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ROOTHAAN–HARTREE–FOCK GROUND-STATE ATOMIC WAVE FUNCTIONS: SLATER-TYPE ORBITAL EXPANSIONS AND EXPECTATION VALUES FOR $Z = 2$–54

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Roothaan–Hartree–Fock orbitals expressed in a Slater-type basis are reported for the ground states of He through Xe. Energy accuracy ranges between 8 and 10 significant figures, reducing by between 21 and 2770 times the energy errors of the previous such compilation (E. Clementi and C. Roetti, Atomic Data and Nuclear Data Tables **14,** 177, 1974). For each atom, the total energy, kinetic energy, potential energy, virial ratio, electron density at the nucleus, and the Kato cusp are given together with radial expectation values $\langle r^n \rangle$ with n from -3 to 2 for each orbital, orbital energies, and orbital expansion coefficients.

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CONTENTS

INTRODUCTION

The first compilation[1] of Roothaan–Hartree–Fock (RHF) atomic wave functions constituted a major event for atomic physics and quantum chemistry. Another set of tables, offering an interesting compromise between accuracy and basis set size, was also published.[2] Eventually, Clementi and Roetti[3] produced comprehensive tables of RHF wave functions for ground and certain excited states of neutral and ionized atoms with atomic numbers 2 to 54. More than 2000 citations since their publication attest to their impact.

In 1974 the RHF method was the most accurate technique available to approximate the Hartree–Fock (HF) equations. Two years earlier, however, improved stability methods for the solution of the HF equations were developed,[4] and since the publication of Froese Fischer's book,[5] in which eight-digit numerical-HF energies and orbital expectation values for He through Rn configurations were reported, numerical HF is considered to be markedly superior to RHF.

Nevertheless, RHF wavefunctions offer some advantages over numerical ones, as they can be readily incorporated into various codes for atomic and related calculations. Numerical wave functions, instead, need to be kept on diskettes or generated as needed, and nontrivial software is required for their use.

The past decade witnessed the coming of age of orbital methods in atomic structure calculations.[6–8] The numerical-multiconfiguration-Hartree–Fock (numerical-MCHF) approach[5] became established as the method of choice, although configuration interaction (CI)[9] appeared to be more general and flexible.

The advantages of numerical MCHF come from the transparency with which both occupied and correlation orbitals are obtained by solving the MCHF equations[5] when convergence problems do not occur. In CI, on the other hand, whereas correlation orbitals can be obtained successfully[10] and automatically, with minor human intervention,[11] the inescapable need to use RHF-occupied orbitals poses severe limitations for atoms larger than Ar, as the existing compilation of RHF atomic wave functions[3] is not sufficiently accurate for spectroscopic purposes.[12] For example, energy errors are as large as 32 meV in the first transition metal series, and larger than 352 meV for elements of the second transition series.

The advantages of CI over numerical HF are the absence of MCHF equations and the orders-of-magnitude-larger CI sizes that can be accommodated. When core–valence correlations are important, as in the Ca spectrum,[13] CI optimization of core–valence orbitals can now be carried out by means of a straightforward and automated procedure while the solution of the corresponding MCHF equations is still beyond the scope of current computer codes.[14,15] However, the potential accuracy of CI will not materialize unless RHF atomic wave functions with energy errors not more than 1 meV become available. The Clementi–Roetti energy errors are between 4 and 32 meV for K through Zn, between 10 and 48 meV for Ga through Kr, and between 220 and 1658 meV for Rb through Xe. In this work we report RHF wave functions for the ground states of He through Xe with energy errors not exceeding 0.6 meV.

For each atom, the total energy, kinetic energy, potential energy, virial ratio, and electron density at the nucleus and the Kato cusp[16] are given together with radial expectation values $\langle r^n \rangle$, n from -3 to 2 for each orbital, orbital energies, and orbital expansion coefficients. This

information is most appropriate at a time when the $N = 10$ electron frontier is beginning to be pushed throughout the whole periodic table. Some classes of physical problems which would be better served by the present tables include structure and spectra of the first two transition metal series, electron scattering from atoms, negative ions beyond Ar, and fine- and hyperfine-structure calculations. The new RHF wave functions will also be useful as starting points for calculations of excited states and pseudopotentials, particularly for atoms beyond Ar, and as starting points for relativistic calculations.[17]

The Roothaan-Hartree-Fock Method

Hartree-Fock atomic wave functions are independent-particle-model approximations to the nonrelativistic Schrodinger's equation for stationary states. The use of Slater determinants accounts for the Pauli principle, and for an N-electron system the HF equations yield N Hartree-Fock spin orbitals.

In conventional Hartree-Fock calculation,[5] the spin orbitals are expressed as products of a radial function times a spherical harmonic times a spin function, the radial functions are taken to depend only on the quantum numbers n and l, and the total wave function is required to be an eigenfunction of the total orbital and spin angular momentum; the form of the spin orbitals guarantees that L_z, S_z, and parity are good quantum numbers. Conventional HF is also known as restricted HF.

RHF or analytic self-consistent-field atomic wave functions[18] are approximations to conventional HF wave functions in which the radial atomic orbitals R_{nl} are expanded as a finite superposition of primitive radial functions:

$$R_{nl} = \sum_j S_{jl} C_{jln}. \tag{1}$$

In this work, the normalized primitive basis $\{S_{jl}\}$ is taken as a Slater-type orbital (STO) set,

$$S_{jl} = N_{jl} r^{(n_{jl}-1)} \exp(-Z_{jl} r), \tag{2}$$

where N_{jl} is a normalization factor, n_{jl} is the principal quantum number, Z_{jl} is the orbital exponent, and l is the azimuthal quantum number.

The nonrelativistic atomic Hamiltonian is approximated by

$$H = \sum_a \left(-\frac{1}{2} \nabla_a^2 - \frac{Z}{r_a} \right) + \sum_{a>b} \frac{1}{r_{ab}}. \tag{3}$$

Eq. (3) may be interpreted in units of energy and length that take into account the finite mass of the atom, which we refer to as atomic units (M) in this paper. The infinite mass atomic unit of energy is modified by a factor $(1 + m/M)^{-1}$ and the atomic unit of length by a factor $(1 + m/M)$ where m is the mass of the electron and M is the nuclear mass. The use of atomic units (M) amounts to using the diagonal part of the mass polarization term, neglecting the nondiagonal part.[19] This nondiagonal part is relatively small, is very sensitive to correlation, and, in calculations beyond HF, viz., in CI calculations, is taken up as a perturbation, or even variationally.

The RHF wave function Φ is a linear combination of Slater determinants $\mathbf{D}_\alpha$ with coefficients a_α fixed for each L-S symmetry:

$$\Phi = \sum_\alpha \mathbf{D}_\alpha a_\alpha. \tag{4}$$

The a_α coefficients may be calculated by a variety of methods,[20] but they do not enter the RHF equations[21] explicitly; the RHF equations, instead, are usually expressed in terms of vector coupling coefficients[21,22] which appear in the energy expression after integration over angular coordinates. The RHF equations

$$\mathbf{F}_c\mathbf{C} = \mathbf{eSC} \tag{5a}$$

$$\mathbf{F}_o\mathbf{C} = \mathbf{eSC} \tag{5b}$$

are self-consistent-field equations obtained by minimizing the expectation value of H [Eq. (3)], taken with the trial wave function Φ, subject to the orthonormality of the radial functions with the same quantum number l. In Eqs. (5), $\mathbf{F}_c$ and $\mathbf{F}_o$ are the closed-shell and open-shell Fock matrices, respectively, $\mathbf{S}$ is the overlap matrix, $\mathbf{C}$ collects the orbital expansion coefficients C_{jln} of Eq. (2) in matrix form, and the vector $\mathbf{e}$ holds the orbital energies.

A definitive formulation and derivation of the RHF equations have been given by Roothaan and Bagus,[21] and a stimulating review is provided in Ref. 3. Efficient methods to improve the attainment of self-consistency are well discussed in the work of Carbó et al.[23]

Computational Details

The first tables of RHF atomic wave functions[1] were produced with a program designed and written by Roothaan and Bagus.[21] That program, after undergoing a translation to Fortran,[24] evolved along several paths. One version was used by Clementi and Roetti.[3] A further improved version is part of the MOTECC collection.[25] An extension for handling open f shells was used to obtain RHF atomic wave functions for atomic numbers 55 to 92.[26]

A fourth version incorporates pseudopotentials and has been effectively documented by Daudey.[27] We have used Daudey's version of the RHF program with the following modifications: (i) If a full calculation with the old program is called a macrocycle, the new program runs any number of macrocycles up to an energy convergence threshold. (ii) After each macrocycle, convergence

thresholds are reinitialized; usually, this procedure overcomes most divergence problems, as a new macrocycle uses the orbitals from the previous macrocycle. (iii) The existing Jacobi diagonalization routine was replaced by a more accurate one. Finally, a program error affecting the operator which eliminates the Lagrange multipliers between orbitals of closed and open shells was uncovered. That error did not prevent the reproduction of Clementi and Roetti's energy values to all reported figures; however, it prevented the achievement of further accuracy.

For certain pilot atoms, such as Ca, Zr, and Xe, we tested thousands of initial STO basis sets until arriving at the energy accuracies required by the physical applications mentioned above. These particular calculations took about three months on a dedicated and fully equipped IBM RS/6000 Model 520 computer. We estimate that to reproduce the results for copper, between 2 and 4 hours of Cray-YMP CPU time would be required, if as a starting point STO sets extrapolated from either our Ni or Zn wave functions were used. Seventy minutes of Cray CPU time are required to obtain the same result from an interpolation between Ni and Zn wave functions. On the other hand, a direct assault on Cu is likely to fail or require perhaps 10 times as much investment in human and computer time. For the complete tables we used approximately 2000 hours of IBM and 160 hours of Cray CPU time. Details on STO set selection are given elsewhere.[28]

Accuracy

Our results have not been mass produced but rather have been generated one by one, recalculating everything several times; viz., we carried out successive extrapolations between Ca and Xe twice back and forth. As a consequence, our energy errors follow a smooth pattern, and approximate linear dependencies in the basis sets are kept to a minimum, an essential requirement for correlation calculations beyond Hartree–Fock.

The accuracy of the total RHF energies has been discussed in Ref. 28. The energy errors increase smoothly from 0.002 microhartree in He up to 0.4 microhartree in Ar. Starting with K, the basis set is kept as small as possible, consistent with the sought energy accuracy of 1 meV (37 microhartree).

Energy errors increase from 3.4 microhartree for K up to 19 microhartree for Cu and 14 microhartree for Zn. From Ga to Kr, the necessary addition of further p-type STOs causes the energy errors to be reduced to about 8 microhartree. Beginning with Rb, with an energy error of 11 microhartree, accuracy diminishes smoothly up to Cd, where the energy error reaches its largest value, 22 microhartree. From In onward the energy errors diminish again from 18 microhartree down to 14 microhartree for Xe. If we define an improved accuracy IA as the quotient between present and past RHF energy errors, our IA relative to the energy results of Clementi and Roetti ranges between 21, for V, and 2770, for Cd.[28] Also, our RHF energies are accurate to more than eight digits, which is more accurate than the previous numerical-HF results.[5] In fact, numerical-HF results for the ground states of Cr, Nb, Mo, Ru, and Rh have just become available with the publication of Ref. 28. In all these ground states the outermost s orbital is singly occupied, and these configurations had not been calculated before by numerical HF. For Cu, Pd, and Ag, previous numerical-HF results[29] were accurate to only six figures.

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EXPLANATION OF TABLE

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

In each data block, the first row lists the element, the atomic number Z, and the configuration and term of the ground-state wave function. Complete orbital configurations are abbreviated with the corresponding noble gas symbol. For example, for silicon (Z = 14), [Ne]3s(2)3p(2) 3P means $1s^2 2s^2 2p^6 3s^2 3p^2\ ^3P$. Blocks are arranged in order of increasing Z.

The second row gives the TOTAL, KINETIC, and POTENTIAL ENERGY in atomic units (M) [1 a.u. = 27.2113961 eV and 1 a.u.(M) is 1 a.u. times $(1 + m/M)^{-1}$, where m is the electron mass and M is the nuclear mass] and the VIRIAL RATIO (=POTENTIAL ENERGY/KINETIC ENERGY, which is equal to -2 for the exact HF wave function).

The third row gives RHO at 0, the electron density ρ at the origin in atomic units (M) [1 a.u.(M) = $1/a_\mu^3$, with a_μ equal to the Bohr radius a_0 times $(1 + m/M)$] and the Kato cusp defined as $(-1/Z)d[\ln \rho(r)]/dr$ at the origin. The Kato cusp is equal to 2 a.u.(M) [1 a.u.(M) = $1/a_\mu$] for the exact HF wave function. 1s, 2p, etc., denote RHF orbitals. Below each orbital are listed

ORB.ENERGY	Orbital energy in a.u.(M)
$\langle R \rangle$	Expectation value of r in a.u.(M)
$\langle R^{**}2 \rangle$	Expectation value of r^2 in a.u.(M)
$\langle 1/R \rangle$	Expectation value of 1/r in a.u.(M)
$\langle 1/R^{**}2 \rangle$	Expectation value of $1/r^2$ in a.u.(M).
$\langle 1/R^{**}3 \rangle$	Expectation value of $1/r^3$ in a.u.(M).

The orbital expansion coefficients, C_{jln} in Eq. (1), are listed next under each RHF orbital. 1S, 2P, etc., denote Slater-type orbitals (STOs) $n_{jl}l$. Orbital exponents Z_{jl} are shown following the STO designation. The STO S_{jl} is given by

$$S_{jl} = N_{jl} r^{(n_{jl}-1)} \exp(-Z_{jl} r),$$

and the normalization constant N_{jl} is given by

$$N_{jl} = (2Z_{jl})^{[n_{jl}+1/2]}/[(2n_{jl})!]^{1/2}.$$

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

HELIUM, Z=2 1s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2.861679993	2.861681613	-5.723361606	-1.999999434

RHOat0 = 22.593709 Kato cusp = 1.999972

	1s	
ORB.ENERGY	-0.917955	
<R>	0.927272	
<R**2>	1.184820	
<1/R>	1.687283	
<1/R**2>	5.995503	
1S	1.4595	1.347900
3S	5.3244	-0.001613
2S	2.6298	-0.100506
2S	1.7504	-0.270779

LITHIUM, Z=3 1s(2)2s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-7.432726924	7.432726876	-14.86545380	-2.000000007

RHOat0 = 87.852850 Kato cusp = 2.000847

	1s	2s	
ORB.ENERGY	-2.477741	-0.196323	
<R>	0.573125	3.873661	
<R**2>	0.446803	17.738419	
<1/R>	2.685034	0.345391	
<1/R**2>	14.888309	0.435420	
1S	4.3069	0.141279	-0.022416
1S	2.4573	0.874231	-0.135791
3S	6.7850	-0.005201	0.000389
2S	7.4527	-0.002307	-0.000068
2S	1.8504	0.006985	-0.076544
2S	0.7667	-0.000305	0.340542
2S	0.6364	0.000760	0.715708

BERYLLIUM, Z=4 1s(2)2s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-14.57302313	14.57302427	-29.14604740	-1.999999922

RHOat0 = 222.35057 Kato cusp = 2.000214

	1s	2s	
ORB.ENERGY	-4.732669	-0.309269	
<R>	0.414994	2.649396	
<R**2>	0.232955	8.426147	
<1/R>	3.681877	0.522523	
<1/R**2>	27.753395	1.055640	
1S	5.7531	0.285107	-0.016378
1S	3.7156	0.474813	-0.155066
3S	9.9670	-0.001620	0.000426
3S	3.7128	0.052852	-0.059234
2S	4.4661	0.243499	-0.031925
2S	1.2919	0.000106	0.387968
2S	0.8555	-0.000032	0.685674

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

BORON, Z=5 1s(2)2s(2)2p(1) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-24.52906069	24.52906021	-49.05812090	-2.000000020

RHOat0 = 451.88988 Kato cusp = 1.999917

	1s	2s		2p
ORB.ENERGY	-7.695335	-0.494706	ORB.ENERGY	-0.309856
<R>	0.325866	1.977064	<R>	2.204757
<R**2>	0.143362	4.709128	<R**2>	6.146069
<1/R>	4.674339	0.712882	<1/R>	0.605006
<1/R**2>	44.538014	2.024473	<1/R**2>	0.529888
			<1/R**3>	0.775649

1S	7.0178	0.381607	-0.022549	2P 5.7416	0.007600
1S	3.9468	0.423958	0.321716	2P 2.6341	0.045137
3S	12.7297	-0.001316	-0.000452	2P 1.8340	0.184206
3S	2.7646	-0.000822	-0.072032	2P 1.1919	0.394754
2S	5.7420	0.237016	-0.050313	2P 0.8494	0.432795
2S	1.5436	0.001062	-0.484281		
2S	1.0802	-0.000137	-0.518986		

CARBON, Z=6 1s(2)2s(2)2p(2) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-37.68861890	37.68861825	-75.37723715	-2.000000017

RHOat0 = 800.79993 Kato cusp = 1.999509

	1s	2s		2p
ORB.ENERGY	-11.325519	-0.705627	ORB.ENERGY	-0.433341
<R>	0.268443	1.589344	<R>	1.714495
<R**2>	0.097199	3.052064	<R**2>	3.746800
<1/R>	5.664439	0.896798	<1/R>	0.783503
<1/R**2>	65.234157	3.255303	<1/R**2>	0.892066
			<1/R**3>	1.691945

1S	8.4936	0.352872	-0.071727	2P 7.0500	0.006977
1S	4.8788	0.473621	0.438307	2P 3.2275	0.070877
3S	15.4660	-0.001199	-0.000383	2P 2.1908	0.230802
2S	7.0500	0.210887	-0.091194	2P 1.4413	0.411931
2S	2.2640	0.000886	-0.393105	2P 1.0242	0.350701
2S	1.4747	0.000465	-0.579121		
2S	1.1639	-0.000119	-0.126067		

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

NITROGEN, Z=7 1s(2)2s(2)2p(3) 4S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-54.40093415	54.40093494	-108.8018691	-1.999999985

RHOat0 = 1294.1163 Kato cusp = 1.999832

	1s	2s		2p
ORB.ENERGY	-15.629060	-0.945324	ORB.ENERGY	-0.567589
<R>	0.228297	1.332277	<R>	1.409631
<R**2>	0.070265	2.149438	<R**2>	2.547642
<1/R>	6.653236	1.078176	<1/R>	0.957690
<1/R**2>	89.841896	4.753583	<1/R**2>	1.336287
			<1/R**3>	3.099879

1S	9.9051	0.354839	-0.067498	2P 8.3490	0.006323
1S	5.7429	0.472579	0.434142	2P 3.8827	0.082938
3S	17.9816	-0.001038	-0.000315	2P 2.5920	0.260147
2S	8.3087	0.208492	-0.080331	2P 1.6946	0.418361
2S	2.7611	0.001687	-0.374128	2P 1.1914	0.308272
2S	1.8223	0.000206	-0.522775		
2S	1.4191	0.000064	-0.207735		

OXYGEN, Z=8 1s(2)2s(2)2p(4) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-74.80939840	74.80940128	-149.6187997	-1.999999961

RHOat0 = 1958.2230 Kato cusp = 1.999979

	1s	2s		2p
ORB.ENERGY	-20.668657	-1.244315	ORB.ENERGY	-0.631906
<R>	0.198589	1.141964	<R>	1.232198
<R**2>	0.053146	1.581223	<R**2>	1.974976
<1/R>	7.642171	1.265272	<1/R>	1.111111
<1/R**2>	118.382497	6.591548	<1/R**2>	1.818717
			<1/R**3>	4.974380

1S	11.2970	0.360063	-0.064363	2P 9.6471	0.005626
1S	6.5966	0.466625	0.433186	2P 4.3323	0.126618
3S	20.5019	-0.000918	-0.000275	2P 2.7502	0.328966
2S	9.5546	0.208441	-0.072497	2P 1.7525	0.395422
2S	3.2482	0.002018	-0.369900	2P 1.2473	0.231788
2S	2.1608	0.000216	-0.512627		
2S	1.6411	0.000133	-0.227421		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$-54

See page 118 for Explanation of Table

FLUORINE, Z=9 1s(2)2s(2)2p(5) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-99.40934928	99.40935019	-198.8186995	-1.999999991

RHOat0 = 2816.8876 Kato cusp = 1.999963

	1s	2s		2p
ORB.ENERGY	-26.382760	-1.572535	ORB.ENERGY	-0.730018
<R>	0.175747	1.001094	<R>	1.084786
<R**2>	0.041612	1.216565	<R**2>	1.543524
<1/R>	8.630362	1.449751	<1/R>	1.271674
<1/R**2>	150.834051	8.697213	<1/R**2>	2.394771
			<1/R**3>	7.545578

1S	12.6074	0.377498	-0.058489	2P	11.0134	0.004879
1S	7.4101	0.443947	0.426450	2P	4.9962	0.130794
3S	23.2475	-0.000797	-0.000274	2P	3.1540	0.337876
2S	10.7416	0.213846	-0.063457	2P	1.9722	0.396122
2S	3.7543	0.002183	-0.358939	2P	1.3632	0.225374
2S	2.5009	0.000335	-0.516660			
2S	1.8577	0.000147	-0.239143			

NEON, Z=10 1s(2)2s(2)2p(6) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-128.5470980	128.5471001	-257.0941980	-1.999999984

RHOat0 = 3895.0667 Kato cusp = 1.999933

	1s	2s		2p
ORB.ENERGY	-32.772442	-1.930391	ORB.ENERGY	-0.850410
<R>	0.157631	0.892113	<R>	0.965273
<R**2>	0.033470	0.967082	<R**2>	1.228454
<1/R>	9.618054	1.632554	<1/R>	1.435350
<1/R**2>	187.196960	11.071475	<1/R**2>	3.058859
			<1/R**3>	10.906781

1S	13.9074	0.392290	-0.053023	2P	12.3239	0.004391
1S	8.2187	0.425817	0.419502	2P	5.6525	0.133955
3S	26.0325	-0.000702	-0.000263	2P	3.5570	0.342978
2S	11.9249	0.217206	-0.055723	2P	2.2056	0.395742
2S	4.2635	0.002300	-0.349457	2P	1.4948	0.221831
2S	2.8357	0.000463	-0.523070			
2S	2.0715	0.000147	-0.246038			

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

SODIUM, Z=11 [Ne]3s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-161.8589113	161.8589125	-323.7178237	-1.999999993

RHOat0 = 5241.9865 Kato cusp = 2.000003

	1s	2s	3s		2p
ORB.ENERGY	-40.478500	-2.797026	-0.182102	ORB.ENERGY	-1.518140
<R>	0.142858	0.779068	4.208762	<R>	0.798485
<R**2>	0.027481	0.731495	20.704809	<R**2>	0.822132
<1/R>	10.607384	1.867338	0.301399	<1/R>	1.696598
<1/R**2>	227.533756	14.453227	0.398424	<1/R**2>	4.187710
				<1/R**3>	17.005671
1S 15.3319	0.387167	0.053722	0.011568		
1S 9.0902	0.434278	-0.430794	-0.072430	2P 13.6175	0.004308
2S 13.2013	0.213027	0.053654	0.011164	2P 6.2193	0.157824
2S 4.7444	0.002205	0.347971	0.057679	2P 3.8380	0.388545
2S 3.1516	0.000627	0.608890	0.089837	2P 2.3633	0.489339
2S 2.4047	-0.000044	0.157462	0.042114	2P 1.5319	0.039759
3S 28.4273	-0.000649	0.000280	-0.000001		
3S 1.3179	0.000026	-0.000492	-0.182627		
3S 0.8911	-0.000023	0.000457	-0.471631		
3S 0.6679	0.000008	0.000016	-0.408817		

MAGNESIUM, Z=12 [Ne]3s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-199.6146361	199.6146406	-399.2292767	-1.999999978

RHOat0 = 6872.1659 Kato cusp = 2.000211

	1s	2s	3s		2p
ORB.ENERGY	-49.031735	-3.767721	-0.253052	ORB.ENERGY	-2.282225
<R>	0.130594	0.690335	3.252938	<R>	0.684998
<R**2>	0.022956	0.571084	12.418454	<R**2>	0.597695
<1/R>	11.597954	2.107821	0.399388	<1/R>	1.951690
<1/R**2>	271.847496	18.382421	0.788544	<1/R**2>	5.469817
				<1/R**3>	24.921147
1S 17.0241	0.352464	0.059265	0.016053		
1S 10.0727	0.481225	-0.447481	-0.096426	2P 14.9021	0.004178
2S 14.6751	0.198592	0.055907	0.014785	2P 6.8076	0.175692
2S 5.1514	0.002259	0.355163	0.077390	2P 4.1426	0.420054
2S 3.4870	0.000556	0.696633	0.110979	2P 2.7152	0.456246
2S 2.5249	-0.000136	0.058440	0.082870	2P 1.4623	0.012155
3S 29.9018	-0.000669	0.000283	0.000010		
3S 1.7568	0.000056	-0.001173	-0.232777		
3S 1.1659	-0.000033	0.000277	-0.494745		
3S 0.8244	0.000011	-0.000059	-0.378869		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

ALUMINIUM, Z=13 [Ne]3s(2)3p(1) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-241.8767070	241.8767064	-483.7534134	-2.000000003

RHOat0 = 8814.3490 Kato cusp = 2.000007

	1s	2s	3s		2p	3p
ORB.ENERGY	-58.501026	-4.910672	-0.393420	ORB.ENERGY	-3.218303	-0.209951
<R>	0.120258	0.620026	2.599278	<R>	0.600543	3.433889
<R**2>	0.019459	0.458897	7.890667	<R**2>	0.455357	14.006188
<1/R>	12.589248	2.349007	0.506786	<1/R>	2.205108	0.379283
<1/R**2>	320.129355	22.797434	1.359520	<1/R**2>	6.915864	0.310543
				<1/R**3>	34.939997	1.088227
1S 18.1792	0.373865	0.061165	0.020024			
1S 10.8835	0.456146	-0.460373	-0.119051	2P 14.4976	0.015480	-0.001690
2S 15.7593	0.202560	0.055062	0.017451	2P 6.6568	0.204774	-0.048903
2S 5.7600	0.001901	0.297052	0.079185	2P 4.2183	0.474317	-0.058101
2S 4.0085	0.000823	0.750997	0.130917	2P 3.0026	0.339646	-0.090680
2S 2.8676	-0.000267	0.064079	0.139113	3P 11.0822	0.024290	-0.001445
3S 33.5797	-0.000560	0.000270	0.000038	3P 1.6784	0.003529	0.234760
3S 2.1106	0.000083	-0.001972	-0.303750	3P 1.0788	-0.000204	0.496072
3S 1.3998	-0.000044	0.000614	-0.547941	3P 0.7494	0.000199	0.359277
3S 1.0003	0.000013	-0.000064	-0.285949			

SILICON, Z=14 [Ne]3s(2)3p(2) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-288.8543622	288.8543624	-577.7087246	-1.999999999

RHOat0 = 11093.598 Kato cusp = 1.999953

	1s	2s	3s		2p	3p
ORB.ENERGY	-68.812456	-6.156538	-0.539842	ORB.ENERGY	-4.256054	-0.297114
<R>	0.111431	0.562941	2.207085	<R>	0.535408	2.752216
<R**2>	0.016701	0.377257	5.676239	<R**2>	0.359681	8.980888
<1/R>	13.581150	2.590401	0.603231	<1/R>	2.456382	0.478031
<1/R**2>	372.382095	27.691054	1.997988	<1/R**2>	8.520346	0.501188
				<1/R**3>	47.269455	2.053873
1S 19.5017	0.377006	0.064222	0.023528			
1S 11.7539	0.454461	-0.472631	-0.136207	2P 15.7304	0.015661	-0.001966
2S 16.9664	0.200676	0.055383	0.019663	2P 7.2926	0.196557	-0.057175
2S 6.3693	0.001490	0.233799	0.074362	2P 4.6514	0.510448	-0.068127
2S 4.5748	0.001201	0.781919	0.122580	2P 3.3983	0.303956	-0.114298
2S 3.3712	-0.000454	0.096627	0.206180	3P 12.0786	0.025586	-0.001976
3S 36.5764	-0.000507	0.000257	0.000048	3P 2.0349	0.003153	0.263703
3S 2.4996	0.000103	-0.001832	-0.319063	3P 1.3221	0.000167	0.522698
3S 1.6627	-0.000053	0.000879	-0.562578	3P 0.9143	0.000156	0.314467
3S 1.1812	0.000013	-0.000033	-0.280471			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

PHOSPHORUS, Z=15 [Ne]3s(2)3p(3) 4S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-340.7187806	340.7187797	-681.4375603	-2.000000003

RHOat0 = 13736.907 Kato cusp = 1.999907

	1s	2s	3s		2p	3p
ORB.ENERGY	-79.969714	-7.511095	-0.696416	ORB.ENERGY	-5.400958	-0.391708
<R>	0.103805	0.515660	1.932685	<R>	0.483401	2.322712
<R**2>	0.014488	0.315921	4.347087	<R**2>	0.291798	6.389634
<1/R>	14.573553	2.831708	0.694730	<1/R>	2.706271	0.570153
<1/R**2>	428.606263	33.056704	2.712832	<1/R**2>	10.284011	0.715755
				<1/R**3>	62.146721	3.311089
1S 20.8264	0.378728	0.067068	0.026409			
1S 12.6329	0.454633	-0.483053	-0.149611	2P 20.2974	0.000934	0.000893
2S 18.1768	0.198318	0.055573	0.021237	2P 9.3161	0.158097	-0.048486
2S 6.9865	0.001102	0.172637	0.065512	2P 5.5199	0.499724	-0.088168
2S 5.1340	0.001500	0.826915	0.119933	2P 3.9517	0.389661	-0.136009
2S 3.7311	-0.000594	0.114274	0.273929	3P 15.5633	-0.004175	0.004247
3S 39.5397	-0.000464	0.000249	0.000057	3P 2.2826	0.003823	0.325638
3S 2.9558	0.000130	-0.003280	-0.321673	3P 1.4968	-0.000307	0.522331
3S 1.9407	-0.000057	0.001381	-0.583392	3P 1.0527	0.000144	0.255540
3S 1.3616	0.000011	-0.000023	-0.293770			

SULFUR, Z=16 [Ne]3s(2)3p(4) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-397.5048955	397.5048994	-795.0097949	-1.999999990

RHOat0 = 16772.672 Kato cusp = 1.999916

	1s	2s	3s		2p	3p
ORB.ENERGY	-92.004449	-9.004288	-0.879527	ORB.ENERGY	-6.682508	-0.437368
<R>	0.097151	0.475772	1.720722	<R>	0.441042	2.060717
<R**2>	0.012686	0.268530	3.443200	<R**2>	0.242088	5.065187
<1/R>	15.566448	3.073197	0.786103	<1/R>	2.954448	0.650667
<1/R**2>	488.806411	38.899462	3.534613	<1/R**2>	12.202777	0.941922
				<1/R**3>	79.777512	4.839939
1S 22.2949	0.367468	0.070509	0.028833			
1S 13.5666	0.471254	-0.492518	-0.160596	2P 22.6414	-0.000466	0.001263
2S 19.4969	0.192030	0.056472	0.022476	2P 10.4197	0.141231	-0.047039
2S 7.5145	0.000539	0.114779	0.056607	2P 6.1160	0.501894	-0.090305
2S 5.7222	0.002074	0.846899	0.107272	2P 4.4156	0.403324	-0.159888
2S 4.2264	-0.000864	0.150553	0.326955	3P 17.3448	-0.006509	0.005017
3S 42.1787	-0.000442	0.000233	0.000067	3P 2.6496	0.004375	0.341230
3S 3.3088	0.000163	-0.002483	-0.337632	3P 1.6975	0.000225	0.519259
3S 2.1707	-0.000073	0.001580	-0.602710	3P 1.1477	0.000315	0.262504
3S 1.5140	0.000014	0.000045	-0.272978			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

CHLORINE, Z=17 [Ne]3s(2)3p(5) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-459.4820719	459.4820743	-918.9641462	-1.999999995

RHOat0 = 20226.726 Kato cusp = 1.999961

	1s	2s	3s		2p	3p
ORB.ENERGY	-104.884420	-10.607480	-1.072912	ORB.ENERGY	-8.072227	-0.506400
<R>	0.091295	0.441714	1.555630	<R>	0.405715	1.842024
<R**2>	0.011200	0.231193	2.812958	<R**2>	0.204326	4.059178
<1/R>	16.559692	3.314397	0.874884	<1/R>	3.201537	0.733287
<1/R**2>	552.979453	45.207640	4.434507	<1/R**2>	14.277874	1.201129
				<1/R**3>	100.397663	6.768657
1S 23.7918	0.357615	0.072699	0.032061			
1S 14.4872	0.484997	-0.499909	-0.172436	2P 24.4396	-0.001409	0.001525
2S 20.8326	0.187615	0.056841	0.024503	2P 11.4909	0.129060	-0.045154
2S 9.4342	-0.000352	0.013158	0.018179	2P 6.6724	0.511775	-0.095725
2S 6.4160	0.002796	0.883708	0.140693	2P 4.8559	0.404231	-0.176763
2S 4.7671	-0.001073	0.214427	0.342425	3P 18.9808	-0.007959	0.005308
3S 44.4484	-0.000427	0.000223	0.000064	3P 2.9926	0.004770	0.354699
3S 3.5704	0.000168	-0.001859	-0.353160	3P 1.8970	0.000703	0.523394
3S 2.3743	-0.000089	0.002000	-0.600895	3P 1.2586	0.000479	0.257066
3S 1.6610	0.000017	0.000024	-0.254301			

ARGON, Z=18 [Ne]3s(2)3p(6) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-526.8175122	526.8175160	-1053.635028	-1.999999993

RHOat0 = 24125.995 Kato cusp = 1.999967

	1s	2s	3s		2p	3p
ORB.ENERGY	-118.610349	-12.322152	-1.277352	ORB.ENERGY	-9.571464	-0.591016
<R>	0.086104	0.412280	1.422172	<R>	0.375330	1.662954
<R**2>	0.009960	0.201226	2.350427	<R**2>	0.174342	3.310795
<1/R>	17.553229	3.555317	0.961985	<1/R>	3.449989	0.814074
<1/R**2>	621.125483	51.979437	5.414514	<1/R**2>	16.525595	1.473630
				<1/R**3>	124.380679	8.974675
1S 25.5708	0.316405	0.079148	0.035512			
1S 15.6262	0.542760	-0.507823	-0.181267	2P 26.6358	0.002436	0.001854
2S 22.3994	0.167691	0.059900	0.026500	2P 12.7337	-0.114774	-0.042064
2S 10.5300	0.000408	-0.026389	0.006280	2P 7.3041	-0.503175	-0.095603
2S 7.0534	0.002431	0.832638	0.111836	2P 5.3353	-0.427033	-0.194233
2S 5.4120	-0.000861	0.295522	0.385604	3P 20.7765	0.009669	0.005891
3S 46.7052	-0.000422	0.000217	0.000070	3P 3.3171	-0.004825	0.366141
3S 3.7982	0.000066	0.002203	-0.376901	3P 2.0947	0.000231	0.526490
3S 2.5495	-0.000061	0.001423	-0.593561	3P 1.3780	-0.000098	0.249866
3S 1.7965	0.000009	0.000186	-0.229971			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

POTASSIUM, Z=19 [Ar]4s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-599.1647831	599.1647844	-1198.329567	-1.999999998

RHOat0 = 28528.062 Kato cusp = 2.002065

	1s	2s	3s	4s
ORB.ENERGY	-133.533046	-14.489955	-1.748779	-0.147475
<R>	0.081466	0.386389	1.277058	5.243652
<R**2>	0.008913	0.176593	1.883466	31.542823
<1/R>	18.547363	3.797705	1.074858	0.236590
<1/R**2>	693.279202	59.265263	6.818406	0.295293
1S 16.9317	1.160058	-0.333245	-0.109835	0.021207
2S 23.6708	-0.107236	-0.019653	-0.009458	0.001900
2S 6.7720	0.001693	1.155997	0.451036	-0.088672
3S 20.5358	-0.079291	-0.033718	-0.016074	0.003193
3S 4.0061	-0.000214	0.018576	-0.397462	0.092956
3S 2.4110	-0.000052	0.002574	-0.569061	0.106797
4S 8.4209	-0.000393	-0.079850	0.037800	-0.009891
4S 3.7899	0.000116	-0.007017	-0.187652	0.045670
4S 1.4301	0.000008	-0.000286	-0.007578	-0.168271
4S 0.9450	-0.000005	0.000178	0.001939	-0.520283
4S 0.6607	0.000002	-0.000064	-0.000781	-0.402360

	2p	3p
ORB.ENERGY	-11.519278	-0.954422
<R>	0.349427	1.436846
<R**2>	0.150801	2.440647
<1/R>	3.697028	0.939014
<1/R**2>	18.926828	1.946475
<1/R**3>	151.814137	12.954567
2P 26.2044	0.001861	0.000437
2P 11.1009	0.366438	0.078509
2P 5.6095	0.380621	0.398893
2P 2.4374	0.002983	-0.769498
3P 8.7158	0.311226	0.016842
3P 1.9702	-0.000488	-0.404117
3P 1.3184	0.000071	-0.039862

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

CALCIUM, Z=20 [Ar]4s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-676.7581817	676.7581767	-1353.516358	-2.000000007

RHOat0 = 33430.819 Kato cusp = 2.001880

		1s	2s	3s	4s
ORB.ENERGY		-149.363724	-16.822743	-2.245375	-0.195529
<R>		0.077301	0.363504	1.159424	4.218469
<R**2>		0.008023	0.156172	1.546005	20.453178
<1/R>		19.541934	4.040857	1.188772	0.299738
<1/R**2>		769.407364	67.045590	8.399576	0.535034
1S	17.6670	1.176575	-0.341543	-0.117803	0.028125
2S	24.5295	-0.119414	-0.019904	-0.010168	0.002534
2S	7.2525	0.000730	1.150570	0.468206	-0.113880
3S	21.3493	-0.086509	-0.033142	-0.016715	0.004109
3S	3.6185	0.000185	-0.000762	-0.640251	0.179379
3S	2.6126	-0.000097	0.001467	-0.441778	0.115506
4S	8.7808	0.000145	-0.068959	0.043103	-0.014022
4S	6.0113	-0.000317	0.016219	-0.064309	0.020813
4S	1.5770	0.000021	-0.000184	-0.001947	-0.331747
4S	1.0566	-0.000015	0.000124	0.000314	-0.522462
4S	0.7584	0.000005	-0.000044	-0.000058	-0.257798

		2p	3p
ORB.ENERGY		-13.629270	-1.340706
<R>		0.326869	1.274550
<R**2>		0.131725	1.908061
<1/R>		3.944088	1.058811
<1/R**2>		21.491321	2.462364
<1/R**3>		183.014479	17.738971
2P	28.8909	0.001400	-0.000342
2P	11.9319	0.348898	-0.076856
2P	6.0967	0.406540	-0.433592
2P	2.5605	0.003420	0.877080
3P	9.4272	0.300142	-0.015449
3P	2.1782	-0.000861	0.312083
3P	1.3295	0.000083	0.020164

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

SCANDIUM, Z=21 [Ar]3d(1)4s(2) 2D

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-759.7357123	759.7356951	-1519.471407	-2.000000023

RHOat0 = 38852.665 Kato cusp = 2.001901

	1s	2s	3s	4s
ORB.ENERGY	-165.899895	-19.080617	-2.567322	-0.210108
<R>	0.073535	0.343178	1.079391	3.959716
<R**2>	0.007259	0.139111	1.339906	18.070522
<1/R>	20.537537	4.284364	1.281937	0.320317
<1/R**2>	849.570335	75.317010	9.816080	0.617022
1S	21.7237	0.929286	-0.272325	-0.095941	0.022762
2S	18.5964	0.076816	-0.165926	-0.066543	0.016069
2S	8.5331	0.001804	1.008339	0.413734	-0.100051
3S	26.6635	0.010320	-0.001551	-0.001264	0.000291
3S	6.3629	0.000323	0.085949	0.116177	-0.031040
3S	4.4087	-0.000281	-0.006473	-0.567549	0.162661
3S	2.9836	0.000073	0.002830	-0.638451	0.169417
4S	10.0558	-0.000626	0.066049	0.079945	-0.022175
4S	1.7339	-0.000024	-0.000346	-0.008505	-0.303304
4S	1.1548	0.000018	0.000234	0.002704	-0.526693
4S	0.8074	-0.000007	-0.000082	-0.000727	-0.286745

	2p	3p		3d
ORB.ENERGY	-15.668246	-1.574546	ORB.ENERGY	-0.343712
<R>	0.307067	1.174391	<R>	1.675431
<R**2>	0.116092	1.619875	<R**2>	3.634183
<1/R>	4.191507	1.152125	<1/R>	0.798980
<1/R**2>	24.224866	2.911805	<1/R**2>	0.886337
<1/R**3>	218.317138	22.409699	<1/R**3>	1.429405
2P	31.2091	0.001156	-0.000287	3D	9.8549	0.015123
2P	12.6896	0.341553	-0.074761	3D	4.8498	0.159653
2P	6.5469	0.415271	-0.457411	3D	2.9200	0.359860
2P	2.7945	0.003830	0.888499	3D	1.7389	0.434880
3P	10.0778	0.296715	-0.013956	3D	1.0594	0.199419
3P	2.3661	-0.000849	0.311816			
3P	1.4540	0.000109	0.021060			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

TITANIUM, Z=22 [Ar]3d(2)4s(2) 3F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-848.4059907	848.4059678	-1696.811958	-2.000000027

RHOat0 = 44828.283 Kato cusp = 2.001810

	1s	2s	3s	4s
ORB.ENERGY	-183.272754	-21.422910	-2.873395	-0.220787
<R>	0.070116	0.325038	1.013029	3.778855
<R**2>	0.006598	0.124734	1.180623	16.500594
<1/R>	21.533643	4.527617	1.370325	0.336131
<1/R**2>	933.739186	84.056728	11.258644	0.679622
1S 22.7314	0.931729	-0.275337	-0.098438	0.022864
2S 19.4596	0.074430	-0.169269	-0.069318	0.016391
2S 8.9861	0.001498	1.018751	0.426684	-0.101044
3S 27.9364	0.009843	-0.001341	-0.001204	0.000273
3S 6.6279	0.000199	0.082054	0.113142	-0.030640
3S 4.6765	-0.000228	-0.007982	-0.591312	0.167643
3S 3.1621	0.000055	0.003062	-0.621860	0.159930
4S 10.6755	-0.000431	0.063448	0.084353	-0.022705
4S 1.8546	-0.000019	-0.000370	-0.008255	-0.292090
4S 1.2210	0.000013	0.000236	0.002364	-0.531732
4S 0.8395	-0.000005	-0.000081	-0.000615	-0.295994

	2p	3p		3d
ORB.ENERGY	-17.791186	-1.795085	ORB.ENERGY	-0.440655
<R>	0.289587	1.093772	<R>	1.459746
<R**2>	0.103139	1.405774	<R**2>	2.737442
<1/R>	4.438401	1.239883	<1/R>	0.907419
<1/R**2>	27.117452	3.369362	<1/R**2>	1.129237
<1/R**3>	257.845159	27.542913	<1/R**3>	2.016343
2P 33.3883	0.000991	0.000249	3D 10.4755	0.016004
2P 13.4246	0.337047	0.073107	3D 5.2370	0.172840
2P 6.9860	0.419748	0.475457	3D 3.1849	0.375781
2P 3.0695	0.004328	-0.866201	3D 1.9290	0.424201
3P 10.7125	0.294936	0.013483	3D 1.1952	0.170623
3P 2.5803	-0.000789	-0.343747		
3P 1.6116	0.000126	-0.025352		

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

VANADIUM, Z=23 [Ar]3d(3)4s(2) 4F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-942.8843308	942.8842963	-1885.768627	-2.000000037

RHOat0 = 51386.879 Kato cusp = 2.001712

	1s	2s	3s	4s
ORB.ENERGY	-201.502829	-23.874650	-3.183183	-0.230578
<R>	0.067000	0.308744	0.955586	3.626288
<R**2>	0.006023	0.112497	1.050952	15.232270
<1/R>	22.530118	4.770636	1.456687	0.350652
<1/R**2>	1021.909309	93.265045	12.761267	0.738393
1S 23.7265	0.934724	-0.278303	-0.100645	0.022861
2S 20.2915	0.071260	-0.173527	-0.072332	0.016726
2S 9.4802	0.001198	1.022901	0.435733	-0.100913
3S 29.1499	0.009527	-0.001124	-0.001135	0.000256
3S 6.9463	0.000121	0.080937	0.102976	-0.028627
3S 4.9127	-0.000187	-0.008467	-0.611858	0.172058
3S 3.3257	0.000044	0.003140	-0.599875	0.147853
4S 11.2844	-0.000270	0.065688	0.090418	-0.023449
4S 1.9549	-0.000015	-0.000372	-0.007592	-0.291512
4S 1.2721	0.000011	0.000230	0.002016	-0.534471
4S 0.8656	-0.000004	-0.000078	-0.000520	-0.295890

	2p	3p		3d
ORB.ENERGY	-20.022490	-2.019223	ORB.ENERGY	-0.509619
<R>	0.274031	1.025157	<R>	1.323232
<R**2>	0.092273	1.235619	<R**2>	2.247763
<1/R>	4.684842	1.325483	<1/R>	0.998468
<1/R**2>	30.168656	3.847820	<1/R**2>	1.361091
<1/R**3>	301.826879	33.272118	<1/R**3>	2.645475
2P 35.8086	0.000832	0.000208	3D 10.9640	0.017413
2P 14.1832	0.330153	0.070957	3D 5.5057	0.198643
2P 7.4366	0.429318	0.488333	3D 3.3114	0.404320
2P 3.2971	0.004908	-0.867911	3D 2.0094	0.399309
3P 11.3721	0.290389	0.013393	3D 1.2637	0.137710
3P 2.7500	-0.000823	-0.348957		
3P 1.7235	0.000157	-0.025660		

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

CHROMIUM, Z=24 [Ar]3d(5)4s(1) 7S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1043.356368	1043.356356	-2086.712724	-2.000000011

RHOat0 = 58544.339 Kato cusp = 2.001644

	1s	2s	3s	4s
ORB.ENERGY	-220.386394	-26.209624	-3.285149	-0.222046
<R>	0.064146	0.294014	0.912445	3.675012
<R**2>	0.005520	0.101988	0.960479	15.719869
<1/R>	23.527254	5.013676	1.529583	0.346492
<1/R**2>	1114.107459	102.950459	14.107917	0.712154
1S 24.7292	0.937075	0.280906	-0.101688	-0.021485
2S 21.1386	0.068919	0.177565	-0.074243	-0.015920
2S 9.9971	0.000859	-1.021993	0.436116	0.093634
3S 30.4212	0.009143	0.001001	-0.001037	-0.000219
3S 7.3629	0.000019	-0.083861	0.108518	0.031754
3S 5.1830	-0.000126	0.007943	-0.632268	-0.170396
3S 3.4391	0.000025	-0.003056	-0.583503	-0.128499
4S 11.9538	-0.000067	-0.068373	0.090243	0.020770
4S 2.1124	-0.000010	0.000328	-0.011065	0.225866
4S 1.3241	0.000006	-0.000305	0.002196	0.541426
4S 0.8703	-0.000002	0.000000	-0.000417	0.358079

	2p	3p		3d
ORB.ENERGY	-22.139845	-2.050921	ORB.ENERGY	-0.373597
<R>	0.260079	0.977756	<R>	1.367969
<R**2>	0.083058	1.128508	<R**2>	2.505590
<1/R>	4.931331	1.394535	<1/R>	1.003726
<1/R**2>	33.384703	4.266269	<1/R**2>	1.415314
<1/R**3>	350.594041	38.785815	<1/R**3>	2.893424
2P 37.4230	0.000786	0.000199	3D 11.4813	0.016904
2P 14.8415	0.333715	0.070569	3D 5.8159	0.198001
2P 7.8404	0.420845	0.496567	3D 3.4526	0.403137
2P 3.6199	0.005346	-0.823061	3D 1.9741	0.392975
3P 11.9471	0.294186	0.014369	3D 1.1473	0.182481
3P 2.9491	-0.000612	-0.389092		
3P 1.9545	0.000251	-0.049588		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

MANGANESE, Z=25 [Ar]3d(5)4s(2)

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1149.866243	1149.866199	-2299.732442	-2.000000038

RHOat0 = 66362.197 Kato cusp = 2.001568

	1s	2s	3s	4s
ORB.ENERGY	-240.533986	-29.109469	-3.816640	-0.247867
<R>	0.061527	0.280660	0.860445	3.381917
<R**2>	0.005077	0.092907	0.852852	13.308367
<1/R>	24.523973	5.256006	1.624910	0.376551
<1/R**2>	1210.253676	113.083563	15.952716	0.845322
1S 25.6998	0.940989	-0.283798	0.104332	0.022617
2S 21.8567	0.064731	-0.187870	0.079962	0.017628
2S 10.7524	0.000286	0.993354	-0.430390	-0.094991
3S 31.6095	0.008989	-0.000781	0.000892	0.000191
3S 7.9533	-0.000098	0.100053	-0.116416	-0.031656
3S 5.4792	-0.000071	-0.007203	0.619299	0.167891
3S 3.6809	0.000007	0.003047	0.596542	0.138100
4S 12.6273	0.000257	0.096877	-0.102035	-0.024434
4S 2.1701	-0.000006	-0.000357	0.008247	-0.272491
4S 1.3884	0.000004	0.000212	-0.002062	-0.538366
4S 0.9204	-0.000001	-0.000071	0.000527	-0.315216

	2p	3p		3d
ORB.ENERGY	-24.812585	-2.479526	ORB.ENERGY	-0.638843
<R>	0.247530	0.913715	<R>	1.130052
<R**2>	0.075182	0.982773	<R**2>	1.640618
<1/R>	5.176571	1.491987	<1/R>	1.167041
<1/R**2>	36.746089	4.869761	<1/R**2>	1.850666
<1/R**3>	404.076937	46.651894	<1/R**3>	4.152144
2P 39.7636	0.000680	0.000175	3D 12.1103	0.018122
2P 15.5794	0.329684	0.070131	3D 6.2285	0.214643
2P 8.2726	0.425128	0.510669	3D 3.7645	0.417697
2P 3.9144	0.005727	-0.801936	3D 2.2778	0.384751
3P 12.5884	0.292622	0.015885	3D 1.4273	0.120919
3P 3.2243	-0.000552	-0.422222		
3P 2.1059	0.000178	-0.044967		

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

IRON, Z=26 [Ar]3d(6)4s(2) 5D

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1262.443656	1262.443629	-2524.887285	-2.000000022

RHOat0 = 74836.676 Kato cusp = 2.001497

	1s	2s	3s	4s
ORB.ENERGY	-261.373415	-31.935515	-4.169434	-0.258178
<R>	0.059112	0.268461	0.819236	3.258487
<R**2>	0.004685	0.084984	0.773333	12.381160
<1/R>	25.521201	5.498549	1.709910	0.391396
<1/R**2>	1310.420410	123.698534	17.698933	0.914094
1S 26.7103	0.942524	-0.285853	0.105891	0.022650
2S 22.7394	0.063210	-0.189028	0.081539	0.017743
2S 11.1579	0.000162	1.008545	-0.442968	-0.096526
3S 32.8592	0.008635	-0.000649	0.000883	0.000194
3S 8.2265	-0.000114	0.093973	-0.101287	-0.028327
3S 5.7011	-0.000058	-0.007693	0.635102	0.171358
3S 3.8393	0.000005	0.003112	0.577033	0.129599
4S 13.2036	0.000297	0.087617	-0.103885	-0.024523
4S 2.2676	-0.000005	-0.000360	0.007684	-0.275750
4S 1.4378	0.000003	0.000209	-0.001785	-0.539740
4S 0.9462	-0.000001	-0.000070	0.000454	-0.312861

	2p	3p		3d
ORB.ENERGY	-27.413707	-2.742193	ORB.ENERGY	-0.646883
<R>	0.236132	0.865859	<R>	1.072733
<R**2>	0.068377	0.882855	<R**2>	1.489969
<1/R>	5.422092	1.576545	<1/R>	1.236916
<1/R**2>	40.273502	5.433663	<1/R**2>	2.085959
<1/R**3>	462.827450	54.596391	<1/R**3>	4.978801
2P 42.2924	0.000583	0.000148	3D 12.7458	0.017645
2P 16.3351	0.323715	0.068651	3D 6.6281	0.216184
2P 8.7201	0.434152	0.516640	3D 4.0177	0.414852
2P 4.0978	0.006165	-0.821240	3D 2.4057	0.383883
3P 13.2514	0.288160	0.017006	3D 1.4774	0.129854
3P 3.3690	-0.000634	-0.407245		
3P 2.1919	0.000215	-0.041825		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

COBALT, Z=27 [Ar]3d(7)4s(2) 4F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1381.414542	1381.414516	-2762.829058	-2.000000019

RHOat0 = 84002.354 Kato cusp = 2.001413

	1s	2s	3s	4s
ORB.ENERGY	-283.065494	-34.868323	-4.524279	-0.267415
<R>	0.056878	0.257290	0.782377	3.153572
<R**2>	0.004337	0.078042	0.705537	11.620654
<1/R>	26.518656	5.740891	1.793467	0.404875
<1/R**2>	1414.588048	134.778776	19.502609	0.976951
1S 27.7200	0.943995	-0.287759	0.107248	0.022574
2S 23.6470	0.061559	-0.187848	0.082163	0.017611
2S 11.4491	0.000242	1.037770	-0.462596	-0.099332
3S 34.0340	0.008379	-0.000495	0.000918	0.000208
3S 8.3235	-0.000061	0.080271	-0.069603	-0.021162
3S 5.8668	-0.000079	-0.008894	0.656282	0.176287
3S 3.9712	0.000014	0.003249	0.544100	0.116449
4S 13.7147	0.000194	0.068031	-0.104310	-0.024406
4S 2.3510	-0.000007	-0.000376	0.006522	-0.281087
4S 1.4789	0.000004	0.000212	-0.001372	-0.539890
4S 0.9682	-0.000002	-0.000072	0.000344	-0.308876

	2p	3p		3d
ORB.ENERGY	-30.120165	-3.006235	ORB.ENERGY	-0.675411
<R>	0.225755	0.823547	<R>	1.016039
<R**2>	0.062466	0.799031	<R**2>	1.342867
<1/R>	5.667323	1.659533	<1/R>	1.310209
<1/R**2>	43.958994	6.017521	<1/R**2>	2.343520
<1/R**3>	526.962559	63.257174	<1/R**3>	5.928037
2P 44.2550	-0.000537	-0.000138	3D 13.3848	0.017145
2P 17.0241	-0.324287	-0.068746	3D 7.0420	0.215033
2P 9.1323	-0.431492	-0.524198	3D 4.2891	0.412560
2P 4.3892	-0.006429	0.802168	3D 2.5511	0.385376
3P 13.8562	-0.289377	-0.018893	3D 1.5435	0.135684
3P 3.5952	0.000501	0.427837		
3P 2.3606	-0.000226	0.050135		

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

NICKEL, Z=28 [Ar]3d(8)4s(2) 3F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1506.870896	1506.870821	-3013.741717	-2.000000050

RHOat0 = 93887.427 Kato cusp = 2.001330

	1s	2s	3s	4s
ORB.ENERGY	-305.619027	-37.917819	-4.887827	-0.276245
<R>	0.054807	0.247019	0.748942	3.059109
<R**2>	0.004027	0.071923	0.646731	10.956617
<1/R>	27.516295	5.983089	1.876340	0.417810
<1/R**2>	1522.756155	146.325009	21.376966	1.038551
1S 28.7266	0.945523	0.289565	-0.108484	0.022468
2S 24.5237	0.059970	0.187069	-0.083030	0.017547
2S 11.7009	0.000155	-1.073281	0.486257	-0.102978
3S 35.2606	0.008101	0.000139	-0.000950	0.000219
3S 8.3190	-0.000099	-0.063716	0.003334	-0.004844
3S 5.8931	-0.000046	0.009081	-0.685620	0.182371
3S 4.0420	0.000008	-0.003291	-0.475026	0.094382
4S 14.1323	0.000226	-0.043470	0.106095	-0.024948
4S 2.4332	-0.000005	0.000399	-0.004158	-0.283769
4S 1.5225	0.000003	-0.000214	0.000568	-0.538297
4S 0.9912	-0.000001	0.000071	-0.000119	-0.308953

	2p	3p		3d
ORB.ENERGY	-32.941726	-3.277669	ORB.ENERGY	-0.706924
<R>	0.216263	0.785486	<R>	0.964703
<R**2>	0.057298	0.727199	<R**2>	1.215301
<1/R>	5.912332	1.741835	<1/R>	1.383487
<1/R**2>	47.802900	6.626055	<1/R**2>	2.615216
<1/R**3>	596.721392	72.719398	<1/R**3>	6.985085
2P 46.7514	-0.000470	-0.000119	3D 13.9008	0.017517
2P 17.7675	-0.319845	-0.067683	3D 7.3628	0.225100
2P 9.5726	-0.438165	-0.527884	3D 4.4602	0.419212
2P 4.5914	-0.006828	0.810679	3D 2.6365	0.376659
3P 14.5116	-0.285978	-0.020283	3D 1.5875	0.130041
3P 3.7535	0.000547	0.421372		
3P 2.4658	-0.000255	0.049664		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$-54

See page 118 for Explanation of Table

COPPER, Z=29 [Ar]3d(10)4s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1638.963723	1638.963674	-3277.927397	-2.000000030

RHOat0 = 104492.35 Kato cusp = 2.001282

	1s	2s	3s	4s
ORB.ENERGY	-328.792952	-40.818928	-5.011952	-0.238481
<R>	0.052880	0.237540	0.722765	3.330979
<R**2>	0.003748	0.066499	0.603463	13.081296
<1/R>	28.514383	6.225289	1.947498	0.382211
<1/R**2>	1634.950447	158.345718	23.064777	0.807793
1S 29.6964	0.948723	0.291804	-0.109162	0.018928
2S 25.2508	0.056347	0.197199	-0.087326	0.015368
2S 12.5550	-0.000132	-1.032643	0.465300	-0.082080
3S 36.3548	0.008076	0.000189	-0.000831	0.000180
3S 9.2482	-0.000094	-0.085466	0.045865	-0.014992
3S 6.2646	-0.000058	0.005789	-0.684743	0.155119
3S 4.1881	0.000009	-0.002676	-0.499518	0.077800
4S 14.8890	0.000346	-0.078044	0.114174	-0.020952
4S 2.4698	-0.000004	0.000278	-0.006857	-0.229694
4S 1.4684	0.000003	-0.000149	0.000964	-0.534263
4S 0.9292	-0.000001	0.000054	-0.000379	-0.370075

	2p	3p		3d
ORB.ENERGY	-35.617918	-3.324793	ORB.ENERGY	-0.491208
<R>	0.207536	0.757481	<R>	0.991125
<R**2>	0.052747	0.678316	<R**2>	1.334835
<1/R>	6.157564	1.810480	<1/R>	1.391231
<1/R**2>	51.812525	7.168310	<1/R**2>	2.702492
<1/R**3>	672.476798	81.840087	<1/R**3>	7.503998
2P 48.7948	0.000433	0.000109	3D 14.1915	0.018641
2P 18.4738	0.318485	0.067352	3D 7.5450	0.239705
2P 9.9976	0.440209	0.525020	3D 4.4604	0.427410
2P 4.7454	0.007102	-0.832540	3D 2.5096	0.365471
3P 15.1401	0.284462	0.022690	3D 1.4098	0.148151
3P 3.8217	-0.000579	-0.397454		
3P 2.5167	0.000353	-0.053274		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

ZINC, Z=30 [Ar]3d(10)4s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1777.848102	1777.848093	-3555.696194	-2.000000005

RHOat0 = 115925.72 Kato cusp = 2.001265

	1s	2s	3s	4s
ORB.ENERGY	-353.304524	-44.361702	-5.637799	-0.292499
<R>	0.051085	0.228773	0.690586	2.897648
<R**2>	0.003497	0.061672	0.550224	9.867948
<1/R>	29.512053	6.467081	2.040101	0.441879
<1/R**2>	1751.093680	170.819077	25.330405	1.155444
1S 30.7026	0.950023	0.293360	-0.110788	0.022191
2S 26.0605	0.055373	0.203764	-0.090902	0.018507
2S 13.2539	-0.000597	-1.012933	0.459095	-0.093638
3S 37.7395	0.007693	0.000174	-0.000721	0.000170
3S 9.8590	-0.000202	-0.099869	0.072788	-0.021745
3S 6.6334	-0.000014	0.005685	-0.664296	0.171174
3S 4.4668	-0.000007	-0.002788	-0.532662	0.105412
4S 15.6259	0.000616	-0.093558	0.116494	-0.025059
4S 2.6384	-0.000001	0.000306	-0.006730	-0.273189
4S 1.6263	0.000001	-0.000170	0.001318	-0.542094
4S 1.0391	0.000000	0.000058	-0.000334	-0.320316

	2p	3p		3d
ORB.ENERGY	-38.924823	-3.839357	ORB.ENERGY	-0.782523
<R>	0.199514	0.719787	<R>	0.874864
<R**2>	0.048729	0.611170	<R**2>	1.004942
<1/R>	6.401756	1.904423	<1/R>	1.530540
<1/R**2>	55.965534	7.914870	<1/R**2>	3.202585
<1/R**3>	754.039092	94.149404	<1/R**3>	9.449971
2P 51.3224	-0.000384	-0.000097	3D 15.0303	0.017396
2P 19.2139	-0.314928	-0.066963	3D 8.1007	0.230530
2P 10.4311	-0.445010	-0.532060	3D 4.9123	0.421574
2P 5.0040	-0.007426	0.823000	3D 2.8828	0.372225
3P 15.7917	-0.282257	-0.024274	3D 1.7108	0.130294
3P 4.0672	0.000573	0.413856		
3P 2.6701	-0.000295	0.048684		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

GALLIUM, Z=31 [Ar]3d(10)4s(2)4p(1) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-1923.261001	1923.260945	-3846.521946	-2.000000029

RHOat0 = 128176.14 Kato cusp = 2.001229

	1s	2s	3s	4s
ORB.ENERGY	-378.818414	-48.168415	-6.394648	-0.424587
<R>	0.049408	0.220632	0.660472	2.488873
<R**2>	0.003271	0.057352	0.502651	7.206665
<1/R>	30.509723	6.708766	2.135134	0.515590
<1/R**2>	1871.221001	183.757673	27.764789	1.671365
1S 31.7059	0.951369	-0.294851	0.112463	0.026164
2S 26.8956	0.054085	-0.208641	0.093784	0.022235
2S 13.9060	-0.000810	0.999302	-0.455774	-0.108184
3S 39.0025	0.007436	-0.000181	0.000654	0.000156
3S 10.3974	-0.000213	0.111737	-0.098559	-0.029450
3S 7.0296	-0.000014	-0.006240	0.636679	0.186235
3S 4.7718	-0.000006	0.003025	0.572674	0.144131
4S 16.3515	0.000699	0.103312	-0.116529	-0.029905
4S 2.8372	-0.000002	-0.000369	0.007303	-0.313648
4S 1.8235	0.000001	0.000210	-0.001607	-0.554658
4S 1.2004	0.000000	-0.000070	0.000434	-0.262151

	2p	3p	4p		3d
ORB.ENERGY	-42.494022	-4.482360	-0.208497	ORB.ENERGY	-1.193363
<R>	0.192085	0.684090	3.424103	<R>	0.787885
<R**2>	0.045150	0.550701	13.898110	<R**2>	0.796141
<1/R>	6.645971	2.002594	0.372133	<1/R>	1.664871
<1/R**2>	60.278558	8.731266	0.342328	<1/R**2>	3.730031
<1/R**3>	841.922736	108.094710	2.891166	<1/R**3>	11.655110
2P 30.9647	0.079671	-0.015325	-0.002333	3D 15.7448	0.016981
2P 11.6838	0.667452	-0.422019	-0.071040	3D 8.5680	0.230981
3P 25.4398	0.175535	-0.025182	-0.003629	3D 5.2654	0.423088
3P 8.2598	0.015771	0.273334	0.048418	3D 3.1808	0.376129
3P 5.5111	0.000196	0.616186	0.123582	3D 1.9710	0.104017
3P 3.7958	0.000646	0.285565	0.025765		
4P 20.5257	0.119573	0.000699	0.000350		
4P 2.2879	-0.000029	0.003673	-0.265238		
4P 1.3751	0.000015	0.000157	-0.533374		
4P 0.8682	-0.000006	0.000039	-0.331517		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$-54

See page 118 for Explanation of Table

GERMANIUM, Z=32 [Ar]3d(10)4s(2)4p(2) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2075.359726	2075.359733	-4150.719459	-1.999999996

RHOat0 = 141264.57 Kato cusp = 2.001189

	1s	2s	3s	4s
ORB.ENERGY	-405.244442	-52.150327	-7.190990	-0.553360
<R>	0.047837	0.213048	0.632246	2.225804
<R**2>	0.003066	0.053468	0.460062	5.730932
<1/R>	31.507381	6.950515	2.232786	0.578893
<1/R**2>	1995.331847	197.169775	30.382780	2.191665
1S 32.7208	0.952125	-0.296096	-0.114120	-0.029258
2S 27.8041	0.053372	-0.209251	-0.094825	-0.024840
2S 14.4020	-0.000842	0.998859	0.458992	0.120324
3S 40.2593	0.007163	-0.000219	-0.000620	-0.000142
3S 10.8267	-0.000171	0.116798	0.121081	0.036502
3S 7.4435	-0.000034	-0.007409	-0.609201	-0.191413
3S 5.0894	0.000000	0.003297	-0.613648	-0.182649
4S 17.0698	0.000678	0.100296	0.111808	0.032523
4S 3.0282	-0.000003	-0.000427	-0.008224	0.352753
4S 1.9965	0.000003	0.000245	0.001917	0.546670
4S 1.3445	-0.000001	-0.000082	-0.000560	0.232419

	2p	3p	4p		3d
ORB.ENERGY	-46.236154	-5.161593	-0.287351	ORB.ENERGY	-1.634891
<R>	0.185185	0.650885	2.866859	<R>	0.721233
<R**2>	0.041948	0.497423	9.655894	<R**2>	0.657080
<1/R>	6.890252	2.103809	0.445517	<1/R>	1.793329
<1/R**2>	64.752319	9.613220	0.511519	<1/R**2>	4.277804
<1/R**3>	936.405701	123.721151	4.801440	<1/R**3>	14.106197
2P 32.3720	0.074659	-0.013603	-0.002241	3D 16.4691	0.016414
2P 12.2227	0.685414	-0.435326	-0.090957	3D 9.0439	0.229546
3P 26.6070	0.165218	-0.021515	-0.002950	3D 5.6272	0.422554
3P 8.7258	0.018146	0.252229	0.056839	3D 3.4888	0.381489
3P 5.8410	-0.000114	0.623458	0.145276	3D 2.1980	0.086376
3P 4.0849	0.000755	0.297367	0.045219		
4P 21.4919	0.112519	0.003214	0.001935		
4P 2.5444	-0.000060	0.003686	-0.299040		
4P 1.5873	0.000027	0.000284	-0.543013		
4P 1.0280	-0.000010	0.000030	-0.283008		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$-54

See page 118 for Explanation of Table

ARSENIC, Z=33 [Ar]3d(10)4s(2)4p(3) 4S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2234.238647	2234.238611	-4468.477258	-2.000000016

RHOat0 = 155219.44 Kato cusp = 2.001147

	1s	2s	3s	4s
ORB.ENERGY	-432.586199	-56.309822	-8.029618	-0.685893
<R>	0.046363	0.205963	0.605962	2.029704
<R**2>	0.002879	0.049964	0.422160	4.747468
<1/R>	32.505042	7.192370	2.332275	0.637555
<1/R**2>	2123.428160	211.057520	33.171895	2.735285
1S 33.7071	0.954050	-0.297645	-0.115924	0.031925
2S 28.5493	0.051397	-0.217749	-0.099930	0.028203
2S 15.1540	-0.001136	0.983785	0.457387	-0.129153
3S 41.4602	0.007024	-0.000102	-0.000574	0.000125
3S 11.3318	-0.000228	0.127118	0.124070	-0.037218
3S 7.7302	-0.000016	-0.007865	-0.596101	0.195492
3S 5.3683	-0.000005	0.003541	-0.624965	0.211438
4S 17.6911	0.000804	0.117619	0.121421	-0.038577
4S 3.2155	-0.000002	-0.000491	-0.008075	-0.393306
4S 2.1464	0.000002	0.000277	0.001685	-0.536125
4S 1.4740	0.000000	-0.000094	-0.000549	-0.206671

	2p	3p	4p
ORB.ENERGY	-50.153741	-5.880690	-0.369480
<R>	0.178758	0.620229	2.512233
<R**2>	0.039071	0.450758	7.371187
<1/R>	7.134625	2.207111	0.509991
<1/R**2>	69.387334	10.555878	0.686379
<1/R**3>	1037.721550	141.058163	6.958306
2P 33.8306	0.069915	-0.011491	-0.001866
2P 12.7682	0.700126	-0.453070	-0.108812
3P 27.7931	0.156149	-0.016656	-0.001656
3P 9.3346	0.021050	0.219149	0.058080
3P 6.2386	0.000000	0.630930	0.161657
3P 4.4077	0.000760	0.322694	0.068207
4P 22.4504	0.106708	0.007328	0.003906
4P 2.7882	-0.000067	0.004166	-0.325259
4P 1.7792	0.000029	0.000064	-0.546313
4P 1.1706	-0.000010	-0.000022	-0.253975

	3d
ORB.ENERGY	-2.112654
<R>	0.667450
<R**2>	0.556641
<1/R>	1.917759
<1/R**2>	4.848005
<1/R**3>	16.818814
3D 17.0538	0.016674
3D 9.4108	0.239639
3D 5.8490	0.435884
3D 3.7033	0.369917
3D 2.3465	0.062948

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

SELENIUM, Z=34 [Ar]3d(10)4s(2)4p(4) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2399.867604	2399.867576	-4799.735180	-2.000000012

RHOat0 = 170070.73 Kato cusp = 2.001117

	1s	2s	3s	4s
ORB.ENERGY	-460.867399	-60.668866	-8.932097	-0.837378
<R>	0.044978	0.199330	0.581534	1.869230
<R**2>	0.002710	0.046790	0.388447	4.015443
<1/R>	33.502730	7.434387	2.433149	0.695413
<1/R**2>	2255.512617	225.425059	36.125092	3.331164
1S 34.7125	0.955079	-0.298867	-0.117604	-0.034379
2S 29.3786	0.050500	-0.221711	-0.102968	-0.030932
2S 15.7400	-0.001361	0.981133	0.461461	0.138682
3S 42.7575	0.006777	-0.000034	-0.000545	-0.000114
3S 11.7494	-0.000279	0.131114	0.126802	0.037692
3S 8.0222	0.000006	-0.008785	-0.586337	-0.197476
3S 5.6528	-0.000012	0.003839	-0.635716	-0.240944
4S 18.3237	0.000911	0.121953	0.125109	0.042941
4S 3.4106	0.000000	-0.000550	-0.008229	0.430881
4S 2.2896	0.000001	0.000298	0.001502	0.532759
4S 1.5845	0.000000	-0.000102	-0.000557	0.178817

	2p	3p	4p		3d
ORB.ENERGY	-54.268896	-6.661518	-0.402851	ORB.ENERGY	-2.649622
<R>	0.172757	0.592268	2.299617	<R>	0.622432
<R**2>	0.036478	0.410405	6.195873	<R**2>	0.480001
<1/R>	7.379110	2.311199	0.562826	<1/R>	2.039610
<1/R**2>	74.184149	11.550310	0.857377	<1/R**2>	5.443420
<1/R**3>	1146.116676	160.058270	9.280218	<1/R**3>	19.814292
2P 35.2165	0.064815	-0.008694	-0.001192	3D 17.6906	0.016536
2P 13.3691	0.719004	-0.474977	-0.125022	3D 9.8167	0.244834
3P 28.9584	0.144057	-0.009411	0.000418	3D 6.1051	0.448354
3P 10.0638	0.026166	0.181185	0.054010	3D 3.9379	0.358333
3P 6.6718	0.000188	0.636415	0.173494	3D 2.4892	0.047754
3P 4.7438	0.000765	0.354144	0.093637		
4P 23.4246	0.097238	0.013955	0.006379		
4P 3.0297	-0.000071	0.005093	-0.358802		
4P 1.9218	0.000023	0.000316	-0.538721		
4P 1.2451	-0.000011	0.000151	-0.242599		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

BROMINE, Z=35 [Ar]3d(10)4s(2)4p(5) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2572.441325	2572.441351	-5144.882675	-1.999999990

RHOat0 = 185843.56 Kato cusp = 2.001075

	1s	2s	3s	4s
ORB.ENERGY	-490.060332	-65.199950	-9.871887	-0.992675
<R>	0.043672	0.193107	0.558860	1.738860
<R**2>	0.002554	0.043907	0.358460	3.467913
<1/R>	34.500432	7.676539	2.534994	0.750675
<1/R**2>	2391.582918	240.271720	39.234690	3.952880
1S 35.7147	0.956178	0.300065	-0.119257	-0.036545
2S 30.2313	0.049303	0.224065	-0.105248	-0.033223
2S 16.2817	-0.001379	-0.981012	0.466489	0.147307
3S 43.9396	0.006623	-0.000003	-0.000526	-0.000106
3S 12.1552	-0.000241	-0.133963	0.130322	0.038175
3S 8.3109	-0.000016	0.009815	-0.579501	-0.196982
3S 5.9392	-0.000002	-0.004183	-0.644361	-0.269614
4S 18.9651	0.000876	-0.122802	0.126778	0.046308
4S 3.6167	-0.000002	0.000613	-0.008641	0.459442
4S 2.4340	0.000003	-0.000317	0.001333	0.530326
4S 1.6936	0.000000	0.000109	-0.000566	0.160145

	2p	3p	4p		3d
ORB.ENERGY	-58.554216	-7.478203	-0.457082	ORB.ENERGY	-3.220169
<R>	0.167142	0.566611	2.111601	<R>	0.584099
<R**2>	0.034132	0.375144	5.223555	<R**2>	0.419895
<1/R>	7.623705	2.416064	0.616846	<1/R>	2.159167
<1/R**2>	79.142919	12.596986	1.046922	<1/R**2>	6.063313
<1/R**3>	1261.838536	180.807646	11.999778	<1/R**3>	23.100843
2P 36.6717	0.059746	-0.005460	-0.000217	3D 18.4910	0.015518
2P 13.9922	0.734105	-0.499743	-0.142598	3D 10.2980	0.242791
3P 30.1518	0.132860	-0.000944	0.003309	3D 6.4197	0.459169
3P 10.8966	0.033198	0.148906	0.049718	3D 4.2010	0.351558
3P 7.0906	0.000750	0.643268	0.184443	3D 2.6377	0.039199
3P 5.0673	0.000664	0.379137	0.118116		
4P 24.3902	0.088869	0.022016	0.009707		
4P 3.2746	-0.000063	0.005992	-0.380018		
4P 2.0783	0.000011	0.000647	-0.537214		
4P 1.3411	-0.000011	0.000313	-0.232420		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$-54

See page 118 for Explanation of Table

KRYPTON, Z=36 [Ar]3d(10)4s(2)4p(6) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2752.054969	2752.054983	-5504.109952	-1.999999995

RHOat0 = 202566.04 Kato cusp = 2.001035

	1s	2s	3s	4s
ORB.ENERGY	-520.165459	-69.903072	-10.849459	-1.152929
<R>	0.042441	0.187256	0.537802	1.629392
<R**2>	0.002412	0.041280	0.331729	3.040358
<1/R>	35.498151	7.918829	2.637556	0.804187
<1/R**2>	2531.640192	255.598355	42.495905	4.603723
1S 36.7205	0.957077	-0.301159	0.120838	0.038487
2S 31.1118	0.048295	-0.224630	0.106713	0.035084
2S 16.7539	-0.001340	0.985238	-0.473731	-0.155808
3S 45.1135	0.006469	0.000027	0.000517	0.000102
3S 12.5170	-0.000192	0.134207	-0.131052	-0.037482
3S 8.5715	-0.000043	-0.011226	0.580549	0.196315
3S 6.2171	0.000010	0.004686	0.644535	0.295835
4S 19.6005	0.000816	0.119437	-0.126985	-0.048888
4S 3.8388	-0.000004	-0.000706	0.009105	-0.476243
4S 2.5911	0.000005	0.000347	-0.001109	-0.530291
4S 1.8100	-0.000001	-0.000119	0.000560	-0.151842

	2p	3p	4p		3d
ORB.ENERGY	-63.009777	-8.331494	-0.524182	ORB.ENERGY	-3.825228
<R>	0.161876	0.542627	1.951590	<R>	0.550880
<R**2>	0.032004	0.343537	4.454829	<R**2>	0.371478
<1/R>	7.868429	2.522775	0.669220	<1/R>	2.276940
<1/R**2>	84.264195	13.706161	1.238775	<1/R**2>	6.708298
<1/R**3>	1385.133258	203.553552	14.886597	<1/R**3>	26.691863
2P 38.0283	0.054135	-0.001435	0.001213	3D 19.1294	0.015286
2P 14.6932	0.751976	-0.526859	-0.160462	3D 10.7158	0.245430
3P 31.3136	0.118384	0.009958	0.007447	3D 6.6805	0.473937
3P 11.7833	0.044500	0.120509	0.045141	3D 4.4322	0.335752
3P 7.4972	0.001287	0.646740	0.191368	3D 2.7599	0.031469
3P 5.3888	0.000557	0.401547	0.141683		
4P 25.3638	0.076875	0.032338	0.014153		
4P 3.5216	-0.000045	0.006341	-0.393849		
4P 2.2424	0.000013	-0.000025	-0.538338		
4P 1.4475	-0.000004	0.000066	-0.225021		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

RUBIDIUM, Z=37 [Kr]5s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-2938.357442	2938.357361	-5876.714803	-2.000000028

RHOat0 = 220301.72 Kato cusp = 2.000922

	1s	2s	3s	4s	5s
ORB.ENERGY	-551.457326	-75.049333	-12.133188	-1.523539	-0.137862
<R>	0.041276	0.181742	0.518105	1.499207	5.631401
<R**2>	0.002281	0.038879	0.307673	2.557226	36.167879
<1/R>	36.495965	8.161488	2.741239	0.876306	0.217763
<1/R**2>	2675.688377	271.418660	45.924228	5.560444	0.280591
1S 37.6597	0.960467	0.303005	-0.122718	0.041454	0.008728
2S 31.9404	0.042932	0.221238	-0.111462	0.038866	0.008204
2S 16.8617	-0.000093	-1.026270	0.524563	-0.183063	-0.038612
3S 45.3535	0.007109	-0.000245	-0.000825	0.000256	0.000042
3S 12.0916	0.000159	-0.100557	-0.215183	0.080032	0.016335
3S 6.6424	0.000125	-0.004612	-0.773124	0.372057	0.084781
4S 19.9148	-0.000059	-0.102291	0.167082	-0.065728	-0.014138
4S 3.9717	-0.000028	0.000640	-0.010285	-0.562841	-0.146431
4S 2.6062	0.000018	-0.000266	0.001188	-0.573101	-0.109368
5S 11.5420	-0.000211	0.010396	-0.210462	0.070777	0.013149
5S 1.7303	-0.000008	0.000116	-0.000540	-0.023626	0.175390
5S 1.0853	0.000005	-0.000066	0.000267	0.003312	0.556025
5S 0.7168	-0.000002	0.000024	-0.000091	-0.001164	0.394524

	2p	3p	4p		3d
ORB.ENERGY	-67.906220	-9.487684	-0.810061	ORB.ENERGY	-4.732282
<R>	0.156927	0.520757	1.734937	<R>	0.521335
<R**2>	0.030066	0.316060	3.477698	<R**2>	0.331036
<1/R>	8.113293	2.629144	0.752058	<1/R>	2.394259
<1/R**2>	89.548558	14.858936	1.577857	<1/R**2>	7.383580
<1/R**3>	1516.271831	228.065929	20.096797	<1/R**3>	30.625668
2P 40.4071	0.043079	0.002918	0.002888	3D 19.9656	0.014081
2P 15.5458	0.779487	-0.545128	-0.184729	3D 11.2720	0.233527
3P 33.1343	0.095670	0.020706	0.012302	3D 7.1489	0.455528
3P 12.7443	0.063827	0.085175	0.039095	3D 4.8701	0.349694
3P 7.9163	0.001775	0.646495	0.207397	3D 3.1960	0.042870
3P 5.7101	0.000499	0.425641	0.174300		
4P 26.7299	0.060229	0.042147	0.019670		
4P 3.7718	-0.000051	0.006843	-0.424584		
4P 2.4254	0.000017	-0.000099	-0.581322		
4P 1.6089	-0.000005	0.000028	-0.145948		

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

STRONTIUM, Z=38 [Kr]5s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-3131.545674	3131.545574	-6263.091248	-2.000000032

RHOat0 = 239052.25 Kato cusp = 2.000923

		1s	2s	3s	4s	5s
ORB.ENERGY		-583.687877	-80.390786	-13.475021	-1.896804	-0.178452
<R>		0.040174	0.176536	0.499698	1.390924	4.632850
<R**2>		0.002161	0.036678	0.286029	2.191496	24.494709
<1/R>		37.493847	8.404429	2.845715	0.948079	0.268683
<1/R**2>		2823.738208	287.731813	49.511285	6.606805	0.484018
1S	38.6766	0.960803	0.303862	0.124165	0.044153	0.011387
2S	32.7622	0.043118	0.227987	0.115932	0.042508	0.010991
2S	17.6638	-0.000546	-1.005014	-0.518144	-0.190100	-0.049113
3S	46.8232	0.006721	-0.000192	0.000757	0.000230	0.000042
3S	12.7979	0.000081	-0.115623	0.175185	0.064281	0.015585
3S	6.9740	0.000104	-0.004700	0.805787	0.420637	0.118647
4S	20.6858	0.000184	-0.118775	-0.172787	-0.070827	-0.018671
4S	4.2125	-0.000025	0.000708	0.011784	-0.569917	-0.187386
4S	2.8491	0.000017	-0.000299	-0.001591	-0.577559	-0.139266
5S	12.1086	-0.000172	0.010249	0.204433	0.067732	0.014814
5S	1.8492	-0.000007	0.000126	0.000624	-0.015972	0.289906
5S	1.2152	0.000005	-0.000079	-0.000339	0.002941	0.558928
5S	0.8188	-0.000002	0.000028	0.000114	-0.000680	0.288435

		2p	3p	4p			3d
ORB.ENERGY		-72.996030	-10.699969	-1.098155	ORB.ENERGY		-5.694389
<R>		0.152268	0.500521	1.577614	<R>		0.495014
<R**2>		0.028297	0.291693	2.857242	<R**2>		0.297162
<1/R>		8.358311	2.735976	0.829072	<1/R>		2.510862
<1/R**2>		94.996384	16.062791	1.931624	<1/R**2>		8.087616
<1/R**3>		1655.482351	254.543524	25.894968	<1/R**3>		34.909486
2P	42.7301	0.030306	0.009319	0.005483	3D	20.7700	0.013127
2P	16.6389	0.811617	-0.569292	-0.209108	3D	11.8072	0.224304
3P	35.0112	0.064192	0.038033	0.019826	3D	7.5922	0.440334
3P	13.8073	0.097475	0.047280	0.028810	3D	5.2871	0.359256
3P	8.2941	0.002506	0.654407	0.225194	3D	3.5961	0.053222
3P	5.9989	0.000332	0.436187	0.199730			
4P	28.1756	0.034102	0.059016	0.027842			
4P	4.0091	-0.000040	0.006535	-0.451600			
4P	2.6162	0.000012	-0.000021	-0.611309			
4P	1.6854	-0.000003	-0.000065	-0.090744			

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

YTTRIUM, Z=39 [Kr]4d(1)5s(2) 2D

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-3331.684158	3331.684150	-6663.368307	-2.000000002

RHOat0 = 258825.47 Kato cusp = 2.000948

	1s	2s	3s	4s	5s
ORB.ENERGY	-616.749339	-85.810931	-14.758905	-2.168866	-0.196137
<R>	0.039129	0.171618	0.482564	1.311714	4.299870
<R**2>	0.002050	0.034657	0.266604	1.946802	21.136058
<1/R>	38.491889	8.647529	2.950163	1.009637	0.290899
<1/R**2>	2975.796354	304.529052	53.229252	7.576340	0.584767
1S 39.7224	0.960080	0.304345	0.125399	0.046138	0.012247
2S 33.6027	0.045175	0.233833	0.119821	0.045391	0.012074
2S 18.3793	-0.001567	-0.993114	-0.516076	-0.195574	-0.051987
3S 48.7440	0.006033	-0.000202	0.000700	0.000199	0.000038
3S 13.3446	-0.000219	-0.124424	0.153637	0.052859	0.012518
3S 7.2830	0.000014	-0.004980	0.824075	0.461392	0.134763
4S 21.3822	0.000855	-0.129631	-0.177748	-0.074774	-0.020203
4S 4.4484	-0.000005	0.000788	0.012444	-0.581457	-0.199281
4S 3.0474	0.000005	-0.000337	-0.001672	-0.575339	-0.145438
5S 12.5609	-0.000022	0.010524	0.200249	0.062477	0.013467
5S 2.0044	-0.000002	0.000134	0.000618	-0.016837	0.296136
5S 1.3112	0.000001	-0.000079	-0.000310	0.002621	0.559777
5S 0.8747	0.000000	0.000027	0.000101	-0.000609	0.288710

	2p	3p	4p		3d	4d
ORB.ENERGY	-78.164460	-11.854181	-1.301177	ORB.ENERGY	-6.599469	-0.249843
<R>	0.147874	0.481793	1.471165	<R>	0.471362	2.435117
<R**2>	0.026679	0.270039	2.480385	<R**2>	0.268432	7.264053
<1/R>	8.603493	2.842924	0.892449	<1/R>	2.626972	0.545592
<1/R**2>	100.608702	17.314274	2.250015	<1/R**2>	8.821104	0.566309
<1/R**3>	1803.049876	282.998630	31.490662	<1/R**3>	39.561154	1.711655
2P 45.1959	0.015985	0.013658	0.007526	3D 20.9990	0.014824	-0.002992
2P 17.8974	0.849353	-0.563739	-0.219184	3D 11.9070	0.258493	-0.056375
3P 37.1587	0.026725	0.048327	0.025116	3D 7.2875	0.601413	-0.241729
3P 14.7946	0.138567	-0.006137	0.011431	3D 4.6011	0.129384	0.512516
3P 8.7835	0.003167	0.620845	0.219417	4D 5.7904	0.084425	-0.365269
3P 6.3922	0.000262	0.487291	0.238060	4D 2.7134	0.002942	0.400153
4P 29.9120	0.001671	0.067300	0.033146	4D 1.6373	-0.000449	0.472371
4P 4.2354	-0.000040	0.008332	-0.473272	4D 0.9993	0.000143	0.213171
4P 2.7964	0.000009	-0.000445	-0.605988			
4P 1.7852	-0.000003	0.000043	-0.080554			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

ZIRCONIUM, Z=40 [Kr]4d(2)5s(2) 3F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-3538.995053	3538.995042	-7077.990095	-2.000000003

RHOat0 = 279659.35 Kato cusp = 2.001009

	1s	2s	3s	4s	5s
ORB.ENERGY	-650.704975	-91.377678	-16.055019	-2.419186	-0.207288
<R>	0.038137	0.166963	0.466569	1.245628	4.091705
<R**2>	0.001947	0.032798	0.249103	1.754744	19.179063
<1/R>	39.490031	8.890788	3.054716	1.067325	0.306527
<1/R**2>	3131.857499	321.811868	57.083949	8.541645	0.657415
1S 40.7891	0.958661	0.304575	-0.126474	0.047779	0.012672
2S 34.4609	0.048443	0.240401	-0.123985	0.048124	0.012781
2S 19.1696	-0.002967	-0.976241	0.510824	-0.198339	-0.052635
3S 51.1760	0.005199	-0.000180	-0.000621	0.000172	0.000028
3S 14.0056	-0.000632	-0.137458	-0.125183	0.037812	0.008034
3S 7.5966	-0.000109	-0.004954	-0.845727	0.497570	0.146263
4S 22.1375	0.001762	-0.141960	0.182541	-0.077806	-0.020961
4S 4.6587	0.000024	0.000801	-0.013029	-0.604867	-0.209688
4S 3.2070	-0.000011	-0.000338	0.001754	-0.561753	-0.139697
5S 13.0607	0.000172	0.010060	-0.196198	0.058290	0.011697
5S 2.1201	0.000004	0.000129	-0.000626	-0.015948	0.302034
5S 1.3752	-0.000003	-0.000073	0.000300	0.002170	0.559795
5S 0.9098	0.000000	0.000025	-0.000097	-0.000494	0.287194

	2p	3p	4p		3d	4d
ORB.ENERGY	-83.478533	-13.019759	-1.487587	ORB.ENERGY	-7.515832	-0.336752
<R>	0.143725	0.464443	1.385566	<R>	0.450089	2.104484
<R**2>	0.025195	0.250756	2.198369	<R**2>	0.243963	5.359532
<1/R>	8.848787	2.949831	0.950890	<1/R>	2.742175	0.627586
<1/R**2>	106.384524	18.611844	2.563936	<1/R**2>	9.581306	0.744770
<1/R**3>	1959.203195	313.471604	37.312794	<1/R**3>	44.579961	2.439249
2P 47.2894	0.007920	0.014954	0.008380	3D 21.6043	0.014903	0.003282
2P 18.9113	0.864740	-0.548594	-0.222193	3D 11.8740	0.398441	0.099488
3P 39.0617	0.006156	0.049948	0.026809	3D 5.6325	0.359142	0.090782
3P 15.5797	0.166347	-0.041392	-0.000868	4D 9.1444	0.314611	0.068680
3P 9.1966	0.003864	0.600526	0.214836	4D 4.1290	0.015434	-0.208862
3P 6.7401	0.000095	0.517300	0.268717	4D 2.6333	0.000045	-0.440798
4P 31.4855	-0.015667	0.067124	0.034677	4D 1.6878	0.000151	-0.393876
4P 4.4650	-0.000029	0.009447	-0.491131	4D 1.1008	0.000001	-0.134919
4P 2.9661	0.000000	-0.000625	-0.598899			
4P 1.8952	-0.000002	0.000106	-0.077406			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

NIOBIUM, Z=41 [Kr]4d(4)5s(1) 6D

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-3753.597716	3753.597739	-7507.195454	-1.999999994

RHOat0 = 301563.83 Kato cusp = 2.000908

	1s	2s	3s	4s	5s
ORB.ENERGY	-685.444011	-96.974820	-17.247057	-2.537468	-0.215590
<R>	0.037194	0.162551	0.451645	1.193620	3.985219
<R**2>	0.001852	0.031083	0.233323	1.611986	18.212711
<1/R>	40.488326	9.134143	3.158977	1.117520	0.314471
<1/R**2>	3291.914304	339.575942	61.059110	9.423756	0.686875
1S 41.7434	0.961175	0.306025	0.127992	0.049152	0.012664
2S 35.3327	0.044322	0.237409	0.123668	0.048721	0.012565
2S 19.4788	-0.001834	-0.990557	-0.522977	-0.206092	-0.053088
3S 51.3713	0.005628	-0.000221	0.000642	0.000186	0.000023
3S 14.2959	-0.000262	-0.130816	0.132276	0.035236	0.006551
3S 7.8700	0.000005	-0.005172	0.842402	0.523528	0.151392
4S 22.6990	0.000984	-0.129732	-0.178513	-0.076873	-0.020174
4S 4.8823	-0.000002	0.000811	0.012585	-0.624565	-0.211147
4S 3.3343	0.000004	-0.000327	-0.001334	-0.552565	-0.132947
5S 13.3478	-0.000005	0.010382	0.198121	0.054469	0.009289
5S 2.2445	-0.000001	0.000125	0.000543	-0.019527	0.280113
5S 1.4324	0.000000	-0.000062	-0.000250	0.004724	0.569278
5S 0.9392	0.000000	0.000024	0.000069	0.000858	0.301898

	2p	3p	4p		3d	4d
ORB.ENERGY	-88.823116	-14.081419	-1.556984	ORB.ENERGY	-8.329286	-0.300639
<R>	0.139800	0.448341	1.324287	<R>	0.430775	2.071214
<R**2>	0.023830	0.233523	2.011649	<R**2>	0.222841	5.289530
<1/R>	9.094202	3.056550	0.998663	<1/R>	2.856822	0.647834
<1/R**2>	112.324514	19.953619	2.836612	<1/R**2>	10.369634	0.800651
<1/R**3>	2124.210204	345.991793	42.723444	<1/R**3>	49.986809	2.723784
2P 49.4286	0.005451	0.014169	0.008213	3D 22.1877	0.014904	0.003283
2P 19.6324	0.862731	-0.536114	-0.222053	3D 12.2251	0.409835	0.100591
3P 40.7909	0.001179	0.047220	0.026290	3D 5.7876	0.327950	0.162213
3P 16.1936	0.178498	-0.057793	-0.006556	3D 3.4029	0.011875	-0.348773
3P 9.5298	0.004367	0.594477	0.211376	4D 9.3914	0.335209	0.065185
3P 7.0510	-0.000114	0.527609	0.289486	4D 2.5965	-0.000669	-0.394496
4P 32.8210	-0.018878	0.063583	0.034165	4D 1.6522	0.000234	-0.366588
4P 4.6928	-0.000015	0.010034	-0.506457	4D 1.0605	-0.000018	-0.141878
4P 3.1130	-0.000015	-0.000586	-0.580540			
4P 2.0122	-0.000002	0.000212	-0.091582			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

MOLYBDENUM, Z=42 [Kr]4d(5)5s(1) 7S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-3975.549487	3975.549493	-7951.098980	-1.999999998

RHOat0 = 324598.90 Kato cusp = 2.000873

	1s	2s	3s	4s	5s
ORB.ENERGY	-721.202191	-102.850591	-18.584528	-2.762907	-0.222725
<R>	0.036296	0.158364	0.437613	1.142377	3.841740
<R**2>	0.001763	0.029498	0.218970	1.476363	16.968563
<1/R>	41.486632	9.377695	3.263694	1.171270	0.327047
<1/R**2>	3455.966236	357.829927	65.186319	10.415942	0.748298
1S 42.7425	0.962070	0.306935	-0.129261	0.050557	0.012933
2S 36.2098	0.043169	0.237253	-0.124528	0.049874	0.012760
2S 19.9247	-0.001678	-0.995992	0.529678	-0.212208	-0.054220
3S 52.4536	0.005573	-0.000250	-0.000626	0.000193	0.000020
3S 14.6520	-0.000202	-0.129301	-0.130879	0.028878	0.004143
3S 8.1505	0.000029	-0.005610	-0.842359	0.551495	0.160091
4S 23.3229	0.000864	-0.125168	0.176789	-0.076744	-0.019965
4S 5.1157	-0.000007	0.000881	-0.012580	-0.634721	-0.214823
4S 3.4917	0.000007	-0.000347	0.001082	-0.553088	-0.132312
5S 13.6857	-0.000038	0.011029	-0.200425	0.051443	0.007496
5S 2.3571	-0.000002	0.000128	-0.000482	-0.019802	0.282363
5S 1.4897	0.000001	-0.000060	0.000206	0.004878	0.568779
5S 0.9661	0.000000	0.000024	-0.000057	0.001027	0.305619

	2p	3p	4p		3d	4d
ORB.ENERGY	-94.444083	-15.286558	-1.723626	ORB.ENERGY	-9.284218	-0.357912
<R>	0.136081	0.433332	1.260413	<R>	0.413218	1.875157
<R**2>	0.022573	0.218033	1.821849	<R**2>	0.204535	4.308556
<1/R>	9.339690	3.163304	1.052205	<1/R>	2.970616	0.713442
<1/R**2>	118.427110	21.342240	3.155945	<1/R**2>	11.183813	0.965543
<1/R**3>	2298.252225	380.677986	49.191240	<1/R**3>	55.781037	3.481440
2P 51.2736	0.002347	0.013908	0.008232	3D 22.9005	0.014298	0.003366
2P 20.4266	0.862806	-0.522435	-0.221257	3D 12.6580	0.410590	0.108254
3P 42.4402	-0.006158	0.045257	0.025846	3D 6.0525	0.321217	0.176427
3P 16.8366	0.193670	-0.077421	-0.014486	3D 3.5536	0.010376	-0.395951
3P 9.8793	0.004935	0.585780	0.208525	4D 9.7486	0.340238	0.071509
3P 7.3678	-0.000336	0.541100	0.312120	4D 2.7024	-0.000597	-0.410929
4P 34.1870	-0.024536	0.060287	0.033403	4D 1.7351	0.000143	-0.335730
4P 4.9234	0.000000	0.010869	-0.519055	4D 1.1346	-0.000036	-0.110648
4P 3.2697	-0.000028	-0.000628	-0.576360			
4P 2.1185	0.000000	0.000255	-0.090868			

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

TECHNETIUM, Z=43 [Kr]4d(5)5s(2) 6S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-4204.788722	4204.788677	-8409.577399	-2.000000011

RHOat0 = 348792.97 Kato cusp = 2.000866

	1s	2s	3s	4s	5s
ORB.ENERGY	-758.043040	-109.069778	-20.131826	-3.152181	-0.231268
<R>	0.035440	0.154384	0.424391	1.091530	3.684647
<R**2>	0.001681	0.028030	0.205872	1.347033	15.641489
<1/R>	42.484927	9.621442	3.368888	1.229587	0.341743
<1/R**2>	3624.007856	376.575106	69.468169	11.549029	0.824194
1S 43.7613	0.962275	0.307603	-0.130405	0.052081	0.013283
2S 37.0818	0.043292	0.239744	-0.126665	0.051665	0.013157
2S 20.5473	-0.001947	-0.989486	0.529567	-0.216073	-0.054962
3S 53.9182	0.005310	-0.000230	-0.000589	0.000189	0.000023
3S 15.1937	-0.000257	-0.135846	-0.114905	0.016662	0.000108
3S 8.4476	0.000011	-0.005741	-0.852057	0.582808	0.170032
4S 24.0307	0.001012	-0.128482	0.177528	-0.077501	-0.019908
4S 5.3489	-0.000003	0.000911	-0.013016	-0.640499	-0.220526
4S 3.6757	0.000004	-0.000339	0.001006	-0.558426	-0.127369
5S 14.1204	-0.000011	0.010992	-0.200850	0.048669	0.006109
5S 2.4102	-0.000001	0.000115	-0.000429	-0.015715	0.305203
5S 1.5279	0.000000	-0.000061	0.000185	0.002098	0.560859
5S 0.9884	0.000000	0.000021	-0.000060	-0.000493	0.290453

	2p	3p	4p
ORB.ENERGY	-100.406084	-16.699570	-2.041209
<R>	0.132553	0.419294	1.193030
<R**2>	0.021411	0.204040	1.628439
<1/R>	9.585252	3.270182	1.113717
<1/R**2>	124.692426	22.778770	3.540576
<1/R**3>	2481.573939	417.620145	57.128767
2P 52.9821	0.001500	0.013626	0.008186
2P 21.0486	0.860433	-0.519116	-0.224913
3P 43.8578	-0.007648	0.044111	0.025642
3P 17.3646	0.198804	-0.083868	-0.018115
3P 10.1141	0.005092	0.609595	0.220385
3P 7.6073	-0.000539	0.519096	0.324748
4P 35.3274	-0.025053	0.058553	0.033083
4P 5.1799	0.000013	0.010590	-0.526097
4P 3.4522	-0.000037	-0.000366	-0.591749
4P 2.2236	0.000003	0.000153	-0.075879

	3d	4d
ORB.ENERGY	-10.444631	-0.543944
<R>	0.397210	1.620236
<R**2>	0.188595	3.142838
<1/R>	3.083493	0.814479
<1/R**2>	12.022897	1.241283
<1/R**3>	61.968839	4.797754
3D 23.5175	0.014099	0.003718
3D 13.0453	0.416170	0.123034
3D 6.2613	0.304613	0.197914
3D 3.7227	0.007879	-0.464963
4D 10.0555	0.351461	0.084609
4D 2.8086	-0.000165	-0.463260
4D 1.8327	0.000023	-0.271624
4D 1.2458	0.000002	-0.041969

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

RUTHENIUM, Z=44 [Kr]4d(7)5s(1) 5F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-4441.539471	4441.539417	-8883.078888	-2.000000012

RHOat0 = 374131.21 Kato cusp = 2.000845

	1s	2s	3s	4s	5s
ORB.ENERGY	-795.513463	-115.158783	-21.413875	-3.257117	-0.222424
<R>	0.034624	0.150598	0.412017	1.054738	3.735235
<R**2>	0.001604	0.026669	0.193987	1.258968	16.140221
<1/R>	43.483425	9.865207	3.473377	1.275814	0.337123
<1/R**2>	3796.066238	395.797963	73.852058	12.484313	0.785489
1S 44.7676	0.962878	0.308369	-0.131520	0.052994	-0.012642
2S 37.9473	0.042691	0.241207	-0.128366	0.052661	-0.012529
2S 21.1032	-0.001991	-0.987658	0.532288	-0.218427	0.051886
3S 55.1696	0.005176	-0.000234	-0.000565	0.000184	-0.000013
3S 15.7100	-0.000255	-0.139581	-0.106262	0.006347	0.002992
3S 8.7353	0.000014	-0.005705	-0.856572	0.607303	-0.167177
4S 24.6978	0.001020	-0.128097	0.177879	-0.077079	0.018510
4S 5.5734	-0.000003	0.000887	-0.013147	-0.652721	0.210064
4S 3.7938	0.000004	-0.000311	0.000766	-0.554377	0.117438
5S 14.5125	-0.000016	0.010610	-0.202916	0.044636	-0.003639
5S 2.5155	-0.000001	0.000105	-0.000406	-0.019362	-0.272330
5S 1.5531	0.000000	-0.000048	0.000156	0.003030	-0.562346
5S 0.9861	0.000000	0.000019	-0.000050	0.000062	-0.327039

	2p	3p	4p
ORB.ENERGY	-106.239384	-17.848743	-2.101237
<R>	0.129203	0.406183	1.150563
<R**2>	0.020337	0.191402	1.517294
<1/R>	9.830944	3.376726	1.158209
<1/R**2>	131.122920	24.257276	3.836005
<1/R**3>	2674.513995	456.767228	63.761114
2P 55.3565	0.000623	0.012338	0.007580
2P 21.7256	0.853588	-0.506203	-0.221231
3P 45.6880	-0.008811	0.040497	0.024093
3P 17.9535	0.207881	-0.096627	-0.023526
3P 10.4294	0.005614	0.607484	0.216321
3P 7.9116	-0.000815	0.524132	0.341837
4P 36.6952	-0.025164	0.054331	0.031441
4P 5.4132	0.000032	0.011449	-0.533904
4P 3.5961	-0.000052	-0.000348	-0.580315
4P 2.3285	0.000002	0.000274	-0.089681

	3d	4d
ORB.ENERGY	-11.343334	-0.412767
<R>	0.382504	1.630109
<R**2>	0.174579	3.259047
<1/R>	3.195826	0.824848
<1/R**2>	12.888866	1.289621
<1/R**3>	68.576385	5.142827
3D 24.1687	0.013758	0.003579
3D 13.4515	0.419226	0.121318
3D 6.5053	0.292226	0.213964
3D 4.0439	0.007494	-0.455974
4D 10.3841	0.359007	0.082299
4D 2.9873	0.000548	-0.440806
4D 1.8815	0.000087	-0.308210
4D 1.2184	0.000068	-0.084621

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, Z = 2-54

See page 118 for Explanation of Table

RHODIUM, Z=45 [Kr]4d(8)5s(1) 4F

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-4685.881686	4685.881624	-9371.763310	-2.000000013

RHOat0 = 400684.70 Kato cusp = 2.000831

	1s	2s	3s	4s	5s
ORB.ENERGY	-834.039464	-121.563637	-22.879601	-3.503878	-0.221613
<R>	0.033844	0.146991	0.400322	1.016687	3.702057
<R**2>	0.001533	0.025403	0.183085	1.169999	15.898379
<1/R>	44.481916	10.109146	3.578229	1.326834	0.340218
<1/R**2>	3972.114072	415.511754	78.385935	13.558832	0.790115
1S 45.7788	0.963300	0.309058	-0.132580	0.054073	-0.012384
2S 38.8162	0.042397	0.244158	-0.130512	0.054017	-0.012320
2S 21.7902	-0.002115	-0.977603	0.528972	-0.218980	0.049849
3S 56.5086	0.005005	-0.000199	-0.000533	0.000178	-0.000004
3S 16.2941	-0.000265	-0.148954	-0.082985	-0.009239	0.007077
3S 9.0435	0.000013	-0.005830	-0.872709	0.633984	-0.168794
4S 25.4412	0.001061	-0.133289	0.177565	-0.076562	0.017614
4S 5.7859	-0.000003	0.000908	-0.013738	-0.665080	0.207481
4S 3.9281	0.000004	-0.000309	0.000731	-0.550367	0.107292
5S 14.9903	-0.000015	0.010662	-0.199602	0.040465	-0.001585
5S 2.5691	-0.000001	0.000101	-0.000395	-0.018196	-0.271487
5S 1.5698	0.000000	-0.000048	0.000151	0.002464	-0.559488
5S 0.9897	0.000000	0.000018	-0.000051	-0.000258	-0.331979

	2p	3p	4p		3d	4d
ORB.ENERGY	-112.386169	-19.179583	-2.291136	ORB.ENERGY	-12.421280	-0.450183
<R>	0.126016	0.393875	1.104031	<R>	0.368927	1.531455
<R**2>	0.019341	0.179916	1.396909	<R**2>	0.162142	2.873215
<1/R>	10.076687	3.483279	1.209582	<1/R>	3.307609	0.878699
<1/R**2>	137.715931	25.782000	4.188646	<1/R**2>	13.781017	1.460626
<1/R**3>	2877.213116	498.268393	71.746275	<1/R**3>	75.610039	6.086010
2P 57.1592	0.000108	0.011910	0.007352	3D 24.9328	0.013008	0.003491
2P 22.3381	0.850632	-0.502207	-0.221625	3D 13.9092	0.416960	0.124544
3P 47.1396	-0.009588	0.039104	0.023422	3D 6.7910	0.290073	0.240728
3P 18.4771	0.212153	-0.102857	-0.027131	3D 4.3808	0.008045	-0.461136
3P 10.6701	0.005752	0.630166	0.224562	4D 10.7708	0.361199	0.083280
3P 8.1551	-0.001016	0.503167	0.351346	4D 3.2220	0.000880	-0.448582
4P 37.8449	-0.025177	0.052362	0.030544	4D 2.0251	0.000162	-0.313926
4P 5.6674	0.000042	0.011550	-0.538045	4D 1.2974	0.000098	-0.086941
4P 3.7624	-0.000061	-0.000140	-0.584071			
4P 2.4396	0.000003	0.000275	-0.091491			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

PALLADIUM, Z=46 [Kr]4d(10) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-4937.921004	4937.921032	-9875.842036	-1.999999994

RHOat0 = 428395.15 Kato cusp = 2.000808

	1s	2s	3s	4s
ORB.ENERGY	-873.315913	-127.966552	-24.209082	-3.587289
<R>	0.033099	0.143552	0.389298	0.985959
<R**2>	0.001466	0.024225	0.173103	1.101818
<1/R>	45.480522	10.353164	3.682831	1.371555
<1/R**2>	4152.168880	435.708975	83.040800	14.537300
1S	46.7974	0.963477	-0.309644	-0.133550	-0.054815
2S	39.7609	0.042281	-0.241461	-0.123434	-0.052756
2S	22.2661	-0.002125	0.972158	0.501753	0.214648
3S	57.8248	0.004837	0.000190	-0.000331	-0.000069
3S	17.1695	-0.000218	0.166151	0.174110	0.063272
3S	10.4876	-0.000076	-0.015150	-1.041445	-0.323329
3S	7.6059	0.000074	0.012539	-0.215033	-0.632043
4S	26.2283	0.001060	0.120928	0.128957	0.065935
4S	7.0968	-0.000036	-0.005154	0.010786	0.630734
4S	4.6932	0.000010	0.000654	-0.002595	0.712527
4S	3.1874	-0.000002	-0.000147	-0.000254	0.151216

	2p	3p	4p
ORB.ENERGY	-118.531082	-20.374264	-2.330069
<R>	0.122981	0.382314	1.068566
<R**2>	0.018416	0.169459	1.311048
<1/R>	10.322528	3.589665	1.253042
<1/R**2>	144.473329	27.350491	4.501777
<1/R**3>	3089.985637	542.141531	79.271902
2P	58.8127	-0.000956	0.011820	0.007233
2P	23.0155	0.848032	-0.497355	-0.219932
3P	48.5886	-0.011945	0.038274	0.022796
3P	19.0380	0.219542	-0.111306	-0.031602
3P	10.9139	0.006054	0.652935	0.231305
3P	8.3975	-0.001285	0.482199	0.357808
4P	39.0467	-0.026699	0.050845	0.029584
4P	5.9151	0.000060	0.011737	-0.542403
4P	3.9120	-0.000073	0.000059	-0.579630
4P	2.5168	0.000001	0.000348	-0.103448

	3d	4d
ORB.ENERGY	-13.363420	-0.335984
<R>	0.356139	1.533028
<R**2>	0.150821	2.951405
<1/R>	3.420148	0.892660
<1/R**2>	14.708093	1.519603
<1/R**3>	83.143427	6.506021
3D	25.6291	0.012542	0.003306
3D	14.3366	0.417949	0.122300
3D	7.0434	0.282174	0.259777
3D	4.7075	0.007467	-0.458744
4D	11.1238	0.367116	0.080472
4D	3.3993	0.000776	-0.450081
4D	2.0532	-0.000099	-0.331187
4D	1.2286	0.000030	-0.115963

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

SILVER, Z=47 [Kr]4d(10)5s(1) 2S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-5197.698452	5197.698391	-10395.39684	-2.000000012

RHOat0 = 457506.91 Kato cusp = 2.000809

	1s	2s	3s	4s	5s
ORB.ENERGY	-913.835587	-134.878402	-25.917812	-4.001481	-0.219972
<R>	0.032386	0.140268	0.378839	0.949403	3.655961
<R**2>	0.001403	0.023127	0.163895	1.020639	15.577450
<1/R>	46.479064	10.597352	3.787881	1.427064	0.344268
<1/R**2>	4336.204776	456.400145	87.852441	15.794289	0.782627
1S 47.8514	0.962576	0.309871	-0.134351	0.055923	0.011744
2S 40.9787	0.043178	0.228566	-0.118518	0.051198	0.010877
2S 22.0035	-0.001792	-1.017441	0.533350	-0.230754	-0.048947
3S 59.2334	0.004598	0.000077	-0.000484	0.000190	0.000002
3S 14.2658	-0.000095	-0.229517	0.240470	-0.109861	-0.017119
3S 9.8321	-0.000064	0.207153	-1.582931	0.833102	0.170582
4S 26.8874	0.000892	-0.105288	0.128920	-0.065026	-0.014950
4S 6.1462	-0.000005	-0.001975	-0.011704	-0.694923	-0.200263
4S 4.1628	0.000005	0.000556	0.000035	-0.526878	-0.085225
5S 12.0237	0.000047	-0.097011	0.272133	-0.057381	0.000512
5S 2.6653	-0.000002	-0.000103	-0.000238	-0.015230	0.266367
5S 1.6001	0.000000	0.000045	0.000089	0.001617	0.554588
5S 0.9964	0.000000	-0.000015	-0.000027	-0.000589	0.343864

	2p	3p	4p		3d	4d
ORB.ENERGY	-125.181574	-21.945422	-2.676802	ORB.ENERGY	-14.678189	-0.537384
<R>	0.120088	0.371418	1.023203	<R>	0.344428	1.369800
<R**2>	0.017555	0.159896	1.199843	<R**2>	0.140869	2.291413
<1/R>	10.568378	3.696050	1.310063	<1/R>	3.531194	0.981689
<1/R**2>	151.392127	28.964882	4.921961	<1/R**2>	15.654430	1.809902
<1/R**3>	3312.961384	588.488911	89.227741	<1/R**3>	91.081757	8.136570
2P 59.6755	-0.000486	0.012015	0.007326	3D 26.5320	0.011443	0.003198
2P 23.4442	0.852285	-0.504748	-0.225437	3D 14.8584	0.408967	0.127221
3P 49.2846	-0.010777	0.038779	0.023026	3D 7.4089	0.293527	0.292865
3P 19.4073	0.212194	-0.108002	-0.031813	3D 5.0317	0.010359	-0.473484
3P 11.1133	0.005206	0.693682	0.248680	4D 11.5827	0.360675	0.081591
3P 8.5884	-0.001057	0.442503	0.362284	4D 3.6742	0.000592	-0.461096
4P 39.6983	-0.025296	0.050594	0.029300	4D 2.3057	-0.000043	-0.323613
4P 6.1921	0.000004	0.011693	-0.544134	4D 1.4594	0.000013	-0.089292
4P 4.0980	-0.000056	0.000268	-0.593807			
4P 2.6664	-0.000002	0.000287	-0.097203			

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

CADMIUM, Z=48 [Kr]4d(10)5s(2) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-5465.133119	5465.133066	-10930.26618	-2.000000010

RHOat0 = 487877.14 Kato cusp = 2.000792

	1s	2s	3s	4s	5s
ORB.ENERGY	-955.315341	-142.006812	-27.708607	-4.450517	-0.264844
<R>	0.031703	0.137128	0.368910	0.914133	3.237216
<R**2>	0.001345	0.022100	0.155390	0.945138	12.166505
<1/R>	47.477627	10.841708	3.893205	1.484941	0.390406
<1/R**2>	4524.234370	477.582300	92.811103	17.160652	1.070592
1S 48.8593	-0.963076	0.310527	-0.135316	0.057161	0.013586
2S 41.8698	-0.042646	0.228857	-0.119308	0.052306	0.012564
2S 22.4790	0.001795	-1.019867	0.537403	-0.235995	-0.056626
3S 60.4880	-0.004491	0.000076	-0.000469	0.000199	0.000016
3S 14.3001	0.000057	-0.259887	0.288963	-0.139049	-0.027410
3S 10.1202	0.000109	0.254786	-1.653006	0.889261	0.209002
4S 27.5563	-0.000878	-0.103810	0.128363	-0.065501	-0.016811
4S 6.4013	0.000007	-0.002567	-0.011693	-0.685578	-0.225422
4S 4.3771	-0.000006	0.000722	-0.000097	-0.544565	-0.106966
5S 12.3302	-0.000072	-0.114971	0.296330	-0.068777	-0.003003
5S 2.8247	0.000002	-0.000139	-0.000218	-0.014236	0.305107
5S 1.7468	-0.000001	0.000062	0.000081	0.001843	0.559228
5S 1.0996	0.000000	-0.000020	-0.000026	-0.000446	0.299847

	2p	3p	4p
ORB.ENERGY	-132.047005	-23.597219	-3.053486
<R>	0.117327	0.361119	0.980384
<R**2>	0.016753	0.151114	1.099649
<1/R>	10.814311	3.802547	1.368985
<1/R**2>	158.474708	30.626741	5.375469
<1/R**3>	3546.474693	637.431377	100.266914
2P 61.2693	-0.003491	0.012056	0.007329
2P 24.3867	0.846774	-0.487592	-0.220421
3P 51.0214	-0.017899	0.037082	0.022058
3P 20.1418	0.233029	-0.129977	-0.042937
3P 11.4415	0.006386	0.692790	0.248783
3P 8.8868	-0.001657	0.447228	0.381672
4P 41.2731	-0.031025	0.047556	0.027784
4P 6.4430	0.000083	0.012624	-0.547540
4P 4.2737	-0.000088	0.000261	-0.608051
4P 2.7729	0.000006	0.000230	-0.084838

	3d	4d
ORB.ENERGY	-16.071957	-0.763640
<R>	0.333489	1.252086
<R**2>	0.131895	1.884727
<1/R>	3.642018	1.064243
<1/R**2>	16.628547	2.105655
<1/R**3>	99.496539	9.903393
3D 27.1187	0.011362	0.003372
3D 15.2353	0.415382	0.134092
3D 7.5671	0.273191	0.410853
3D 5.7574	0.008574	-0.530026
4D 11.8823	0.374807	0.080051
4D 4.0763	0.001446	-0.492902
4D 2.6003	-0.000168	-0.337277
4D 1.6781	0.000035	-0.079483

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

INDIUM, Z=49 [Kr]4d(10)5s(2)5p(1) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-5740.169136	5740.169085	-11480.33822	-2.000000009

RHOat0 = 519574.86 Kato cusp = 2.000773

	1s	2s	3s	4s	5s
ORB.ENERGY	-997.800440	-149.395427	-29.624647	-4.976682	-0.372649
<R>	0.031048	0.134125	0.359491	0.881300	2.844453
<R**2>	0.001290	0.021140	0.147532	0.877587	9.304171
<1/R>	48.476204	11.086132	3.998535	1.543153	0.444787
<1/R**2>	4716.256388	499.249788	97.904761	18.591183	1.468225
1S 49.8562	-0.963874	0.311262	-0.136287	0.058380	0.015733
2S 42.7396	-0.041635	0.232797	-0.121521	0.054098	0.014736
2S 23.3252	0.001644	-0.998250	0.526341	-0.234633	-0.063871
3S 61.5834	-0.004461	0.000146	-0.000472	0.000173	0.000019
3S 15.4101	-0.000167	-0.246350	0.292647	-0.136020	-0.032213
3S 10.5039	0.000414	0.211167	-1.611645	0.868222	0.234704
4S 28.3599	-0.000714	-0.116182	0.130254	-0.067856	-0.019619
4S 6.6346	0.000008	-0.002366	-0.014751	-0.672160	-0.251912
4S 4.5945	-0.000008	0.000716	0.000660	-0.559666	-0.133245
5S 12.8800	-0.000229	-0.100060	0.265628	-0.043432	0.002168
5S 2.9947	0.000003	-0.000144	-0.000375	-0.013547	0.343640
5S 1.9172	-0.000002	0.000067	0.000169	0.001819	0.566475
5S 1.2425	0.000000	-0.000021	-0.000051	-0.000457	0.246558

	2p	3p	4p	5p
ORB.ENERGY	-139.171910	-25.374265	-3.507196	-0.197279
<R>	0.114689	0.351365	0.939852	3.777242
<R**2>	0.016005	0.143028	1.008733	16.634893
<1/R>	11.060332	3.909187	1.429675	0.331864
<1/R**2>	165.721288	32.336681	5.862263	0.313803
<1/R**3>	3790.740322	689.033986	112.429693	4.457480
2P 50.3601	0.069930	-0.000716	0.020255	-0.004135
2P 19.8835	0.714310	0.656646	-0.471830	0.094945
3P 42.1272	0.149803	-0.017882	0.064433	-0.013104
3P 12.3717	0.001067	-0.901074	0.706386	-0.141370
3P 8.9588	0.000149	-0.451270	0.168541	-0.039221
4P 34.7384	0.105796	-0.041099	0.082715	-0.016775
4P 6.0595	-0.000141	-0.005543	-0.679925	0.174014
4P 4.0228	-0.000010	-0.000663	-0.485366	0.073620
5P 18.7753	0.006026	0.130590	-0.191612	0.038641
5P 2.5200	-0.000005	0.000011	-0.015790	-0.269992
5P 1.5365	0.000002	-0.000003	0.001286	-0.555145
5P 0.9534	0.000000	0.000004	-0.000517	-0.333057

	3d	4d
ORB.ENERGY	-17.589547	-1.063118
<R>	0.323243	1.156916
<R**2>	0.123768	1.590773
<1/R>	3.752678	1.144702
<1/R**2>	17.630750	2.416159
<1/R**3>	108.403669	11.856480
3D 27.9290	0.010541	-0.003594
3D 15.7710	0.402123	-0.103601
3D 8.4278	0.174209	-1.002117
3D 7.3906	0.135450	0.859764
4D 12.3645	0.357445	0.037696
4D 4.7206	0.002120	0.529715
4D 3.0048	-0.000091	0.396615
4D 1.9243	0.000007	0.082009

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

TIN, Z=50 [Kr]4d(10)5s(2)5p(2) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-6022.931678	6022.931640	-12045.86332	-2.000000006

RHOat0 = 552621.73 Kato cusp = 2.000769

		1s	2s	3s	4s	5s
ORB.ENERGY		1041.223339	-156.977572	-31.598969	-5.512489	-0.476426
<R>		0.030419	0.131250	0.350534	0.850435	2.585885
<R**2>		0.001238	0.020241	0.140251	0.816477	7.646049
<1/R>		49.474791	11.330667	4.104012	1.602228	0.490494
<1/R**2>		4912.272590	521.406227	103.140624	20.102124	1.851116
1S	50.8848	-0.963742	0.311679	-0.137098	0.059535	0.017407
2S	43.6518	-0.042158	0.232593	-0.122055	0.055090	0.016260
2S	23.7600	0.001971	-1.003187	0.531834	-0.240399	-0.070946
3S	63.1844	-0.004214	0.000149	-0.000468	0.000181	0.000038
3S	15.3000	0.000076	-0.281509	0.349803	-0.169197	-0.046567
3S	10.7843	0.000092	0.270107	-1.701531	0.933273	0.277739
4S	29.0062	-0.000941	-0.113792	0.130124	-0.068648	-0.021206
4S	6.9275	0.000008	-0.003118	-0.014337	-0.648826	-0.265073
4S	4.8462	-0.000007	0.000912	0.000313	-0.591938	-0.165573
5S	13.1566	-0.000064	-0.122197	0.299228	-0.057389	-0.003124
5S	3.1710	0.000003	-0.000182	-0.000288	-0.014377	0.371340
5S	2.0784	-0.000002	0.000086	0.000144	0.002015	0.562270
5S	1.3745	0.000000	-0.000027	-0.000039	-0.000545	0.222868

		2p	3p	4p	5p
ORB.ENERGY		-146.489258	-27.209033	-3.969043	-0.265035
<R>		0.112165	0.342112	0.902128	3.248093
<R**2>		0.015304	0.135565	0.927899	12.191397
<1/R>		11.306439	4.015986	1.491373	0.386575
<1/R**2>		173.132173	34.095123	6.378493	0.445571
<1/R**3>		4046.070155	743.401042	125.701866	6.832151
2P	52.0165	0.065285	-0.000395	0.018150	-0.004624
2P	20.4432	0.731458	0.646815	-0.454590	0.110016
3P	43.4868	0.140962	-0.015665	0.058174	-0.014678
3P	12.6049	0.000357	-0.902956	0.699907	-0.168847
3P	9.1725	0.000268	-0.432953	0.171411	-0.045190
4P	35.8464	0.100039	-0.037195	0.075210	-0.018836
4P	6.3115	-0.000171	-0.005180	-0.672221	0.203400
4P	4.2560	-0.000002	-0.000768	-0.498300	0.094435
5P	19.3198	0.006952	0.120041	-0.178466	0.044257
5P	2.7011	-0.000007	0.000042	-0.015496	-0.313546
5P	1.7056	0.000004	-0.000013	0.001276	-0.561331
5P	1.0938	-0.000001	0.000008	-0.000511	-0.273972

		3d	4d
ORB.ENERGY		-19.163348	-1.369034
<R>		0.313622	1.080402
<R**2>		0.116380	1.377097
<1/R>		3.863205	1.221482
<1/R**2>		18.661202	2.733849
<1/R**3>		117.818962	13.957697
3D	28.8714	0.009551	-0.003436
3D	16.3132	0.391196	-0.098746
3D	8.8904	0.185799	-0.973948
3D	7.6656	0.143279	0.796256
4D	12.8390	0.347738	0.055998
4D	4.9306	0.002084	0.548357
4D	3.1899	-0.000128	0.387795
4D	2.0484	0.000005	0.061893

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

ANTIMONY, Z=51 [Kr]4d(10)5s(2)5p(3) 4S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-6313.485304	6313.485364	-12626.97067	-1.999999990

RHOat0 = 587044.44 Kato cusp = 2.000752

	1s	2s	3s	4s	5s
ORB.ENERGY	1085.589032	-164.757946	-33.636206	-6.063172	-0.581765
<R>	0.029816	0.128494	0.342004	0.821515	2.390153
<R**2>	0.001189	0.019398	0.133489	0.761324	6.506819
<1/R>	50.473390	11.575314	4.209629	1.661857	0.532141
<1/R**2>	5112.280230	544.052180	108.518628	21.687379	2.237688
1S 51.8877	-0.964330	0.312314	-0.137982	0.060711	-0.018852
2S 44.5213	-0.041502	0.235156	-0.123689	0.056632	-0.017743
2S 24.4600	0.001952	-0.992428	0.527160	-0.241679	0.075737
3S 64.3876	-0.004143	0.000160	-0.000461	0.000161	-0.000046
3S 16.0100	-0.000017	-0.280646	0.361794	-0.173010	0.052605
3S 11.1348	0.000222	0.256053	-1.690278	0.932230	-0.298252
4S 29.7459	-0.000889	-0.119544	0.130614	-0.070282	0.022826
4S 7.1903	0.000009	-0.003210	-0.016561	-0.626505	0.272024
4S 5.0920	-0.000009	0.000969	0.000808	-0.617304	0.195900
5S 13.6191	-0.000129	-0.117797	0.285046	-0.041765	-0.000107
5S 3.3489	0.000003	-0.000192	-0.000364	-0.015234	-0.393283
5S 2.2326	-0.000002	0.000092	0.000200	0.002101	-0.556743
5S 1.5001	0.000000	-0.000028	-0.000052	-0.000613	-0.209339

	2p	3p	4p	5p
ORB.ENERGY	-154.003778	-29.106134	-4.444706	-0.334705
<R>	0.109749	0.333323	0.867077	2.901067
<R**2>	0.014649	0.128664	0.855986	9.667023
<1/R>	11.552631	4.122931	1.553756	0.433785
<1/R**2>	180.707339	35.902001	6.922127	0.576437
<1/R**3>	4312.681007	800.596117	140.076276	9.345140
2P 53.7047	0.061335	-0.000059	0.016559	-0.005130
2P 20.9836	0.744974	0.638631	-0.443368	0.123457
3P 44.8533	0.133912	-0.013587	0.053525	-0.016292
3P 12.8322	0.000023	-0.911119	0.703768	-0.196548
3P 9.3659	0.000314	-0.411288	0.168629	-0.045694
4P 36.9427	0.095844	-0.033699	0.069735	-0.020924
4P 6.5539	-0.000192	-0.004469	-0.667082	0.224069
4P 4.4870	0.000004	-0.000920	-0.508060	0.114248
5P 19.8592	0.007501	0.110887	-0.168885	0.050016
5P 2.8844	-0.000009	0.000082	-0.015231	-0.345604
5P 1.8640	0.000005	-0.000032	0.001432	-0.560641
5P 1.2205	-0.000001	0.000012	-0.000380	-0.239545

	3d	4d
ORB.ENERGY	-20.798064	-1.687854
<R>	0.304568	1.016399
<R**2>	0.109644	1.212421
<1/R>	3.973620	1.295656
<1/R**2>	19.719955	3.060008
<1/R**3>	127.755391	16.216641
3D 18.7549	0.178452	0.009818
3D 11.7256	0.720283	-0.753495
3D 8.1288	0.234244	0.146216
4D 25.4647	-0.018179	0.008944
4D 14.9735	-0.066416	0.284152
4D 5.6954	0.001380	0.515789
4D 3.7082	0.000355	0.474863
4D 2.3636	-0.000101	0.089348

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, Z = 2–54

See page 118 for Explanation of Table

TELLURIUM, Z=52 [Kr]4d(10)5s(2)5p(4) 3P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-6611.784043	6611.784050	-13223.56809	-1.999999999

RHOat0 = 622874.99 Kato cusp = 2.000737

		1s	2s	3s	4s	5s
ORB.ENERGY		1130.916996	-172.755400	-35.754883	-6.647011	-0.700555
<R>		0.029236	0.125850	0.333871	0.794422	2.227963
<R**2>		0.001143	0.018606	0.127199	0.711487	5.637959
<1/R>		51.472008	11.820079	4.315393	1.721886	0.572717
<1/R**2>		5316.282203	567.189131	114.039411	23.344190	2.651395
1S	52.8991	-0.964664	0.312852	-0.138803	0.061845	0.020204
2S	45.4465	-0.041115	0.233815	-0.123500	0.057243	0.018858
2S	24.8600	0.001902	-0.997672	0.532103	-0.246978	-0.081399
3S	65.6488	-0.004049	0.000167	-0.000437	0.000163	0.000055
3S	16.0400	-0.000139	-0.310341	0.420965	-0.210337	-0.069302
3S	11.4242	0.000378	0.304298	-1.778781	1.000308	0.339745
4S	30.4485	-0.000844	-0.114638	0.128010	-0.069568	-0.023624
4S	7.4618	0.000011	-0.003957	-0.016045	-0.610764	-0.280046
4S	5.3315	-0.000011	0.001178	0.000516	-0.641036	-0.223822
5S	13.9235	-0.000205	-0.135154	0.316904	-0.058386	-0.006221
5S	3.4919	0.000004	-0.000228	-0.000262	-0.015384	0.433791
5S	2.3444	-0.000002	0.000111	0.000169	0.002097	0.549980
5S	1.5918	0.000000	-0.000034	-0.000040	-0.000673	0.179374

		2p	3p	4p	5p
ORB.ENERGY		-161.734370	-31.084040	-4.952561	-0.359827
<R>		0.107434	0.324966	0.834979	2.691328
<R**2>		0.014034	0.122270	0.793022	8.338314
<1/R>		11.798907	4.229998	1.615914	0.471710
<1/R**2>		188.446948	37.757092	7.485997	0.701608
<1/R**3>		4590.820851	860.684837	155.430526	11.936268
2P	55.4092	0.057722	0.000214	0.015790	-0.005407
2P	21.5212	0.757303	0.631491	-0.440349	0.133015
3P	46.2296	0.127432	-0.011784	0.051263	-0.017209
3P	13.0584	-0.000208	-0.921065	0.723399	-0.219879
3P	9.5469	0.000342	-0.388965	0.154219	-0.043211
4P	38.0429	0.092022	-0.030576	0.067070	-0.022171
4P	6.7573	-0.000210	-0.003564	-0.671899	0.243368
4P	4.6933	0.000011	-0.001050	-0.504924	0.126850
5P	20.4079	0.007976	0.102147	-0.164779	0.053565
5P	3.0444	-0.000009	0.000121	-0.014301	-0.394122
5P	1.9579	0.000005	-0.000035	0.000655	-0.547374
5P	1.2735	-0.000001	0.000018	-0.000455	-0.215262

		3d	4d
ORB.ENERGY		-22.512343	-2.038281
<R>		0.296029	0.961176
<R**2>		0.103481	1.079909
<1/R>		4.083956	1.368189
<1/R**2>		20.807251	3.396734
<1/R**3>		138.230493	18.648071
3D	19.1502	0.189945	0.004940
3D	11.9116	0.696808	-0.781454
3D	8.2893	0.217717	0.182028
4D	26.1132	-0.017243	0.008693
4D	15.2954	-0.037499	0.280698
4D	5.8285	0.000343	0.536227
4D	3.8606	0.000478	0.456122
4D	2.4677	-0.000134	0.070461

TABLE. Roothaan-Hartree-Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

IODINE, Z=53 [Kr]4d(10)5s(2)5p(5) 2P

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-6917.980881	6917.980928	-13835.96181	-1.999999993

RHOat0 = 660139.50 Kato cusp = 2.000727

		1s	2s	3s	4s	5s
ORB.ENERGY		1177.186285	-180.949210	-37.934455	-7.244349	-0.821109
<R>		0.028678	0.123312	0.326110	0.769050	2.094420
<R**2>		0.001100	0.017861	0.121338	0.666420	4.971697
<1/R>		52.470639	12.064949	4.421281	1.782144	0.611070
<1/R**2>		5524.278168	590.816463	119.702508	25.068477	3.073379
1S	53.9232	-0.964645	0.313262	0.139548	0.062924	0.021403
2S	46.3778	-0.041350	0.233029	0.123356	0.057894	0.019834
2S	25.3200	0.002077	-0.998597	-0.533745	-0.250833	-0.086007
3S	67.1360	-0.003875	0.000169	0.000411	0.000140	0.000065
3S	16.5300	-0.000063	-0.304908	-0.436540	-0.219917	-0.078592
3S	11.7430	0.000273	0.292959	1.788202	1.016648	0.365055
4S	31.1982	-0.000950	-0.111008	-0.124327	-0.068867	-0.024011
4S	7.7564	0.000011	-0.003955	0.017184	-0.581290	-0.275646
4S	5.5959	-0.000010	0.001165	-0.000621	-0.675335	-0.261359
5S	14.3135	-0.000153	-0.130049	-0.315258	-0.051735	-0.006855
5S	3.6876	0.000004	-0.000215	0.000244	-0.017394	0.442124
5S	2.5058	-0.000002	0.000101	-0.000177	0.002308	0.549606
5S	1.7111	0.000000	-0.000030	0.000037	-0.000779	0.178244

		2p	3p	4p	5p
ORB.ENERGY		-169.660337	-33.122299	-5.473347	-0.403173
<R>		0.105213	0.317010	0.805271	2.501704
<R**2>		0.013457	0.116335	0.737040	7.200318
<1/R>		12.045262	4.337185	1.678107	0.510301
<1/R**2>		196.350971	39.660476	8.071898	0.837936
<1/R**3>		4880.731149	923.737857	171.835965	14.871083
2P	57.1079	0.053730	0.000290	0.014308	-0.005622
2P	22.0921	0.773329	0.624253	-0.427468	0.140976
3P	47.6375	0.119094	-0.010507	0.046630	-0.017855
3P	13.2707	-0.000909	-0.932085	0.726136	-0.243155
3P	9.7063	0.000538	-0.363922	0.148233	-0.038653
4P	39.2034	0.086139	-0.027814	0.061235	-0.022967
4P	6.9871	-0.000264	-0.002337	-0.671132	0.255316
4P	4.9206	0.000031	-0.001284	-0.509596	0.147401
5P	20.9853	0.008997	0.092541	-0.153148	0.056485
5P	3.2522	-0.000013	0.000175	-0.014932	-0.410935
5P	2.1021	0.000008	-0.000040	-0.000020	-0.543892
5P	1.3652	-0.000002	0.000025	-0.000577	-0.210766

		3d	4d
ORB.ENERGY		-24.285681	-2.401195
<R>		0.287964	0.913033
<R**2>		0.097830	0.971471
<1/R>		4.194206	1.439107
<1/R**2>		21.922969	3.742982
<1/R**3>		149.256705	21.250066
3D	19.5616	0.206457	-0.004338
3D	12.0593	0.645959	-0.795614
3D	8.4937	0.205748	0.222659
4D	26.9243	-0.015706	0.008081
4D	15.6155	0.009349	0.263784
4D	5.9399	0.000011	0.566249
4D	3.9812	0.000439	0.427834
4D	2.5304	-0.000133	0.052510

TABLE. Roothaan–Hartree–Fock Ground-State Atomic Wave Functions, $Z = 2$–54

See page 118 for Explanation of Table

XENON, Z=54 [Kr]4d(10)5s(2)5p(6) 1S

TOTAL ENERGY	KINETIC ENERGY	POTENTIAL ENERGY	VIRIAL RATIO
-7232.138349	7232.138386	-14464.27673	-1.999999995

RHOat0 = 698865.13 Kato cusp = 2.000711

		1s	2s	3s	4s	5s
ORB.ENERGY		1224.397767	-189.340111	-40.175652	-7.856291	-0.944407
<R>		0.028141	0.120873	0.318696	0.745267	1.980955
<R**2>		0.001059	0.017160	0.115870	0.625571	4.440087
<1/R>		53.469284	12.309921	4.527285	1.842538	0.647891
<1/R**2>		5736.266145	614.934856	125.507901	26.858025	3.506821
1S	54.9179	-0.965401	0.313912	-0.140382	0.064020	-0.022510
2S	47.2500	-0.040350	0.236118	-0.125401	0.059550	-0.021077
2S	26.0942	0.001890	-0.985333	0.528161	-0.251138	0.088978
3S	68.1771	-0.003868	0.000229	-0.000435	0.000152	-0.000081
3S	16.8296	-0.000263	-0.346825	0.494492	-0.252274	0.095199
3S	12.0759	0.000547	0.345786	-1.855445	1.063559	-0.398492
4S	31.9030	-0.000791	-0.120941	0.128637	-0.071737	0.025623
4S	8.0145	0.000014	-0.005057	-0.017980	-0.563072	0.274471
4S	5.8396	-0.000013	0.001528	0.000792	-0.697466	0.291110
5S	14.7123	-0.000286	-0.151508	0.333907	-0.058009	0.011171
5S	3.8555	0.000005	-0.000281	-0.000228	-0.018353	-0.463123
5S	2.6343	-0.000003	0.000134	0.000191	0.002292	-0.545266
5S	1.8124	0.000001	-0.000040	-0.000037	-0.000834	-0.167779

		2p	3p	4p	5p
ORB.ENERGY		-177.782438	-35.221651	-6.008328	-0.457283
<R>		0.103082	0.309425	0.777023	2.337950
<R**2>		0.012915	0.110816	0.685527	6.276430
<1/R>		12.291694	4.444510	1.741492	0.547155
<1/R**2>		204.419530	41.612611	8.690096	0.970729
<1/R**3>		5182.670677	989.845535	189.572708	17.825267
2P	58.7712	0.051242	0.000264	0.013769	-0.005879
2P	22.6065	0.781070	0.622357	-0.426955	0.149040
3P	48.9702	0.114910	-0.009861	0.045088	-0.018716
3P	13.4997	-0.000731	-0.952677	0.748434	-0.266839
3P	9.8328	0.000458	-0.337900	0.132850	-0.031096
4P	40.2591	0.083993	-0.026340	0.059406	-0.024100
4P	7.1841	-0.000265	-0.000384	-0.679569	0.267374
4P	5.1284	0.000034	-0.001665	-0.503653	0.161460
5P	21.5330	0.009061	0.087491	-0.149635	0.059721
5P	3.4469	-0.000014	0.000240	-0.014193	-0.428353
5P	2.2384	0.000006	-0.000083	0.000528	-0.542284
5P	1.4588	-0.000002	0.000026	-0.000221	-0.201667

		3d	4d
ORB.ENERGY		-26.118859	-2.777871
<R>		0.280333	0.870451
<R**2>		0.092633	0.880863
<1/R>		4.304379	1.508735
<1/R**2>		23.067118	4.099141
<1/R**3>		160.847940	24.028996
3D	19.9787	0.220185	-0.013758
3D	12.2129	0.603140	-0.804573
3D	8.6994	0.194682	0.260624
4D	27.7398	-0.014369	0.007490
4D	15.9410	0.049865	0.244109
4D	6.0580	-0.000300	0.597018
4D	4.0990	0.000418	0.395554
4D	2.5857	-0.000133	0.039786