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

CARLOS F. BUNGE and JOSÉ A. BARRIENTOS

Instituto de Física, Universidad Nacional Autónoma de México
Apartado Postal 20-364, 01000 México D.F., México

and

ANNIK VIVIER BUNGE

Departamento de Química, Universidad Autónoma Metropolitana
Apartado Postal 55-534, Iztapalapa, 09340 México D.F., México

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. © 1993 Academic Press, Inc.

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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 correla-

tion 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:

$$R_{nl} = \sum_j S_{jl} C_{jln}. \qquad (1)$$

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

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

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

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

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 D_α with coefficients a_α fixed for each L-S symmetry:

$$\Phi = \sum_\alpha D_\alpha a_\alpha. \qquad (4)$$

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

$$F_c C = eSC \qquad (5a)$$

$$F_o C = eSC \qquad (5b)$$

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), F_c and F_o are the closed-shell and open-shell Fock matrices, respectively, S is the overlap matrix, C collects the orbital expansion coefficients C_{jln} of Eq. (2) in matrix form, and the vector 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 $1s^2 2s^2 2p^6 3s^2 3p^2$ ^{3}P. 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
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HELIUM, Z=2   1s(2)   1S

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

RHOatO = 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

RHOatO = 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

RHOatO = 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
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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
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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
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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			