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Intra-Atomic Electric Field Radial Potentials in Step-Like Presentation

Levan Chkhartishvili, Tamar Berberashvili

Department of Physics, Georgian Technical University, Tbilisi, Georgia.
Email: chkharti2003@yahoo.com

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ABSTRACT

Within the frames of semiclassical approach, intra-atomic electric field potentials are parameterized in form of radial step-like functions. Corresponding parameters for 80 *chemical elements are tabulated by fitting of the semiclassical energy levels of atomic electrons to their first principle values. In substance binding energy and electronic structure calculations, superposition of the semiclassically parameterized constituent-atomic potentials can serve as a good initial approximation of its inner potential: the estimated errors of the determined structural and energy parameters make up a few percent.*

***Keywords*:** *Electric Field Potential, Atoms, Step-Like Radial Functions*

1. Introduction

Because the electron mass is negligible in comparison with masses of atomic nuclei, substances, *i.e.* atoms and polyatomic bound systems – molecules or condensed matters – can be considered as one-electron systems in almost stationary self-consistent electric field generated by nuclei fixed at their equilibrium positions and space-averaged electron charge density. For this reason, electronic structure, which includes both electron energy spectrum and electron density space distribution, determines practically all principal physical properties of a substance. From its part, theoretical prediction of the substance electronic structure should be primarily based on the inner electric field potential, so that appropriate choice of the initial potential for such kind calculations greatly increases their accuracy.

When isolated atoms associate forming molecular or condensed forms of substance only part of electrons (called as valence electrons) redistributes. And what is more, corresponding changes in the electron density distribution are so weak that usually a simple superposition of the free atom's radial potentials centered at the corresponding sites of the atomic structure serves as a good initial approximation of the inner potential in any polyatomic system. At the worst, initial inner electric field potentials can be presented by superposition of the atomic-like radial potentials with different centers. Thus, in this line the key problem consists in construction of the effective atomic potentials in relevant functional form.

Relatively recently, with that end in view we have proposed piece-wise analytical and, in particular, step-like radial atomic potentials obtained within initial quasi-classical, *i.e.*, semiclassical approximation. They have been successfully used in binding energy and electronic structure calculations carried out for some polyatomic systems like the sodium diatomic molecule and crystals [1], boron-containing diatomic molecules [2,3], and mainly for boron nitride molecular, crystalline, and nano-structures [3-16]. In addition, semiclassical interatomic boron-boron pair potentials have explained some ground-state parameters of the boron nanotubes [17-19], as well as main features of the isotopic effects in boron-rich solids [20-23].

But, above cited studies exploited semiclassical potentials only of certain, namely, some light atoms, whereas full-scale calculations performed for any wide class of materials need a quantity of appropriate effective atomic potentials. Present work aims to build up semiclassical atomic potentials for the stable chemical elements in most convenient form of radial step-like functions.

The paper is organized as follows. At first, sense of the semiclassicality for the substance-electron-system is clarified. Then, a semiclassical parameterization scheme is introduced for charge distributions in atoms and atomic potentials as well. Next section presents results and brief discussion of the performed numerical calculations based on fitting of the semiclassical electron-energy spectra with these obtained from first principles. And finally, accuracies of the constructed step-like radial atomic po-

tentials are estimated for energy and expansion parameters of a material.

2. Substance as a Semiclassical Electron System

Beginning from Bohr's fundamental work [24] semiclassically describing electronic spectrum of the one-electron hydrogen-like atom with Coulomb potential up to nowadays, similar analysis is widely used for light atoms. Due to exact quantum-mechanical solvability of the Coulomb potential, exact wave functions of electron-states in a hydrogen-like atom can be obtained directly from the corresponding classical orbits [25]. And therefore, quantum dynamics of the electron in a hydrogen-like atom is wholly expressed by its classical dynamics.

Classically a two-electron helium-like atom can be represented as a pair of electrons placed at the opposite ends of the straight line with nucleus at the midpoint (see e.g. [26]). This classical model added with quantization condition for electron orbital moment leads to the almost hydrogen-like electron energy spectra, where atomic number Z is substituted for the reduced value Z–1/4 (it means that another electron effectively screens nuclear electric charge). Ground state energies calculated from the obtained relation for some helium-like systems differ from the experimental ones only by 3-6% [27]. Even entirely classical model of helium atom can be successfully explored numerically to obtain its possible configurations [28]: most of the orbits are found to cause auto-ionization via chaotic transients. As for the modern semiclassical approach based on the conception of periodic classical orbits, it allow visually interpret physical meaning of special quantum numbers inherent to this three-particle system between ground and fragmented states [29].

For many-electron atoms, a reasonable accuracy can be achieved in terms of the self-consistent-field approximation, within which a minimum of the total energy is sought in the class of quasi-classical wave functions [30]. As is well known, many-electron systems such as heavy atoms are characterized by some quantum properties like the electron-shell effects, fluctuations in parameters' values, discrete electron energy spectrum etc, which are averaged and, therefore, invisible in semiclassical atomic models. However, it was demonstrated that semiclassical treatment of the atomic many-electron system, when it is combined with information-theory-method, reveals resources to describe such kind effects as well [31].

It was demonstrated how based on purely classical notions it is possible to reproduce general trends in inelastic scattering atomic form-factors dependences upon quantum numbers [32]. Besides, starting from classical relations together with energy conservation law and classical-quantum correspondence principle, it was found expressions of intensity-distribution and line-width of the electron–ion recombination X-ray spectrum, which is in unexpectedly good agreement with these resulted from the accurate quantum-mechanical calculations [33].

Semiclassical quantization rule leading to the exact electron energies in a hydrogen-like atom with Coulomb potential at the same time provides good accuracy of the valence electron energy value in a many-electron atom with model potential in form of sum of the nucleus Coulomb potential and a screening term [34]. Substitutions of the electron quantum numbers for their analogues in Thomas–Fermi semiclassical statistical model of atom can be applied for investigation of the excited and ionized electron states [35]. Semiclassical electron energy spectrum of Thomas–Fermi atom, which was described in terms of an effective kinetic energy obtained from the corresponding quantization rule formulated in momentum space, was found to agree essentially with that in the standard formalism employing an effective potential energy [36].

Semiclassical evaluation of sums over quantum numbers of electron states in many-electron atoms is known to be an effective tool of obtaining of the integrated atomic characteristics (see e.g. [37]) like the shell and subshell electron densities [38] or averaged electron momentum density [39] in atoms etc. Introducing of the semiclassical self-consistent intra-atomic electric field yields the relative error not more than $\sim 1/\pi^2 n^2$ in determining of the electronic energies, where n is the principal quantum number of the highest occupied electron state [40]. Then, accuracy of the semiclassical approximation should quite satisfactory even for light atoms.

Effectiveness of the Bohr-type analytical models to the description of the periodic motion of electrons in small-sized molecules also was demonstrated [41]. For a long time, semiclassical asymptotic form was known to provide a fundamental device for studying quantum systems in which non-perturbative effects play an essential role. But, the crucial step was advanced for the bound-state quantization of fermions few-body systems such as molecules. Semiclassical quantization rules were successfully applied to describe elastic interatomic scattering [42] in spectroscopy of diatomic molecules [43]. Using path integration as a relevant mathematical tool for semiclassical asymptotic form it was obtained semiclassical quantization rule for the periodic mean-field solutions [44]. Therm energies of diatomic K_2 molecule calculated by the semiclassical method showed absolute deviations of only ~ 0.05 cm^{-1} from the quantum-mechanical results [45]. Same approach was found to be a strong method for generating the interatomic potential energy curve for diatomic molecules. It was provided a semiclassical description of the shell-structure in fermions-system: level densities and shell-corrections were obtained from the

periodic orbit theory [46]. The semiclassical quantification method has raised increasing interest in relation to approximated method in various physical systems such as not only atoms, but molecules etc. It would serve as a general device for evaluating the bound-state spectra, once the exact or approximate solutions for the mean-field equation are known. Usually, different methods all use only periodic and/or non-closed quasi-periodic classical orbitals as basis for the quantization. Contrary to them, in [47] it was introduced an adapted version of the semiclassical quantization method applied to molecular orbitals into path integrals formalism, and it also gives an alternative procedure for the calculation of the electronic correlation energy of a molecular system.

Primitive semiclassical treatment even reveals existence of a classical contribution to the chemical bond in small molecules: ground state electron is found to be exchanged classically between two nuclei [48]. Proceeding classical limit for a one-electron orbital model of such many-electron systems with electron periodic motion leads to visualization of its quantum description [49]. Quantum description also can be introduced starting from the formal correspondence between classical harmonics of an electron periodic motion and its quantum jumps, *i.e.* Fourier-analysis added by the simple quantization condition directly yields steady-state electron energies [50]. Even formation of the electron spin, which is considered as essentially quantum characteristic, can be explained within a classical model [51].

In case of multidimensional systems, the globally uniform semiclassical approximation for energy eigenstates can be derived explicitly [52]. This is a true semiclassical approximation producing almost accurate wave functions providing with considerable degree of overlap (more than 0.98) between semiclassical and exact quantum eigenstates. Semiclassical method of calculation was used to describe electronic super-shells in metallic clusters [53]. Later, it was supposed a general method of the quasi-classical spectral analysis useful for central potentials with Coulomb singularity or finite value at the center which are characteristic for isolated atoms and spherical clusters, respectively [54]. Atomic clusters and condensed phases can be calculated in framework of the density-functional theory (DFT) using a quasi-classical expansion of the energy functional [55].

However, as substance is considered as a non-relativistic electron system affected by the external field of nuclei fixed at their sites in structure, its inner potential do not satisfy the standard Wentzel-Kramers-Brillouin (WKB) quasi-classical condition on spatial smoothness due to singularities at nuclear sites and electron shell effects. The success of the above approaches can be explained on the basis of the quasi-classical expressions obtained by Maslov [56] for the energies of bound electronic states. It follows from these expressions that the exact and quasi-classical spectra are similar to each other irrespective of the potential smoothness at $2\Phi_0 R_0^2 >> 1$, where Φ_0 and R_0 are the characteristic values of the potential and its effective range, respectively (hereafter, all relationships will be given in the atomic system of units (a.u.)).

3. Semiclassical Parameterization of the Electric Charge Density and Electric Field Potential Distributions in an Atom

The semiclassical parameterization of the atomic electric charge density and electric field potential distributions (see e.g. [57]) can be performed in analytical form if the effective fields acting on any i th electron in a neutral atom (*i.e.*, $i = 1,2,3,...,Z$ with Z as the nucleus charge) are represented by Coulomb-like potentials

$$\Phi_i(r) = \frac{Z_i}{r} \tag{1}$$

where

$$Z_i = n_i \sqrt{2 \mid E_i \mid} \tag{2}$$

is the effective charge of the nucleus screened by other electrons' cloud dependent on the electron-state principal quantum number n_i and its energy $E_i < 0$.

Electron charge equals to -1. Therefore, classical turning points radii r_i' and r_i'' ($r_i' < r_i''$) of the i th electron with orbital quantum number l_i can be found as the roots of the equation

$$E_i = -\Phi_i(r) + \frac{l_i(l_i+1)}{2r^2} \tag{3}$$

As a result, we obtain

$$r_i' = \frac{n_i - \sqrt{n_i^2 - l_i(l_i+1)}}{\sqrt{2 \mid E_i \mid}} \tag{4}$$

$$r_i'' = \frac{n_i + \sqrt{n_i^2 - l_i(l_i+1)}}{\sqrt{2 \mid E_i \mid}} \tag{5}$$

Let $\widetilde{\Phi}_i(r)$ be the potential of the effective electric field induced by the i th electron. Then, potential $\widetilde{\Phi}(r)$ of the electric field induced by the whole electron cloud can be written as the sum of the potentials $\widetilde{\Phi}_i(r)$:

$$\widetilde{\Phi}(r) = \sum_{i=1}^{i=Z} \widetilde{\Phi}_i(r) \tag{6}$$

Potential of the electric field acting on an arbitrary i th electron of the atom is equal to the sum of the potentials of the nucleus Coulomb field and the field induced by all the electrons, except for the potential of the electron under consideration:

$$\frac{Z_i}{r} = \frac{Z}{r} + \widetilde{\Phi}(r) - \widetilde{\Phi}_i(r) \tag{7}$$

Now, we sum up such potentials over electrons. As a result, the terms independent of the electron number on the right-hand sides are multiplied by the total number Z of electrons in the atom and the sum of the potentials $\widetilde{\Phi}_i(r)$ gives $\widetilde{\Phi}(r)$. The solution of the obtained equation with respect to $\widetilde{\Phi}(r)$ has the form

$$\widetilde{\Phi}(r) = -\frac{Z^2 - \sum_{i=1}^{i=Z} Z_i}{Z-1}\frac{1}{r} \tag{8}$$

i.e. in this case, effective field of the interaction between nucleus and electron cloud also turns out to be a Coulomb-like field.

Nucleus charge equals to $+Z$ and in the ground state its relative (to the electron cloud) motion corresponds to a zero orbital quantum number. Therefore, the radius of one classical turning point for nucleus is equal to 0 and the radius $\widetilde{r}$ of another turning point is a root of the equation

$$\widetilde{E} = Z\widetilde{\Phi}(r) \tag{9}$$

where $\widetilde{E}$ is the eigenvalue of the energy associated with the relative motion electron cloud and nucleus. Under the assumption that the nucleus has an infinite mass the reduced mass of the system nucleus – electron cloud with *Z* electrons equals to the cloud total mass *Z*. Therefore, energy and, consequently, turning point radius for the nucleus motion with respect to the electron cloud are given by the formulas

$$\widetilde{E} = -\frac{Z^3(Z^2 - \sum_{i=1}^{i=Z} Z_i)^2}{2(Z-1)^2} \tag{10}$$

$$\widetilde{r} = \frac{2(Z-1)}{Z^2(Z^2 - \sum_{i=1}^{i=Z} Z_i)} \tag{11}$$

The semiclassical, *i.e.*, initial quasi-classical approximation implies that exponentially decaying partial electron densities are disregarded in the classically forbidden regions and that oscillations of these densities are ignored in classically allowed regions. As a result, the radial dependence of the direction-averaged partial charge density of the i th electron state in atom is represented by a piecewise constant function:

$$\begin{aligned} \rho_i(r) &= 0 && r < r_i' \\ &= -\frac{3}{4\pi(r_i''^3 - r_i'^3)} && r_i' \le r \le r_i'' \\ &= 0 && r_i'' < r \end{aligned} \tag{12}$$

A similar averaging for the nucleus motion with respect to the electron cloud nucleus is equivalent to averaging the nuclear charge over a sphere of radius $\tilde{r}$:

$$\begin{aligned} \tilde{\rho}(r) &= \frac{3Z}{4\pi\tilde{r}^3} && 0 \le r \le \tilde{r} \\ &= 0 && \tilde{r} < r \end{aligned} \tag{13}$$

Summation of similar contributions gives the distribution of the total density of the electric charge in the atom in the form of a step radial function

$$\rho(r) = \tilde{\rho}(r) + \sum_{i=1}^{i=Z} \rho_i(r) = \rho_k$$
$$R_{k-1} \le r < R_k \quad k = 1,2,3,...,q \tag{14}$$

where ρ_k are constants determined from the radii of the classical turning points and R_k coincide with these radii. Here, $0 \equiv R_0 < R_1 < R_2 < \cdots < R_q < R_{q+1} \equiv \infty$ and $q \le 2Z$ is the number of layers with uniform charge densities. Parameter R_q plays the role of the quasi-classical atomic radius (the charge density is equal to zero at $r > R_q$). Mathematically, this representation is equivalent to the volume averaging in layers $R_{k-1} \le r < R_k$.

Next, we calculate the fields induced by the charged layers with densities ρ_k on the basis of the Gauss theorem and sum these fields. Then, the atomic potential can be written in the form of the continuously differentiable piecewise analytical function

$$\begin{aligned} \phi(r) &= \frac{a_k}{r} + b_k r^2 + c_k && R_{k-1} \le r < R_k \qquad k = 1,2,3,...,q \\ a_k &= \frac{4\pi}{3}\sum_{i=1}^{i=k-1} \rho_i(R_i^3 - R_{i-1}^3) - \frac{4\pi}{3}\rho_k R_{k-1}^3 \\ b_k &= -\frac{2\pi}{3}\rho_k \\ c_k &= 2\pi\sum_{i=k+1}^{i=q} \rho_i(R_i^2 - R_{i-1}^2) + 2\pi\rho_k R_k^2 \end{aligned} \tag{15}$$

However, since the energy of the electronic system is a single-valued functional of the electron density, it is expedient to approximate the above potential by a step function too. Averaging over the volume can adequately perform this:

$$\varphi(r) = \frac{3a_k(R_k^2 - R_{k-1}^2)}{2(R_k^3 - R_{k-1}^3)} + \frac{3b_k(R_k^5 - R_{k-1}^5)}{5(R_k^3 - R_{k-1}^3)} + c_k = \varphi_k$$
$$R_{k-1} \le r < R_k \quad k = 1,2,3,...,q \tag{16}$$

4. Tables

The numerical values of parameters R_k, ρ_k, and φ_k can be found by fitting quasi-classical energetic levels E_i to the Hartree–Fock (HF) ab initio ones [58]. Results of calculation are presented in **Table 1** below for each

chemical element taken separately. Origin of a radial layer radius is identified in parenthesis after the layer number: is it a classical turning point radius of nucleus or an electron-state? Note that inner turning points of nucleus and *s*-electron states coincide with effective atomic electric field center, *i.e.* corresponding radii equal to 0. Radii of inner and outer classical turning points for rest electron-states are distinguished by single and double priming.

Values are shown with seven significant digits in accordance with the input data (HF energies) accuracy. Such high accuracy is useful in interim calculations. As for the final results, they should be expressed in round numbers to the three or four significant digits because the relative errors of the semiclassical calculations aiming to found structural and energy parameters for polyatomic systems usually make up a few percent.

Table 1. Calculated semiclassical parameters of the atoms

k	1 (**1 H**)	1 (1*s*)
R_k	1.000000 E + 00	2.000000 E + 00
ρ_k	2.088909 E + 01	−2.984155 E − 02
φ_k	4.875000 E − 01	5.892857 E − 02

k	1 (**2 He**)	2 (1*s*)
R_k	3.875716 E − 01	1.476061 E + 00
ρ_k	8.052884 E + 00	−1.484666 E − 01
φ_k	4.187991 E + 00	3.082284 E − 01

k	1 (**3 Li**)	2 (1*s*)	3 (2*s*)
R_k	1.349014 E − 01	8.984357 E − 01	6.383510 E + 00
ρ_k	2.910724 E + 02	−6.593034 E − 01	− 9.177675 E − 04
φ_k	2.312713 E + 01	2.009273 E + 00	4.311415 E − 02

k	1 (**4 Be**)	2 (1*s*)	3 (2*s*)
R_k	5.596220 E − 02	6.500727 E − 01	5.086001 E + 00
ρ_k	5.446885 E + 03	−1.741653 E + 00	3.629210 E − 03
φ_k	8.057431 E + 01	4.887950 E + 00	1.097914 E − 01

k	1 (**5 B**)	2 (1*s*)	3 (2*p*')	4 (2*s*)	5 (2*p*")
R_k	2.758476 E − 02	5.098016 E − 01	7.441219 E − 01	4.021346 E + 00	4.337060 E + 00
ρ_k	5.686514 E + 04	− 3.610951 E + 00	− 7.342212 E − 03	− 1.028341 E − 02	− 2.941197 E − 03
φ_k	2.105468 E + 02	8.882329 E + 00	3.652920 E + 00	2.060720 E − 01	6.135348 E − 04

k	1 (**6 C**)	2 (1*s*)	3 (2*p*')	4 (2*s*)	5 (2*p*")
R_k	1.542721 E − 02	4.202289 E − 01	6.292303 E − 01	3.367110 E + 00	3.667423 E + 00
ρ_k	3.901153 E + 05	−6.446545 E + 00	− 1.250747 E − 02	− 2.223623 E − 02	− 9.728757 E − 03
φ_k	578818 E + 02	1.399183 E + 01	5.842260 E + 00	3.410756 E − 01	1.835877 E−03

k	1 (**7 N**)	2 (1*s*)	3 (2*p*')	4 (2*s*)	5 (2*p*")
R_k	9.446222 E − 03	3.577244 E − 01	5.498034 E − 01	2.909074 E + 00	3.204489 E + 00
ρ_k	1.982589 E + 06	− 1.044967 E + 01	− 1.939444 E − 02	− 4.126981 E − 02	− 2.187537 E − 02
φ_k	8.784581 E + 02	2.022523 E + 01	8.464698 E + 00	5.096684 E − 01	3.993358 E − 03

k	1 (**8 O**)	2 (1s)	3 (2p')	4 (2s)	5 (2p")
R_k	6.103946 E − 03	3.110705 E −01	5.210723 E − 01	2.535595 E + 00	3.037032 E + 00
ρ_k	8.397857 E + 06	− 1.589154 E + 01	− 2.928881 E − 02	− 6.355156 E − 02	− 3.426275 E − 02
φ_k	1.559999 E + 03	2.773984 E + 01	1.102222 E + 01	7.898878 E − 01	1.796550 E − 02

k	1 (**9 F**)	2 (1s)	3 (2p')	4 (2s)	5 (2p")
R_k	4.176561 E − 03	2.753309 E − 01	4.847945 E − 01	2.255511 E + 00	2.825589 E + 00
ρ_k	2.949151 E + 07	− 2.291743 E + 01	− 4.161086 E − 02	− 9.479146 E − 02	− 5.318060 E − 02
φ_k	2.571045 E + 03	3.638866 E + 01	1.405815 E + 01	1.114922 E + 00	3.595575 E − 02

k	1 (**10 Ne**)	2 (1s)	3 (2p')	4 (2s)	5 (2p")
R_k	2.985142 E − 03	2.470362 E − 01	4.491695 E − 01	2.035740 E + 00	2.617951 E + 00
ρ_k	8.974622 E + 07	− 3.172744 E + 01	− 5.659451 E − 02	− 1.368319 E − 01	− 8.023741 E − 02
φ_k	4.002938 E + 03	4.617305 E + 01	1.754276 E + 01	1.481199 E + 00	5.649046 E − 02

k	1 (**11 Na**)	2 (1s)	3 (2p')
R_k	2.333813 E − 03	2.222812 E − 01	3.361773 E − 01
ρ_k	2.065883 E + 08	− 4.357330 E + 01	− 9.895069 E − 02
φ_k	5.636078 E + 03	5.702576 E + 01	2.540262 E + 01

4 (2s)	5 (2p")	6 (3s)
1.691207 E + 00	1.959385 E + 00	9.942100 E + 00
− 2.903333 E − 01	− 1.916255 E − 01	− 2.429277 E − 04
2.264005 E + 00	4.264542 E − 01	2.565704 E − 02

k	1 (**12 Mg**)	2 (1s)	3 (2p')
R_k	1.833883 E − 03	2.019651 E − 01	2.741860 E − 01
ρ_k	4.644914 E + 08	− 5.811295 E + 01	− 1.551165 E − 01
φ_k	7.829429 E + 03	6.933347 E + 01	3.379468 E + 01

4 (2s)	5 (2p")	6 (3s)
1.457155 E + 00	1.598073 E + 00	8.433944 E + 00
− 5.078705 E − 01	− 3.535498 E − 01	− 7.958830 E − 04
3.315594 E + 00	9.711561 E − 01	6.118891 E − 02

k	1 (**13 Al**)	2 (1s)	3 (2p')	4 (3p')
R_k	1.462229 E − 03	1.848984 E − 01	2.308930 E − 01	5.466816 E − 01
ρ_k	9.926781 E + 08	− 7.576501 E + 01	− 2.311670 E − 01	− 8.218780 E − 01
φ_k	1.064293 E + 04	8.299728 E + 01	4.322824 E + 01	1.753508 E + 01

5 (2s)	6 (2p")	7 (3s)	8 (3p")
1.276364 E + 00	1.345743 E + 00	6.764067 E + 00	8.712604 E + 00
− 8.222391 E − 01	− 5.926148 E − 01	− 1.903885 E − 03	− 3.610562 E − 04
3.600567 E + 00	1.684978 E + 00	1.386415 E − 01	2.846971 E − 03

k	1 (**14 Si**)	2 (1s)	3 (2p')	4 (3p')
R_k	1.177767 E − 03	1.704832 E − 01	2.007802 E − 01	4.595484 E − 01
ρ_k	2.045794 E + 09	− 9.668486 E + 01	− 3.248175 E − 01	− 1.223166 E + 00
φ_k	1.423563 E + 04	9.804605 E + 01	5.346299 E + 01	2.372269 E + 01

5 (2s)	6 (2p")	7 (3s)	8 (3p")
1.139926 E + 00	1.170233 E + 00	5.774354 E + 00	7.323940 E + 00
− 1.224381 E + 00	− 9.020437 E − 01	− 3.695549 E − 03	− 1.215666 E − 03
5.013770 E + 00	2.545996 E + 00	2.317236 E − 01	6.068273 E − 03

k	1 (**15 P**)	2 (1s)	3 (2p')	4 (3p')
R_k	9.593563 E − 04	1.581438 E − 01	1.782334 E − 01	4.002321 E − 01
ρ_k	4.055672 E + 09	− 1.211595 E + 02	− 4.380049 E − 01	− 1.722228 E + 00
φ_k	1.873096 E + 04	1.144569 E + 02	6.457731 E + 01	3.040964 E + 01

5 (2s)	6 (2p")	7 (3s)	8 (3p")
1.032033 E + 00	1.038820 E + 00	5.083961 E + 00	6.378601 E + 00
− 1.724988 E + 00	− 1.290617 E + 00	− 6.393927 E − 03	− 2.760347 E − 03
6.608240 E + 00	3.548359 E + 00	3.396463 E − 01	9.624267 E − 03

k	1 (**16 S**)	2 (1s)	3 (2p')	4 (3p')
R_k	7.873147 E − 04	1.474384 E − 01	1.602340 E − 01	3.787647 E − 01
ρ_k	7.826836 E + 09	− 1.495490 E + 02	− 5.752957 E − 01	− 2.342732 E + 00
φ_k	2.435211 E + 04	1.322761 E + 02	7.674520 E + 01	3.528555 E + 01

5 (2p")	6 (2s)	7 (3s)	8 (3p")
9.339120 E − 01	9.425845 E − 01	4.523887 E + 00	6.036469 E + 00
− 2.347074 E + 00	− 5.796381 E − 01	− 9.499509 E − 03	− 4.342400 E − 03
8.375741 E + 00	4.756158 E + 00	5.098488 E − 01	2.058169 E − 02

k	1 (**17 Cl**)	2 (1s)	3 (2p')	4 (3p')
R_k	6.532226 E − 04	1.380891 E − 01	1.457901 E − 01	3.520031 E − 01
ρ_k	1.456052 E + 10	− 1.820631 E + 02	− 7.359436 E − 01	− 3.082461 E + 00
φ_k	3.119221 E + 04	1.514459 E + 02	8.983302 E + 01	4.146700 E + 01

5 (2p")	6 (2s)	7 (3s)	8 (3p")
8.497267 E − 01	8.684381 E − 01	4.095949 E + 00	5.609963 E + 00
− 3.089224 E + 00	− 7.427061 E − 01	− 1.371081 E − 02	− 6.762524 E − 03
1.047479 E + 01	6.101408 E + 00	6.943084 E − 01	3.204793 E − 02

k	1 (**18 Ar**)	2 (1s)	3 (2p')	4 (3p')
R_k	5.474781 E − 04	1.298535 E − 01	1.338860 E − 01	3.258315 E − 01
ρ_k	2.618688 E + 10	− 2.189839 E + 02	− 9.217434 E − 01	− 3.951462 E + 00
φ_k	3.941303 E + 04	1.719603 E + 02	1.038562 E + 02	4.862917 E + 01

5 (2*p*'')	6 (2*s*)	7 (3*s*)	8 (3*p*'')
7.803446 E − 01	8.057526 E − 01	3.753883 E + 00	5.192860 E + 00
− 3.961694 E + 00	− 9.319752 E − 01	− 1.925783 E − 02	− 1.023175 E − 02
1.282209 E + 01	7.582522 E + 00	8.919572 E − 01	4.376578 E − 02

k	1 (**19 K**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (2*p*'')
R_k	4.727958 E − 04	1.220427 E − 01	1.223829 E − 01	2.564030 E − 01	7.113169 E − 01
ρ_k	4.291847 E + 10	− 2.616615 E + 02	− 2.656616 E + 02	− 5.178522 E + 00	− 5.199519 E + 00
φ_k	4.817966 E + 04	1.942944 E + 02	1.195273 E + 02	6.680192 E + 01	1.623827 E + 01

6 (2*s*)	7 (3*s*)	8 (3*p*'')	9 (4*s*)
7.430389 E − 01	3.208255 E + 00	4.086360 E + 00	1.473043 E + 01
− 1.199407 E + 00	− 3.553070 E − 02	− 2.107182 E − 02	− 7.469050 E − 05
9.178612 E + 00	1.258072 E + 00	2.068058 E − 01	1.499003 E − 02

k	1 (**20 Ca**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (2*p*'')
R_k	4.088020 E − 04	1.121988 E − 01	1.157157 E − 01	2.163349 E − 01	6.539423 E − 01
ρ_k	6.988798 E + 10	− 3.096286 E + 02	− 3.147766 E + 02	− 6.625287 E + 00	− 6.660246 E + 00
φ_k	5.866054 E + 04	2.246811 E + 02	1.363192 E + 02	8.373755 E + 01	1.982931 E + 01

6 (2*s*)	7 (3*s*)	8 (3*p*'')	9 (4*s*)
6.895990 E − 01	2.831339 E + 00	3.447784 E + 00	1.279289 E + 01
− 1.512189 E + 00	− 5.622245 E − 02	− 3.518632 E − 02	− 2.280529 E − 04
1.103673 E + 01	1.726474 E + 00	4.329498 E − 01	3.507845 E − 02

k	1 (**21 Sc**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.495658 E − 04	1.046439 E − 01	1.097974 E − 01	1.996252 E − 01
ρ_k	1.173664 E + 11	− 3.625008 E + 02	− 3.688463 E + 02	− 8.130180 E + 00
φ_k	7.203863 E + 04	2.552117 E + 02	1.537630 E + 02	9.620138 E + 01

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
6.099095 E − 01	6.475133 E − 01	1.529288 E + 00	2.647865 E + 00
− 8.174672 E + 00	− 1.829179 E + 00	− 7.046518 E − 02	− 7.177448 E − 02
2.333772 E + 01	1.310249 E + 01	5.350410 E + 00	1.412970 E + 00

9 (3*p*'')	10 (4*s*)	11 (3*d*'')
3.181477 E + 00	5.707379 E + 00	1.234108 E + 01
− 4.605550 E − 02	− 1.563323 E − 03	− 2.540280 E − 04
5.766749 E − 01	2.237779 E − 01	2.179856 E − 02

k	1 (**22 Ti**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.013518 E − 04	9.820236 E − 02	1.044639 E − 01	1.869609 E − 01
ρ_k	1.919167 E + 11	− 4.209588 E + 02	− 4.286367 E + 02	− 9.801412 E + 00
φ_k	8.755133 E + 04	2.872142 E + 02	1.721800 E + 02	1.087104 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
5.723653 E − 01	6.110909 E − 01	1.908091 E + 00	2.502871 E + 00
− 9.855572 E + 00	− 2.177684 E + 00	− 8.538408 E − 02	− 8.673223 E − 02
2.709414 E + 01	1.537353 E + 01	4.186494 E + 00	1.335356 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.979643 E + 00	7.121092 E + 00	8.521671 E + 00
− 5.627954 E − 02	− 2.119704 E − 03	− 7.715554 E − 04
7.476607 E − 01	1.196428 E − 01	3.156347 E − 03

k	1 (**23 V**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	2.601095 E − 04	9.256893 E − 02	9.962640 E − 02	1.762791 E − 01
ρ_k	3.120117 E + 11	− 4.853546 E + 02	− 4.945213 E + 02	− 1.166471 E + 01
φ_k	1.060522 E + 05	3.209083 E + 02	1.916313 E + 02	1.217554 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
5.395313 E − 01	5.788639 E − 01	1.867140 E + 00	2.377964 E + 00
− 1.172932 E + 01	− 2.562651 E + 00	− 1.010817 E − 01	− 1.032399 E − 01
3.114340 E + 01	1.785930 E + 01	4.730460 E + 00	1.618205 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.809404 E + 00	6.968261 E + 00	7.924130 E + 00
− 6.773191 E − 02	− 3.117812 E − 03	− 9.595919 E − 04
9.784493 E − 01	1.402956 E − 01	1.832263 E − 03

k	1 (**24 Cr**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	2.257520 E − 04	8.758647 E − 02	9.521818 E − 02	1.670378 E − 01
ρ_k	4.979986 E + 11	− 5.559828 E + 02	− 5.668046 E + 02	− 1.373243 E + 01
φ_k	1.275136 E + 05	3.562990E + 02	2.121004E + 02	1.353698E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
5.104914 E − 01	5.500740 E − 01	1.831115 E + 00	2.268075 E + 00
− 1.380838 E + 01	− 2.986651 E + 00	− 1.179983 E − 01	− 1.210491 E − 01
3.546478 E + 01	2.053528 E + 01	5.299796 E + 00	1.929230 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.662124 E + 00	6.833814 E + 00	7.498190 E + 00
− 8.012597 E − 02	− 4.183420 E − 03	− 1.132588 E − 03
1.243684 E + 00	1.661301 E − 01	1.045829 E − 03

k	1 (**25 Mn**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.970173 E − 04	8.315498 E − 02	9.118571 E − 02	1.590773 E − 01
ρ_k	7.804374 E + 11	− 6.331017 E + 02	− 6.457474 E + 02	− 1.600771 E + 01
φ_k	1.522077 E + 05	3.933287 E + 02	2.335698 E + 02	1.494468 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
4.846627 E − 01	5.242371 E − 01	1.800835 E + 00	2.171677 E + 00
− 1.609563 E + 01	− 3.449931 E + 00	− 1.358885 E − 01	− 1.398977 E − 01
4.004232 E + 01	2.339427 E + 01	5.880152 E + 00	2.258767 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.535256 E + 00	6.720807 E + 00	7.077436 E + 00
− 9.327942 E − 02	− 5.355993 E − 03	− 1.346833 E − 03
1.535328 E + 00	1.929413 E − 01	3.586332 E − 04

k	1 (**26 Fe**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.728400 E − 04	7.911165 E − 02	8.747507 E − 02	1.512669 E − 01
ρ_k	1.202131 E + 12	− 7.171896 E + 02	− 7.318750 E + 02	− 1.854820 E + 01
φ_k	1.804475 E + 05	4.323994 E + 02	2.561417 E + 02	1.647530 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
4.610965 E − 01	5.005045 E − 01	1.764513 E + 00	2.077770 E + 00
− 1.865046 E + 01	− 3.965039 E + 00	− 1.568596 E − 01	− 1.619738 E − 01
4.495410 E + 01	2.645283 E + 01	6.529329 E + 00	2.639717 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.410779 E + 00	6.585254 E + 00	7.033322 E + 00
− 1.087447 E − 01	− 6.486578 E − 03	− 1.372334 E − 03
1.883139 E + 00	2.331049 E − 01	5.767085 E − 04

k	1 (**27 Co**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.524057 E − 04	7.547369 E − 02	8.405654 E − 02	1.444711 E − 01
ρ_k	1.820837 E + 12	− 8.083521 E + 02	− 8.252652 E + 02	− 2.131927 E + 01
φ_k	2.125211 E + 05	4.731134 E + 02	2.797123 E + 02	1.805247 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
4.398929 E − 01	4.789933 E − 01	1.733761 E + 00	1.994624 E + 00
− 2.143665 E + 01	− 4.523643 E + 00	− 1.790090 E − 01	− 1.852988 E − 01
5.011827 E + 01	2.969002 E + 01	7.183303 E + 00	3.034107 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.302473 E + 00	6.470483 E + 00	6.883165 E + 00
− 1.251318 E − 01	− 7.753902 E − 03	− 1.464120 E − 03
2.253930 E + 00	2.716290 E − 01	5.219691 E − 04

k	1 (**28 Ni**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.350222 E − 04	7.216906 E − 02	8.089558 E − 02	1.383599 E − 01
ρ_k	2.715524 E + 12	− 9.069139 E + 02	− 9.262582 E + 02	− 2.434036 E + 01
φ_k	2.487756 E + 05	5.155529 E + 02	3.043036 E + 02	1.969151 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
4.206321 E − 01	4.593284 E − 01	1.705828 E + 00	1.919013 E + 00
− 2.447399 E + 01	− 5.129635 E + 00	− 2.027591 E − 01	− 2.103064 E − 01
5.555121 E + 01	3.311022 E + 01	7.853485 E + 00	3.448915 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.205076 E + 00	6.366238 E + 00	6.728001 E + 00
− 1.427436 E − 01	− 9.115030 E − 03	− 1.567773 E − 03
2.654621 E + 00	3.114798 E − 01	4.295498 E − 04

k	1 (**29 Cu**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.220837 E − 04	6.915185 E − 02	7.796404 E − 02	1.328183 E − 01
ρ_k	3.804836 E + 12	− 1.013164 E + 03	− 1.035152 E + 03	− 2.762119 E + 01
φ_k	2.849738 E + 05	5.586503 E + 02	3.288432 E + 02	2.128615 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
4.030465 E − 01	4.412704 E − 01	1.042111 E + 00	1.849776 E + 00
− 2.777226 E + 01	− 5.783729 E + 00	− 2.269000 E − 01	− 2.641396 E − 01
6.017921 E + 01	3.563878 E + 01	1.517850 E + 01	4.534901 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.116759 E + 00	3.889212 E + 00	1.060109 E + 01
− 1.887026 E − 01	− 3.764039 E − 02	− 4.007654 E − 04
2.139620 E + 00	6.068395 E − 01	3.377457 E − 02

k	1 (**30 Zn**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	1.093014 E − 04	6.639125 E − 02	7.523854 E − 02	1.278388 E − 01
ρ_k	5.484732 E + 12	− 1.127357 E + 03	− 1.152204 E + 03	− 3.116592 E + 01
φ_k	3.292847 E + 05	6.042967 E + 02	3.552648 E + 02	2.302047 E + 02

5 (2*p*'')	6 (2*s*)	7 (3*d*')	8 (3*s*)
3.869566 E − 01	4.246594 E − 01	1.013522 E + 00	1.786819 E + 00
− 3.133533 E + 01	− 6.488273 E + 00	− 2.535231 E − 01	− 2.985017 E − 01
6.593855 E + 01	3.922154 E + 01	1.655417 E + 01	5.018828 E + 00

9 (3*p*'')	10 (3*d*'')	11 (4*s*)
2.037400 E + 00	3.782514 E + 00	1.045940 E + 01
− 2.148067 E − 01	− 4.539589 E − 02	− 4.172736 E − 04
2.411364 E + 00	6.624929 E − 01	3.470547 E − 02

k	1 (**31 Ga**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (2*p*'')
R_k	9.999056 E − 05	6.354192 E − 02	7.266068 E − 02	1.183149 E − 01	3.703495 E − 01
ρ_k	7.402800 E + 12	− 1.251794 E + 03	− 1.280136 E + 03	− 3.549781 E + 01	− 3.571151 E + 01
φ_k	3.719511 E + 05	6.541462 E + 02	3.827763 E + 02	2.556463 E + 02	7.203164 E + 01

6 (4*p*')	7 (2*s*)	8 (3*d*')	9 (3*s*)
4.000629 E − 01	4.075339 E − 01	8.207280 E − 01	1.677752 E + 00
− 7.369772 E + 00	− 7.369910 E + 00	− 3.156732 E − 01	− 4.003778 E − 01
4.294966 E + 01	4.044939 E + 01	2.158163 E + 01	5.860955 E + 00

10 (3*p*")	11 (3*d*")	12 (4*s*)	13 (4*p*")
1.885615 E + 00	3.062999 E + 00	8.681390 E + 00	1.198854 E + 01
− 2.992761 E − 01	− 8.557296 E − 02	− 8.683064 E − 04	− 1.385572 E − 04
2.525737 E + 00	9.701396 E − 01	8.953004 E − 02	3.130941 E − 03

k	1 (**32 Ge**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	9.152975 E − 05	6.091629 E − 02	7.025164 E − 02	1.102557 E − 01	3.407788 E − 01
ρ_k	9.962644 E + 12	− 1.385189 E + 03	− 1.417356 E + 03	− 4.023520 E + 01	− 4.049928 E + 01
φ_k	4.194475 E + 05	7.062215 E + 02	4.114887 E + 02	2.818673 E + 02	8.232897 E + 01

6 (2*p*")	7 (2*s*)	8 (3*d*')	9 (3*s*)
3.550461 E − 01	3.916665 E − 01	7.011994 E − 01	1.582128 E + 00
− 4.049972 E + 01	− 8.332968 E + 00	− 3.861721 E − 01	− 5.219974 E − 01
5.031343 E + 01	4.588502 E + 01	2.635623 E + 01	6.739995 E + 00

10 (3*p*")	11 (3*d*")	12 (4*s*)	13 (4*p*")
1.757173 E + 00	2.616912 E + 00	7.604480 E + 00	1.021199 E + 01
− 4.014337 E − 01	− 1.373594 E − 01	− 1.534117 E − 03	− 4.483593 E − 04
2.784645 E + 00	1.339787 E + 00	1.525060 E − 01	6.312235 E − 03

k	1 (**33 As**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	8.390709 E − 05	5.848880 E − 02	6.799527 E − 02	1.032950 E − 01	3.005274 E − 01
ρ_k	1.333612 E + 13	− 1.527877 E + 03	− 1.564217 E + 03	− 4.540040 E + 01	− 4.572154 E + 01
φ_k	4.718582 E + 05	7.604931 E + 02	4.413606 E + 02	3.089537 E + 02	9.868202 E + 01

6 (2*p*")	7 (2*s*)	8 (3*d*')	9 (3*s*)
3.408977 E − 01	3.769232 E − 01	6.168400 E − 01	1.497231 E + 00
− 4.572252 E + 01	− 9.382132 E + 00	− 4.658747 E − 01	− 6.653952 E − 01
5.747501 E + 01	4.960630 E + 01	3.109604 E + 01	7.683508 E + 00

10 (3*p*")	11 (3*d*")	12 (4*s*)	13 (4*p*")
1.646238 E + 00	2.302078 E + 00	6.830392 E + 00	9.005793 E + 00
− 5.231378 E − 01	− 2.019994 E − 01	− 2.478899 E − 03	− 9.805796 E − 04
3.142610 E + 00	1.769067 E + 00	2.236234 E − 01	9.621769 E − 03

k	1 (**34 Se**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	7.701127 E − 05	5.622750 E − 02	6.587597 E − 02	9.705244 E − 02	2.878107 E − 01
ρ_k	1.777164 E + 13	− 1.680309 E + 03	− 1.721213 E + 03	− 5.104387 E + 01	− 5.143105 E + 01
φ_k	5.296960 E + 05	8.171156 E + 02	4.724217 E + 02	3.373356 E + 02	1.075189 E + 02

6 (2*p*'')	7 (2*s*)	8 (3*d*'')	9 (3*s*)
3.277179 E − 01	3.631299 E − 01	5.508007 E − 01	1.419578 E + 00
− 5.143254 E + 01	− 1.052897 E + 01	− 5.575898 E − 01	− 8.378243 E − 01
6.232486 E + 01	5.356944 E + 01	3.603637 E + 01	8.745636 E + 00

10 (3*p*'')	11 (3*d*'')	12 (4*s*)	13 (4*p*'')
1.546749 E + 00	2.055616 E + 00	6.181776 E + 00	8.624716 E + 00
− 6.709217 E − 01	− 2.837442 E − 01	− 3.509678 E − 03	− 1.488515 E − 03
3.616572 E + 00	2.303229 E + 00	3.376347 E − 01	1.833763 E − 02

k	1 (**35 Br**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	7.079964 E − 05	5.413089 E − 02	6.388372 E − 02	9.159978 E − 02	2.701979 E − 01
ρ_k	2.354433 E + 13	− 1.842653 E + 03	− 1.888496 E + 03	− 5.714848 E + 01	− 5.760900 E + 01
φ_k	5.931226 E + 05	8.758716 E + 02	5.046158 E + 02	3.665159 E + 02	1.196651 E + 02

6 (2*p*'')	7 (2*s*)	8 (3*d*'')	9 (3*s*)
3.154980 E − 01	3.502848 E − 01	4.996283 E − 01	1.350318 E + 00
− 5.761125 E + 01	− 1.176836 E + 01	− 6.593011 E − 01	− 1.034761 E + 00
6.833061 E + 01	5.776175 E + 01	4.103985 E + 01	9.882824 E + 00

10 (3*p*'')	11 (3*d*'')	12 (4*s*)	13 (4*p*'')
1.459849 E + 00	1.864638 E + 00	5.676813 E + 00	8.096922 E + 00
− 8.408365 E − 01	− 3.803189 E − 01	− 4.858655 E − 03	− 2.248732 E − 03
4.163553 E + 00	2.892445 E + 00	4.591730 E − 01	2.713501 E − 02

k	1 (**36 Kr**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	6.520398 E − 05	5.218195 E − 02	6.200750 E − 02	8.678239 E − 02	2.523121 E − 01
ρ_k	3.100213 E + 13	− 2.015226 E + 03	− 2.066399 E + 03	− 6.373287 E + 01	− 6.427441 E + 01
φ_k	6.624313 E + 05	9.367502 E + 02	5.379329 E + 02	3.965350 E + 02	1.337821 E + 02

6 (2*p*'')	7 (2*s*)	8 (3*d*'')	9 (3*s*)
3.041387 E − 01	3.382960 E − 01	4.584139 E − 01	1.288048 E + 00
− 6.427773 E + 01	− 1.310405 E + 01	− 7.715564 E − 01	− 1.257663 E + 00
7.503190 E + 01	6.217318 E + 01	4.615233 E + 01	1.109493 E + 01

10 (3*p*'')	11 (3*d*'')	12 (4*s*)	13 (4*p*'')
1.383073 E + 00	1.710824 E + 00	5.268325 E + 00	7.560943 E + 00
− 1.034231 E + 00	− 4.926861 E − 01	− 6.579293 E − 03	− 3.313988 E − 03
4.773982 E + 00	3.534833 E + 00	5.868131 E − 01	3.586672 E − 02

k	1 (**37 Rb**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	6.070802 E − 05	5.026544 E − 02	6.022254 E − 02	8.132292 E − 02	2.029644 E − 01
ρ_k	3.947980 E + 13	− 2.200059 E + 03	− 2.257313 E + 03	− 7.124147 E + 01	− 7.189957 E + 01
φ_k	7.312598 E + 05	1.001329 E + 03	5.724190 E + 02	4.312196 E + 02	1.753015 E + 02

6 (2*p*'')	7 (2*s*)	8 (3*d*')	9 (3*s*)	10 (3*p*'')
2.929685E − 01	3.264912 E − 01	4.121461 E − 01	1.218004 E + 00	1.296064 E + 00
− 7.190594E + 01	− 1.465283 E + 01	− 9.336976 E − 01	− 1.602583 E + 00	− 1.338345 E + 00
8.859241E + 01	6.646259 E + 01	5.220725 E + 01	1.238409 E + 01	5.373080 E + 00

11 (3*d*'')	12 (4*s*)	13 (4*p*'')	14 (5*s*)
1.538150 E + 00	4.582967 E + 00	6.082158 E + 00	1.904387 E + 01
− 6.802465 E − 01	− 1.136136 E − 02	− 6.401139 E − 03	− 3.456575 E − 05
4.252708 E + 00	8.138172 E − 01	1.393163 E − 01	1.057707 E − 02

k	1 (**38 Sr**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	5.649045 E − 05	4.848135 E − 02	5.853622 E − 02	7.657762 E − 02	1.743202 E − 01
ρ_k	5.032339 E + 13	− 2.396022 E + 03	− 2.459831 E + 03	− 7.933502 E + 01	− 8.012319 E + 01
φ_k	8.071016 E + 05	1.068257 E + 03	6.081450 E + 02	4.667447 E + 02	2.124328 E + 02

6 (2*p*'')	7 (2*s*)	8 (3*d*')	9 (3*s*)	10 (3*p*'')
2.825700 E − 01	3.154582 E − 01	3.757189 E − 01	1.155770 E + 00	1.220437 E + 00
− 8.013324 E + 01	− 1.632401 E + 01	− 1.114481 E + 00	− 1.997390 E + 00	− 1.688127 E + 00
1.001483 E + 02	7.106794 E + 01	5.837499 E + 01	1.384092 E + 01	6.125594 E + 00

11 (3*d*'')	12 (4*s*)	13 (4*p*'')	14 (5*s*)
1.402202 E + 00	4.107361 E + 00	5.223789 E + 00	1.673859 E + 01
− 8.999501 E − 01	− 1.704132 E − 02	− 1.015079 E − 02	− 1.018086 E − 04
5.104113 E + 00	1.102047 E + 00	2.781945 E − 01	2.447504 E − 02

k	1 (**39 Y**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	5.236921 E − 05	4.685108 E − 02	5.694566 E − 02	7.275406 E − 02
ρ_k	6.482580 E + 13	− 2.602725 E + 03	− 2.673430 E + 03	− 8.784124 E + 01
φ_k	8.935358 E + 05	1.136812 E + 03	6.450321 E + 02	5.017009 E + 02

5 (4*p*')	6 (2*p*'')	7 (2*s*)	8 (3*d*')
1.601441 E − 01	2.730681 E − 01	3.053329 E − 01	3.490053 E − 01
− 8.876033 E + 01	− 8.877329 E + 01	− 1.806852 E + 01	− 1.295142 E + 00
2.395223 E + 02	1.095471 E + 02	7.606533 E + 01	6.442781 E + 01

9 (3*s*)	10 (3*p*'')	11 (3*d*'')	12 (4*d*')
1.104356 E + 00	1.159500 E + 00	1.302505 E + 00	1.337515 E + 00
− 2.396705 E + 00	− 2.042206 E + 00	− 1.123117 E + 00	− 2.155444 E − 02
1.542110 E + 01	7.004576 E + 00	6.043694 E + 00	5.413486 E + 00

13 (4*s*)	14 (4*p*'')	15 (4*d*'')	16 (5*s*)
3.841116 E + 00	4.798980 E + 00	1.143536 E + 01	1.414640 E + 01
− 2.171434 E − 02	− 1.328936 E − 02	− 3.285598 E − 04	− 1.686566 E − 04
1.360085 E + 00	3.863704 E − 01	6.436441 E − 02	2.580686 E − 03

k	1 (**40 Zr**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	4.854586 E − 05	4.533534 E − 02	5.543996 E − 02	6.942112 E − 02
ρ_k	8.346702 E + 13	− 2.820873 E + 03	− 2.898909 E + 03	− 9.688049 E + 01
φ_k	9.886325 E + 05	1.207368 E + 03	6.830739 E + 02	5.371539 E + 02

5 (4*p*')	6 (2*p*")	7 (2*s*)	8 (3*d*')
1.497748 E − 01	2.642337 E − 01	2.958863 E − 01	3.270379 E − 01
− 9.793841 E + 01	− 9.795425 E + 01	− 1.991792 E + 01	− 1.486163 E + 00
2.648215 E + 02	1.187383 E + 02	8.135216 E + 01	7.060441 E + 01

9 (3*s*)	10 (3*p*")	11 (3*d*")	12 (4*d*')
1.058841 E + 00	1.106382 E + 00	1.220522 E + 00	1.301045 E + 00
− 2.824948 E + 00	− 2.422741 E + 00	− 1.364817 E + 00	− 2.603216 E − 02
1.711908 E + 01	7.983580 E + 00	7.073825 E + 00	6.258831 E + 00

13 (4*s*)	14 (4*p*")	15 (4*d*")	16 (5*s*)
3.636969 E + 00	4.488245 E + 00	1.112355 E + 01	1.218499 E + 01
− 2.637962 E − 02	− 1.645480 E − 02	− 6.113773 E − 04	− 2.639161 E − 04
1.634497 E + 00	5.108769 E − 01	6.803978 E − 02	6.220605 E − 04

k	1 (**41 Nb**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	4.501991 E − 05	4.391736 E − 02	5.401178 E − 02	6.643865 E − 02
ρ_k	1.072707 E + 14	− 3.050890 E + 03	− 3.136732 E + 03	− 1.064995 E + 02
φ_k	1.092722 E + 06	1.280030 E + 03	7.222732 E + 02	5.733900 E + 02

5 (4*p*')	6 (2*p*")	7 (2*s*)	8 (3*d*')
1.412630 E − 01	2.559691 E − 01	2.870219 E − 01	3.082248 E − 01
− 1.077064 E + 02	− 1.077253 E + 02	− 2.188346 E + 01	− 1.690672 E + 00
2.899560 E + 02	1.280690 E + 02	8.690561 E + 01	7.697269 E + 01

9 (3*s*)	10 (3*p*")	11 (3*d*")	12 (4*d*')
1.017632 E + 00	1.058850 E + 00	1.150311 E + 00	1.272790 E + 00
− 3.289871 E + 00	− 2.836797 E + 00	− 1.629909 E + 00	− 3.070995 E − 02
1.893695 E + 01	9.059018 E + 00	8.198586 E + 00	7.145154 E + 00

13 (4*s*)	14 (4*p*")	15 (4*d*")	16 (5*s*)
3.464973 E + 00	4.233175 E + 00	1.088198 E + 01	1.109917 E + 01
− 3.126663 E − 02	− 1.978928 E − 02	− 9.058751 E − 04	− 3.491964 E − 04
1.940829 E + 00	6.632702 E − 01	7.957632 E − 02	3.449854 E − 05

k	1 (**42 Mo**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	4.178552 E − 05	4.258720 E − 02	5.265520 E − 02	6.374337 E − 02
ρ_k	1.374305 E + 14	− 3.293107 E + 03	− 3.387246 E + 03	− 1.167202 E + 02
φ_k	1.206027 E + 06	1.354802 E + 03	7.626188 E + 02	6.104650 E + 02

5 (4*p*')	6 (2*p*")	7 (2*s*)	8 (3*d*')
1.340394 E − 01	2.482164 E − 01	2.786829 E − 01	2.918330 E − 01
− 1.180867 E + 02	− 1.181088 E + 02	− 2.396970 E + 01	− 1.909450 E + 00
3.152121 E + 02	1.376027 E + 02	9.271058 E + 01	8.354308 E + 01

9 (3*s*)	10 (3*p*")	11 (3*d*")	12 (4*d*')
9.800179 E − 01	1.015894 E + 00	1.089135 E + 00	1.249745 E + 00
− 3.793542 E + 00	− 3.286271 E + 00	− 1.919725 E + 00	− 3.563374 E − 02
2.086513 E + 01	1.021983 E + 01	9.409282 E + 00	8.064772 E + 00

13 (4*s*)	14 (4*p*")	15 (5*s*)	16 (4*d*")
3.316004 E + 00	4.016708 E + 00	1.031409 E + 01	1.068495 E + 01
− 3.641780 E − 02	− 2.332308 E − 02	− 1.219220 E − 03	− 7.840598 E − 04
2.272332 E + 00	8.374436 E − 01	1.059247 E − 01	2.258214 E − 04

k	1 (**43 Tc**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.882324 E − 05	4.133751 E − 02	5.136509 E − 02	6.129718 E − 02
ρ_k	1.754303 E + 14	− 3.547815 E + 03	− 3.650753 E + 03	− 1.275539 E + 02
φ_k	1.328965 E + 06	1.431661 E + 03	8.041074 E + 02	6.483741 E + 02

5 (4*p*')	6 (2*p*")	7 (2*s*)	8 (3*d*')
1.278604 E − 01	2.409326 E − 01	2.708275 E − 01	2.774215 E − 01
− 1.290906 E + 02	− 1.291161 E + 02	− 2.617834 E + 01	− 2.142288 E + 00
3.405277 E + 02	1.473462 E + 02	9.876592 E + 01	9.031936 E + 01

9 (3*s*)	10 (3*p*")	11 (3*d*")	12 (4*d*')
9.455719 E − 01	9.769087 E − 01	1.035351 E + 00	1.231746 E + 00
− 4.335521 E + 00	− 3.770769 E + 00	− 2.234002 E + 00	− 4.076921 E − 02
2.289872 E + 01	1.146057 E + 01	1.070110 E + 01	9.005113 E + 00

13 (4*s*)	14 (4*p*")	15 (5*s*)	16 (4*d*")
3.186168 E + 00	3.831546 E + 00	9.587477 E + 00	1.053106 E + 01
− 4.179288 E − 02	− 2.703122 E − 02	− 1.565457 E − 03	− 1.023670 E − 03
2.622872 E + 00	1.028803 E + 00	1.492681 E − 01	2.032708 E − 03

k	1 (**44 Ru**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.611369 E − 05	4.015578 E − 02	5.013584 E − 02	5.902079 E − 02
ρ_k	2.230224 E + 14	− 3.815532 E + 03	− 3.927828 E + 03	− 1.390723 E + 02
φ_k	1.461909 E + 06	1.510763 E + 03	8.467422 E + 02	6.874083 E + 02

5 (4*p*')	6 (2*p*")	7 (2*s*)	8 (3*d*')
1.220143 E − 01	2.340450 E − 01	2.633820 E − 01	2.643215 E − 01
− 1.407939 E + 02	− 1.408232 E + 02	− 2.852738 E + 01	− 2.394761 E + 00
3.673248 E + 02	1.575063 E + 02	1.050439 E + 02	9.734860 E + 01

9 (3*s*)	10 (3*p*'')	11 (3*d*'')	12 (4*d*')
9.133153 E − 01	9.406294 E − 01	9.864613 E − 01	1.209399 E + 00
− 4.930517 E + 00	− 4.303789 E + 00	− 2.582260 E + 00	− 4.650346 E − 02
2.504522 E + 01	1.278456 E + 01	1.208312 E + 01	1.002162 E + 01

13 (4*s*)	14 (4*p*'')	15 (5*s*)	16 (4*d*'')
3.062729 E + 00	3.656358 E + 00	9.373947 E + 00	1.034000 E + 01
− 4.780123 E − 02	− 3.118181 E − 02	− 1.877428 E − 03	− 1.297767 E − 03
3.014346 E + 00	1.252608 E + 00	1.818008 E − 01	2.533380 E − 03

k	1 (**45 Rh**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.363296 E − 05	3.904164 E − 02	4.896407 E − 02	5.693585 E − 02
ρ_k	2.823766 E + 14	− 4.096380 E + 03	− 4.218567 E + 03	− 1.512420 E + 02
φ_k	1.605423 E + 06	1.591948 E + 03	8.905132 E + 02	7.273057 E + 02

5 (4*p*')	6 (2*p*'')	7 (3*d*')	8 (2*s*)
1.169241 E − 01	2.275514 E − 01	2.526218 E − 01	2.563458 E − 01
− 1.531597 E + 02	− 1.531930 E + 02	− 3.100646 E + 01	− 3.391110 E + 01
3.942567 E + 02	1.678941 E + 02	1.127274 E + 02	1.045915 E + 02

9 (3*s*)	10 (3*p*'')	11 (3*d*'')	12 (4*d*')
8.835513 E − 01	9.074011 E − 01	9.427974 E − 01	1.191622 E + 00
− 5.567006 E + 00	− 4.874783 E + 00	− 2.957121 E + 00	− 5.247938 E − 02
2.720889 E + 01	1.418261 E + 01	1.354179 E + 01	1.105142 E + 01

13 (4*s*)	14 (4*p*'')	15 (5*s*)	16 (4*d*'')
2.953454 E + 00	3.503823 E + 00	9.043605 E + 00	1.018801 E + 01
− 5.406222 E − 02	− 3.552900 E − 02	− 2.228368 E − 03	− 1.582837 E − 03
3.420811 E + 00	1.490568 E + 00	2.257527 E − 01	4.333491 E − 03

k	1 (**46 Pd**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	3.135993 E − 05	3.798848 E − 02	4.784571 E − 02	5.501025 E − 02
ρ_k	3.560771 E + 14	− 4.390715 E + 03	− 4.523348 E + 03	− 1.640911 E + 02
φ_k	1.760059 E + 06	1.675240 E + 03	9.354178 E + 02	7.681297 E + 02

5 (4*p*')	6 (2*p*'')	7 (3*d*')	8 (2*s*)
1.123683 E − 01	2.214131 E − 01	2.420456 E − 01	2.496803 E − 01
− 1.662173 E + 02	− 1.662548 E + 02	− 3.362176 E + 01	− 3.692404 E + 01
4.216182 E + 02	1.785547 E + 02	1.209265 E + 02	1.120601 E + 02

9 (3*s*)	10 (3*p*'')	11 (3*d*'')	12 (4*d*')
8.558870 E − 01	8.767124 E − 01	9.033265 E − 01	1.176168 E + 00
− 6.248755 E + 00	− 5.487216 E + 00	− 3.361044 E + 00	− 5.876710 E − 02
2.945320 E + 01	1.565481 E + 01	1.507872 E + 01	1.210346 E + 01

13 (4*s*)	14 (4*p*'')	15 (5*s*)	16 (4*d*'')
2.854421 E + 00	3.367301 E + 00	8.721407 E + 00	1.005589 E + 01
− 6.064830 E − 02	− 4.011839 E − 02	− 2.600952 E − 03	− 1.881202 E − 03
3.846500 E + 00	1.746075 E + 00	2.771911 E − 01	6.997619 E − 03

k	1 (**47 Ag**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	2.952782 E − 05	3.699131 E − 02	4.677718 E − 02	5.322435 E − 02
ρ_k	4.358279 E + 14	− 4.698854 E + 03	− 4.842505 E + 03	− 1.776379 E + 02
φ_k	1.909909 E + 06	1.759912 E + 03	9.807244 E + 02	8.091657 E + 02

5 (4*p*')	6 (2*p*'')	7 (3*d*'')	8 (2*s*)
1.082510 E − 01	2.156012 E − 01	2.324222 E − 01	2.433561 E − 01
− 1.799854 E + 02	− 1.800274 E + 02	− 3.637649 E + 01	− 4.010617 E + 01
4.487302 E + 02	1.887680 E + 02	1.286466 E + 02	1.190270 E + 02

9 (4*d*')	10 (3*s*)	11 (3*p*'')	12 (3*d*'')
7.049601 E − 01	8.300820 E − 01	8.482500 E − 01	8.674116 E − 01
− 6.976692 E + 00	− 6.986521 E + 00	− 6.151728 E + 00	− 3.804267 E + 00
3.908188 E + 01	1.891337 E + 01	1.646990 E + 01	1.596332 E + 01

13 (4*s*)	14 (4*p*'')	15 (4*d*'')	16 (5*s*)
2.763928 E + 00	3.243917 E + 00	6.027200 E + 00	1.387693 E + 01
− 7.458398 E − 02	− 5.197082 E − 02	− 1.000752 E − 02	− 1.786739 E − 04
4.016741 E + 00	1.410594 E + 00	3.639316 E − 01	2.123996 E − 02

k	1 (**48 Cd**)	2 (2*p*')	3 (1*s*)	4 (3*p*')
R_k	2.764401 E − 05	3.604624 E − 02	4.575532 E − 02	5.156591 E − 02
ρ_k	5.424374 E + 14	− 5.022756 E + 03	− 5.176336 E + 03	− 1.918938 E + 02
φ_k	2.083482 E + 06	1.853729 E + 03	1.034221 E + 03	8.581836 E + 02

5 (4*p*')	6 (2*p*'')	7 (3*d*'')	8 (2*s*)
1.045398 E − 01	2.100929 E − 01	2.236414 E − 01	2.373506 E − 01
− 1.944751 E + 02	− 1.945217 E + 02	− 3.927316 E + 01	− 4.345964 E + 01
4.832583 E + 02	2.063170 E + 02	1.436819 E + 02	1.332878 E + 02

9 (4*d*')	10 (3*s*)	11 (3*p*'')	12 (3*d*'')
6.778536 E − 01	8.059884 E − 01	8.218190 E − 01	8.346412 E − 01
− 5.182215 E + 00	− 7.763532 E + 00	− 6.851616 E + 00	− 4.270299 E + 00
4.795679 E + 01	2.494971 E + 01	2.186001 E + 01	2.135897 E + 01

13 (4*s*)	14 (4*p*'')	15 (4*d*'')	16 (5*s*)
2.681445 E + 00	3.132706 E + 00	5.795447 E + 00	1.373979 E + 01
− 8.382595 E − 02	− 5.906115 E − 02	− 1.246825 E − 02	− 1.840775 E − 04
6.073621 E + 00	2.658194 E + 00	1.097410 E + 00	3.335212 E − 01

k	1 (**49 In**)	2 (2p')	3 (1s)	4 (3p')	5 (4p')
R_k	2.611485 E − 05	3.511143 E − 02	4.477062 E − 02	4.972748 E − 02	9.754386 E − 02
ρ_k	6.568177 E + 14	− 5.360185 E + 03	− 5.528167 E + 03	− 2.075506 E + 02	− 2.104289 E + 02
φ_k	2.251429 E + 06	1.938178 E + 03	1.075775 E + 03	8.976829 E + 02	5.220315 E + 02

6 (2p'')	7 (3d')	8 (2s)	9 (5p')	10 (4d')
2.046444 E − 01	2.137762 E − 01	2.314069 E − 01	3.250338 E − 01	5.745003 E − 01
− 2.104863 E + 02	− 4.250458 E + 01	− 4.729780 E + 01	− 8.766608 E + 00	− 8.766671 E + 00
2.130830 E + 02	1.462519 E + 02	1.349310 E + 02	9.904672 E + 01	4.714387 E + 01

11 (3s)	12 (3p'')	13 (3d'')	14 (4s)
7.794883 E − 01	7.925194 E − 01	7.978237 E − 01	2.535737 E + 00
− 8.786849 E + 00	− 7.778728 E + 00	− 4.900401 E + 00	− 1.071865 E − 01
2.418580 E + 01	1.920578 E + 01	1.889586 E + 01	4.776507 E + 00

15 (4p'')	16 (4d'')	17 (5s)	18 (5p'')
2.923061 E + 00	4.911808 E + 00	1.158315 E + 01	1.559485 E + 01
− 7.790259 E − 02	− 2.054839 E − 02	− 3.701749 E − 04	− 6.294652 E − 05
1.688160 E + 00	5.692079 E − 01	5.639479 E − 02	2.097238 E − 03

k	1 (**50 Sn**)	2 (2p')	3 (1s)	4 (3p')	5 (4p')
R_k	2.467213 E − 05	3.422326 E − 02	4.382713 E − 02	4.802160 E − 02	9.169330 E − 02
ρ_k	7.948065 E + 14	− 5.714333 E + 03	− 5.895736 E + 03	− 2.240491 E + 02	− 2.272451 E + 02
φ_k	2.431725 E + 06	2.031427 E + 03	1.125036 E + 03	9.447684 E + 02	5.671729 E + 02

6 (2p'')	7 (3d')	8 (2s)	9 (5p')	10 (4d')
1.994678 E − 01	2.048100 E − 01	2.257492 E − 01	2.804256 E − 01	5.062632 E − 01
− 2.273142 E + 02	− 4.591169 E + 01	− 5.136238 E + 01	− 9.860977 E + 00	− 9.861173 E + 00
2.264465 E + 02	1.556454 E + 02	1.433694 E + 02	1.153567 E + 02	5.888310 E + 01

11 (3s)	12 (3d'')	13 (3p'')	14 (4s)
7.547442 E − 01	7.643613 E − 01	7.653325 E − 01	2.409355 E + 00
− 9.890659 E + 00	− 8.780099 E + 00	− 3.329406 E + 00	− 1.333130 E − 01
2.747505 E + 01	2.064088 E + 01	2.044099 E + 01	5.225673 E + 00

15 (4p'')	16 (4d'')	17 (5s)	18 (5p'')
2.747739 E + 00	4.328401 E + 00	1.024433 E + 01	1.345458 E + 01
− 9.917492 E − 02	− 3.012673 E − 02	− 6.401462 E − 04	− 1.960355 E − 04
1.880047 E + 00	7.646722 E − 01	9.464658 E − 02	4.190133 E − 03

k	1 (**51 Sb**)	2 (2p')	3 (1s)	4 (3p')	5 (4p')
R_k	2.332088 E − 05	3.337787 E − 02	4.292223 E − 02	4.643023 E − 02	8.664807 E − 02
ρ_k	9.599455 E + 14	− 6.083905 E + 03	− 6.279443 E + 03	− 2.414227 E + 02	− 2.449588 E + 02
φ_k	2.624084 E + 06	2.126981 E + 03	1.175481 E + 03	9.929617 E + 02	6.127320 E + 02

6 (2*p*'')	7 (3*d*')	8 (2*s*)	9 (5*p*')	10 (4*d*')
1.945405 E − 01	1.965963 E − 01	2.203544 E − 01	2.495391 E − 01	4.559489 E − 01
− 2.450406 E + 02	− 4.950237 E + 01	− 5.566519 E + 01	− 1.104041 E + 01	− 1.104083 E + 01
2.399941 E + 02	1.653418 E + 02	1.520799 E + 02	1.300246 E + 02	7.044826 E + 01

11 (3*s*)	12 (3*d*'')	13 (3*p*'')	14 (4*s*)
7.315308 E − 01	7.337072 E − 01	7.399704 E − 01	2.297336 E + 00
− 1.108120 E + 01	− 9.861523 E + 00	− 3.698705 E + 00	− 1.625863 E − 01
3.066017 E + 01	2.227480 E + 01	2.209584 E + 01	5.720609 E + 00

15 (4*p*'')	16 (4*d*'')	17 (5*s*)	18 (5*p*'')
2.596551 E + 00	3.898228 E + 00	9.270607 E + 00	1.197267 E + 01
− 1.232070 E − 01	− 4.138160 E − 02	− 1.016576 E − 03	− 4.173142 E − 04
2.112967 E + 00	9.840578 E − 01	1.370464 E − 01	6.326601 E − 03

k	1 (**52 Te**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	2.205345 E − 05	3.257040 E − 02	4.205326 E − 02	4.492876 E − 02	8.208538 E − 02
ρ_k	1.157405 E + 15	− 6.469406 E + 03	− 6.679851 E + 03	− 2.597405 E + 02	− 2.636431 E + 02
φ_k	2.829311 E + 06	2.224939 E + 03	1.227111 E + 03	1.042414 E + 03	6.598953 E + 02

6 (3*d*')	7 (2*p*'')	8 (2*s*)	9 (5*p*')	10 (4*d*')
1.889628 E − 01	1.898342 E − 01	2.151935 E − 01	2.406710 E − 01	4.149085 E − 01
− 2.637394 E + 02	− 2.776199 E + 02	− 6.023488 E + 01	− 1.232182 E + 01	− 1.232244 E + 01
2.550619 E + 02	1.753634 E + 02	1.606489 E + 02	1.377109 E + 02	8.029383 E + 01

11 (3*d*'')	12 (3*s*)	13 (3*p*'')	14 (4*s*)
7.052189 E − 01	7.095263 E − 01	7.160411 E − 01	2.194126 E + 00
− 1.237601 E + 01	− 5.435748 E + 00	− 4.099042 E + 00	− 1.964236 E − 01
3.412204 E + 01	2.401900 E + 01	2.376272 E + 01	6.286788 E + 00

15 (4*p*'')	16 (4*d*'')	17 (5*s*)	18 (5*p*'')
2.459822 E + 00	3.547345 E + 00	8.448161 E + 00	1.154719 E + 01
− 1.512217 E − 01	− 5.497902 E − 02	− 1.412092 E − 03	− 6.202203 E − 04
2.405228 E + 00	1.258944 E + 00	2.074935 E − 01	1.204640 E − 02

k	1 (**53 I**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	2.086803 E − 05	3.180051 E − 02	4.121852 E − 02	4.352442 E − 02	7.808259 E − 02
ρ_k	1.392332 E + 15	− 6.870988 E + 03	− 7.097090 E + 03	− 2.789775 E + 02	− 2.832702 E + 02
φ_k	3.047541 E + 06	2.325207 E + 03	1.279941 E + 03	1.092975 E + 03	7.075875 E + 02

6 (3*d*')	7 (2*p*'')	8 (2*s*)	9 (5*p*')	10 (4*d*')
1.819331 E − 01	1.853470 E − 01	2.102648 E − 01	2.273653 E − 01	3.822704 E − 01
− 2.833820 E + 02	− 2.911583 E + 02	− 6.505592 E + 01	− 1.369398 E + 01	− 1.369489 E + 01
2.731331 E + 02	1.857106 E + 02	1.685551 E + 02	1.479557 E + 02	9.094124 E + 01

11 (3*d*'')	12 (3*s*)	13 (3*p*'')	14 (4*s*)
6.789834 E − 01	6.888415 E − 01	6.936597 E − 01	2.101721 E + 00
− 1.376339 E + 01	− 5.987138 E + 00	− 4.526363 E + 00	− 2.336622 E − 01
3.772690 E + 01	2.586681 E + 01	2.548103 E + 01	6.899952 E + 00

15 (4*p*'')	16 (4*d*'')	17 (5*s*)	18 (5*p*'')
2.339872 E + 00	3.268298 E + 00	7.803381 E + 00	1.090880 E + 01
− 1.822322 E − 01	− 7.041664 E − 02	− 1.924337 E − 03	− 9.195065 E − 04
2.730047 E + 00	1.556790 E + 00	2.824270 E − 01	1.830144 E − 02

k	1 (**54 Xe**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	1.976032 E − 05	3.106561 E − 02	4.041604 E − 02	4.220737 E − 02	7.452533 E − 02
ρ_k	1.670796 E + 15	− 7.288990 E + 03	− 7.531521 E + 03	− 2.991585 E + 02	− 3.038657 E + 02
φ_k	3.279111 E + 06	2.427739 E + 03	1.333923 E + 03	1.144606 E + 03	7.559227 E + 02

6 (3*d*')	7 (2*p*'')	8 (2*s*)	9 (5*p*')	10 (4*d*')
1.754323 E − 01	1.810636 E − 01	2.055529 E − 01	2.134902 E − 01	3.554090 E − 01
− 3.039943 E + 02	− 3.126674 E + 02	− 7.013605 E + 01	− 1.516040 E + 01	− 1.516174 E + 01
2.916489 E + 02	1.963378 E + 02	1.766887 E + 02	1.594076 E + 02	1.021463 E + 02

11 (3*d*'')	12 (3*s*)	13 (3*p*'')	14 (4*s*)
6.547224 E − 01	6.693523 E − 01	6.726696 E − 01	2.018208 E + 00
− 1.524696 E + 01	− 6.573828 E + 00	− 4.981703 E + 00	− 2.744835 E − 01
4.139147 E + 01	2.780050 E + 01	2.727882 E + 01	7.550129 E + 00

15 (4*p*'')	16 (4*d*'')	17 (5*s*)	18 (5*p*'')
2.233273 E + 00	3.038641 E + 00	7.276186 E + 00	1.024308 E + 01
− 2.164013 E − 01	− 8.779759 E − 02	− 2.572283 E − 03	− 1.332830 E − 03
3.079605 E + 00	1.873818 E + 00	3.598366 E − 01	2.419956 E − 02

k	1 (**55 Cs**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	1.882567 E − 05	3.034583 E − 02	3.964060 E − 02	4.085289 E − 02	7.021561 E − 02
ρ_k	1.967990 E + 15	− 7.725818 E + 03	− 7.986020 E + 03	− 3.208696 E + 02	− 3.260607 E + 02
φ_k	3.505658 E + 06	2.533596 E + 03	1.388984 E + 03	1.198794 E + 03	8.156654 E + 02

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)	10 (4*d*')
1.687565 E − 01	1.746273 E − 01	1.768685 E − 01	2.009346 E − 01	3.222227 E − 01
− 3.262145 E + 02	− 3.359582 E + 02	− 3.359606 E + 02	− 7.575875 E + 01	− 1.690460 E + 01
3.125647 E + 02	2.091124 E + 02	2.029666 E + 02	1.847288 E + 02	1.168266 E + 02

11 (3*d*'')	12 (3*s*)	13 (3*p*'')	14 (4*s*)	15 (4*p*'')
6.298078 E − 01	6.493185 E − 01	6.510829 E − 01	1.918350 E + 00	2.104125 E + 00
− 1.701896 E + 01	− 7.275268 E + 00	− 5.531181 E + 00	− 3.400614 E − 01	− 2.724285 E − 01
4.560922 E + 01	2.963468 E + 01	2.894976 E + 01	8.178919 E + 00	3.407417 E + 00

16 (4*d*'')	17 (5*s*)	18 (5*p*'')	19 (6*s*)
2.754908 E + 00	6.371605 E + 00	8.378469 E + 00	2.412889 E + 01
− 1.186612 E − 01	− 4.298250 E − 03	− 2.452407 E − 03	− 1.699414 E − 05
2.230443 E + 00	5.019411 E − 01	9.493183 E − 02	7.804349 E − 03

k	1 (**56 Ba**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	1.792580 E − 05	2.965819 E − 02	3.889412 E − 02	3.958653 E − 02	6.648555 E − 02
ρ_k	2.320937 E + 15	− 8.179920 E + 03	− 8.458643 E + 03	− 3.436230 E + 02	− 3.493284 E + 02
φ_k	3.748586 E + 06	2.641857 E + 03	1.445293 E + 03	1.254123 E + 03	8.757556 E + 02

6 (5*p*')	7 (3*d*')	8 (2*p*'')	9 (2*s*)	10 (4*d*')
1.518527 E − 01	1.626049 E − 01	1.728606 E − 01	1.965160 E − 01	2.961243 E − 01
− 3.495095 E + 02	− 3.495132 E + 02	− 3.604051 E + 02	− 8.168176 E + 01	− 1.876769 E + 01
3.578978 E + 02	2.377281 E + 02	2.187389 E + 02	1.930848 E + 02	1.294398 E + 02

11 (3*d*'')	12 (3*s*)	13 (3*p*'')	14 (4*s*)	15 (4*p*'')
6.068497 E − 01	6.304911 E − 01	6.309005 E − 01	1.829902 E + 00	1.992348 E + 00
− 1.891503 E + 01	− 8.023115 E + 00	− 6.118073 E + 00	− 4.126575 E − 01	− 3.347359 E − 01
4.988457 E + 01	3.163095 E + 01	3.077654 E + 01	8.913591 E + 00	3.824103 E + 00

16 (4*d*'')	17 (5*s*)	18 (5*p*'')	19 (6*s*)
2.531775 E + 00	5.749176 E + 00	7.285766 E + 00	2.137902 E + 01
− 1.536089 E − 01	− 6.265215 E − 03	− 3.752607 E − 03	− 4.886279 E − 05
2.660332 E + 00	6.818691 E − 01	1.877558 E − 01	1.790125 E − 02

k	1 (**57 La**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	1.692451 E − 05	2.902829 E − 02	3.818004 E − 02	3.859718 E − 02	6.475144 E − 02
ρ_k	2.806973 E + 15	− 8.648024 E + 03	− 8.945288 E + 03	− 3.663737 E + 02	− 3.725292 E + 02
φ_k	4.041273 E + 06	2.750477 E + 03	1.502852 E + 03	1.307546 E + 03	9.178818 E + 02

6 (5*p*')	7 (3*d*')	8 (2*p*'')	9 (2*s*)
1.492569 E − 01	1.579506 E − 01	1.691893 E − 01	1.924604 E − 01
− 3.727252 E + 02	− 3.727291 E + 02	− 3.846125 E + 02	− 8.734805 E + 01
3.729340 E + 02	2.494777 E + 02	2.300989 E + 02	2.021814 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.863917 E − 01	5.894798 E − 01	6.151331 E − 01	6.155785 E − 01
− 2.037232 E + 01	− 2.053520 E + 01	− 8.651790 E + 00	− 2.496299 E + 00
1.372805 E + 02	5.348854 E + 01	3.393667 E + 01	3.292557 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.785570 E + 00	1.940382 E + 00	2.298301 E + 00	2.448564 E + 00
− 4.494250 E − 01	− 3.655542 E − 01	− 1.694816 E − 01	− 1.702380 E − 01
9.680064 E + 00	4.253781 E + 00	3.240094 E + 00	2.588716 E + 00

18 (5*s*)	19 (4*f*")	20 (5*p*")	21 (6*s*)
5.648357 E + 00	6.894903 E + 00	7.161220 E + 00	2.121609 E + 01
− 7.356273 E − 03	− 4.706705 E − 03	− 3.950365 E − 03	− 4.999715 E − 05
7.526164 E − 01	2.064493 E − 01	1.488919 E − 01	1.818341 E − 02

k	1 (**58 Ce**)	2 (2*p*')	3 (1*s*)	4 (3*p*')	5 (4*p*')
R_k	1.599118 E − 05	2.842692 E − 02	3.749201 E − 02	3.767547 E − 02	6.322577 E − 02
ρ_k	3.386083 E + 15	− 9.133412 E + 03	− 9.449945 E + 03	− 3.900092 E + 02	− 3.966276 E + 02
φ_k	4.352190 E + 06	2.861066 E + 03	1.561513 E + 03	1.361690 E + 03	9.593886 E + 02

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)
1.472617 E − 01	1.536583 E − 01	1.656842 E − 01	1.885836 E − 01
− 3.968383 E + 02	− 3.968423 E + 02	− 4.097497 E + 02	− 9.321721 E + 01
3.867739 E + 02	2.608374 E + 02	2.416580 E + 02	2.115025 E + 02

10 (4*d*')	11 (3*d*")	12 (3*p*")	13 (3*s*)
2.781337 E − 01	5.734605 E − 01	6.004435 E − 01	6.016325 E − 01
− 2.202548 E + 01	− 2.220331 E + 01	− 9.295950 E + 00	− 2.677542 E + 00
1.449479 E + 02	5.710741 E + 01	3.630382 E + 01	3.511709 E + 01

14 (4*s*)	15 (4*p*")	16 (4*f*')	17 (4*d*")
1.746119 E + 00	1.894663 E + 00	2.055460 E + 00	2.377961 E + 00
− 4.850018 E − 01	− 3.953169 E − 01	− 1.847051 E − 01	− 1.868198 E − 01
1.043088 E + 01	4.660491 E + 00	3.931914 E + 00	3.110304 E + 00

18 (5*s*)	19 (4*f*")	20 (5*p*")	21 (6*s*)
5.566603 E + 00	6.166379 E + 00	7.065490 E + 00	2.108081 E + 01
− 8.994719 E − 03	− 6.226691 E − 03	− 4.112028 E − 03	− 5.096590 E − 05
7.995669 E − 01	2.456582 E − 01	1.710934 E − 01	1.840633 E − 02

k	1 (**59 Pr**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.512190 E − 05	2.785126 E − 02	3.680808 E − 02	3.682849 E − 02	6.183397 E − 02
ρ_k	4.073279 E + 15	− 9.636514 E + 03	− 9.973082 E + 03	− 9.980179 E + 03	− 4.216776 E + 02
φ_k	4.681737 E + 06	2.973704 E + 03	1.621891 E + 03	1.416684 E + 03	1.000719 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)
1.455508 E − 01	1.496529 E − 01	1.623291 E − 01	1.848684 E − 01
− 4.219028 E + 02	− 4.219070 E + 02	− 4.358787 E + 02	− 9.931069 E + 01
4.001429 E + 02	2.720948 E + 02	2.534467 E + 02	2.210478 E + 02

10 (4*d*')	11 (3*p*")	12 (3*d*")	13 (3*s*)
2.707756 E − 01	5.585121 E − 01	5.866197 E − 01	5.884677 E − 01
− 2.373995 E + 01	− 2.393267 E + 01	− 9.960942 E + 00	− 2.863529 E + 00
1.526084 E + 02	6.078199 E + 01	3.872898 E + 01	3.736104 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.709870 E + 00	1.852956 E + 00	1.908274 E + 00	2.315051 E + 00
− 5.205225 E − 01	− 4.250118 E − 01	− 1.998558 E − 01	− 2.038198 E − 01
1.118484 E + 01	5.061475 E + 00	4.525381 E + 00	3.569309 E + 00

18 (5*s*)	19 (4*f*'')	20 (5*p*'')	21 (6*s*)
5.494347 E + 00	5.724821 E + 00	6.983402 E + 00	2.095775 E + 01
− 1.110054 E − 02	− 8.221864 E − 03	− 4.257831 E − 03	− 5.186893 E − 05
8.379122 E − 01	2.752646 E − 01	1.889244 E − 01	1.860202 E − 02

k	1 (**60 Nd**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.429845 E − 05	2.729903 E − 02	3.598534 E − 02	3.618805 E − 02	6.052815 E − 02
ρ_k	4.899993 E + 15	− 1.015774 E + 04	− 1.051515 E + 04	− 1.052275 E + 04	− 4.477293 E + 02
φ_k	5.035292 E + 06	3.088887 E + 03	1.688947 E + 03	1.473064 E + 03	1.041376 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*'')	9 (2*s*)
1.439487 E − 01	1.458807 E − 01	1.591104 E − 01	1.813003 E − 01
− 4.479693 E + 02	− 4.479737 E + 02	− 4.630575 E + 02	− 1.056481 E + 02
4.139305 E + 02	2.838705 E + 02	2.659183 E + 02	2.312467 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.639634 E − 01	5.444343 E − 01	5.735075 E − 01	5.759484 E − 01
− 2.552730 E + 01	− 2.573532 E + 01	− 1.065151 E + 01	− 3.056072 E + 00
1.608111 E + 02	6.497240 E + 01	4.165075 E + 01	4.009460 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*d*'')	17 (4*f*')
1.675726 E + 00	1.813825 E + 00	1.832209 E + 00	2.256809 E + 00
− 5.569315 E − 01	− 3.168863 E − 01	− 2.154176 E − 01	− 2.213890 E − 01
1.238404 E + 01	5.893310 E + 00	5.410196 E + 00	4.318720 E + 00

18 (5*s*)	19 (5*p*'')	20 (4*f*'')	21 (6*s*)
5.426173 E + 00	5.496626 E + 00	6.906539 E + 00	2.083995 E + 01
− 1.336062 E − 02	− 1.037207 E − 02	− 4.400710 E − 03	− 5.275352 E − 05
1.059656 E + 00	4.268438 E − 01	3.170839 E − 01	6.749257 E − 02

k	1 (**61 Pm**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.355498 E − 05	2.676874 E − 02	3.520315 E − 02	3.556952 E − 02	5.929694 E − 02
ρ_k	5.847159 E + 15	− 1.069743 E + 04	− 1.107650 E + 04	− 1.108461 E + 04	− 4.748046 E + 02
φ_k	5.400008 E + 06	3.205363 E + 03	1.756347 E + 03	1.529583 E + 03	1.081710 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.423181 E − 01	1.424408 E − 01	1.560196 E − 01	1.778704 E − 01
− 4.750599 E + 02	− 4.913051 E + 02	− 4.913096 E + 02	− 1.122356 E + 02
4.272666 E + 02	2.949123 E + 02	2.776764 E + 02	2.408401 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.576158 E − 01	5.311385 E − 01	5.610415 E − 01	5.640176 E − 01
− 2.738987 E + 01	− 2.761365 E + 01	− 1.136849 E + 01	− 3.255421 E + 00
1.683087 E + 02	6.842279 E + 01	4.381140 E + 01	4.205992 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.643422 E + 00	1.776930 E + 00	1.784150 E + 00	2.202538 E + 00
− 5.943078 E − 01	− 4.867371 E − 01	− 2.314269 E − 01	− 2.395107 E − 01
1.277106 E + 01	5.915201 E + 00	5.450483 E + 00	4.332152 E + 00

18 (4*f*'')	19 (5*s*)	20 (5*p*'')	21 (6*s*)
5.352450 E + 00	5.361529 E + 00	6.834191 E + 00	2.072706 E + 01
− 1.572286 E − 02	− 7.639086 E − 03	− 4.541128 E − 03	− 5.362020 E − 05
9.264694 E − 01	3.046666 E − 01	2.061615 E − 01	1.896759 E − 02

k	1 (**62 Sm**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.284936 E − 05	2.625936 E − 02	3.446021 E − 02	3.497183 E − 02	5.814608 E − 02
ρ_k	6.976837 E + 15	− 1.125583 E + 04	− 1.165740 E + 04	− 1.166605 E + 04	− 5.029050 E + 02
φ_k	5.789945 E + 06	3.324344 E + 03	1.825273 E + 03	1.587449 E + 03	1.122785 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.389563 E − 01	1.410812 E − 01	1.530507 E − 01	1.745725 E − 01
− 5.031758 E + 02	− 5.206288 E + 02	− 5.206335 E + 02	− 1.190690 E + 02
4.468028 E + 02	3.063691 E + 02	2.878084 E + 02	2.510747 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.517731 E − 01	5.185918 E − 01	5.492012 E − 01	5.526584 E − 01
− 2.932322 E + 01	− 2.956295 E + 01	− 1.210992 E + 01	− 3.460731 E + 00
1.762967 E + 02	7.236629 E + 01	4.645429 E + 01	4.450105 E + 01

14 (4*s*)	15 (4*f*')	16 (4*p*'')	17 (4*d*'')
1.613085 E + 00	1.732378 E + 00	1.742442 E + 00	2.152586 E + 00
− 6.321350 E − 01	− 5.183802 E − 01	− 5.289767 E − 01	− 2.582047 E − 01
1.358776 E + 01	6.391937 E + 00	5.920541 E + 00	4.697597 E + 00

18 (4*f*'')	19 (5*s*)	20 (5*p*'')	21 (6*s*)
5.197135 E + 00	5.301955 E + 00	6.768956 E + 00	2.062113 E + 01
− 1.847299 E - 02	− 7.876521 E − 03	− 4.672957 E − 03	− 5.445075 E − 05
1.005250 E + 00	3.186345 E − 01	2.091799 E − 01	1.913206 E − 02

k	1 (**63 Eu**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.219082 E − 05	2.576970 E − 02	3.375364 E − 02	3.439396 E − 02	5.706899 E − 02
ρ_k	8.301428 E + 15	− 1.183327 E + 04	− 1.225816 E + 04	− 1.226736 E + 04	− 5.320452 E + 02
φ_k	6.201154 E + 06	3.445400E + 03	1.895290 E + 03	1.646235 E + 03	1.164159 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.357784 E − 01	1.398620 E − 01	1.501968 E − 01	1.713991 E − 01
− 5.323316 E + 02	− 5.510390 E + 02	− 5.510438 E + 02	− 1.261507 E + 02
4.666162 E + 02	3.178006 E + 02	2.979675 E + 02	2.615256 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.463879 E − 01	5.067318 E − 01	5.379403 E − 01	5.418307 E − 01
− 3.132728 E + 01	− 3.158308 E + 01	− 1.287570 E + 01	− 3.671886 E + 00
1.843447 E + 02	7.637629 E + 01	4.915445 E + 01	4.699317 E + 01

14 (4*s*)	15 (4*f*')	16 (4*p*'')	17 (4*d*'')
1.584561 E + 00	1.676329 E + 00	1.710165 E + 00	2.106543 E + 00
− 6.703014 E − 01	− 5.502921 E − 01	− 5.639366 E − 01	− 2.775422 E − 01
1.440904 E + 01	6.931056 E + 00	6.421800 E + 00	5.042089 E + 00

18 (4*f*'')	19 (5*s*)	20 (5*p*'')	21 (6*s*)
5.028988 E + 00	5.247153 E + 00	6.710462 E + 00	2.052170 E + 01
− 2.174508 E − 02	− 8.100574 E − 03	− 4.795583 E − 03	− 5.524607 E − 05
1.093016 E + 00	3.350770 E − 01	2.119955 E − 01	1.928248 E − 02

k	1 (**64 Gd**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.157214 E − 05	2.529679 E − 02	3.306830 E − 02	3.383459 E − 02	5.597565 E − 02
ρ_k	9.859391 E + 15	− 1.243045 E + 04	− 1.287962 E + 04	− 1.288941 E + 04	− 5.623746 E + 02
φ_k	6.636392 E + 06	3.568843 E + 03	1.966987 E + 03	1.706333 E + 03	1.207276 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.327075 E − 01	1.383863 E − 01	1.474405 E − 01	1.683315 E − 01
− 5.626781 E + 02	− 5.827144 E + 02	− 5.827193 E + 02	− 1.335489 E + 02
4.871441 E + 02	3.299331 E + 02	3.087194 E + 02	2.722655 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.408313 E − 01	4.952712 E − 01	5.270179 E − 01	5.313159 E − 01
− 3.344636 E + 01	− 3.372027 E + 01	− 1.368393 E + 01	− 3.895931 E + 00
1.929045 E + 02	8.062657 E + 01	5.201204 E + 01	4.963145 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.555765 E + 00	1.677401 E + 00	1.696154 E + 00	2.059036 E + 00
− 7.125924 E − 01	− 5.857953 E − 01	− 2.822890 E − 01	− 2.973424 E − 01
1.534610 E + 01	7.325831 E + 00	6.736773 E + 00	5.441206 E + 00

18 (4*f*'')	19 (5*s*)	20 (5*p*'')	21 (6*s*)
5.088462 E + 00	5.185206 E + 00	6.639659 E + 00	2.041409 E + 01
− 2.342792 E − 02	− 8.374598 E − 03	− 4.949733 E − 03	− 5.612436 E − 05
1.110918 E + 00	3.285374 E − 01	2.153353 E − 01	1.946442 E − 02

k	1 (**65 Tb**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.099388 E − 05	2.484157 E − 02	3.241524 E − 02	3.329320 E − 02	5.495105 E − 02
ρ_k	1.167810 E + 16	− 1.304731 E + 04	− 1.352163 E + 04	− 1.353202 E + 04	− 5.937848 E + 02
φ_k	7.094619 E + 06	3.694361 E + 03	2.039781 E + 03	1.767355 E + 03	1.250692 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*")	9 (2*s*)
1.297977 E − 01	1.370587 E − 01	1.447873 E − 01	1.653759 E − 01
− 5.941056 E + 02	− 6.155199 E + 02	− 6.155250 E + 02	− 1.412059 E + 02
5.079517 E + 02	3.420359 E + 02	3.194925 E + 02	2.832223 E + 02

10 (4*d*')	11 (3*d*")	12 (3*p*")	13 (3*s*)
2.357027 E − 01	4.844117 E − 01	5.166100 E − 01	5.212751 E − 01
− 3.563983 E + 01	− 3.593202 E + 01	− 1.451773 E + 01	− 4.126144 E + 00
2.015240 E + 02	8.494418 E + 01	5.492782 E + 01	5.232165 E + 01

14 (4*s*)	15 (4*p*")	16 (4*f*')	17 (4*d*")
1.528655 E + 00	1.646698 E + 00	1.695881 E + 00	2.015188 E + 00
− 7.552868 E − 01	− 6.216232 E − 01	− 3.008211 E − 01	− 3.177642 E − 01
1.628864 E + 01	7.862463 E + 00	7.114606 E + 00	5.792547 E + 00

18 (4*f*")	19 (5*s*)	20 (5*p*")	21 (6*s*)
5.087643 E + 00	5.128200 E + 00	6.575961 E + 00	2.031322 E + 01
− 2.557768 E − 02	− 8.634514 E − 03	− 5.094160 E − 03	− 5.696462 E − 05
1.149220 E + 00	3.282643 E − 01	2.184604 E − 01	1.963136 E − 02

k	1 (**66 Dy**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	1.045269 E − 05	2.440289 E − 02	3.179110 E − 02	3.276889 E − 02	5.398232 E − 02
ρ_k	1.379658 E + 16	− 1.368419 E + 04	− 1.418455 E + 04	− 1.419557 E + 04	− 6.263047 E + 02
φ_k	7.576753 E + 06	3.821960 E + 03	2.113703 E + 03	1.829316 E + 03	1.294514 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*")	9 (2*s*)
1.270311 E − 01	1.358371 E − 01	1.422305 E − 01	1.625253 E − 01
− 6.266431 E + 02	− 6.494872 E + 02	− 6.494924 E + 02	− 1.491312 E + 02
5.290553 E + 02	3.541427 E + 02	3.303080 E + 02	2.943813 E + 02

10 (4*d*')	11 (3*d*")	12 (3*p*")	13 (3*s*)
2.309114 E − 01	4.740864 E − 01	5.066629 E − 01	5.116604 E − 01
− 3.791227 E + 01	− 3.822303 E + 01	− 1.537886 E + 01	− 4.363147 E + 00
2.102216 E + 02	8.932320 E + 01	5.788990 E + 01	5.505145 E + 01

14 (4*s*)	15 (4*p*")	16 (4*f*')	17 (4*d*")
1.502929 E + 00	1.617668 E + 00	1.686402 E + 00	1.974224 E + 00
− 7.986697 E − 01	− 6.580243 E − 01	− 3.196398 E − 01	− 3.387848 E − 01
1.722567 E + 01	8.385086 E + 00	7.508497 E + 00	6.148345 E + 00

18 (4*f*'')	19 (5*s*)	20 (5*p*'')	21 (6*s*)
5.059205 E + 00	5.074819 E + 00	6.517351 E + 00	2.021750 E + 01
− 2.803033 E − 02	− 8.885350 E − 03	− 5.232098 E − 03	− 5.777754 E − 05
1.178608 E + 00	3.118441 E − 01	2.048830 E − 01	1.315337 E − 02

k	1 (**67 Ho**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	9.945252 E − 06	2.397961 E − 02	3.119218 E − 02	3.226082 E − 02	5.305342 E − 02
ρ_k	1.626068 E + 16	− 1.434149 E + 04	− 1.486882 E + 04	− 1.488048 E + 04	− 6.599750 E + 02
φ_k	8.084010 E + 06	3.951747 E + 03	2.188906 E + 03	1.892339 E + 03	1.339029 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.243882 E − 01	1.346577 E − 01	1.397634 E − 01	1.597724 E − 01
− 6.603314 E + 02	− 6.846629 E + 02	− 6.846682 E + 02	− 1.573397 E + 02
5.505829 E + 02	3.664274 E + 02	3.413134 E + 02	3.058120 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.263474 E − 01	4.642232 E − 01	4.971177 E − 01	5.024187 E − 01
− 4.027217 E + 01	− 4.060211 E + 01	− 1.627070 E + 01	− 4.608181 E + 00
2.191267 E + 02	9.384923 E + 01	6.097224 E + 01	5.789403 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.478214 E + 00	1.589832 E + 00	1.680044 E + 00	1.935203 E + 00
− 8.433617 E − 01	− 6.955431 E − 01	− 3.390715 E − 01	− 3.603710 E − 01
1.823287 E + 01	8.969195 E + 00	7.941848 E + 00	6.547806 E + 00

18 (5*s*)	19 (4*f*'')	20 (5*p*'')	21 (6*s*)
5.023137 E + 00	5.040132 E + 00	6.460761 E + 00	2.012445 E + 01
− 3.043672 E − 02	− 2.666954 E − 02	− 5.370063 E − 03	− 5.858267 E − 05
1.254156 E + 00	3.325995 E − 01	2.233961 E − 01	1.994078 E − 02

k	1 (**68 Er**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	9.469073 E − 06	2.357091 E − 02	3.061683 E − 02	3.176825 E − 02	5.216126 E − 02
ρ_k	1.912044 E + 16	− 1.501953 E + 04	− 1.557477 E + 04	− 1.558710 E + 04	− 6.948161 E + 02
φ_k	8.617273 E + 06	4.083653 E + 03	2.265324 E + 03	1.956354 E + 03	1.384176 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.218603 E − 01	1.335162 E − 01	1.373813 E − 01	1.571122 E − 01
− 6.951912 E + 02	− 7.210684 E + 02	− 7.210739 E + 02	− 1.658366 E + 02
5.724670 E + 02	3.788218 E + 02	3.524393 E + 02	3.174441 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.219906 E − 01	4.547890 E − 01	4.879482 E − 01	4.935263 E − 01
− 4.272134 E + 01	− 4.307108 E + 01	− 1.719384 E + 01	− 4.861411 E + 00
2.281714 E + 02	9.845260 E + 01	6.410479 E + 01	6.077933 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.454434 E + 00	1.563097 E + 00	1.676339 E + 00	1.897953 E + 00
− 8.894001 E − 01	− 7.342118 E − 01	− 3.591345 E − 01	− 3.825247 E − 01
1.924028 E + 01	9.544839 E + 00	8.344504 E + 00	6.920616 E + 00

18 (5*s*)	19 (4*f*'')	20 (5*p*'')	21 (6*s*)
4.973004 E + 00	5.029016 E + 00	6.405994 E + 00	2.003387 E + 01
− 3.278073 E − 02	− 3.272135 E − 02	− 5.508257 E − 03	− 5.938094 E − 05
1.310607 E + 00	3.202432 E − 01	2.122952 E − 01	1.541445 E − 02

k	1 (**69 Tm**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	9.022326 E − 06	2.317622 E − 02	3.006476 E − 02	3.129052 E − 02	5.131126 E − 02
ρ_k	2.242874 E + 16	− 1.571857 E + 04	− 1.630266 E + 04	− 1.631569 E + 04	− 7.308296 E + 02
φ_k	9.176975 E + 06	4.217696 E + 03	2.342943 E + 03	2.021375 E + 03	1.429839 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.194452 E − 01	1.324514 E − 01	1.350809 E − 01	1.545411 E − 01
− 7.312236 E + 02	− 7.587025 E + 02	− 7.587081 E + 02	− 1.746181 E + 02
5.947097 E + 02	3.912844 E + 02	3.636650 E + 02	3.293243 E + 02

10 (4*d*')	11 (3*d*'')	12 (3*p*'')	13 (3*s*)
2.178790 E − 01	4.457756 E − 01	4.791497 E − 01	4.849797 E − 01
− 4.525532 E + 01	− 4.562524 E + 01	− 1.814636 E + 01	− 5.122005 E + 00
2.373568 E + 02	1.031677 E + 02	6.733126 E + 01	6.375168 E + 01

14 (4*s*)	15 (4*p*'')	16 (4*f*')	17 (4*d*'')
1.431713 E + 00	1.537626 E + 00	1.667520 E + 00	1.862801 E + 00
− 9.362794 E − 01	− 7.735846 E − 01	− 3.795567 E − 01	− 4.053003 E − 01
2.029026 E + 01	1.015463 E + 01	8.798674 E + 00	7.337621 E + 00

18 (5*s*)	19 (4*f*'')	20 (5*p*'')	21 (6*s*)
4.925525 E + 00	5.002560 E + 00	6.354907 E + 00	1.994718 E + 01
− 3.538065 E − 02	− 3.138504 E − 02	− 5.641505 E − 03	− 6.015851 E − 05
1.391601 E + 00	3.364342 E − 01	2.255136 E − 01	2.023324 E − 02

k	1 (**70 Yb**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	8.533454 E − 06	2.279488 E − 02	2.953483 E − 02	3.082698 E − 02	5.050267 E − 02
ρ_k	2.689273 E + 16	− 1.643892 E + 04	− 1.705282 E + 04	− 1.706656 E + 04	− 7.680314 E + 02
φ_k	9.843350 E + 06	4.356263 E + 03	2.424143 E + 03	2.089788 E + 03	1.478365 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*'')	9 (2*s*)
1.171367 E − 01	1.314809 E − 01	1.328583 E − 01	1.520552 E − 01
− 7.684410 E + 02	− 7.975768 E + 02	− 7.975825 E + 02	− 1.836854 E + 02
6.196960 E + 02	4.061612 E + 02	3.773473 E + 02	3.438525 E + 02

10 (4*d*')	11 (3*d*")	12 (3*p*")	13 (3*s*)
2.140080 E − 01	4.371600 E − 01	4.707041 E − 01	4.767629 E − 01
− 4.787355 E + 01	− 4.826391 E + 01	− 1.912814 E + 01	− 5.390067 E + 00
2.490679 E + 02	1.103905 E + 02	7.305095 E + 01	6.921061 E + 01

14 (4*s*)	15 (4*p*")	16 (4*d*")	17 (4*f*')
1.410030 E + 00	1.513395 E + 00	1.652496 E + 00	1.829705 E + 00
− 9.841722 E − 01	− 8.138557 E − 01	− 4.005970 E − 01	− 4.046665 E − 01
2.378244 E + 01	1.319903 E + 01	1.171609 E + 01	1.020663 E + 01

18 (5*s*)	19 (5*p*")	20 (6*s*)	21 (4*f*")
4.880889 E + 00	4.957488 E + 00	6.308344 E + 00	1.986459 E + 01
− 1.430803 E − 02	− 1.020179 E − 02	− 6.132236 E − 03	− 4.263839 E − 04
3.435089 E + 00	1.892657 E + 00	1.467032 E + 00	1.425577 E − 01

k	1 (**71 Lu**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	8.266763 E − 06	2.241482 E − 02	2.895126 E − 02	3.037472 E − 02	4.909457 E − 02
ρ_k	3.000290 E + 16	− 1.718498 E + 04	− 1.783064 E + 04	− 1.784522 E + 04	− 8.077731 E + 02
φ_k	1.030606 E + 07	4.493213 E + 03	2.505109 E + 03	2.156018 E + 03	1.536383 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
1.145729 E − 01	1.230806 E − 01	1.306431 E − 01	1.495764 E − 01	2.060470 E − 01
− 8.082229 E + 02	− 8.393586 E + 02	− 8.393656 E + 02	− 1.937087 E + 02	− 5.103228 E + 01
6.427891 E + 02	4.323445 E + 02	3.989907 E + 02	3.527581 E + 02	2.592397 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
4.275920 E − 01	4.614035 E − 01	4.677554 E − 01	9.189539 E − 01	1.362795 E + 00
− 5.146966 E + 01	− 2.033393 E + 01	− 5.748237 E + 00	− 1.082878 E + 00	− 1.082977 E + 00
1.129170 E + 02	7.322243 E + 01	6.907144 E + 01	3.719560 E + 01	1.636277 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.374502 E + 00	1.471199 E + 00	1.761641 E + 00	4.088386 E + 00
− 1.133767 E + 00	− 9.498991 E − 01	− 5.000522 E − 01	− 6.267649 E − 02
1.166921 E + 01	1.081014 E + 01	8.408322 E + 00	1.930121 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
4.645356 E + 00	5.905303 E + 00	1.341504 E + 01	1.902817 E + 01
− 1.188695 E − 02	− 7.123908 E − 03	− 1.682207 E − 04	− 6.930276 E − 05
5.542266 E − 01	3.295314 E − 01	6.708647 E − 02	4.500897 E − 03

k	1 (**72 Hf**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	7.942153 E − 06	2.204711 E − 02	2.838944 E − 02	2.993548 E − 02	4.777245 E − 02
ρ_k	3.431067 E + 16	− 1.795337 E + 04	− 1.863188 E + 04	− 1.864735 E + 04	− 8.488828 E + 02
φ_k	1.087839 E + 07	4.634963 E + 03	2.590096 E + 03	2.225943 E + 03	1.597709 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
1.121167 E − 01	1.166256 E − 01	1.285000 E − 01	1.471763 E − 01	1.987707 E − 01
− 8.493792 E + 02	− 8.825983 E + 02	− 8.826065 E + 02	− 2.041024 E + 02	− 5.433133 E + 01
6.689327 E + 02	4.589846 E + 02	4.212568 E + 02	3.644445 E + 02	2.720719 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
4.184252 E − 01	4.524498 E − 01	4.590678 E − 01	7.958842 E − 01	1.182512 E + 00
− 5.481852 E + 01	− 2.159127 E + 01	− 6.122393 E + 00	− 1.187123 E + 00	− 1.187427 E + 00
1.181039 E + 02	7.603467 E + 01	7.156347 E + 01	4.406821 E + 01	2.099441 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.340888 E + 00	1.431579 E + 00	1.699431 E + 00	3.547535 E + 00
− 1.265168 E + 00	− 1.067123 E + 00	− 5.788844 E − 01	− 9.169640 E − 02
1.329924 E + 01	1.101342 E + 01	8.611454 E + 00	2.453383 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
4.454872 E + 00	5.595599 E + 00	1.161845 E + 01	1.856056 E + 01
− 1.395547 E − 02	− 8.554943 E − 03	− 3.792083 E − 04	− 7.467376 E − 05
7.626280 E − 01	4.153868 E − 01	9.719603 E − 02	7.325306 E − 03

k	1 (**73 Ta**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	7.631713 E − 06	2.169085 E − 02	2.784660 E − 02	2.950866 E − 02	4.651300 E − 02
ρ_k	3.920741 E + 16	− 1.874457 E + 04	− 1.945706 E + 04	− 1.947345 E + 04	− 8.914216 E + 02
φ_k	1.147814 E + 07	4.779089 E + 03	2.676727 E + 03	2.297139 E + 03	1.660270 E + 03

6 (3*d*')	7 (5*p*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
1.097535 E − 01	1.111061 E − 01	1.264236 E − 01	1.448492 E − 01	1.919797 E − 01
− 8.919505 E + 02	− 9.273707 E + 02	− 9.273802 E + 02	− 2.148920 E + 02	− 5.778574 E + 01
6.957360 E + 02	4.852762 E + 02	4.430852 E + 02	3.764243 E + 02	2.852119 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
4.096055 E − 01	4.437983 E − 01	4.506598 E − 01	7.279785 E − 01	1.052722 E + 00
− 5.832648 E + 01	− 2.280348 E + 01	− 6.515035 E + 00	− 1.298346 E + 00	− 1.298943 E + 00
1.234953 E + 02	7.900383 E + 01	7.420106 E + 01	4.903137 E + 01	2.527371 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.308684 E + 00	1.393838 E + 00	1.641369 E + 00	3.158166 E + 00
− 1.409128 E + 00	− 1.196100 E + 00	− 6.671165 E − 01	− 1.263770 E − 01
1.484975 E + 01	1.131803 E + 01	8.915607 E + 00	3.000450 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
4.287157 E + 00	5.330777 E + 00	1.062715 E + 01	1.819478 E + 01
− 1.619138 E − 02	− 1.013193 E − 02	− 6.761963 E − 04	− 7.926851 E − 05
9.792991 E − 01	5.038921 E − 01	1.234208 E − 01	9.712115 E − 03

k	1 (**74 W**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	7.335294 E − 06	2.134557 E − 02	2.732218 E − 02	2.909372 E − 02	4.531461 E − 02
ρ_k	4.476005 E + 16	− 1.955890 E + 04	− 2.030652 E + 04	− 2.032387 E + 04	− 9.354103 E + 02
φ_k	1.210557 E + 07	4.925515 E + 03	2.764911 E + 03	2.369521 E + 03	1.723925 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
1.062835 E − 01	1.074799 E − 01	1.244111 E − 01	1.425921 E − 01	1.856389 E − 01
− 9.359824 E + 02	− 9.359932 E + 02	− 9.737090 E + 02	− 2.260828 E + 02	− 6.139738 E + 01
7.309494 E + 02	5.113910 E + 02	4.618265 E + 02	3.886275 E + 02	2.985765 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
4.011205 E − 01	4.354405 E − 01	4.425243 E − 01	6.785347 E − 01	9.535360 E − 01
− 6.199545 E + 01	− 2.427965 E + 01	− 6.926302 E + 00	− 1.416575 E + 00	− 1.417558 E + 00
1.290182 E + 02	8.205992 E + 01	7.691620 E + 01	5.342073 E + 01	2.945134 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.277873 E + 00	1.357926 E + 00	1.587157 E + 00	2.860608 E + 00
− 1.565828 E + 00	− 1.337016 E + 00	− 7.649445 E − 01	− 1.668816 E − 01
1.633277 E + 01	1.168801 E + 01	9.286319 E + 00	3.565638 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
4.137164 E + 00	5.099395 E + 00	9.905362 E + 00	1.789615 E + 01
− 1.861103 E − 02	− 1.186834 E − 02	− 1.066182 E − 03	− 8.330332 E − 05
1.197595 E + 00	5.905312 E − 01	1.466285 E − 01	1.066271 E − 02

k	1 (**75 Re**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	7.052590 E − 06	2.101090 E − 02	2.681617 E − 02	2.869023 E − 02	4.417950 E − 02
ρ_k	5.104189 E + 16	− 2.039662 E + 04	− 2.118055 E + 04	− 2.119890 E + 04	− 9.808544 E + 02
φ_k	1.276098 E + 07	5.074261 E + 03	2.854636 E + 03	2.443103 E + 03	1.788532 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
1.020708 E − 01	1.052952 E − 01	1.224605 E − 01	1.404029 E − 01	1.797421 E − 01
− 9.814717 E + 02	− 9.814839 E + 02	− 1.021596 E + 03	− 2.376730 E + 02	− 6.516340 E + 01
7.738094 E + 02	5.373127 E + 02	4.779253 E + 02	4.011031 E + 02	3.121685 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.929669 E − 01	4.273761 E − 01	4.346616 E − 01	6.321120 E − 01	8.751885 E − 01
− 6.582227 E + 01	− 2.570976 E + 01	− 7.355407 E + 00	− 1.541238 E + 00	− 1.542757 E + 00
1.347099 E + 02	8.524797 E + 01	7.975271 E + 01	5.819505 E + 01	3.383441 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.248527 E + 00	1.323911 E + 00	1.536742 E + 00	2.625565 E + 00
− 1.734519 E + 00	− 1.489190 E + 00	− 8.718813 E − 01	− 2.130049 E − 01
1.778149 E + 01	1.212521 E + 01	9.722206 E + 00	4.151119 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
4.003368 E + 00	4.897269 E + 00	9.227675 E + 00	1.766722 E + 01
− 2.124345 E − 02	− 1.380188 E − 02	− 1.606236 E − 03	− 8.658389 E − 05
1.415530 E + 00	6.732158 E − 01	1.719958 E − 01	1.225940 E − 02

k	1 (**76 W**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	6.782561 E − 06	2.068583 E − 02	2.632472 E − 02	2.829760 E − 02	4.307877 E − 02
ρ_k	5.814921 E + 16	− 2.125837 E + 04	− 2.207983 E + 04	− 2.209924 E + 04	− 1.027866 E + 03
φ_k	1.344595 E + 07	5.225432 E + 03	2.946108 E + 03	2.517994 E + 03	1.854817 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
9.799526 E − 02	1.031804 E − 01	1.205659 E − 01	1.382751 E − 01	1.740920 E − 01
− 1.028532 E + 03	− 1.028545 E + 03	− 1.071175 E + 03	− 2.497110 E + 02	− 6.911444 E + 01
8.191251 E + 02	5.643502 E + 02	4.943785 E + 02	4.138285 E + 02	3.261744 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.850746 E − 01	4.195437 E − 01	4.270153 E − 01	6.193245 E − 01	8.085513 E − 01
− 6.983957 E + 01	− 2.720979 E + 01	− 7.808158 E + 00	− 1.676031 E + 00	− 1.677970 E + 00
1.405995 E + 02	8.855556 E + 01	8.269640 E + 01	6.040299 E + 01	3.733654 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.219978 E + 00	1.290925 E + 00	1.488435 E + 00	2.425654 E + 00
− 1.921159 E + 00	− 1.658201 E + 00	− 9.923529 E − 01	− 2.672200 E − 01
1.927409 E + 01	1.264124 E + 01	1.024084 E + 01	4.810809 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
3.872806 E + 00	4.701730 E + 00	9.041002 E + 00	1.736408 E + 01
− 2.403135 E − 02	− 1.581149 E − 02	− 2.030086 E − 03	− 9.119816 E − 05
1.678574 E + 00	7.911883 E − 01	1.919439 E − 01	1.255294 E − 02

k	1 (**77 Ir**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	6.524992 E − 06	2.037057 E − 02	2.585066 E − 02	2.791552 E − 02	4.203832 E − 02
ρ_k	6.617015 E + 16	− 2.214417 E + 04	− 2.300436 E + 04	− 2.302485 E + 04	− 1.076373 E + 03
φ_k	1.416063 E + 07	5.378885 E + 03	3.039060 E + 03	2.594036 E + 03	1.921907 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
9.440459 E − 02	1.011485 E − 01	1.187284 E − 01	1.362102 E − 01	1.688400 E − 01
− 1.077089 E + 03	− 1.077105 E + 03	− 1.122356 E + 03	− 2.621587 E + 02	− 7.322356 E + 01
8.638821 E + 02	5.912136 E + 02	5.111503 E + 02	4.268041 E + 02	3.403589 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.774915 E − 01	4.119886 E − 01	4.196280 E − 01	5.983490 E − 01	7.535920 E − 01
− 7.401849 E + 01	− 2.876770 E + 01	− 8.279000 E + 00	− 1.817282 E + 00	− 1.819790 E + 00
1.466288 E + 02	9.197084 E + 01	8.573813 E + 01	6.355893 E + 01	4.117309 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.192849 E + 00	1.259747 E + 00	1.443532 E + 00	2.260776 E + 00
− 2.120161 E + 00	− 1.838851 E + 00	− 1.122330 E + 00	− 3.274016 E − 01
2.075273 E + 01	1.320819 E + 01	1.080825 E + 01	5.489014 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
3.755672 E + 00	4.529453 E + 00	8.734797 E + 00	1.712980 E + 01
− 2.703104 E − 02	− 1.801785 E − 02	− 2.603355 E − 03	− 9.499142 E − 05
1.938918 E + 00	9.033696 E − 01	2.149277 E − 01	1.326012 E − 02

k	1 (**78 Pt**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	6.279256 E − 06	2.006461 E − 02	2.539271 E − 02	2.754356 E − 02	4.104965 E − 02
ρ_k	7.521102 E + 16	− 2.305439 E + 04	− 2.395454 E + 04	− 2.397616 E + 04	− 1.126414 E + 03
φ_k	1.490592 E + 07	5.534636 E + 03	3.133523 E + 03	2.671247 E + 03	1.989927 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
9.115679 E − 02	9.919285 E − 02	1.169451 E − 01	1.342048 E − 01	1.639215 E − 01
− 1.127184 E + 03	− 1.127201 E + 03	− 1.175181 E + 03	− 2.750300 E + 02	− 7.749827 E + 01
9.087151 E + 02	6.181979 E + 02	5.282418 E + 02	4.400267 E + 02	3.547585 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.701928 E − 01	4.046900 E − 01	4.124811 E − 01	5.775879 E − 01	7.069320 E − 01
− 7.836692 E + 01	− 3.038651 E + 01	− 8.769163 E + 00	− 1.965711 E + 00	− 1.968898 E + 00
1.528042 E + 02	9.549197 E + 01	8.887572 E + 01	6.694126 E + 01	4.511803 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.166953 E + 00	1.230120 E + 00	1.401480 E + 00	2.120796 E + 00
− 2.332757 E + 00	− 2.032301 E + 00	− 1.262751 E + 00	− 3.940994 E − 01
2.224029 E + 01	1.382535 E + 01	1.142476 E + 01	6.196621 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
3.648215 E + 00	4.373626 E + 00	8.431724 E + 00	1.692784 E + 01
− 3.024032 E − 02	− 2.040700 E − 02	− 3.285504 E − 03	− 9.843213 E − 05
2.205280 E + 00	1.017173 E + 00	2.390923 E − 01	1.402244 E − 02

k	1 (**79 Au**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	6.044821 E − 06	1.976755 E − 02	2.495013 E − 02	2.718132 E − 02	4.010913 E − 02
ρ_k	8.538629 E + 16	− 2.398938 E + 04	− 2.493072 E + 04	− 2.495351 E + 04	− 1.178013 E + 03
φ_k	1.568253 E + 07	5.692682 E + 03	3.229489 E + 03	2.749620 E + 03	2.058871 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
8.819474 E − 02	9.730951 E − 02	1.152137 E − 01	1.322567 E − 01	1.593048 E − 01
− 1.178838 E + 03	− 1.178857 E + 03	− 1.229677 E + 03	− 2.883314 E + 02	− 8.194135 E + 01
9.537326 E + 02	6.453641 E + 02	5.456497 E + 02	4.534934 E + 02	3.693735 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.631640 E − 01	3.976366 E − 01	4.055643 E − 01	5.576508 E − 01	6.666796 E − 01
− 8.288773 E + 01	− 3.206721 E + 01	− 9.278955 E + 00	− 2.121442 E + 00	− 2.125426 E + 00
1.591232 E + 02	9.911578 E + 01	9.210602 E + 01	7.048931 E + 01	4.916488 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.142212 E + 00	1.201935 E + 00	1.362009 E + 00	2.000039 E + 00
− 2.559251 E + 00	− 2.238845 E + 00	− 1.413880 E + 00	− 4.674971 E − 01
2.374419 E + 01	1.448861 E + 01	1.208641 E + 01	6.934115 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
3.548987 E + 00	4.231509 E + 00	8.140679 E + 00	1.675164 E + 01
− 3.367208 E − 02	− 2.299068 E − 02	− 4.085500 E − 03	− 1.015709 E − 04
2.477770 E + 00	1.132656 E + 00	2.642118 E − 01	1.480553 E − 02

k	1 (**80 Hg**)	2 (2*p*')	3 (3*p*')	4 (1*s*)	5 (4*p*')
R_k	5.821331 E − 06	1.947908 E − 02	2.452258 E − 02	2.682846 E − 02	3.921587 E − 02
ρ_k	9.681318 E + 16	− 2.494941 E + 04	− 2.593320 E + 04	− 2.595720 E + 04	− 1.231179 E + 03
φ_k	1.649075 E + 07	5.852996 E + 03	3.326914 E + 03	2.829128 E + 03	2.128635 E + 03

6 (5*p*')	7 (3*d*')	8 (2*p*")	9 (2*s*)	10 (4*d*')
8.550357 E − 02	9.549643 E − 02	1.135324 E − 01	1.303637 E − 01	1.549764 E − 01
− 1.232061 E + 03	− 1.232082 E + 03	− 1.285853 E + 03	− 3.020634 E + 02	− 8.655148 E + 01
9.986890 E + 02	6.726233 E + 02	5.633633 E + 02	4.671986 E + 02	3.841763 E + 02

11 (3*d*")	12 (3*p*")	13 (3*s*)	14 (5*d*')	15 (4*f*')
3.563975 E − 01	3.908226 E − 01	3.988730 E − 01	5.364145 E − 01	6.316740 E − 01
− 8.757939 E + 01	− 3.380894 E + 01	− 9.807862 E + 00	− 2.284060 E + 00	− 2.289033 E + 00
1.655741 E + 02	1.028348 E + 02	9.542193 E + 01	7.446016 E + 01	5.345713 E + 01

16 (4*s*)	17 (4*p*")	18 (4*d*")	19 (4*f*")
1.118616 E + 00	1.175167 E + 00	1.325003 E + 00	1.895022 E + 00
− 2.799053 E + 00	− 2.457940 E + 00	− 1.575308 E + 00	− 5.473941 E − 01
2.525985 E + 01	1.518807 E + 01	1.278284 E + 01	7.692339 E + 00

20 (5*s*)	21 (5*p*")	22 (5*d*")	23 (6*s*)
3.457738 E + 00	4.102389 E + 00	7.830668 E + 00	1.660763 E + 01
− 3.737423 E − 02	− 2.582468 E − 02	− 5.077650 E − 03	− 1.042362 E − 04
2.748177 E + 00	1.242705 E + 00	2.904978 E − 01	1.570841 E − 02

From the presented results one can drew following conclusions. In accordance with well-known ionization potential – atomic number relationship, quasi-classical atomic radius R_q reveals a quasi-periodic dependence upon the parameter Z with maxima at hydrogen H and typical metals (including all alkali elements) Li, Na, Al, K, Ga, Rb, Ag, In, Cs, Tl corresponding to the atomic ionization potentials' minima.

Schematic-plots of the obtained $\rho(r)$ and $-\varphi(r)$ functions in the step-like form are shown in **Figures 1** and **2**, respectively. Electric-charge-density reveals sharp and positive main maximum in the vicinity of center, which corresponds to the nucleus vibrations' region, broad negative minimum, which corresponds to the electron-density main maximum located at relatively short distance from the center, and a few extremes at relatively

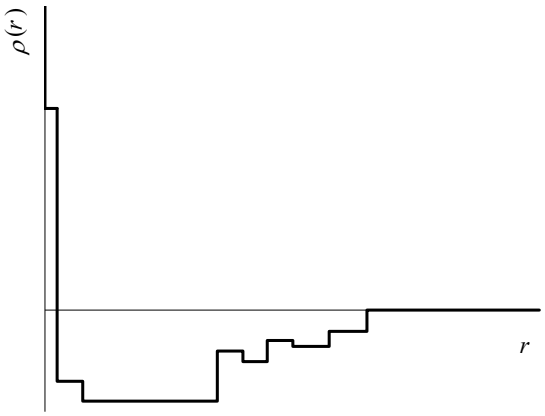

Figure 1. Schematic-plot of the electric-charge-density step-like radial distribution in atoms

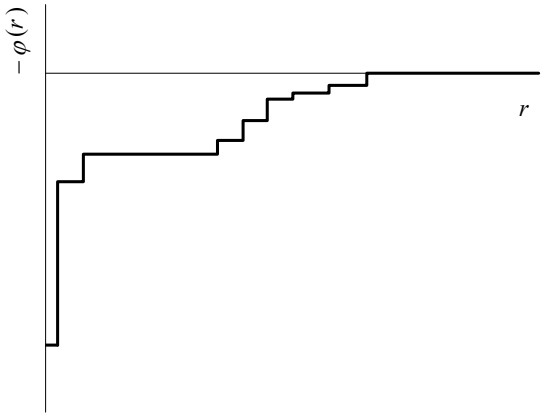

Figure 2. Schematic-plot of the electron-potential-energy step-like radial distribution in atoms

long distance, which are characteristic for the shell-structure of atoms. As for the electron-potential-energy-function, anywhere it is negative and monotonously rises. Thus, it posses only minimum at the center (an additional minimum may be revealed in effective-potential-function). Of course, behind the atomic radius both $\rho(r)$ and $-\varphi(r)$ functions in the step-like presentation are identically zero.

5. Accuracy of Binding-Energy and Electronic-Structure Calculations Based on Radial Step-Like Atomic Potentials

It is not out of place to consider accuracy of the binding energy and electronic-structure calculations carried out within the semiclassical approximation, *i.e.* on the basis of above introduced radial step-like atomic potentials. It is most convenient to estimate the method accuracy for Thomas-Fermi (TF) statistical semiclassical atomic model starting from the only analytical solution

$$\varphi(r) = \frac{81\pi^2}{8r^4} - F \tag{17}$$

of the TF equation. Here F is the Fermi-energy for intra-atomic electron gas, *i.e.* higher occupied electron level. Corresponding electron charge density is expressed by the function

$$\rho(r) = -\frac{243\pi}{8r^6} \tag{18}$$

As electron charge equals to -1 its potential energy in atom $U(r) = -\varphi(r) \to -1/r^4 \to -\infty$ when $r \to 0$. Then, inner turning point radius $r' = 0$ for any electron bound in TF "atom". As for the outer turning point radius r'' of the electron with energy $E \le F$, it can be found as only real positive root of the equation $E = U_{eff}(r)$, where $U_{eff}(r) = U(r) + l(l+1)/2r^2$ is the effective potential energy of the electron with orbital quantum number l, *i.e.*

$$E = F - \frac{81\pi^2}{8r^4} + \frac{l(l+1)}{2r^2} \tag{19}$$

Because differences between semiclassical electron energies are negligible if compared with their depth, one can suppose that approximately all of them coincide with Fermi-energy, $E = F$. In that case, the product $l(l+1)$ also should be substituted for its standard semiclassical expression $(l+1/2)^2$. As a result, we get

$$r'' = \frac{9\pi}{2l+1} \tag{20}$$

Consequently, averaged partial charge density of a l-electron-subshell equals to

$$\rho_l(r) = \frac{-1}{4\pi r''^3/3} = -\frac{(2l+1)^3}{972\pi^4} \tag{21}$$

and 0, respectively, inside and outside the r''-sphere.

As is known, when summation over the principal and orbital quantum numbers n and l characterizing electron motion in central-symmetric electric field is substituted for semiclassical integration the combinations $\nu = n - 1/2$ and $\lambda = l + 1/2$ serve as integration variables. As $l \le n-1$ the limit of integration over λ should be taken equal to $n - 1 + 1/2 = \nu$. As for the degeneracy factor, it equals to $2(2l+1) = 4\lambda$. Note that partial electron charge density takes on a nonzero value $-2\lambda^3/243\pi^4$ if $r \le r'' = 9\pi/2\lambda$. Consequently,

$\lambda \le 9\pi/2r$. But, $\nu_{\max} = \lambda_{\max}$ and, then, the ratio $9\pi/2r$ should serve as the limit of integration over ν too.

Now we can found total electron charge density by means of semiclassical integration:

$$\rho_{Semiclassical}(r) = -\int_0^{\frac{9\pi}{2r}} d\nu \int_0^{\nu} d\lambda \; 4\lambda \; \frac{2\lambda^3}{243\pi^4} = -\frac{729\pi^2}{80r^6} \quad (22)$$

It yields semiclassical atomic potential in following form

$$\varphi_{Semiclassical}(r) = \frac{81\pi^2(90\pi^2)^{1/3}}{80r^4} - F \quad (23)$$

Variable parts of the obtained semiclassical expressions reveal same radial dependences ($\sim -1/r^6$ and $\sim 1/r^6$, respectively, for electron charge density and potential) as corresponding exact analytical solutions, but differ from them by the multipliers $3\pi/10$ and $(3\pi/10)^{2/3}$. Therefore, semiclassically determined structural and energy parameters are expected to be distinguished from their exact values by the multipliers of order of magnitude $\sim(10/3\pi)^{1/3} \approx 1.02 \sim 1$ and $\sim(3\pi/10)^{2/3} \approx 0.96 \sim 1$, respectively. Thus the estimated errors of the semiclassical approach make up a few percent. This conclusion is actually proved by the above cited calculations performed for some one-, two-, and three-dimensional real polyatomic structures.

6. Conclusions

Obtained results, numerically reflected in presented tables, vividly show that an effective method of parameterization of the intra-atomic electric field can by based on semiclassical approach. Such possibility follows from the Maslov criterion, according to which the exact and semiclassical atomic electron-energy spectra should be similar to each other irrespective of the atomic potentials' smoothness properties. Within the semiclassical approximation, intra-atomic eclectic charge density and electric field potential distributions can be presented by the step-like radial functions, where nucleus and electron-states classical turning point radii play role of the steps' limits, while charge density and potential inside a step are substituted for their volume averaged values. Superposition of the semiclassical atomic step-like radial potentials can serve as an initial approximation for the substance inner potential. Binding energy and electronic structure calculations based on such potential allow determining of the substance structural and energy parameters with relative accuracy making up a few percent, what is quite sufficient for materials science purposes.

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