0.94	181 686	181 533.3	1.07e−06	1.11e−06
17	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4F_{9/2}$	0.95	182 360	182 195.6	1.40e−01	1.36e−01
18	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{5/2}$	$0.38 + 0.30\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D + 0.26\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	187 234		1.91e−07	1.92e−07
19	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{1/2}$	0.94	187 477	187 290.4	1.54e−07	1.48e−07
20	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{7/2}$	$0.59 + 0.21\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	187 506	188 824.5	5.55e−05	4.31e−05
21	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{3/2}$	0.94	187 575	187 397.5	1.19e−07	1.17e−07
22	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D_{5/2}$	$0.64 + 0.18\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F + 0.13\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	188 019	187 821.3	1.18e−07	1.18e−07
23	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F_{7/2}$	$0.35 + 0.35\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4D + 0.24\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F$	189 057		7.89e−07	7.76e−07
24	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2G_{7/2}$	0.94	208 246	207 760.7	1.93e−07	1.94e−07
25	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2G_{9/2}$	0.94	208 374	207 859.3	1.26e−01	1.24e−01
26	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{5/2}$	$0.81 + 0.11\ 3s\,^2S\,3p^4(^3_2P)\,^4P$	221 139	220 786.8	3.07e−11	3.05e−11
27	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{3/2}$	$0.80 + 0.11\ 3s\,^2S\,3p^4(^3_2P)\,^4P$	221 654	221 300.9	3.05e−11	3.03e−11
28	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^4P_{1/2}$	$0.81 + 0.11\ 3s\,^2S\,3p^4(^3_2P)\,^4P$	222 001	221 627.4	3.03e−11	3.01e−11
29	$3s\,^2S\,3p^4(^3_2P)\,^2P_{3/2}$	$0.44 + 0.36\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P + 0.09\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P$	223 805	222 956.1	4.46e−11	4.36e−11
30	$3s\,^2S\,3p^4(^3_2P)\,^2P_{1/2}$	$0.43 + 0.41\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P + 0.08\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P$	224 891	224 019.3	4.41e−11	4.32e−11
31	$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{3/2}$	$0.46 + 0.41\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D + 0.02\ 3s\,^2S\,3p^4(^1_2D)\,^2D$	225 349		2.73e−10	2.69e−10
32	$3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D_{5/2}$	$0.47 + 0.42\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D + 0.03\ 3s\,^2S\,3p^4(^1_2D)\,^2D$	226 733		2.65e−10	2.61e−10
33	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D_{5/2}$	$0.64 + 0.16\ 3s\,^2S\,3p^4(^1_2D)\,^2D + 0.06\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D$	239 358	238 674	3.84e−11	3.80e−11
34	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D_{3/2}$	$0.65 + 0.17\ 3s\,^2S\,3p^4(^1_2D)\,^2D + 0.05\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D$	239 738	239 050	3.69e−11	3.65e−11
35	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P_{1/2}$	$0.44 + 0.30\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P + 0.15\ 3s\,^2S\,3p^4(^3_2P)\,^2P$	246 701		3.64e−11	3.59e−11
36	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2P_{3/2}$	$0.47 + 0.30\ 3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2P + 0.14\ 3s\,^2S\,3p^4(^3_2P)\,^2P$	247 150		3.66e−11	3.61e−11
37	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F_{5/2}$	$0.53 + 0.37\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F$	247 182	246 628	2.61e−11	2.61e−11
38	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2F_{7/2}$	$0.54 + 0.37\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2F$	247 316	246 737.6	2.61e−11	2.61e−11
39	$3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S_{1/2}$	$0.48 + 0.27\ 3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P + 0.14\ 3s\,^2S\,3p^4(^1_0S)\,^2S$	250 005		5.31e−11	5.26e−11
40	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{1/2}$	$0.66 + 0.20\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2S + 0.06\ 3s\,^2S\,3p^4(^1_0S)\,^2S$	250 061	250 215.2	1.14e−10	1.13e−10
41	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{3/2}$	0.92	250 721	250 902.16	4.87e−10	4.81e−10
42	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^4P_{5/2}$	0.93	251 782	251 967.35	4.85e−10	4.79e−10
43	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^2P_{1/2}$	0.91	255 973	256 087.8	1.19e−10	1.18e−10
44	$3s^2\,3p^2(^3_2P)\,^3P\,4s\,^2P_{3/2}$	0.91	257 213	257 343.58	1.17e−10	1.16e−10
45	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D_{5/2}$	$0.43 + 0.35\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.07\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D$	257 224		2.91e−11	2.90e−11
46	$3s^2\,3p^2(^3_2P)\,^3P\,3d\,^2D_{3/2}$	$0.43 + 0.37\ 3s^2\,3p^2(^1_0S)\,^1S\,3d\,^2D + 0.05\ 3s^2\,3p^2(^1_2D)\,^1D\,3d\,^2D$	257 667		2.93e−11	2.92e−11
47	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^6D^\circ_{3/2}$	0.98	259 721		1.72e−06	1.65e−06
48	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^6D^\circ_{1/2}$	0.98	259 730		1.47e−06	1.38e−06
49	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^6D^\circ_{5/2}$	0.98	259 731		2.42e−06	2.41e−06
50	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^6D^\circ_{7/2}$	0.98	259 755		4.51e−06	4.67e−06
51	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^6D^\circ_{9/2}$	0.98	259 799		1.12e−05	9.38e−06
52	$3s^2\,3p^2(^1_2D)\,^1D\,4s\,^2D_{5/2}$	$0.92 + 0.02\ 3s\,^2S\,3p^2(^3_2P)\,^2P\,3d\,^1D\,4s\,^2D$	267 750	267 741.3	2.31e−10	2.29e−10
53	$3s^2\,3p^2(^1_2D)\,^1D\,4s\,^2D_{3/2}$	$0.92 + 0.02\ 3s\,^2S\,3p^2(^3_2P)\,^2P\,3d\,^1D\,4s\,^2D$	267 774	267 762	2.29e−10	2.26e−10
54	$3p^5\,^2P^\circ_{3/2}$	$0.48 + 0.34\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^2P^\circ + 0.06\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^2P^\circ$	275 778		1.01e−09	9.51e−10
55	$3p^5\,^2P^\circ_{1/2}$	$0.47 + 0.35\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^2P^\circ + 0.06\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^2P^\circ$	277 251		1.04e−09	9.78e−10

Notes. Energy levels are given relative to the ground state. The states 57 and 58 are indicated in bold. The labels for these levels were not assigned with largest contribution to the composition.

Table A.3. continued.

56	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2S^\circ_{1/2}$	0.92	280 888		9.69e−10	9.64e−10
57	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ_{1/2}$	**0.24** + $0.45\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ + 0.20\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ$	283 959		1.17e−09	1.17e−09
58	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ_{3/2}$	**0.28** + $0.36\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ + 0.25\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ$	284 080		1.46e−09	1.47e−09
59	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ_{5/2}$	$0.33 + 0.31\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.23\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ$	284 232		2.15e−09	2.16e−09
60	$3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ_{7/2}$	$0.37 + 0.36\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ$	284 368		3.40e−09	3.39e−09
61	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{1/2}$	$0.47 + 0.25\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.18\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	286 149	285 956.2	9.93e−10	9.90e−10
62	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{3/2}$	$0.56 + 0.20\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.14\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	286 336	286 224.5	8.45e−10	8.43e−10
63	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{5/2}$	$0.68 + 0.14\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.08\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	286 778	286 747.8	7.14e−10	7.14e−10
64	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4D^\circ_{7/2}$	$0.79 + 0.09\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.04\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	287 525	287 550.8	6.38e−10	6.38e−10
65	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{1/2}$	0.92	289 025	289 122.3	5.42e−10	5.43e−10
66	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{3/2}$	$0.80 + 0.06\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ + 0.04\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4S^\circ$	289 132	289 233.9	5.58e−10	5.58e−10
67	$3s^2\,3p^2(^1_0S)\,^1S\,4s\,^2S_{1/2}$	$0.90 + 0.03\ 3p^4(^1_0S)\,^1S\,4s\,^2S$	289 489		2.27e−10	2.25e−10
68	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ_{5/2}$	$0.78 + 0.10\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ + 0.04\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ$	289 727	289 830.5	5.70e−10	5.70e−10
69	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ_{3/2}$	$0.68 + 0.17\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ + 0.07\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ$	290 224	290 251.5	8.10e−10	8.02e−10
70	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ_{3/2}$	$0.70 + 0.15\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ + 0.11\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4F^\circ$	291 322		5.69e−09	5.36e−09
71	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ_{5/2}$	$0.69 + 0.14\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ + 0.11\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4F^\circ$	291 519		5.02e−09	4.76e−09
72	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ_{5/2}$	$0.62 + 0.14\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ$	291 628	291 663.1	7.95e−10	7.88e−10
73	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4S^\circ_{3/2}$	$0.86 + 0.05\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^4P^\circ + 0.02\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,4s\,^4S^\circ$	291 667	291 744	5.64e−10	5.60e−10
74	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ_{7/2}$	$0.71 + 0.14\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ + 0.11\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4F^\circ$	291 804		5.87e−09	5.52e−09
75	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ_{9/2}$	$0.72 + 0.14\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ + 0.11\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4F^\circ$	292 173		6.02e−09	5.66e−09
76	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ_{1/2}$	$0.75 + 0.14\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ + 0.02\ 3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ$	295 743	295 670.2	6.98e−10	6.89e−10
77	$3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ_{3/2}$	$0.73 + 0.17\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ$	295 849	295 802.2	7.03e−10	6.94e−10
78	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2F^\circ_{5/2}$	$0.91 + 0.02\ 3s\,^2S\,3p^2(^3_2P)\,^2P\,3d\,^1D\,4p\,^2F^\circ$	303 802	303 665.4	6.34e−10	6.32e−10
79	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2F^\circ_{7/2}$	$0.92 + 0.02\ 3s\,^2S\,3p^2(^3_2P)\,^2P\,3d\,^1D\,4p\,^2F^\circ$	304 125	303 989.1	6.29e−10	6.28e−10
80	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^2S^\circ_{1/2}$	$0.61 + 0.18\ 3s^2\,3p\,^2P\,3d^2(^3_2P)\,^2S^\circ + 0.17\ 3s\,^2S\,3p^3(^2_3D)\,^1D\,3d\,^2S^\circ$	304 259		2.52e−09	2.40e−09
81	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ_{5/2}$	$0.71 + 0.18\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ$	306 032	305 827.4	7.72e−10	7.52e−10
82	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2D^\circ_{3/2}$	$0.72 + 0.17\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2D^\circ$	306 112	305 899.6	7.65e−10	7.46e−10
83	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4G^\circ_{5/2}$	$0.88 + 0.07\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4G^\circ$	306 552		2.17e−09	2.04e−09
84	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4G^\circ_{7/2}$	$0.88 + 0.07\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4G^\circ$	306 623		2.19e−09	2.06e−09
85	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4G^\circ_{9/2}$	$0.88 + 0.07\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4G^\circ$	306 732		2.21e−09	2.08e−09
86	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4G^\circ_{11/2}$	$0.88 + 0.07\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^4G^\circ$	306 871		2.23e−09	2.09e−09
87	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{1/2}$	$0.76 + 0.14\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ$	312 019		4.92e−10	4.85e−10
88	$3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ_{3/2}$	$0.71 + 0.17\ 3s^2\,3p^2(^3_2P)\,^3P\,4p\,^2P^\circ$	312 497		4.95e−10	4.88e−10
89	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^2G^\circ_{7/2}$	$0.80 + 0.15\ 3s^2\,3p\,^2P\,3d^2(^1_2G)\,^2G^\circ$	317 986		5.06e−09	4.74e−09
90	$3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^2G^\circ_{9/2}$	$0.80 + 0.14\ 3s^2\,3p\,^2P\,3d^2(^1_2G)\,^2G^\circ$	318 047		5.29e−09	4.93e−09
91	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4D^\circ_{1/2}$	$0.37 + 0.30\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.18\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	324 720		3.76e−10	3.72e−10
92	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4D^\circ_{3/2}$	$0.35 + 0.29\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.18\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	324 958		3.72e−10	3.68e−10
93	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4D^\circ_{5/2}$	$0.33 + 0.28\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.17\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	325 417		3.66e−10	3.61e−10
94	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4P^\circ_{1/2}$	$0.73 + 0.12\ 3s^2\,3p\,^2P\,3d^2(^3_2P)\,^4P^\circ + 0.11\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4P^\circ$	326 067		7.89e−10	7.72e−10
95	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4D^\circ_{7/2}$	$0.36 + 0.30\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4D^\circ + 0.19\ 3s\,^2S\,3p^3(^4_3S)\,^5S\,3d\,^4D^\circ$	326 249		3.40e−10	3.36e−10
96	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4P^\circ_{3/2}$	$0.69 + 0.11\ 3s^2\,3p\,^2P\,3d^2(^3_2P)\,^4P^\circ + 0.08\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4P^\circ$	326 277		5.84e−10	5.73e−10
97	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4P^\circ_{5/2}$	$0.48 + 0.14\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^2D^\circ + 0.08\ 3s^2\,3p\,^2P\,3d^2(^3_2P)\,^4P^\circ$	326 678		5.25e−10	5.16e−10
98	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^2D^\circ_{3/2}$	$0.41 + 0.13\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^2D^\circ + 0.11\ 3s\,^2S\,3p^3(^2_3D)\,^1D\,3d\,^2D^\circ$	326 881		7.97e−10	7.78e−10
99	$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{1/2}$	$0.87 + 0.03\ 3p^4(^1_0S)\,^1S\,4p\,^2P^\circ$	327 235		6.24e−10	6.21e−10
100	$3s^2\,3p^2(^1_0S)\,^1S\,4p\,^2P^\circ_{3/2}$	$0.87 + 0.03\ 3p^4(^1_0S)\,^1S\,4p\,^2P^\circ + 0.02\ 3s^2\,3p^2(^1_2D)\,^1D\,4p\,^2P^\circ$	327 351		6.18e−10	6.14e−10
101	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^2D^\circ_{5/2}$	$0.30 + 0.28\ 3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4P^\circ + 0.09\ 3s^2\,3p\,^2P\,3d^2(^3_2F)\,^2D^\circ$	327 371		5.88e−10	5.76e−10
102	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ_{9/2}$	$0.77 + 0.15\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4F^\circ$	329 302		7.89e−10	7.52e−10
103	$3s\,^2S\,3p^3(^2_1P)\,^3P\,3d\,^4F^\circ_{7/2}$	$0.76 + 0.16\ 3s\,^2S\,3p^3(^2_3D)\,^3D\,3d\,^4F^\circ + 0.03\ 3s^2\,3p^2(^3_2P)\,^3P\,4f\,^4F^\circ$	329 535		7.53e−10	7.19e−10