K-shell photoabsorption and photoionization of trace elements

III. Isoelectronic sequences with electron number $19 \leq N \leq 26$

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ABSTRACT

Context. This is the final report of a three-paper series on the K-shell photoabsorption and photoionization of trace elements (low cosmic abundance), namely F, Na, P, Cl, K, Sc, Ti, V, Cr, Mn, Co, Cu and Zn. K lines and edges from such elements are observed in the X-ray spectra of supernova remnants, galaxy clusters and accreting black holes and neutron stars, their diagnostic potential being limited by poor atomic data.

Aims. We are completing the previously reported radiative datasets with new photoabsorption and photoionization cross sections for isoelectronic sequences with electron number $19 \leq N \leq 26$. We are also giving attention to the access, integrity and usability of the whole resulting atomic database.

Methods. Target representations are obtained with the atomic structure code AUTOSTRUCTURE. Where possible, cross sections for ground-configuration states are computed with the Breit–Pauli $R$-matrix method (RPRM) in either intermediate or LS coupling including damping effects; otherwise and more generally, they are generated in the isolated-resonance approximation with AUTOSTRUCTURE.

Results. Cross sections were computed with bprm only for the K ($N = 19$) and Ca ($N = 20$) isoelectronic sequences, the latter in LS coupling. For the rest of the sequences ($21 \leq N \leq 26$), AUTOSTRUCTURE was run in LS-coupling mode taking into account damping effects. Comparisons between these two methods for K-like Zn xii and Ca-like Zn xiii show that, to ensure reasonable accuracy, the LS calculations must be performed taking into account the non-fine-structure relativistic corrections. The original data structures of the bprm and AUTOSTRUCTURE output files, namely photoabsorption and total and partial photoionization cross sections, are maintained but supplemented with files detailing the target $(N_{\gamma}-e)$ representations and photon states $(N-e)$ system.

Conclusions. We conclude that, due to large target size, the photoionization of ions with $N > 20$ involving inner-shell excitations rapidly leads to untractable bprm calculations, and is then more effectively treated in the isolated resonance approximation with AUTOSTRUCTURE. This latter approximation by no means involves small calculations as Auger damping must be explicitly specified in the intricate decay routes.

Key words. atomic data -- X-rays: general

1. Introduction

The present project is concerned with the computation of atomic data to improve the diagnostic capabilities of the spectral K lines and edges of chemical elements with low cosmic abundance (trace elements) - namely F, Na, P, Cl, K, Sc, Ti, V, Cr, Mn, Co, Cu and Zn. In spite of their low abundances, they are nevertheless observed in the X-ray spectra of supernova remnants, galaxy clusters and accreting black holes and neutron stars (see, for instance, Hwang et al. 2000, Miller et al. 2006, Badenes et al. 2008, Kallman et al. 2009, Tamura et al. 2009, Ueda et al. 2004, Nobukawa et al. 2010, Park et al. 2013), from which they can be used to constrain the plasma characteristics. For this purpose level energies, radiative and Auger widths and fluorescence yields for K-vacancy levels in ions of the aforementioned isonuclear sequences were computed by Palmeri et al. (2012), hereafter PQM12, with hfr (a Hartree–Fock code with relativistic corrections by Cowan 1981). Their atomic target representations were subsequently used by Palmeri et al. (2016), hereafter Paper I, and Mendoza et al. (2017), hereafter Paper II, to calculate with the Breit–Pauli $R$-matrix method (bprm, Berrington et al. 1995) intermediate-coupling photoabsorption and photoionization cross sections for isoelectronic sequences with electron number $N \leq 18$. In this context, the resonance structures associated with the L and K ionization edges were studied in detail, particularly the radiation and spectator-Auger damping effects that lead to K-edge smearing (Palmeri et al. 2002).

In the present and final report of this project, we compute with the multi-purpose atomic structure code AUTOSTRUCTURE $LS$-...
coupling photoabsorption and photoionization cross sections for trace ions in isoelectronic sequences with $19 \leq N \leq 26$ assuming the isolated resonance approximation. This latter approach has been adopted because bprm has proven to be ineffective due to the large target sizes involved. Autostructure accuracy has been previously shown to be reasonable for this purpose (see Paper II), and is further examined here for the simpler K ($N = 19$) and Ca ($N = 20$) isoelectronic sequences.

An important part of this report is the curation aspects of the voluminous database that has been generated in this project, which is to become available online from the Centre de Données astronomiques de Strasbourg (CDS1). We emphasize, however, that the datasets have been computed with different numerical methods and angular couplings, and their content and structures may thus nominally vary.

2. Numerical methods

The main task of the present project is to compute photoabsorption and total and partial photoionization cross sections for ions of the isonuclear series P, Cl, K, Sc, Ti, V, Cr, Mn, Co, Cu and Zn with electron numbers $N < Z < 1$, where $Z$ is the atomic number identifying the sequence. As previously mentioned in Paper I, species with $Z = 1 \leq N \leq Z$ will be treated elsewhere. Cross sections for isoelectronic sequences with $N \leq 11$ were reported in Paper I and with $12 \leq N \leq 18$ in Paper II. We discuss here the details of the computations for fourth-row ions with $19 \leq N \leq 26$.

The cross sections reported in Paper I and Paper II were carried out in intermediate coupling (IC) with the relativistic (Breit–Pauli) bprm method, which allows the inclusion of radiative and spectator-Auger damping (Robicheaux et al. 1993; Gorczyca & Badnell 1996, 2000). The target representations listed in Table 9 of PQM12 were used but, for ions with $12 \leq N \leq 18$, levels from the 2s-hole configurations [2s] were additionally included. Electronic orbitals were generated in a Thomas–Fermi–Dirac statistical potential with the Autostructure atomic structure code (Eissner et al. 1974; Badnell 2011).

Due to the large target sizes required for species with $19 \leq N \leq 26$, specially those bearing ground configurations $3p^33d^m_{\text{ff}}$ with $m > 2$, the bprm approach is no longer practical. Exploratory calculations in Paper II revealed that LS cross sections could be adequately generated for such larger ions with a distorted-wave approach in the isolated-resonance approximation implemented in Autostructure. Target models are still those from PQM12 but, as previously shown (Paper II), they are complemented with levels from configurations of the type [2s]~$\mu$. Radiative damping is taken into account by Autostructure but, in contrast to bprm, the Auger decay branches must be explicitly specified in the configuration list thus leading to lengthy calculations. The key feature of this approach is the decoupling of the photoionization and photoexcitation processes that enables the treatment of larger systems.

3. Results

For the trace elements there are hardly any previously multi-channel photoabsorption cross sections for fourth-row ions with ground configurations $3p^33d^n$; therefore, cross sections are calculated from the ionization threshold up to the monotonic decreasing tail beyond the K edge. We illustrate the main findings of our analysis in terms of the Zn ions. For the potassium isoelectronic sequence ($N = 19$) it is still possible, although involved, to perform a bprm calculation in IC to compare with Autostructure. Such a comparison is carried out in Fig. 1 for the $3p^33d^2_{\text{D1/2}}$ ground state of Zn xi, where the bprm data below the L edge ($\sim 103\text{ Ryd}$) have been convolved for clarity with a Gaussian of width $\Delta E/E = 0.001$. (b) K-edge region; the Autostructure energy scale has been shifted by 0.9 Ryd to obtain resonance positional matching.

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the laboratory and observational energy scales that are deterrents in a reliable choice. As a consequence, no attempt is made here to adjust the energy scales.

4. Database content and conventions

As previously mentioned, the datasets generated in the present project are to become available online from the CDS. We give here a concise description of the adopted data conventions and structures to identify the files and facilitate the extraction of their content.

4.1. Summary

Following the close-coupling (R-matrix) convention, where a scattering system is conceived as a target plus a colliding electron, we identify the N-electron ionic species to be photoionized with the 2-tuple \((Z, N_f)\), where \(Z\) is the atomic number and \(N_f = N - 1\) is the number of target electrons. In the present project we have been mainly concerned with photoabsorption and photoionization cross sections of states in the ionic ground configuration that will be referred to as photon states. The latter are identified by the 4-tuple \((0, 2J, \pi, \text{lev})\) in IC and \((2S+1, L, \pi, \text{lev})\) in \(LS\), where \(J\) and \(L\) are respectively the total and orbital angular momentum quantum numbers, \(2S+1\) the spin multiplicity, \(\pi\) the parity (\(\pi = 0\) for even, \(\pi = 1\) for odd) and \(\text{lev}\) the level index within the \(J\pi/S\pi L\pi\) series. A summary of the database content in terms of these identifiers is given in Table 4. It may be seen therein that 24 isoelectronic sequences with target electron numbers \(2 \leq N_f \leq 25\) have been considered encompassing elements with atomic numbers \(9 \leq Z \leq 30\). Sequences with \(N_f \geq 19\) have been treated in \(LS\) coupling, and for \(N_f \geq 20\), Ni species have also been included to complement previous work by Wittkof et al. (2011a).

4.2. Target data

IC energy-level data for \((Z, N_f)\) targets in isoelectronic sequences with \(2 \leq N_f \leq 18\) and \(LS\) energy-level data for those with \(19 \leq N_f \leq 25\) are listed in Table 2 and Table 3 respectively. Energies in Rydbergs are given relative to the ground state, the latter listing the total ion energy. Table 2 is very similar to Table 9 of [Dom12] but, since it is generated by \texttt{bprm-strg3}, the level order may vary; moreover, for sequences with \(N_f > 10\), the level number is greater since additional configurations were taken into account. Tables 2–3 are essential when considering the partial photoionization cross sections that, for a specific N-electron photon state, are tabulated in \(i\) order.

4.3. Photon-state data

The N-electron photon states for which cross sections have been computed are listed in Table 4 (isoelectronic sequences with \(3 \leq N \leq 19\) in IC) and Table 5 (sequences with \(20 \leq N \leq 26\), in \(LS\)); they essentially correspond to states within the ionic ground configuration. Energies are given in Rydbergs relative to the ionization potential. In systems with several photon states, IC cross sections for ions with \(N \leq 19\) are tabulated in \(i\) order.

4.4. Photoabsorption and photoionization cross sections

Cross sections have been computed using the serial version of the Breit–Pauli R-matrix codes for isoelectronic sequences with target electron numbers \(N_f \leq 19\) and with \texttt{autostructure} for \(20 \leq N_f \leq 25\) (see Table 4). Since the output files produced by these two suites of codes are somewhat different, we have kept the original nomenclature, structure and formats rather than making an attempt to unify them. We have also avoided the conversion of cross sections computed in \(LS\) coupling to intermediate coupling. For an ionic species identified with the target tuple \((Z, N_f) \equiv (\text{zz}, \text{nn})\), the following files have been included in the database.

For isoelectronic sequences with \(2 \leq N_f \leq 19\),

- \texttt{zznn.xpaot}: total photoabsorption cross sections.
- \texttt{zznn.xpisum}: sum of the partial photoionization cross sections. It must be noted that this sum does not take into account the Auger damped component since it is treated in \texttt{bprm} by means of a model potential that does not specify parental branching.
- \texttt{zznn.xpipar}: partial photoionization cross sections.

For isoelectronic sequences with \(20 \leq N_f \leq 25\),

- \texttt{zznn.xdpaot}: total photoabsorption cross sections.
- \texttt{zznn.xd9isum}: sum of the direct partial photoionization cross sections. It must be noted that in \texttt{autostructure} the direct photoionization and photoexcitation processes are computed separately, and for the larger ions with \(N_f > 19\), different target representations are implemented for each step that cannot be collated into a single unified target; therefore, the resonance component is neglected.
- \texttt{zznn.xd9par}: direct partial photoionization cross sections.

5. Conclusions

Photoabsorption and photoionization cross sections have been computed for ions of the trace elements (elements with low cosmic abundance) F, Na, P, Cl, K, Sc, Ti, V, Cr, Mn, Co, Cu and Zn with electron number \(N \leq 26\). Cross sections were computed...
in intermediate coupling with the Breit–Pauli $R$-matrix method $bprm$ for sequences with $N \leq 20$; for the rest of the sequences ($21 \leq N \leq 26$), they were obtained, due to large target sizes, with autostructure in $LS$ coupling assuming the isolated resonance approximation. Comparisons between these two methods for K-like and Ca-like ions show that, to ensure reasonable accuracy, it is vital to perform the $LS$ calculations taking into account the non-fine-structure relativistic corrections. Curation procedures performed on the datasets stored at the CDS have been described to facilitate their download and use. These datasets will also be processed to be included in the atomic database of the xstar modeling code that calculates the physical conditions and emission spectra of photoionized gases (Bautista & Kallman 2001; Kallman et al. 2009).

As shown in Fig. 5b of Paper II, the $bprm$ photoabsorption cross section of Ar-like Sc iv in the K-edge region shows a small discontinuity at $\approx 331.5$ Ryd where the optical potential associated with Auger damping is switched on. This feature will be found in most $bprm$ curves in the K-edge region. Similarly, the discontinuous AUTOSTRUCTURE cross section across the K-edge spectral head is due to the finite number of rendered resonances. This broad dip will be present in most of the cross sections computed with this code as appreciated in Fig. 1b, Fig. 2b,c and Fig. 3 (right column) of the present report. Such numerical artifacts should be borne in mind.

There are hardly any previous calculations or experiments to reliably evaluate the accuracy of the present datasets. However, our target and collisional models have been extensively benchmarked with experiment and astronomical observations of K-line spectra involving ionic species from cosmic abundant iononuclear series and, in some cases, assessed by independent calculations with more refined approximations (e.g. the $R$-matrix plus pseudo-states framework). More precisely, we can cite the following sequences: N (García et al. 2009; Gharibeh et al. 2011; Sant’Anna et al. 2011; Shorman et al. 2013; Gharibeh et al. 2014); O (García et al. 2005, 2011; Gharibeh et al. 2013; Gharibeh et al. 2014; McLaughlin et al. 2013a, b; Gatuzz et al. 2013a, b; Gorczyca et al. 2013; McLaughlin et al. 2013a, b; McLaughlin et al. 2014; Bizau et al. 2015; McLaughlin et al. 2015; Ne, Mg, Si, S, Ar, and Ca (Palmeri et al. 2008a; Witthoeft et al. 2011b); Al (Palmeri et al. 2011; Witthoeft et al. 2013) and Ni (Palmeri et al. 2008b; Witthoeft et al. 2011a).

The L-edge structure in ions with electron number $N > 12$, as discussed in Paper II, is not expected to be fully converged in contrast to that of the K edge. Moreover, as shown by Gorczyca et al. (2013) for O i, theoretical K resonance positions are always subject to small wavelength adjustments to fit astronomical or laboratory measurements, which for this specific system have been shown to be discrepant. Therefore, the present data sets should be treated with due caution until they are independently verified.

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Table 2. Summary of the ionic systems studied in the present work identified by the 2-tuple \((Z, N_T)\), where \(Z\) is the atomic number and \(N_T = N - 1\) the number of target electrons. Photon states of the \(N\)-electron systems for which cross sections have been calculated are identified with the 4-tuple \((0, 2J, \pi, elev)\) in IC and \((2S + 1, L, \pi, elev)\) in LS. Isoelectronic sequences with \(2 \leq N_T \leq 18\) were treated in IC and those with \(19 \leq N_T \leq 25\) in LS.

| \(N_T\) | \(Z\) | N-electron photon states | Photon state identifiers |
|-------|-------|---------------------------|------------------------|
| 2     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 1s²2s¹2p²/2, 2s²2p⁰/2 | (0, 1, 0, 1) |
| 3     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 1s²2s²2p⁰/2, 3p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 1) |
| 4     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p⁰/2, 2p⁰/2, 3s²2p⁰/2 | (0, 1, 0, 1) |
| 5     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p²/2, 3p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 1) |
| 6     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p¹/2, 3p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 0) |
| 7     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p¹/2, 3p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 0) |
| 8     | 9, 11, 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p¹/2, 3p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 0) |
| 9     | 15, 17, 19, 21–25, 27, 29, 30 | 2s²2p⁰/2, 3s²2p⁰/2 | (0, 0, 0, 0) |
| 10    | 15, 17, 19, 21–25, 27, 29, 30 | 2p³3s²2p²/2, 3s²2p⁰/2 | (0, 1, 0, 1) |
| 11    | 15, 17, 19, 21–25, 27, 29, 30 | 2p³3s²2p⁰/2, 3p³2s²2p⁰/2 | (0, 1, 0, 1) |
| 12    | 15, 17, 19, 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 1, 0, 1) |
| 13    | 17, 19, 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 0, 0, 1) |
| 14    | 17, 19, 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 0, 0, 0) |
| 15    | 19, 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 0, 0, 0) |
| 16    | 19, 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 0, 0, 0) |
| 17    | 21–25, 27, 29, 30 | 3s²3p², 3p²3d², 3p³2s²2p⁰/2 | (0, 0, 0, 0) |
| 18    | 21–25, 27, 29, 30 | 3p³3d², 3p³3d², 3p³3d² | (0, 0, 0, 0) |
| 19    | 22–25, 27, 29, 30 | 3p³3d², 3p³3d², 3p³3d² | (3, 3, 0, 1) |
| 20    | 23–25, 27, 30 | 3p³3d², 3p³3d², 3p³3d² | (3, 3, 0, 1) |
| 21    | 24, 25, 27–30 | 3p³3d², 3p³3d², 3p³3d² | (2, 2, 0, 1) |
| 22    | 25, 27–30 | 3p³3d², 3p³3d², 3p³3d² | (2, 2, 0, 1) |
| 23    | 27–30 | 3p³3d², 3p³3d², 3p³3d² | (2, 2, 0, 1) |
| 24    | 27–30 | 3p³3d², 3p³3d², 3p³3d² | (2, 2, 0, 1) |
| 25    | 28–30 | 3p³3d², 3p³3d², 3p³3d² | (2, 2, 0, 1) |

Table 2. IC energy-level data for target ions \((Z, N_T)\) with \(N_T \leq 18\). The listed ground-state energy is the total ion energy while, for the rest of the levels, the level energy relative to the ground state is tabulated. Note: A complete version of this table is available electronically.
Table 3. $L_S$ energy-level data for target ions ($Z, N_T$) with $19 \leq N_T \leq 25$. The listed ground-state energy is the total ion energy while, for the rest of the levels, the level energy relative to the ground state is tabulated. Note: A complete version of this table is available electronically.

| $Z$ | $N_T$ | $i$ | $2S + 1$ | $L$ | $Pi$ | Conf | Term | $E$ (Ryd) |
|-----|-------|-----|---------|-----|------|------|------|-----------|
| 22  | 19    | 1   | 2       | 2   | 0    | 3p6.3d | 2d   | -1701.498049 |
| 22  | 19    | 2   | 2       | 2   | 0    | 3p6.4s | 2s   | 0.60370 |
| 22  | 19    | 3   | 4       | 2   | 1    | [3p]3d2 | 4d   | 2.268570 |
| 22  | 19    | 4   | 4       | 4   | 1    | [3p]3d2 | 4g   | 2.414790 |
| 22  | 19    | 5   | 4       | 4   | 1    | [3p]3d2 | 4p   | 2.425060 |
| 22  | 19    | 6   | 4       | 3   | 1    | [3p]3d2 | 4f   | 2.503180 |
| 22  | 19    | 7   | 2       | 2   | 1    | [3p]3d2 | 2d   | 2.523660 |
| 22  | 19    | 8   | 2       | 3   | 1    | [3p]3d2 | 2f   | 2.537130 |
| 22  | 19    | 9   | 2       | 2   | 1    | [3p]3d2 | 2p   | 2.591330 |
| 22  | 19    | 10  | 2       | 5   | 1    | [3p]3d2 | 2h   | 2.640820 |
| 22  | 19    | 11  | 2       | 4   | 1    | [3p]3d2 | 2g   | 2.660690 |
| 22  | 19    | 12  | 2       | 3   | 1    | [3p]3d2 | 2f   | 2.668140 |
| 22  | 19    | 13  | 4       | 2   | 1    | [3p]3d2 | 4d   | 2.725970 |
| 22  | 19    | 14  | 4       | 4   | 1    | [3p]3d2 | 4s   | 2.858760 |
| 22  | 19    | 15  | 4       | 4   | 4    | [3p]3d2 | 4g   | 2.889300 |
| 22  | 19    | 16  | 4       | 4   | 2    | [3p]3d2 | 4p   | 3.059900 |
| 22  | 19    | 17  | 2       | 4   | 1    | [3p]3d2 | 2g   | 2.904600 |
| 22  | 19    | 18  | 4       | 4   | 1    | [3p]3d2 | 4p   | 3.059900 |
| 22  | 19    | 19  | 2       | 2   | 1    | [3p]3d2 | 2p   | 3.119540 |
| 22  | 19    | 20  | 2       | 1   | 1    | [3p]3d2 | 2f   | 3.156530 |
| 22  | 19    | 21  | 4       | 3   | 1    | [3p]3d2 | 4f   | 3.156530 |

Table 4. IC energy-level data for photon states of ($Z, N$) systems for which cross sections have been computed ($N \leq 19$). Level energies are given relative to the ionization potential. Note: A complete version of this table is available electronically.

| $Z$ | $N$ | $i$ | $2S + 1$ | $L$ | $Pi$ | Lev | Conf | Term | $E$ (Ryd) |
|-----|-----|-----|---------|-----|------|-----|------|------|-----------|
| 9   | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -13.610382 |
| 11  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -22.040222 |
| 15  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -44.973266 |
| 17  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -59.496210 |
| 19  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -76.703846 |
| 21  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -94.756868 |
| 22  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -104.878480 |
| 23  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -115.529476 |
| 24  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -126.713523 |
| 25  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -138.436465 |
| 27  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -163.519500 |
| 29  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -190.819322 |
| 30  | 3   | 1   | 0       | 1   | 0    | 1s2.2s | 2s   | -205.243438 |

Table 5. $L_S$ energy-level data for photon states of ($Z, N$) systems for which cross sections have been computed ($20 \leq N \leq 26$). Level energies are given relative to the ionization potential. Note: A complete version of this table is available electronically.

| $Z$ | $N$ | $i$ | $2S + 1$ | $L$ | $Pi$ | Lev | Conf | Term | $E$ (Ryd) |
|-----|-----|-----|---------|-----|------|-----|------|------|-----------|
| 22  | 20  | 1   | 3       | 1   | 0    | 1s2.3d2 | 3p   | -2.612760 |
| 22  | 20  | 2   | 3       | 2   | 0    | 1s2.3d2 | 3d   | -2.358835 |
| 22  | 20  | 3   | 3       | 3   | 0    | 1s2.3d2 | 3f   | -2.734018 |
| 22  | 20  | 4   | 1       | 0    | 0    | 1s2.3d2 | 3s   | -2.296660 |
| 22  | 20  | 5   | 1       | 2    | 0    | 1s2.3d2 | 3d   | -2.629597 |
| 22  | 20  | 6   | 1       | 2    | 2    | 1s2.3d2 | 3d   | -2.314143 |
| 22  | 20  | 7   | 1       | 4    | 0    | 1s2.3d2 | 3d   | -2.585943 |
| 23  | 20  | 1   | 3       | 1    | 0    | 1s2.3d2 | 3p   | -4.065680 |
| 23  | 20  | 2   | 3       | 2    | 0    | 1s2.3d2 | 3d   | -3.298038 |
| 23  | 20  | 3   | 3       | 3    | 0    | 1s2.3d2 | 3f   | -4.210251 |
| 23  | 20  | 4   | 1       | 0    | 0    | 1s2.3d2 | 3s   | -3.675538 |
| 23  | 20  | 5   | 1       | 2    | 0    | 1s2.3d2 | 3d   | -4.083912 |
| 23  | 20  | 6   | 1       | 2    | 2    | 1s2.3d2 | 3d   | -3.253742 |
| 23  | 20  | 7   | 1       | 4    | 0    | 1s2.3d2 | 3d   | -4.031014 |