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Pseudopotentials that work: From H to Pu

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Recent developments have enabled pseudopotential methods to reproduce accurately the results of all-electron calculations for the self-consistent electronic structure of atoms, molecules, and solids. The properties of these potentials are discussed in the context of earlier approaches, and their numerous recent successful applications are summarized. While the generation of these pseudopotentials from all-electron atom calculations is straightforward in principle, detailed consideration of the differences in physics of various groups of atoms is necessary to achieve pseudopotentials with the most desirable attributes. One important attribute developed here is optimum transferability to various systems. Another is the ability to be fitted with a small set of analytic functions useful with a variety of wave-function representations. On the basis of these considerations, a consistent set of pseudopotentials has been developed for the entire Periodic Table. Relativistic effects are included in a way that enables the potentials to be used in nonrelativistic formulations. The scheme used to generate the numerical potentials, the fitting procedure, and the testing of the fit are discussed. Representative examples of potentials are shown that display attributes spanning the set. A complete tabulation of the fitted potentials is given along with a guide to its use.

I. INTRODUCTION

Pseudopotentials were originally introduced to simplify electronic structure calculations by eliminating the need to include atomic core states and the strong potentials responsible for binding them. Considerable success was achieved in describing the band structure of semiconductors and simple metals with the use of the empirical pseudopotential method. In this approach, the total effective potential acting on the electrons, including Coulomb and exchange-correlation contributions as well as the ionic parts, was represented by just a few terms in a Fourier expansion. The coefficients were adjusted to agree with some experimentally determined features of the energy bands.[1] In an alternative approach, a simple function representing the ion-core potential was adjusted to fit the experimental ionization potential of the hydrogenic ion. The function typically consisted of a Coulombic tail at large radius discontinuously changing to a constant inside some "core radius." These potentials were then screened using a linear dielectric function method, and gave band structures in reasonable agreement with the empirical potentials, provided the poorly convergent higher Fourier components were set at zero.[1]

Aspects of these two approaches were combined to deal with more complicated systems such as surfaces. A parametrized smooth model potential, with the appropriate Coulomb tail and a rapidly convergent Fourier expansion, was adjusted to fit experimental band energies in a fully self-consistent calculation.[2,3] The charge density given by the square of the pseudo-wave-functions was treated as the real valence charge, and used directly to compute the Coulomb and exchange-correlation potentials (the latter within the local-density-functional approximation[4]). These model potentials were then assumed to be transferable, that is, able to accurately represent the ion potential in other geometries such as surfaces, where the potential cannot be represented by a few Fourier components, and where a self-consistent treatment of the screening is essential. Considerable success was achieved in describing the electronic properties of such systems,[5] and the current work is an outgrowth of this approach to the use of model potentials.

Paralleling the application of pseudopotentials, a theoretical justification for their use was developed.[1] This was initially based upon the orthogonalized-plane-wave (OPW) method of band structure.[6] In this method, plane waves were combined with Bloch sums of core wave functions in such proportion that each basis function was orthogonal to the core states. These combinations then formed a rapidly convergent basis for the valence wave functions. If the linear combination of OPW's forming a band eigenstate was taken without including its core orthogonalization terms, the resulting smooth wave function could be identified with the pseudo-wave-function. Phillips and Kleinman showed that the effective potential which has such plane-wave pseudo-wave-functions as its eigenstates could be derived from the all-electron potential and the core-state wave functions and energies.[7] Thus a nonempirical approach to finding a pseudopotential was introduced. This potential was nonlocal, in the sense that each angular-momentum component of the valence pseudo-wave-function about an atomic center felt a different potential (arising from different core states). Approximate self-consistent band-structure calculations were carried out for Si and other semiconductors with the use of this approach.[8]

The wave functions of Phillips-Kleinman pseudopotentials have a certain problem. The normalized pseudo-wave-function and the normalized OPW eigenfunction have the same shape in the region of space outside the cores, but have different amplitudes. The pseudo-wave-function is typically smaller than the OPW because neglect of the so-called "orthogonality hole" puts too much of its total charge in the core region.[1] This problem is serious in the case of a self-consistent calculation, since the incorrect distribution of valence charge between the valence and core regions will cause errors in the Coulomb potential. In principle, the pseudo-wave-function can be orthogonalized to the cores before the charge density is calculated, but this cumbersome procedure obviates most of the advantages of using a pseudopotential.

The problem of the orthogonality hole is not, in fact, a necessary consequence of replacing an all-electron potential by a valence pseudopotential. It is a consequence of the Phillips-Kleinman construction, but that is by no means unique. Suppose we have a self-consistent local density calculation for the ground state of some atom at hand. A pseudo-wave-function for the atom need have just two properties to be consistent with our intentions: it should be nodeless, and it should, *when normalized,* become identical to the true valence wave function beyond some "core radius," R_c. Such a function can be constructed in arbitrarily many ways. For any particular such pseudo-wave-function, the radial Schrödinger equation can be inverted to yield a pseudopotential which has the function as its eigenfunction at the correct eigenvalue. (Note that the nodeless property permits inversion with no further constraints on the function.) By this construction, it is clear that the pseudopotential and full potential are identical beyond R_c. The pseudopotential inside R_c correctly mimics the scattering property of the full potential inside R_c *at the eigenvalue energy* (and, of course, for the particular angular momentum of the wave function under discussion). We have used the term "norm-conserving" to describe pseudopotentials constructed in this fashion.[9]

The ability of a pseudopotential to reproduce a single atomic state alone does not make it useful. To be useful, the core portion of the pseudopotential must be *transferable* to other situations where the external potential has changed, such as in molecules, solids, or for excited atomic configurations, and where the eigenstates of interest are at different energies. An identity related to the Friedel sum rule, and previously discussed in connection with pseudopotentials by Shaw and Harrison[10] and Topp and Hopfield,[11] can be used to show that any norm-conserving pseudopotential satisfies an important transferability criterion. The identity is (in atomic units)

$$-2\pi\left[(r\phi)^2\frac{d}{d\epsilon}\frac{d}{dr}\ln\phi\right]_R=4\pi\int_0^R\phi^2r^2dr\ , \tag{1.1}$$

where ϕ is the solution of the radial Schrödinger equation at energy ϵ (not necessarily an eigenvalue) which is regular at $r=0$. The radial logarithmic derivative of ϕ is simply related to the scattering phase shift.[12] The consequence of (1.1) is that if two potentials v_1 and v_2 yield solutions ϕ_1 and ϕ_2 which have the same integrated charge inside a sphere of radius R [for $\phi_1(R)=\phi_2(R)$], the linear energy variation around ϵ of their scattering phase shifts (at R) is identical. The requirement on the atomic pseudo-wave-function that it agree identically with the full wave function for $R>R_c$ when both are normalized guarantees that the integrated charge is identical for $R>R_c$, and thus that the scattering properties of the pseudopotential and full potential have the same energy variation to first order when transferred to other systems. Since a given atomic valence state participates with the most weight in molecular orbitals or energy bands that are distributed around the atomic energy level, this optimizes transferability to leading order. Band-structure methods based on muffin-tin potentials such as the augmented-plane-wave (APW) method and Korringa-Kohn-Rostoker (KKR) method depend only on the logarithmic derivatives of the potential at the muffin-tin radius. While such methods are not customarily used for pseudopotentials, it is clear that the energy range over which the pseudopotential logarithmic derivatives track those of the full potential directly measures the range over which the pseudopotential bands are accurate. The norm-conserving construction as defined so far does not guarantee that the logarithmic derivatives track over any useful range. The loosely defined constraint that the pseudo-wave-function and the potential be smooth and physically reasonable in shape in fact yields logarithmic derivative agreement over a wide energy range.[9,13] This close tracking for practical pseudopotentials ensures, through (1.1), that the core-region integrated charge is accurately reproduced over a range of states. Conditions for exactly matching the second energy derivatives have recently been derived, and may be useful for further refinement.[14]

Wave functions of norm-conserving pseudopotentials are designed to reproduce full-potential wave functions accurately in the valence regions. Their definition makes no reference to the core states. Orthogonalization of these wave functions to the core states *will not yield a well-defined object,* in contrast to the Phillips-Kleinman case. While it may be desirable to reproduce the core-region structure of the all-electron wave function in some after-the-fact manner to address questions like nuclear hyperfine coupling, a rigorous procedure consistent with the use of norm-conserving pseudopotentials has not yet been devised.

The first use of the norm-conservation concept was carried out within an empirical model potential framework for Na by Topp and Hopfield.[11] A smooth function with a $1/r$ tail for large r was fit to reproduce the experimental $3s$-electron binding energy. It was then observed that the lowest excited states had approximately correct energies, and that this constituted a finite-difference approximation to the energy derivative in (1.1). The importance of obtaining the correct valence-region amplitude for the normalized pseudo-wave-function was discussed in the context of chemical bonding.[11]

Systematic development of pseudopotentials based on *ab initio* atomic all-electron calculations was first undertaken by Goddard and co-workers.[15,16] They followed the Phillips-Kleinman approach and expressed the pseudo-wave-function as a linear combination of the valence function and core functions. The coefficients of the core functions were chosen to satisfy smoothness and expandability conditions, which included the requirement that $\phi_l(r)$ go to zero as r^{l+1} at small r (the centrifugal barrier enforces only r^l behavior). The *ab initio* calculations on which these pseudopotentials are based are Hartree-Fock calculations, so that the radial equations for the wave functions contain nonlocal exchange operators. This complicates the problem of finding a local pseudopotential to replace the core. These authors dealt with this complexity and the need to find a practical representation for the pseudopotential by introducing a pseudopotential basis set (powers of r times Gaussians). They vary the coefficients to minimize the error in integrals of the nonlocal Schrödinger equation satisfied by the pseudo-wave-function with members of the wave-function basis set used for the atom calculations[15,16] This criterion for a fit also allows them to ignore the r^{-2} divergence at small r of the exact pseudopotential (which arises from the r^{l+1} behavior of the wave function) with minimum error.

The above method for choosing pseudo-wave-functions was introduced in the context of calculations based on the local-density-functional approach[4] by Topiol *et al.*[17] These authors dealt directly with the numerical potential produced by inverting the Schrödinger equation, which is local in this case.

In both of the above approaches, the "orthogonality-hole" problem persists, since the pseudo-wave-function is strictly a sum of orthogonal core and valence wave functions. In both cases, norm conservation was later introduced with a minimum departure from the original approach. Redondo *et al.* modified the Goddard group's approach by a method which explicitly depends on the use of a basis-function set in the original all-electron atom calculation.[18] The basis functions are partitioned into two groups, with longer and shorter range. The coefficients of the longer-range basis functions are fixed at their values in the normalized valence wave function. Members of the shorter-range groups are added with coefficients varied to satisfy nodelessness, normalization, r^{l+1} behavior and smoothness for the resulting pseudo-wave-function. The fitted potential is then found as previously described.[18] This construction makes no explicit use of the core functions (which are particular linear combinations of the short-range basis set). The pseudo-wave-function converges smoothly to the valence function around a radius determined by the division of the basis-function set. This in principle provides additional flexibility in optimizing the pseudo-wave-function, but this was not discussed by the authors.[18]

Zunger retained the Phillips-Kleinman construction used in his earlier work with Topiol and

Ratner[17] in adding norm conservation to local-density-functional pseudopotentials.[19] The linear combination of core states added to the valence state was fixed to satisfy r^{l+1} behavior and smoothness. A function of the form $r^{l+1}e^{-\alpha r}$ was then added with a coefficient varied to give the correct tail amplitude for the normalized pseudo-wave-function. Choice of α gives some control over the smooth transition to the valence function, but a minimum radius is set by the range of the least-bound core function.[19]

An alternative approach to pseudopotential construction was introduced by Christiansen *et al.*[20] specifically in the context of treating the norm-conservation problem. These authors chose the pseudo-wave-function to be identically the Hartree-Fock valence function beyond some matching radius, and to be a polynomial inside. A five-term polynomial with r^{l+1} as the leading power was chosen to give the correct normalization, and to match the value and first three derivatives of the valence function at the matching radius. The matched derivatives ensure continuous behavior of the pseudopotential, but some kinks may occur in the potential in the core region.[21] This construction does not guarantee a nodeless pseudo-wave-function, but the choice of matching radius can be varied to achieve this goal.[20]

All the above constructions give pseudopotentials which diverge with repulsive r^{-2} behavior at small r. This is a consequence of the r^{l+1} behavior of the pseudo-wave-function, which appears to be an arbitrary requirement. For pseudo-wave-functions which are based on linear combinations of the valence (and possibly core) functions, however, the alternative to relaxing this condition is a $-Z/r$ attractive singularity at small r, where Z is the nuclear charge, due to the cusp condition satisfied by the wave functions.[16] In addition, the r^{l+1} requirement serves to minimize the core content of a Phillips—Kleinman-type pseudo-wave-function,[17,19] and hence minimize the orthogonality hole problem. The retention of the r^{l+1} requirement in norm-conserving methods which do not use eigenfunctions of the full potential at small r (the Redondo *et al.*[18] and Christiansen *et al.*[20] methods) seems to have purely historical origins.

A method very similar to that of Christiansen *et al.*[20] was applied to local-density-functional atoms by Kerker[22] with attention to the above issue. Choosing polynomial or exponential of polynomial functions with $ar^{l}+br^{l+2}$ leading behavior inside the matching radius guaranteed a nonsingular pseudopotential, which is a significant advantage whenever a basis-function expansion of this potential is to be used. Pseudo-wave-function convergence is also improved. The use of the exponential form guarantees nodelessness,[22] but the matching radius cannot be too small if a physically reasonable pseudo-wave-function is to be obtained.

The pseudopotentials which are presented in this paper, which were introduced by two of the authors,[9] are nonsingular and intended for use in density-functional calculations. They are constructed in two steps from the results of an all-electron atom calculation. First, the full potential at large r is smoothly merged into a parametrized potential inside a radius r_c. The (single) parameter is adjusted to reproduce the valence eigenvalue, and hence eigenfunction for $r > r_c$, for the highest-energy bound state of each angular momentum l. The norm is then corrected by the addition of a short-range term to this eigenfunction, and the Schrödinger equation for the resulting pseudo-wave-function is analytically inverted, yielding a (typically small) correction to the potential. Nonsingular pseudopotentials can also be constructed for coreless (hence nodeless) valence states.[9]

Pseudopotentials constructed according to this prescription have been used in self-consistent band-structure calculations, and shown to accurately reproduce the results of all-electron calculations. Self-consistent band energies have been compared for Si,[9,23,24] Nb,[25] and CsAu,[26] with errors in the range of 0.05 eV for Si and 0.1—0.2 eV in the other cases.

More extensive use has been made of these pseudopotentials in total-energy calculations. They have been shown to yield lattice constants, cohesive energies, bulk modulii, and phonon frequencies with accuracies of a few percent *compared to experiment* for Si,[27,28] diamond,[28,29] Ge,[30] GaP,[28] GaAs,[31] AlAs,[31] the Si_2 molecule,[32] and others. The excellent results obtained in these studies depend, of course, on much more than the ability of the pseudopotentials to reproduce all-electron calculations. The accuracy of the local-density approximation itself for such systems is critically tested by these comparisons.[4] In addition the rigid-core approximation, which is central to any pseudopotential, must be accurate. This has been established analytically by showing that first-order corrections to the total energy associated with core relaxation cancel identically,[33] and numerical tests indicate errors in the 0.05-eV range for the more difficult case of transition metals.[33] Moreover, the nonlinear density functional of the exchange and correlation potential induces errors if the pseudopotentials are used for different systems than the reference atom. This, too, leads to second-order corrections in the total energy. We shall come back to these problems below.

In treating heavier atoms, it is necessary to consider relativistic effects. For valence states in the valence region, the relativistic Dirac equation reduces to the nonrelativistic Schrödinger equation. This suggests that relativistic effects on the valence electrons, which occur in the core region, can be lumped together with other properties of the core in creating a pseudopotential which can be used to treat heavy atoms in a nonrelativistic formalism. This approach was applied to relativistic Hartree-Fock calculations by several groups using a Phillips-Kleinman construction.[34,35] The method used in this paper to construct norm-conserving pseudopotentials for local-density-approximation calculations was generalized to the relativistic case by Kleinman[36] and subsequently tested for a variety of atoms.[37]

For the relativistic atom, each electron's orbital angular momentum and spin must be coupled, and different energies and wave functions are found for the two possible values of the total angular-momentum quantum number, $j=l+\frac{1}{2}$ and $j=l-\frac{1}{2}$. Two different pseudopotentials are thus found for each l. The most convenient form for application is to take the weighted sum and difference of these potentials.[36–38] The j-average potential then yields results which are similar to those obtained using a "scalar" version of the Dirac equation in which the spin-orbit term is removed.[39] We have carried out tests on heavy atoms comparing the valence levels based on the j-average potential (derived from the fully relativistic atom) with those of completely "scalar relativistic" atoms. The results typically agree within a few hundredths of an eV. This also establishes the fact that the scalar method closely reproduces the fully relativistic core charge. A further test of the j-average pseudopotential was carried out by comparing the self-consistent band structure of CsAu with the use of this potential and with a scalar relativistic full-potential method.[27] The agreement found, typically 0.1–0.3 eV, was excellent.

The "difference" pseudopotential is in fact a spin-orbit pseudopotential which should formally appear multiplying the operator $\vec{L}\cdot\vec{S}$.[36–38] It reduces to zero outside the core, since the pseudopotentials for all j converge to the full potential. Unlike the true spin-orbit potential, which diverges as r^{-3} at small r,[40] the spin-orbit pseudopotential can be smooth and nonsingular in the core region. (Note that it would be completely inconsistent to apply the full potential spin-orbit operator to a pseudo-wave-function.) The approach used here gives spin-orbit pseudopotentials which are often nearly constant over most of the core region.

A number of workers have already successfully constructed and used pseudopotentials based on Ref. 9. It is clear, however, that experience is very helpful in choosing all-electron atom reference configurations, core radii, cutoff functions, etc., and that extensive testing is mandatory for the best results. The principal purpose of this paper is to make a good set of these pseudopotentials for all the elements in the Periodic Table available to others. For many applications, analytic fits to the potentials are necessary. Here again, much experimentation and testing is necessary to find an accurate but economical fitting basis. The quality of fit which could be achieved played an important role in guiding the choices to be made in the construction of the numerical pseudopotential. The fitted form was also devised to permit its publication in a compact table without loss of accuracy.

In Sec. II, the physics involved in choosing reference configurations and pseudopotential construction details for various groups of elements are discussed. The fitting approach is motivated, and the testing procedure for the tabulated results is described. Section III presents examples illustrating the several classes of behavior encountered in various groups of elements. Section IV explains the arrangement and use of the pseudopotential tables. In Sec. V some cases with ambiguous core-valence separation are discussed. Section VI concludes the paper.

II. THE CONSTRUCTION OF PSEUDOPOTENTIALS

This section is divided into three parts: the description of full-core atom calculations from which the pseudopotentials will be derived, the construction of numerical pseudopotentials from energies, wave functions, and potential of a reference full-core atom, and the procedure of fitting simple analytical functions to the set of numerical pseudopotentials.

For both the underlying full-core atom and the subsequently constructed pseudoatom, electron interaction effects are described in the local-density-functional framework.[4] In this scheme the ground-state energy of a system of interacting electrons in an external (nuclear) potential is written as functional of the electron density $\rho(r)$:

$$
\begin{aligned}
E[\rho] = T[\rho] + E_{\rm Coul}[\rho] \\
+ \int V_{\rm ext}(r)\rho(r)dr + E_{\rm xc}[\rho]\,,
\end{aligned}
\tag{2.1}
$$

where $T[\rho]$ is the kinetic energy of the noninteracting electrons,

$$E_{\rm Coul}[\rho] = \tfrac{1}{2}\int\int \frac{\rho(r)\rho(r')}{|r-r'|}dr\,dr'\,,$$

the usual electrostatic Coulomb energy of the electrons, $V_{\rm ext}(r) = -Z/r$, the nuclear potential, and $E_{\rm xc}[\rho]$, the exchange-correlation energy. According to Kohn and Sham,[4] a variational solution of Eq. (2.1) can be obtained by solving a set of Schrödinger-type equations self-consistently:

$$
\begin{gathered}
[T+V(r)]\psi_i(r) = \epsilon_i\psi_i(r)\,, \\
V(r) = \int \frac{\rho(r')}{|r-r'|}dr' + \frac{\delta E_{\rm xc}[\rho]}{\delta\rho(r)} + V_{\rm ext}(r)\,, \\
\rho(r) = \sum_{\substack{\text{occupied}\\ \text{states } i}} |\psi_i(r)|^2\,,
\end{gathered}
\tag{2.2}
$$

To account for relativistic effects in a consistent way for all atoms in the Periodic Table we use Dirac's formulation of the kinetic energy.[41] Thus, the Schrödinger equation [Eq. (2.2)] is replaced by a pair of coupled equations for minor and major wave-function components $G_i(r)$ and $F_i(r)$, respectively, which in their radial form are

$$
\begin{gathered}
\frac{dF_i(r)}{dr} - \frac{\kappa}{r}F_i(r) + \alpha[\epsilon_i - V(r)]G_i(r) = 0\,, \\
\frac{dG_i(r)}{dr} + \frac{\kappa}{r}G_i(r) - \alpha\left[\frac{2}{\alpha^2} + \epsilon_i - V(r)\right]F_i(r) = 0\,.
\end{gathered}
\tag{2.3}
$$

We use atomic units $\hbar = m = e = 1$ and $c = \alpha^{-1} = 137.04$. κ is a nonzero integer quantum number

$$
\kappa = \begin{cases} l, & \text{for } j = l - \frac{1}{2} \\ -(l+1), & \text{for } j = l + \frac{1}{2}\,. \end{cases}
\tag{2.4}
$$

The charge density is given by summing over both components, i.e.,

$$\rho(r) = \sum_{\substack{\text{occupied}\\ \text{states } i}} [\,|G_i(r)|^2 + |F_i(r)|^2\,]\,.$$

For one-electron potentials Dirac's equation includes all relativistic effects and yields spin-orbit splitting energies.

The use of reliable approximations for the exchange-correlation energy $E_{\rm xc}[\rho]$ in Eqs. (2.1) and (2.2) is of central importance. In the local-density approximation,

$$E_{\rm xc}[\rho] = \int \rho(r)\epsilon_{\rm xc}(\rho(r))dr\,, \tag{2.5}$$

where $\epsilon_{\rm xc}(\rho)$ is the exchange-correlation energy per electron of a homogeneous system with density ρ. Among a variety[42] of interpolation formulas available for $\epsilon_{\rm xc}(\rho)$ here we use the recent results of Ceperly and Alder[42] as parametrized by Perdew and Zunger.[43] This choice was motivated by several factors: (i) Ceperley and Alder's results are based on a stochastic sampling of an exact solution of the interacting electron gas, (ii) their results are interpolated by Perdew and Zunger to yield correct high- and low-density limits, and (iii) a consistent extension to finite spin-polarization exists.[44]

For the unpolarized gas we have (in a.u.)

$$
\begin{gathered}
\epsilon_{\rm xc} = \epsilon_x + \epsilon_c \quad \text{with } \epsilon_x = -\frac{0.4582}{r_s}\,, \\
\epsilon_c = \begin{cases} \dfrac{-0.1432}{1 + 1.0529\sqrt{r_s} + 0.3334 r_s} & \text{for } r_s \ge 1 \\ -0.0480 + 0.0311\ln r_s - 0.0116 r_s \\ +0.0020 r_s \ln r_s \quad \text{for } r_s < 1\,. \end{cases}
\end{gathered}
\tag{2.6}
$$

Here r_s is related to the density through $\rho^{-1} = (4\pi/3)r_s^3$. The exchange-correlation potential can be obtained from Eq. (2.6) as

$$\mu_{\rm xc} = \epsilon_{\rm xc} - r_s/3\frac{d\epsilon_{\rm xc}}{dr_s}\,. \tag{2.7}$$

A detailed comparison of the interpolation formula for ϵ_c given above and other existing prescriptions (i.e., Wigner, Hedin-Lundquist, Gunnarson-Lundquist, etc.) can be found in Ref. 43. On the basis of several test calculations for atoms and solids we found only very small differences between using, e.g., Ceperley-Alder or Wigner expressions. The two expressions intersect each other for $r_s \approx 2$, i.e., for average atomic or crystalline densities, while they deviate significantly from each other in the low- and high-density regimes.

To account for relativistic quantum-electrodynamical corrections to the Coulomb interaction, and to be consistent with the Dirac treatment of the free-particle kinetic energy, we modify the nonrelativistic density-functional exchange-correlation energy $\epsilon_{\rm xc}$ as proposed by MacDonald and Vosko.[45] This amounts to multiplying exchange energy ϵ_x and potential μ_x by density-dependent correction factors f_ϵ and f_μ, respectively,

$$f_\epsilon(r_s)=1-\frac{3}{2}\left[\frac{(1+\beta)^{1/2}}{\beta}-\frac{\ln[\beta+(1+\beta^2)^{1/2}]}{\beta^2}\right]^2 ,$$

$$f_\mu(r_s)=-\frac{1}{2}+\frac{3}{2}\frac{\ln[\beta+(1+\beta^2)^{1/2}]}{\beta(1+\beta^2)} , \tag{2.8}$$

where the dimensionless expansion parameter $\beta=0.0140/r_s$ measures the density-dependent Fermi velocity in units of the speed of light. The correction which is due to retardation and magnetic effects decreases the effective exchange interaction appreciably only for rather high densities, i.e., in the atomic core. For example, inclusion of the correction increases the total energy of atomic Pb by about 44 a.u. of which 42 a.u. result from the 1*s* electrons. The 6*s* valence electrons are affected by less than 0.1 eV. We nevertheless include the correction consistently in all atomic calculations.

For the full-core atom the Dirac equations [Eqs. (2.3)] are solved using a modified version of the original Liberman-Waber-Cromer program[46] which uses a logarithmically spaced radial integration mesh. The numerical accuracy is about 10^{-5} a.u. Atomic states are specified as usual by orbital occupation numbers. The atomic ground state within the local-density-functional (LDF) framework is defined by occupying the lowest-lying orbitals. For the purpose, however, of obtaining eigensolutions for both spin-orbit components, $j=l\pm\frac{1}{2}$, we always occupy both components, regardless of their orbital energies, weighted by noninteger values according to their multiplicities. Valence-electron wave functions and energies with angular momenta that are present in the ground state are obtained from ground-state[47] calculations. Higher-angular-momentum wave functions are calculated from appropriately excited atomic states (see also below and Table II). For convenience, the atomic core charge is allowed to relax. The most consistent way to generate these excited configurations would be to keep the core charge frozen in its ground-state form. However, tests indicated that allowing core relaxation in the excited-state configurations which we used had negligible effect on the pseudopotentials. Valence-electron eigenfunctions and eigenvalues for $j=l\pm\frac{1}{2}$ up to $l=2$ ($l=3$ for elements with $Z>55$), as well as the corresponding self-consistent potentials $V(r)$ [Eqs. (2.2)], are calculated for all elements from $Z=1$(H) to $Z=94$ (Pu).

The norm-conserving pseudopotentials are constructed in five steps.

(i) Dirac's equations are solved for a chosen atomic reference configuration labeled by ν. The output is a set of one-electron eigenvalues (for the valence states) and radial wave functions (F and G) as well as the self-consistent LDF potential. As pointed out by Kleinman[36] and later elaborated by Bachelet and Schlüter,[37] Dirac's equations [Eqs. (2.3)] can formally be replaced for valence electrons *outside* the core region by a Schrödinger-type equation for the major wave-function component $G_\kappa(r)$:

$$\left[\frac{1}{2}\frac{d^2}{dr^2}-\frac{\kappa(\kappa+1)}{2r^2}+V^\nu(r)\right]G_\kappa(r)=\epsilon G_\kappa(r) , \tag{2.9}$$

with κ given in Eq. (2.4). This replacement is correct up to terms of order α^2. The minor wave-function component $F_\kappa(r)$ is strongly admixed with $G_\kappa(r)$ only in the core region of heavy atoms. Equation (2.9) can thus be thought of as the starting point for the construction of pseudopotentials and pseudo-wave-functions. The construction steps are carried out independently for each angular-momentum (lj) quantum state. For convenience this state is labeled by j only in the following discussion.

(ii) We construct a first-step pseudopotential $\hat{V}^\nu_{1j}$ by cutting off the singularity near $r\approx 0$ in the screened full-core potential V^ν:

$$\hat{V}^\nu_{1j}(r)=V^\nu(r)\left[1-f\left[\frac{r}{r_{cj}}\right]\right]+c_j^\nu f\left[\frac{r}{r_{cj}}\right] , \tag{2.10}$$

where $f(r/r_{cj})$ is a smooth cutoff function which approaches 0 as $x\rightarrow\infty$, cutting off around $r\approx r_{cj}$ and approaching 1 as $r\rightarrow 0$. The constant c_j^ν is adjusted, so that the lowest nodeless solution $w^\nu_{1j}(r)$ of the radial Schrödinger equation containing $\hat{V}^\nu_{1j}$ has an energy equal to the original eigenvalue ϵ^ν_j. The normalized function $w^\nu_{1j}(r)$ agrees with the full-core valence wave function beyond r_{cj} within a multiplicative constant γ^ν_j,

$$\gamma^\nu_j w^\nu_{1j}(r)\rightarrow G_j(r) , \quad r>r_{cj} , \tag{2.11}$$

since both satisfy the same differential equation and homogeneous boundary conditions for $r>r_{cj}$. The choice of the cut-off function,

TABLE I. List of parameters cc_l that determine the optimum pseudopotential cutoff radii r_{cl} through $r_{cl}=r_{\max}/cc_l$, where $r_{\max}$ is the radius of the outermost peak in the radial wave function.

Elements	$l=0$	$l=1$	$l=2$	$l=3$
${}_1\text{H}\rightarrow{}_2\text{He}$	3.0	3.6	3.6	
${}_3\text{Li}$	2.0	3.0	3.5	
${}_4\text{Be}\rightarrow{}_{10}\text{Ne}$	1.8	3.0	3.5	
${}_{11}\text{Na}$	2.0	1.8	3.5	
${}_{12}\text{Mg}\rightarrow{}_{18}\text{Ar}$	1.8	1.45	2.2	
${}_{19}\text{K}\rightarrow{}_{30}\text{Zn}$	1.8	1.6	3.0	
${}_{31}\text{Ga}\rightarrow{}_{36}\text{Kr}$	1.8	1.7	2.0	
${}_{37}\text{Rb}\rightarrow{}_{48}\text{Cd}$	1.8	1.7	1.6	
${}_{49}\text{In}\rightarrow{}_{54}\text{Xe}$	1.6	1.7	2.0	
${}_{55}\text{Cs}$	1.8	1.7	1.45	4.5
${}_{56}\text{Ba}$	1.8	1.7	1.45	3.0
${}_{57}\text{La}\rightarrow{}_{71}\text{Lu}$	1.45	1.6	1.45	3.0
${}_{72}\text{Hf}\rightarrow{}_{80}\text{Hg}$	1.6	1.6	1.45	3.0
${}_{81}\text{Tl}\rightarrow{}_{86}\text{Rn}$	1.6	1.7	2.2	3.0
${}_{87}\text{Fr}$	1.6	1.6	1.45	4.5
${}_{88}\text{Ra}\rightarrow{}_{94}\text{Pu}$	1.6	1.6	1.45	2.0

$$f(r/r_{cj})=\exp[-(r/r_{cj})^{\lambda}]\ , \qquad (2.12)$$

with $\lambda=3.5$ was found to yield optimum results in tests on a variety of atoms. The exponent $\lambda=3.5$ guarantees nonsingular pseudopotentials for $r=0$ and was found to allow better analytic fits than larger λ values. The "quality parameter" or cutoff radius r_{cj} defines the range over which pseudo-wave-function and full-core wave functions are allowed to deviate from each other. It is *not* to be regarded as an adjustable parameter but can be used to define the "quality" of the pseudopotential. Large r_{cj} values produce rather smooth and $j(l)$-independent pseudopotentials at the expense of larger inaccuracies of the pseudo-wave-function away from the core region. Small r_{cj} values produce stronger and more $j(l)$-dependent pseudopotentials with maximum accuracy. A strict lower limit for r_{cj} is the position of the outermost node in the full-core valence wave function, but numerical instabilities appear already for slightly larger r_{cj} values. Optimum r_{cj} values are obtained by scaling down from the radius ($r_{\max}$) of the outermost peak in the radial function G_κ, $r_{cj}=r_{\max}/cc$, where cc is typically in the range of $1.5-2$. We present in Table I a complete list of optimum cc values used for the present calculations. Cutoff radii for the two spin-orbit components $j=l\pm\frac{1}{2}$ were chosen to be identical and equal to the average obtained from $r_{\max}/cc$.

(iii) The second step involves a modification at short range of the intermediate pseudo-wave-function $w^v_{1j}(r)$ to

$$w^v_{2j}(r)=\gamma^v_j[w^v_{1j}(r)+\delta^v_j r^{l+1}f(r/r_{cj})]\ , \qquad (2.13)$$

such that the *normalized* function $w^v_{2j}(r)$ agrees with the full-core valence wave function for $r>r_{cj}$. This requires that δ^v_j be the smaller solution of the quadratic equation

$$(\gamma^v_j)^2\int[w^v_{1j}(r)+\delta^v_j r^{l+1}f(r/r_{cj})]^2dr=1\ . \qquad (2.14)$$

The magnitude of the norm correction $(\gamma^v_j)^2-1$ is typically small ($\sim 10^{-2}-10^{-3}$). While the existence of a solution δ^v_j is guaranteed, unphysical results can occur for weakly bound and therefore extended excited states. "Bumpy" pseudo-wave-functions (and potentials) for angular momenta present only in excited states (e.g., $l=2$ for Si) can be avoided by using appropriately ionized excited-atom configurations (e.g., for Si $3s^{1.25}3p^{0.75}3d^{0.25}$) which tend to increase wave-function localization. This improves the transferability of the pseudopotential to systems of interest where the wave-function components corresponding to excited states are confined by surrounding atoms. Nevertheless, the high-l-component potentials are less accurate and should *not* be used as local reference potentials. Note that the atomic ground state is used for all angular momenta present in the ground state. This also minimizes systematic transferability errors. Table II contains a list of atom reference configurations used in the present work.

(iv) In the third step the final screened pseudopotentials $\hat{V}^v_{2j}(r)$, producing the nodeless eigenfunctions $w^v_{2j}(r)$ at eigenvalues ϵ_j, are found by inverting the radial Schrödinger equation. This can be done analytically, knowing $\hat{V}^v_{1j}(r)$ and $w^v_{2j}(r)$:

$$\hat{V}^v_{2j}(r)=\hat{V}^v_{1j}(r)+\frac{\delta^v_j r^{l+1}f}{2w^v_{2j}(r)}\times\left\{\frac{\lambda^2\left[\frac{r}{r_{cj}}\right]^{2\lambda}-[2\lambda l+\lambda(\lambda+1)]\left[\frac{r}{r_{cj}}\right]^{\lambda}}{r^2}+2\epsilon_j-2\hat{V}^v_{1j}(r)\right\}\ . \qquad (2.15)$$

TABLE II. Atomic valence configurations (ν) used to derive the l,j-dependent pseudopotentials. Only excited-state configurations are shown. Angular momenta present in the (assumed) ground state are derived from the ground state given in the Sargent-Welch table (Ref. 47) and no configuration is indicated here. Potentials for $l=3$ are derived only for elements with $Z \geq 55$. The symbol (*) indicates the systematic increase by 1 electron per increasing nuclear charge, i.e., for Si one has $s^1p^{0.75}d^{0.5}$ while for Ar the configuration is $s^1p^{4.75}d^{0.5}$. Ground states of the Sargent-Welch table are modified for the following few exceptions: $_{46}$Pd from s^0d^{10} to s^1d^9, $_{57}$La from d^1f^0 to d^0f^1, and $_{93}$Np from d^1f^4 to d^0f^5. Moreover, for all rare-earth elements ($Z=57-71$) the $6s^2\cdots$ configuration is replaced by the $5s^25p^66s^0\cdots$ configuration (see text).

	Angular momentum		
Elements	$l=1$	$l=2$	$l=3$
$_1$H	$p^{0.5}$	$d^{0.5}$	
$_2$He	$s^{0.8}p^{0.2}$	$s^{0.8}d^{0.2}$	
$_3$Li→$_4$Be	$p^{0.25}d^{0.25}$	as $l=1$	
$_5$B		$s^1d^{0.2}$	
$_6$C		$s^{0.75}p^1d^{0.25}$	
$_7$N→$_8$O		$s^1p^{1.75}d^{0.25}$	
$_9$F		$s^{1.25}p^{2.5}d^{0.25}$	
$_{10}$Ne		$s^1p^{2.75}d^{0.25}$	
$_{11}$Na	$p^{0.25}d^{0.25}$	as $l=1$	
$_{12}$Mg	$s^{0.5}p^{0.25}d^{0.25}$	as $l=1$	
$_{13}$Al		$s^{0.75}d^{0.25}$	
$_{14}$Si→$_{18}$Ar		$s^1p^{0.75*}d^{0.25}$	
$_{19}$K	$p^{0.25}$	$d^{0.25}$	
$_{20}$Ca	$s^{0.5}p^{0.25}d^{0.25}$	as $l=1$	
$_{21}$Sc→$_{30}$Zn	$s^{0.75}p^{0.25}d^{1*}$		
$_{31}$Ga		$s^{0.75}d^{0.25}$	
$_{32}$Ge→$_{36}$Kr		$s^1p^{0.75*}d^{0.25}$	
$_{37}$Rb	$p^{0.25}$	$d^{0.25}$	
$_{38}$Sr	$s^{0.5}p^{0.25}d^{0.25}$	as $l=1$	
$_{39}$Y→$_{48}$Cd	$s^{0.75}p^{0.25}d^{1*}$		
$_{49}$In		$s^{0.75}d^{0.25}$	
$_{50}$Sn→$_{54}$Xe		$s^1p^{0.75*}d^{0.25}$	
$_{55}$Cs	$p^{0.25}$	$d^{0.25}$	$f^{0.25}$
$_{56}$Ba	$s^{0.75}p^{0.25}$	$s^{0.75}d^{0.25}$	$s^{0.75}f^{0.25}$
$_{57}$La→$_{71}$Lu		$s^2p^6d^1f^{1*}$	
$_{72}$Hf→$_{80}$Hg	$s^{0.75}p^{0.25}d^{2*}$		$s^{0.75}d^{1*}f^{0.25}$
$_{81}$Tl		$s^{0.75}d^{0.25}$	$s^{0.75}f^{0.25}$
$_{82}$Pb→$_{86}$Rn		$s^1p^{0.75*}d^{0.25}$	$s^{0.75}p^{0.75*}f^{0.25}$
$_{87}$Fr	$p^{0.25}$	$d^{0.25}$	$f^{0.25}$
$_{88}$Ra	$s^{0.75}p^{0.25}$	$s^{0.75}d^{0.25}$	$s^{0.75}f^{0.25}$
$_{89}$Ac	$s^{0.75}p^{0.25}d^1$	as $l=1$	$s^{0.75}d^1f^{0.25}$
$_{90}$Th	$p^{0.25}d^{1.5}f^{0.25}$	as $l=1$	as $l=1$
$_{91}$Pa→$_{92}$U	$s^1p^{0.5}d^{0.5}f^{1*}$		
$_{93}$Np→$_{94}$Pu	$s^{0.5}p^{0.5}d^{0.5}f^{3.5*}$		

The second term in Eq. (2.15) is a smooth correction which cuts off

$$\sim f = \exp\left[-\left(\frac{r}{r_{cj}}\right)^{\lambda}\right] .$$

No numerical instabilities are associated with this procedure.

(v) Finally, in the last step the screened potentials $\hat{V}^{\nu}_{2j}(R)$ are *unscreened* using the nodeless pseudo-wave-functions $w^{\nu}_{2j}(r)$:

$$\hat{V}^{\text{ion}}_{l\pm 1/2}(r) = \hat{V}^{\nu}_{2j}(r) - \int \frac{\rho^{\nu}(r')}{|r-r'|}dr' - \frac{\delta E_{xc}[\rho^{\nu}]}{\delta\rho^{\nu}(r)} , \tag{2.16}$$

$$\rho^{\nu}(r) = \sum_{\substack{\text{occupied}\\ \text{valence states}}} \left|\frac{w^{\nu}_{2j}(r)}{r}\right|^2 .$$

As pointed out in Ref. 48, this valence-unscreening procedure, though exact by definition for the reference atom, represents a linearization of the exchange-correlation energy as a function of charge density. The systematic error occurring for different valence configurations, though small for paramagnetic systems, increases with decreasing valence electron density in the reference state. For systems with few valence electrons such as the alkali atoms, highly ionized reference configurations should thus be avoided.[48] The bare-ion pseudopotentials $\hat{V}_{l\pm 1/2}^{\mathrm{ion}}(r)$ of Eq. (2.16) are, to first order, independent of changes in the atomic prototype configuration ν. We therefore drop the index ν in all further discussions.

It is convenient to define an average pseudopotential

$$\hat{V}_l^{\mathrm{ion}}(r)=\frac{1}{2l+1}[l\hat{V}_{l-1/2}^{\mathrm{ion}}(r)+(l+1)\hat{V}_{l+1/2}^{\mathrm{ion}}] \tag{2.17}$$

weighted by the different j degeneracies of the $l\pm\frac{1}{2}$ states. This average potential is appropriate for scalar relativistic use. Note, that the definition of $\hat{V}_l^{\mathrm{ion}}(r)$ in Eq. (2.17) differs from Eq. (2.12) of Ref. 36; it is, however, consistent with Eq. (13) of Ref. 37. A difference potential $\hat{V}_l^{\mathrm{so}}(r)$ describing the strength of spin-orbit effects can accordingly be defined as

$$\hat{V}_l^{\mathrm{so}}(r)=\frac{2}{2l+1}(\hat{V}_{l+1/2}^{\mathrm{ion}}-\hat{V}_{l-1/2}^{\mathrm{ion}}) . \tag{2.18}$$

Thus the total ionic pseudopotential to be used in relativistic calculations is

$$\hat{V}_{\mathrm{ps}}^{\mathrm{ion}}(r)=\sum_l |l\rangle[\hat{V}_l^{\mathrm{ion}}(r)+\hat{V}_l^{\mathrm{so}}(r)\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}]\langle l| . \tag{2.19}$$

The potential is appropriate for Schrödinger equations yet contains relativistic effects to order α^2.

The pseudopotentials [Eqs. (2.17) and (2.18)], two (one for $l=0$) for each angular momentum for a given atom, are derived on a numerical radial grid. To facilitate their tabulation and use, however, it is desirable to find high-precision fits involving few analytic functions. For this purpose we decompose $\hat{V}_l^{\mathrm{ion}}(r)$ into a long-range Coulomb part (l independent) and a short-range l-dependent pseudopotential part. We have

$$\hat{V}_l^{\mathrm{ion}}=\hat{V}_{\mathrm{core}}(r)+\Delta\hat{V}_l^{\mathrm{ion}} . \tag{2.20}$$

The core potential is thought of as originating from Gaussian-type effective core charges:

$$\hat{V}_{\mathrm{core}}(r)=-\frac{Z_v}{r}\left[\sum_{i=1}^{2} c_i^{\mathrm{core}}\,\mathrm{erf}[(\alpha_i^{\mathrm{core}})^{1/2}r]\right] , \tag{2.21}$$

and therefore smoothly approaches a finite value for $r\to 0$. Z_v denotes the valence charge. The remaining potentials $\Delta\hat{V}_l^{\mathrm{ion}}(r)$ and $\hat{V}_l^{\mathrm{so}}(r)$ are both expanded in Gaussian-type functions, e.g.,

$$\Delta\hat{V}_l^{\mathrm{ion}}(r)=\sum_{i=1}^{3}(A_i+r^2A_{i+3})e^{-\alpha_i\cdot r^2} . \tag{2.22}$$

Thus each atom is characterized by

(i) a valence charge Z_v and two sets of linear coefficients and decay constants describing the core, $c_i^{\mathrm{core}},\alpha_i^{\mathrm{core}}$, $i=1,2$. Note that $c_1^{\mathrm{core}}+c_2^{\mathrm{core}}=1$.

(ii) for each l value two sets of three linear coefficients each, A_i and A_{i+3} corresponding to the decay constants α_i, $i=1,2,3$ for the average potential, and

(iii) a similar set as (ii) for each spin-orbit difference potential, provided the spin-orbit splitting of the eigenvalues is larger than a chosen threshold value of 0.05 eV.

The choice of error function, Gaussian, and r^2 times Gaussian functions was made to maximize the number of calculational techniques which can make direct use of the fitted form. Plane-wave matrix elements can be calculated analytically. The one-, two-, and three-center integrals needed for Gaussian linear combination of atomic orbitals (LCAO) calculations can be expanded as sums of analytic functions, as can mixed-basis Gaussian-plane-wave matrix elements.

The core parameters are the starting point of the fitting procedure. For this purpose the self-consistent full-core potential $V^{\nu}(R)$ is first formally unscreened by the valence electrons. We write

$$V_{\mathrm{ion}}(r)=V^{\nu}(r)-\int\frac{\rho_{\mathrm{val}}(r')}{|r-r'|}dr'-\frac{\delta E_{\mathrm{xc}}[\rho_{\mathrm{val}}]}{\delta\rho_{\mathrm{val}}(r)} . \tag{2.23}$$

$V_{\mathrm{ion}}(r)$ has the form $-Z_v/r$ for large r, but deviates from this form in the core region to attain a $-Z_{\mathrm{full}}/r$ behavior for $r\to 0$. The function $\hat{V}_{\mathrm{core}}(r)$ [Eq. (2.21)] is then fitted to $V_{\mathrm{ion}}(r)$ using the cutoff function

$$g\equiv 1-f=1-\exp[-(r/\bar{r}_{cj})^{\lambda}]$$

as a weighting function. Here $\bar{r}_{cj}$ denotes the atom average over the angular-momentum-dependent cutoff radii r_{cj} given in Table I. $\hat{V}_{\rm core}(r)$ thus has the built-in feature of simulating shallow core charges that may extend beyond the pseudopotential cutoff radii r_{cj}. Examples, such as Cs, shall be described below. Note that $\hat{V}_{\rm core}(r)$ is not uniquely defined but determines the remainder $\Delta\hat{V}_l^{\rm ion}$ through Eq. (2.20). The choice of $\hat{V}_{\rm core}(r)$ discussed here both simplifies the shape and reduces the range of $\Delta\hat{V}_l^{\rm ion}$. In the context of a solid-state or molecular calculation, matrix elements of an ion pseudopotential must be taken between wave-function components which have angular momenta about that center which are higher than the largest l value given. The most consistent procedure is to use the potential for the largest l given for all higher l. However, the construction of $\hat{V}_{\rm core}$ given here enables this term alone to be used as a "local" l-dependent potential for higher l's with little loss of accuracy. (Both approaches depend on the centrifugal barrier to keep the high-l components out of the core region).

The nonlocal short-range components $\Delta\hat{V}_l^{\rm ion}(r)$ and $\hat{V}_l^{\rm so}(r)$ are each fitted by nonlinear least-squares procedures constraining the longest-range components to remain roughly within r_{cj}.

The weighting of the fits was chosen to minimize the error in potential matrix elements, i.e.,

$$\int (V_{\rm num}-V_{\rm fit})^2 r^{-2}\,|\,w_{2j}^{v}\,|^4 dr \;, \tag{2.24}$$

except in some special cases, like some excited states with a relatively long range where the wave-function weighting $r^{-2}|\,w_{2j}^{v}\,|^4$ was replaced by 1. Equation (2.24) exhibits strong nonlinearities as a function of the independent parameters and exhibits a large number of nearly equivalent minima. Random search and conventional simplex procedures were used to find satisfactory solutions.

Linear dependencies of the fitting functions can lead to large values for some of the fitting coefficients A_i in (2.22). This effect is reduced by constraining the nonlinear fit to maintain a finite spacing of the α_i. Nonetheless, too many significant figures must be retained in the A_i's for practical tabulation. To solve this problem we have transformed the coefficients A_i, A_{i+3}, $i=1,3$ of Eq. (2.22) into a set of coefficients C_i, $i=1,6$ for an orthonormal basis set,

$$C_i = -\sum_{l=1}^{6} A_l Q_{il} \;, \tag{2.25}$$

where the orthogonality matrix

$$Q_{il} = \begin{cases} 0 \quad \text{for } i>l \\ \left[S_{il} - \sum\limits_{k=1}^{i-1} Q_{ki}^2 \right]^{1/2} \quad \text{for } i=l \\ \dfrac{\left[S_{il} - \sum\limits_{k=1}^{i-1} Q_{ki} Q_{kl} \right]}{Q_{ii}} \quad \text{for } i<l \;. \end{cases} \tag{2.26}$$

The overlap matrix is defined by

$$S_{il} = \int_0^\infty r^2 \Phi_i(r)\Phi_l(r)\,dr \;,$$

with

$$\Phi_i(r) = \begin{cases} e^{-\alpha_i r^2} \quad \text{for } i=1,2,3 \\ r^2 e^{-\alpha_i r^2} \quad \text{for } i=4,5,6 \end{cases} . \tag{2.27}$$

The Gaussian exponents α_i are rounded to two decimal places prior to a final linear fit determining the A_i. The coefficients C_i in Eq. (2.25) are rounded to four digits. To test the overall accuracy of the fitting procedure including the rounding as tabulated, the potentials are reassembled by first performing an inverse matrix transformation,

$$A_i = -\sum_{l=1}^{6} C_l Q_{il}^{-1} \;, \tag{2.28}$$

and then using Eqs. (2.20), (2.21), and (2.22).

The minus signs in Eqs. (2.25) and (2.28) correspond to a particular choice of phase. The quality of the fits can then be assessed by comparing two independent pseudoatom calculations for identical configurations using the original numerical pseudopotentials and the fitted analytical version. Typical results for a variety of atoms are shown in Table III. The test results illustrate two different and unrelated features: (i) transferability, i.e., the quality of describing atomic excitations (eigenvalues and total energies) by pseudopotentials that have been derived from a different reference state, usually the ground state, and (ii) the quality of the fitted potentials.

The issue of pseudopotential transferability has been discussed before.[9,33,48] Transferability is determined by the "frozen-core" approximation underlying the construction of all pseudopotentials, by the linearization of core and valence exchange-correlation contributions, and by the norm-conservation feature. As can be seen from Table III, transferability is generally excellent. The error increases typically for "two-shell" systems, in par-

TABLE III. Results of test calculations for a variety of representative atoms. State 1 is reference state for the pseudopotential construction, state 2 represents the (de-) excited state. Differences in total energy are given in columns 4 (full-core atom), 5 (numerical pseudopotential atom), and 6 (fitted pseudopotential atom). Columns 7 and 8 show the differences in eigenvalues between the numerical pseudopotential case and the fitted pseudopotential case for states 1 and 2, respectively. All energies are given in eV.

			Excitation energies			Eigenvalues	
Element	State 1	State 2	Full core ΔE_{tot} (eV)	Pseudo ΔE_{tot} (eV)	Pseudo and fit ΔE_{tot} (eV)	$\Delta\epsilon$ (eV) State 1	$\Delta\epsilon$ (eV) State 2
C	s^2p^2	sp^3	8.23	8.22	8.25	s 5×10^{-4}	4×10^{-3}
						p 2×10^{-3}	3×10^{-2}
Si	s^2p^2	sp^3	6.79	6.79	6.79	s 1×10^{-3}	1×10^{-3}
						p 2×10^{-2}	3×10^{-2}
Ge	s^2p^2	sp^3	8.01	8.00	7.97	s 4×10^{-2}	4×10^{-2}
						p 1×10^{-2}	1×10^{-2}
Sn	s^2p^2	sp^3	7.02	7.01	6.96	s 7×10^{-2}	7×10^{-2}
						p 2×10^{-2}	2×10^{-2}
Ni	d^8s^2	d^9s^1	-1.66	-1.57	-1.36	s 3×10^{-2}	4×10^{-2}
						d 2×10^{-1}	2×10^{-1}
Pd	d^9s^1	$d^{10}s^0$	-1.47	-1.43	-1.17	s 1×10^{-2}	3×10^{-2}
						d 2×10^{-1}	1×10^{-1}
Pt	d^9s^1	$d^{10}s^0$	-0.03	-0.003	$+0.06$	s 1×10^{-2}	1×10^{-2}
						d 5×10^{-2}	3×10^{-2}
Sm^{2+}	f^6d^0	f^5d^1	4.32	4.56	4.43	d 2×10^{-2}	3×10^{-2}
						f 2×10^{-1}	2×10^{-1}

ticular for the $3d$ transition elements and the $4f$ rare-earth elements. The extreme localization of $4f$ electrons in the rare-earth series necessitates the inclusion of the $5s,5p$ "core" electrons into the valence shell (see Sec. V). This inclusion restores a core which remains "frozen" to a much better approximation and decreases the error for a $4f$-$5d$ valence excitation from 1.7 to 0.2 eV.[49]

The error due to fitting the analytical functions generally varies between 10^{-2} and 10^{-4} eV. Exceptions are again the $3d$ and $4f$ elements whose $d(f)$ pseudopotentials are extremely strong. Absolute errors in the $d(f)$ eigenvalues range from 0.1 to 0.3 eV for the $3d$ elements and from 0.2 to 1.1 eV for the $4f$ elements. These errors illustrate the limitations given by the small set of six Gaussian-type fitting functions. Relative errors, however, in both excitation energies and changes in eigenvalues are considerably smaller. Note that the neglect of spin-polarization for the magnetic $3d$ and $4f$ elements amounts to systematic errors of equal or larger magnitude. We point out in this context that the present pseudopotentials which are derived for paramagnetic reference atoms *cannot* be used for spin-polarized situations. The strong non linearities associated with the spin-polarized exchange-correlation functionals[43] require systematic modifications.[48,50] An extended version of the present work to include spin-polarization effects and improved fits involving more parameters will be published shortly for $3d$ and $4f$ elements.[51]

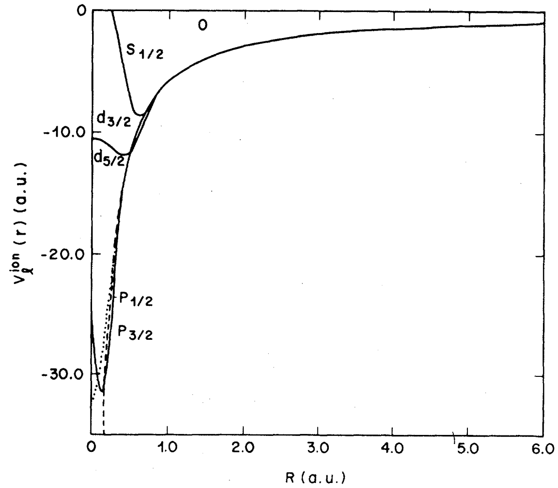

FIG. 1. Ion-core pseudopotential for oxygen. Dashed line corresponds to $-Z_v/r$, the dotted line to $\hat{V}^{\text{core}}(r)$ as defined in the text.

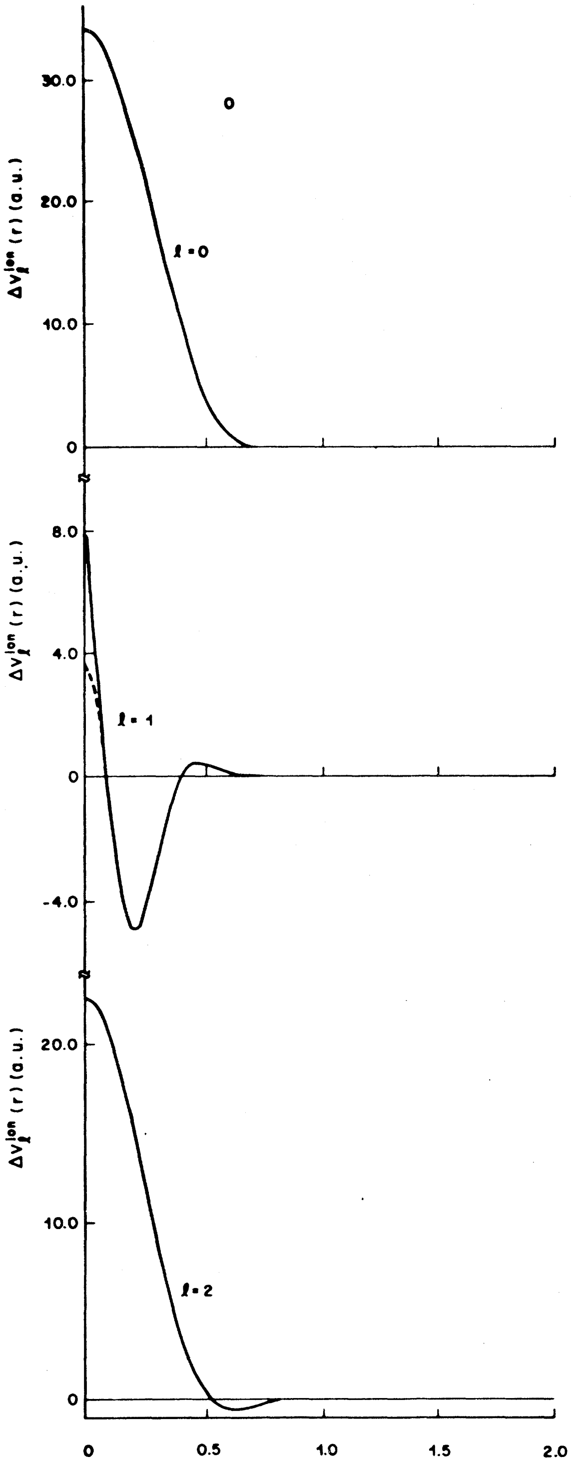

FIG. 2. Angular-momentum-dependent pseudopotential components $\Delta\hat{V}_l^{\rm ion}(r)$ for oxygen. $\Delta V_l^{\mathrm{ion}(r)} = \hat{V}_l^{\rm ion}(r) - \hat{V}^{\rm core}(r)$. Numerical potentials are given by the full lines, the analytical fits by the dashed lines.

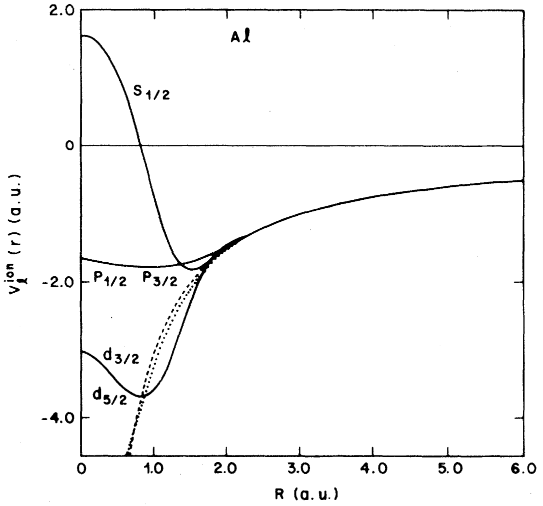

FIG. 3. Ion-core pseudopotentials for aluminum. Conventions as in Fig. 1.

III. EXAMPLES OF REPRESENTATIVE PSEUDOPOTENTIALS

In this section we present some illustrative examples of pseudopotential behavior. Figure 1 shows the ion-core potentials ($l = 0,1,2$) for oxygen. The nonlocality or l dependence is strong since only s valence electrons experience orthogonality repulsion in the core region. The dashed curve corresponds to $-Z_v/r$. Spin-orbit splitting is smaller than the chosen threshold value of 0.05 eV and only one potential $\hat{V}_{l\pm 1/2}^{\rm ion}$ for both $j = l \pm \frac{1}{2}$ is shown. Fitted and original numerical potentials cannot be distinguished on the scale of the plot.

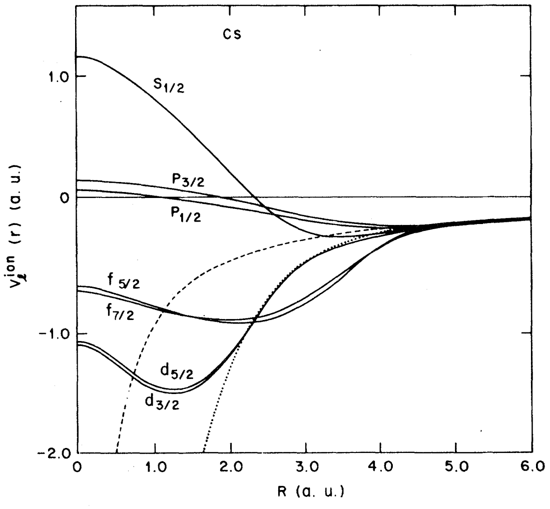

FIG. 4. Ion-core pseudopotentials for cesium. Conventions as in Fig. 1.

Figure 2 shows the nonlocal differences $\Delta \hat{V}_l^{\text{ion}}$ for oxygen as defined in Eq. (2.20) and as fitted to the Gaussian-type series.

A weakly l-dependent example is shown in Fig. 3 for Al. The remaining weak nonlocality is a consequence of optimizing the quality of the pseudo-wave-functions, i.e., minimizing the range (r_{cj}) of nonlocality. Relaxing this constraint from a range of ~ 2.5 a.u. (present case) to ~ 3.0 a.u. decreases the l dependence dramatically. The Al potentials are representative for "free-electron"-like *s-p* materials in the upper right-hand side of the Periodic Table.

In Fig. 4 we show an extreme example of a large alkali atom, Cs. The pseudopotentials are weak but long range. Spin-orbit splitting effects give rise to different potentials for different values $j = l \pm \frac{1}{2}$. Cs exhibits shallow (~ -13.6 eV) $5p$ "core" electrons. The charge density due to these electrons extends to ~ 5 a.u. as is illustrated by the large difference in the $-Z_v/r$ potential (dashed curve) and $\hat{V}^{\text{core}}(r)$ (dotted curve). In spite of this large core radius, core polarization and exchange nonlinearity effects are relatively small since the valence states ($6s, 6p^*, 5d^*, 4f^*$, etc.) are also spatially rather extended and core overlap is small. This is in contrast to the rare-earth series which begins with La only two atomic numbers higher than Cs. As mentioned in Sec. II for rare-earth elements even $5s$ and $5p$ "core states" are strongly polarized by $4f$ valence excitations.

Figure 5 shows the ion-core pseudopotentials for Au. The $5d$ electrons experience a strongly attractive potential. This potential, however, is considerably less attractive than for $3d$ or $4d$ transition or noble elements due to increased orthogonality effects. Strong spin-orbit-splitting effects are present with decreasing amplitude for p, d, and f electrons. The Au valence wave functions are illustrated in Fig. 6. The $6s$ and $5d$ wave functions are calculated from the atomic ground state ($5d^{10}6s^1$) while the $6p$ and $5f$ states are obtained from excited states, respectively (Table II). Only the $j = l - \frac{1}{2}$ spin-orbit components are shown. The multishell behavior, typical for transition- noble-, and rare-earth elements is clearly visible.

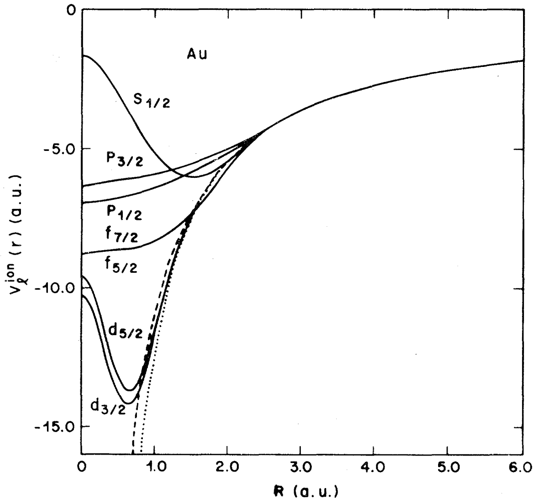

FIG. 5. Ion-core pseudopotentials for gold. Conventions as in Fig. 1.

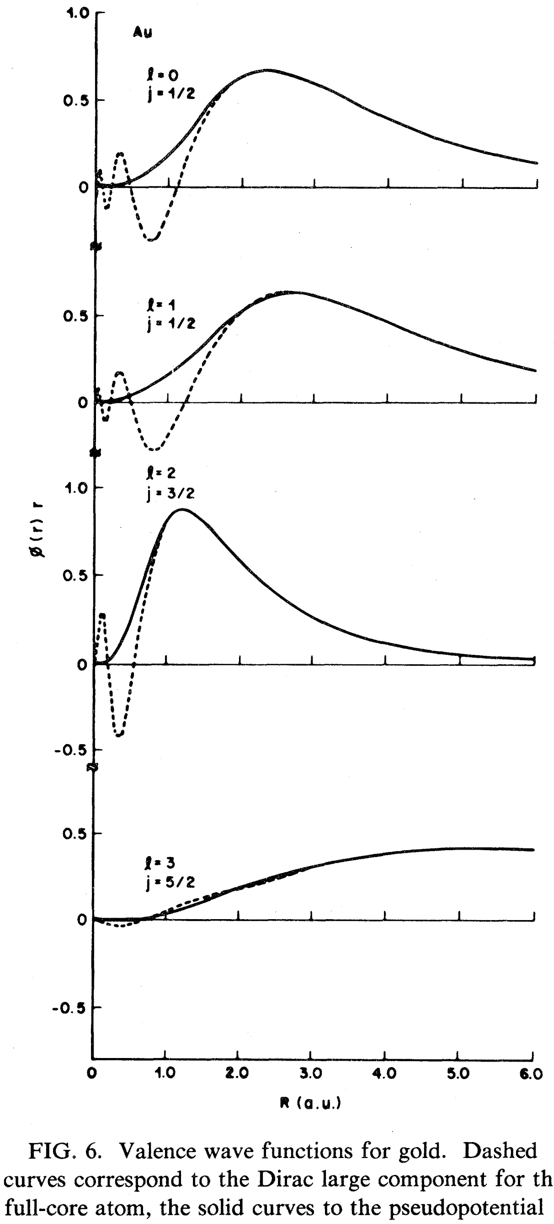

FIG. 6. Valence wave functions for gold. Dashed curves correspond to the Dirac large component for the full-core atom, the solid curves to the pseudopotential (see Fig. 5) atom.

TABLE IV. Pseudopotential parameters for atoms hydrogen through plutonium. Use of the table is explained in detail in Sec. IV in the text.

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
H	1	1	core	16.22	5.55		1.1924	-0.1924				
			0	17.08	23.54	25.42	0.0950	-0.0842	-0.0443	-0.0519	0.0084	0.0122
			1	1.71	3.86	8.08	-0.2475	-0.2727	-0.0301	-0.0094	-0.0291	0.0018
			2	2.44	3.30	4.47	-0.6887	0.0913	-0.1809	-0.0881	-0.0541	0.0058
He	2	2	core	56.23	19.24		1.1998	-0.1998				
			0	65.16	80.72	89.81	0.1418	-0.1252	-0.0670	-0.0749	0.0110	0.0166
			1	7.89	22.12	25.92	-0.5936	-0.2780	0.0535	0.1278	0.0246	0.0124
			2	0.93	15.09	23.06	-1.1044	-0.6780	0.0847	0.2954	-0.0699	0.0057
Li	3	1	core	1.84	0.73		2.9081	-1.9081				
			0	1.10	1.23	1.42	-1.4520	0.2543	0.0381	0.0581	-0.0004	-0.0114
			1	2.48	7.47	8.20	-0.0046	-0.1402	0.1055	0.1259	0.0241	0.0122
			2	0.33	0.46	0.62	-0.6347	-0.5406	-0.1712	-0.0055	-0.0300	0.0316
Be	4	2	core	2.61	1.00		1.5280	-0.5280				
			0	2.20	2.46	2.74	-1.5794	0.4081	0.0459	0.0746	-0.0007	-0.0157
			1	2.45	15.31	24.62	0.5140	-0.0694	-0.0457	-0.1549	-0.0300	0.0033
			2	1.14	1.31	1.47	-0.5444	-0.3612	-0.0488	-0.0664	0.0129	0.0156
B	5	3	core	6.21	2.47		1.6546	-0.6546				
			0	3.85	4.24	4.78	-2.1425	0.4462	0.0505	0.0894	0.0031	-0.0166
			1	2.71	2.98	7.48	0.2076	0.0707	-0.1583	0.0919	-0.0411	0.0048
			2	1.97	2.46	2.77	-0.8961	-0.5528	-0.0688	-0.0508	-0.0069	0.0226
C	6	4	core	9.28	3.69		1.5222	-0.5222				
			0	5.99	6.75	7.84	-2.4586	0.5262	0.0468	0.0913	0.0037	-0.0171
			1	4.31	4.74	11.92	0.2520	0.0952	-0.1687	0.1009	-0.0447	0.0046
			2	2.97	3.63	3.97	-0.9890	-0.6244	-0.1027	-0.0602	0.0118	0.0223
N	7	5	core	12.87	5.12		1.4504	-0.4504				
			0	7.70	9.13	11.46	-2.7030	0.4479	0.0930	0.1109	-0.0006	-0.0208
			1	6.47	7.12	17.92	0.3085	0.1260	-0.1754	0.1091	-0.0483	0.0050
			2	4.15	4.95	5.36	-1.1252	-0.6889	-0.1081	-0.0669	0.0147	0.0292
O	8	6	core	18.09	7.19		1.4224	-0.4224				
			0	11.13	13.29	16.72	-3.0282	0.5619	0.0579	0.1023	0.0040	-0.0187
			1	9.31	10.24	26.07	0.3311	0.1360	-0.1867	0.1150	-0.0504	0.0051
			2	5.87	7.12	8.05	-1.2035	-0.7542	-0.1158	-0.0806	0.0128	0.0274
F	9	7	core	23.78	9.45		1.3974	-0.3974				
			0	14.86	17.23	20.40	-3.2328	0.6759	0.0344	0.1089	0.0108	-0.0196
			1	13.00	14.30	36.72	0.3796	0.1601	-0.1932	0.1203	-0.0524	0.0054
			2	7.78	9.02	10.17	-1.3425	-0.8033	-0.1176	-0.0850	0.0047	0.0285
			so 1	15.51	22.39	28.43	-0.0044	-0.0008	0.0002	0.0000	0.0000	0.0000
Ne	10	8	core	29.13	11.58		1.3711	-0.3711				
			0	17.61	20.97	26.47	-3.4264	0.6156	0.0747	0.1241	0.0070	-0.0226
			1	16.05	17.66	45.22	0.4077	0.1726	-0.2057	0.1283	-0.0560	0.0054
			2	9.17	11.32	12.33	-1.4102	-0.8951	-0.1337	-0.0911	0.0255	0.0450
			so 1	17.64	25.73	34.05	-0.0056	-0.0013	0.0002	0.0000	0.0000	0.0000
Na	11	1	core	1.71	0.50		5.1815	-4.1815				
			0	0.99	1.10	1.24	-2.4718	0.3334	0.0619	0.0890	-0.0014	-0.0123
			1	0.51	0.65	0.84	-1.6202	-0.4908	-0.0861	0.0375	-0.0161	0.0070
			2	0.38	0.55	0.73	-0.9415	-0.9710	-0.2336	-0.0593	-0.0228	0.0455

TABLE IV. *(Continued.)*

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Mg	12	2	core	2.04	0.81		3.5602	-2.5602				
			0	1.38	1.49	1.81	-2.8667	0.4554	0.0723	0.0876	-0.0015	-0.0142
			1	0.82	1.29	1.60	-1.9343	-0.2867	-0.0215	0.0264	0.0097	0.0038
			2	0.47	0.66	0.88	-1.1475	-1.0778	-0.3055	-0.0719	-0.0330	0.0588
Al	13	3	core	1.77	0.70		1.7905	-0.7905				
			0	1.92	2.10	2.39	-2.6670	0.7075	0.0251	0.0608	-0.0134	-0.0161
			1	0.82	1.13	1.51	-1.5706	-0.2352	0.0327	0.0262	-0.0090	-0.0047
			2	1.36	1.59	1.77	-0.2574	-0.5358	-0.0668	-0.1835	0.0187	0.0551
Si	14	4	core	2.16	0.86		1.6054	-0.6054				
			0	2.48	2.81	3.09	-3.0575	0.8096	0.0012	0.0511	-0.0217	-0.0128
			1	1.24	1.60	2.12	-1.7966	-0.0986	0.0424	0.0284	-0.0030	-0.0039
			2	1.89	2.22	2.48	-0.1817	-0.5634	-0.0944	-0.2168	0.0215	0.0588
P	15	5	core	2.59	1.03		1.4995	-0.4995				
			0	2.82	3.21	4.19	-3.3940	0.7363	0.0787	0.0639	-0.0318	-0.0103
			1	1.83	2.15	2.51	-2.0001	0.0851	0.0377	0.0271	-0.0008	-0.0044
			2	2.39	2.78	3.16	-0.1719	-0.6077	-0.1112	-0.2485	0.0206	0.0634
			so 1	0.43	0.53	0.70	-0.0073	-0.0042	-0.0008	-0.0011	0.0003	-0.0016
S	16	6	core	2.99	1.19		1.4261	-0.4261				
			0	3.37	3.71	4.69	-3.6230	0.8028	0.1087	0.0697	-0.0439	-0.0062
			1	2.09	2.67	3.51	-2.1440	0.0083	0.0601	0.0318	-0.0038	-0.0053
			2	2.97	3.48	3.97	-0.1018	-0.6482	-0.1307	-0.2799	0.0200	0.0672
			so 1	0.54	0.66	0.87	-0.0090	-0.0051	-0.0011	-0.0013	0.0003	-0.0020
Cl	17	7	core	3.48	1.38		1.3860	-0.3860				
			0	4.94	9.61	15.05	-3.6651	1.2609	-0.5528	-0.3237	0.0368	0.0150
			1	2.41	3.16	4.73	-2.3089	-0.0556	0.0784	0.0357	-0.0080	-0.0060
			2	4.04	4.83	5.40	0.0968	-0.6838	-0.1482	-0.3090	0.0218	0.0735
			so 1	0.70	0.86	1.10	-0.0112	-0.0059	-0.0010	-0.0015	0.0005	-0.0020
Ar	18	8	core	3.99	1.59		1.3622	-0.3622				
			0	4.67	5.28	6.26	-4.1009	0.9478	0.1062	0.0805	-0.0524	-0.0079
			1	2.91	3.69	6.16	-2.4688	-0.0363	0.0854	0.0374	-0.0108	-0.0067
			2	5.10	5.92	6.62	0.1771	-0.7316	-0.1536	-0.3351	0.0117	0.0742
			so 1	0.90	1.10	1.45	-0.0139	-0.0068	-0.0008	-0.0016	0.0009	-0.0018
K	19	1	core	1.42	0.26		6.3140	-5.3140				
			0	0.58	0.64	0.71	-3.9287	0.2938	-0.0613	0.1062	0.0000	-0.0092
			1	0.39	0.56	0.73	-3.2276	-0.4254	-0.1754	0.0803	0.0067	0.0111
			2	2.84	3.12	55.36	2.0774	-0.7044	-0.1248	-0.3174	-0.0802	-0.0004
Ca	20	2	core	1.61	0.45		4.8360	-3.8360				
			0	0.75	1.19	2.08	-4.7576	0.3179	-0.1286	0.0279	0.0520	0.0054
			1	0.67	2.23	2.99	-4.1513	0.0156	-0.1494	-0.2563	-0.0404	-0.0179
			2	6.92	24.35	86.59	3.0392	-1.0190	0.2634	0.4961	-0.0295	0.0089
Sc	21	3	core	3.96	0.69		3.7703	-2.7703				
			0	0.93	1.25	1.65	-6.0205	-0.3209	-0.4627	0.1373	0.0055	0.0174
			1	0.72	1.08	1.20	-5.0131	-0.9627	-0.7049	0.1062	-0.0850	0.0803
			2	5.01	5.96	6.78	2.3518	0.4640	-0.3980	0.2076	-0.1778	0.0562

TABLE IV. (*Continued.*)

atom	Z_a	Z_v		L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Ti	22	4		core	4.68	0.94		3.3889	-2.3889				
				0	1.10	1.43	1.88	-6.4327	-0.3723	-0.5592	0.1547	-0.0074	0.0191
				1	0.85	1.28	1.42	-5.3910	-1.1136	-0.8023	0.1263	-0.1034	0.0851
				2	4.47	2.03	14.24	2.2908	-0.9185	0.4398	-0.5087	-0.1470	0.3404
			so	1	0.22	0.30	0.36	-0.0202	-0.0054	0.0011	-0.0007	0.0005	-0.0004
V	23	5		core	5.14	1.11		2.9680	-1.9680				
				0	1.23	1.54	1.97	-6.6485	-0.3951	-0.5795	0.1797	-0.0151	0.0176
				1	1.03	1.33	1.43	-5.5539	-0.9047	-0.8758	0.1629	-0.1369	0.0810
				2	4.60	3.28	17.66	2.4040	-1.2280	0.4141	-0.4851	-0.2405	0.3451
			so	1	0.57	1.30	1.36	-0.0221	0.0064	-0.0025	-0.0011	-0.0001	0.0000
			so	2	9.12	12.58	16.56	-0.0074	-0.0022	0.0011	-0.0004	0.0000	0.0002
Cr	24	6		core	5.19	1.37		2.8897	-1.8897				
				0	1.24	1.52	1.92	-6.5839	-0.7164	-0.6117	0.2379	-0.0291	0.0185
				1	0.89	1.33	1.67	-5.4905	-1.6271	-0.9456	0.2477	-0.1257	0.1132
				2	1.42	14.49	13.04	1.3296	2.4992	0.6775	0.2743	0.3172	0.1432
			so	1	0.23	0.34	0.45	-0.0237	-0.0091	0.0010	-0.0011	0.0012	-0.0005
			so	2	9.86	13.42	18.09	-0.0084	-0.0026	0.0013	-0.0005	0.0000	0.0002
Mn	25	7		core	6.03	1.63		2.7024	-1.7024				
				0	1.39	1.81	2.42	-7.0281	-0.8509	-0.6464	0.2240	-0.0292	0.0157
				1	1.17	1.64	1.77	-5.7836	-1.3330	-0.9789	0.2018	-0.1250	0.1188
				2	1.73	16.13	16.75	1.3989	2.5937	-0.6073	0.2667	-0.3079	0.1595
			so	1	0.26	0.37	0.47	-0.0261	-0.0094	0.0011	-0.0015	0.0013	-0.0006
			so	2	12.01	16.16	20.96	-0.0097	-0.0027	0.0012	-0.0005	0.0000	0.0002
Fe	26	8		core	6.51	1.91		2.6179	-1.6179				
				0	1.67	2.06	2.33	-7.2356	-0.5601	-0.6868	0.2287	-0.0271	0.0198
				1	1.22	1.77	1.96	-5.8685	-1.5627	-1.0392	0.2321	-0.1459	0.1258
				2	1.95	20.17	19.00	1.4849	2.7562	0.7649	0.2481	0.2996	0.1639
			so	1	0.28	0.40	0.51	-0.0283	-0.0104	0.0012	-0.0018	0.0015	-0.0007
			so	2	15.25	23.70	30.81	-0.0108	-0.0023	0.0009	0.0000	-0.0001	0.0001
Co	27	9		core	6.95	2.38		2.7407	-1.7407				
				0	1.67	2.15	2.82	-7.3964	-1.0257	-0.7633	0.2532	-0.0369	0.0198
				1	0.98	6.55	9.51	-5.5862	-2.7886	0.6251	0.2217	-0.1988	-0.0636
				2	2.41	23.76	18.38	1.5732	2.6419	0.8724	0.3015	0.3376	0.1447
			so	1	0.25	0.32	0.41	-0.0273	-0.0124	-0.0008	-0.0022	0.0021	-0.0019
			so	2	11.21	13.48	15.68	-0.0103	-0.0048	-0.0012	0.0000	0.0001	-0.0001
Ni	28	10		core	7.60	2.74		2.6949	-1.6949				
				0	1.80	2.38	3.17	-7.5612	-1.1512	-0.8213	0.2546	-0.0351	0.0228
				1	1.18	2.10	2.59	-5.8322	-2.4306	-1.2453	0.2729	-0.1929	0.1633
				2	2.53	23.55	26.60	1.5867	2.9229	-0.6560	0.2811	-0.2986	0.1867
			so	1	0.51	1.29	1.50	-0.0324	0.0022	0.0034	0.0025	-0.0008	-0.0003
			so	2	18.01	24.17	31.75	-0.0155	-0.0044	0.0016	-0.0008	0.0001	0.0002
Cu	29	11		core	7.59	3.02		2.6959	-1.6959				
				0	1.75	2.32	3.09	-7.2915	-1.4275	-0.8717	0.3180	-0.0558	0.0289
				1	1.25	7.80	10.93	-5.8592	-2.6799	0.6113	0.1380	-0.2028	-0.0691
				2	2.78	25.70	27.47	1.7433	3.0657	-0.7516	0.2519	-0.2938	0.1973
			so	1	0.54	1.44	1.73	-0.0347	0.0022	0.0035	0.0029	-0.0008	-0.0003
			so	2	19.55	28.16	37.61	-0.0158	-0.0042	0.0012	-0.0004	0.0000	0.0001

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Zn	30	12	core	8.78	3.49		2.6313	-1.6313				
			0	2.11	2.80	3.67	-7.8453	-1.2476	-0.9016	0.2734	-0.0392	0.0280
			1	1.38	2.54	3.12	-6.0406	-2.6215	-1.3062	0.2663	-0.2050	0.1599
			2	3.09	32.58	30.83	1.7225	3.1083	0.9207	0.2519	0.2946	0.1898
			so 1	0.58	1.48	1.72	-0.0374	0.0024	0.0041	0.0029	-0.0009	-0.0004
			so 2	16.48	18.18	25.99	-0.0165	-0.0077	-0.0025	0.0000	0.0001	-0.0001
Ga	31	3	core	2.01	0.80		4.0433	-3.0433				
			0	2.01	2.23	2.59	-3.9018	0.8835	0.0370	0.1642	0.0385	-0.0110
			1	1.23	1.71	2.29	-2.9715	0.0100	0.0161	0.0992	0.0525	0.0134
			2	1.10	1.30	1.48	-3.1017	-0.1879	0.0293	-0.0140	-0.0692	-0.0181
			so 1	0.34	0.45	0.61	-0.0369	-0.0168	0.0001	-0.0043	0.0031	-0.0032
Ge	32	4	core	2.28	0.91		3.1110	-2.1110				
			0	2.22	2.45	2.87	-4.2628	0.8653	0.0826	0.1446	0.0039	-0.0226
			1	1.79	2.29	2.72	-3.2382	0.5131	-0.1044	0.0547	0.0545	0.0175
			2	1.42	1.53	2.07	-3.2171	0.0215	0.0052	-0.0495	-0.0816	-0.0175
			so 1	0.48	0.69	0.88	-0.0487	-0.0181	0.0025	-0.0040	0.0026	-0.0021
As	33	5	core	2.60	1.03		2.6218	-1.6218				
			0	2.41	2.77	3.52	-4.7162	0.7952	0.1146	0.1326	-0.0152	-0.0269
			1	1.74	1.92	2.42	-3.7141	0.1877	0.0987	0.0830	-0.0171	-0.0106
			2	1.67	1.93	2.22	-3.3845	0.0948	-0.0020	-0.0478	-0.0789	-0.0227
			so 1	0.67	1.10	1.37	-0.0624	-0.0173	0.0054	-0.0023	0.0012	-0.0014
Se	34	6	core	2.88	1.14		2.2934	-1.2934				
			0	2.64	3.16	4.27	-5.1201	0.7585	0.1318	0.1236	-0.0295	-0.0280
			1	2.04	2.30	2.83	-4.0006	0.3139	0.0941	0.0789	-0.0179	-0.0122
			2	1.90	2.32	2.59	-3.5118	0.1192	-0.0001	-0.0485	-0.0758	-0.0224
			so 1	0.78	1.22	1.51	-0.0715	-0.0191	0.0048	-0.0021	0.0004	-0.0017
Br	35	7	core	3.20	1.27		2.1007	-1.1007				
			0	3.07	3.66	4.89	-5.5059	0.9501	0.0931	0.1101	-0.0322	-0.0279
			1	2.37	2.76	3.29	-4.3404	0.4232	0.0832	0.0741	-0.0192	-0.0121
			2	2.26	2.66	2.97	-3.6741	0.2350	-0.0095	-0.0527	-0.0789	-0.0247
			so 1	0.91	1.53	1.90	-0.0806	-0.0191	0.0064	-0.0009	-0.0005	-0.0018
Kr	36	8	core	3.49	1.39		1.9478	-0.9478				
			0	3.45	3.99	4.73	-5.6969	1.1088	0.0608	0.1088	-0.0277	-0.0306
			1	2.70	3.28	3.97	-4.6594	0.5027	0.0713	0.0671	-0.0210	-0.0113
			2	2.62	3.05	3.45	-3.8018	0.3188	-0.0171	-0.0609	-0.0845	-0.0267
			so 1	0.66	0.73	0.93	-0.0811	-0.0419	-0.0132	0.0041	0.0065	0.0027
			so 2	0.60	0.74	0.97	-0.0115	-0.0053	-0.0005	-0.0009	0.0009	-0.0003
Rb	37	1	core	1.37	0.21		6.8301	-5.8301				
			0	0.37	0.41	0.57	-4.6310	-0.5824	-0.0743	0.1298	-0.0764	0.0240
			1	0.35	0.54	0.71	-4.0288	-0.4084	-0.2697	0.0623	0.0150	0.0192
			2	1.05	1.17	1.52	-1.4261	-0.4197	0.2694	0.0335	-0.1074	-0.0399
			so 1	0.08	0.10	0.13	-0.0499	-0.0176	-0.0011	-0.0033	-0.0013	0.0003
Sr	38	2	core	1.52	0.33		4.8514	-3.8514				
			0	0.61	0.97	2.17	-5.4936	0.3031	-0.1884	-0.0028	0.0727	0.0092
			1	0.55	1.05	1.36	-5.0728	0.1477	-0.3858	-0.2429	-0.0199	0.0028
			2	2.02	2.26	2.56	-1.4177	-0.0612	0.1422	-0.0207	-0.1026	-0.0369
			so 1	0.15	0.23	0.28	-0.0551	0.0022	0.0085	0.0027	-0.0039	0.0009
			so 2	0.53	0.80	0.98	-0.0083	-0.0030	0.0023	-0.0014	0.0003	0.0009

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Y	39	3	core	2.06	0.49		4.1719	-3.1719				
			0	0.68	1.24	1.98	-6.3823	-0.0887	-0.2111	0.0629	0.0746	0.0165
			1	0.60	1.00	1.30	-5.8849	-0.3215	-0.4611	-0.1168	0.0024	0.0164
			2	2.18	3.16	4.15	-2.0082	-0.1203	0.1371	0.0065	-0.0849	-0.0434
			so 1	0.17	0.26	0.32	-0.0643	-0.0024	0.0092	0.0016	-0.0033	0.0009
			so 2	0.68	1.12	1.40	-0.0105	-0.0038	0.0027	-0.0010	0.0002	0.0015
Zr	40	4	core	2.28	0.66		3.9162	-2.9162				
			0	0.77	1.40	2.52	-6.8451	-0.1478	-0.2403	0.0514	0.0956	0.0188
			1	0.85	1.24	1.41	-6.3813	0.2719	-0.6486	-0.2569	-0.0428	0.0025
			2	3.15	4.09	4.77	-2.2570	0.2031	0.0482	-0.0127	-0.0734	-0.0457
			so 1	0.20	0.30	0.37	-0.0685	0.0012	0.0113	0.0020	-0.0039	0.0015
			so 2	1.09	1.48	1.60	-0.0136	-0.0024	0.0030	-0.0010	-0.0002	0.0013
Nb	41	5	core	2.41	0.82		3.7419	-2.7419				
			0	0.83	1.69	2.01	-7.2106	-0.3737	-0.1856	0.0776	0.0762	0.0198
			1	0.68	1.03	1.35	-6.6026	-0.8640	-0.5452	0.0161	0.0149	0.0212
			2	3.62	4.74	5.57	-2.3809	0.2602	0.0288	-0.0238	-0.0757	-0.0479
			so 1	0.17	0.22	0.29	-0.0799	-0.0241	0.0036	-0.0033	0.0007	0.0008
			so 2	0.72	0.78	0.92	-0.0134	-0.0081	-0.0021	0.0002	0.0026	-0.0024
Mo	42	6	core	2.57	1.02		3.8044	-2.8044				
			0	1.00	1.55	2.17	-7.6953	-0.1283	-0.3159	0.0214	0.0723	0.0147
			1	0.74	1.07	1.36	-6.8483	-1.0260	-0.6387	0.0532	0.0128	0.0265
			2	4.23	5.56	6.47	-2.5781	0.3659	-0.0090	-0.0332	-0.0734	-0.0487
			so 1	0.31	0.87	1.04	-0.0933	0.0030	0.0032	0.0037	0.0016	0.0010
			so 2	0.77	0.85	1.07	-0.0145	-0.0088	-0.0038	-0.0044	-0.0043	-0.0074
Tc	43	7	core	2.82	1.12		3.3669	-2.3669				
			0	1.32	1.66	2.02	-7.9427	0.8094	-0.5052	-0.0255	0.0585	0.0144
			1	0.81	1.16	1.53	-7.1478	-1.0526	-0.6331	0.0629	0.0107	0.0183
			2	4.26	6.15	8.18	-2.6530	0.2013	0.0267	-0.0522	-0.0924	-0.0489
			so 1	0.20	0.25	0.33	-0.0931	-0.0313	0.0012	-0.0048	0.0004	-0.0004
			so 2	0.86	0.95	1.37	-0.0167	-0.0106	-0.0044	-0.0018	-0.0011	-0.0049
Ru	44	8	core	3.00	1.19		3.0213	-2.0213				
			0	1.22	1.75	2.82	-8.1233	0.1070	-0.3548	-0.0128	0.0818	0.0112
			1	0.85	1.13	1.42	-7.2337	-1.1230	-0.6771	0.1463	-0.0095	0.0235
			2	4.85	6.67	9.05	-2.6367	0.2226	0.0153	-0.0886	-0.1145	-0.0537
			so 1	0.30	0.48	0.54	-0.1068	-0.0140	0.0086	0.0006	-0.0003	-0.0014
			so 2	1.06	1.19	1.63	-0.0195	-0.0115	-0.0039	-0.0021	-0.0004	-0.0044
Rh	45	9	core	3.21	1.28		2.7857	-1.7857				
			0	1.26	1.45	1.84	-8.3853	-0.0860	-0.3080	0.1507	0.0181	-0.0144
			1	0.86	1.17	1.57	-7.2953	-1.3860	-0.7192	0.1676	-0.0091	0.0217
			2	5.53	7.41	9.84	-2.6828	0.2534	-0.0003	-0.1204	-0.1344	-0.0573
			so 1	0.29	0.49	0.60	-0.1129	-0.0246	0.0091	-0.0006	0.0006	-0.0016
			so 2	1.47	1.65	1.84	-0.0235	-0.0108	-0.0017	-0.0021	0.0011	-0.0028
Pd	46	10	core	3.31	1.32		2.5256	-1.5256				
			0	1.39	1.58	1.90	-8.4880	0.1180	-0.2996	0.1352	0.0299	-0.0156
			1	1.02	1.18	1.36	-7.3583	-0.8758	-0.7000	0.2071	-0.0150	0.0246
			2	5.67	7.48	9.90	-2.5474	0.1555	0.0320	-0.1258	-0.1435	-0.0551
			so 1	0.29	0.50	0.61	-0.1179	-0.0320	0.0091	-0.0019	0.0016	-0.0019
			so 2	1.30	1.47	1.86	-0.0234	-0.0134	-0.0045	-0.0024	-0.0008	-0.0052

TABLE IV. (*Continued.*)

atom	Z_a	Z_v		L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Ag	47	11		core	3.53	1.41		2.3857	-1.3857				
				0	1.37	1.66	2.10	-8.6835	-0.3273	-0.2831	0.1536	0.0235	-0.0201
				1	1.06	1.23	1.38	-7.4504	-1.0227	-0.7357	0.2462	-0.0283	0.0285
				2	6.39	8.34	11.05	-2.6206	0.1731	0.0226	-0.1551	-0.1601	-0.0569
			so	1	0.29	0.49	0.64	-0.1220	-0.0388	0.0082	-0.0033	0.0025	-0.0023
			so	2	1.54	1.83	2.34	-0.0269	-0.0147	-0.0040	-0.0020	0.0004	-0.0035
Cd	48	12		core	3.91	1.56		2.3128	-1.3128				
				0	1.56	1.87	2.35	-9.1206	-0.0844	-0.3042	0.1489	0.0246	-0.0192
				1	1.16	1.38	1.54	-7.8625	-1.0969	-0.7517	0.2497	-0.0418	0.0235
				2	7.28	9.47	12.62	-2.8771	0.2491	-0.0034	-0.1818	-0.1768	-0.0596
			so	1	0.48	1.36	1.63	-0.1396	-0.0013	0.0081	0.0059	0.0018	0.0014
			so	2	1.84	2.25	2.96	-0.0308	-0.0156	-0.0035	-0.0018	0.0008	-0.0022
In	49	3		core	1.79	0.71		6.7251	-5.7251				
				0	1.09	1.66	2.96	-6.3577	-0.3902	0.2686	0.3024	0.0096	-0.0218
				1	0.99	1.24	1.53	-5.1150	-0.0727	-0.0221	0.1552	0.0791	0.0139
				2	0.64	0.72	0.91	-5.2975	-1.1521	-0.3480	0.0497	-0.0493	0.0448
			so	1	0.31	0.49	0.61	-0.1208	-0.0381	0.0107	-0.0080	0.0054	-0.0041
			so	2	0.20	0.29	0.39	-0.0203	-0.0060	-0.0001	0.0005	-0.0011	-0.0006
Sn	50	4		core	1.97	0.78		5.0086	-4.0086				
				0	1.48	1.93	2.82	-6.7306	0.4760	0.1040	0.2141	0.0298	-0.0166
				1	1.28	1.59	1.94	-5.5160	0.5027	-0.0915	0.1143	0.0767	0.0122
				2	1.06	1.32	1.49	-5.6362	0.0969	-0.2082	-0.0945	-0.0746	-0.0179
			so	1	0.41	0.77	0.94	-0.1525	-0.0372	0.0173	-0.0036	0.0036	-0.0036
			so	2	0.24	0.29	0.38	-0.0203	-0.0047	0.0005	0.0004	-0.0014	0.0011
Sb	51	5		core	2.12	0.85		4.0534	-3.0534				
				0	1.81	2.19	2.81	-7.0275	1.0069	-0.0067	0.1620	0.0202	-0.0189
				1	1.51	1.90	2.29	-5.7588	0.8375	-0.1826	0.0699	0.0757	0.0149
				2	1.27	1.42	1.57	-5.7899	0.4770	-0.2460	-0.0974	-0.0660	-0.0104
			so	1	0.57	0.93	0.97	-0.1759	-0.0179	0.0166	-0.0029	0.0038	-0.0035
			so	2	0.28	0.34	0.45	-0.0233	-0.0060	0.0004	0.0001	-0.0010	0.0007
Te	52	6		core	2.37	0.95		3.5696	-2.5696				
				0	2.07	2.46	3.08	-7.4702	1.3178	-0.0530	0.1393	0.0120	-0.0217
				1	1.61	1.84	2.40	-6.5344	0.7242	-0.0138	0.1103	0.0171	-0.0121
				2	1.48	1.85	2.15	-6.1700	0.5686	-0.2999	-0.1996	-0.1109	-0.0218
			so	1	0.48	0.63	0.84	-0.1852	-0.0511	0.0105	-0.0064	0.0008	0.0043
			so	2	0.37	0.48	0.62	-0.0194	0.0016	0.0040	0.0010	-0.0027	0.0021
I	53	7		core	2.52	1.01		3.0856	-2.0856				
				0	2.08	2.47	3.13	-7.7267	1.0339	0.0336	0.1559	-0.0105	-0.0262
				1	1.80	2.11	2.63	-6.8333	0.9051	-0.0462	0.0953	0.0055	-0.0101
				2	1.70	2.12	2.47	-6.3176	0.8200	-0.3541	-0.2309	-0.1198	-0.0235
			so	1	0.40	0.70	2.64	-0.1789	-0.0723	0.0216	-0.0041	-0.0162	0.0105
			so	2	0.42	0.58	0.77	-0.0206	0.0026	0.0051	0.0012	-0.0029	0.0021
Xe	54	8		core	2.63	1.05		2.6837	-1.6837				
				0	2.47	2.85	3.29	-7.7726	1.6588	-0.0902	0.1167	-0.0116	-0.0293
				1	1.81	2.13	2.70	-6.8951	0.7362	0.0358	0.1124	-0.0019	-0.0182
				2	1.83	2.13	2.31	-6.4148	0.9902	-0.3344	-0.1465	-0.0759	-0.0148
			so	1	0.42	0.46	0.63	-0.2015	-0.0957	-0.0233	-0.0063	0.0113	-0.0062
			so	2	0.44	0.64	0.85	-0.0302	-0.0059	0.0031	-0.0001	-0.0010	0.0007

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Cs	55	1	core	1.29	0.17		7.8924	-6.8924				
			0	0.38	0.70	0.89	-5.7556	-0.0946	-0.2594	0.0450	0.0541	0.0198
			1	0.27	0.46	0.58	-4.8922	-0.7649	-0.4366	0.0622	0.0028	0.0469
			2	0.47	0.52	0.67	-2.3938	-0.9885	-0.1755	0.0125	0.0751	0.0712
			3	0.36	0.41	0.48	-1.2582	-2.6006	-0.7020	-0.7802	0.3752	0.5278
			so 1	0.10	0.29	0.35	-0.1297	-0.0030	0.0090	0.0061	0.0007	0.0007
			so 2	0.21	0.32	0.39	-0.0156	-0.0058	0.0045	-0.0028	0.0005	0.0018
Ba	56	2	core	1.34	0.25		5.3338	-4.3338				
			0	0.57	0.72	0.87	-6.5072	0.8849	-0.4698	-0.0209	0.0373	0.0135
			1	0.46	0.72	0.90	-6.1261	0.2875	-0.6345	-0.2950	-0.0459	0.0019
			2	0.72	0.79	1.18	-2.9066	-0.6623	-0.0283	-0.0097	0.0316	0.0372
			3	4.48	11.55	17.54	10.4771	1.7858	-0.1905	0.8932	-0.2398	0.3013
			so 1	0.11	0.17	0.21	-0.1239	0.0107	0.0291	0.0021	-0.0074	0.0043
			so 2	0.33	0.57	0.69	-0.0234	-0.0073	0.0057	-0.0023	0.0000	0.0013
			so 3	13.56	19.09	20.63	-0.1393	0.0474	0.1806	-0.0608	-0.0421	0.0630
La	57	11	core	5.00	2.00		3.2494	-2.2494				
			0	2.56	2.79	3.40	-10.6839	0.0617	0.0545	0.2446	-0.0025	-0.0350
			1	2.55	3.03	3.81	-10.0938	0.4797	-0.1510	0.1225	0.0262	-0.0149
			2	1.50	2.79	3.32	-8.3844	-1.8837	-0.3217	0.0580	0.0317	0.0179
			3	4.64	9.39	30.90	5.0661	3.1425	-0.7802	0.4424	-0.5445	0.1727
			so 1	0.55	1.59	1.65	-0.2335	-0.0690	0.0741	-0.0095	-0.0049	0.0028
			so 2	0.41	0.56	0.66	-0.0249	-0.0048	0.0056	-0.0018	-0.0001	0.0025
			so 3	11.37	15.03	19.99	-0.0272	-0.0065	0.0089	-0.0016	-0.0019	0.0022
Ce	58	12	core	5.32	2.13		3.0538	-2.0538				
			0	2.95	3.31	3.97	-11.2263	0.5418	0.0074	0.2271	0.0132	-0.0307
			1	2.66	3.16	3.95	-10.2554	0.4195	-0.1454	0.1292	0.0305	-0.0182
			2	1.59	2.92	3.40	-8.5475	-1.9114	-0.3301	0.0719	0.0353	0.0202
			3	5.44	11.16	38.88	5.5065	3.1187	-0.9227	0.3404	-0.4913	0.0987
			so 1	0.70	0.80	0.90	-0.2686	-0.0795	0.0154	-0.0245	0.0205	-0.0062
			so 2	0.35	0.59	0.73	-0.0247	-0.0084	0.0059	-0.0020	0.0005	0.0030
			so 3	13.01	17.35	23.09	-0.0301	-0.0073	0.0086	-0.0015	-0.0018	0.0020
Pr	59	13	core	5.53	2.21		2.8422	-1.8422				
			0	2.95	3.45	4.30	-11.2831	0.2599	0.0406	0.2377	0.0103	-0.0342
			1	2.79	3.28	4.05	-10.2961	0.4690	-0.1388	0.1338	0.0338	-0.0204
			2	0.83	1.27	3.92	-7.3276	-4.5230	-1.9614	-0.0697	-0.0213	-0.0179
			3	5.48	12.47	36.99	5.7790	3.5755	-0.8505	0.3427	-0.6118	0.2323
			so 1	0.86	1.23	1.60	-0.2966	-0.0571	0.0381	-0.0160	-0.0014	-0.0022
			so 2	0.36	0.57	0.71	-0.0251	-0.0087	0.0060	-0.0026	0.0016	0.0033
			so 3	15.00	20.26	26.28	-0.0382	-0.0082	0.0126	-0.0020	-0.0026	0.0027
Nd	60	14	core	5.69	2.28		2.6639	-1.6639				
			0	3.07	3.62	4.52	-11.2815	0.2837	0.0442	0.2418	0.0171	-0.0362
			1	2.85	3.39	4.25	-10.3011	0.3799	-0.1090	0.1422	0.0351	-0.0236
			2	0.96	1.20	3.92	-7.6071	-4.0643	-2.0017	-0.0662	-0.0387	-0.0086
			3	5.67	13.03	39.55	5.9335	3.6380	-0.8933	0.3147	-0.6081	0.2074
			so 1	0.92	1.38	1.77	-0.3183	-0.0626	0.0371	-0.0132	-0.0033	-0.0050
			so 2	0.37	0.59	0.73	-0.0258	-0.0091	0.0062	-0.0027	0.0016	0.0036
			so 3	15.35	20.51	27.37	-0.0329	-0.0085	0.0071	-0.0014	-0.0014	0.0016

TABLE IV. (*Continued.*)

atom	Z_a	Z_v		L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Pm	61	15		core	5.91	2.36		2.5202	-1.5202				
				0	3.19	3.78	4.74	-11.3168	0.2798	0.0443	0.2472	0.0227	-0.0376
				1	2.86	3.49	4.44	-10.3472	0.1553	-0.0743	0.1570	0.0311	-0.0269
				2	0.85	1.45	3.63	-7.2561	-4.8386	-1.8650	0.0453	-0.1202	0.0318
				3	6.47	15.12	45.49	6.4562	3.6610	-0.9714	0.2472	-0.6095	0.1915
			so	1	0.96	1.45	1.85	-0.3384	-0.0732	0.0340	-0.0132	-0.0033	-0.0070
			so	2	0.39	0.65	0.79	-0.0270	-0.0092	0.0067	-0.0023	0.0004	0.0037
			so	3	17.63	23.78	31.49	-0.0386	-0.0096	0.0082	-0.0016	-0.0015	0.0017
Sm	62	16		core	6.07	2.43		2.3958	-1.3958				
				0	2.98	3.72	5.53	-11.2993	-0.4408	0.1275	0.2692	-0.0008	-0.0461
				1	2.92	3.58	4.60	-10.3462	0.0665	-0.0513	0.1662	0.0287	-0.0292
				2	0.88	1.48	3.69	-7.2714	-4.8568	-1.8893	0.0443	-0.1299	0.0379
				3	7.25	15.09	66.56	6.7894	3.4372	-1.0144	0.2271	-0.5059	-0.0087
			so	1	0.98	1.48	1.91	-0.3568	-0.0880	0.0299	-0.0145	-0.0033	-0.0087
			so	2	0.39	0.65	0.81	-0.0275	-0.0101	0.0068	-0.0027	0.0011	0.0040
			so	3	18.09	24.34	32.44	-0.0376	-0.0100	0.0066	-0.0015	-0.0012	0.0014
Eu	63	17		core	6.24	2.50		2.2886	-1.2886				
				0	3.21	4.09	5.57	-11.2950	-0.1543	0.1098	0.2707	0.0230	-0.0448
				1	2.95	3.63	4.86	-10.3464	-0.0883	-0.0251	0.1764	0.0249	-0.0323
				2	0.91	1.58	3.92	-7.2842	-4.9156	-1.8075	0.0301	-0.1176	0.0220
				3	7.15	16.06	65.19	6.8341	3.6642	-1.0629	0.1867	-0.5247	0.0133
			so	1	1.00	1.46	1.84	-0.3752	-0.1035	0.0222	-0.0170	-0.0037	-0.0103
			so	2	0.41	0.67	0.84	-0.0285	-0.0102	0.0071	-0.0027	0.0008	0.0042
			so	3	18.63	24.42	32.39	-0.0351	-0.0100	0.0037	-0.0013	-0.0004	0.0008
Gd	64	18		core	6.47	2.59		2.2076	-1.2076				
				0	3.23	4.13	6.14	-11.3219	-0.3734	0.1301	0.2828	0.0210	-0.0494
				1	3.09	3.78	4.94	-10.3903	-0.0394	-0.0334	0.1793	0.0281	-0.0326
				2	0.94	1.44	3.72	-7.3243	-4.8653	-2.1397	0.0450	-0.1612	0.0740
				3	6.09	20.42	52.53	6.6458	4.7028	-1.2897	-0.0164	-0.6041	0.2209
			so	1	1.09	1.63	2.03	-0.3951	-0.0976	0.0279	-0.0153	-0.0022	-0.0122
			so	2	0.50	0.73	0.77	-0.0305	-0.0069	0.0078	-0.0025	-0.0003	0.0041
			so	3	21.53	28.93	38.31	-0.0443	-0.0115	0.0068	-0.0015	-0.0011	0.0014
Tb	65	19		core	7.15	2.86		2.2267	-1.2267				
				0	4.01	4.85	6.06	-12.1597	0.5455	-0.0178	0.2425	0.0331	-0.0375
				1	3.78	4.86	5.79	-11.0516	0.7319	-0.2260	0.1016	0.0552	-0.0174
				2	0.89	1.13	4.80	-7.3381	-5.1014	-3.1648	-0.2815	-0.0193	-0.0042
				3	8.09	19.92	63.65	6.9653	3.8278	-1.1642	0.1398	-0.5686	0.0998
			so	1	1.41	1.81	1.93	-0.3912	-0.0063	0.0578	-0.0148	-0.0044	-0.0012
			so	2	0.41	0.61	0.72	-0.0281	-0.0099	0.0075	-0.0033	0.0019	0.0057
			so	3	22.20	29.71	38.86	-0.0484	-0.0120	0.0095	-0.0020	-0.0016	0.0019
Dy	66	20		core	7.34	2.94		2.1510	-1.1510				
				0	3.94	4.90	6.48	-12.1853	0.1544	0.0476	0.2623	0.0186	-0.0420
				1	3.60	4.46	6.43	-11.0914	0.1925	-0.0897	0.1503	0.0384	-0.0288
				2	0.98	1.07	4.95	-7.5499	-4.8079	-3.2512	-0.3080	-0.0226	-0.0046
				3	8.61	19.67	77.81	7.1684	3.7722	-1.1300	0.1562	-0.5380	0.0147
			so	1	1.29	1.99	2.49	-0.4123	-0.0485	0.0612	-0.0107	-0.0066	-0.0044
			so	2	0.49	0.64	0.69	-0.0302	-0.0074	0.0079	-0.0028	0.0009	0.0063
			so	3	22.54	30.35	40.40	-0.0418	-0.0123	0.0028	-0.0011	-0.0003	0.0005

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Ho	67	21	core	7.61	3.04		2.0909	-1.0909				
			0	4.30	5.13	6.43	-12.2311	0.5302	-0.0108	0.2540	0.0334	-0.0391
			1	3.74	4.54	6.51	-11.1537	0.1971	-0.0920	0.1570	0.0362	-0.0296
			2	1.00	1.12	4.98	-7.5630	-4.9238	-3.2952	-0.2738	-0.0489	0.0187
			3	9.47	22.29	67.95	7.6062	3.8647	-1.0828	0.1853	-0.6586	0.1766
			so 1	1.39	1.97	2.37	-0.4390	-0.0516	0.0543	-0.0134	-0.0056	-0.0054
			so 2	0.46	0.63	0.73	-0.0302	-0.0094	0.0081	-0.0039	0.0021	0.0061
			so 3	26.02	34.97	46.35	-0.0529	-0.0141	0.0064	-0.0017	-0.0009	0.0012
Er	68	22	core	7.81	3.12		2.0304	-1.0304				
			0	4.43	5.33	6.72	-12.2358	0.5076	-0.0062	0.2585	0.0377	-0.0401
			1	4.07	4.86	6.27	-11.1562	0.5467	-0.1428	0.1454	0.0442	-0.0260
			2	1.03	1.13	4.91	-7.5853	-4.9303	-3.3638	-0.2337	-0.0844	0.0554
			3	10.49	22.24	96.01	7.9047	3.6124	-1.1072	0.1830	-0.5547	-0.0141
			so 1	1.30	1.95	2.51	-0.4587	-0.0952	0.0492	-0.0166	-0.0052	-0.0060
			so 2	0.47	0.65	0.75	-0.0311	-0.0098	0.0084	-0.0041	0.0022	0.0064
			so 3	26.84	36.06	47.83	-0.0523	-0.0144	0.0047	-0.0014	-0.0006	0.0008
Tm	69	23	core	8.00	3.20		1.9772	-0.9772				
			0	4.33	5.37	7.25	-12.2384	0.0973	0.0615	0.2781	0.0234	-0.0452
			1	4.16	5.01	6.32	-11.1663	0.4813	-0.1266	0.1557	0.0407	-0.0272
			2	0.99	1.09	4.76	-7.4010	-5.0757	-3.6580	-0.2274	-0.1009	0.1168
			3	10.70	23.01	97.41	8.0188	3.7007	-1.1219	0.1746	-0.5675	-0.0096
			so 1	1.63	2.12	2.44	-0.4907	-0.0433	0.0484	-0.0127	-0.0049	-0.0093
			so 2	0.46	0.82	1.03	-0.0329	-0.0119	0.0088	-0.0014	-0.0036	0.0052
			so 3	27.19	36.08	47.95	-0.0507	-0.0151	0.0022	-0.0013	0.0000	0.0004
Yb	70	24	core	8.21	3.28		1.9271	-0.9271				
			0	4.75	5.66	7.29	-12.2213	0.5562	-0.0038	0.2658	0.0464	-0.0411
			1	4.28	5.16	6.51	-11.1769	0.4612	-0.1191	0.1603	0.0419	-0.0283
			2	0.92	1.01	5.25	-7.1961	-5.2544	-4.0282	-0.4326	-0.0233	0.0352
			3	10.84	23.34	104.93	8.1067	3.8237	-1.1214	0.1763	-0.5767	-0.0296
			so 1	1.80	2.35	2.52	-0.5165	-0.0274	0.0481	-0.0093	-0.0027	-0.0100
			so 2	0.39	0.59	0.75	-0.0296	-0.0137	0.0082	-0.0043	0.0049	0.0083
			so 3	28.40	38.60	53.04	-0.0513	-0.0151	0.0015	-0.0009	0.0000	0.0002
Lu	71	25	core	8.50	3.40		1.8919	-0.8919				
			0	4.14	5.46	8.81	-12.2748	-0.7498	0.1571	0.3173	0.0005	-0.0580
			1	4.37	5.26	6.65	-11.2713	0.3629	-0.0966	0.1760	0.0399	-0.0307
			2	1.43	2.07	5.11	-8.1746	-4.8216	-2.0022	0.0534	-0.1323	0.0657
			3	10.00	27.95	77.78	8.1099	4.6874	-1.1615	0.0700	-0.7321	0.2595
			so 1	1.43	2.17	2.78	-0.5342	-0.1358	0.0406	-0.0209	-0.0045	-0.0146
			so 2	0.73	1.03	1.14	-0.0448	-0.0103	0.0103	-0.0043	0.0016	0.0049
			so 3	32.21	44.08	58.94	-0.0613	-0.0177	0.0028	-0.0013	-0.0001	0.0004
Hf	72	4	core	2.02	0.80		5.8921	-4.8921				
			0	0.96	1.28	1.51	-7.5055	0.1785	-0.2739	0.0967	0.0822	0.0337
			1	0.47	0.87	1.30	-6.3572	-2.0326	-0.5975	0.1046	0.0384	0.0356
			2	1.48	1.66	2.10	-3.1747	-0.7669	0.0457	-0.0085	0.0513	0.0490
			3	1.04	1.17	1.33	-4.8138	-1.0321	0.2355	0.0761	-0.0860	-0.0208
			so 1	0.17	0.26	0.32	-0.2748	-0.0769	0.0173	-0.0104	0.0076	-0.0054
			so 2	0.76	1.09	1.17	-0.0462	-0.0101	0.0113	-0.0049	0.0004	0.0047

TABLE IV. *(Continued.)*

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Ta	73	5	core	2.16	0.86		4.7264	-3.7264				
			0	0.68	0.75	1.35	-7.7044	-1.6658	-0.3376	0.1727	-0.0935	0.0128
			1	0.63	0.94	1.21	-6.8198	-1.2014	-0.6058	0.0729	0.0285	0.0385
			2	1.65	1.82	2.53	-3.2040	-0.6699	0.0252	-0.0195	0.0403	0.0407
			3	1.02	1.19	1.47	-4.8229	-1.2430	0.1775	0.0635	-0.0915	-0.0207
			so 1	0.18	0.30	0.39	-0.2984	-0.0938	0.0193	-0.0086	0.0068	-0.0057
			so 2	0.76	1.24	1.49	-0.0512	-0.0161	0.0115	-0.0045	0.0016	0.0051
W	74	6	core	2.26	0.90		3.9028	-2.9028				
			0	0.70	0.77	1.38	-7.7271	-1.7108	-0.3426	0.1751	-0.0995	0.0111
			1	0.64	0.95	1.22	-6.8405	-1.2895	-0.6084	0.1061	0.0304	0.0404
			2	1.90	2.32	2.60	-3.1992	-0.4925	0.0550	-0.0235	0.0222	0.0360
			3	1.07	1.21	1.45	-4.8452	-1.2223	0.1783	0.0535	-0.0999	-0.0256
			so 1	0.19	0.29	0.36	-0.3033	-0.0960	0.0159	-0.0132	0.0103	-0.0074
			so 2	0.56	0.63	0.75	-0.0503	-0.0304	-0.0130	-0.0144	-0.0142	-0.0248
Re	75	7	core	2.44	0.98		3.5075	-2.5075				
			0	0.80	0.88	1.26	-8.2984	-1.5845	-0.2659	0.1969	-0.1164	0.0271
			1	0.84	1.03	1.17	-7.3294	-0.5431	-0.6469	0.0843	0.0255	0.0401
			2	3.49	4.52	5.24	-3.3902	0.6188	-0.1286	-0.0317	-0.0240	-0.0112
			3	1.14	1.25	1.46	-5.0854	-1.2739	0.1765	0.0644	-0.1049	-0.0289
			so 1	0.22	0.33	0.40	-0.3363	-0.0973	0.0171	-0.0116	0.0087	-0.0086
			so 2	0.63	0.70	0.91	-0.0573	-0.0336	-0.0163	-0.0188	-0.0200	-0.0266
Os	76	8	core	2.47	0.99		2.9996	-1.9996				
			0	0.82	0.91	1.24	-8.2345	-1.5905	-0.2208	0.1894	-0.1200	0.0269
			1	0.73	1.05	1.37	-7.1957	-1.2059	-0.5669	0.1161	0.0402	0.0300
			2	3.20	4.02	4.94	-3.2781	0.3440	-0.0168	-0.0203	-0.0415	-0.0116
			3	1.02	1.19	1.41	-5.0871	-1.6048	0.1234	0.0652	-0.1268	-0.0371
			so 1	0.23	0.35	0.43	-0.3415	-0.0994	0.0206	-0.0140	0.0115	-0.0067
			so 2	0.61	0.69	0.91	-0.0576	-0.0369	-0.0180	-0.0148	-0.0181	-0.0267
Ir	77	9	core	2.67	1.07		2.8089	-1.8089				
			0	1.06	1.16	1.39	-8.9278	-0.7827	-0.0945	0.2077	-0.0766	0.0004
			1	0.84	1.12	1.23	-7.4725	-0.9830	-0.6357	0.1348	0.0252	0.0400
			2	3.26	4.26	5.63	-3.5581	0.2703	-0.0036	-0.0238	-0.0415	-0.0083
			3	1.07	1.22	1.41	-5.3733	-1.7325	0.0969	0.0796	-0.1406	-0.0410
			so 1	0.55	1.27	1.36	-0.3470	0.0921	-0.0279	-0.0111	-0.0032	-0.0019
			so 2	0.73	0.82	1.21	-0.0669	-0.0401	-0.0160	-0.0117	-0.0082	-0.0200
Pt	78	10	core	2.71	1.08		2.5166	-1.5166				
			0	1.14	1.25	1.44	-8.8888	-0.5626	-0.0692	0.2058	-0.0575	-0.0091
			1	0.96	1.08	1.34	-7.7003	-0.5239	-0.5936	0.1341	0.0364	0.0254
			2	3.23	4.09	5.46	-3.4567	0.1513	0.0239	-0.0393	-0.0516	-0.0071
			3	0.97	1.14	1.37	-5.4558	-2.0590	-0.0027	0.0952	-0.1650	-0.0438
			so 1	0.26	0.40	0.49	-0.3813	-0.1176	0.0202	-0.0154	0.0116	-0.0094
			so 2	0.75	0.84	1.13	-0.0680	-0.0405	-0.0179	-0.0165	-0.0161	-0.0259
Au	79	11	core	2.85	1.14		2.3778	-1.3778				
			0	1.09	1.24	1.62	-8.9867	-1.0964	-0.1164	0.2108	-0.0732	-0.0077
			1	1.02	1.12	1.34	-7.8473	-0.5246	-0.6230	0.1483	0.0363	0.0278
			2	3.34	3.78	4.97	-3.6440	0.0850	0.0286	-0.0597	-0.0456	0.0047
			3	1.03	1.17	1.39	-5.6797	-2.0821	-0.0032	0.1156	-0.1733	-0.0507
			so 1	0.26	0.39	0.49	-0.3833	-0.1289	0.0164	-0.0189	0.0144	-0.0110
			so 2	0.89	1.04	1.39	-0.0791	-0.0452	-0.0148	-0.0113	-0.0058	-0.0191

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Hg	80	12	core	2.99	1.20		2.2533	-1.2533				
			0	1.24	1.41	1.84	-9.5486	-0.8291	-0.0650	0.2058	-0.0641	-0.0092
			1	1.02	1.12	1.40	-7.9485	-0.7733	-0.6648	0.1799	0.0346	0.0315
			2	3.33	3.79	5.37	-3.7392	-0.0139	0.0408	-0.0636	-0.0453	0.0064
			3	0.94	1.07	1.18	-5.8931	-2.5065	-0.2075	0.1636	-0.2383	-0.0339
			so 1	0.66	1.52	1.63	-0.3943	0.1059	-0.0317	-0.0117	-0.0036	-0.0023
			so 2	0.89	1.00	1.39	-0.0796	-0.0457	-0.0193	-0.0181	-0.0157	-0.0257
Tl	81	3	core	1.77	0.59		6.7158	-5.7158				
			0	1.24	1.89	5.07	-7.6582	-0.0300	0.1161	0.3351	0.0637	-0.0059
			1	0.71	0.96	1.30	-5.8681	-1.0109	0.0245	0.2286	0.0178	-0.0129
			2	0.70	0.81	1.04	-6.0798	-0.8199	-0.5486	-0.1761	0.0331	0.1048
			3	0.91	1.09	1.21	-4.1125	-1.3267	0.4578	0.1868	-0.0910	-0.0456
			so 1	0.31	0.52	0.62	-0.3984	-0.1040	0.0451	-0.0222	0.0174	-0.0109
			so 2	0.20	0.24	0.32	0.0288	0.0753	0.0435	0.0094	-0.0219	0.0369
Pb	82	4	core	1.92	0.76		6.5444	-5.5444				
			0	1.40	1.98	3.57	-8.3628	0.1094	0.1191	0.3305	0.0557	0.0032
			1	0.95	1.21	1.77	-6.9590	-0.5127	0.0637	0.2131	0.0485	-0.0143
			2	0.79	0.91	1.20	-6.8182	-0.8903	-0.6033	-0.1888	0.0154	0.0916
			3	1.35	1.62	1.82	-4.0362	-1.0178	0.5641	0.1487	-0.1291	-0.0624
			so 1	0.45	0.71	0.82	-0.5058	-0.0654	0.0487	-0.0128	0.0136	-0.0117
			so 2	0.24	0.30	0.40	0.0257	0.0759	0.0376	0.0130	-0.0275	0.0245
Bi	83	5	core	2.03	0.81		5.2104	-4.2104				
			0	1.62	2.16	3.24	-8.6521	0.5682	0.0727	0.2679	0.0221	-0.0041
			1	1.23	1.48	1.75	-7.2503	0.3928	-0.0127	0.1712	0.0669	-0.0059
			2	0.92	1.04	1.34	-7.0492	-0.4597	-0.5518	-0.2095	0.0055	0.0813
			3	1.70	1.92	2.19	-3.6420	-0.7705	0.5327	0.0841	-0.1722	-0.0752
			so 1	0.47	0.77	0.89	-0.5574	-0.0931	0.0509	-0.0114	0.0107	-0.0147
			so 2	0.28	0.34	0.45	0.0246	0.0777	0.0401	0.0112	-0.0261	0.0260
Po	84	6	core	2.17	0.87		4.4190	-3.4190				
			0	1.90	2.72	3.20	-8.8296	1.2562	-0.0868	0.1922	0.0340	-0.0101
			1	1.46	1.82	2.27	-7.6222	0.9054	-0.1548	0.1081	0.0857	0.0076
			2	1.03	1.17	1.51	-7.3062	-0.2355	-0.5527	-0.2228	0.0158	0.0829
			3	2.28	2.58	2.99	-3.0770	-0.5522	0.4418	0.0114	-0.1948	-0.0717
			so 1	0.46	0.77	0.96	-0.6012	-0.1455	0.0494	-0.0116	0.0019	-0.0156
			so 2	0.31	0.40	0.52	0.0263	0.0854	0.0441	0.0114	-0.0277	0.0277
At	85	7	core	2.29	0.92		3.8179	-2.8179				
			0	1.94	2.25	2.85	-9.1942	0.9723	0.0808	0.2203	-0.0377	-0.0100
			1	1.70	2.13	2.67	-7.9335	1.3792	-0.3076	0.0369	0.0789	0.0139
			2	1.20	1.42	1.78	-7.4567	0.1638	-0.5722	-0.3036	-0.0089	0.0768
			3	3.37	3.81	4.33	-2.2899	-0.3680	0.2809	-0.1026	-0.2173	-0.0672
			so 1	0.40	0.51	0.72	-0.6197	-0.2427	-0.0158	-0.0265	0.0068	-0.0022
			so 2	0.35	0.46	0.60	0.0338	0.0977	0.0488	0.0138	-0.0318	0.0304
			so 3	0.96	1.47	1.85	-0.0207	-0.0058	0.0114	-0.0050	-0.0015	0.0046
Rn	86	8	core	2.45	0.98		3.4235	-2.4235				
			0	2.28	2.66	3.34	-9.2586	1.8254	-0.0335	0.1692	-0.0066	-0.0247
			1	2.11	2.58	2.80	-8.2305	2.1388	-0.6641	-0.0823	0.0514	0.0221
			2	1.39	1.61	1.99	-7.6190	0.5216	-0.6703	-0.3719	-0.0121	0.0857
			3	4.35	6.11	11.37	-1.8307	-0.7487	0.1902	-0.2562	-0.3020	-0.0472
			so 1	0.40	0.44	0.48	-0.6370	-0.2736	-0.0112	0.0834	0.1677	0.0721
			so 2	0.40	0.52	0.67	0.0462	0.1135	0.0536	0.0175	-0.0383	0.0353
			so 3	2.13	2.85	3.04	-0.0620	-0.0072	0.0296	-0.0124	-0.0069	0.0071

TABLE IV. (*Continued.*)

atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Fr	87	1	core	1.23	0.16		8.4416	-7.4416				
			0	0.36	0.53	0.69	-5.8904	-0.1647	-0.3018	0.1280	0.0584	0.0342
			1	0.16	0.31	0.96	-4.8581	-1.9964	-0.6630	0.0699	0.0869	0.0008
			2	0.36	0.40	0.63	-3.0529	-1.2715	-0.2513	0.0931	0.0451	0.0666
			3	0.38	0.43	0.52	-3.0166	-1.8140	0.5796	0.4211	-0.1318	-0.0554
			so 1	0.06	0.09	0.11	-0.3418	-0.1079	0.0164	-0.0148	0.0090	-0.0102
			so 2	0.17	0.27	0.33	-0.0454	-0.0141	0.0121	-0.0057	0.0001	0.0035
Ra	88	2	core	0.99	0.24		6.1114	-5.1114				
			0	0.49	0.63	0.74	-6.6907	0.5888	-0.2960	0.0687	0.0641	0.0304
			1	0.29	0.44	0.56	-6.0767	-0.6269	-0.4742	0.0163	0.0270	0.0352
			2	0.50	0.55	1.36	-3.4169	-0.8443	-0.0162	0.0274	0.0222	0.0217
			3	4.09	4.68	5.19	2.2350	-2.4528	0.9112	0.1423	-0.0204	0.0303
			so 1	0.13	0.28	0.32	-0.4357	0.0239	0.0183	0.0086	0.0045	0.0032
			so 2	0.19	0.24	0.31	-0.0583	-0.0278	0.0011	-0.0084	0.0076	0.0001
			so 3	1.45	2.17	2.74	-0.0441	-0.0127	0.0412	-0.0203	-0.0025	0.0205
Ac	89	3	core	1.49	0.31		4.7270	-3.7270				
			0	0.54	0.77	1.02	-8.2168	0.0920	-0.3962	0.0779	0.0604	0.0275
			1	0.25	0.43	1.28	-6.9513	-2.1603	-0.8600	-0.0054	0.1271	0.0022
			2	0.56	0.62	1.23	-4.4657	-1.3359	-0.1864	0.0158	0.0018	0.0184
			3	5.40	6.13	6.91	1.3312	-2.5472	0.8208	0.0024	0.0587	0.1169
			so 1	0.15	0.31	0.33	-0.4745	0.0254	0.0224	0.0063	0.0042	0.0039
			so 2	0.17	0.19	0.25	-0.0590	-0.0361	-0.0133	-0.0101	-0.0071	-0.0220
			so 3	1.84	2.26	2.98	-0.0409	-0.0195	-0.0022	-0.0031	0.0029	-0.0010
Th	90	4	core	1.59	0.40		4.3902	-3.3902				
			0	0.62	0.77	1.35	-9.0342	0.2160	-0.4277	0.0541	0.0790	0.0243
			1	0.44	0.48	0.55	-8.4035	-0.5210	-0.8289	0.2778	-0.0169	0.0888
			2	0.71	0.78	1.39	-5.1907	-1.1444	-0.0440	0.0631	0.0061	0.0126
			3	6.10	6.99	7.92	0.9203	-2.4893	0.8255	-0.0430	0.0225	0.1112
			so 1	0.13	0.25	0.33	-0.4753	0.0100	0.0973	0.0201	-0.0170	0.0018
			so 2	0.23	0.27	0.36	-0.0754	-0.0409	-0.0109	-0.0118	-0.0029	-0.0174
			so 3	2.08	2.55	3.36	-0.0449	-0.0206	-0.0025	-0.0029	0.0026	-0.0010
Pa	91	5	core	2.06	0.45		3.8349	-2.8349				
			0	0.56	0.80	1.07	-9.5369	-1.1466	-0.5565	0.2043	0.0460	0.0300
			1	0.56	0.66	0.75	-9.4357	-0.2689	-1.1084	0.0661	-0.0646	0.0446
			2	0.65	0.73	0.94	-5.8109	-2.0532	-0.3147	0.1394	-0.0207	0.0288
			3	7.31	8.53	11.54	0.2527	-2.0863	0.8840	0.0351	-0.1739	0.1578
			so 1	0.15	0.29	0.38	-0.4599	0.0881	0.1202	0.0314	-0.0267	0.0042
			so 2	0.20	0.23	0.29	-0.0656	-0.0390	-0.0133	-0.0131	-0.0080	-0.0240
			so 3	1.80	4.20	11.43	-0.0460	-0.0306	-0.0002	-0.0012	-0.0008	0.0012
U	92	6	core	2.08	0.50		3.5183	-2.5183				
			0	0.60	0.76	1.06	-9.6565	-1.0562	-0.6184	0.2244	0.0435	0.0270
			1	0.52	0.62	0.70	-9.5702	-0.9102	-1.1087	0.2426	-0.0947	0.0639
			2	0.66	0.75	0.86	-5.8926	-2.2312	-0.3447	0.1552	-0.0291	0.0317
			3	7.27	8.62	12.50	0.3088	-2.0827	0.8200	0.0050	-0.1939	0.1305
			so 1	0.16	0.30	0.39	-0.5079	0.0599	0.1053	0.0283	-0.0202	0.0011
			so 2	0.20	0.22	0.29	-0.0656	-0.0414	-0.0128	-0.0018	0.0019	-0.0199
			so 3	1.84	2.15	2.34	-0.0490	-0.0311	-0.0134	0.0041	-0.0002	-0.0007

TABLE IV. (*Continued.*)

atom	Z_a	Z_v		L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Np	93	7		core	2.72	0.60		3.5099	-2.5099				
				0	0.62	0.91	1.17	-10.4153	-2.0222	-0.9596	0.3000	-0.0075	0.0778
				1	0.50	0.82	1.03	-10.1156	-2.4063	-1.4851	0.1011	-0.1430	0.1141
				2	0.83	0.92	1.06	-7.3516	-2.4042	-0.3586	0.2802	-0.0396	0.0466
				3	10.07	13.17	17.30	-1.1744	-1.4501	0.9518	0.2863	-0.2900	-0.1468
			so	1	0.14	0.21	0.26	-0.5832	-0.0985	0.0640	-0.0126	0.0003	-0.0065
			so	2	0.30	0.35	0.43	-0.0880	-0.0427	-0.0064	-0.0079	0.0083	-0.0076
			so	3	2.07	3.81	15.69	-0.0504	-0.0319	-0.0044	-0.0027	-0.0004	0.0014
Pu	94	8		core	2.76	0.62		3.1671	-2.1671				
				0	0.59	0.94	1.25	-10.2963	-2.4940	-0.9263	0.3236	-0.0057	0.0676
				1	0.59	0.83	0.92	-10.2746	-1.6981	-1.5450	0.1102	-0.1780	0.1118
				2	0.93	1.02	3.49	-7.5476	-2.1067	-0.3096	0.0732	0.1190	-0.0164
				3	10.23	13.36	17.64	-1.0461	-1.4985	0.9908	0.3096	-0.2679	-0.1382
			so	1	0.15	0.23	0.27	-0.6093	-0.0944	0.0628	-0.0075	0.0029	-0.0069
			so	2	0.33	0.41	0.54	-0.0987	-0.0487	-0.0066	-0.0083	0.0087	-0.0075
			so	3	2.12	4.64	13.73	-0.0520	-0.0335	-0.0004	-0.0019	-0.0005	0.0010

TABLE V. Silicon $l=0,1,2$ pseudopotentials on a real space mesh as derived from the coefficients in Table IV. All units in a.u.

R	$l=0$	$l=1$	$l=2$
0.0	2.2360	−2.4805	−4.6679
0.1	2.1929	−2.4857	−4.7191
0.2	2.0610	−2.5009	−4.8554
0.3	1.8327	−2.5258	−5.0375
0.4	1.5002	−2.5588	−5.2249
0.5	1.0598	−2.5971	−5.3899
0.6	0.5170	−2.6366	−5.5125
0.7	−0.1078	−2.6724	−5.5657
0.8	−0.7729	−2.7000	−5.5108
0.9	−1.4175	−2.7158	−5.3107
1.0	−1.9743	−2.7175	−4.9543
1.1	−2.3894	−2.7037	−4.4725
1.2	−2.6395	−2.6737	−3.9321
1.3	−2.7354	−2.6275	−3.4117
1.4	−2.7133	−2.5655	−2.9730
1.5	−2.6181	−2.4895	−2.6438
1.6	−2.4893	−2.4018	−2.4182
1.7	−2.3534	−2.3058	−2.2690
1.8	−2.2245	−2.2054	−2.1641
1.9	−2.1071	−2.1043	−2.0782
2.0	−2.0016	−2.0057	−1.9966
2.1	−1.9062	−1.9119	−1.9143
2.2	−1.8196	−1.8244	−1.8319
2.3	−1.7403	−1.7436	−1.7518
2.4	−1.6676	−1.6695	−1.6762
2.5	−1.6007	−1.6016	−1.6063

IV. PERIODIC TABLE OF PSEUDOPOTENTIALS AND A GUIDE TO USE IT

In Table IV we compile the parameters necessary to synthesize ion-core pseudopotentials for the elements hydrogen through plutonium. Each element is identified by its symbol, its atomic number, and its valence charge (i.e., the number of electrons chosen to be treated as valence electrons in the ground state) in columns 1−3. Column 4, denoted L, indicates the particular potential, i.e., $\hat{V}^{\rm core}(r)$ [Eq. (2.21)] or $l=0,1,2,3$ for $\Delta\hat{V}_l^{\rm ion}(r)$ [Eq. (2.22)] or the spin-orbit potential $\Delta\hat{V}_l^{\rm so}$ for $l=1,2,3$. The nonlinear-fit parameters $\alpha_i^{\rm core}$, $i=1,2$, or α_i, $i=1,2,3$ are given in columns 5, 6, 7, respectively, in atomic units, i.e., $a_{\rm Bohr}^{-2}$. The linear coefficients $c_i^{\rm core}$, $i=1,2$ or C_i, $i=1,6$ defined through Eqs. (2.21), (2.22), and (2.25) are given in columns 8−13 in *atomic units,* i.e., 27.2116 eV. This table is computer generated to eliminate transcription errors.

For the potentials $\Delta\hat{V}_l^{\rm ion}(r)$ and $\Delta\hat{V}_l^{\rm so}(r)$, but *not* for $\hat{V}^{\rm core}(r)$, the coefficients C_i have to be transformed by an inverse orthogonality transformation [Eq. (2.28)] to obtain the linear coefficients A_i and A_{i+3} to be used in Eq. (2.22). This transformation either necessitates the inversion of a 6×6 matrix Q_{il} defined recursively in Eq. (2.26) based on the analytical overlap matrix S_{il} and the subsequent use of Eq. (2.28) or a direct solution of the linear equation system Eq. (2.25). Due to the inherent nonorthogonality of the fitting functions $\Phi_i(r)$ [Eq. (2.27)] high numerical accuracy, i.e., double precision on a 32-bit computer or single precision on a 64-bit computer, is required for the computation. We found that computer routines performing least-squares approximations to the solutions of the linear equation system (2.25) gave the most stable answers. To provide the user with an independent check on the accuracy of his own inverse orthogonalization procedure we list in Table V the $l=0,1,2$ ion-core pseudopotentials of Si. The results are obtained with single-precision routines on a CRAY-1 computer.

V. AMBIGUOUS CASES

The separation into a well-isolated core and into a valence shell is not always unambiguously possible. It may, therefore, be convenient in certain cases to have a choice of pseudopotentials available with more or less expanded valence shells. In the following we briefly discuss four typical cases of ambiguous behavior.

(i) The heavy I*A* alkali atoms show relatively shallow $(n-1)p$ core shells. The eigenvalues of $3p$, $4p$, $5p$, and $6p$ for K, Rb, Cs, and Fr are, respectively, −18.8, −16.3, −13.6, and −10.9 eV. Accordingly, as discussed in the case of Cs in Sec. III, the spatial extent of these p functions can be large. However, the overlap with excited ns, p, or d states in the valence shell is small due to strong orthogonality effects. Test calculations on Cs atoms and also for the semiconducting compound CsAu[25] show that errors due to $5p$ core polarization and exchange nonlinearities amount to less than 0.2 eV. We therefore present only pseudopotentials for I*A* atoms with the $(n-1)p$ shell included in the core (Table IV). Note that the $l=0$ potentials are derived from the neutral ground-state configurations to minimize transferability errors due to the nonlinear charge dependence of the exchange-correlation potential.

(ii) The group II*B* atoms Zn, Cd, and Hg immediately following the transition and noble elements, show $3d$, $4d$, or $5d$ electrons with eigenvalues of −10.3, 11.6, and 9.5 eV, respectively, which put them into an ambiguous situation. While they are corelike in the elemental metals, they may fall within the valence-band region in compounds and play a role in bonding. In Table IV we present potentials for these atoms which include the $(n-1)d$ electrons into the valence shell, just as the preceding noble elements. The resulting d potentials are very strong and may lead to difficulties for certain applications, e.g., where plane-wave expansions are used. We therefore present in Table VI alternative potentials which assume the $(n-1)d$ shell to be included in the core. These potentials are smooth and only weakly l dependent, similar to those for the neighboring group-III atoms.

(iii) As mentioned in the Sec. II the rare-earth elements La through Lu show extremely localized $4f$ wave functions ($r_{\rm max}\approx 0.5$ a.u.). This wave-function "collapse" which occurs between Ba and Ce is well documented in the literature and leads to a number of curious effects.[52] From the point of view of pseudopotentials the collapse places the $4f$ charge not only well inside the $5d$,$6s$ valence electrons, but also inside the $5s$ and $5p$ core electrons ($r_{\rm max}\approx 1.5$ a.u.) with eigenvalues at about −50 and −30 eV, respectively. The result is that excitations involving changes in the $4f$ occupation will alter the screening for the $5s$ and $5p$ electrons dramatically, such that a frozen core is no longer a good approximation. We therefore included the $5s$ and $5p$ electrons into the valence shell for all rare-

TABLE VI. Pseudopotential parameters for the atoms Zn, Cd, and Hg which were constructed *without* 3*d*, 4*d*, and 5*d* electrons, respectively, in the valence shell. Table is to be used as Table IV.

Atom	Z_a	Z_v	L	α_1	α_2	α_3	c_1	c_2	c_3	c_4	c_5	c_6
Zn	30	2	core	2.51	0.75		6.1450	-5.1450				
			0	1.52	2.06	7.62	-4.8062	0.0120	0.1552	0.2804	0.0430	-0.0133
			1	1.02	1.13	1.28	-3.6742	-0.6484	0.0752	0.1188	-0.0161	0.0266
			2	0.52	0.72	1.30	-2.9756	-1.8692	-0.5538	-0.0237	-0.0331	0.0837
			so 1	0.46	0.70	0.86	-0.0443	-0.0129	0.0030	-0.0017	0.0011	-0.0007
Cd	48	2	core	2.19	0.60		8.5331	-7.5331				
			0	1.20	1.32	1.44	-7.0001	-0.1006	0.2713	0.1929	-0.0352	0.0675
			1	0.81	0.90	1.01	-5.8819	-1.0097	0.0258	0.2006	-0.0416	0.0287
			2	0.52	0.59	1.22	-5.1735	-2.0936	-0.7797	0.0217	-0.0286	0.0880
			so 1	0.38	0.64	0.79	-0.1366	-0.0241	0.0114	0.0014	-0.0009	-0.0022
Hg	80	2	core	2.09	0.51		8.9048	-7.9048				
			0	1.10	1.21	1.33	-7.7678	-0.5451	0.2376	0.2223	-0.0396	0.0890
			1	0.79	0.87	0.99	-6.7759	-0.9047	0.0686	0.2543	-0.0154	0.0443
			2	0.44	0.48	1.32	-5.9821	-2.3858	-1.0888	-0.0186	-0.0040	0.0730
			3	0.41	0.51	0.97	-3.7143	-3.3954	-0.9322	0.0991	-0.1363	0.1480
			so 1	0.36	0.66	0.81	-0.4562	-0.0772	0.0455	0.0065	-0.0017	-0.0066
			so 2	0.15	0.18	0.23	-0.0218	0.0191	0.0150	0.0076	-0.0078	0.0174

earth atom potentials given in Table IV. This decreases the error for a 4*f*-5*d* excitation associated with the frozen-core approximation from 1.7 to 0.2 eV.

VI. CONCLUSIONS

We have developed a comprehensive and consistent set of pseudopotentials using guidelines which have been found through extensive testing to maximize transferability. Our chief goal has been the publication of these potentials in a convenient form for application. A second aim was to discuss the physics of the pseudopotentials thoroughly, and explain the reasons underlying the many choices made in the development process. We anticipate that the potentials will continue to be useful in many contexts. When at some future time improved exchange-correlation density functionals or further improvements in pseudopotential formalism are developed, the results reported here on reference configurations, radii, and fitting strategy should greatly simplify the task of producing new potentials.

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