# Relativistic calculations of screening parameters and atomic radii of neutral atoms

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**Abstract**

Calculations of the effective nuclear charge for elements with $1 \leq Z \leq 118$ have been performed in a Dirac-Fock approach including all relativistic effects as well as contributions from quantum electrodynamics. Maximum charge density for every subshell of every element in the periodic table were also computed in the same framework as well as atomic radii based on the total charge density. Results were compared with the extensively cited works of Clementi *et al.*, obtained in the 1960's with Roothan's self-consistent-field method.

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**Contents**



## 1. Introduction

The usefulness of simple analytical functions for describing the electronic orbitals has been demonstrated long ago [1], and even now, with very high computer processing power, some codes rely on them to obtain physical properties that range from $g$-factors [2] and crystallographic defect structures [3], electron-hole interactions in layered materials [4] to molecular equilibrium structures and force constants [5]. In fact, the materials science community has been very active in searching new materials with targeted properties using state-of-the-art codes that still rely on atomic radii calculated with Slater-type-orbitals (STO) [6]. Quantum chemistry program packages, for instance, rely heavily on these analytical functions, with libraries of basis sets that span over several types of wavefunctions, from single STO to linear combinations of Gaussian-Type functions [7]. Electron and photon scattering are some of the physical processes in which screening parameters are still very much in use [8], with several calculations relying on atomic radii obtained through the use of screened potentials [9]. Scattering cross sections of both neutral atoms and ions make use of the effective nuclear charge [10–12] and atomic form factors that can be evaluated in the independent particle model using screened

hydrogenic wavefuntions [13]. Tong *et al.* [14], for instance, have investigated two-photon transitions in atomic inner shells by evaluating the relativistic and atomic-screening effects on the decay rates, and found that electron screening has a sizable effect in the two-photon decay rate by expanding the outer-shell wavefunctions, hence decreasing orbital overlap. Multielectron quantum electrodynamic (QED) computations still employ several approaches that rely on the screening of the nuclear potential in order to evaluate the electron's self-energy by providing a scaling factor to the hydrogenic expression [15–17]. Also, atomic and covalent radii are usually calculated on several codes with simple analytical expressions based on $Z_{\text{eff}}$ [18, 19], which also renders this method as a versatile tool for teaching periodic trends in the classroom [20].

The definition of atomic radii varies greatly within the literature (see [15] and references therein), dating back as far as the work of Slater which noticed a correlation between the maximum charge density of the outermost electron shell and ionic radius of an atom [21]. Other authors, however, have chosen either the simple [22] or weighted [23] mean radius of specific orbitals to infer the atom size, while others defined it as half the distance of the molecular single bond length in heteronuclear diatomic molecules [18, 24]. One particular use of the atomic radii is in the measuring of drift times of atoms in gases, which are used in velocity filters, for example in the isolation of superheavy elements in buffer-gas traps [25, 26]. Although the radii data of superheavy elements is scarce, the experimental results of the ionic radii of $Am^+$, $Pu^+$, $Fm^+$ and $Cf^+$ seem to favor a mean spherical radius description over the mean atomic radius based on the total electronic density [15].

The STO functions, which are still very useful, especially in codes that calculate solid state properties, due to the large number of evaluated orbitals, can be written as

$$\psi_{n,l,m} = N r^{n-1} e^{-\frac{Z_{\text{eff}}}{n} r} Y_{l,m}(\theta, \phi), \tag{1}$$

where $n, l, m$ are, respectively, the principal, orbital and magnetic hydrogenic quantum numbers, $N$ is the normalization factor, and $Y_{l,m}(\theta, \phi)$ are the spherical harmonics, whereas the effective nuclear charge $Z_{\text{eff}}$ is just the nuclear charge, $Z$, minus the screening constant $\sigma_{n,l}$

$$Z_{\text{eff}} = Z - \sigma_{n,l}. \tag{2}$$

Clementi *et al.* [27, 28] performed a systematic calculation in the 1960's of the screening constants of all orbitals for neutral atoms with $1 \leq Z \leq 86$, using Roothan-Hartree-Fock (RHF) Self-Consistent-Method with STO, and their results are still a reference, as seen not only by the sheer number of citations of both papers (more than 3000), but also their substantial increase in the last decade. The fact that the STO, used in their HF computation, lack radial nodes by definition, will result in drastically different average radius and $Z_{\text{eff}}$ for wavefunctions with one or more nodes.

In this work, we have calculated screening constants, effective nuclear charges and atomic radii for every shell of neutral atoms with $1 \leq Z \leq 118$, using the relativistic Multiconfiguration Dirac-Fock General Matrix Element (MCDFGME) program package [29, 30] in the monoconfiguration mode. The effective nuclear charge is obtained through a routine that evaluates many-electron radiative corrections, being $Z_{\text{eff}}$ deduced from the comparison of the mean value of the radius of the Dirac-Fock (DF) orbital with that of the hydrogenic one [31]. These QED contributions, such as the vacuum polarization and electron self-energy, contribute to the high reliability of this code in obtaining high precision level energies and radiative and radiationless transition rates [32, 33]. The fact that our calculations are fully relativistic result in wavefunctions that, in some orbitals, deviate quite strongly from the non-relativistic calculations of Clementi

*et al.* [27, 28], which in turn result in different atomic radii and screening constants.

## 2. The Dirac-Fock method

The Dirac-Fock (DF) method implemented in the MCDFGME computer code has been thoroughly described elsewhere [29, 30, 34], and it starts from a no-pair Hamiltonian, which is written as

$$\mathcal{H}^{\text{nopair}} = \sum_{i=1}^{N} \mathcal{H}_{\text{D}}(r_i) + \sum_{i<j} \upsilon(r_{ij}), \tag{3}$$

where $\mathcal{H}_{\text{D}}$ is a one-electron Dirac operator and $\upsilon$ is an operator that represents the two-body interaction and $r_{ij}$ is the inter-electronic distance ($|r_i - r_j|$). The operator $\upsilon$ combines the Coulomb potential with retardation and magnetic interactions, as well as projection operators [35]. The total wave function is then calculated with the help of the variational principle. We can write the total energy of the ion as

$$\mathcal{H}^{\text{nopair}} \left|\Psi_{\Pi,J,M}(r_1,...,r_N)\right\rangle = E_{\Pi,J,M} \left|\Psi_{\Pi,J,M}(r_1,...,r_N)\right\rangle, \tag{4}$$

where $\Pi$ is the parity, $J$ is the total angular momentum eigenvalue, and $M$ is the eigenvalue of its projection on the $z$ axis. **The DF method is then defined by the particular choice of the trial functions to solve Eq. (4), which are linear combinations of configuration state functions (CSF):**

$$\left|\Psi_{\Pi,J,M}\right\rangle = \sum_{\nu} c_\nu \left|\nu \Pi J M\right\rangle. \tag{5}$$

**These trial functions are eigenfunctions of the parity $\Pi$, the total angular momentum $J^2$, and its projection $J_z$. The label $\nu$ stands for all other numbers (principal quantum number,...) necessary to define unambiguously the CSF. The $c_\nu$ are called the mixing coefficients and are obtained by diagonalization of the Hamiltonian matrix coming from the minimization of the energy in Eq. (4) with respect to the $c_\nu$. In the present work, since we remain at the DF level, those coefficients will only account for the intermediate coupling. The configuration state functions are antisymmetric products of one-electron wave functions expressed as a linear combination of Slater determinants of Dirac 4-spinors, whose coefficients, $d_i$, are evaluated by requiring that the configuration state functions are eigenstates of $J^2$ and $J_z$,**

$$\left|\nu \Pi J M\right\rangle = \sum_i d_i \begin{vmatrix} \Phi_1^i(r_1) & \cdots & \Phi_N^i(r_1) \\ \vdots & \ddots & \vdots \\ \Phi_1^i(r_N) & \cdots & \Phi_N^i(r_N) \end{vmatrix}, \tag{6}$$

**where the $\Phi$-s are the one-electron wave functions. In the relativistic case, the one-electron wave functions are the Dirac four-component spinors:**

$$\boldsymbol{\Phi_{n\kappa\mu}(r)} = \frac{\mathbf{1}}{\boldsymbol{r}} \begin{bmatrix} \boldsymbol{P_{n\kappa}(r)\chi_{\kappa\mu}(\theta,\phi)} \\ \boldsymbol{iQ_{n\kappa}(r)\chi_{-\kappa\mu}(\theta,\phi)} \end{bmatrix}, \tag{7}$$

**where $\chi_{\kappa\mu}(\theta,\phi)$ is a two component Pauli spherical spinors [36], and $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and the small radial components of the wave function, respectively. The functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the solutions of coupled integro-differential equations obtained by minimizing the energy as defined in Eq. (4) with respect to each radial wave function.**

*2.1. Atomic radii and effective atomic number definitions*

**There are several different ways of defining the atomic radius of an atom or ion. In this work, we follow the definitions of Indelicato *et al.* [15], where besides the usual definition of the mean radius of a specific orbital as**

$$\langle r \rangle_{\mathrm{DF}} = \langle \Phi_{n\kappa\mu} | \, r \, | \Phi_{n\kappa\mu} \rangle \, , \tag{8}$$

**and the radii of maximum density of every subshell, $r_{\mathbf{max}}$, defined as the radius where $|r\Psi(r)|^2$ is maximum, we also define the mean atom radius $\langle r_{\mathbf{at.}} \rangle$ and the mean spherical radius $\sqrt{\langle r^2_{\mathbf{at.}} \rangle}$. These two last quantities are based on the total electronic density, and the radial electronic density is defined as [15]**

$$r^2 \rho(r) = \int r^2 \rho(r, \Omega) d\Omega = \sum_{i \in \mathrm{occ.orb.}} \varpi_i \left( P_i(r)^2 + Q_i(r)^2 \right) , \tag{9}$$

**where $P$ and $Q$ are defined in Eq. (7). The $\varpi_i$ are the orbital effective occupation numbers,**

$$\varpi_i = \sum_j c_j^2 n_j^i, \tag{10}$$

**and the sum extends over all configurations containing orbital $i$, whereas $n_j^i$ is the occupation number of this orbital in the configuration $j$. The total density is then normalized to**

$$\int_0^\infty r^2 \rho(r) dr = N_e, \tag{11}$$

**where $N_e$ is the number of electrons in the atom. In this way, the mean atom radius is represented as**

$$\left\langle r_{\mathrm{at.}}^{(p)} \right\rangle = \frac{1}{N_e} \int_0^\infty r^{(p)} r^2 \rho(r) dr, \tag{12}$$

**for $p = 1$, and the mean spherical radius is obtained as $\sqrt{\left\langle r_{\mathbf{at.}}^{(p)} \right\rangle}$ for $p = 2$.**

**The effective nuclear charge, $Z_{\mathbf{eff}}$, is then calculated by solving numerically the equation**

$$\langle r \rangle_{\mathrm{DF}} = \langle r \left( Z_{\mathrm{eff}} \right) \rangle_{\mathrm{Hydr.}} \, , \tag{13}$$

**where the point-nucleus, Dirac hydrogenic mean orbital radius is given by [37–40]**

$$\langle r(Z) \rangle_{\mathrm{Hydr.}} = \frac{(n - |\kappa| + \gamma) \left( 3N^2 - \kappa^2 \right) - \kappa N}{2ZN}, \tag{14}$$

with $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$ and $N = \sqrt{(n - |\kappa| + \gamma)^2 + (Z\alpha)^2}$.

## 3. Results and discussion

*3.1. Effective Z*

The effective nuclear charge values of all subshells of elements with $1 \leq Z \leq 118$ obtained in this work are presented in Fig. 1. The overall behavior is as expected, with inner shells presenting smoother curves as higher shells become filled. As can be seen from Fig. 2, where the $Z_{\mathrm{eff}}$ for the $L_1$, $L_2$ and $L_3$ subshells are plotted as a function of $Z$, there are some differences that can be quite substantial in the obtained $Z_{\mathrm{eff}}$ when compared to the results of Clementi *et al.*. These differences arise not only from the fact that their calculation is nonrelativistic, resulting in orbitals that deviate

strongly from the DF orbitals due to the relativistic contraction of the wavefunction, but also because they employed minimum basis sets composed of nodeless STO. **Although each STO is a nodeless function, due to orthogonality constraints in the SCF computation, the wavefunctions of the same symmetry are coupled. This means that the final wavefunctions will have the right number of nodes, but at the same time it means that the correspondence between the optimized orbital exponents and the screening parameters cannot be performed unambiguously. This is one of the reasons for the discrepancies observed in Fig. 3** where the $Z_{\text{eff}}$ for every subshell of Kr, Xe and Rn are compared to the results of Clementi *et al.*. The DF calculated $Z_{\text{eff}}$ values for every subshell of elements with $1 \leq Z \leq 118$ are presented in Tables 1, 2 and 3. QED contributions such as self-energy and vacuum polarization were included self consistently in our calculations, however their effect is almost negligible, contributing only with a maximum of 0.2% to the $Z_{\text{eff}}$. Note, however, that we have used configurations corresponding to the ground state of a Dirac-Fock calculation (i.e., without correlation), as given in [41]. For a few elements, the ground state configuration, as given for example on several databases, can be different. Nevertheless, as shown in [15] the lack of electronic correlation can give rise to variations in the atomic radii of less than 1% for high-Z elements.

### *3.2. Atomic radii*

The use of nodeless wavefunctions combined with the absence of relativistic effects in their calculation will result in radii of maximum charge density of the valence orbital that deviate from our results by around 3% for He, increasing to 40% for Hg. For La and Ce the radii show an even greater disparity, which is due to the fact that Clementi *et al.* had convergence problems due to the extreme broadness of the 4f orbital. For individual orbital radii, the differences can be even higher for some subshells, especially those which are not well described by a single STO. The divergence of results can be traced to the quality of the wavefunctions, as demonstrated in Fig. 4 since the definition of the $\mathrm{r}_{max}$ is the same in both works. In Table A the average radii of the $1s$, $2s$, $2p_{1/2}$, $2p_{3/2}$ and $3s$ subshells of Rn calculated both with the DF and HF methods, are also compared with the $< r >$ values of STO calculated with the optimized exponents of Clementi *et al.*, illustrating not only the effect of the relativistic treatment of the wavefunction, but also the quality of the STO wavefunctions.

As can be readily seen, the $2p_{3/2}$ wavefunction is very similar in both the DF and HF approach calculated in this work, and, since it has no nodes, it compares very well to the results of Clementi *et al.*. However for subshells in which the relativistic contraction is more evident and especially for wavefunctions with one or more nodes, the results deviate substantially. The radii of maximum charge density of every subshell, $r_{\max}$, are also presented in Tables 4, 5 and 6. In Table 7 we present the ground state mean atomic radius and the atom mean spherical radius, calculated using the total charge distribution, as described by Indelicato *et al.* [15] for all the elements of the periodic table. These values can be important in atomic drift spectroscopy as the drift time of an atom in a gas cell depends on its initial velocity and its charge distribution radius, while the maximum charge density of the valence orbital is of greater importance in molecular bonding for example.

In Fig. 5 we present the comparison of the average radius of the outer shell of neutral elements and compare them with the results of Clementi *et al.* as well as with the covalent radii values of Cordero *et al.* [19] and Pyykkö *et al.* [24]. The covalent radii of Cordero *et al.* and Pyykkö *et al.* were calculated having in mind the additive rule of the atomic radii for bond length calculation, and hence their results are highly dependent on the orbital hybridization,

| $< r >$ | DF | HF | [28] |
|---|---|---|---|
| $1s$ | 0.0151 | 0.0176 | 0.0176 |
| $2s$ | 0.0626 | 0.0738 | 0.0788 |
| $2p_{1/2}$ | 0.05126 | 0.06235 | |
| $2p_{3/2}$ | 0.06062 | 0.06235 | 0.0614 |
| $3s$ | 0.1625 | 0.1846 | 0.1389 |

Table A

Average radius, $< r >$ for the $1s$, $2s$, $2p_{1/2}$, $2p_{3/2}$ and 3s orbitals of Rn calculated using the Dirac-Fock and Hartree-Fock methods. The $< r >$ values are also compared with the ones computed with a single STO with orbital exponents obtained by Clementi *et al.*.

molecular bond type, coordination number and whether they show a single- or multiple-bond character [24, 42]. In fact, it is well known that the cationic radius of an element is typically at least 0.5 Å shorter than its covalent radius, while the opposite situation occurs with the anionic radii, showing how strongly the effective radius of an atom depends on its electronegativity relative to that of the atom to which it is bonded. Note, however, that our values correspond to the radial values of the probability distribution maximum of the valence shell, which should not be compared directly with the covalent radii of every element, as the features described above can be very important for different groups of elements in the periodic table. For instance, the bonds between transition metals and halides tend to show a multiple-bond character, and in fact the triple bond covalent radii of Pyykkö *et al.* [42] show better agreement with our halogens results than their single bond data [24]. We emphasize the fact that we have used the configurations corresponding to the ground state of a DF calculation (i.e., without correlation), as given in [41]. For some elements, the ground state configuration obtained through HF calculations as well as those given for example on the NIST database [43], can be different.

As can be readily seen in Fig. 5, our results compare very well with the values of Cordero *et al.* except for the halogens and rare gases, for which our values are substantially lower. This can be traced back to the fact that the molecular bonds of compounds with such elements do not usually involve one single orbital, having a multiple-bond character. On the other hand, our results for the radii of alkali metals are somewhat higher than those of both Cordero *et al.* and Pyykkö *et al.* but lower than those of Clementi *et al.* which can be attributed to relativistic effects. For Pd (Z=46) we notice a huge discrepancy with all the compared results, as the DF ground state configuration, which also corresponds to the one presented in the NIST database [43], is $[Kr]4d^{10}$ in contrast with its neighbors which have in their ground state configuration the 5s orbital. In fact, the calculated ground state configuration with the HF method of Clementi *et al.* [28] is $[Kr]4d^{8}5s^{2}$, which explains the smoothness of their curve near Z=46. The fact that the covalent radii also presents the same smoothness, is due to the mixing of the 4d and 5s orbitals in the HOMO of Pd complexes [44].

## 4. Conclusions

We have calculated the effective nuclear charge and maximum charge density radii for every subshell of elements with $1 \leq Z \leq 118$ using the Dirac-Fock formalism. The results were compared to those of Clementi *et al.* which have been ubiquitously used for several decades, and the radii data with the results of Cordero *et al.* and Pyykkö *et al.*. Deviations up to 30% were found in the $Z_{\text{eff}}$, especially for the multiple node orbitals of high $Z$ elements, and differences up to 40% have been found in the radii of maximum charge density of the valence orbitals with the results of Clementi *et al.*, while greater disparities were found in the comparison with the covalent radii of Cordero *et al.* and Pyykkö *et al.*. Although some of the physical properties that are usually calculated from the parameters discussed in this work are not very sensitive to changes in the mentioned parameters, others (such as covalent radii, vacuum polarization, self-energy, etc.) can be severely influenced by changes in the $Z_{\text{eff}}$ and $r_{\max}$. Consequently, we believe that our work could prove invaluable in updating the databases in which the Clementi *et al.* results are used.

## Acknowledgments

M. Guerra and P. Amaro acknowledge the support of the FCT, under Contracts No. SFRH/BPD/92455/2013 and SFRH/BPD/92329/2013, respectively. This work was supported in part by the research center grant no. UID/FIS/04559/2013 to LIBPhys-UNL, from the FCT/MCTES/PIDDAC.

Laboratoire Kastler Brossel (LKB) is "Unité Mixte de Recherche du CNRS, de l'ENS et de l'UPMC n° 8552". P.I. thanks the Allianz Program of the Helmholtz Association, contract n° EMMI HA-216 "Extremes of Density and Temperature: Cosmic Matter in the Laboratory".

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## Figures

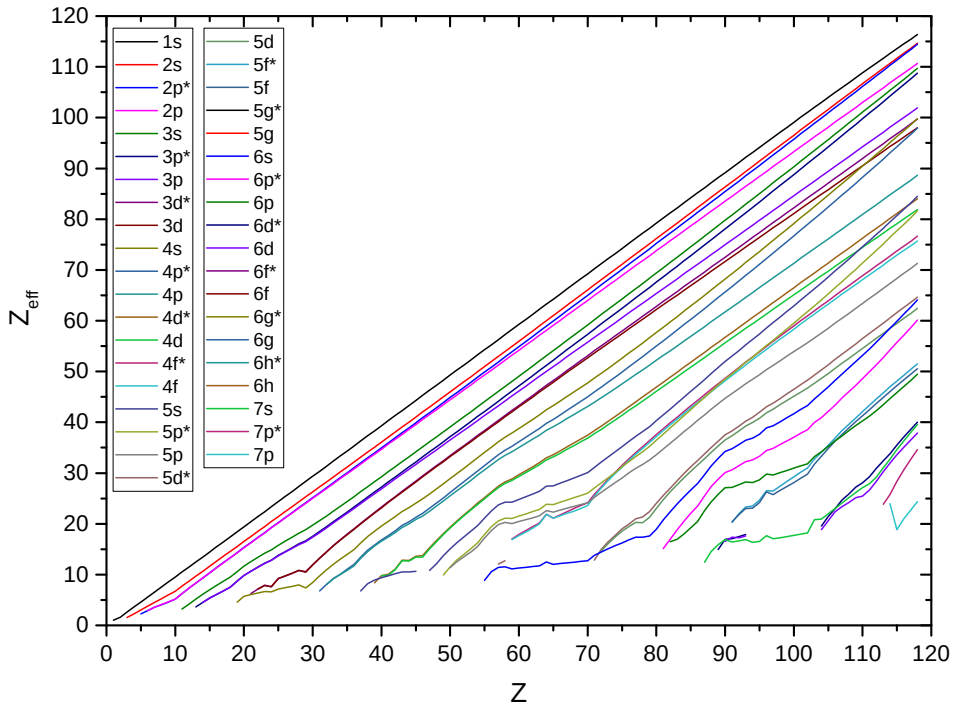



**Fig. 1**: Dirac-Fock effective nuclear charge as a function of the atomic number. Stared orbital labels correspond to the orbital with $j = l - \frac{1}{2}$.

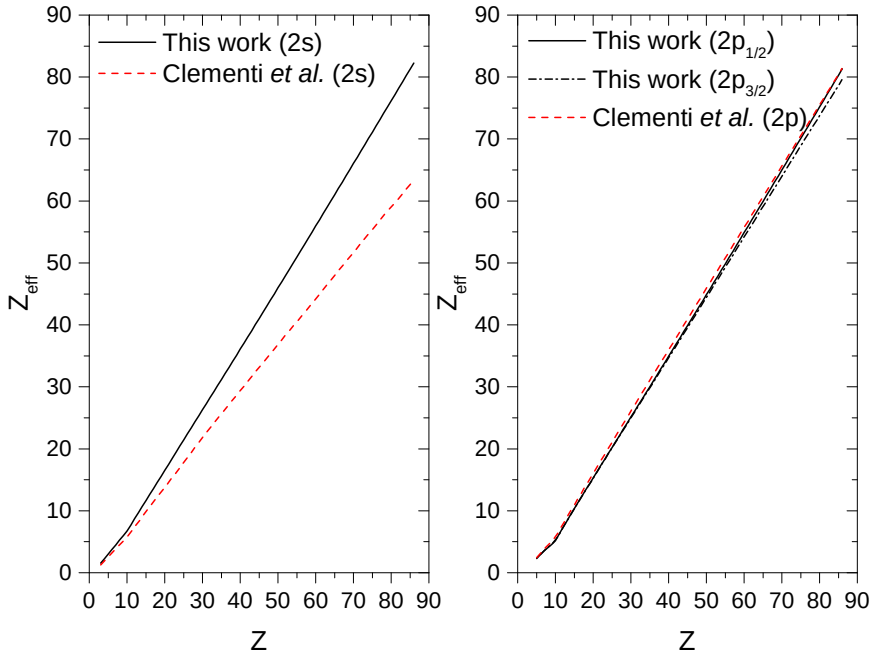



**Fig. 2**: Comparison of the effective nuclear charge calculated in this work with the results of Clementi *et al.* [27, 28]

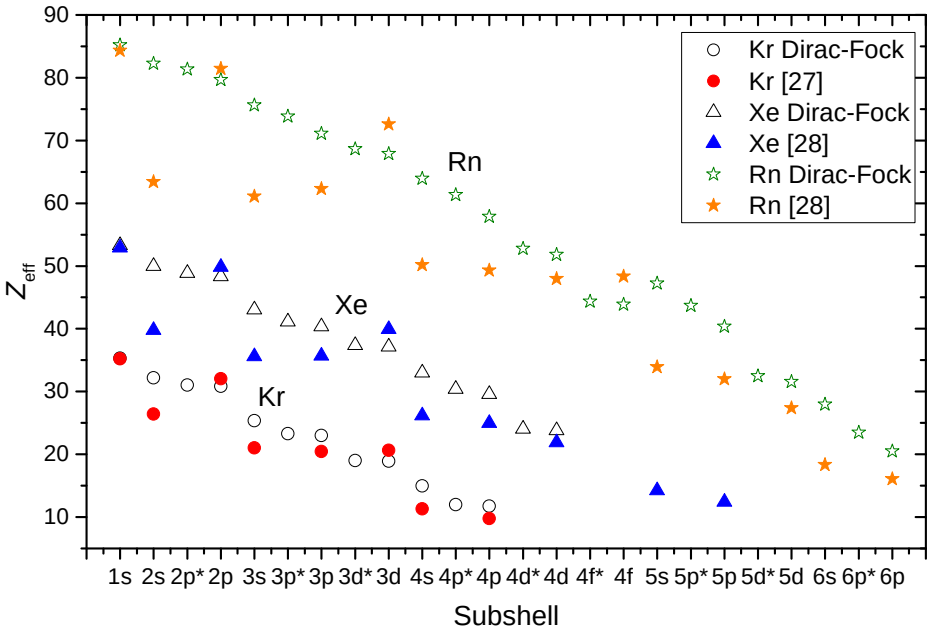



**Fig. 3**: Comparison of the Dirac-Fock and Hartree-Fock effective nuclear charge calculated in this work for all subshells of Kr, Xe and Rn. Stared orbital labels correspond to the orbital with $j = l - \frac{1}{2}$.

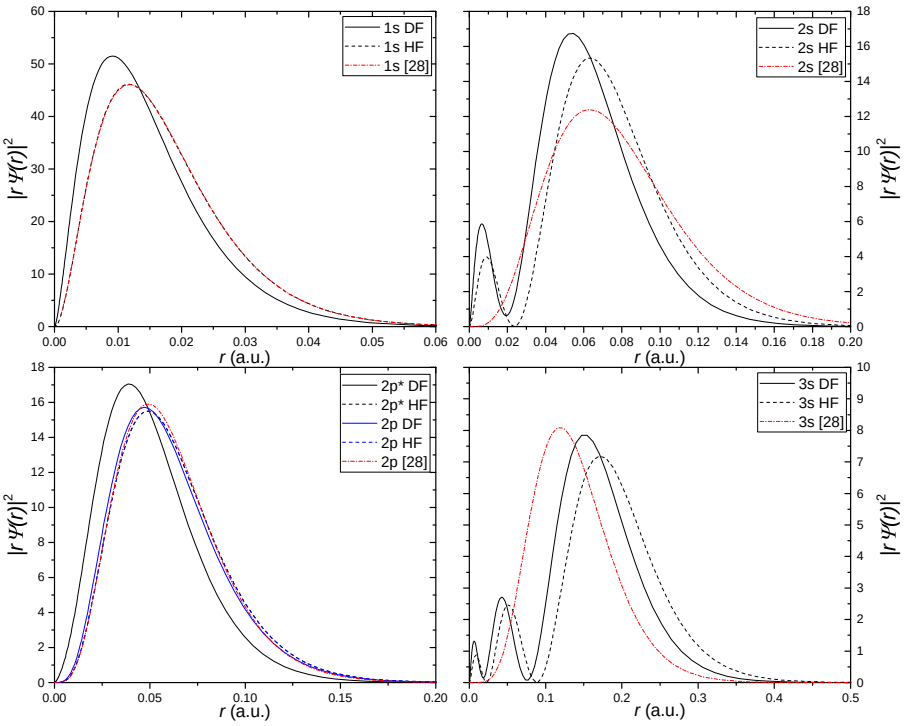



**Fig. 4**: Hartree-Fock and Dirac-Fock radial probability densities for the $1s$, $2s$, $2p_{1/2}$, $2p_{3/2}$ and $3s$ subshells of Rn. Shown also are STO with the orbital exponents obtained by Clementi *et al.* [27, 28].

### Explanation of Tables

**Table 1. Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from $1s$ to $4s$.**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $1s, 2s, 2p_{1/2}, ...$ | Atomic subshells. |

**Table 2. Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from $4p_{1/2}$ to $5f_{7/2}$.**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $4p_{1/2}, 4p_{3/2}, 4d_{3/2}, ...$ | Atomic subshells. |

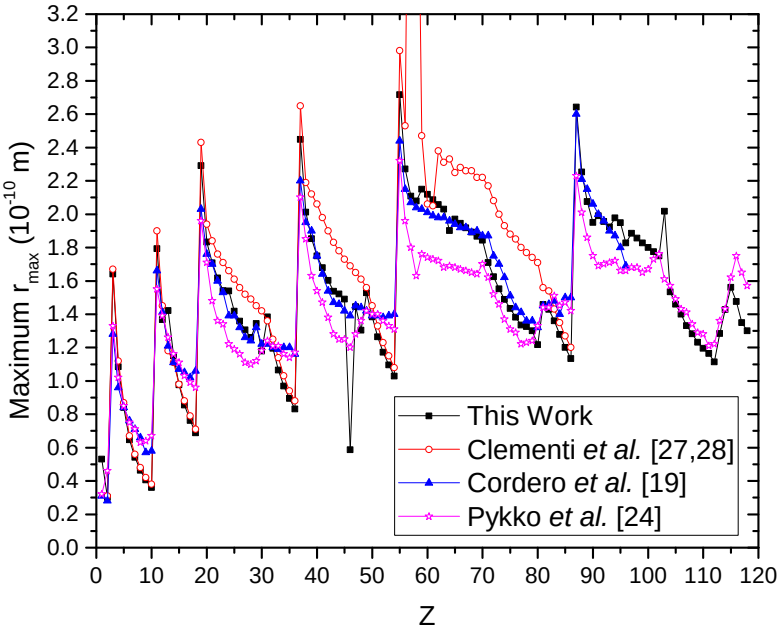



**Fig. 5**: Radii of maximum charge distribution, $r_{\max}$, of the valence shell of elements with $1 \leq Z \leq 118$. Presented also are the maximum charge distribution values of Clementi *et al.* [27, 28], as well as the single-bond covalent radii of Cordero *et al.* [19] and Pyykö *et al.* [24].

**Table 3. Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from $6s$ to $7p_{3/2}$.**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $6s, 6p_{1/2}, 6p_{3/2}, ...$ | Atomic subshells. |

**Table 4. Radii of maximum charge density, $r_{\max}$, calculated with the Dirac-Fock method for subshells ranging from 1s to 4s ($a_0$).**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $1s, 2s, 2p_{1/2}, ...$ | Atomic subshells. |

**Table 5. Radii of maximum charge density, $r_{\max}$, calculated with the Dirac-Fock method for subshells ranging from $4p_{1/2}$ to $5f_{7/2}$ ($a_0$).**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $4p_{1/2}, 4p_{3/2}, 4d_{3/2}, ...$ | Atomic subshells. |

**Table 6. Radii of maximum charge density, $r_{\mathbf{max}}$, calculated with the Dirac-Fock method for subshells ranging from $6s$ to $7p_{3/2}$ ($a_0$).**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| $6s, 6p_{1/2}, 6p_{3/2}, ...$ | Atomic subshells. |

**Table 7. Atom mean radius, $\langle r_{\mathbf{at}} \rangle$, using the total charge density and atom mean spherical radius, $\sqrt{\langle r_{\mathbf{at}}^{\mathbf{2}} \rangle}$, of neutral elements with $1 \leq Z \leq 118$ ($a_0$).**

| | |
|---|---|
| Configuration | Ground state configuration, obtained from reference [41], for which the calculation was performed. |
| Atom mean radius | Atomic radius, $\langle r_{\mathrm{at}} \rangle$, using total charge density from Eq. (12) |
| Atom mean spherical radius | Atomic spherical radius obtained as $\sqrt{\langle r_{\mathrm{at}}^2 \rangle}$ from Eq. (12) |

**Explanation of Graphs**

**Graph 1. Dirac-Fock effective nuclear charge.**

| | |
|---|---|
| $Z$ | Atomic number |
| $Z_{\text{eff}}$ | Effective nuclear charge |
| $*$ | Stared orbital labels correspond to the orbital with $j = l - \frac{1}{2}$. |

**Graph 2. Comparison of the $n = 2$ $Z_{\text{eff}}$ with the results of Clementi *et al.* [27, 28].**

| | |
|---|---|
| $Z_{\text{eff}}$ | Effective nuclear charge. |
| $Z$ | Atomic number. |

**Graph 3. Comparison of the Dirac-Fock and Hartree-Fock effective nuclear charge calculated in this work for all subshells of Kr, Xe and Rn.**

| | |
|---|---|
| $Z_{\text{eff}}$ | Effective nuclear charge. |
| $*$ | Stared orbital labels correspond to the orbital with $j = l - \frac{1}{2}$. |

**Graph 4. Hartree-Fock and Dirac-Fock wavefunctions for the $1s$, $2s$, $2p_{1/2}$, $2p_{3/2}$ and $3s$ subshells of Rn.**

| | |
|---|---|
| $\lvert r\Psi(r)\rvert^2$ | Radial probability density. |
| $r$ | Distance to the nucleus in $a_0$ |
| $DF, HF$ | Dirac-Fock and Hartree-Fock values, respectively. |

**Graph 5. Radii of maximum charge distribution of the valence shell of elements with $1 \leq Z \leq 118$.**

| | |
|---|---|
| $Z$ | Atomic number |
| Maximum $r_{\max}$ | Maximum charge density of the valence shell. |

**Table 1**
Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from 1s to 4s.

| Atomic Number | Configuration | $1s$ | $2s$ | $2p_{1/2}$ | $2p_{3/2}$ | 3s | $3p_{1/2}$ | $3p_{3/2}$ | $3d_{3/2}$ | $3d_{5/2}$ | 4s |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $1s$ | 1.000 | | | | | | | | | |
| 2 | $1s^2$ | 1.618 | | | | | | | | | |
| 3 | $1s^2 2s$ | 2.617 | 1.550 | | | | | | | | |
| 4 | $1s^2 2s^2$ | 3.614 | 2.266 | | | | | | | | |
| 5 | $1s^2 2s^2 2p$ | 4.603 | 3.036 | 2.268 | | | | | | | |
| 6 | $1s^2 2s^2 2p^2$ | 5.587 | 3.776 | 2.916 | 2.916 | | | | | | |
| 7 | $1s^2 2s^2 2p^3$ | 6.570 | 4.505 | 3.547 | 3.546 | | | | | | |
| 8 | $1s^2 2s^2 2p^4$ | 7.553 | 5.257 | 4.022 | 4.082 | | | | | | |
| 9 | $1s^2 2s^2 2p^5$ | 8.534 | 5.997 | 4.598 | 4.615 | | | | | | |
| 10 | $1s^2 2s^2 2p^6$ | 9.515 | 6.731 | 5.185 | 5.175 | | | | | | |
| 11 | [Ne]$3s$ | 10.498 | 7.708 | 6.268 | 6.256 | 3.211 | | | | | |
| 12 | [Ne]$3s^2$ | 11.484 | 8.699 | 7.306 | 7.292 | 4.156 | | | | | |
| 13 | [Ne]$3s^2 3p$ | 12.471 | 9.686 | 8.343 | 8.313 | 5.201 | 3.642 | | | | |
| 14 | [Ne]$3s^2 3p^2$ | 13.459 | 10.669 | 9.362 | 9.323 | 6.127 | 4.543 | 4.541 | | | |
| 15 | [Ne]$3s^2 3p^3$ | 14.448 | 11.648 | 10.355 | 10.332 | 6.999 | 5.386 | 5.376 | | | |
| 16 | [Ne]$3s^2 3p^4$ | 15.437 | 12.625 | 11.356 | 11.321 | 7.863 | 6.041 | 6.083 | | | |
| 17 | [Ne]$3s^2 3p^5$ | 16.427 | 13.599 | 12.357 | 12.306 | 8.699 | 6.789 | 6.781 | | | |
| 18 | [Ne]$3s^2 3p^6$ | 17.417 | 14.572 | 13.340 | 13.304 | 9.519 | 7.541 | 7.502 | | | |
| 19 | [Ar]$4s$ | 18.408 | 15.550 | 14.330 | 14.289 | 10.601 | 8.726 | 8.685 | | | 4.593 |
| 20 | [Ar]$4s^2$ | 19.400 | 16.530 | 15.320 | 15.275 | 11.677 | 9.837 | 9.791 | | | 5.709 |
| 21 | [Ar]$3d4s^2$ | 20.394 | 17.510 | 16.303 | 16.262 | 12.549 | 10.673 | 10.633 | 6.216 | | 6.090 |
| 22 | [Ar]$3d^2 4s^2$ | 21.388 | 18.490 | 17.286 | 17.244 | 13.377 | 11.471 | 11.415 | 7.146 | 7.139 | 6.388 |
| 23 | [Ar]$3d^3 4s^2$ | 22.382 | 19.468 | 18.270 | 18.222 | 14.189 | 12.251 | 12.178 | 7.904 | 7.845 | 6.664 |
| 24 | [Ar]$3d^5 4s$ | 23.378 | 20.446 | 19.264 | 19.193 | 14.875 | 12.864 | 12.774 | 7.631 | 7.608 | 6.615 |
| 25 | [Ar]$3d^5 4s^2$ | 24.372 | 21.421 | 20.244 | 20.165 | 15.776 | 13.766 | 13.666 | 9.246 | 9.225 | 7.161 |
| 26 | [Ar]$3d^6 4s^2$ | 25.368 | 22.397 | 21.218 | 21.140 | 16.578 | 14.537 | 14.422 | 9.670 | 9.779 | 7.442 |
| 27 | [Ar]$3d^7 4s^2$ | 26.364 | 23.373 | 22.194 | 22.112 | 17.370 | 15.297 | 15.163 | 10.240 | 10.300 | 7.699 |
| 28 | [Ar]$3d^8 4s^2$ | 27.360 | 24.348 | 23.172 | 23.081 | 18.157 | 16.053 | 15.898 | 10.829 | 10.805 | 7.948 |
| 29 | [Ar]$3d^{10} 4s$ | 28.357 | 25.324 | 24.161 | 24.045 | 18.835 | 16.667 | 16.495 | 10.584 | 10.479 | 7.351 |
| 30 | [Ar]$3d^{10} 4s^2$ | 29.353 | 26.298 | 25.137 | 25.011 | 19.719 | 17.544 | 17.356 | 11.978 | 11.886 | 8.416 |
| 31 | [Ar]$3d^{10} 4s^2 4p$ | 30.349 | 27.273 | 26.114 | 25.976 | 20.623 | 18.468 | 18.257 | 13.272 | 13.228 | 9.782 |
| 32 | [Ar]$3d^{10} 4s^2 4p^2$ | 31.345 | 28.248 | 27.093 | 26.942 | 21.549 | 19.420 | 19.184 | 14.501 | 14.457 | 10.934 |
| 33 | [Ar]$3d^{10} 4s^2 4p^3$ | 32.341 | 29.224 | 28.071 | 27.909 | 22.489 | 20.370 | 20.136 | 15.694 | 15.613 | 11.995 |
| 34 | [Ar]$3d^{10} 4s^2 4p^4$ | 33.337 | 30.201 | 29.051 | 28.876 | 23.439 | 21.342 | 21.083 | 16.822 | 16.751 | 13.023 |
| 35 | [Ar]$3d^{10} 4s^2 4p^5$ | 34.333 | 31.179 | 30.033 | 29.844 | 24.397 | 22.324 | 22.037 | 17.929 | 17.850 | 14.003 |
| 36 | [Ar]$3d^{10} 4s^2 4p^6$ | 35.329 | 32.158 | 31.014 | 30.813 | 25.359 | 23.298 | 23.012 | 19.018 | 18.924 | 14.950 |
| 37 | [Kr]$5s$ | 36.325 | 33.139 | 31.998 | 31.782 | 26.331 | 24.283 | 23.977 | 20.096 | 19.998 | 16.241 |
| 38 | [Kr]$5s^2$ | 37.322 | 34.121 | 32.983 | 32.752 | 27.308 | 25.271 | 24.946 | 21.166 | 21.062 | 17.503 |
| 39 | [Kr]$4d5s^2$ | 38.318 | 35.105 | 33.968 | 33.723 | 28.285 | 26.261 | 25.914 | 22.234 | 22.117 | 18.574 |
| 40 | [Kr]$4d^2 5s^2$ | 39.315 | 36.089 | 34.955 | 34.695 | 29.264 | 27.250 | 26.882 | 23.290 | 23.160 | 19.575 |
| 41 | [Kr]$4d^4 5s$ | 40.311 | 37.074 | 35.943 | 35.666 | 30.240 | 28.238 | 27.848 | 24.335 | 24.199 | 20.463 |
| 42 | [Kr]$4d^5 5s$ | 41.308 | 38.060 | 36.932 | 36.637 | 31.220 | 29.226 | 28.812 | 25.361 | 25.232 | 21.403 |
| 43 | [Kr]$4d^5 5s^2$ | 42.305 | 39.048 | 37.922 | 37.610 | 32.203 | 30.214 | 29.776 | 26.384 | 26.247 | 22.398 |
| 44 | [Kr]$4d^7 5s$ | 43.302 | 40.036 | 38.912 | 38.582 | 33.181 | 31.201 | 30.738 | 27.406 | 27.251 | 23.217 |
| 45 | [Kr]$4d^8 5s$ | 44.299 | 41.025 | 39.903 | 39.555 | 34.163 | 32.189 | 31.698 | 28.416 | 28.253 | 24.107 |
| 46 | [Kr]$4d^{10}$ | 45.296 | 42.014 | 40.897 | 40.528 | 35.143 | 33.176 | 32.656 | 29.429 | 29.271 | 24.893 |
| 47 | [Kr]$4d^{10} 5s$ | 46.294 | 43.005 | 41.890 | 41.501 | 36.127 | 34.164 | 33.614 | 30.430 | 30.264 | 25.864 |
| 48 | [Kr]$4d^{10} 5s^2$ | 47.291 | 43.997 | 42.884 | 42.474 | 37.113 | 35.152 | 34.573 | 31.428 | 31.254 | 26.871 |
| 49 | [Kr]$4d^{10} 5s^2 5p$ | 48.288 | 44.989 | 43.879 | 43.447 | 38.100 | 36.144 | 35.531 | 32.424 | 32.242 | 27.877 |
| 50 | [Kr]$4d^{10} 5s^2 5p^2$ | 49.285 | 45.982 | 44.875 | 44.421 | 39.088 | 37.138 | 36.491 | 33.419 | 33.228 | 28.896 |
| 51 | [Kr]$4d^{10} 5s^2 5p^3$ | 50.282 | 46.976 | 45.872 | 45.395 | 40.079 | 38.131 | 37.454 | 34.413 | 34.212 | 29.922 |
| 52 | [Kr]$4d^{10} 5s^2 5p^4$ | 51.280 | 47.971 | 46.869 | 46.370 | 41.071 | 39.129 | 38.416 | 35.405 | 35.195 | 30.951 |
| 53 | [Kr]$4d^{10} 5s^2 5p^5$ | 52.277 | 48.967 | 47.868 | 47.345 | 42.064 | 40.128 | 39.379 | 36.396 | 36.176 | 31.984 |
| 54 | [Kr]$4d^{10} 5s^2 5p^6$ | 53.274 | 49.963 | 48.867 | 48.319 | 43.060 | 41.128 | 40.344 | 37.387 | 37.157 | 33.017 |
| 55 | [Xe]$6s$ | 54.271 | 50.960 | 49.867 | 49.295 | 44.058 | 42.130 | 41.309 | 38.377 | 38.137 | 34.056 |
| 56 | [Xe]$6s^2$ | 55.269 | 51.958 | 50.868 | 50.270 | 45.058 | 43.134 | 42.275 | 39.368 | 39.116 | 35.099 |
| 57 | [Xe]$5d6s^2$ | 56.266 | 52.957 | 51.870 | 51.245 | 46.059 | 44.140 | 43.241 | 40.358 | 40.094 | 36.137 |
| 58 | [Xe]$4f5d6s^2$ | 57.264 | 53.960 | 52.876 | 52.225 | 47.065 | 45.148 | 44.211 | 41.345 | 41.078 | 37.059 |
| 59 | [Xe]$4f^3 6s^2$ | 58.262 | 54.966 | 53.886 | 53.209 | 48.075 | 46.159 | 45.186 | 42.322 | 42.068 | 37.871 |
| 60 | [Xe]$4f^4 6s^2$ | 59.259 | 55.971 | 54.894 | 54.189 | 49.081 | 47.170 | 46.153 | 43.308 | 43.044 | 38.775 |
| 61 | [Xe]$4f^5 6s^2$ | 60.257 | 56.976 | 55.903 | 55.170 | 50.089 | 48.182 | 47.120 | 44.294 | 44.016 | 39.676 |
| 62 | [Xe]$4f^6 6s^2$ | 61.255 | 57.982 | 56.913 | 56.151 | 51.097 | 49.195 | 48.085 | 45.280 | 44.985 | 40.572 |
| 63 | [Xe]$4f^7 6s^2$ | 62.252 | 58.989 | 57.924 | 57.132 | 52.106 | 50.214 | 49.047 | 46.275 | 45.944 | 41.464 |
| 64 | [Xe]$4f^7 5d6s^2$ | 63.250 | 59.994 | 58.933 | 58.111 | 53.112 | 51.224 | 50.008 | 47.253 | 46.907 | 42.431 |
| 65 | [Xe]$4f^9 6s^2$ | 64.248 | 61.004 | 59.947 | 59.095 | 54.126 | 52.238 | 50.978 | 48.220 | 47.886 | 43.263 |
| 66 | [Xe]$4f^{10} 6s^2$ | 65.246 | 62.013 | 60.960 | 60.077 | 55.137 | 53.253 | 51.942 | 49.196 | 48.851 | 44.158 |
| 67 | [Xe]$4f^{11} 6s^2$ | 66.244 | 63.023 | 61.973 | 61.058 | 56.150 | 54.272 | 52.904 | 50.176 | 49.811 | 45.055 |

**Table 1** (continued)

| Atomic Number | Configuration | $1s$ | $2s$ | $2p_{1/2}$ | $2p_{3/2}$ | 3s | $3p_{1/2}$ | $3p_{3/2}$ | $3d_{3/2}$ | $3d_{5/2}$ | 4s |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 68 | $[Xe]4f^{12}6s^2$ | 67.241 | 64.033 | 62.988 | 62.040 | 57.163 | 55.292 | 53.865 | 51.156 | 50.768 | 45.953 |
| 69 | $[Xe]4f^{13}6s^2$ | 68.239 | 65.044 | 64.003 | 63.021 | 58.178 | 56.313 | 54.825 | 52.138 | 51.723 | 46.851 |
| 70 | $[Xe]4f^{14}6s^2$ | 69.237 | 66.055 | 65.019 | 64.003 | 59.193 | 57.337 | 55.785 | 53.121 | 52.674 | 47.748 |
| 71 | $[Xe]4f^{14}5d6s^2$ | 70.234 | 67.065 | 66.034 | 64.983 | 60.207 | 58.356 | 56.742 | 54.092 | 53.626 | 48.697 |
| 72 | $[Xe]4f^{14}5d^26s^2$ | 71.232 | 68.076 | 67.049 | 65.962 | 61.222 | 59.377 | 57.699 | 55.062 | 54.578 | 49.659 |
| 73 | $[Xe]4f^{14}5d^36s^2$ | 72.230 | 69.087 | 68.065 | 66.941 | 62.238 | 60.398 | 58.656 | 56.032 | 55.528 | 50.633 |
| 74 | $[Xe]4f^{14}5d^46s^2$ | 73.227 | 70.099 | 69.082 | 67.919 | 63.256 | 61.421 | 59.613 | 57.001 | 56.479 | 51.617 |
| 75 | $[Xe]4f^{14}5d^56s^2$ | 74.225 | 71.111 | 70.099 | 68.897 | 64.275 | 62.446 | 60.569 | 57.969 | 57.430 | 52.610 |
| 76 | $[Xe]4f^{14}5d^66s^2$ | 75.222 | 72.123 | 71.116 | 69.875 | 65.296 | 63.473 | 61.527 | 58.939 | 58.379 | 53.610 |
| 77 | $[Xe]4f^{14}5d^76s^2$ | 76.220 | 73.136 | 72.135 | 70.853 | 66.318 | 64.501 | 62.484 | 59.908 | 59.329 | 54.618 |
| 78 | $[Xe]4f^{14}5d^96s$ | 77.217 | 74.149 | 73.154 | 71.830 | 67.341 | 65.531 | 63.440 | 60.876 | 60.279 | 55.629 |
| 79 | $[Xe]4f^{14}5d^{10}6s$ | 78.214 | 75.163 | 74.173 | 72.807 | 68.367 | 66.563 | 64.398 | 61.844 | 61.228 | 56.648 |
| 80 | $[Xe]4f^{14}5d^{10}6s^2$ | 79.211 | 76.177 | 75.193 | 73.784 | 69.395 | 67.598 | 65.356 | 62.813 | 62.177 | 57.676 |
| 81 | $[Xe]4f^{14}5d^{10}6s^26p$ | 80.208 | 77.192 | 76.214 | 74.761 | 70.425 | 68.635 | 66.314 | 63.782 | 63.125 | 58.708 |
| 82 | $[Xe]4f^{14}5d^{10}6s^26p^2$ | 81.204 | 78.207 | 77.236 | 75.737 | 71.456 | 69.674 | 67.273 | 64.752 | 64.074 | 59.745 |
| 83 | $[Xe]4f^{14}5d^{10}6s^26p^3$ | 82.200 | 79.222 | 78.258 | 76.713 | 72.489 | 70.715 | 68.233 | 65.721 | 65.022 | 60.788 |
| 84 | $[Xe]4f^{14}5d^{10}6s^26p^4$ | 83.197 | 80.238 | 79.281 | 77.689 | 73.525 | 71.759 | 69.193 | 66.691 | 65.970 | 61.836 |
| 85 | $[Xe]4f^{14}5d^{10}6s^26p^5$ | 84.192 | 81.254 | 80.304 | 78.665 | 74.562 | 72.805 | 70.154 | 67.661 | 66.918 | 62.888 |
| 86 | $[Xe]4f^{14}5d^{10}6s^26p^6$ | 85.186 | 82.270 | 81.329 | 79.640 | 75.601 | 73.853 | 71.115 | 68.632 | 67.866 | 63.945 |
| 87 | $[Rn]7s$ | 86.182 | 83.287 | 82.354 | 80.615 | 76.642 | 74.904 | 72.076 | 69.602 | 68.814 | 65.008 |
| 88 | $[Rn]7s^2$ | 87.176 | 84.304 | 83.380 | 81.590 | 77.685 | 75.957 | 73.038 | 70.573 | 69.762 | 66.076 |
| 89 | $[Rn]6d7s^2$ | 88.171 | 85.322 | 84.406 | 82.565 | 78.730 | 77.012 | 74.001 | 71.545 | 70.709 | 67.147 |
| 90 | $[Rn]6d^27s^2$ | 89.165 | 86.340 | 85.434 | 83.539 | 79.777 | 78.069 | 74.963 | 72.516 | 71.657 | 68.222 |
| 91 | $[Rn]5f^26d7s^2$ | 90.158 | 87.359 | 86.463 | 84.515 | 80.827 | 79.130 | 75.927 | 73.487 | 72.606 | 69.296 |
| 92 | $[Rn]5f^36d7s^2$ | 91.149 | 88.376 | 87.492 | 85.489 | 81.876 | 80.193 | 76.891 | 74.459 | 73.554 | 70.375 |
| 93 | $[Rn]5f^46d7s^2$ | 92.143 | 89.397 | 88.523 | 86.464 | 82.930 | 81.258 | 77.855 | 75.431 | 74.502 | 71.459 |
| 94 | $[Rn]5f^67s^2$ | 93.134 | 90.416 | 89.554 | 87.439 | 83.985 | 82.327 | 78.819 | 76.403 | 75.450 | 72.542 |
| 95 | $[Rn]5f^77s^2$ | 94.123 | 91.435 | 90.586 | 88.413 | 85.041 | 83.398 | 79.783 | 77.379 | 76.395 | 73.632 |
| 96 | $[Rn]5f^76d7s^2$ | 95.115 | 92.455 | 91.618 | 89.386 | 86.100 | 84.470 | 80.747 | 78.351 | 77.341 | 74.728 |
| 97 | $[Rn]5f^97s^2$ | 96.105 | 93.476 | 92.652 | 90.361 | 87.161 | 85.546 | 81.712 | 79.322 | 78.288 | 75.824 |
| 98 | $[Rn]5f^{10}7s^2$ | 97.093 | 94.495 | 93.687 | 91.334 | 88.222 | 86.624 | 82.676 | 80.295 | 79.233 | 76.924 |
| 99 | $[Rn]5f^{11}7s^2$ | 98.081 | 95.515 | 94.722 | 92.307 | 89.286 | 87.706 | 83.641 | 81.268 | 80.178 | 78.029 |
| 100 | $[Rn]5f^{12}7s^2$ | 99.067 | 96.534 | 95.757 | 93.279 | 90.352 | 88.789 | 84.605 | 82.242 | 81.122 | 79.137 |
| 101 | $[Rn]5f^{13}7s^2$ | 100.051 | 97.552 | 96.794 | 94.251 | 91.418 | 89.876 | 85.570 | 83.215 | 82.066 | 80.249 |
| 102 | $[Rn]5f^{14}7s^2$ | 101.034 | 98.571 | 97.831 | 95.223 | 92.487 | 90.965 | 86.535 | 84.189 | 83.009 | 81.364 |
| 103 | $[Rn]5f^{14}7s^27p$ | 102.017 | 99.589 | 98.868 | 96.194 | 93.558 | 92.057 | 87.499 | 85.161 | 83.952 | 82.485 |
| 104 | $[Rn]5f^{14}6d^27s^2$ | 102.997 | 100.607 | 99.906 | 97.164 | 94.629 | 93.151 | 88.463 | 86.133 | 84.893 | 83.610 |
| 105 | $[Rn]5f^{14}6d^37s^2$ | 103.976 | 101.623 | 100.945 | 98.134 | 95.702 | 94.248 | 89.427 | 87.105 | 85.835 | 84.740 |
| 106 | $[Rn]5f^{14}6d^47s^2$ | 104.941 | 102.631 | 101.982 | 99.103 | 96.770 | 95.346 | 90.391 | 88.077 | 86.776 | 85.868 |
| 107 | $[Rn]5f^{14}6d^57s^2$ | 105.914 | 103.644 | 103.021 | 100.072 | 97.844 | 96.448 | 91.355 | 89.048 | 87.716 | 87.005 |
| 108 | $[Rn]5f^{14}6d^67s^2$ | 106.884 | 104.656 | 104.061 | 101.040 | 98.920 | 97.554 | 92.319 | 90.020 | 88.656 | 88.147 |
| 109 | $[Rn]5f^{14}6d^77s^2$ | 107.851 | 105.666 | 105.101 | 102.007 | 99.997 | 98.662 | 93.283 | 90.991 | 89.595 | 89.293 |
| 110 | $[Rn]5f^{14}6d^97s$ | 108.815 | 106.674 | 106.141 | 102.974 | 101.074 | 99.772 | 94.246 | 91.961 | 90.534 | 90.442 |
| 111 | $[Rn]5f^{14}6d^{10}7s$ | 109.775 | 107.680 | 107.181 | 103.940 | 102.151 | 100.886 | 95.209 | 92.932 | 91.472 | 91.595 |
| 112 | $[Rn]5f^{14}6d^{10}7s^2$ | 110.731 | 108.684 | 108.220 | 104.905 | 103.230 | 102.003 | 96.172 | 93.902 | 92.409 | 92.754 |
| 113 | $[Rn]5f^{14}6d^{10}7s^27p$ | 111.684 | 109.684 | 109.260 | 105.870 | 104.308 | 103.122 | 97.135 | 94.872 | 93.346 | 93.917 |
| 114 | $[Rn]5f^{14}6d^{10}7s^27p^2$ | 112.631 | 110.682 | 110.299 | 106.834 | 105.386 | 104.245 | 98.098 | 95.842 | 94.282 | 95.083 |
| 115 | $[Rn]5f^{14}6d^{10}7s^27p^3$ | 113.574 | 111.676 | 111.337 | 107.797 | 106.464 | 105.370 | 99.060 | 96.811 | 95.217 | 96.253 |
| 116 | $[Rn]5f^{14}6d^{10}7s^27p^4$ | 114.511 | 112.666 | 112.374 | 108.759 | 107.541 | 106.497 | 100.023 | 97.781 | 96.151 | 97.427 |
| 117 | $[Rn]5f^{14}6d^{10}7s^27p^5$ | 115.442 | 113.651 | 113.410 | 109.721 | 108.617 | 107.627 | 100.984 | 98.749 | 97.085 | 98.605 |
| 118 | $[Rn]5f^{14}6d^{10}7s^27p^6$ | 116.367 | 114.631 | 114.444 | 110.682 | 109.691 | 108.759 | 101.946 | 99.718 | 98.018 | 99.786 |

**Table 2**
Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from $4p_{1/2}$ to $5f_{7/2}$.

| Atomic Number | Configuration | $4p_{1/2}$ | $4p_{3/2}$ | $4d_{3/2}$ | $4d_{5/2}$ | $4f_{5/2}$ | $4f_{7/2}$ | $5s$ | $5p_{1/2}$ | $5p_{3/2}$ | $5d_{3/2}$ | $5d_{5/2}$ | $5f_{5/2}$ | $5f_{7/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $1s$ | | | | | | | | | | | | | |
| 2 | $1s^2$ | | | | | | | | | | | | | |
| 3 | $1s^2 2s$ | | | | | | | | | | | | | |
| 4 | $1s^2 2s^2$ | | | | | | | | | | | | | |
| 5 | $1s^2 2s^2 2p$ | | | | | | | | | | | | | |
| 6 | $1s^2 2s^2 2p^2$ | | | | | | | | | | | | | |
| 7 | $1s^2 2s^2 2p^3$ | | | | | | | | | | | | | |
| 8 | $1s^2 2s^2 2p^4$ | | | | | | | | | | | | | |
| 9 | $1s^2 2s^2 2p^5$ | | | | | | | | | | | | | |
| 10 | $1s^2 2s^2 2p^6$ | | | | | | | | | | | | | |
| 11 | [Ne]$3s$ | | | | | | | | | | | | | |
| 12 | [Ne]$3s^2$ | | | | | | | | | | | | | |
| 13 | [Ne]$3s^2 3p$ | | | | | | | | | | | | | |
| 14 | [Ne]$3s^2 3p^2$ | | | | | | | | | | | | | |
| 15 | [Ne]$3s^2 3p^3$ | | | | | | | | | | | | | |
| 16 | [Ne]$3s^2 3p^4$ | | | | | | | | | | | | | |
| 17 | [Ne]$3s^2 3p^5$ | | | | | | | | | | | | | |
| 18 | [Ne]$3s^2 3p^6$ | | | | | | | | | | | | | |
| 19 | [Ar]$4s$ | | | | | | | | | | | | | |
| 20 | [Ar]$4s^2$ | | | | | | | | | | | | | |
| 21 | [Ar]$3d4s^2$ | | | | | | | | | | | | | |
| 22 | [Ar]$3d^2 4s^2$ | | | | | | | | | | | | | |
| 23 | [Ar]$3d^3 4s^2$ | | | | | | | | | | | | | |
| 24 | [Ar]$3d^5 4s$ | | | | | | | | | | | | | |
| 25 | [Ar]$3d^5 4s^2$ | | | | | | | | | | | | | |
| 26 | [Ar]$3d^6 4s^2$ | | | | | | | | | | | | | |
| 27 | [Ar]$3d^7 4s^2$ | | | | | | | | | | | | | |
| 28 | [Ar]$3d^8 4s^2$ | | | | | | | | | | | | | |
| 29 | [Ar]$3d^{10} 4s$ | | | | | | | | | | | | | |
| 30 | [Ar]$3d^{10} 4s^2$ | | | | | | | | | | | | | |
| 31 | [Ar]$3d^{10} 4s^2 4p$ | 6.779 | | | | | | | | | | | | |
| 32 | [Ar]$3d^{10} 4s^2 4p^2$ | 8.076 | 8.052 | | | | | | | | | | | |
| 33 | [Ar]$3d^{10} 4s^2 4p^3$ | 9.240 | 9.137 | | | | | | | | | | | |
| 34 | [Ar]$3d^{10} 4s^2 4p^4$ | 10.076 | 10.000 | | | | | | | | | | | |
| 35 | [Ar]$3d^{10} 4s^2 4p^5$ | 11.040 | 10.849 | | | | | | | | | | | |
| 36 | [Ar]$3d^{10} 4s^2 4p^6$ | 11.983 | 11.731 | | | | | | | | | | | |
| 37 | [Kr]$5s$ | 13.463 | 13.209 | | | | | 6.760 | | | | | | |
| 38 | [Kr]$5s^2$ | 14.798 | 14.531 | | | | | 8.210 | | | | | | |
| 39 | [Kr]$4d5s^2$ | 15.841 | 15.618 | 8.401 | | | | 8.891 | | | | | | |
| 40 | [Kr]$4d^2 5s^2$ | 16.826 | 16.595 | 9.795 | 9.752 | | | 9.372 | | | | | | |
| 41 | [Kr]$4d^4 5s$ | 17.663 | 17.374 | 10.028 | 9.859 | | | 9.751 | | | | | | |
| 42 | [Kr]$4d^5 5s$ | 18.619 | 18.243 | 11.066 | 10.968 | | | 10.162 | | | | | | |
| 43 | [Kr]$4d^5 5s^2$ | 19.666 | 19.265 | 12.824 | 12.730 | | | 10.498 | | | | | | |
| 44 | [Kr]$4d^7 5s$ | 20.405 | 20.004 | 12.759 | 12.644 | | | 10.518 | | | | | | |
| 45 | [Kr]$4d^8 5s$ | 21.296 | 20.848 | 13.641 | 13.429 | | | 10.649 | | | | | | |
| 46 | [Kr]$4d^{10}$ | 22.078 | 21.543 | 13.718 | 13.417 | | | | | | | | | |
| 47 | [Kr]$4d^{10} 5s$ | 23.060 | 22.493 | 15.295 | 15.038 | | | 10.848 | | | | | | |
| 48 | [Kr]$4d^{10} 5s^2$ | 24.068 | 23.468 | 16.714 | 16.470 | | | 12.118 | | | | | | |
| 49 | [Kr]$4d^{10} 5s^2 5p$ | 25.114 | 24.472 | 18.049 | 17.877 | | | 13.711 | 9.943 | | | | | |
| 50 | [Kr]$4d^{10} 5s^2 5p^2$ | 26.180 | 25.489 | 19.321 | 19.167 | | | 15.048 | 11.485 | 11.382 | | | | |
| 51 | [Kr]$4d^{10} 5s^2 5p^3$ | 27.222 | 26.524 | 20.586 | 20.369 | | | 16.275 | 12.907 | 12.549 | | | | |
| 52 | [Kr]$4d^{10} 5s^2 5p^4$ | 28.282 | 27.539 | 21.756 | 21.556 | | | 17.440 | 13.955 | 13.503 | | | | |
| 53 | [Kr]$4d^{10} 5s^2 5p^5$ | 29.346 | 28.557 | 22.916 | 22.696 | | | 18.546 | 15.116 | 14.478 | | | | |
| 54 | [Kr]$4d^{10} 5s^2 5p^6$ | 30.397 | 29.598 | 24.054 | 23.807 | | | 19.609 | 16.228 | 15.498 | | | | |
| 55 | [Xe]$6s$ | 31.453 | 30.616 | 25.183 | 24.928 | | | 21.088 | 17.916 | 17.193 | | | | |
| 56 | [Xe]$6s^2$ | 32.510 | 31.634 | 26.301 | 26.038 | | | 22.517 | 19.423 | 18.675 | | | | |
| 57 | [Xe]$5d6s^2$ | 33.569 | 32.650 | 27.420 | 27.137 | | | 23.700 | 20.564 | 19.872 | 12.047 | | | |
| 58 | [Xe]$4f5d6s^2$ | 34.477 | 33.508 | 28.258 | 27.968 | | | 24.275 | 21.122 | 20.297 | 12.736 | 12.609 | | |
| 59 | [Xe]$4f^3 6s^2$ | 35.243 | 34.218 | 28.831 | 28.549 | 16.980 | 16.876 | 24.283 | 21.039 | 20.034 | | | | |
| 60 | [Xe]$4f^4 6s^2$ | 36.137 | 35.047 | 29.643 | 29.336 | 17.887 | 17.663 | 24.820 | 21.507 | 20.432 | | | | |
| 61 | [Xe]$4f^5 6s^2$ | 37.027 | 35.870 | 30.448 | 30.113 | 18.686 | 18.371 | 25.352 | 21.967 | 20.823 | | | | |
| 62 | [Xe]$4f^6 6s^2$ | 37.912 | 36.683 | 31.241 | 30.877 | 19.439 | 19.163 | 25.869 | 22.406 | 21.198 | | | | |
| 63 | [Xe]$4f^7 6s^2$ | 38.798 | 37.487 | 32.028 | 31.628 | 20.154 | 20.004 | 26.375 | 22.808 | 21.567 | | | | |
| 64 | [Xe]$4f^7 5d6s^2$ | 39.771 | 38.396 | 32.986 | 32.563 | 21.882 | 21.903 | 27.411 | 23.817 | 22.616 | 13.486 | 13.396 | | |
| 65 | [Xe]$4f^9 6s^2$ | 40.567 | 39.114 | 33.598 | 33.160 | 21.127 | 21.083 | 27.456 | 23.785 | 22.327 | | | | |
| 66 | [Xe]$4f^{10} 6s^2$ | 41.451 | 39.917 | 34.375 | 33.909 | 21.757 | 21.575 | 27.982 | 24.245 | 22.691 | | | | |
| 67 | [Xe]$4f^{11} 6s^2$ | 42.338 | 40.717 | 35.153 | 34.654 | 22.385 | 22.044 | 28.511 | 24.697 | 23.060 | | | | |

**Table 2** (continued)

| Atomic Number | Configuration | $4p_{1/2}$ | $4p_{3/2}$ | $4d_{3/2}$ | $4d_{5/2}$ | $4f_{5/2}$ | $4f_{7/2}$ | $5s$ | $5p_{1/2}$ | $5p_{3/2}$ | $5d_{3/2}$ | $5d_{5/2}$ | $5f_{5/2}$ | $5f_{7/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 68 | [Xe]$4f^{12}6s^2$ | 43.226 | 41.516 | 35.929 | 35.397 | 23.007 | 22.507 | 29.043 | 25.150 | 23.429 | | | | |
| 69 | [Xe]$4f^{13}6s^2$ | 44.115 | 42.311 | 36.699 | 36.134 | 23.606 | 23.029 | 29.572 | 25.593 | 23.790 | | | | |
| 70 | [Xe]$4f^{14}6s^2$ | 45.004 | 43.101 | 37.463 | 36.866 | 24.162 | 23.625 | 30.093 | 26.025 | 24.141 | | | | |
| 71 | [Xe]$4f^{14}5d6s^2$ | 45.954 | 43.966 | 38.355 | 37.731 | 25.810 | 25.464 | 31.122 | 27.037 | 25.212 | 12.841 | | | |
| 72 | [Xe]$4f^{14}5d^26s^2$ | 46.922 | 44.847 | 39.273 | 38.621 | 27.322 | 27.058 | 32.142 | 28.044 | 26.214 | 14.961 | 14.694 | | |
| 73 | [Xe]$4f^{14}5d^36s^2$ | 47.902 | 45.741 | 40.208 | 39.528 | 28.764 | 28.514 | 33.164 | 29.083 | 27.185 | 16.475 | 16.107 | | |
| 74 | [Xe]$4f^{14}5d^46s^2$ | 48.893 | 46.645 | 41.158 | 40.447 | 30.129 | 29.892 | 34.185 | 30.107 | 28.144 | 17.741 | 17.410 | | |
| 75 | [Xe]$4f^{14}5d^56s^2$ | 49.890 | 47.558 | 42.098 | 41.386 | 31.507 | 31.165 | 35.209 | 31.251 | 29.044 | 19.047 | 18.553 | | |
| 76 | [Xe]$4f^{14}5d^66s^2$ | 50.900 | 48.476 | 43.057 | 42.315 | 32.756 | 32.453 | 36.234 | 32.245 | 30.005 | 19.945 | 19.430 | | |
| 77 | [Xe]$4f^{14}5d^76s^2$ | 51.917 | 49.400 | 44.021 | 43.250 | 33.989 | 33.687 | 37.253 | 33.268 | 30.933 | 20.991 | 20.284 | | |
| 78 | [Xe]$4f^{14}5d^96s$ | 52.939 | 50.332 | 44.992 | 44.194 | 35.205 | 34.856 | 38.152 | 34.216 | 31.680 | 21.362 | 20.247 | | |
| 79 | [Xe]$4f^{14}5d^{10}6s$ | 53.966 | 51.265 | 45.956 | 45.159 | 36.401 | 36.019 | 39.146 | 35.269 | 32.569 | 22.394 | 21.296 | | |
| 80 | [Xe]$4f^{14}5d^{10}6s^2$ | 54.999 | 52.199 | 46.924 | 46.103 | 37.574 | 37.186 | 40.298 | 36.423 | 33.622 | 24.026 | 22.990 | | |
| 81 | [Xe]$4f^{14}5d^{10}6s^26p$ | 56.041 | 53.138 | 47.894 | 47.050 | 38.729 | 38.335 | 41.433 | 37.626 | 34.728 | 25.563 | 24.724 | | |
| 82 | [Xe]$4f^{14}5d^{10}6s^26p^2$ | 57.089 | 54.080 | 48.866 | 47.998 | 39.871 | 39.470 | 42.581 | 38.864 | 35.843 | 26.997 | 26.271 | | |
| 83 | [Xe]$4f^{14}5d^{10}6s^26p^3$ | 58.140 | 55.026 | 49.841 | 48.948 | 41.000 | 40.591 | 43.738 | 40.057 | 36.978 | 28.491 | 27.683 | | |
| 84 | [Xe]$4f^{14}5d^{10}6s^26p^4$ | 59.198 | 55.975 | 50.818 | 49.900 | 42.119 | 41.701 | 44.902 | 41.270 | 38.094 | 29.853 | 29.035 | | |
| 85 | [Xe]$4f^{14}5d^{10}6s^26p^5$ | 60.260 | 56.928 | 51.797 | 50.852 | 43.227 | 42.800 | 46.069 | 42.482 | 39.208 | 31.190 | 30.322 | | |
| 86 | [Xe]$4f^{14}5d^{10}6s^26p^6$ | 61.327 | 57.883 | 52.777 | 51.806 | 44.325 | 43.890 | 47.240 | 43.686 | 40.349 | 32.483 | 31.563 | | |
| 87 | [Rn]$7s$ | 62.400 | 58.840 | 53.759 | 52.761 | 45.416 | 44.971 | 48.415 | 44.893 | 41.452 | 33.763 | 32.829 | | |
| 88 | [Rn]$7s^2$ | 63.477 | 59.798 | 54.742 | 53.717 | 46.500 | 46.046 | 49.594 | 46.099 | 42.550 | 35.022 | 34.074 | | |
| 89 | [Rn]$6d7s^2$ | 64.560 | 60.758 | 55.729 | 54.674 | 47.577 | 47.113 | 50.769 | 47.309 | 43.648 | 36.276 | 35.300 | | |
| 90 | [Rn]$6d^27s^2$ | 65.647 | 61.720 | 56.716 | 55.632 | 48.647 | 48.173 | 51.944 | 48.518 | 44.740 | 37.511 | 36.501 | | |
| 91 | [Rn]$5f^26d7s^2$ | 66.734 | 62.679 | 57.696 | 56.584 | 49.719 | 49.215 | 53.024 | 49.563 | 45.663 | 38.311 | 37.356 | 20.293 | 20.370 |
| 92 | [Rn]$5f^36d7s^2$ | 67.825 | 63.639 | 58.678 | 57.537 | 50.778 | 50.254 | 54.134 | 50.672 | 46.630 | 39.264 | 38.307 | 21.982 | 21.803 |
| 93 | [Rn]$5f^46d7s^2$ | 68.921 | 64.599 | 59.658 | 58.487 | 51.828 | 51.286 | 55.242 | 51.782 | 47.582 | 40.214 | 39.228 | 23.296 | 23.019 |
| 94 | [Rn]$5f^67s^2$ | 70.018 | 65.558 | 60.634 | 59.435 | 52.880 | 52.310 | 56.307 | 52.827 | 48.451 | 40.960 | 39.984 | 23.470 | 23.095 |
| 95 | [Rn]$5f^77s^2$ | 71.121 | 66.519 | 61.614 | 60.380 | 53.896 | 53.345 | 57.410 | 53.971 | 49.364 | 41.973 | 40.822 | 24.705 | 24.185 |
| 96 | [Rn]$5f^76d7s^2$ | 72.230 | 67.480 | 62.594 | 61.327 | 54.923 | 54.357 | 58.547 | 55.124 | 50.353 | 43.051 | 41.845 | 26.548 | 26.306 |
| 97 | [Rn]$5f^97s^2$ | 73.341 | 68.440 | 63.567 | 62.271 | 55.946 | 55.353 | 59.616 | 56.164 | 51.211 | 43.770 | 42.592 | 26.455 | 25.775 |
| 98 | [Rn]$5f^{10}7s^2$ | 74.456 | 69.400 | 64.543 | 63.214 | 56.962 | 56.353 | 60.719 | 57.273 | 52.116 | 44.680 | 43.441 | 27.406 | 26.569 |
| 99 | [Rn]$5f^{11}7s^2$ | 75.576 | 70.360 | 65.519 | 64.154 | 57.969 | 57.350 | 61.824 | 58.391 | 53.014 | 45.596 | 44.277 | 28.341 | 27.351 |
| 100 | [Rn]$5f^{12}7s^2$ | 76.701 | 71.320 | 66.494 | 65.093 | 58.968 | 58.339 | 62.932 | 59.512 | 53.906 | 46.505 | 45.104 | 29.250 | 28.120 |
| 101 | [Rn]$5f^{13}7s^2$ | 77.829 | 72.280 | 67.468 | 66.030 | 59.984 | 59.322 | 64.041 | 60.638 | 54.792 | 47.408 | 45.923 | 30.123 | 28.932 |
| 102 | [Rn]$5f^{14}7s^2$ | 78.963 | 73.239 | 68.442 | 66.965 | 60.976 | 60.340 | 65.154 | 61.768 | 55.672 | 48.304 | 46.732 | 30.961 | 29.780 |
| 103 | [Rn]$5f^{14}7s^27p$ | 80.103 | 74.199 | 69.415 | 67.900 | 61.970 | 61.319 | 66.298 | 62.926 | 56.609 | 49.279 | 47.669 | 32.753 | 31.739 |
| 104 | [Rn]$5f^{14}6d^27s^2$ | 81.248 | 75.160 | 70.391 | 68.836 | 62.960 | 62.296 | 67.454 | 64.105 | 57.570 | 50.311 | 48.645 | 34.089 | 33.326 |
| 105 | [Rn]$5f^{14}6d^37s^2$ | 82.400 | 76.121 | 71.366 | 69.771 | 63.948 | 63.269 | 68.619 | 65.292 | 58.532 | 51.334 | 49.620 | 35.529 | 34.835 |
| 106 | [Rn]$5f^{14}6d^47s^2$ | 83.556 | 77.082 | 72.343 | 70.706 | 64.935 | 64.240 | 69.788 | 66.490 | 59.499 | 52.376 | 50.599 | 36.874 | 36.271 |
| 107 | [Rn]$5f^{14}6d^57s^2$ | 84.718 | 78.044 | 73.316 | 71.643 | 65.920 | 65.208 | 70.968 | 67.690 | 60.474 | 53.383 | 51.599 | 38.336 | 37.556 |
| 108 | [Rn]$5f^{14}6d^67s^2$ | 85.887 | 79.006 | 74.292 | 72.577 | 66.901 | 66.174 | 72.158 | 68.908 | 61.449 | 54.413 | 52.579 | 39.600 | 38.880 |
| 109 | [Rn]$5f^{14}6d^77s^2$ | 87.062 | 79.969 | 75.268 | 73.512 | 67.881 | 67.138 | 73.355 | 70.134 | 62.428 | 55.443 | 53.565 | 40.872 | 40.135 |
| 110 | [Rn]$5f^{14}6d^97s$ | 88.243 | 80.932 | 76.243 | 74.448 | 68.860 | 68.099 | 74.555 | 71.368 | 63.419 | 56.475 | 54.557 | 42.122 | 41.297 |
| 111 | [Rn]$5f^{14}6d^{10}7s$ | 89.430 | 81.895 | 77.219 | 75.383 | 69.836 | 69.058 | 75.767 | 72.610 | 64.403 | 57.499 | 55.568 | 43.355 | 42.479 |
| 112 | [Rn]$5f^{14}6d^{10}7s^2$ | 90.624 | 82.858 | 78.194 | 76.316 | 70.811 | 70.015 | 76.992 | 73.862 | 65.380 | 58.520 | 56.549 | 44.571 | 43.688 |
| 113 | [Rn]$5f^{14}6d^{10}7s^27p$ | 91.825 | 83.821 | 79.170 | 77.249 | 71.784 | 70.971 | 78.220 | 75.128 | 66.361 | 59.540 | 57.530 | 45.768 | 44.874 |
| 114 | [Rn]$5f^{14}6d^{10}7s^27p^2$ | 93.034 | 84.785 | 80.145 | 78.181 | 72.755 | 71.925 | 79.457 | 76.406 | 67.344 | 60.559 | 58.511 | 46.949 | 46.044 |
| 115 | [Rn]$5f^{14}6d^{10}7s^27p^3$ | 94.249 | 85.749 | 81.121 | 79.113 | 73.725 | 72.877 | 80.702 | 77.692 | 68.330 | 61.582 | 59.490 | 48.111 | 47.195 |
| 116 | [Rn]$5f^{14}6d^{10}7s^27p^4$ | 95.472 | 86.713 | 82.097 | 80.045 | 74.693 | 73.827 | 81.955 | 78.988 | 69.318 | 62.605 | 60.468 | 49.261 | 48.334 |
| 117 | [Rn]$5f^{14}6d^{10}7s^27p^5$ | 96.702 | 87.678 | 83.074 | 80.976 | 75.660 | 74.776 | 83.216 | 80.297 | 70.307 | 63.627 | 61.446 | 50.399 | 49.460 |
| 118 | [Rn]$5f^{14}6d^{10}7s^27p^6$ | 97.939 | 88.643 | 84.050 | 81.906 | 76.625 | 75.722 | 84.485 | 81.617 | 71.298 | 64.650 | 62.422 | 51.526 | 50.574 |

**Table 3**
Effective nuclear charge calculated with the Dirac-Fock method for subshells ranging from $6s$ to $7p_{3/2}$.

| Atomic Number | Configuration | $6s$ | $6p_{1/2}$ | $6p_{3/2}$ | $6d_{3/2}$ | $6d_{5/2}$ | $7s$ | $7p_{1/2}$ | $7p_{3/2}$ |
|---|---|---|---|---|---|---|---|---|---|
| 55 | [Xe]$6s$ | 8.869 | | | | | | | |
| 56 | [Xe]$6s^2$ | 10.612 | | | | | | | |
| 57 | [Xe]$5d6s^2$ | 11.407 | | | | | | | |
| 58 | [Xe]$4f5d6s^2$ | 11.539 | | | | | | | |
| 59 | [Xe]$4f^36s^2$ | 11.134 | | | | | | | |
| 60 | [Xe]$4f^46s^2$ | 11.285 | | | | | | | |
| 61 | [Xe]$4f^56s^2$ | 11.434 | | | | | | | |
| 62 | [Xe]$4f^66s^2$ | 11.577 | | | | | | | |
| 63 | [Xe]$4f^76s^2$ | 11.714 | | | | | | | |
| 64 | [Xe]$4f^75d6s^2$ | 12.493 | | | | | | | |
| 65 | [Xe]$4f^96s^2$ | 12.019 | | | | | | | |
| 66 | [Xe]$4f^{10}6s^2$ | 12.164 | | | | | | | |
| 67 | [Xe]$4f^{11}6s^2$ | 12.310 | | | | | | | |
| 68 | [Xe]$4f^{12}6s^2$ | 12.457 | | | | | | | |
| 69 | [Xe]$4f^{13}6s^2$ | 12.601 | | | | | | | |
| 70 | [Xe]$4f^{14}6s^2$ | 12.741 | | | | | | | |
| 71 | [Xe]$4f^{14}5d6s^2$ | 13.770 | | | | | | | |
| 72 | [Xe]$4f^{14}5d^26s^2$ | 14.473 | | | | | | | |
| 73 | [Xe]$4f^{14}5d^36s^2$ | 15.109 | | | | | | | |
| 74 | [Xe]$4f^{14}5d^46s^2$ | 15.691 | | | | | | | |
| 75 | [Xe]$4f^{14}5d^56s^2$ | 16.244 | | | | | | | |
| 76 | [Xe]$4f^{14}5d^66s^2$ | 16.843 | | | | | | | |
| 77 | [Xe]$4f^{14}5d^76s^2$ | 17.391 | | | | | | | |
| 78 | [Xe]$4f^{14}5d^96s$ | 17.381 | | | | | | | |
| 79 | [Xe]$4f^{14}5d^{10}6s$ | 17.586 | | | | | | | |
| 80 | [Xe]$4f^{14}5d^{10}6s^2$ | 18.926 | | | | | | | |
| 81 | [Xe]$4f^{14}5d^{10}6s^26p$ | 20.761 | 15.075 | | | | | | |
| 82 | [Xe]$4f^{14}5d^{10}6s^26p^2$ | 22.352 | 16.953 | 16.455 | | | | | |
| 83 | [Xe]$4f^{14}5d^{10}6s^26p^3$ | 23.877 | 18.820 | 16.925 | | | | | |
| 84 | [Xe]$4f^{14}5d^{10}6s^26p^4$ | 25.293 | 20.474 | 17.956 | | | | | |
| 85 | [Xe]$4f^{14}5d^{10}6s^26p^5$ | 26.640 | 22.040 | 19.199 | | | | | |
| 86 | [Xe]$4f^{14}5d^{10}6s^26p^6$ | 27.925 | 23.495 | 20.478 | | | | | |
| 87 | [Rn]$7s$ | 29.695 | 25.518 | 22.568 | | | 12.400 | | |
| 88 | [Rn]$7s^2$ | 31.412 | 27.334 | 24.327 | | | 14.583 | | |
| 89 | [Rn]$6d7s^2$ | 32.882 | 28.768 | 25.811 | 14.908 | | 15.886 | | |
| 90 | [Rn]$6d^27s^2$ | 34.258 | 30.108 | 27.125 | 16.952 | 16.547 | 16.894 | | |
| 91 | [Rn]$5f^26d7s^2$ | 34.764 | 30.610 | 27.175 | 17.074 | 17.393 | 16.414 | | |
| 92 | [Rn]$5f^36d7s^2$ | 35.611 | 31.432 | 27.733 | 17.495 | 17.245 | 16.657 | | |
| 93 | [Rn]$5f^46d7s^2$ | 36.442 | 32.223 | 28.272 | 17.903 | 17.599 | 16.897 | | |
| 94 | [Rn]$5f^67s^2$ | 36.857 | 32.609 | 28.144 | | | 16.345 | | |
| 95 | [Rn]$5f^77s^2$ | 37.658 | 33.288 | 28.666 | | | 16.553 | | |
| 96 | [Rn]$5f^76d7s^2$ | 38.864 | 34.438 | 29.814 | 18.068 | 17.781 | 17.687 | | |
| 97 | [Rn]$5f^97s^2$ | 39.287 | 34.855 | 29.621 | | | 17.041 | | |
| 98 | [Rn]$5f^{10}7s^2$ | 40.086 | 35.598 | 30.076 | | | 17.270 | | |
| 99 | [Rn]$5f^{11}7s^2$ | 40.889 | 36.332 | 30.532 | | | 17.501 | | |
| 100 | [Rn]$5f^{12}7s^2$ | 41.695 | 37.068 | 30.980 | | | 17.735 | | |
| 101 | [Rn]$5f^{13}7s^2$ | 42.498 | 37.797 | 31.411 | | | 17.964 | | |
| 102 | [Rn]$5f^{14}7s^2$ | 43.298 | 38.518 | 31.825 | | | 18.190 | | |
| 103 | [Rn]$5f^{14}7s^27p$ | 44.623 | 39.985 | 33.252 | | | 20.817 | 15.583 | |
| 104 | [Rn]$5f^{14}6d^27s^2$ | 45.762 | 40.916 | 34.169 | 19.549 | 18.825 | 20.956 | | |
| 105 | [Rn]$5f^{14}6d^37s^2$ | 47.000 | 42.144 | 35.254 | 21.453 | 20.607 | 22.031 | | |
| 106 | [Rn]$5f^{14}6d^47s^2$ | 48.231 | 43.322 | 36.329 | 22.973 | 22.386 | 23.018 | | |
| 107 | [Rn]$5f^{14}6d^57s^2$ | 49.496 | 44.791 | 37.307 | 24.688 | 23.360 | 24.111 | | |
| 108 | [Rn]$5f^{14}6d^67s^2$ | 50.745 | 46.003 | 38.357 | 25.886 | 24.188 | 25.151 | | |
| 109 | [Rn]$5f^{14}6d^77s^2$ | 52.001 | 47.298 | 39.362 | 27.209 | 25.159 | 26.174 | | |
| 110 | [Rn]$5f^{14}6d^97s$ | 53.159 | 48.589 | 40.255 | 28.041 | 25.440 | 27.143 | | |
| 111 | [Rn]$5f^{14}6d^{10}7s$ | 54.386 | 49.929 | 41.222 | 29.284 | 26.668 | 27.870 | | |
| 112 | [Rn]$5f^{14}6d^{10}7s^2$ | 55.794 | 51.317 | 42.272 | 30.895 | 28.358 | 29.225 | | |
| 113 | [Rn]$5f^{14}6d^{10}7s^27p$ | 57.152 | 52.774 | 43.453 | 32.398 | 30.259 | 31.028 | 23.835 | |
| 114 | [Rn]$5f^{14}6d^{10}7s^27p^2$ | 58.525 | 54.247 | 44.630 | 33.800 | 31.942 | 32.734 | 25.759 | 23.952 |
| 115 | [Rn]$5f^{14}6d^{10}7s^27p^3$ | 59.901 | 55.717 | 45.838 | 35.498 | 33.592 | 34.631 | 28.378 | 18.858 |
| 116 | [Rn]$5f^{14}6d^{10}7s^27p^4$ | 61.288 | 57.163 | 47.052 | 37.082 | 35.107 | 36.352 | 30.646 | 20.984 |
| 117 | [Rn]$5f^{14}6d^{10}7s^27p^5$ | 62.685 | 58.658 | 48.253 | 38.586 | 36.537 | 37.987 | 32.686 | 22.716 |
| 118 | [Rn]$5f^{14}6d^{10}7s^27p^6$ | 64.092 | 60.136 | 49.485 | 40.026 | 37.895 | 39.547 | 34.580 | 24.366 |

**Table 4**
Radii of maximum charge density calculated with the Dirac-Fock method for subshells ranging from 1s to 4s ($a_0$).

| Atomic Number | Configuration | $1s$ | $2s$ | $2p_{1/2}$ | $2p_{3/2}$ | 3s | $3p_{1/2}$ | $3p_{3/2}$ | $3d_{3/2}$ | $3d_{5/2}$ | 4s |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $1s$ | 1.000 | | | | | | | | | |
| 2 | $1s^2$ | 0.570 | | | | | | | | | |
| 3 | $1s^2 2s$ | 0.364 | 3.101 | | | | | | | | |
| 4 | $1s^2 2s^2$ | 0.267 | 2.051 | | | | | | | | |
| 5 | $1s^2 2s^2 2p$ | 0.211 | 1.525 | 1.587 | | | | | | | |
| 6 | $1s^2 2s^2 2p^2$ | 0.174 | 1.222 | 1.212 | 1.212 | | | | | | |
| 7 | $1s^2 2s^2 2p^3$ | 0.149 | 1.022 | 0.984 | 0.984 | | | | | | |
| 8 | $1s^2 2s^2 2p^4$ | 0.129 | 0.875 | 0.834 | 0.831 | | | | | | |
| 9 | $1s^2 2s^2 2p^5$ | 0.115 | 0.766 | 0.720 | 0.720 | | | | | | |
| 10 | $1s^2 2s^2 2p^6$ | 0.103 | 0.683 | 0.633 | 0.635 | | | | | | |
| 11 | $[Ne]3s$ | 0.093 | 0.607 | 0.548 | 0.550 | 3.387 | | | | | |
| 12 | $[Ne]3s^2$ | 0.085 | 0.546 | 0.483 | 0.484 | 2.583 | | | | | |
| 13 | $[Ne]3s^2 3p$ | 0.078 | 0.495 | 0.431 | 0.433 | 2.096 | 2.685 | | | | |
| 14 | $[Ne]3s^2 3p^2$ | 0.073 | 0.453 | 0.389 | 0.391 | 1.796 | 2.168 | 2.172 | | | |
| 15 | $[Ne]3s^2 3p^3$ | 0.068 | 0.417 | 0.355 | 0.357 | 1.581 | 1.841 | 1.846 | | | |
| 16 | $[Ne]3s^2 3p^4$ | 0.063 | 0.387 | 0.326 | 0.328 | 1.416 | 1.613 | 1.616 | | | |
| 17 | $[Ne]3s^2 3p^5$ | 0.060 | 0.360 | 0.302 | 0.304 | 1.286 | 1.436 | 1.441 | | | |
| 18 | $[Ne]3s^2 3p^6$ | 0.056 | 0.338 | 0.281 | 0.282 | 1.178 | 1.295 | 1.302 | | | |
| 19 | $[Ar]4s$ | 0.053 | 0.317 | 0.262 | 0.264 | 1.077 | 1.158 | 1.164 | | | 4.328 |
| 20 | $[Ar]4s^2$ | 0.050 | 0.299 | 0.246 | 0.248 | 0.992 | 1.048 | 1.054 | | | 3.463 |
| 21 | $[Ar]3d4s^2$ | 0.048 | 0.283 | 0.231 | 0.233 | 0.925 | 0.969 | 0.974 | 1.125 | | 3.226 |
| 22 | $[Ar]3d^2 4s^2$ | 0.046 | 0.268 | 0.219 | 0.221 | 0.869 | 0.903 | 0.909 | 0.997 | 0.999 | 3.055 |
| 23 | $[Ar]3d^3 4s^2$ | 0.044 | 0.255 | 0.207 | 0.209 | 0.819 | 0.847 | 0.852 | 0.905 | 0.908 | 2.912 |
| 24 | $[Ar]3d^5 4s$ | 0.042 | 0.243 | 0.197 | 0.199 | 0.778 | 0.800 | 0.807 | 0.861 | 0.863 | 2.908 |
| 25 | $[Ar]3d^5 4s^2$ | 0.040 | 0.232 | 0.187 | 0.189 | 0.737 | 0.753 | 0.760 | 0.772 | 0.775 | 2.680 |
| 26 | $[Ar]3d^6 4s^2$ | 0.038 | 0.222 | 0.179 | 0.181 | 0.701 | 0.714 | 0.720 | 0.723 | 0.724 | 2.567 |
| 27 | $[Ar]3d^7 4s^2$ | 0.037 | 0.213 | 0.171 | 0.173 | 0.670 | 0.678 | 0.685 | 0.678 | 0.680 | 2.469 |
| 28 | $[Ar]3d^8 4s^2$ | 0.035 | 0.204 | 0.164 | 0.166 | 0.640 | 0.646 | 0.653 | 0.639 | 0.642 | 2.381 |
| 29 | $[Ar]3d^{10} 4s$ | 0.034 | 0.196 | 0.157 | 0.159 | 0.615 | 0.619 | 0.626 | 0.614 | 0.617 | 2.540 |
| 30 | $[Ar]3d^{10} 4s^2$ | 0.033 | 0.189 | 0.151 | 0.153 | 0.589 | 0.591 | 0.599 | 0.574 | 0.577 | 2.227 |
| 31 | $[Ar]3d^{10} 4s^2 4p$ | 0.032 | 0.182 | 0.145 | 0.148 | 0.565 | 0.564 | 0.573 | 0.539 | 0.542 | 1.967 |
| 32 | $[Ar]3d^{10} 4s^2 4p^2$ | 0.031 | 0.176 | 0.140 | 0.142 | 0.543 | 0.540 | 0.548 | 0.508 | 0.511 | 1.787 |
| 33 | $[Ar]3d^{10} 4s^2 4p^3$ | 0.030 | 0.170 | 0.135 | 0.138 | 0.522 | 0.518 | 0.526 | 0.480 | 0.483 | 1.648 |
| 34 | $[Ar]3d^{10} 4s^2 4p^4$ | 0.029 | 0.164 | 0.130 | 0.133 | 0.502 | 0.497 | 0.505 | 0.455 | 0.458 | 1.533 |
| 35 | $[Ar]3d^{10} 4s^2 4p^5$ | 0.028 | 0.159 | 0.126 | 0.129 | 0.484 | 0.477 | 0.485 | 0.433 | 0.436 | 1.437 |
| 36 | $[Ar]3d^{10} 4s^2 4p^6$ | 0.027 | 0.154 | 0.122 | 0.125 | 0.466 | 0.459 | 0.467 | 0.413 | 0.415 | 1.353 |
| 37 | $[Kr]5s$ | 0.026 | 0.150 | 0.118 | 0.121 | 0.450 | 0.442 | 0.450 | 0.394 | 0.397 | 1.270 |
| 38 | $[Kr]5s^2$ | 0.026 | 0.145 | 0.114 | 0.117 | 0.435 | 0.426 | 0.434 | 0.378 | 0.380 | 1.196 |
| 39 | $[Kr]4d5s^2$ | 0.025 | 0.141 | 0.111 | 0.114 | 0.421 | 0.411 | 0.419 | 0.362 | 0.365 | 1.135 |
| 40 | $[Kr]4d^2 5s^2$ | 0.024 | 0.137 | 0.107 | 0.111 | 0.408 | 0.397 | 0.406 | 0.348 | 0.350 | 1.082 |
| 41 | $[Kr]4d^4 5s$ | 0.024 | 0.133 | 0.104 | 0.108 | 0.395 | 0.384 | 0.393 | 0.335 | 0.337 | 1.036 |
| 42 | $[Kr]4d^5 5s$ | 0.023 | 0.130 | 0.101 | 0.105 | 0.383 | 0.372 | 0.380 | 0.322 | 0.325 | 0.992 |
| 43 | $[Kr]4d^5 5s^2$ | 0.022 | 0.126 | 0.098 | 0.102 | 0.372 | 0.360 | 0.369 | 0.311 | 0.314 | 0.952 |
| 44 | $[Kr]4d^7 5s$ | 0.022 | 0.123 | 0.096 | 0.100 | 0.361 | 0.349 | 0.358 | 0.301 | 0.303 | 0.918 |
| 45 | $[Kr]4d^8 5s$ | 0.021 | 0.120 | 0.093 | 0.097 | 0.351 | 0.339 | 0.348 | 0.291 | 0.293 | 0.885 |
| 46 | $[Kr]4d^{10}$ | 0.021 | 0.117 | 0.091 | 0.095 | 0.341 | 0.329 | 0.338 | 0.281 | 0.284 | 0.856 |
| 47 | $[Kr]4d^{10} 5s$ | 0.020 | 0.114 | 0.089 | 0.093 | 0.332 | 0.320 | 0.329 | 0.273 | 0.276 | 0.827 |
| 48 | $[Kr]4d^{10} 5s^2$ | 0.020 | 0.111 | 0.086 | 0.091 | 0.324 | 0.311 | 0.320 | 0.265 | 0.268 | 0.799 |
| 49 | $[Kr]4d^{10} 5s^2 5p$ | 0.019 | 0.109 | 0.084 | 0.088 | 0.315 | 0.302 | 0.312 | 0.257 | 0.260 | 0.773 |
| 50 | $[Kr]4d^{10} 5s^2 5p^2$ | 0.019 | 0.106 | 0.082 | 0.087 | 0.307 | 0.295 | 0.304 | 0.250 | 0.253 | 0.748 |
| 51 | $[Kr]4d^{10} 5s^2 5p^3$ | 0.018 | 0.104 | 0.080 | 0.085 | 0.300 | 0.287 | 0.297 | 0.243 | 0.246 | 0.724 |
| 52 | $[Kr]4d^{10} 5s^2 5p^4$ | 0.018 | 0.102 | 0.078 | 0.083 | 0.293 | 0.280 | 0.290 | 0.237 | 0.240 | 0.702 |
| 53 | $[Kr]4d^{10} 5s^2 5p^5$ | 0.018 | 0.099 | 0.076 | 0.081 | 0.285 | 0.273 | 0.283 | 0.230 | 0.233 | 0.682 |
| 54 | $[Kr]4d^{10} 5s^2 5p^6$ | 0.017 | 0.097 | 0.075 | 0.079 | 0.279 | 0.266 | 0.276 | 0.224 | 0.228 | 0.662 |
| 55 | $[Xe]6s$ | 0.017 | 0.095 | 0.073 | 0.078 | 0.272 | 0.260 | 0.270 | 0.219 | 0.222 | 0.643 |
| 56 | $[Xe]6s^2$ | 0.016 | 0.093 | 0.071 | 0.076 | 0.266 | 0.254 | 0.264 | 0.214 | 0.217 | 0.625 |
| 57 | $[Xe]5d6s^2$ | 0.016 | 0.091 | 0.070 | 0.075 | 0.260 | 0.248 | 0.259 | 0.209 | 0.212 | 0.609 |
| 58 | $[Xe]4f5d6s^2$ | 0.016 | 0.089 | 0.068 | 0.073 | 0.255 | 0.242 | 0.253 | 0.204 | 0.207 | 0.594 |
| 59 | $[Xe]4f^3 6s^2$ | 0.015 | 0.087 | 0.067 | 0.072 | 0.249 | 0.237 | 0.248 | 0.199 | 0.202 | 0.580 |
| 60 | $[Xe]4f^4 6s^2$ | 0.015 | 0.086 | 0.065 | 0.071 | 0.244 | 0.231 | 0.242 | 0.195 | 0.198 | 0.566 |
| 61 | $[Xe]4f^5 6s^2$ | 0.015 | 0.084 | 0.064 | 0.069 | 0.239 | 0.226 | 0.238 | 0.190 | 0.193 | 0.553 |
| 62 | $[Xe]4f^6 6s^2$ | 0.015 | 0.082 | 0.063 | 0.068 | 0.234 | 0.221 | 0.233 | 0.186 | 0.189 | 0.541 |
| 63 | $[Xe]4f^7 6s^2$ | 0.014 | 0.081 | 0.061 | 0.067 | 0.229 | 0.217 | 0.228 | 0.182 | 0.185 | 0.529 |
| 64 | $[Xe]4f^7 5d6s^2$ | 0.014 | 0.079 | 0.060 | 0.066 | 0.224 | 0.212 | 0.224 | 0.178 | 0.182 | 0.517 |
| 65 | $[Xe]4f^9 6s^2$ | 0.014 | 0.078 | 0.059 | 0.065 | 0.220 | 0.208 | 0.220 | 0.175 | 0.178 | 0.506 |
| 66 | $[Xe]4f^{10} 6s^2$ | 0.013 | 0.076 | 0.058 | 0.064 | 0.216 | 0.203 | 0.216 | 0.171 | 0.175 | 0.496 |
| 67 | $[Xe]4f^{11} 6s^2$ | 0.013 | 0.075 | 0.056 | 0.063 | 0.211 | 0.199 | 0.212 | 0.168 | 0.171 | 0.485 |

**Table 4** (continued)

| Atomic Number | Configuration | $1s$ | $2s$ | $2p_{1/2}$ | $2p_{3/2}$ | 3s | $3p_{1/2}$ | $3p_{3/2}$ | $3d_{3/2}$ | $3d_{5/2}$ | 4s |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 68 | $[Xe]4f^{12}6s^2$ | 0.013 | 0.073 | 0.055 | 0.062 | 0.207 | 0.195 | 0.208 | 0.165 | 0.168 | 0.475 |
| 69 | $[Xe]4f^{13}6s^2$ | 0.013 | 0.072 | 0.054 | 0.061 | 0.203 | 0.192 | 0.204 | 0.161 | 0.165 | 0.466 |
| 70 | $[Xe]4f^{14}6s^2$ | 0.012 | 0.071 | 0.053 | 0.060 | 0.200 | 0.188 | 0.201 | 0.158 | 0.162 | 0.457 |
| 71 | $[Xe]4f^{14}5d6s^2$ | 0.012 | 0.070 | 0.052 | 0.059 | 0.196 | 0.184 | 0.198 | 0.156 | 0.159 | 0.448 |
| 72 | $[Xe]4f^{14}5d^26s^2$ | 0.012 | 0.068 | 0.051 | 0.058 | 0.192 | 0.181 | 0.194 | 0.153 | 0.156 | 0.439 |
| 73 | $[Xe]4f^{14}5d^36s^2$ | 0.012 | 0.067 | 0.050 | 0.057 | 0.189 | 0.178 | 0.191 | 0.150 | 0.154 | 0.430 |
| 74 | $[Xe]4f^{14}5d^46s^2$ | 0.011 | 0.066 | 0.049 | 0.056 | 0.186 | 0.174 | 0.188 | 0.147 | 0.151 | 0.422 |
| 75 | $[Xe]4f^{14}5d^56s^2$ | 0.011 | 0.065 | 0.048 | 0.055 | 0.182 | 0.171 | 0.185 | 0.145 | 0.149 | 0.414 |
| 76 | $[Xe]4f^{14}5d^66s^2$ | 0.011 | 0.064 | 0.047 | 0.054 | 0.179 | 0.168 | 0.182 | 0.142 | 0.146 | 0.406 |
| 77 | $[Xe]4f^{14}5d^76s^2$ | 0.011 | 0.063 | 0.046 | 0.054 | 0.176 | 0.165 | 0.179 | 0.140 | 0.144 | 0.398 |
| 78 | $[Xe]4f^{14}5d^96s$ | 0.011 | 0.062 | 0.046 | 0.053 | 0.173 | 0.162 | 0.176 | 0.138 | 0.142 | 0.391 |
| 79 | $[Xe]4f^{14}5d^{10}6s$ | 0.010 | 0.060 | 0.045 | 0.052 | 0.170 | 0.159 | 0.174 | 0.136 | 0.140 | 0.384 |
| 80 | $[Xe]4f^{14}5d^{10}6s^2$ | 0.010 | 0.059 | 0.044 | 0.051 | 0.167 | 0.156 | 0.171 | 0.133 | 0.137 | 0.377 |
| 81 | $[Xe]4f^{14}5d^{10}6s^26p$ | 0.010 | 0.058 | 0.043 | 0.051 | 0.164 | 0.154 | 0.169 | 0.131 | 0.135 | 0.370 |
| 82 | $[Xe]4f^{14}5d^{10}6s^26p^2$ | 0.010 | 0.057 | 0.042 | 0.050 | 0.161 | 0.151 | 0.166 | 0.129 | 0.133 | 0.364 |
| 83 | $[Xe]4f^{14}5d^{10}6s^26p^3$ | 0.010 | 0.057 | 0.041 | 0.049 | 0.159 | 0.148 | 0.164 | 0.127 | 0.131 | 0.357 |
| 84 | $[Xe]4f^{14}5d^{10}6s^26p^4$ | 0.009 | 0.056 | 0.041 | 0.049 | 0.156 | 0.146 | 0.161 | 0.125 | 0.130 | 0.351 |
| 85 | $[Xe]4f^{14}5d^{10}6s^26p^5$ | 0.009 | 0.055 | 0.040 | 0.048 | 0.154 | 0.143 | 0.159 | 0.123 | 0.128 | 0.345 |
| 86 | $[Xe]4f^{14}5d^{10}6s^26p^6$ | 0.009 | 0.054 | 0.039 | 0.047 | 0.151 | 0.141 | 0.157 | 0.122 | 0.126 | 0.339 |
| 87 | $[Rn]7s$ | 0.009 | 0.053 | 0.038 | 0.047 | 0.149 | 0.139 | 0.155 | 0.120 | 0.124 | 0.333 |
| 88 | $[Rn]7s^2$ | 0.009 | 0.052 | 0.038 | 0.046 | 0.146 | 0.136 | 0.153 | 0.118 | 0.123 | 0.327 |
| 89 | $[Rn]6d7s^2$ | 0.009 | 0.051 | 0.037 | 0.045 | 0.144 | 0.134 | 0.151 | 0.116 | 0.121 | 0.322 |
| 90 | $[Rn]6d^27s^2$ | 0.008 | 0.050 | 0.036 | 0.045 | 0.142 | 0.132 | 0.149 | 0.115 | 0.119 | 0.316 |
| 91 | $[Rn]5f^26d7s^2$ | 0.008 | 0.049 | 0.036 | 0.044 | 0.139 | 0.130 | 0.147 | 0.113 | 0.118 | 0.311 |
| 92 | $[Rn]5f^36d7s^2$ | 0.008 | 0.049 | 0.035 | 0.044 | 0.137 | 0.127 | 0.145 | 0.112 | 0.116 | 0.306 |
| 93 | $[Rn]5f^46d7s^2$ | 0.008 | 0.048 | 0.034 | 0.043 | 0.135 | 0.125 | 0.143 | 0.110 | 0.115 | 0.301 |
| 94 | $[Rn]5f^67s^2$ | 0.008 | 0.047 | 0.034 | 0.043 | 0.133 | 0.123 | 0.141 | 0.109 | 0.113 | 0.295 |
| 95 | $[Rn]5f^77s^2$ | 0.008 | 0.046 | 0.033 | 0.042 | 0.131 | 0.121 | 0.139 | 0.107 | 0.112 | 0.291 |
| 96 | $[Rn]5f^76d7s^2$ | 0.008 | 0.046 | 0.032 | 0.042 | 0.129 | 0.119 | 0.138 | 0.106 | 0.110 | 0.286 |
| 97 | $[Rn]5f^97s^2$ | 0.007 | 0.045 | 0.032 | 0.041 | 0.127 | 0.117 | 0.136 | 0.104 | 0.109 | 0.281 |
| 98 | $[Rn]5f^{10}7s^2$ | 0.007 | 0.044 | 0.031 | 0.041 | 0.125 | 0.115 | 0.134 | 0.103 | 0.108 | 0.277 |
| 99 | $[Rn]5f^{11}7s^2$ | 0.007 | 0.043 | 0.030 | 0.040 | 0.123 | 0.113 | 0.133 | 0.101 | 0.106 | 0.272 |
| 100 | $[Rn]5f^{12}7s^2$ | 0.007 | 0.043 | 0.030 | 0.040 | 0.121 | 0.111 | 0.131 | 0.100 | 0.105 | 0.268 |
| 101 | $[Rn]5f^{13}7s^2$ | 0.007 | 0.042 | 0.029 | 0.039 | 0.119 | 0.110 | 0.129 | 0.099 | 0.104 | 0.264 |
| 102 | $[Rn]5f^{14}7s^2$ | 0.007 | 0.041 | 0.029 | 0.039 | 0.117 | 0.108 | 0.128 | 0.098 | 0.103 | 0.260 |
| 103 | $[Rn]5f^{14}7s^27p$ | 0.007 | 0.041 | 0.028 | 0.038 | 0.115 | 0.106 | 0.126 | 0.096 | 0.102 | 0.256 |
| 104 | $[Rn]5f^{14}6d^27s^2$ | 0.006 | 0.040 | 0.027 | 0.038 | 0.113 | 0.104 | 0.125 | 0.095 | 0.100 | 0.252 |
| 105 | $[Rn]5f^{14}6d^37s^2$ | 0.006 | 0.039 | 0.027 | 0.037 | 0.112 | 0.103 | 0.124 | 0.094 | 0.099 | 0.248 |
| 106 | $[Rn]5f^{14}6d^47s^2$ | 0.006 | 0.039 | 0.026 | 0.037 | 0.110 | 0.101 | 0.122 | 0.093 | 0.098 | 0.244 |
| 107 | $[Rn]5f^{14}6d^57s^2$ | 0.006 | 0.038 | 0.026 | 0.037 | 0.108 | 0.099 | 0.121 | 0.092 | 0.097 | 0.240 |
| 108 | $[Rn]5f^{14}6d^67s^2$ | 0.006 | 0.037 | 0.025 | 0.036 | 0.106 | 0.098 | 0.119 | 0.091 | 0.096 | 0.236 |
| 109 | $[Rn]5f^{14}6d^77s^2$ | 0.006 | 0.037 | 0.024 | 0.036 | 0.105 | 0.096 | 0.118 | 0.090 | 0.095 | 0.232 |
| 110 | $[Rn]5f^{14}6d^97s$ | 0.006 | 0.036 | 0.024 | 0.035 | 0.103 | 0.094 | 0.117 | 0.088 | 0.094 | 0.229 |
| 111 | $[Rn]5f^{14}6d^{10}7s$ | 0.005 | 0.035 | 0.023 | 0.035 | 0.102 | 0.093 | 0.116 | 0.087 | 0.093 | 0.225 |
| 112 | $[Rn]5f^{14}6d^{10}7s^2$ | 0.005 | 0.035 | 0.023 | 0.035 | 0.100 | 0.091 | 0.114 | 0.086 | 0.092 | 0.222 |
| 113 | $[Rn]5f^{14}6d^{10}7s^27p$ | 0.005 | 0.034 | 0.022 | 0.034 | 0.098 | 0.090 | 0.113 | 0.085 | 0.091 | 0.218 |
| 114 | $[Rn]5f^{14}6d^{10}7s^27p^2$ | 0.005 | 0.033 | 0.022 | 0.034 | 0.097 | 0.088 | 0.112 | 0.084 | 0.090 | 0.215 |
| 115 | $[Rn]5f^{14}6d^{10}7s^27p^3$ | 0.005 | 0.033 | 0.021 | 0.034 | 0.095 | 0.086 | 0.111 | 0.083 | 0.089 | 0.211 |
| 116 | $[Rn]5f^{14}6d^{10}7s^27p^4$ | 0.005 | 0.032 | 0.021 | 0.033 | 0.094 | 0.085 | 0.109 | 0.083 | 0.088 | 0.208 |
| 117 | $[Rn]5f^{14}6d^{10}7s^27p^5$ | 0.005 | 0.032 | 0.020 | 0.033 | 0.092 | 0.083 | 0.108 | 0.082 | 0.087 | 0.205 |
| 118 | $[Rn]5f^{14}6d^{10}7s^27p^6$ | 0.005 | 0.031 | 0.019 | 0.033 | 0.091 | 0.082 | 0.107 | 0.081 | 0.087 | 0.202 |

**Table 5**
Radii of maximum charge density calculated with the Dirac-Fock method for subshells ranging from $4p_{1/2}$ to $5f_{7/2}$ ($a_0$).

| Atomic Number | Configuration | $4p_{1/2}$ | $4p_{3/2}$ | $4d_{3/2}$ | $4d_{5/2}$ | $4f_{5/2}$ | $4f_{7/2}$ | $5s$ | $5p_{1/2}$ | $5p_{3/2}$ | $5d_{3/2}$ | $5d_{5/2}$ | $5f_{5/2}$ | $5f_{7/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $1s$ | | | | | | | | | | | | | |
| 2 | $1s^2$ | | | | | | | | | | | | | |
| 3 | $1s^2 2s$ | | | | | | | | | | | | | |
| 4 | $1s^2 2s^2$ | | | | | | | | | | | | | |
| 5 | $1s^2 2s^2 2p$ | | | | | | | | | | | | | |
| 6 | $1s^2 2s^2 2p^2$ | | | | | | | | | | | | | |
| 7 | $1s^2 2s^2 2p^3$ | | | | | | | | | | | | | |
| 8 | $1s^2 2s^2 2p^4$ | | | | | | | | | | | | | |
| 9 | $1s^2 2s^2 2p^5$ | | | | | | | | | | | | | |
| 10 | $1s^2 2s^2 2p^6$ | | | | | | | | | | | | | |
| 11 | $[Ne]3s$ | | | | | | | | | | | | | |
| 12 | $[Ne]3s^2$ | | | | | | | | | | | | | |
| 13 | $[Ne]3s^2 3p$ | | | | | | | | | | | | | |
| 14 | $[Ne]3s^2 3p^2$ | | | | | | | | | | | | | |
| 15 | $[Ne]3s^2 3p^3$ | | | | | | | | | | | | | |
| 16 | $[Ne]3s^2 3p^4$ | | | | | | | | | | | | | |
| 17 | $[Ne]3s^2 3p^5$ | | | | | | | | | | | | | |
| 18 | $[Ne]3s^2 3p^6$ | | | | | | | | | | | | | |
| 19 | $[Ar]4s$ | | | | | | | | | | | | | |
| 20 | $[Ar]4s^2$ | | | | | | | | | | | | | |
| 21 | $[Ar]3d4s^2$ | | | | | | | | | | | | | |
| 22 | $[Ar]3d^2 4s^2$ | | | | | | | | | | | | | |
| 23 | $[Ar]3d^3 4s^2$ | | | | | | | | | | | | | |
| 24 | $[Ar]3d^5 4s$ | | | | | | | | | | | | | |
| 25 | $[Ar]3d^5 4s^2$ | | | | | | | | | | | | | |
| 26 | $[Ar]3d^6 4s^2$ | | | | | | | | | | | | | |
| 27 | $[Ar]3d^7 4s^2$ | | | | | | | | | | | | | |
| 28 | $[Ar]3d^8 4s^2$ | | | | | | | | | | | | | |
| 29 | $[Ar]3d^{10} 4s$ | | | | | | | | | | | | | |
| 30 | $[Ar]3d^{10} 4s^2$ | | | | | | | | | | | | | |
| 31 | $[Ar]3d^{10} 4s^2 4p$ | 2.615 | | | | | | | | | | | | |
| 32 | $[Ar]3d^{10} 4s^2 4p^2$ | 2.234 | 2.257 | | | | | | | | | | | |
| 33 | $[Ar]3d^{10} 4s^2 4p^3$ | 1.984 | 2.011 | | | | | | | | | | | |
| 34 | $[Ar]3d^{10} 4s^2 4p^4$ | 1.804 | 1.832 | | | | | | | | | | | |
| 35 | $[Ar]3d^{10} 4s^2 4p^5$ | 1.658 | 1.689 | | | | | | | | | | | |
| 36 | $[Ar]3d^{10} 4s^2 4p^6$ | 1.538 | 1.570 | | | | | | | | | | | |
| 37 | $[Kr]5s$ | 1.414 | 1.442 | | | | | 4.627 | | | | | | |
| 38 | $[Kr]5s^2$ | 1.314 | 1.339 | | | | | 3.803 | | | | | | |
| 39 | $[Kr]4d5s^2$ | 1.236 | 1.258 | 1.801 | | | | 3.500 | | | | | | |
| 40 | $[Kr]4d^2 5s^2$ | 1.170 | 1.190 | 1.600 | 1.612 | | | 3.305 | | | | | | |
| 41 | $[Kr]4d^4 5s$ | 1.113 | 1.136 | 1.506 | 1.521 | | | 3.174 | | | | | | |
| 42 | $[Kr]4d^5 5s$ | 1.061 | 1.084 | 1.388 | 1.400 | | | 3.028 | | | | | | |
| 43 | $[Kr]4d^5 5s^2$ | 1.012 | 1.034 | 1.267 | 1.278 | | | 2.905 | | | | | | |
| 44 | $[Kr]4d^7 5s$ | 0.973 | 0.995 | 1.212 | 1.225 | | | 2.875 | | | | | | |
| 45 | $[Kr]4d^8 5s$ | 0.934 | 0.956 | 1.144 | 1.157 | | | 2.818 | | | | | | |
| 46 | $[Kr]4d^{10}$ | 0.900 | 0.923 | 1.096 | 1.109 | | | | | | | | | |
| 47 | $[Kr]4d^{10} 5s$ | 0.866 | 0.889 | 1.033 | 1.046 | | | 2.729 | | | | | | |
| 48 | $[Kr]4d^{10} 5s^2$ | 0.834 | 0.857 | 0.977 | 0.988 | | | 2.465 | | | | | | |
| 49 | $[Kr]4d^{10} 5s^2 5p$ | 0.804 | 0.827 | 0.928 | 0.938 | | | 2.236 | 2.889 | | | | | |
| 50 | $[Kr]4d^{10} 5s^2 5p^2$ | 0.776 | 0.799 | 0.884 | 0.893 | | | 2.071 | 2.547 | 2.614 | | | | |
| 51 | $[Kr]4d^{10} 5s^2 5p^3$ | 0.750 | 0.773 | 0.844 | 0.853 | | | 1.938 | 2.309 | 2.387 | | | | |
| 52 | $[Kr]4d^{10} 5s^2 5p^4$ | 0.725 | 0.748 | 0.808 | 0.817 | | | 1.828 | 2.130 | 2.213 | | | | |
| 53 | $[Kr]4d^{10} 5s^2 5p^5$ | 0.701 | 0.724 | 0.775 | 0.784 | | | 1.731 | 1.986 | 2.069 | | | | |
| 54 | $[Kr]4d^{10} 5s^2 5p^6$ | 0.679 | 0.702 | 0.745 | 0.754 | | | 1.649 | 1.866 | 1.945 | | | | |
| 55 | $[Xe]6s$ | 0.659 | 0.681 | 0.718 | 0.726 | | | 1.562 | 1.738 | 1.808 | | | | |
| 56 | $[Xe]6s^2$ | 0.639 | 0.662 | 0.693 | 0.701 | | | 1.483 | 1.634 | 1.697 | | | | |
| 57 | $[Xe]5d6s^2$ | 0.621 | 0.644 | 0.669 | 0.677 | | | 1.419 | 1.552 | 1.610 | 2.220 | | | |
| 58 | $[Xe]4f5d6s^2$ | 0.604 | 0.627 | 0.650 | 0.657 | 0.715 | 0.721 | 1.383 | 1.510 | 1.572 | 2.115 | 2.144 | | |
| 59 | $[Xe]4f^3 6s^2$ | 0.590 | 0.613 | 0.634 | 0.642 | 0.697 | 0.702 | 1.370 | 1.501 | 1.573 | | | | |
| 60 | $[Xe]4f^4 6s^2$ | 0.575 | 0.599 | 0.617 | 0.625 | 0.667 | 0.673 | 1.340 | 1.467 | 1.540 | | | | |
| 61 | $[Xe]4f^5 6s^2$ | 0.561 | 0.585 | 0.601 | 0.609 | 0.641 | 0.647 | 1.310 | 1.433 | 1.507 | | | | |
| 62 | $[Xe]4f^6 6s^2$ | 0.547 | 0.572 | 0.586 | 0.594 | 0.618 | 0.623 | 1.281 | 1.402 | 1.477 | | | | |
| 63 | $[Xe]4f^7 6s^2$ | 0.535 | 0.560 | 0.571 | 0.580 | 0.597 | 0.601 | 1.254 | 1.373 | 1.449 | | | | |
| 64 | $[Xe]4f^7 5d6s^2$ | 0.523 | 0.547 | 0.556 | 0.565 | 0.570 | 0.574 | 1.213 | 1.322 | 1.393 | 1.909 | 1.931 | | |
| 65 | $[Xe]4f^9 6s^2$ | 0.511 | 0.537 | 0.545 | 0.553 | 0.560 | 0.564 | 1.201 | 1.313 | 1.394 | | | | |
| 66 | $[Xe]4f^{10} 6s^2$ | 0.500 | 0.526 | 0.532 | 0.541 | 0.543 | 0.548 | 1.177 | 1.286 | 1.370 | | | | |
| 67 | $[Xe]4f^{11} 6s^2$ | 0.489 | 0.515 | 0.521 | 0.529 | 0.527 | 0.533 | 1.154 | 1.261 | 1.344 | | | | |

**Table 5** (continued)

| Atomic Number | Configuration | $4p_{1/2}$ | $4p_{3/2}$ | $4d_{3/2}$ | $4d_{5/2}$ | $4f_{5/2}$ | $4f_{7/2}$ | $5s$ | $5p_{1/2}$ | $5p_{3/2}$ | $5d_{3/2}$ | $5d_{5/2}$ | $5f_{5/2}$ | $5f_{7/2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 68 | $[Xe]4f^{12}6s^2$ | 0.479 | 0.505 | 0.510 | 0.518 | 0.512 | 0.518 | 1.131 | 1.235 | 1.322 | | | | |
| 69 | $[Xe]4f^{13}6s^2$ | 0.469 | 0.496 | 0.499 | 0.508 | 0.499 | 0.505 | 1.110 | 1.212 | 1.299 | | | | |
| 70 | $[Xe]4f^{14}6s^2$ | 0.459 | 0.487 | 0.489 | 0.497 | 0.486 | 0.492 | 1.089 | 1.189 | 1.278 | | | | |
| 71 | $[Xe]4f^{14}5d6s^2$ | 0.450 | 0.477 | 0.478 | 0.487 | 0.471 | 0.476 | 1.058 | 1.152 | 1.236 | 1.847 | | | |
| 72 | $[Xe]4f^{14}5d^26s^2$ | 0.441 | 0.468 | 0.468 | 0.477 | 0.456 | 0.461 | 1.030 | 1.116 | 1.196 | 1.675 | 1.723 | | |
| 73 | $[Xe]4f^{14}5d^36s^2$ | 0.431 | 0.459 | 0.458 | 0.468 | 0.442 | 0.448 | 1.001 | 1.081 | 1.159 | 1.560 | 1.606 | | |
| 74 | $[Xe]4f^{14}5d^46s^2$ | 0.423 | 0.451 | 0.449 | 0.458 | 0.430 | 0.434 | 0.974 | 1.048 | 1.125 | 1.472 | 1.511 | | |
| 75 | $[Xe]4f^{14}5d^56s^2$ | 0.414 | 0.443 | 0.440 | 0.449 | 0.417 | 0.422 | 0.949 | 1.016 | 1.093 | 1.396 | 1.436 | | |
| 76 | $[Xe]4f^{14}5d^66s^2$ | 0.406 | 0.435 | 0.431 | 0.440 | 0.406 | 0.411 | 0.924 | 0.987 | 1.062 | 1.332 | 1.374 | | |
| 77 | $[Xe]4f^{14}5d^76s^2$ | 0.398 | 0.428 | 0.422 | 0.432 | 0.395 | 0.400 | 0.901 | 0.959 | 1.034 | 1.275 | 1.318 | | |
| 78 | $[Xe]4f^{14}5d^96s$ | 0.391 | 0.420 | 0.414 | 0.423 | 0.385 | 0.390 | 0.879 | 0.933 | 1.009 | 1.235 | 1.280 | | |
| 79 | $[Xe]4f^{14}5d^{10}6s$ | 0.383 | 0.413 | 0.406 | 0.416 | 0.375 | 0.380 | 0.858 | 0.908 | 0.983 | 1.189 | 1.231 | | |
| 80 | $[Xe]4f^{14}5d^{10}6s^2$ | 0.376 | 0.405 | 0.399 | 0.408 | 0.366 | 0.371 | 0.837 | 0.883 | 0.958 | 1.139 | 1.177 | | |
| 81 | $[Xe]4f^{14}5d^{10}6s^26p$ | 0.369 | 0.399 | 0.391 | 0.401 | 0.358 | 0.362 | 0.816 | 0.859 | 0.933 | 1.094 | 1.128 | | |
| 82 | $[Xe]4f^{14}5d^{10}6s^26p^2$ | 0.362 | 0.392 | 0.384 | 0.394 | 0.349 | 0.354 | 0.797 | 0.836 | 0.909 | 1.054 | 1.084 | | |
| 83 | $[Xe]4f^{14}5d^{10}6s^26p^3$ | 0.355 | 0.386 | 0.377 | 0.386 | 0.342 | 0.346 | 0.778 | 0.815 | 0.887 | 1.016 | 1.045 | | |
| 84 | $[Xe]4f^{14}5d^{10}6s^26p^4$ | 0.349 | 0.380 | 0.370 | 0.380 | 0.334 | 0.338 | 0.759 | 0.793 | 0.865 | 0.982 | 1.010 | | |
| 85 | $[Xe]4f^{14}5d^{10}6s^26p^5$ | 0.342 | 0.373 | 0.364 | 0.373 | 0.327 | 0.331 | 0.742 | 0.774 | 0.844 | 0.950 | 0.978 | | |
| 86 | $[Xe]4f^{14}5d^{10}6s^26p^6$ | 0.336 | 0.368 | 0.358 | 0.367 | 0.320 | 0.324 | 0.726 | 0.755 | 0.825 | 0.921 | 0.948 | | |
| 87 | $[Rn]7s$ | 0.330 | 0.362 | 0.352 | 0.361 | 0.313 | 0.318 | 0.709 | 0.736 | 0.806 | 0.893 | 0.920 | | |
| 88 | $[Rn]7s^2$ | 0.324 | 0.356 | 0.345 | 0.355 | 0.307 | 0.312 | 0.694 | 0.719 | 0.788 | 0.868 | 0.893 | | |
| 89 | $[Rn]6d7s^2$ | 0.318 | 0.351 | 0.340 | 0.349 | 0.301 | 0.305 | 0.678 | 0.703 | 0.771 | 0.844 | 0.869 | | |
| 90 | $[Rn]6d^27s^2$ | 0.313 | 0.346 | 0.334 | 0.344 | 0.295 | 0.300 | 0.665 | 0.686 | 0.754 | 0.821 | 0.846 | | |
| 91 | $[Rn]5f^26d7s^2$ | 0.307 | 0.341 | 0.329 | 0.339 | 0.290 | 0.294 | 0.651 | 0.672 | 0.740 | 0.804 | 0.826 | 1.110 | 1.124 |
| 92 | $[Rn]5f^36d7s^2$ | 0.302 | 0.336 | 0.324 | 0.334 | 0.284 | 0.289 | 0.637 | 0.658 | 0.725 | 0.786 | 0.808 | 1.055 | 1.071 |
| 93 | $[Rn]5f^46d7s^2$ | 0.297 | 0.331 | 0.319 | 0.328 | 0.279 | 0.284 | 0.625 | 0.644 | 0.712 | 0.769 | 0.790 | 1.012 | 1.028 |
| 94 | $[Rn]5f^67s^2$ | 0.292 | 0.326 | 0.314 | 0.323 | 0.274 | 0.279 | 0.613 | 0.630 | 0.698 | 0.753 | 0.775 | 0.985 | 1.001 |
| 95 | $[Rn]5f^77s^2$ | 0.287 | 0.321 | 0.309 | 0.319 | 0.270 | 0.274 | 0.601 | 0.617 | 0.687 | 0.736 | 0.760 | 0.950 | 0.966 |
| 96 | $[Rn]5f^76d7s^2$ | 0.282 | 0.317 | 0.304 | 0.314 | 0.265 | 0.269 | 0.590 | 0.605 | 0.674 | 0.721 | 0.744 | 0.911 | 0.925 |
| 97 | $[Rn]5f^97s^2$ | 0.278 | 0.312 | 0.300 | 0.310 | 0.261 | 0.265 | 0.578 | 0.593 | 0.663 | 0.708 | 0.730 | 0.890 | 0.908 |
| 98 | $[Rn]5f^{10}7s^2$ | 0.273 | 0.308 | 0.295 | 0.305 | 0.256 | 0.261 | 0.568 | 0.581 | 0.652 | 0.694 | 0.717 | 0.865 | 0.882 |
| 99 | $[Rn]5f^{11}7s^2$ | 0.268 | 0.304 | 0.291 | 0.301 | 0.252 | 0.257 | 0.557 | 0.571 | 0.641 | 0.681 | 0.703 | 0.840 | 0.858 |
| 100 | $[Rn]5f^{12}7s^2$ | 0.264 | 0.300 | 0.287 | 0.297 | 0.248 | 0.253 | 0.547 | 0.559 | 0.631 | 0.668 | 0.691 | 0.818 | 0.836 |
| 101 | $[Rn]5f^{13}7s^2$ | 0.259 | 0.296 | 0.283 | 0.293 | 0.244 | 0.249 | 0.537 | 0.549 | 0.620 | 0.656 | 0.679 | 0.797 | 0.814 |
| 102 | $[Rn]5f^{14}7s^2$ | 0.255 | 0.292 | 0.279 | 0.289 | 0.241 | 0.245 | 0.528 | 0.538 | 0.611 | 0.644 | 0.668 | 0.778 | 0.795 |
| 103 | $[Rn]5f^{14}7s^27p$ | 0.251 | 0.288 | 0.275 | 0.285 | 0.237 | 0.241 | 0.518 | 0.529 | 0.601 | 0.633 | 0.656 | 0.756 | 0.772 |
| 104 | $[Rn]5f^{14}6d^27s^2$ | 0.247 | 0.285 | 0.271 | 0.282 | 0.233 | 0.238 | 0.509 | 0.519 | 0.591 | 0.621 | 0.645 | 0.736 | 0.750 |
| 105 | $[Rn]5f^{14}6d^37s^2$ | 0.243 | 0.281 | 0.268 | 0.278 | 0.230 | 0.234 | 0.501 | 0.509 | 0.583 | 0.611 | 0.634 | 0.716 | 0.731 |
| 106 | $[Rn]5f^{14}6d^47s^2$ | 0.239 | 0.278 | 0.264 | 0.275 | 0.227 | 0.231 | 0.492 | 0.500 | 0.574 | 0.600 | 0.623 | 0.698 | 0.712 |
| 107 | $[Rn]5f^{14}6d^57s^2$ | 0.235 | 0.274 | 0.261 | 0.271 | 0.223 | 0.228 | 0.483 | 0.491 | 0.565 | 0.590 | 0.613 | 0.681 | 0.695 |
| 108 | $[Rn]5f^{14}6d^67s^2$ | 0.231 | 0.271 | 0.257 | 0.268 | 0.220 | 0.225 | 0.475 | 0.481 | 0.556 | 0.580 | 0.603 | 0.665 | 0.678 |
| 109 | $[Rn]5f^{14}6d^77s^2$ | 0.227 | 0.268 | 0.254 | 0.264 | 0.217 | 0.222 | 0.467 | 0.473 | 0.549 | 0.571 | 0.593 | 0.650 | 0.663 |
| 110 | $[Rn]5f^{14}6d^97s$ | 0.224 | 0.264 | 0.250 | 0.261 | 0.214 | 0.219 | 0.459 | 0.464 | 0.541 | 0.561 | 0.583 | 0.636 | 0.648 |
| 111 | $[Rn]5f^{14}6d^{10}7s$ | 0.220 | 0.261 | 0.247 | 0.258 | 0.211 | 0.216 | 0.451 | 0.456 | 0.533 | 0.552 | 0.575 | 0.622 | 0.635 |
| 112 | $[Rn]5f^{14}6d^{10}7s^2$ | 0.216 | 0.258 | 0.244 | 0.255 | 0.209 | 0.213 | 0.443 | 0.448 | 0.526 | 0.543 | 0.565 | 0.609 | 0.621 |
| 113 | $[Rn]5f^{14}6d^{10}7s^27p$ | 0.213 | 0.255 | 0.241 | 0.252 | 0.206 | 0.210 | 0.436 | 0.440 | 0.518 | 0.535 | 0.557 | 0.596 | 0.609 |
| 114 | $[Rn]5f^{14}6d^{10}7s^27p^2$ | 0.209 | 0.252 | 0.238 | 0.249 | 0.203 | 0.208 | 0.428 | 0.432 | 0.511 | 0.527 | 0.549 | 0.585 | 0.596 |
| 115 | $[Rn]5f^{14}6d^{10}7s^27p^3$ | 0.206 | 0.249 | 0.235 | 0.246 | 0.201 | 0.205 | 0.421 | 0.424 | 0.504 | 0.518 | 0.541 | 0.574 | 0.585 |
| 116 | $[Rn]5f^{14}6d^{10}7s^27p^4$ | 0.202 | 0.246 | 0.232 | 0.243 | 0.198 | 0.203 | 0.414 | 0.417 | 0.497 | 0.511 | 0.533 | 0.563 | 0.574 |
| 117 | $[Rn]5f^{14}6d^{10}7s^27p^5$ | 0.199 | 0.244 | 0.229 | 0.241 | 0.195 | 0.200 | 0.407 | 0.409 | 0.490 | 0.503 | 0.525 | 0.553 | 0.564 |
| 118 | $[Rn]5f^{14}6d^{10}7s^27p^6$ | 0.196 | 0.241 | 0.227 | 0.238 | 0.193 | 0.198 | 0.400 | 0.402 | 0.484 | 0.496 | 0.518 | 0.543 | 0.554 |

**Table 6**
Radii of maximum charge density calculated with the Dirac-Fock method for subshells ranging from $6s$ to $7p_{3/2}(a_0)$.

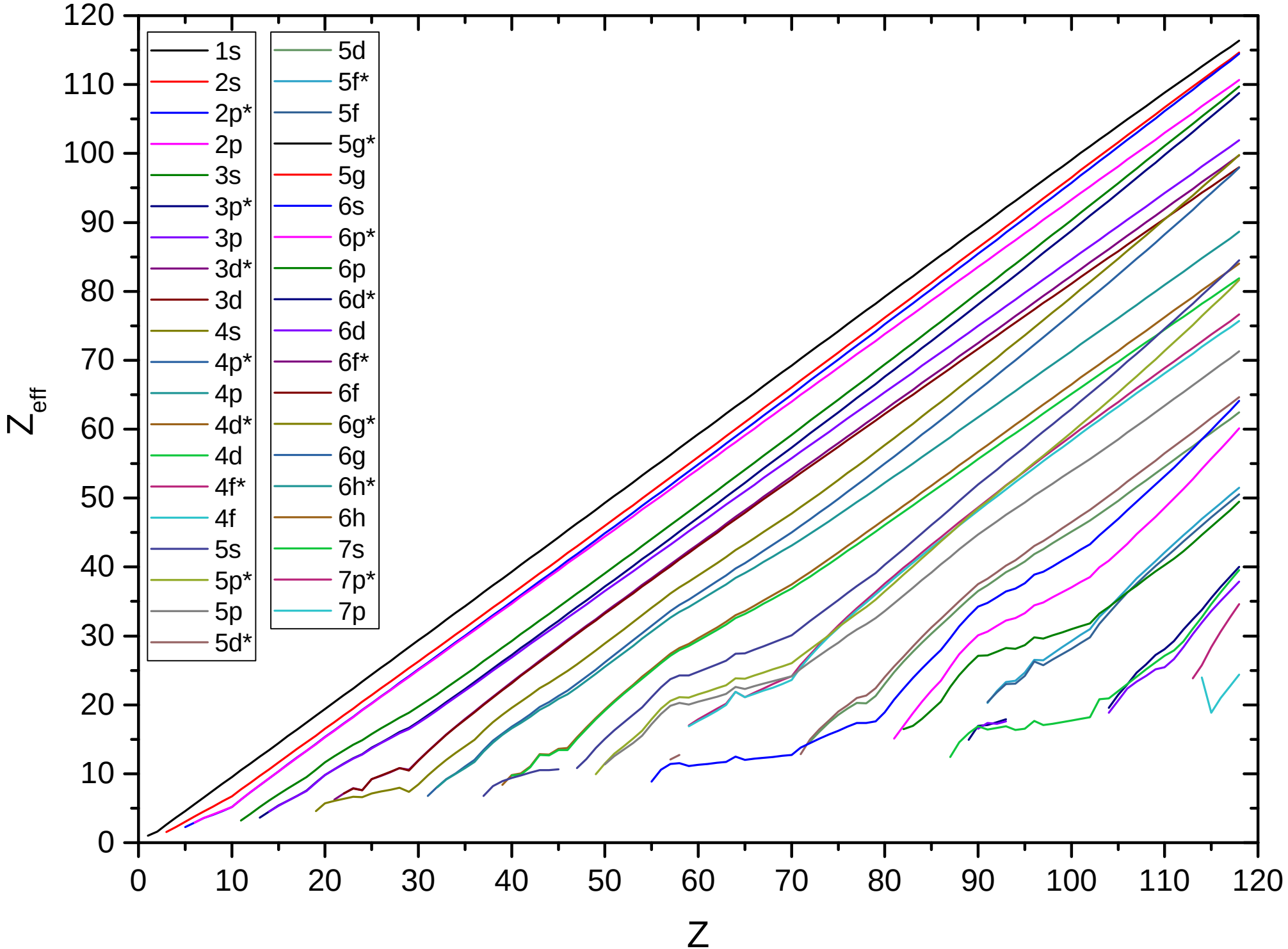
| Atomic Number | Configuration | $6s$ | $6p_{1/2}$ | $6p_{3/2}$ | $6d_{3/2}$ | $6d_{5/2}$ | $7s$ | $7p_{1/2}$ | $7p_{3/2}$ |
|---|---|---|---|---|---|---|---|---|---|
| 55 | $[Xe]6s$ | 5.135 | | | | | | | |
| 56 | $[Xe]6s^2$ | 4.292 | | | | | | | |
| 57 | $[Xe]5d6s^2$ | 3.985 | | | | | | | |
| 58 | $[Xe]4f5d6s^2$ | 3.927 | | | | | | | |
| 59 | $[Xe]4f^36s^2$ | 4.063 | | | | | | | |
| 60 | $[Xe]4f^46s^2$ | 4.003 | | | | | | | |
| 61 | $[Xe]4f^56s^2$ | 3.942 | | | | | | | |
| 62 | $[Xe]4f^66s^2$ | 3.886 | | | | | | | |
| 63 | $[Xe]4f^76s^2$ | 3.836 | | | | | | | |
| 64 | $[Xe]4f^75d6s^2$ | 3.592 | | | | | | | |
| 65 | $[Xe]4f^96s^2$ | 3.725 | | | | | | | |
| 66 | $[Xe]4f^{10}6s^2$ | 3.674 | | | | | | | |
| 67 | $[Xe]4f^{11}6s^2$ | 3.625 | | | | | | | |
| 68 | $[Xe]4f^{12}6s^2$ | 3.575 | | | | | | | |
| 69 | $[Xe]4f^{13}6s^2$ | 3.530 | | | | | | | |
| 70 | $[Xe]4f^{14}6s^2$ | 3.484 | | | | | | | |
| 71 | $[Xe]4f^{14}5d6s^2$ | 3.232 | | | | | | | |
| 72 | $[Xe]4f^{14}5d^26s^2$ | 3.069 | | | | | | | |
| 73 | $[Xe]4f^{14}5d^36s^2$ | 2.932 | | | | | | | |
| 74 | $[Xe]4f^{14}5d^46s^2$ | 2.814 | | | | | | | |
| 75 | $[Xe]4f^{14}5d^56s^2$ | 2.711 | | | | | | | |
| 76 | $[Xe]4f^{14}5d^66s^2$ | 2.610 | | | | | | | |
| 77 | $[Xe]4f^{14}5d^76s^2$ | 2.522 | | | | | | | |
| 78 | $[Xe]4f^{14}5d^96s$ | 2.505 | | | | | | | |
| 79 | $[Xe]4f^{14}5d^{10}6s$ | 2.458 | | | | | | | |
| 80 | $[Xe]4f^{14}5d^{10}6s^2$ | 2.301 | | | | | | | |
| 81 | $[Xe]4f^{14}5d^{10}6s^26p$ | 2.147 | 2.754 | | | | | | |
| 82 | $[Xe]4f^{14}5d^{10}6s^26p^2$ | 2.026 | 2.495 | 2.699 | | | | | |
| 83 | $[Xe]4f^{14}5d^{10}6s^26p^3$ | 1.920 | 2.293 | 2.569 | | | | | |
| 84 | $[Xe]4f^{14}5d^{10}6s^26p^4$ | 1.831 | 2.134 | 2.415 | | | | | |
| 85 | $[Xe]4f^{14}5d^{10}6s^26p^5$ | 1.753 | 2.007 | 2.269 | | | | | |
| 86 | $[Xe]4f^{14}5d^{10}6s^26p^6$ | 1.683 | 1.902 | 2.144 | | | | | |
| 87 | $[Rn]7s$ | 1.609 | 1.794 | 2.009 | | | 4.992 | | |
| 88 | $[Rn]7s^2$ | 1.541 | 1.703 | 1.898 | | | 4.258 | | |
| 89 | $[Rn]6d7s^2$ | 1.483 | 1.629 | 1.810 | 2.627 | | 3.921 | | |
| 90 | $[Rn]6d^27s^2$ | 1.432 | 1.565 | 1.735 | 2.389 | 2.474 | 3.684 | | |
| 91 | $[Rn]5f^26d7s^2$ | 1.404 | 1.533 | 1.717 | 2.347 | 2.355 | 3.762 | | |
| 92 | $[Rn]5f^36d7s^2$ | 1.370 | 1.493 | 1.679 | 2.282 | 2.339 | 3.698 | | |
| 93 | $[Rn]5f^46d7s^2$ | 1.338 | 1.456 | 1.644 | 2.223 | 2.282 | 3.634 | | |
| 94 | $[Rn]5f^67s^2$ | 1.315 | 1.431 | 1.634 | | | 3.738 | | |
| 95 | $[Rn]5f^77s^2$ | 1.286 | 1.398 | 1.602 | | | 3.681 | | |
| 96 | $[Rn]5f^76d7s^2$ | 1.252 | 1.357 | 1.553 | 2.128 | 2.189 | 3.455 | | |
| 97 | $[Rn]5f^97s^2$ | 1.232 | 1.335 | 1.546 | | | 3.562 | | |
| 98 | $[Rn]5f^{10}7s^2$ | 1.206 | 1.306 | 1.518 | | | 3.508 | | |
| 99 | $[Rn]5f^{11}7s^2$ | 1.182 | 1.277 | 1.494 | | | 3.455 | | |
| 100 | $[Rn]5f^{12}7s^2$ | 1.158 | 1.252 | 1.469 | | | 3.402 | | |
| 101 | $[Rn]5f^{13}7s^2$ | 1.135 | 1.225 | 1.447 | | | 3.353 | | |
| 102 | $[Rn]5f^{14}7s^2$ | 1.113 | 1.201 | 1.425 | | | 3.305 | | |
| 103 | $[Rn]5f^{14}7s^27p$ | 1.086 | 1.167 | 1.384 | | | 2.959 | 3.813 | |
| 104 | $[Rn]5f^{14}6d^27s^2$ | 1.061 | 1.139 | 1.348 | 1.893 | 2.010 | 2.898 | | |
| 105 | $[Rn]5f^{14}6d^37s^2$ | 1.035 | 1.110 | 1.315 | 1.777 | 1.881 | 2.759 | | |
| 106 | $[Rn]5f^{14}6d^47s^2$ | 1.011 | 1.082 | 1.281 | 1.687 | 1.778 | 2.644 | | |
| 107 | $[Rn]5f^{14}6d^57s^2$ | 0.988 | 1.052 | 1.251 | 1.603 | 1.713 | 2.517 | | |
| 108 | $[Rn]5f^{14}6d^67s^2$ | 0.965 | 1.025 | 1.221 | 1.540 | 1.640 | 2.422 | | |
| 109 | $[Rn]5f^{14}6d^77s^2$ | 0.944 | 1.000 | 1.195 | 1.479 | 1.580 | 2.328 | | |
| 110 | $[Rn]5f^{14}6d^97s$ | 0.924 | 0.975 | 1.169 | 1.436 | 1.532 | 2.258 | | |
| 111 | $[Rn]5f^{14}6d^{10}7s$ | 0.904 | 0.953 | 1.145 | 1.389 | 1.485 | 2.200 | | |
| 112 | $[Rn]5f^{14}6d^{10}7s^2$ | 0.884 | 0.930 | 1.120 | 1.340 | 1.430 | 2.104 | | |
| 113 | $[Rn]5f^{14}6d^{10}7s^27p$ | 0.863 | 0.906 | 1.096 | 1.297 | 1.377 | 2.008 | 2.425 | |
| 114 | $[Rn]5f^{14}6d^{10}7s^27p^2$ | 0.846 | 0.885 | 1.072 | 1.259 | 1.330 | 1.922 | 2.273 | 2.697 |
| 115 | $[Rn]5f^{14}6d^{10}7s^27p^3$ | 0.827 | 0.864 | 1.049 | 1.217 | 1.286 | 1.835 | 2.097 | 2.949 |
| 116 | $[Rn]5f^{14}6d^{10}7s^27p^4$ | 0.810 | 0.844 | 1.028 | 1.184 | 1.247 | 1.768 | 2.002 | 2.790 |
| 117 | $[Rn]5f^{14}6d^{10}7s^27p^5$ | 0.793 | 0.825 | 1.006 | 1.147 | 1.212 | 1.701 | 1.894 | 2.551 |
| 118 | $[Rn]5f^{14}6d^{10}7s^27p^6$ | 0.777 | 0.806 | 0.987 | 1.121 | 1.180 | 1.647 | 1.820 | 2.456 |

**Table 7**
Atom mean radius using the total charge density and atom mean spherical radius of neutral elements with $1 \leq Z \leq 118$.

| Atomic Number | Configuration | Atom mean radius ($a_0$) | Atom mean spherical radius ($a_0$) |
|---|---|---|---|
| 1 | $1s$ | 1.501 | |
| 2 | $1s^2$ | 0.927 | |
| 3 | $1s^2 2s$ | 1.673 | 2.492 |
| 4 | $1s^2 2s^2$ | 1.532 | 2.081 |
| 5 | $1s^2 2s^2 2p$ | 1.362 | 1.780 |
| 6 | $1s^2 2s^2 2p^2$ | 1.191 | 1.516 |
| 7 | $1s^2 2s^2 2p^3$ | 1.050 | 1.314 |
| 8 | $1s^2 2s^2 2p^4$ | 0.951 | 1.181 |
| 9 | $1s^2 2s^2 2p^5$ | 0.864 | 1.066 |
| 10 | $1s^2 2s^2 2p^6$ | 0.789 | 0.968 |
| 11 | $[Ne]3s$ | 0.985 | 1.570 |
| 12 | $[Ne]3s^2$ | 1.020 | 1.569 |
| 13 | $[Ne]3s^2 3p$ | 1.054 | 1.603 |
| 14 | $[Ne]3s^2 3p^2$ | 1.033 | 1.517 |
| 15 | $[Ne]3s^2 3p^3$ | 0.997 | 1.420 |
| 16 | $[Ne]3s^2 3p^4$ | 0.966 | 1.349 |
| 17 | $[Ne]3s^2 3p^5$ | 0.929 | 1.274 |
| 18 | $[Ne]3s^2 3p^6$ | 0.892 | 1.201 |
| 19 | $[Ar]4s$ | 1.021 | 1.638 |
| 20 | $[Ar]4s^2$ | 1.059 | 1.677 |
| 21 | $[Ar]3d4s^2$ | 1.020 | 1.586 |
| 22 | $[Ar]3d^2 4s^2$ | 0.979 | 1.504 |
| 23 | $[Ar]3d^3 4s^2$ | 0.940 | 1.431 |
| 24 | $[Ar]3d^5 4s$ | 0.852 | 1.248 |
| 25 | $[Ar]3d^5 4s^2$ | 0.868 | 1.306 |
| 26 | $[Ar]3d^6 4s^2$ | 0.838 | 1.251 |
| 27 | $[Ar]3d^7 4s^2$ | 0.808 | 1.200 |
| 28 | $[Ar]3d^8 4s^2$ | 0.780 | 1.154 |
| 29 | $[Ar]3d^{10} 4s$ | 0.724 | 1.047 |
| 30 | $[Ar]3d^{10} 4s^2$ | 0.730 | 1.071 |
| 31 | $[Ar]3d^{10} 4s^2 4p$ | 0.751 | 1.141 |
| 32 | $[Ar]3d^{10} 4s^2 4p^2$ | 0.752 | 1.133 |
| 33 | $[Ar]3d^{10} 4s^2 4p^3$ | 0.747 | 1.110 |
| 34 | $[Ar]3d^{10} 4s^2 4p^4$ | 0.743 | 1.094 |
| 35 | $[Ar]3d^{10} 4s^2 4p^5$ | 0.735 | 1.070 |
| 36 | $[Ar]3d^{10} 4s^2 4p^6$ | 0.725 | 1.043 |
| 37 | $[Kr]5s$ | 0.799 | 1.344 |
| 38 | $[Kr]5s^2$ | 0.830 | 1.399 |
| 39 | $[Kr]4d5s^2$ | 0.823 | 1.357 |
| 40 | $[Kr]4d^2 5s^2$ | 0.810 | 1.312 |
| 41 | $[Kr]4d^4 5s$ | 0.770 | 1.191 |
| 42 | $[Kr]4d^5 5s$ | 0.755 | 1.149 |
| 43 | $[Kr]4d^5 5s^2$ | 0.768 | 1.195 |
| 44 | $[Kr]4d^7 5s$ | 0.731 | 1.097 |
| 45 | $[Kr]4d^8 5s$ | 0.719 | 1.071 |
| 46 | $[Kr]4d^{10}$ | 0.682 | 0.967 |
| 47 | $[Kr]4d^{10} 5s$ | 0.694 | 1.023 |
| 48 | $[Kr]4d^{10} 5s^2$ | 0.700 | 1.045 |
| 49 | $[Kr]4d^{10} 5s^2 5p$ | 0.716 | 1.099 |
| 50 | $[Kr]4d^{10} 5s^2 5p^2$ | 0.720 | 1.104 |
| 51 | $[Kr]4d^{10} 5s^2 5p^3$ | 0.722 | 1.099 |
| 52 | $[Kr]4d^{10} 5s^2 5p^4$ | 0.722 | 1.093 |
| 53 | $[Kr]4d^{10} 5s^2 5p^5$ | 0.719 | 1.081 |
| 54 | $[Kr]4d^{10} 5s^2 5p^6$ | 0.715 | 1.065 |
| 55 | $[Xe]6s$ | 0.770 | 1.305 |
| 56 | $[Xe]6s^2$ | 0.795 | 1.360 |
| 57 | $[Xe]5d6s^2$ | 0.792 | 1.331 |
| 58 | $[Xe]4f5d6s^2$ | 0.778 | 1.303 |
| 59 | $[Xe]4f^3 6s^2$ | 0.756 | 1.278 |
| 60 | $[Xe]4f^4 6s^2$ | 0.743 | 1.253 |
| 61 | $[Xe]4f^5 6s^2$ | 0.731 | 1.229 |
| 62 | $[Xe]4f^6 6s^2$ | 0.719 | 1.206 |
| 63 | $[Xe]4f^7 6s^2$ | 0.707 | 1.184 |
| 64 | $[Xe]4f^7 5d6s^2$ | 0.704 | 1.163 |
| 65 | $[Xe]4f^9 6s^2$ | 0.685 | 1.142 |
| 66 | $[Xe]4f^{10} 6s^2$ | 0.674 | 1.122 |
| 67 | $[Xe]4f^{11} 6s^2$ | 0.664 | 1.103 |

**Table 7** (continued)

| Atomic Number | Configuration | Atom mean radius ($a_0$) | Atom mean spherical radius ($a_0$) |
|---|---|---|---|
| 68 | $[Xe]4f^{12}6s^2$ | 0.653 | 1.084 |
| 69 | $[Xe]4f^{13}6s^2$ | 0.643 | 1.066 |
| 70 | $[Xe]4f^{14}6s^2$ | 0.634 | 1.048 |
| 71 | $[Xe]4f^{14}5d6s^2$ | 0.633 | 1.038 |
| 72 | $[Xe]4f^{14}5d^26s^2$ | 0.628 | 1.018 |
| 73 | $[Xe]4f^{14}5d^36s^2$ | 0.623 | 0.998 |
| 74 | $[Xe]4f^{14}5d^46s^2$ | 0.618 | 0.979 |
| 75 | $[Xe]4f^{14}5d^56s^2$ | 0.612 | 0.961 |
| 76 | $[Xe]4f^{14}5d^66s^2$ | 0.607 | 0.945 |
| 77 | $[Xe]4f^{14}5d^76s^2$ | 0.602 | 0.929 |
| 78 | $[Xe]4f^{14}5d^96s$ | 0.587 | 0.885 |
| 79 | $[Xe]4f^{14}5d^{10}6s$ | 0.582 | 0.872 |
| 80 | $[Xe]4f^{14}5d^{10}6s^2$ | 0.584 | 0.882 |
| 81 | $[Xe]4f^{14}5d^{10}6s^26p$ | 0.594 | 0.921 |
| 82 | $[Xe]4f^{14}5d^{10}6s^26p^2$ | 0.598 | 0.932 |
| 83 | $[Xe]4f^{14}5d^{10}6s^26p^3$ | 0.603 | 0.945 |
| 84 | $[Xe]4f^{14}5d^{10}6s^26p^4$ | 0.606 | 0.949 |
| 85 | $[Xe]4f^{14}5d^{10}6s^26p^5$ | 0.607 | 0.949 |
| 86 | $[Xe]4f^{14}5d^{10}6s^26p^6$ | 0.607 | 0.944 |
| 87 | $[Rn]7s$ | 0.640 | 1.105 |
| 88 | $[Rn]7s^2$ | 0.657 | 1.151 |
| 89 | $[Rn]6d7s^2$ | 0.660 | 1.143 |
| 90 | $[Rn]6d^27s^2$ | 0.659 | 1.125 |
| 91 | $[Rn]5f^26d7s^2$ | 0.648 | 1.102 |
| 92 | $[Rn]5f^36d7s^2$ | 0.641 | 1.084 |
| 93 | $[Rn]5f^46d7s^2$ | 0.635 | 1.067 |
| 94 | $[Rn]5f^67s^2$ | 0.623 | 1.048 |
| 95 | $[Rn]5f^77s^2$ | 0.617 | 1.032 |
| 96 | $[Rn]5f^76d7s^2$ | 0.616 | 1.022 |
| 97 | $[Rn]5f^97s^2$ | 0.605 | 1.002 |
| 98 | $[Rn]5f^{10}7s^2$ | 0.598 | 0.987 |
| 99 | $[Rn]5f^{11}7s^2$ | 0.592 | 0.973 |
| 100 | $[Rn]5f^{12}7s^2$ | 0.586 | 0.959 |
| 101 | $[Rn]5f^{13}7s^2$ | 0.580 | 0.946 |
| 102 | $[Rn]5f^{14}7s^2$ | 0.574 | 0.933 |
| 103 | $[Rn]5f^{14}7s^27p$ | 0.587 | 0.984 |
| 104 | $[Rn]5f^{14}6d^27s^2$ | 0.574 | 0.922 |
| 105 | $[Rn]5f^{14}6d^37s^2$ | 0.572 | 0.910 |
| 106 | $[Rn]5f^{14}6d^47s^2$ | 0.569 | 0.898 |
| 107 | $[Rn]5f^{14}6d^57s^2$ | 0.567 | 0.890 |
| 108 | $[Rn]5f^{14}6d^67s^2$ | 0.564 | 0.878 |
| 109 | $[Rn]5f^{14}6d^77s^2$ | 0.561 | 0.868 |
| 110 | $[Rn]5f^{14}6d^97s$ | 0.555 | 0.849 |
| 111 | $[Rn]5f^{14}6d^{10}7s$ | 0.552 | 0.838 |
| 112 | $[Rn]5f^{14}6d^{10}7s^2$ | 0.551 | 0.835 |
| 113 | $[Rn]5f^{14}6d^{10}7s^27p$ | 0.554 | 0.849 |
| 114 | $[Rn]5f^{14}6d^{10}7s^27p^2$ | 0.556 | 0.855 |
| 115 | $[Rn]5f^{14}6d^{10}7s^27p^3$ | 0.573 | 0.932 |
| 116 | $[Rn]5f^{14}6d^{10}7s^27p^4$ | 0.571 | 0.918 |
| 117 | $[Rn]5f^{14}6d^{10}7s^27p^5$ | 0.577 | 0.928 |
| 118 | $[Rn]5f^{14}6d^{10}7s^27p^6$ | 0.574 | 0.916 |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4f
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6g*
6g
6h*
6h
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50
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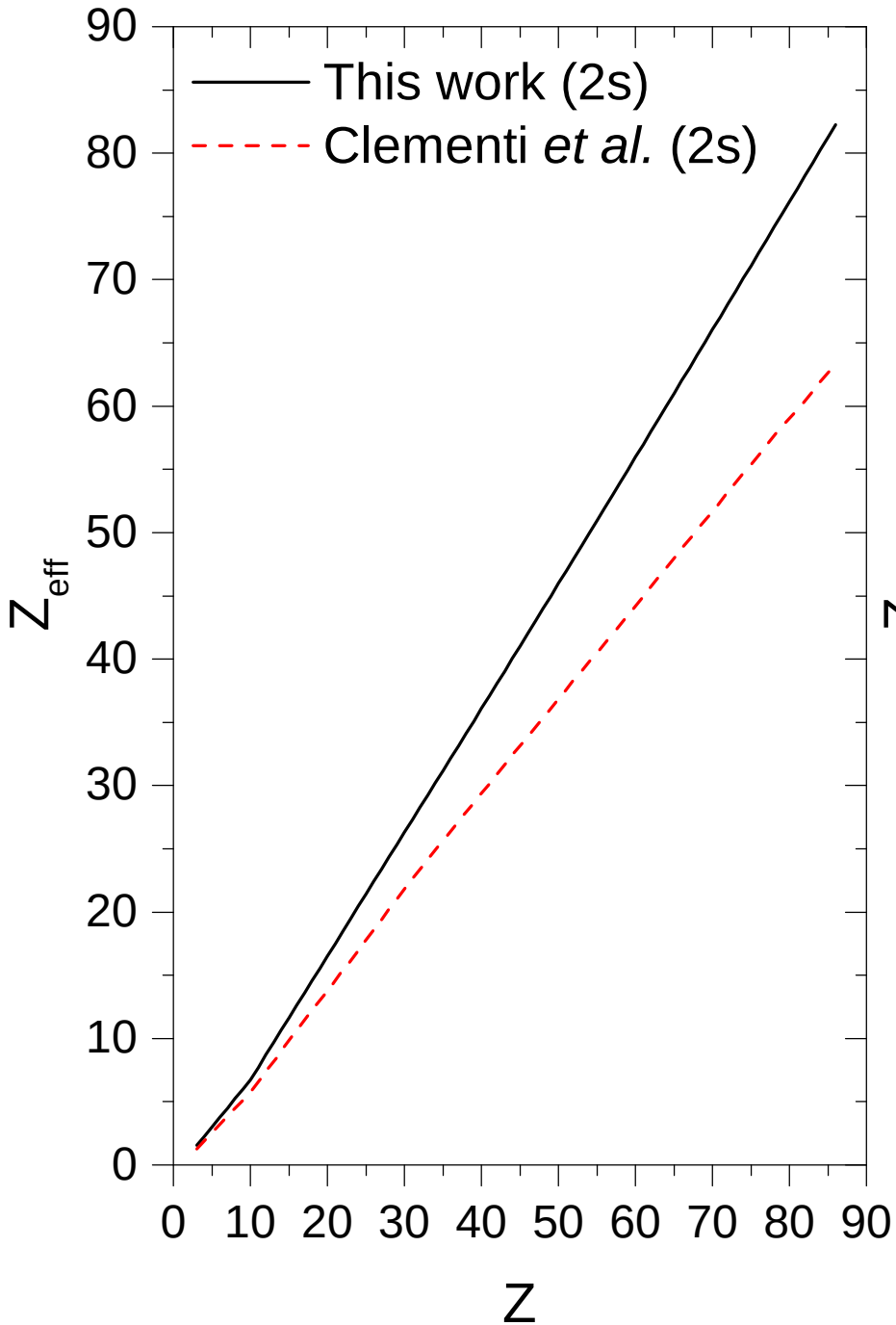
100
110
120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Clementi et al. (2s)
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60
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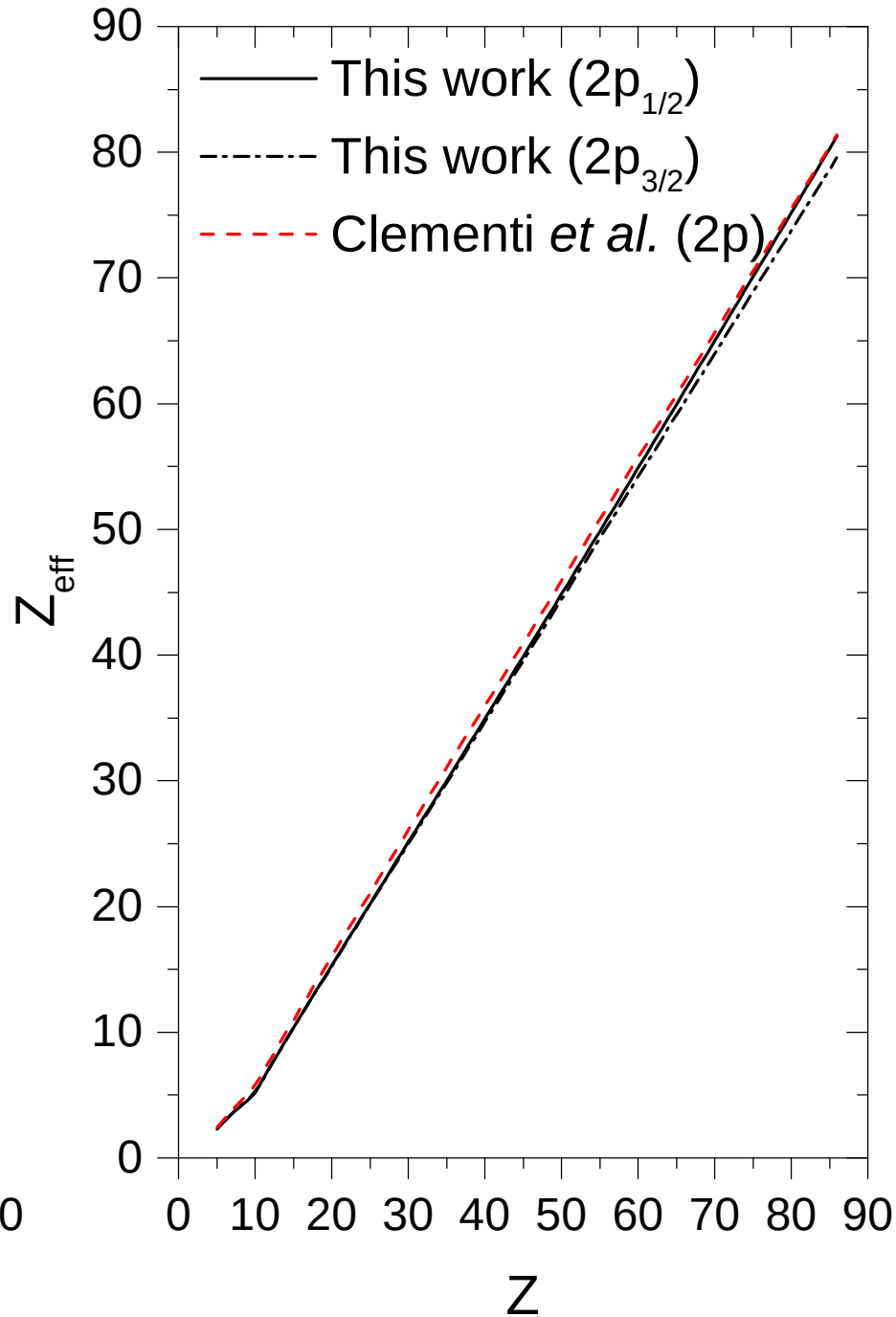
80
90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This work ($2p_{3/2}$)
Clementi et al. (2p)
$Z_{eff}$
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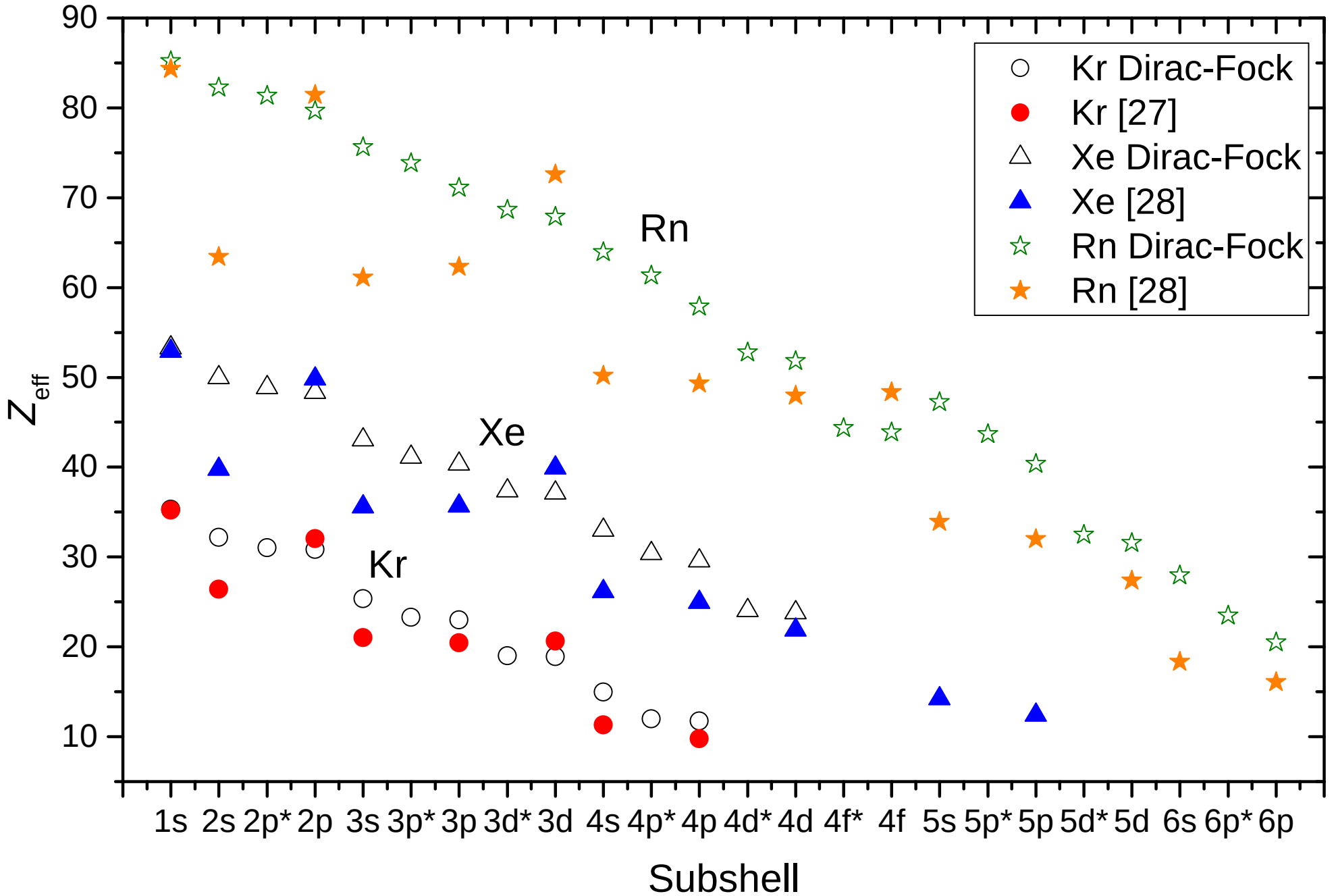
20
30
40
50
60
70
80
90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80
70
60
50
40
30
20
10
$Z_{eff}$
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Subshell
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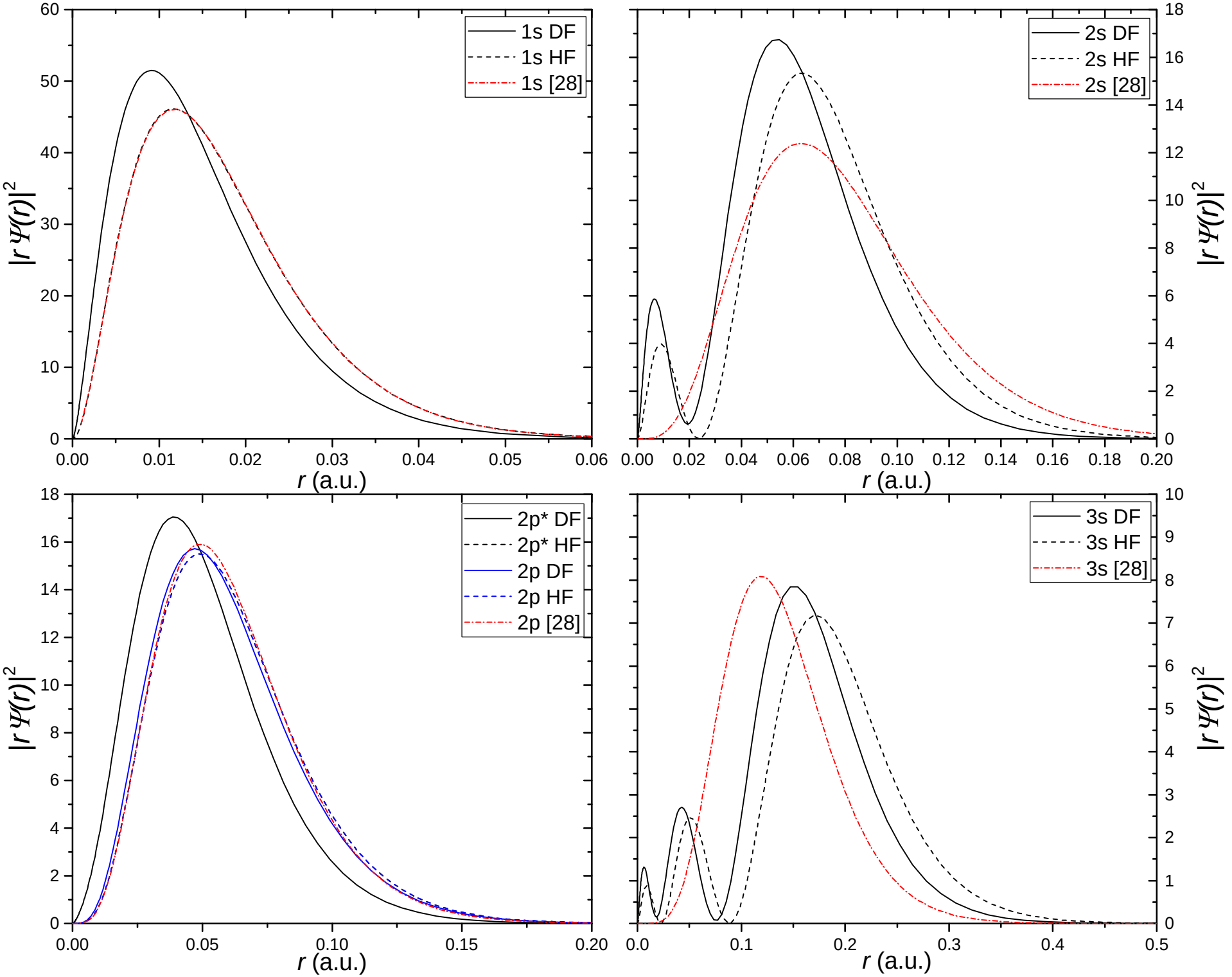
Kr [27]
Xe Dirac-Fock
Xe [28]
Rn Dirac-Fock
Rn [28]
Rn
Xe
Kr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1s HF
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2s DF
2s HF
2s [28]
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2p* HF
2p DF
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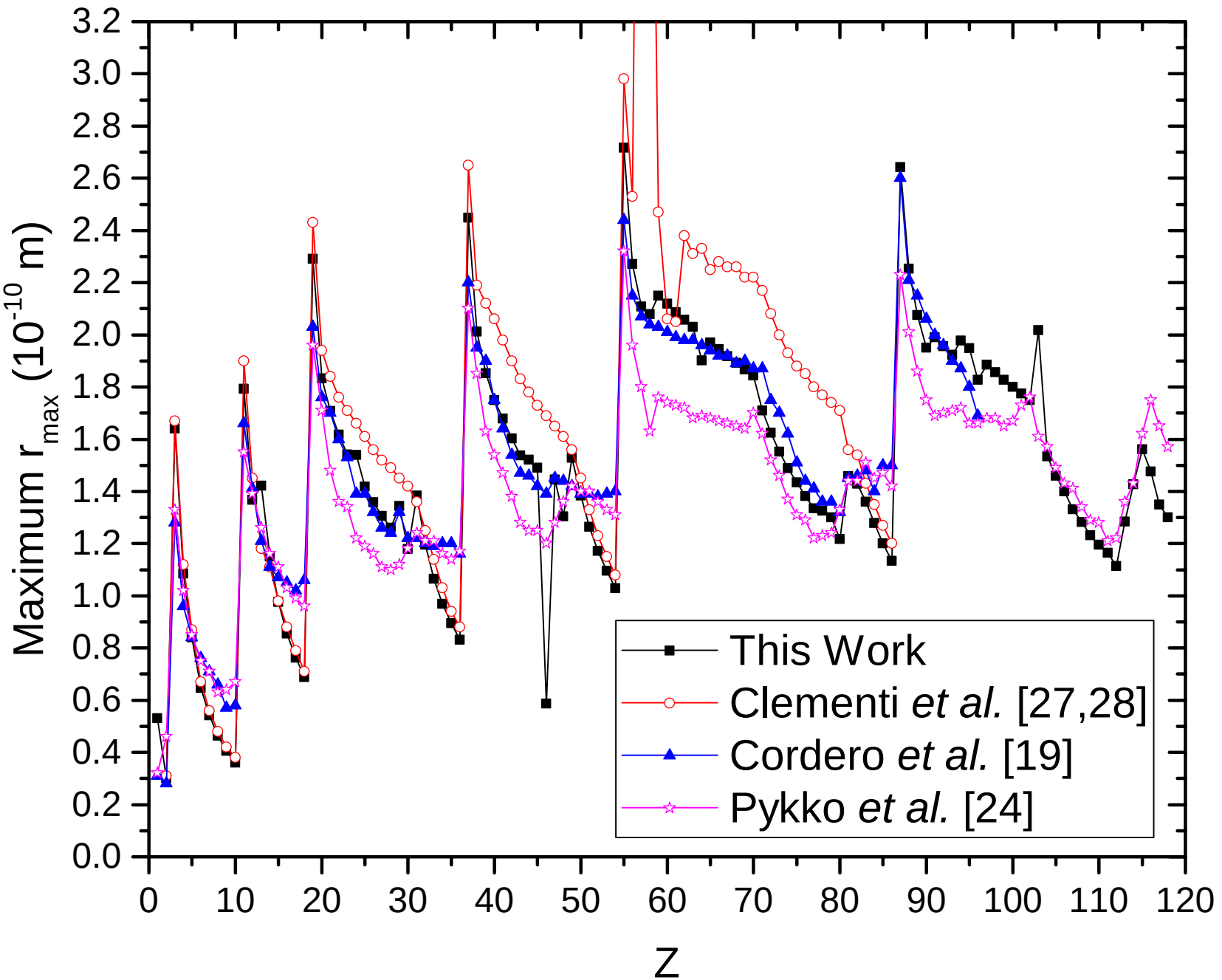
3s DF
3s HF
3s [28]
r (a.u.)
|r Ψ(r)|²


Maximum $r_{max}$ ($10^{-10}$ m)
Z
This Work
Clementi *et al.* [27,28]
Cordero *et al.* [19]
Pykko *et al.* [24]
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0.8
1.0
1.2
1.4
1.6
1.8
2.0
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2.8
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