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RELATIVISTIC MR-MP ENERGY LEVELS FOR L-SHELL IONS OF SULFUR AND ARGON

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Abstract

Calculated level energies for valence and K-vacancy states are provided for the ion series S VII - S XIV and Ar IX - Ar XVI. The calculations were performed with the relativistic Multi-Reference Møller-Plesset Perturbation Theory method (MR-MP). The data set includes all the level energies with configurations $1s^2 2(s, p)^q$, $1s^2 2(s, p)^{q-1} nl$, $1s^1 2(s, p)^{q+1}$, $1s^1 2(s, p)^q nl$, $2(s, p)^{q+2}$ and $2(s, p)^{q+1} nl$, where $1 \leq q \leq 8$, $n \leq 5$ and $l \leq 3$. We have compared our results with data from the National Institute of Standards and Technology (NIST) on-line database and with previous calculations. The average deviation of valence level energies ranges from 0.16 eV in Ne-like ions to 0.01 eV in Li-like ions, showing that the present MR-MP valence level energies are highly accurate. In the case of K-vacancy states, the deviation is generally below 0.3 eV for Li-like S XIV and Ar XVI. The deviation for K-vacancy energies in other L-shell ions (Be-, B-, C-, N- and O-like Ar ions) is higher but likely because the NIST-recommended values have a higher uncertainty. The data set includes many $n = 4$ and $n = 5$ valence and K-vacancy levels in L-shell ions of S and Ar not previously reported. The data can be used for line identification and modeling of L-shell ions of S and Ar in astrophysical and laboratory-generated plasmas, and as energy references in the absence of more accurate laboratory measurements.

Keywords

atomic data; line: identification

1. INTRODUCTION

L-shell ions of Sulfur and Argon play an important role in the study of astrophysical objects. L-shell ions of S have been observed in the spectra of astrophysical objects such as the stellar coronae of Capella (Audard et al. 2001) and Procyon (Raassen et al. 2002; Li et al. 2013), AGNs MCG-6–30–15 (Lee et al. 2001), IRAS 13349+2438 (Holczer et al. 2007) and NGC 3783 (Kaspi et al. 2007), the high-mass X-ray binaries 4U1700–37 (Boroson et al. 2003), Vela X-1 (Watanabe et al. 2006), and Cygnus X-1 (Chang & Cui 2007). L- and K-shell ions of S and Si have been used to establish the nature of stellar wind in Cygnus X-1 (Hell et al. 2013; Miškovičová et al. 2016). The lines of S ions are also valuable tools for analysis of observational data (Keenan et al. 2000, 2002, 2004; Lepson et al. 2005). Moreover, weak lines coming from S ions could be useful for a more accurate and complete description of the 211.3 Å Fe XIV channel of the Atmospheric Imaging Assembly on the *Solar Dynamics Observatory* (Beiersdorfer et al. 2014).

Laboratory measurements and calculations have been carried out throughout several decades to establish the atomic data (level energies, wavelengths, radiative rates, Auger rates, electron impact excitation collision strengths, etc.) of L-shell ions of S needed for the modeling of astrophysical systems. Multiple spectroscopic techniques have been used, including measurements with the beam-foil technique (Langenberg et al. 1980; Yang et al. 1980, 2009), lasers (Fawcett et al. 1970; Fawcett & Hayes 1973, 1987; Faenov et al. 1994), heavy-ion storage rings (Schippers et al. 2012) and electron beam ion traps (EBIT) (Lepson & Beiersdorfer 2005; Beiersdorfer et al. 2014; Hell et al. 2016; Beiersdorfer et al. 2017). On the theoretical/computational side, a large body of work has been performed, from systematic calculations of L-shell ions of S (Bhatia & Landi 2003a,b; Karpuškiene et al. 2005; Landi & Bathia 2008; Palmeri et al. 2008; Luna et al. 2009; Martins et al. 2009; Fan et al. 2009; Liang et al. 2011; Pagan et al. 2011; Elabidi et al. 2012; Li et al. 2013; Hell et al. 2016) to isoelectronic sequence of various L-shell ions (Witthoeft et al. 2007; Jönsson et al. 2011; Liang et al. 2012; Rynkunb et al. 2012; Jönsson et al. 2014; Rynkunb et al. 2014; Nazé et al. 2014; Wang et al. 2014, 2015, 2017); see Fan et al. (2009) and references therein for a short account of other calculations.

Spectral lines from L-shell ions of Ar have also been observed in Procyon (Raassen et al. 2002) and sunspots during a flare (Doschek & Warren 2016). Lines from L-shell ions of Ar are also used for plasma diagnostics (Dere et al. 2001; Landi et al. 2001; Widing & Feldman 2008). Similar to L-shell ions of S, multiple laboratory measurements have been carried out to provide atomic data for highly charged Ar, e.g. EBIT measurements (Träbert et al. 2000; Lepson et al. 2003; Träbert et al. 2005; Beiersdorfer et al. 2014). Calculations have been performed as well, including targeted calculations of selected ions of Ar (McKeown et al. 2004; Eissner et al. 2005; Landi & Bathia 2006; Cheng et al. 2006; Liang et al. 2006; Bhatia & Landi 2008; Ekman et al. 2014), systematic calculations of L-shell ions of Ar (Natarajan & Mulye 2001; Natarajan 2002, 2003; Liang et al. 2004; Mulye & Natarajan 2004; Aggarwal et al. 2005; Palmeri et al. 2008; Ludlow et al. 2010; Bilal et al. 2018) and isoelectronic sequence of various L-shell ions (Witthoeft et al. 2007; Liang et al. 2010; Jönsson et al. 2011; Rynkunb et al. 2012; Jönsson et al. 2014; Rynkunb et al. 2014; Nazé et al. 2014; Wang et al. 2014; Ekman et al. 2014; Wang et al. 2015, 2016, 2017).

A sizable portion of the atomic data generated for L-shell ions of S and Ar has been included in atomic databases like AtomDB (Foster et al. 2017), CHIANTI (Dere et al. 1997; Del Zanna et al. 2015) and the National Institute of Standards and Technology (NIST) on-line database (Kramida et al. 2015). For few-electron systems (H-, He- and Li-like S and Ar) there are data for many transitions, including K-vacancy levels. In the case of multielectron L-shell ions, Be- to Ne-like S and Ar, the data are limited, and the accuracy is often too poor for astrophysical plasma diagnostics (Hell et al. 2016) and laboratory line identification (Lepson et al. 2003; Träbert et al. 2005; Beiersdorfer et al. 2014). The data are particularly limited for K-vacancy levels of multielectron L-shell ions (Hell et al. 2016).

The proper interpretation of astrophysical and laboratory data requires commensurately highly accurate calculations. This is a complex task in the case of multielectron L-shell ions. The complexity comes from the need to fully incorporate electron dynamics, relativistic effects, and quantum electrodynamic effects. Most multiconfiguration Dirac-Fock (MCDF) and configuration interaction (CI) electronic structure methods are fully relativistic and correct for quantum electrodynamic effects. However, they typically fail to properly account for all electron dynamics in multielectron ions because of the rather large configuration expansion required and the associated computational cost. The computational cost can be reduced by including the dominant configurations, but such truncated expansions typically fail to accurately describe core-valence and core-core correlations. The limitations of the MCDF and CI methods can be mitigated by combining CI with Many-Body Perturbation Theory techniques (MBPT) (Dzuba et al. 1996; Vilkas et al. 1999; Gu 2005; Gu et al. 2006; Vilkas & Ishikawa 2005, 2007; Safronova et al. 2009). The CI+MBPT methods accurately account for the core-valence and core-core correlations that are missing in the MCDF and CI methods.

One of the combined methods is the Multi-Reference Møller-Plesset (MR-MP) method developed by Ishikawa (Ishikawa et al. 1991; Vilkas et al. 1999; Vilkas & Ishikawa 2005, 2007). The MR-MP method has been shown to yield highly accurate valence level energies (Vilkas et al. 2005; Santana et al. 2009; Santana & Träbert 2015; Santana 2016) as well as core-excited level energies (Beiersdorfer et al. 2013; Díaz et al. 2013; Beiersdorfer et al. 2017). We recently applied (Santana et al. 2018) this method to calculate both valence and K-vacancy level energies in L-shell ions Si V - Si XII. We compared the calculated level energies with the recommended data listed in NIST on-line database. The absolute deviation of valence level energies ranges from 0.20 eV in Si V to 0.04 eV in Si XII. For K-vacancy levels, the average energy deviation was below 0.3 eV in Si XII and Si XIII, which are the only L-shell ions of Si with recommended K-vacancy level energies in NIST on-line database. These calculations show that the MR-MP method yields highly accurate valence as well as K-vacancy level energies for L-shell ions, providing level energies that can be used as reference values for astrophysical plasma diagnostics, line identification and to confirm level designations.

In the present work, we extend our earlier calculations of Si to the L-shell ions of S and Ar. The computational methods are briefly described in Sec. 2. The results are discussed in Sec. 3, where we compare our calculated level energies with the recommended values listed in the NIST on-line database and perform a statistical analysis to identify potential outlier level

energies in our data set. The potential outlier level energies are then compared with previous theoretical values. We conclude in Sec. 4 with a summary.

2. COMPUTATIONAL METHODS

In the relativistic MR-MP method, the large and small radial components of the bound Dirac spinors are expanded in sets of even-tempered Gaussian-type functions (Ishikawa et al. 1991). The basis sets used were $34s32p30d28f$ Gaussian (G) spinors for angular momentum values up to $L = 3$, 26 G spinors for $L = 4-5$, and 15 G spinors for $L = 6-11$. The basis exponents $\{\zeta_i = \alpha\beta^{i-1}; i = 1, 2, \dots, N_k\}$ are defined by the parameters α and β . The value of β was set to 2.1 and α was set to 0.000770 for S and 0.001240 for Ar. These α -values were chosen such that the maximum exponent of the $34s$ set equals $9.89 \times 10^{10} \left(\frac{Z}{118}\right)^4$ for $\beta = 2.1$.

We arrived at such empirical expression in our previous work (Santana 2016), where we found that an earlier expression from Ishikawa et al. (1997) for α was inadequate at high Z values. From comparisons of calculated and experimental data for $Z = 26$ (Santana et al. 2010) and $Z = 78$ (Santana & Ishikawa 2014), we postulated the new expression (see Santana (2016) for details). Note that our expression for α was not fitted to get better agreement to the NIST level energies of L-shell ions. We have employed the expression for ions in the Mg-isoelectronic sequence (Santana & Träbert 2015; Santana 2016) and L-shell ions of Si (Santana et al. 2018), yielding accurate results in both cases.

In the MR-MP method (Vilkas et al. 1999; Vilkas & Ishikawa 2005), a single set of core and valence spinors in the V^N potential is initially obtained with a state-averaged MCDF for the ground and low lying excited states of the ions. In the present work, we averaged the energies of even- and odd-parity states arising from the nonrelativistic configurations $1s^2(s, p)^q$ and $1s^2(s, p)^{q-1}nl$, where $1 \leq q \leq 8$ and $(n \leq 5 \text{ and } l \leq 3)$. The set of spinors was employed to perform Multi-Reference Configuration Interaction (MR-CI) calculations, including all relativistic configurations arising from the following nonrelativistic configurations: $1s^2(s, p)^q$, $1s^2(s, p)^{q-1}nl$, $1s^12(s, p)^{q+1}$, $1s^12(s, p)^qnl$, $2(s, p)^{q+2}$ and $2(s, p)^{q+1}nl$. After the MR-CI calculations, the CI wavefunction was used as the based for state-specific MR-MP second order perturbation theory calculations, where all electrons were included to accurately account for relativity and electron correlation effects. Radiative corrections, or the lowest-order quantum electrodynamical (QED) effects, were estimated by evaluating (Indelicato et al. 1987) the electron self-energy and vacuum polarization for each state.

3. RESULTS AND DISCUSSION

The calculated level energies are given in Tables 1 and 2 for the L-shell ions of S and Ar, respectively. We assessed the accuracy of the calculated energies by comparing our results with values listed in the NIST on-line database (Kramida et al. 2015). To compare NIST and MR-MP levels, the NIST levels were matched with MR-MP levels by comparing three identifiers: *i)* total angular momentum J , *ii)* parity and *iii)* principal nonrelativistic configuration. In cases where the identifiers are not unique, the NIST level is assigned to the MR-MP level with the closest energy. In general, the comparison between NIST and MR-

MP levels is not trivial because it requires to transform from the jj -coupling into the LS -coupling scheme. However, a formal mapping between the two scheme is complex and it has not been implemented in the MR-MP code. It is also possible to use radiative rates and other properties (e.g. Land g factors, etc) for a better level matching but such properties are outside the scope of the present work. The MR-MP method typically yield level energies in good agreement with the NIST-recommended values and we expect our method to compare NIST and MR-MP levels to be sufficient for the present work. The NIST database lists some valence level energies for all L-shell ions of S and Ar. For K-vacancy level energies, there are NIST-recommended values for S XIV and Ar XVI to Ar XI. We start our discussion with a statistical analysis of the deviation between NIST and MR-MP calculated valence level energies. Such a statistical analysis allows us to quantify systematic errors in the MR-MP data set and to identify potential outlier level energies. Afterward, we focus on the potential outliers, comparing their MR-MP values with previous calculations. We end this section discussing our results for K-vacancy level energies.

3.1. Basic statistics of the deviation between MR-MP and NIST valence level energies

Figure 1 shows the distribution of the deviation between MR-MP valence level energies and the recommended values in the NIST on-line database. For completeness, we have included in Figure 1 the results for the L-shell ions of Si that were previously reported (Santana et al. 2018). The sample size in Figure 1 is $N = 1078$. The deviation data was tested to explore if it follows a normal distribution. A Shapiro-Wilk normality test was performed. At a significance level of $\alpha = 1\%$, the deviation data is not normally distributed (P-value is much less than 0.01). The distribution for the deviation is approximately symmetric, slightly left skewed (skewness value -0.28 with 95 % confidence interval $[-0.42, -0.13]$). Another characteristic of the deviation data distribution is that it is heavy tailed (kurtosis value 43.04), an indication of the presence of outliers. We proceed to detect outliers via informal tests based on boxplot methods. The results of outlier detection can change depending on the outlier detection methods. A method commonly used to detect outliers is the boxplot method of Tukey (1977). Three features makes this method attractive and applicable to our case: it does not require a prior (specific) distributional assumption, it is applicable for approximately symmetric data to skewed data and its quartiles are resistant to extreme values (does not depend on sample mean and variance). Following the method of Tukey (1977), the inner fences, where the possible outliers are located, are estimated at $[-0.65, -0.40]$ and $[0.26, 0.51]$. Deviation values below -0.65 eV or above 0.51 eV (outer fences) are labeled as probable outliers. For skewed data the adjusted boxplot method is suggested (Huberta & Vandervierenb 2008). The adjusted boxplot analysis yield the lower and upper bound at -0.33 eV and 0.34 eV, respectively. The adjusted boxplot method is a more robust method to detect outliers in skewed data. We rounded the lower and upper bounds to -0.3 and 0.3 eV, respectively. Level energies with absolute deviations between 0.3 eV and 0.5 eV were marked as possible outliers and those with absolute deviations outside 0.5 eV were marked as probable outliers.

3.2. Valence level energies: $1s^2 2(s, p)^q$ and $1s^2 2(s, p)^{q-1} nl$

Figure 2 shows box-and-whisker plots for the absolute deviation between MR-MP valence level energies and the values listed in the NIST database for L-shell ions of S and Ar. In the

plot, the lower and upper quartiles are the end of the box, the vertical line inside the box is the median, and the two lines outside the box indicate the highest and lowest absolute deviation. Note that the results in Figure 2 do not include the potential outlier valence level energies, levels with an absolute deviations higher than 0.3 eV. Excluding the potential outliers, the median of the absolute deviation is below 0.16 eV for all ions. The median generally increases with the number of electrons, going from 0.01 eV in Li-like to 0.16 eV in Ne-like ions, which is the expected behavior due to the higher complexity in the less ionized systems. The results for the L-shell ions of S and Ar are in line with our previous results for L-shell ions of Si (Santana et al. 2018), where the median of the absolute deviation was below 0.25 eV. We now turn to discuss the potential outliers.

3.2.1. Potential outlier level energies—We have divided the potential outlier level energies into two groups, those with an absolute deviation above 0.5 eV and those with an absolute deviation between 0.3 and 0.5 eV. The level energies with absolute deviations above 0.5 eV for L-shell ions of S and Ar are listed in Tables 3 and 4, respectively. For the ions of S, there are 13 level energies with deviation higher than 0.5 eV: 4 levels for S XIII, and 3 levels each for S XII, S XI and S X. In the case of the ions of Ar, we found 33 levels with a significant deviation: 2 levels for Ar XIV, 4 levels each for Ar XIII and Ar XII, 6 levels for Ar XI, 5 levels for Ar X and 12 levels for Ar IX. We note that the entries in the NIST database for most of the states in the ions of S in Table 3 indicate that the levels may not be real. Generally, we note that the MR-MP results are highly accurate. Only a small fraction (52/1078) of level energies in L-shell ions of Si (Santana et al. 2018), S and Ar show a significant deviation (> 0.5 eV) from the NIST-recommended values. Deviations above 0.5 eV likely come from misassignment or uncertainties in the values listed in the NIST database.

As pointed out in Sec. 1, there is a large number of previous reports on the level energies of L-shell ions of S and Ar. If the uncertainty in the values listed in the NIST database is causing the large deviation for the states in Tables 3 and 4, previous calculations should also show a significant deviation for those states. Such analysis is worth performing only for highly accurate calculations. Many previous calculations were focused on providing collisional data and the atomic structure was evaluated with CI-based methods (Bhatia & Landi 2003a,b; Witthoef et al. 2007; Landi & Bathia 2008; Ludlow et al. 2010; Liang et al. 2010, 2011, 2012; Elabidi et al. 2012). A large portion of such calculations has been collected in the CHIANTI v8 database (Dere et al. 1997; Del Zanna et al. 2015). We compared the calculated level energies collected in the CHIANTI v8 database with the NIST-recommended values (Kramida et al. 2015) to estimate the accuracy of available CI-based results. Table 5 include the average absolute deviation (eV) between calculated valence level energies and the recommended values in the NIST database for the L-shell ions in Tables 3 and 4. Only NIST level energies present in both the MR-MP calculations and the CHIANTI v8 database were considered in the evaluation of the average deviations listed in Table 5. The MR-MP average deviations given in Table 5 can be higher than the medians shown in Figure 2 because the averages in Table 5 include the outliers. In general, the average absolute deviation of the levels in the CHIANTI v8 database is at least 0.5 eV for the L-shell ions of S and Ar, and as high as 1.06 eV for Ar X. By contrast, the maximum

average absolute deviation in the case of our MR-MP is 0.33 eV and the deviation for most ions are between 0.1 and 0.2 eV. The expected uncertainty in CI-based results is, therefore, too high to be used to identify misassignment in the NIST database.

In addition to CI-based calculations, there are multiple calculations based on the multiconfiguration Dirac-Hartree-Fock (MCDHF) method combined with relativistic CI (RCI) calculations (Jönsson et al. 2011; Rynkunb et al. 2012; Jönsson et al. 2014; Rynkunb et al. 2014). However, such calculations do not include the states in Tables 3 and 4 because the focus was mainly on the $n = 2$ states. The work of Ekman et al. (2014), which employed the same MCDHF+RCI method, included the states of interest in the present work for Ar XIII. Furthermore, there is a small number of calculations with the combined CI+MBPT methods. Of particular interest are the recent works of Wang et al. (2014, 2015, 2016). Wang et al. used the CI+MBPT method implemented in the Flexible Atomic Code (FAC) (Gu 2005; Gu et al. 2006) to calculate level energies and transition properties in Be-like (Wang et al. 2015), C-like (Wang et al. 2014) and N-like (Wang et al. 2016) ions. Results from these recent calculations have been shown to have a lower uncertainty than the CI-base results; see Wang et al. (2014, 2015, 2016) and Ekman et al. (2014) for detailed comparisons between the multiple calculations. Below we compare our results for the states in Tables 3 and 4 with the set of accurate calculations mentioned above.

For the levels in Be-like S XIII, the MR-MP and CI+MBPT (Wang et al. 2015) methods yield energy values within 0.04 eV for the states $2p3d^1P^0_1$, $2p4p^3D_3$, $2p4d^3F^0_3$ and $2s5d^3D_3$. In the case of C-like S XI, Wang et al. (2014) did not include $2s2p^23I$ levels. For C-like Ar XIII, Wang et al. (2014) reported values of 143.97 and 424.58 eV for the states $2p^4^1S_0$ and $2s^22p3d^3D^0_3$, respectively. MR-MP and CI+MBPT differ for the state $2p^4^1S_0$; the source of the discrepancy is unclear. We include in Table 6 MR-MP energies for the state $2p^4^1S_0$ in C-like ions with low- and mid- Z values. Excluding C-like Ar XIII, the deviation from the NIST-recommended values decreases smoothly with increasing atomic number Z . These results suggest that the NIST-recommended energy value for the state $2p^4^1S_0$ in Ar XIII should be slightly higher, by ~ 0.3 eV. Table 6 shows that CI+MBPT yield accurate results but the deviations do not decrease systematically with increasing atomic number Z . Ekman et al. (2014) also reported accurate energies for C-like ions. Excluding the state $2s^22p4d^3D^0_1$, the MR-MP energies and those of Ekman et al. (2014) are within 0.2 eV for the states of C-like Ar XIII in Table 4. Ekman et al. (2014) found an energy of 539.39 eV for $2s^22p4d^3D^0_1$, while our result is 539.06 eV. The other ion with available accurately calculated level energies is N-like Ar XII. Wang et al. (2016) reported energy values of 376.26, 385.48, 387.45, 388.65 and 399.25 eV for the states $2s^22p^2(^3P)3p^4S^o_{3/2}$, $2s^22p^2(^1D)3p^2D^o_{5/2}$, $2s^22p^2(^1D)3p^2P^o_{1/2}$, respectively. Overall, previous $2s^22p^2(^1D)3p^2P^o_{3/2}$ and $2s^22p^2(^3P)3d^2D_{5/2}$ accurate calculations also show a significant deviation for states in Tables 3 and 4.

Tables 7 and 8 show the level energies with deviations between 0.3 and 0.5 eV. The source of the deviation for these level energies can be a combination of the uncertainties in the values listed in the NIST database and limitations of the MR-MP method to fully treat

electron correlation effects. Electron correlation effects play a major role in low- Z ions and decrease with increasing Z (Vilkas et al. 1999). We can use this trend to get an idea of how much correlation is missing in the MR-MP calculations; MR-MP results follow the trend very closely, see Table 6; also see Table 5 in our previous work (Santana et al. 2018). For C- and O-like ions with $Z < 10$, the MR-MP method yields deviations over 0.5 eV, while for ions with $Z > 18$, the deviation is of the order of 0.1 eV. In the case of $Z = 12 - 18$, the deviation ranges from 0.5 to 0.2 eV. Correlation effects are not uniform across the different states in a given ion, but our analysis shows the magnitude of missing correlations effects in our MR-MP results for the L-shell ions of S and Ar. We now discuss the MR-MP results for K-vacancy level energies in L-shell ions of S and Ar.

3.3. K-vacancy level energies: $1s^12(s, p)^{q+1}$ and $1s^12(s, p)^{q+1}nl$

The most complete data set of K-vacancy level energies in the NIST database is available for Li-like S XIV and Ar XVI. Tables 9 and 10 show the K-vacancy level energies in the NIST database that were matched with our MR-MP results. The recommended energy values in the NIST database for Li-like S XIV and Ar XVI are compared with our MR-MP results in Figure 3. We also included in our comparison previous CI-based calculations (Palmeri et al. 2008; Hell et al. 2016) as well as the level energies collected in the CHIANTI v8 database (Dere et al. 1997; Del Zanna et al. 2015). The deviations for these previous calculations are scattered and over 0.5 eV for many levels, including the $1s^2(s, p)^2$ levels. Our MR-MP calculations agree better with the NIST-recommended K-vacancy level energies. The deviation for MR-MP is uniformly below 0.3 eV for the $1s^2(s, p)^2$ levels. For the $1s^12(s, p)^1n/l$ levels, the MR-MP deviation is higher but below 0.7 eV for the majority of states. For some states, the MR-MP deviation is large, 1 eV or higher. Such a large deviation is likely the result of a misassignment. For instance, the states $1s2s(^1S)3d^2D_{3/2}$ and $1s2s(^1S)3d^2D_{5/2}$ in Li-like S XIV have the same energy 2853.61 eV in the NIST database, which is highly unlikely. Similarly, the states $1s2p(^1P^o)3p^2D_{3/2}$ and $1s2p(^1P^o)3p^2P_{1/2}$ are listed with the same energy of 2863.47 eV. The MR-MP method reproduces the NIST-recommended values of K-vacancy level energies for Li-like S XIV and Ar XVI much better than the previous calculations. However, there are correlation effects missing in our MR-MP calculations as shown above for valence level energies. For K-vacancy level energies, correlation effects are expected to be even more significant as these levels are autoionizing. We will explore such correlation effects in the K-vacancy level energies for ions in isoelectronic sequences of Li and Be in future works.

The NIST database also includes K-vacancy level energies for other L-shell ions of Ar. We include in Table 11 the available data for Ar XV to Ar XI with the corresponding MR-MP results. Only $1s^12(s, p)^{q+1}$ level energies are available. We show the deviation of MR-MP from the NIST-recommended values in Figure 4. We include in our comparison previous calculations of $1s^12(s, p)^{q+1}$ level energies in L-shell ions of Ar from Palmeri et al. (2008) and Safronova & Shlyaptseva (1996, 1999). The MR-MP results are closer to the NIST-recommended values than the other calculations, but the overall agreement is poor. Some level energies have been likely misidentified. For instance, all calculations yield deviations over 2 eV for the states $1s2s(^3S)2p^2(^1D) ^3D_2$ in Be-like Ar XV, $1s2s(^3S)2p^4(^3P) ^3P$ in C-like

Ar XIII, and the states $1s2s(^3S)2p^5\ ^4P^o_{3/2}$ and $1s2s(^3S)2p^5\ ^2P^o_{1/2}$ in N-like Ar XII. The poor agreement between calculated K-vacancy level energies and the values recommended in the NIST database stress the need for more measurements.

4. SUMMARY

In the present work, we have calculated valence and K-vacancy level energies of L-shell ions (Li-like to Ne-like) of S and Ar with the Multi-Reference Møller-Plesset method. The calculated energies are highly accurate and can be used to identify level energies with large uncertainty in the NIST database. The average deviation from available measurements is below 0.3 eV for valence level energies. For K-vacancy level energies, the deviation is generally below 0.3 eV for Li-like S XIV and Ar XVI. In the case of K-vacancy states in L-shell ions such as Be-, B-, C-, N- and O-like Ar ions, the deviations can be higher than 2 eV, suggesting that the NIST-recommended level energy values for such states have large uncertainties. More accurate measurements are needed, particularly for K-vacancy level energies. The data set we have presented will be useful for line identification and for confirming level designations, as well as for providing reference values for astrophysical analyses.

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Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

Histogram ($N=1078$) and box-and-whisker plots for the deviation between MR-MP valence level energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for L-shell ions of Si, S and Ar. The results for the L-shell ions of Si were previously reported (Santana et al. 2018) and included here for completeness. The annotations show the statistical parameters determined using the method of Huberta & Vandervierenb (2008).

Figure 2.

Box-and-whisker plots for the absolute deviation between MR-MP valence level energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for the L-shell ions of (a) S and (b) Ar. The number of level energies included in the statistical analysis is given above each box.

Figure 3.

Deviation between MR-MP energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for K-vacancy states in (a) S XIV and (b) Ar XVI. The x -axis corresponds to the index of each level in Tables 9 and 10. Previous calculations are also included for comparison: HFR (Palmeri et al. 2008), FAC (Hell et al. 2016) and AUTOSTRUCTURE as included in the CHIANTI v8 data base (Dere et al. 1997; Del Zanna et al. 2015).

Figure 4.

Deviation between calculated level energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for K-vacancy states in Ar XV to Ar XI. The levels are listed in the x -axis in the same order as they appear in Tables 11 for each ion. Panels a, b and c show results for calculations with the MR-MP, HFR (Palmeri et al. 2008) and Z-expansion (Safronova & Shlyaptseva 1996, 1999) methods, respectively

Table 1.

Valence Level Energies in L-shell Ions of S Evaluated with the MR-MP Method.

<i>N</i>	Index	Configuration ^{<i>a</i>, <i>b</i>}	<i>J</i>	Parity	Energy (eV)
3	1	1s22s	1/2	even	0.00
3	2	1s22p−	1/2	odd	27.82
3	3	1s22p+	3/2	odd	29.69
3	4	1s23s	1/2	even	399.22
3	5	1s23p−	1/2	odd	406.90
3	6	1s23p+	3/2	odd	407.45
3	7	1s23d−	3/2	even	410.31
3	8	1s23d+	5/2	even	410.48
3	9	1s24s	1/2	even	535.56
3	10	1s24p−	1/2	odd	538.71
3	11	1s24p+	3/2	odd	538.95
3	12	1s24d−	3/2	even	540.14
3	13	1s24d+	5/2	even	540.21
3	14	1s24f−	5/2	odd	540.27
3	15	1s24f+	7/2	odd	540.30
3	16	1s25s	1/2	even	597.97
3	17	1s25p−	1/2	odd	599.51
3	18	1s25p+	3/2	odd	599.63
3	19	1s25d−	3/2	even	600.27
3	20	1s25d+	5/2	even	600.31
3	21	1s25f−	5/2	odd	600.32
3	22	1s25f+	7/2	odd	600.34

Note—Note that only 22 levels arising from the $1s^2nl$ ($n < 6$ and $l < 3$) configurations in S XIV ($N = 3$) are shown here.

^{*a*} s = s_{1/2}, p− = p_{1/2}, p+ = p_{3/2}, d− = d_{3/2}, d+ = d_{5/2}, f− = f_{5/2} and f+ = f_{7/2}.

^{*b*} The number after the −/+ symbols is the power of the corresponding configuration. For example, the *jj* configuration of level 15 is $1s_{1/2}^2 4f_{7/2}$.

(Table 1 is published in its entirety in machine-readable format online. A portion is shown here for guidance regarding its form and content.)

Table 2.

Valence Level Energies in L-shell Ions of Ar Evaluated with the MR-MP Method.

<i>N</i>	Index	Configuration ^{a, b}	<i>J</i>	Parity	Energy (eV)
3	1	1s22s	1/2	even	0.00
3	2	1s22p−	1/2	odd	31.87
3	3	1s22p+	3/2	odd	35.04
3	4	1s23s	1/2	even	517.72
3	5	1s23p−	1/2	odd	526.53
3	6	1s23p+	3/2	odd	527.46
3	7	1s23d−	3/2	even	530.78
3	8	1s23d+	5/2	even	531.08
3	9	1s24s	1/2	even	695.02
3	10	1s24p−	1/2	odd	698.62
3	11	1s24p+	3/2	odd	699.01
3	12	1s24d−	3/2	even	700.38
3	13	1s24d+	5/2	even	700.51
3	14	1s24f−	5/2	odd	700.58
3	15	1s24f+	7/2	odd	700.65
3	16	1s25s	1/2	even	776.37
3	17	1s25p−	1/2	odd	778.08
3	18	1s25p+	3/2	odd	778.29
3	19	1s25d−	3/2	even	778.90
3	20	1s25d+	5/2	even	778.97
3	21	1s25f−	5/2	odd	779.02
3	22	1s25f+	7/2	odd	779.05

Note—Note that only 22 levels arising from the $1s^2nl$ ($n < 6$ and $l < 3$) configurations in Ar XVI ($N = 3$) are shown here.

^a s = s_{1/2}, p− = p_{1/2}, p+ = p_{3/2}, d− = d_{3/2}, d+ = d_{5/2}, f− = f_{5/2} and f+ = f_{7/2}.

^b The number after the −/+ symbols is the power of the corresponding configuration. For example, the *jj* configuration of level 15 is $1s_{1/2}^2 4f_{7/2}$.

(Table 2 is published in its entirety in machine-readable format online. A portion is shown here for guidance regarding its form and content.)

Table 3.

Valence Level Energies (eV) of L-shell Ions of S with a Deviation Between the NIST-recommended Values and Our MR-MP Results Higher than 0.5 eV.

Ion	Level	NIST	MR-MP	Deviation
S XIII	$2p3d\ ^1P_1^o$	428.63	429.47	0.84
S XIII	$2p4p\ ^3D_3$	534.12	533.54	-0.59
S XIII	$2p4d\ ^1F_3^o$	537.29	538.46	1.18
S XIII	$2s5d\ ^3D_3$	559.97	559.27	-0.71
S XII	$2s2p(^3P^o)3s\ ^4P_{5/2}^o$	344.02	343.47	-0.55
S XII	$2s2p(^1P^o)3p\ ^2D_{5/2}$	379.52	378.24	-1.28
S XII	$2s2p(^1P^o)3p\ ^2D_{3/2}$	379.52	378.40	-1.11
S XI	$2s2p^2(^4P)3s\ ^3P_2$	321.22	319.44	-1.77
S XI	$2s2p^2(^4P)3p\ ^3D_2^o$	323.29	324.29	1.00
S XI	$2s2p^2(^2D)3s\ ^3D_3$	333.55	331.55	-1.99
S X	$2s2p^3(^5S^o)3d\ ^4D_{3/2}^o$	315.25	316.35	1.10
S X	$2s2p^3(^5S^o)3d\ ^4D_{5/2}^o$	315.57	316.35	0.78
S X	$2s2p^3(^3P^o)3d\ ^4D_{7/2}^o$	342.09	341.49	-0.60

Table 4.

Valence Level Energies (eV) of L-shell Ions of Ar with a Deviation Between the NIST-recommended Values and Our MR-MP Results Higher than 0.5 eV.

Ion	Level	NIST	MR-MP	Deviation
Ar XIV	$2s^2 3p^2 P_{1/2}^o$	438.15	437.61	-0.54
Ar XIV	$2s 2p(^3P^o) 3d^2 F_{7/2}^o$	490.28	489.56	-0.72
Ar XIII	$2p^4 ^1S_0$	143.78	144.41	0.62
Ar XIII	$2s^2 2p 3d^3 D_3^o$	425.17	424.66	-0.51
Ar XIII	$2s 2p^2(^4P) 3d^5 P_3$	451.90	452.67	0.76
Ar XIII	$2s^2 2p 4d^3 D_1^0$	540.38	539.06	-1.32
Ar XII	$2s^2 2p^2(^3P) 3p^4 S_{3/2}^o$	379.27	377.89	-1.38
Ar XII	$2s^2 2p^2(^1D) 3p^2 D_{5/2}^o$	387.43	385.77	-1.66
Ar XII	$2s^2 2p^2(^1D) 3p^2 P_{1/2}^o$	388.54	387.72	-0.82
Ar XII	$2s^2 2p^2(^1D) 3p^2 P_{3/2}^o$	389.62	388.95	-0.67
Ar XII	$2s^2 2p^2(^3P) 3d^2 D_{5/2}$	400.07	399.57	-0.50
Ar XI	$2s^2 2p^3(^2P^o) 3s^1 P_1^o$	328.53	327.58	-0.95
Ar XI	$2s^2 2p^3(^2D^o) 3p^3 F_2$	338.33	337.75	-0.58
Ar XI	$2s^2 2p^3(^2D^o) 3d^3 G_3^0$	359.59	359.02	-0.57
Ar XI	$2s^2 2p^3(^2D^o) 3d^3 S_1^o$	363.71	362.60	-1.10
Ar XI	$2s^2 2p^3(^2P^o) 3d^3 D_1^o$	370.41	373.81	3.40
Ar XI	$2s^2 2p^3(^2D^o) 4d^3 D_3^o$	446.16	445.38	-0.79
Ar X	$2s^2 2p^4(^1D) 4s^2 D_{5/2}$	384.86	384.18	-0.68
Ar X	$2s^2 2p^4(^3P) 4f^4 F_{9/2}^0$	393.72	394.31	0.59
Ar X	$2s^2 2p^4(^3P) 4f^4 F_{7/2}^o$	393.79	394.40	0.62
Ar X	$2s^2 2p^4(^1D) 4d^2 F_{7/2}$	401.04	400.31	-0.74
Ar X	$2s^2 2p^4(^1S) 4f^2 F_{5/2}^o$	412.51	411.74	-0.77
Ar IX	$2s 2p^6 3s^3 S_1$	325.23	326.76	1.53
Ar IX	$2s 2p^6 3s^1 S_0$	327.29	329.96	2.67

Ion	Level	NIST	MR-MP	Deviation
Ar IX	$2s^2 2p^5 4p^3 D_3$	342.32	341.65	-0.67
Ar IX	$2s^2 2p^5 4p^3 P_2$	342.63	341.70	-0.93
Ar IX	$2s 2p^6 3p^3 P_2^o$	345.74	345.02	-0.72
Ar IX	$2s 2p^6 3p^1 P_1^o$	346.01	344.76	-1.25
Ar IX	$2s^2 2p^5 5s^3 P_0^o$	369.19	371.51	2.32
Ar IX	$2s^2 2p^5 5s^3 P_1^o$	370.59	371.58	0.99
Ar IX	$2s 2p^6 3d^3 D_3$	371.08	367.87	-3.21
Ar IX	$2s^2 2p^5 5p^3 D_1$	373.34	372.68	-0.66
Ar IX	$2s^2 2p^5 5p^3 D_2$	374.22	374.88	0.67
Ar IX	$2s^2 2p^5 5p^1 S_0$	376.94	375.56	-1.38

Table 5.

Average Absolute Deviation (eV) Between Calculated Valence Level Energies and the NIST-recommended Values (Kramida et al. 2015) for L-shell Ions of S and Ar.

Ion	MR-MP	CHIANTI v8
S XIII	0.16	0.44
S XII	0.15	0.57
S XI	0.11	0.80
S X	0.09	0.75
Ar XIV	0.14	0.65
Ar XIII	0.06	0.53
Ar XII	0.26	0.77
Ar XI	0.27	0.73
Ar X	0.16	1.06
Ar IX	0.33	0.55

Note—Results are included for level energies from our MR-MP calculations and the CHIANTI v8 database (Dere et al. 1997; Del Zanna et al. 2015).

Table 6.Energy (eV) of the $2p^4\ ^1S_0$ Level in Various C-like Ions.

Ion	NIST	MR-MP	Deviation	CI+MBPT	Deviation
O III	42.56	43.95	1.38	-	
Ne V	62.05	62.70	0.65	-	
Mg VII	81.64	82.12	0.48	-	
Si IX	101.63	102.02	0.39	101.42	-0.21
S XI	122.34	122.66	0.32	122.17	-0.17
Ar XIII	143.78	144.41	0.63	143.97	0.19
Mn XX	237.18	237.34	0.16	237.13	-0.05
Fe XXI	253.94	254.07	0.13	253.83	-0.11

Note—CI+MBPT results from Wang et al. (2014) are included for comparison.

Table 7.

Valence Level Energies (eV) of L-shell ions of S with a Deviation Between the NIST-recommended Values and Our MR-MP Results of 0.3 – 0.5 eV.

Ion	Level	NIST	MR-MP	Deviation
S XIII	$1s^2 2p 3p^3 P_1$	417.28	417.62	0.34
S XIII	$1s^2 2s 4s^3 S_1$	499.02	499.33	0.30
S XII	$2s 2p(^3P^o) 3p^2 P_{1/2}$	352.20	352.64	0.44
S XII	$2s 2p(^3P^o) 3d^4 P_{3/2}^o$	367.85	367.49	-0.36
S XII	$2s 2p(^3P^o) 4p^2 D_{5/2}$	462.71	463.20	0.49
S XII	$2s^2 5d^2 D_{3/2}$	484.90	484.56	-0.34
S XI	$2p^4 ^1S_0$	122.34	122.66	0.32
S XI	$2s 2p^2(^4P) 3d^5 P_2$	341.28	340.79	-0.49
S XI	$2s 2p^2(^2D) 3p^1 F_3^o$	346.54	346.14	-0.40
S XI	$2s 2p^2(^2P) 3d^3 P_2$	378.53	378.97	0.44
S X	$2s^2 2p^2(^3P) 4d^4 P_{5/2}$	361.36	361.00	-0.37
S VIII	$2s^2 2p^4(^3P) 3p^4 S_{3/2}^o$	210.57	210.14	-0.43
S VIII	$2s^2 2p^4(^3P) 3d^2 F_{5/2}$	228.05	227.69	-0.35
S VIII	$2s^2 2p^4(^3P) 4s^2 P_{3/2}$	260.91	260.49	-0.43
S VII	$2s^2 2p^5 3d^3 D_2^o$	204.15	203.76	-0.39
S VII	$2s^2 2p^5(^2P^o) 4f^2 [5/2]_2$	239.17	238.82	-0.34
S VII	$2s^2 2p^5(^2P^o) 4f^2 [7/2]_4$	239.26	238.93	-0.33
S VII	$2s^2 2p^5(^2P^o) 5s^2 [3/2]_1^o$	247.83	247.42	-0.42

Table 8.

Valence Level Energies (eV) of L-shell ions of Ar with a Deviation Between the NIST-recommended Values and Our MR-MP Results of 0.3 – 0.5 eV.

Ion	Level	NIST	MR-MP	Deviation
Ar XV	$1s^2 2s 3d^3 D_1$	509.10	509.40	0.30
Ar XV	$1s^2 2s 3d^3 D_2$	509.99	509.51	-0.48
Ar XIV	$2s^2 4d^2 D_{3/2}$	585.74	585.43	-0.31
Ar XIII	$2s^2 2p 3d^1 F_3^o$	430.13	429.80	-0.33
Ar XII	$2s^2 2p^2(^3P) 3s^4 P_{1/2}$	355.46	355.14	-0.33
Ar XII	$2s^2 2p^2(^3P) 3s^2 P_{3/2}$	361.05	360.61	-0.44
Ar XII	$2s^2 2p^2(^3P) 3p^4 P_{3/2}^o$	373.40	373.07	-0.33
Ar XII	$2s^2 2p^2(^3P) 3d^4 P_{5/2}$	395.18	394.85	-0.33
Ar XI	$2s^2 2p^3(^2P^o) 3d^3 P_1^o$	367.99	368.32	0.33
Ar XI	$2s^2 2p^3(^2P^o) 3d^3 D_2^o$	368.18	367.87	-0.30
Ar X	$2s^2 2p^4(^1D) 3d^2 S_{1/2}$	330.17	329.77	-0.40
Ar X	$2s^2 2p^4(^3P) 4d^4 F_{3/2}$	393.17	392.75	-0.42
ArX	$2s^2 2p^4(^1D) 4d^2 F_{5/2}$	400.91	400.43	-0.48
Ar IX	$2s^2 2p^5 4p^3 S_1$	341.61	341.26	-0.35
Ar IX	$2s^2 2p^5 4p^1 P_1$	342.32	342.01	-0.31
Ar IX	$2s^2 2p^5 4p^1 D_2$	344.54	344.16	-0.38
Ar IX	$2s 2p^6 3p^3 P_1^o$	345.54	346.01	0.47
Ar IX	$2s^2 2p^5 4f^1 F_3$	353.56	353.16	-0.39
Ar IX	$2s^2 2p^5 5d^3 D_3^o$	376.96	376.64	-0.31

Table 9.

K-vacancy Level Energies (eV) of S XIV Recommended in the NIST Database and Calculated with the MR-MP Method.

Index	Level	NIST	MR-MP	FAC	HFR	AS
1	$1s2s^2 2S_{1/2}$	2408.02	2408.19	2407.37	2407.96	2408.01
2	$1s(2S)2s2p(3P^o) 4P^o_{1/2}$	2415.26	2415.21	2414.51	2414.70	2413.37
3	$1s(2S)2s2p(3P^o) 4P^o_{3/2}$	2415.77	2415.71	2415.02	2415.43	2414.06
4	$1s(2S)2s2p(3P^o) 4P^o_{5/2}$	2417.00	2416.96	2416.26	2416.74	2415.32
5	$1s(2S)2s2p(3P^o) 2P^o_{1/2}$	2437.05	2437.07	2436.55	2437.26	2436.56
6	$1s(2S)2s2p(3P^o) 3P^o_{3/2}$	2438.01	2438.08	2437.58	2438.25	2437.56
7	$1s2p^2 4P_{1/2}$	2445.13	2445.08	2444.90	2444.75	2444.81
8	$1s2p^2 4P_{3/2}$	2445.95	2445.91	2445.66	2445.54	2445.59
9	$1s2p^2 4P_{5/2}$	2446.87	2446.84	2446.62	2446.73	2446.75
10	$1s(2S)2s2p(1P^o) 2P^o_{1/2}$	2447.05	2447.14	2447.65	2447.77	2445.99
11	$1s(2S)2s2p(1P^o) 2P^o_{3/2}$	2447.55	2447.51	2448.00	2448.33	2446.49
12	$1s2p^2 2D_{5/2}$	2459.62	2459.54	2460.38	2460.38	2459.76
13	$1s2p^2 2D_{3/2}$	2459.72	2459.65	2460.45	2460.11	2459.50
14	$1s2p^2 2P_{1/2}$	2462.82	2463.00	2463.31	2463.41	2463.29
15	$1s2p^2 2P_{3/2}$	2464.62	2464.81	2465.12	2465.18	2465.01
16	$1s2p^2 2S_{1/2}$	2478.97	2478.98	2479.98	2480.09	2479.03
17	$1s2s(3S)3p^2 P^o_{3/2}$	2829.66	2829.65	2828.80		2829.18
18	$1s2s(3S)3p^2 P^o_{1/2}$	2829.79	2829.80	2828.93		2829.21
19	$1s2s(3S)3d^2 D_{5/2}$	2838.69	2838.43	2837.75		2838.26
20	$1s2s(3S)3d^2 D_{3/2}$	2838.74	2838.47	2837.77		2838.26
21	$1s2s(1S)3p^2 P^o_{1/2}$	2845.12	2844.86	2843.87		2845.04
22	$1s2s(1S)3p^2 P^o_{3/2}$	2845.64	2845.36	2844.38		2845.55
23	$1s2p(3P^o)3p^2 P_{3/2}$	2847.19	2847.43	2846.85		2846.62
21	$1s2p(3P^o)3p^2 P_{1/2}$	2847.31	2847.51	2846.95		2846.67

Index	Level	NIST	MR-MP	FAC	HFR	AS
25	$1s2s(^1S)3d^2D_{3/2}$	2853.61	2852.68	2852.65		2853.49
26	$1s2s(^1S)3d^2D_{5/2}$	2853.61	2852.47	2852.35		2853.16
27	$1s2p(^3P^o)3p^2D_{3/2}$	2854.06	2853.39	2853.28		2853.26
28	$1s2p(^3P^o)3p^2D_{5/2}$	2855.41	2854.84	2854.77		2854.80
29	$1s2p(^1P^o)3s^2P^o_{3/2}$	2856.03	2855.73	2855.15		2855.95
30	$1s2p(^1P^o)3s^2P^o_{1/2}$	2856.27	2855.76	2855.58		2856.35
31	$1s2p(^3P^o)3p^2S_{1/2}$	2859.21	2858.49	2858.51		2858.31
32	$1s2p(^1P^o)3p^2D_{3/2}$	2863.47	2863.53	2862.50		2862.96
33	$1s2p(^1P^o)3p^2P_{1/2}$	2863.47	2862.75	2862.43		2863.80
34	$1s2p(^1P^o)3p^2D_{5/2}$	2863.54	2862.89	2862.52		2863.12
35	$1s2p(^1P^o)3p^2P_{3/2}$	2864.22	2862.83	2863.24		2863.02

Note—Previous calculations are included for comparison: FAC (Hell et al. 2016), HFR (Palmeri et al. 2008), and AUTOSTRUCTURE (AS) (as included in the CHIANTI v8 data base (Dere et al. 1997; Del Zanna et al. 2015)).

Table 10.

K-vacancy level energies (eV) of Ar XVI Recommended in the NIST Database and Calculated with the MR-MP Method.

Index	Level	NIST	MR-MP	HFR	AS
1	$1s2s^2 2S_{1/2}$	3079.30	3079.19	3079.14	3078.93
2	$1s(2S)2s2p(^3P^o)_1 4P^o_{1/2}$	3087.33	3087.10	3086.74	3084.99
3	$1s(2S)2s2p(^3P^o)_3 4P^o_{3/2}$	3088.18	3087.95	3087.92	3086.13
4	$1s(2S)2s2p(^3P^o)_2 2P^o_{1/2}$	3112.53	3112.37	3112.79	3111.82
5	$1s(2S)2s2p(^3P^o)_2 2P^o_{3/2}$	3114.16	3114.08	3114.51	3112.22
6	$1s2p^2 4P_{1/2}$	3122.06	3121.79	3121.60	3121.48
7	$1s2p^2 4P_{3/2}$	3123.45	3123.20	3122.97	3122.80
8	$1s(2S)2s2p(^1P^o)_2 2P^o_{1/2}$	3124.20	3124.02	3124.92	3122.70
9	$1s(2S)2s2p(^1P^o)_2 2P^o_{3/2}$	3124.92	3124.66	3125.79	3124.79
10	$1s2p^2 4P_{5/2}$	3124.99	3124.75	3124.90	3124.69
11	$1s2p^2 2D_{3/2}$	3139.39	3139.19	3139.77	3138.93
12	$1s2p^2 2D_{5/2}$	3139.45	3139.28	3140.38	3139.52
13	$1s2p^2 2P_{1/2}$	3142.58	3142.49	3143.23	3142.95
14	$1s2p^2 2P_{3/2}$	3145.74	3145.67	3146.35	3145.96
15	$1s2p^2 2S_{1/2}$	3161.52	3161.34	3162.65	3161.36
16	$1s2s(^3S)3s^2 2S_{1/2}$	3617.38	3617.76		3617.77
17	$1s2s(^3S)3p^4 P^o_{3/2}$	3620.50	3620.73		3620.59
18	$1s2s(^3S)3p^2 P^o_{3/2}$	3621.88	3622.29		3621.82
19	$1s2s(^3S)3p^2 P^o_{1/2}$	3621.99	3622.50		3621.85
20	$1s2s(^3S)3d^2 D_{3/2}$	3632.08	3632.45		3632.23
21	$1s2s(^3S)3d^2 D_{5/2}$	3632.12	3632.40		3632.24
22	$1s2s(^1S)3s^2 2S_{1/2}$	3632.21	3632.42		3632.26
23	$1s2s(^1S)3p^2 P^o_{3/2}$	3640.28	3640.46		3640.59
24	$1s2s(^1S)3p^2 P^o_{1/2}$	3640.28	3639.57		3639.69

Index	Level	NIST	MR-MP	HFR	AS
25	$1s2p(^3P^o)3p^2P_{3/2}$	3642.91	3642.94		3642.15
26	$1s2p(^3P^o)3p^4D_{3/2}$	3643.54	3645.57		3645.08
27	$1s2p(^3P^o)3p^2D_{3/2}$	3649.63	3649.57		3649.50
28	$1s2p(^3P^o)3p^4S_{3/2}$	3649.63	3640.40		3647.18
29	$1s2p(^3P^o)3p^2D_{5/2}$	3652.06	3651.95		3652.07
30	$1s2p(^3P^o)3p^4P_{3/2}$	3652.38	3660.65		3660.92
31	$1s2p(^3P^o)3p^2S_{1/2}$	3654.86	3655.83		3655.71
32	$1s2p(^1P^o)3p^2D_{3/2}$	3660.80	3661.90		3662.21
33	$1s2p(^1P^o)3p^2D_{5/2}$	3660.95	3660.78		3661.16

Note—Previous calculations are included for comparison: HFR (Palmeri et al. 2008) and AUTOSTRUCTURE (AS) (as included in the CHIANTI v8 data base (Dere et al. 1997; Del Zanna et al. 2015)).

Table 11.

K-vacancy Level Energies (eV) of Ar XV to Ar XI Recommended in the NIST Database and Calculated with the MR-MP Method.

Index	Ion	Level	NIST	MR-MP	HFR	Z-exp
1	Ar XV	$1s2s(^3S)2p^2(^1D)^3D_3$	3115.44	3113.77	3115.30	3114.53
2	Ar XV	$1s2s(^3S)2p^2(^1D)^3D_2$	3118.27	3116.71	3114.74	3114.53
3	Ar XV	$1s2s(^3S)2p^2(^1D)^3S_1$	3128.11	3127.96	3129.27	3128.60
4	Ar XV	$1s2s(^1S)2p^2(^1D)^1D_2$	3134.73	3135.00	3133.98	3133.48
5	Ar XV	$1s2p^3^3D_3^o$	3153.13	3152.48	3154.30	3153.60
6	Ar XV	$1s2p^3^3D_1^o$	3153.68	3152.73	3153.98	3153.86
7	Ar XV	$1s2p^3^3P_1^o$	3166.93	3166.64	3168.37	3167.82
1	Ar XIV	$1s2s^22p^2^2D_{3/2}$	3062.62	3062.57	3062.89	3059.65
2	Ar XIV	$1s2s^22p^2^2D_{5/2}$	3062.78	3062.62	3063.42	3059.73
3	Ar XIV	$1s2s^22p^2^2P_{3/2}$	3067.48	3068.10	3068.55	3065.02
4	Ar XIV	$1s2s(^3S)2p^3(^2D^o)^4D_{7/2}^o$	3084.78	3084.96	3086.38	3082.73
5	Ar XIV	$1s2s(^3S)2p^3(^2D^o)^4D_{5/2}^o$	3085.31	3085.11	3086.07	3082.37
6	Ar XIV	$1s2s(^3S)2p^3(^2P^o)^2P_{3/2}^o$	3117.09	3116.78	3118.39	3110.25
7	Ar XIV	$1s2s(^3S)2p^3(^2D^o)^2D_{5/2}^o$	3120.75	3119.14	3121.68	3116.95
8	Ar XIV	$1s2p^4^2P_{3/2}$	3161.80	3161.38	3163.18	3158.94
1	Ar XIII	$1s2s^22p^3^3D_3^o$	3035.28	3035.66	3037.55	-
2	Ar XIII	$1s2s^22p^3^1D_2^o$	3048.92	3048.76	3050.48	3048.41
3	Ar XIII	$1s2s^22p^3^1P_1^o$	3053.81	3054.95	3056.36	3054.68
4	Ar XIII	$1s2s(^3S)2p^4(^3P)^5P_2$	3059.19	3061.87	3062.55	3062.10
5	Ar XIII	$1s2s(^3S)2p^4(^1D)^3D_3$	3088.20	3088.92	3088.81	3088.92
6	Ar XIII	$1s2s(^3S)2p^4(^3P)^3P_1$	3089.01	3088.30	3091.32	3089.80
7	Ar XIII	$1s2s(^3S)2p^4(^3P)^3P_2$	3098.28	3105.33	3090.59	-
8	Ar XIII	$1s2s(^1S)2p^4(^1D)^1D_2$	3105.00	3107.32	3107.45	3105.82
9	Ar XIII	$1s2p^5^1P_1^o$	3160.95	3161.65	3165.38	3162.00

Index	Ion	Level	NIST	MR-MP	HFR	Z-exp
1	Ar XII	$1s(2s)2s^2 2p^4(1D)^2 D_{3/2}$	3024.45	3025.86	3027.47	3026.25
2	Ar XII	$1s(2s)2s^2 2p^4(3P)^2 P_{1/2}$	3028.46	3030.37	3032.08	3030.70
3	Ar XII	$1s(2s)2s^2 2p^4(3P)^2 P_{3/2}$	3028.60	3029.43	3031.16	3029.76
4	Ar XII	$1s2s(3s)2p^5 4P_{5/2}^o$	3063.54	3065.52	3067.59	3067.94
5	Ar XII	$1s2s(3s)2p^5 4P_{3/2}^o$	3064.73	3067.18	3069.16	3069.60
6	Ar XII	$1s2s(3s)2p^5 2P_{3/2}^o$	3085.60	3087.21	3089.71	3089.36
7	Ar XII	$1s2s(3s)2p^5 2P_{1/2}^o$	3096.54	3100.05	3103.24	3102.71
1	Ar XI	$1s2s^2 2p^5 3P_2^o$	2989.22	2989.91	2992.31	2988.35
2	Ar XI	$1s2s^2 2p^5 3P_1^o$	2991.98	2991.75	2994.04	2990.44
3	Ar XI	$1s2s^2 2p^5 3P_0^o$	2992.76	2993.16	2995.16	2991.95
4	Ar XI	$1s2s^2 2p^5 1P_1^o$	3001.37	3002.42	3004.75	3000.52
5	Ar XI	$1s2s2p^6 3S_1$	3052.90	3055.50	3059.79	3054.64
6	Ar XI	$1s2s2p^6 1S_0$	3070.01	3071.98	3076.93	3071.24

Note—Previous calculations are included for comparison: HFR (Palmeri et al. 2008) and Z-expansion (Safronova & Shlyaptseva 1996, 1999).