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Hartree-Fock and Roothaan-Hartree-Fock energies for the ground states of He through Xe

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We report a compilation of Roothaan-Hartree-Fock (RHF) wave functions for the ground states of He through Xe, with atomic orbitals expressed in terms of Slater-type functions. Slight increases in the size of the basis set with respect to those used in Clementi and Roetti's tables [At. Data Nucl. Data Tables **14**, 177 (1974)] turn out to yield total energies to better than eight figures, reducing between 21 and 2770 times the energy errors in the above tables, and also improving over the previous numerical HF energies computed by Froese Fischer [*The Hartree-Fock Method for Atoms* (Wiley, New York, 1977)]. We also report 10-digit numerical HF energies with different results for Cr, Cu, Nb, Mo, Ru, Rh, Pd, and Ag.

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I. INTRODUCTION

Hartree-Fock (HF) atomic wave functions are independent-particle-model approximations to the nonrelativistic Schrödinger equation for stationary states. The Pauli principle is imposed through the use of Slater determinants. For an N-electron system, the HF equations yield N Hartree-Fock spin orbitals.

In the conventional Hartree-Fock approximation [1], 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. The conventional HF approximation is also known as the restricted HF approximation.

Roothaan-Hartree-Fock (RHF) or analytic self-consistent-field atomic wave functions [2] are approximations to conventional HF wave functions in which the radial atomic orbitals are expanded as a finite superposition of primitive radial functions.

Since Roothaan's papers [2] and through the early 1970s, RHF calculations yielded the most accurate atomic HF energies. Later, numerical HF calculations [1] became more accurate than RHF ones. However, our recent results for Mg [3] suggested that, once again, RHF energies might be more accurate than available numerical HF results. In this paper we communicate a compilation of RHF atomic wave functions for He through Xe [3] that is significantly more accurate than its predecessors. In order to assess the quality of the new RHF wave functions, we report ten-digit numerical HF energies, which may also serve for reference purposes.

Why use RHF atomic wave functions when an efficient code [4] for numerical multiconfiguration Hartree-Fock (MCHF) wave functions is available? The MCHF code of Froese Fischer generates HF atomic wave functions as accurately as physically reasonable, and it can also be used to introduce correlation effects, viz., to go beyond the HF approximation. Nevertheless, RHF wave functions today are very much in demand, as suggested by the 150-odd citations [5] received in 1990 by Clementi and Roetti's tables [6] of RHF atomic wave functions. Another compilation of RHF wave functions [7], less available than the work of Clementi and Roetti, has also proved very useful.

The RHF wave functions offer some advantages over their, in principle more accurate, numerical counterparts as they can be readily incorporated into a variety of codes for atomic calculations, and also for molecular and solid-state calculations by density-functional methods. Numerical wave functions, instead, need to be kept in diskettes or generated as needed, and nontrivial software is required for their use, viz., to calculate expectation and transition values.

Traditionally, RHF atomic wave functions have been expanded in terms of Slater-type orbitals (STO's). More recently, Chakravorty and Clementi [8] reported significantly improved RHF results using a very large basis set of Gaussian-type orbitals (GTO's). Although the latter may be convenient in relativistic (and nonrelativistic) calculations with finite nuclear size [8], there is continued interest in the STO basis set for the study of correlation effects, and also because far fewer STO's than GTO's are needed for a given accuracy.

Our own interest in STO-expanded RHF wave functions stems from atomic structure calculations by the configuration-interaction (CI) method. The RHF approximation is the starting point of the CI method in accurate predictions of atomic spectra and negative ions. In many instances the CI method is more powerful than the MCHF method on account of the relative ease with which basis functions can be generated, for example, for core-excited states and slightly bound negative ions.

To perform these calculations involving highly correlated electronic motions it is convenient to have rather accurate RHF wave functions to start from. In the case of electron affinities, in particular, the energy error in previous RHF results [6] is often orders of magnitude larger than the values of the affinities themselves. For example, electron affinities might be smaller than 100 meV [9], while RHF energy errors of this magnitude and above (1658 meV for Cd) are not uncommon. This observation is also valid for the prediction of atomic spectra in general.

Of course, one could use a RHF code and calculate RHF wave functions as needed. However, it is not just that simple to calculate RHF wave functions of the accuracy already reported in the literature, much less with the accuracy warranted by the applications mentioned above. Also, by considering not a few but a large number of atomic states, systematic trends emerge, allowing for more accurate and rapid results. It is therefore of interest to have a compilation of RHF wave functions with energies in error by not much more than 1 meV.

In Sec. II we report improved numerical HF energies for the ground states of He through Xe. Computer programs to carry out atomic RHF calculations are mentioned in Sec. III. In Sec. IV we discuss our RHF energy results and compare them with the more accurate numerical HF energies.

II. NUMERICAL HARTREE-FOCK CALCULATIONS

We have used a relatively old version [4] of the MCHF program of Froese Fischer to calculate numerical HF energies. The coefficients $f_k(l)$ and $g_k(l,l')$ for the Slater integrals F^k and G^k were taken from Froese Fisher's book [1], except those for Cr, Nb, Mo, Ru, and Rh, which were calculated using the relationship [10] between the $f_k(l)$ and $g_k(l,l')$, and the RHF coupling coefficients discussed by Roothaan and Bagus [11]. The Malli-Olive tabulation of RHF coupling coefficients was used [10].

In Table I we present Hartree-Fock energies for the

TABLE I. Hartree-Fock total energies (in a.u.) for the ground states of He through Xe. Values which are not available are denoted by NA.

Z	Atom	State	Configuration	Previous[a]	Present
2	He	^1S	1s(2)	−2.861 680 0	−2.861 679 995
3	Li	^2S	...2s(1)	−7.432 726 9	−7.432 726 927
4	Be	^1S	...2s(2)	−14.573 023	−14.573 023 16
5	B	^2P	...2s(2)2p(1)	−24.529 061	−24.529 060 72
6	C	^3P	...2s(2)2p(2)	−37.688 619	−37.688 618 95
7	N	^4S	...2s(2)2p(3)	−54.400 934	−54.400 934 19
8	O	^3P	...2s(2)2p(4)	−74.809 398	−74.809 398 45
9	F	^2P	...2s(2)2p(5)	−99.409 349	−99.409 349 33
10	Ne	^1S	...2s(2)2p(6)	−128.547 10	−128.547 098 0
11	Na	^2S	...3s(1)	−161.858 91	−161.858 911 6
12	Mg	^1S	...3s(2)	−199.614 63	−199.614 636 3
13	Al	^2P	...3s(2)3p(1)	−241.876 71	−241.876 707 2
14	Si	^3P	...3s(2)3p(2)	−288.854 36	−288.854 362 4
15	P	^4S	...3s(2)3p(3)	−340.718 78	−340.718 780 8
16	S	^3P	...3s(2)3p(4)	−397.504 90	−397.504 895 8
17	Cl	^2P	...3s(2)3p(5)	−459.482 07	−459.482 072 1
18	Ar	^1S	...3s(2)3p(6)	−526.817 51	−526.817 512 6
19	K	^2S	...4s(1)	−599.164 79	−599.164 786 5
20	Ca	^1S	...4s(2)	−676.758 18	−676.758 185 7
21	Sc	^2D	...3d(1)4s(2)	−759.735 72	−759.735 717 8
22	Ti	^3F	...3d(2)4s(2)	−848.406 00	−848.405 996 7
23	V	^4F	...3d(3)4s(2)	−942.884 33	−942.884 337 4
24	Cr	^7S	...3d(5)4s(1)	NA	−1043.356 376
25	Mn	^6S	...3d(5)4s(2)	−1149.866 2	−1149.866 251
26	Fe	^5D	...3d(6)4s(2)	−1262.443 7	−1262.443 665
27	Co	^4F	...3d(7)4s(2)	−1381.414 6	−1381.414 553
28	Ni	^3F	...3d(8)4s(2)	−1506.870 9	−1506.870 908

TABLE I. (*Continued*).

Z	Atom	State	Configuration	Previous[a]	Present
29	Cu	^2S	. . .3*d*(10)4*s*(1)	−1638.96[b]	−1638.963 742
30	Zn	^1S	. . .3*d*(10)4*s*(2)	−1777.848 1	−1777.848 116
31	Ga	^2P	. . .3*d*(10)4*s*(2)4*p*(1)	−1923.261 0	−1923.261 009
32	Ge	^3P	. . .3*d*(10)4*s*(2)4*p*(2)	−2075.359 7	−2075.359 733
33	As	^4S	. . .3*d*(10)4*s*(2)4*p*(3)	−2234.238 6	−2234.238 654
34	Se	^3P	. . .3*d*(10)4*s*(2)4*p*(4)	−2399.867 6	−2399.867 611
35	Br	^2P	. . .3*d*(10)4*s*(2)4*p*(5)	−2572.441 3	−2572.441 332
36	Kr	^1S	. . .3*d*(10)4*s*(2)4*p*(6)	−2752.055 0	−2752.054 977
37	Rb	^2S	. . .5*s*(1)	−2938.357 4	−2938.357 453
38	Sr	^1S	. . .5*s*(2)	−3131.545 7	−3131.545 686
39	Y	^2D	. . .4*d*(1)5*s*(2)	−3331.684 2	−3331.684 169
40	Zr	^3F	. . .4*d*(2)5*s*(2)	−3538.995 1	−3539.995 064
41	Nb	^6D	. . .4*d*(4)5*s*(1)	NA	−3753.597 727
42	Mo	^7S	. . .4*d*(5)5*s*(1)	NA	−3975.549 499
43	Tc	^6S	. . .4*d*(5)5*s*(2)	−4204.788 7	−4204.788 736
44	Ru	^5F	. . .4*d*(7)5*s*(1)	NA	−4441.539 487
45	Rh	^4F	. . .4*d*(8)5*s*(1)	NA	−4685.881 703
46	Pd	^1S	. . .4*d*(10)	−4937.92[b]	−4937.921 023
47	Ag	^2S	. . .4*d*(10)5*s*(1)	−5197.70[b]	−5197.698 472
48	Cd	^1S	. . .4*d*(10)5*s*(2)	−5465.133 1	−5465.133 141
49	In	^2P	. . .4*d*(10)5*s*(2)5*p*(1)	−5740.169 1	−5740.169 154
50	Sn	^3P	. . .4*d*(10)5*s*(2)5*p*(2)	−6022.931 7	−6022.931 694
51	Sb	^4S	. . .4*d*(10)5*s*(2)5*p*(3)	−6313.485 3	−6313.485 319
52	Te	^3P	. . .4*d*(10)5*s*(2)5*p*(4)	−6611.784 0	−6611.784 058
53	I	^2P	. . .4*d*(10)5*s*(2)5*p*(5)	−6917.980 9	−6917.980 895
54	Xe	^1S	. . .4*d*(10)5*s*(2)5*p*(6)	−7232.138 4	−7232.138 363

[a] Reference [1], except where indicated otherwise.
[b] Reference [12].

ground states of He through Xe and compare them with a previous eight-digit tabulation [1]. A few discrepancies with the old results are observed: in Mg, Ca, V, Mn, As, Rb, In, and Te, always affecting one unit in the eighth digit.

Ten-digit energy accuracy is expected after observing more than ten-digit stability upon increasing mesh sizes both for solving the HF equations and for the evaluation of one- and two-electron integrals. Virial ratios accurate to between eight and ten figures are always obtained.

The solutions of numerical HF equations for open-shell systems are usually plagued by numerical instabilities. The accuracy achieved in this work honors the exceptional quality of Froese Fisher's code [4].

Numerical HF results for the ground states of Cr, Nb, Mo, Ru, and Rh are new in the literature. 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 [12] were only accurate to six figures.

III. ROOTHAAN-HARTREE-FOCK CALCULATIONS

The first comprehensive tables of RHF atomic wave functions were produced by Clementi [13] with a program designed and written by Roothaan and Bagus [11]. That program, after undergoing a translation to FORTRAN [14], evolved along several paths. One version was used by Clementi and Roetti to generate a compilation of RHF atomic wave functions [6]. A further improved version is part of the program collection in Ref. [15]. An extension to handle open *f* shells was used to obtain RHF atomic wave functions for atomic numbers 55–92 [16].

A fourth version incorporates pseudopotentials and has been effectively documented by Daudey [17]. 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, and (iii) the convergence parameters for the Jacobi diagonalization were reduced by a factor of 10 000. Eventually, we had to replace the existing Jacobi subroutine 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 further accuracy.

IV. RESULTS AND DISCUSSION

In Table II we compare the RHF energies of this work with those of Clementi and Roetti and with the "exact" numerical values of Table I. It may be observed that, for all atoms considered, our RHF energies are less than 1 meV in error. In all cases our energies are below recent RHF energies of Chakravorty and Clementi [8] using geometrical Gaussian basis sets. Also, they are accurate to more than eight digits, which is more accurate than the previous numerical HF results [1].

In the last column of Table II we report the improved accuracy (IA) as the quotient between present and past RHF energy errors. The smallest IA is 21, for V, while

TABLE II. Roothaan-Hartree-Fock total energies (in a.u.) for the ground states of He through Xe, comparison with previous RHF results and with exact ones. The last column shows the improved accuracy (IA) defined as the quotient between present and past RHF energy errors.

Z	Atom	State	Previous RHF^a	Present RHF^b	Exact HF^c	IA
2	He	^1S	−2.861 679 9	−2.861 679 993	−2.861 679 995	47
3	Li	^2S	−7.432 725 7	−7.432 726 924	−7.432 726 927	409
4	Be	^1S	−14.573 021	−14.573 023 13	−14.573 023 16	72
5	B	^2P	−24.529 057	−24.529 060 69	−24.529 060 72	124
6	C	^3P	−37.688 612	−37.688 618 90	−37.688 618 95	139
7	N	^4S	−54.400 924	−54.400 934 15	−54.400 934 19	255
8	O	^3P	−74.809 370	−74.809 398 40	−74.809 398 45	569
9	F	^2P	−99.409 300	−999.409 349 28	−99.409 349 33	986
10	Ne	^1S	−128.547 05	−128.547 098 0	−128.547 098 0	533
11	Na	^2S	−161.858 90	−161.858 911 3	−161.858 911 6	39
12	Mg	^1S	−199.614 61	−199.614 636 1	−199.614 636 3	131
13	Al	^2P	−241.876 68	−241.876 707 0	−241.876 707 2	136
14	Si	^3P	−288.854 31	−288.854 362 2	−288.854 362 4	262
15	P	^4S	−340.718 69	−340.718 780 6	−340.718 780 8	454
16	S	^3P	−397.504 85	−397.504 895 5	−397.504 895 8	152
17	Cl	^2P	−459.481 87	−459.482 071 9	−459.482 072 1	1010
18	Ar	^1S	−526.817 39	−526.817 512 2	−526.817 512 6	306
19	K	^2S	−599.164 53	−599.164 783 1	−599.164 786 5	74
20	Ca	^1S	−676.758 03	−676.758 181 7	−676.758 185 7	39
21	Sc	^2D	−759.735 52	−759.735 712 3	−759.735 717 8	36
22	Ti	^3F	−848.405 75	−848.405 990 7	−848.405 996 7	41
23	V	^4F	−942.884 20	−942.884 330 8	−942.884 337 4	21
24	Cr	^7S	−1043.355 2	−1043.356 368	−1043.356 376	147
25	Mn	^6S	−1149.865 7	−1149.866 243	−1149.866 251	69
26	Fe	^5D	−1262.443 2	−1262.443 656	−1262.443 665	52
27	Co	^4F	−1381.414 2	−1381.414 542	−1381.414 553	32
28	Ni	^3F	−1506.870 5	−1506.870 896	−1506.870 908	34
29	Cu	^2S	−1638.962 8	−1638.963 723	−1638.963 742	50
30	Zn	^1S	−1777.847 7	−1777.848 102	−1777.848 116	30
31	Ga	^2P	−1923.260 4	−1923.261 001	−1923.261 009	76
32	Ge	^3P	−2075.359 1	−2075.359 726	−2075.359 733	90
33	As	^4S	−2234.238 2	−2234.238 647	−2234.238 654	65
34	Se	^3P	−2399.865 8	−2399.867 604	−2399.867 611	259
35	Br	^2P	−2572.440 8	−2572.441 325	−2572.441 332	76
36	Kr	^1S	−2752.054 6	−2752.054 969	−2752.054 977	47
37	Rb	^2S	−2938.347 0	−2938.357 442	−2938.357 453	950
38	Sr	^1S	−3131.537 9	−3131.545 674	−3131.545 686	649
39	Y	^2D	−3331.671 2	−3331.684 158	−3331.684 169	1179
40	Zr	^3F	−3538.982 1	−3538.995 053	−3538.995 064	1179
41	Nb	^6D	−3753.584 5	−3753.597 716	−3753.597 727	1202

TABLE II. (*Continued*).

Z	Atom	State	Previous RHF[a]	Present RHF[b]	Exact HF[c]	IA
42	Mo	^7S	−3975.533 8	−3975.549 487	−3975.549 499	1308
43	Tc	^6S	−4204.775 3	−4204.788 722	−4204.788 736	960
44	Ru	^5F	−4441.526 4	−4441.539 471	−4441.539 487	818
45	Rh	^4F	−4685.883 3[d]	−4685.881 686	−4685.881 703	
46	Pd	^1S	−4937.907 1	−4937.921 004	−4937.921 023	819
47	Ag	^2S	−5197.685 2	−5197.698 452	−5197.698 472	664
48	Cd	^1S	−5465.072 2	−5465.133 119	−5465.133 141	2770
49	In	^2P	−5740.157 0	−5740.169 136	−5740.169 154	675
50	Sn	^3P	−6022.922 0	−6022.931 678	−6022.931 694	606
51	Sb	^4S	−6313.475 5	−6313.485 304	−6313.485 319	655
52	Te	^3P	−6611.774 8	−6611.784 043	−6611.784 058	617
53	I	^2P	−6917.972 7	−6917.980 881	−6917.980 895	585
54	Xe	^1S	−7232.130 2	−7232.138 349	−7232.138 363	583

[a] Reference [2].

[b] This work and Ref. [3].

[c] This work.

[d] Wrong value, cannot be reproduced.

the largest one is 2770, for Cd. The energy errors increase smoothly from 0.002 μhartree for He up to 0.4 μhartree for Ar. These errors are much smaller than warranted by most applications, yet they were obtained with moderate-size basis sets.

The potential energies, kinetic energies, orbital energies, orbital exponents of the STO's, and corresponding expansion coefficients will be presented elsewhere [3].

The monumental tables of Clementi-Roetti RHF [6] date from 1974, a time when available computer resources were a small fraction of what we have today. Extensive orbital exponent STO optimizations were not only tedious but also appeared beyond computational reach.

The recent introduction of cheap and powerful workstations such as the IBM RS/6000 series opened the possibility to attempt RHF calculations competitive with the numerical HF results. Our results show that once effective optimization of STO orbital exponents is achieved, RHF energies converge rather fast with increasing basis-set size. Key to the success of RHF calculations is the composition of the STO basis sets, which is defined by the set of principal quantum numbers for STO's of successive angular momentum l.

For He we used one 1*s*, two 2*s* and one 3*s* STO, this combination being denoted hereafter by (121). For Li and Be we used (241) and (232) STO's, respectively. For B through Ne we used (241)(5) sets, the (5) indicating five 2*p* STO's.

In Table III we present the composition of the present STO basis and compare it with those of Bagus, Gilbert, and Roothaan [7], and of Clementi and Roetti [6]. As can be seen, there is a certain resemblance between the first two. The major difference with Clementi and Roetti's calculation is our use of (5) and (44) or (35) *d*-type basis for Rb-Sr and Y-Xe, respectively, instead of

TABLE III. Compositions of STO basis and comparison with the ones of Bagus, Gilbert, and Roothaan (BGR), and of Clementi and Roetti (CR).

	Basis composition		
Atom	Present	BGR	CR
He	(121)	(12)	(5)
Li	(241)	(23)	(24)
Be	(232)	(221)	(24)
B-Ne	(241) (5)	(221) (4)	(24) (4)
Na-Mg	(244) (5)	(123) (3)	(107) (104)
Al-Ar	(244) (44)	(123) (32)	(107) (107)
K-Ca	(1235) (43)	(1232) (32)	(2234) (24)
Sc-Zn	(1244) (43) (5)	(1232) (32) (4)	(2234) (24) (5)
Ga-Kr	(1244) (244) (5)	(1232) (322) (4)	(2233) (234) (5)
Rb-Sr	(12334) (244) (5)		(22223) (223) (3)
Y-Cd	(12334) (244) (44)		(22223) (223) (23)
In-Sn	(12334) (2334) (44)		(22223) (2223) (23)
Sb-Xe	(12334) (2334) (35)		(22223) (2223) (23)

the (3) and (32) basis employed by these authors; this accounts for most of the energy differences between both calculations. The improved accuracy reported in Table II, however, resulted also from a more comprehensive STO optimization within more effective basis-set compositions.

For a few light atoms we used the Bagus-Gilbert-Roothaan STO's [7] as starting points for larger STO optimizations. The other STO optimizations, even those involving most light atoms, started from a linearly extrapolated full basis for the two lighter (or heavier) elements. Also, interpolations were found useful. For example, given accurate RHF wave functions for In and Xe, a straight linear interpolation between them yields RHF energies for Sn, Sb, Te, and I which are in error by no more than 100 μhartree. After optimizing sequentially the STO's with lowest orbital exponents for each nl value, the error is reduced to about 20 μhartree. Further extensive orbital exponent optimization within each harmonic set lowers the energy by another 5 μhartree.

Energy optimization of STO orbital exponents becomes quite cumbersome when there is a discontinuity in the basis-set composition, for example, for In and Sn. For Y through Cd, a (44) d-type basis appears to be better than a (35) basis. For In, a (44) set is better than a (35) set by 4 μhartree but the two $3d$ STO's with smallest orbital exponents become rather close to each other. For Sn, the same energy difference shrinks to 1 μhartree and the two troublesome $3d$ STO's become approximately linearly dependent with each other if full optimization is allowed. For Xe, the (35) basis is better by 1 μhartree and it easily lends itself to extrapolation into I, Te, and Sb; the same is not true of the (44) basis.

In spite of having carried out an extensive search around many local minima in the nonlinear parameter space, we are unable to conclude how far we are from absolute energy minima for the present basis-set compositions, except for the bounds afforded by the numerical HF results. Should future needs warrant improved accuracy the present basis-set composition may serve as a guide for the construction of an enlarged set.

The main conclusion of this work is that RHF atomic wave functions of the accuracy of numerical HF can be obtained and are available [3] for the ground states of He through Xe. Apart from their practical importance, some people will also find them aesthetically satisfying.

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[1] Ch. Froese Fischer, *The Hartree-Fock Method for Atoms* (Wiley, New York, 1977).
[2] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951); **32**, 179 (1960).
[3] C. F. Bunge, J. A. Barrientos, and A. V. Bunge, At. Data Nucl. Data Tables (to be published).
[4] Ch. Froese Fischer, Comput. Phys. Commun. **14**, 145 (1978).
[5] Science Citation Index 1990, Institute for Scientific Information, Inc., Philadelphia.
[6] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).
[7] P. S. Bagus, T. L. Gilbert, and C. C. J. Roothaan, J. Chem. Phys. **56**, 5195 (1972).
[8] S. Chakravorty and E. Clementi, Phys. Rev. A **39**, 2290 (1989); A. Mohanty and E. Clementi, Chem. Phys. Lett. **157**, 348 (1989).
[9] Ch. Froese Fischer, J. B. Lagowski, and S. H. Vosko, Phys. Rev. Lett. **59**, 2263 (1987).
[10] G. L. Malli and J. P. Olive, J. Chem. Phys. **43**, 861 (1965); see also Laboratory of Molecular Structure, University of Chicago, Tech. Report No. 1962-63, Part 2 (unpublished).
[11] C. C. J. Roothaan and P. S. Bagus, in *Methods in Computational Physics,* edited by B. Alder, S. Fernbach, and M. Rotenberg (Academic, New York, 1963), Vol. 2, p. 47.
[12] J. P. Desclaux, Comput. Phys. Commun. **12**, 311 (1973).
[13] E. Clementi, IBM J. Res. Dev. **9**, 2 (1965); IBM J. Res. Dev. Suppl. **9**, 2 (1965).
[14] B. Roos, C. Salez, A. Veillard, and E. Clementi, IBM Tech. Report No. RJ-518, 1968 (unpublished).
[15] *Modern Techniques in Computational Chemistry: MOTECC-90,* edited by E. Clementi (ESCOM Science, Leiden, 1990).
[16] A. D. McLean and R. S. McLean, At. Data Nucl. Data Tables **26**, 197 (1981).
[17] J.-P. Daudey, Instituto de Fisica, Universidad Nacional Autónoma de México Tech. Report 1978 (unpublished).