Atomic Self-Consistent-Field Program by the Basis Set Expansion Method: Columbus Version

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Abstract

A revised and extended (Columbus) version of the Chicago atomic self-consistent-field (Hartree-Fock) program of 1963 is described. Its principal present use is in developing Gaussian basis sets for molecular calculations. Complete memory allocation (using Fortran 90) has been added as well as improved integral formulas and efficient and simple programming features. Energy-expression coefficients have been added sufficient to treat the ground states of all atoms to the extent that Russell-Saunders (LS) coupling applies. Excited states with large angular-momentum orbitals can be treated. Relativistic effects can be included to the extent possible with relativistic effective core potentials. An alternative method of exponent optimization is provided. A review of earlier work is included.

PACS codes and keywords:

31.15.Ar   Ab initio calculations
31.15.Ne   Self-consistent-field methods

I   Introduction

This program carries out atomic self-consistent-field (SCF) calculations for Slater or Gaussian basis sets. Effective core potentials may be used. The number of open shells, with some exceptions, is limited to one for each symmetry.

The antecedents of this program are (1) the original (Chicago) version written by Roothaan and Bagus [1], in assembly language, for the IBM 70xx series computers and (2) the subsequent (San Jose) Fortran II version written by Roos, Salez, Veillard, and Clementi [2].

The present (Columbus) version is written in Fortran 90, and is based on the Bielefeld version [3], written in Fortran 66 (later modified to Fortran 77), which is one of many descendants of the San Jose version. The features of the program will be described principally with respect to the original Chicago version. The principal use of this program has been for developing basis sets for molecular calculations [4, 5, 6].

Since the general exposition of the theory and methods on which this program is based are contained in early references which are difficult to obtain [1, 2], this paper includes a review of the earlier work. The original [1] section numbers and titles are used to facilitate comparison.

II   General Theory

This section is mostly summarized from Roothaan and Bagus [1], but extensions concerning the use of Gaussian basis sets and effective core potentials (ECPs) have been included.

The orbitals $(\phi_{i\lambda\alpha})$ are expressed as linear combinations of basis functions $(\chi_{p\lambda\alpha})$ by

$$\phi_{i\lambda\alpha} = \Sigma_p \chi_{p\lambda\alpha} C_{pi\lambda}$$

where λ designates the orbital angular momentum magnitude quantum number and α designates the orbital angular momentum component quantum number (commonly m_l). The basis functions are expressed as products of radial and angular factors,

$$\chi_{p\lambda\alpha} = R_{p\lambda}(r) Y_{\lambda\alpha}(\theta, \phi)$$

where the $R_{p\lambda}$ (unnormalized) can be either Slater orbitals (STOs)

$$r^{n-1} e^{-\zeta r}$$

or Gaussian orbitals (GTOs)

$$r^{n-1}e^{-\zeta r^2}$$

where, for GTOs,

$$n - \lambda = \text{odd integer}$$

to enable convenient molecular use.

The one-electron integrals needed (overlap, kinetic energy, nuclear attraction) are

$$S_{\lambda pq} = \int_0^\infty R_{\lambda p}(r) R_{\lambda q}(r) r^2 dr$$

$$T_{\lambda pq} = \frac{1}{2} \int_0^\infty [R'_{\lambda p}(r) R'_{\lambda q}(r) r^2 + \lambda(\lambda + 1) R_{\lambda p}(r) R_{\lambda q}(r)] dr$$

$$U_{\lambda pq} = \int_0^\infty R_{\lambda p}(r) R_{\lambda q}(r) r dr$$

In addition, if ECPs are used for each angular momentum, then

$$U_{\lambda pq}^{ECP} = \int_0^\infty R_{\lambda p}(r) \mathbf{U}_\lambda^{\mathbf{ECP}} R_{\lambda q}(r) r^2 dr$$

The energy integrals are combined into

$$H_{\lambda pq} = T_{\lambda pq} - Z U_{\lambda pq} + U_{\lambda pq}^{ECP}$$

(where the last term is optional).

These integrals are stored in one-dimensional arrays with the λpq indices combined into a single index in dictionary order on λpq with $p \geq q$. Such arrays are called *supervectors*.

For self-consistent-field (SCF) calculations, electron-repulsion integrals are needed in which two orbitals have angular momentum λ and two orbitals have angular momentum μ, where λ and μ can be equal. The two ways of arranging these orbitals among the two electrons give the (symmetric) coulomb and exchange *supermatrices*.

$$\mathcal{J}_{\lambda pq, \mu rs, \nu} = \int_0^\infty \int_0^\infty R_{\lambda p}(r_1) R_{\lambda q}(r_1)(r_<^\nu / r_>^{\nu+1}) R_{\mu r}(r_2) R_{\mu s}(r_2) r_1^2 dr_1 r_2^2 dr_2$$

$$\mathcal{K}_{\lambda pq, \mu rs, \nu} = \frac{1}{2} [\int_0^\infty \int_0^\infty R_{\lambda p}(r_1) R_{\lambda q}(r_2)(r_<^\nu / r_>^{\nu+1}) R_{\mu r}(r_1) R_{\mu s}(r_2) r_1^2 dr_1 r_2^2 dr_2$$

$$+ \int_0^\infty \int_0^\infty R_{\lambda p}(r_1) R_{\lambda q}(r_2)(r_<^\nu / r_>^{\nu+1}) R_{\mu r}(r_2) R_{\mu s}(r_1) r_1^2 dr_1 r_2^2 dr_2]$$

These integrals can be evaluated in the form $\int_0^\infty dr_1 \int_0^{r_1} dr_2 (r_2^\nu / r_1^{\nu+1}) \ldots$ or $\int_0^\infty dr_1 \int_{r_1}^\infty dr_2 (r_1^\nu / r_2^{\nu+1}) \ldots$. For both STOs and GTOs the latter form is usually more efficient. Closed-shell calculations require only the linear combination of the shell-averaged coulomb supermatrix less half of the shell-averaged exchange supermatrix, defined as the $\mathcal{P}$ *supermatrix*:

$$\mathcal{P}_{\lambda pq, \mu rs} = \mathcal{J}_{\lambda pq, \mu rs, 0} - \frac{1}{2} \sum_{\nu=|\lambda-\mu|}^{\lambda+\mu,2} A_{\lambda\mu\nu} \mathcal{K}_{\lambda pq, \mu rs, \nu}$$

where the $A_{\lambda\mu\nu}$ appear in the coupling of Legendre polynomials

$$P_\lambda P_\mu = \sum_{\nu=|\lambda-\mu|}^{\lambda+\mu,2} (2\nu+1) A_{\lambda\mu\nu} P_\nu$$

and can be expressed as squares of 3-j coefficients:

$$A_{\lambda\mu\nu} = \left(\begin{array}{ccc} \lambda & \mu & \nu \\ 0 & 0 & 0 \end{array} \right)^2$$

They are most easily computed in terms of particular binomial coefficients:

$$A_{2n} = \left(\begin{array}{c} 2n \\ n \end{array} \right) = \frac{(2n)!}{(n!)^2}$$

where

$$A_0 = 1$$

and

$$A_{2n+2} = 2(2n+1)A_{2n}/(n+1)$$

Then

$$A_{\lambda\mu\nu} = \frac{A_{-\lambda+\mu+\nu} A_{\lambda-\mu+\nu} A_{\lambda+\mu-\nu}}{(\lambda+\mu+\nu+1)A_{\lambda+\mu+\nu}}$$

Open-shell calculations also require the $\mathcal{Q}$ *supermatrix*:

$$\mathcal{Q}_{\lambda pq, \mu rs} = \sum_{\nu=0}^{2(\lambda,\mu)_<,2} J_{\lambda\mu\nu} \mathcal{J}_{\lambda pq, \mu rs, \nu} - \frac{1}{2} \sum_{\nu=|\lambda-\mu|}^{\lambda+\mu,2} K_{\lambda\mu\nu} \mathcal{K}_{\lambda pq, \mu rs, \nu}$$

where the $J_{\lambda\mu\nu}$ and $K_{\lambda\mu\nu}$ are open-shell energy coefficients that depend on the open-shell electron configuration and electronic state of the atom. When $\lambda = \mu$, $J_{\lambda\lambda\nu}$ and $K_{\lambda\lambda\nu}$ are not independent in most cases.

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Table I of ref. [1], containing open-shell energy coefficients for $(s, p)^n$, was extended by Malli and Olive [7] to include $(s, p, d)^n$ and f^n. Additions here include various $(s, p, d, f, g)^n$ cases [8, 9] and include all LS coupling cases needed for the ground states of atoms [10]. Tables of these coefficients are given in Appendix A. These include some cases with two open shells of the same symmetry. All coefficients have been redefined to show the hole-particle equivalence, making the tables more compact. The tables now include Landé (spin-orbit splitting) factors for use in a future version of the program. Some general formulas [11] in terms of the $A_{\lambda\mu\nu}$ are also provided.

The $C_{pi\lambda}$ for all values of p define the vector $\mathbf{c}_{i\lambda}$ for the $i\lambda$ shell. These vectors are orthonormal using $\mathbf{S}_\lambda$, the λ block of the $\mathbf{S}$ matrix,

$$\mathbf{c}_{i\lambda}^\dagger \mathbf{S}_\lambda \mathbf{c}_{j\lambda} = \delta_{ij}$$

The occupation number of the $i\lambda$ shell is denoted by $N_{i\lambda}$. For each value of λ there is only one closed-shell value of $N_{i\lambda}$ and we are only considering one open-shell value of $N_{i\lambda}$ as well, so we also use the notation $N_{C\lambda}$ and $N_{O\lambda}$. A density matrix (supervector) for each shell, $\mathbf{D}_{i\lambda}$ is defined by

$$D_{i\lambda pq} = (2 - \delta_{pq})N_{i\lambda}C_{pi\lambda}C_{qi\lambda}$$

where the factor $(2 - \delta_{pq})$ is required to treat the off-diagonal matrix elements correctly in contractions with integral supervectors and supermatrices. Closed-shell, open-shell, and total-density matrices (supervectors) are defined by summing over the corresponding ranges of i.

$$\mathbf{D}_{\mathbf{C}\lambda} = \Sigma_{i \subset closed} \mathbf{D}_{i\lambda}$$

$$\mathbf{D}_{\mathbf{O}\lambda} = \Sigma_{i \subset open} \mathbf{D}_{i\lambda}$$

$$\mathbf{D}_{\mathbf{T}\lambda} = \mathbf{D}_{\mathbf{C}\lambda} + \mathbf{D}_{\mathbf{O}\lambda}$$

The open-shell sum is usually over one (or zero) shells, but is slightly generalized here to some cases with more than one open shell of the same symmetry where the occupation numbers and open-shell energy coefficients are all the same.

The expression for the total energy, in the general case, contains shell-shell interactions of the closed-closed, closed-open, and open-open types. Since the first two types have the same form (twice as many coulomb integrals

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as exchange integrals), the energy expression has its simplest form when expressed in terms of $\mathbf{D_T}$ and $\mathbf{D_O}$.

$$E = \mathbf{H}^\dagger \mathbf{D_T} + \frac{1}{2}\mathbf{D_T}^\dagger \mathcal{P} \mathbf{D_T} - \frac{1}{2}\mathbf{D_O}^\dagger \mathcal{Q} \mathbf{D_O}$$

Applying the variational principle to this energy expression, using the orthonormality constraints, results in the closed- and open-shell Fock matrices (supervectors),

$$\mathbf{F_C} = \mathbf{H} + \mathbf{P} + \mathbf{R_O}$$

$$\mathbf{F_O} = \mathbf{H} + \mathbf{P} - \mathbf{Q} + \mathbf{R_C}$$

using

$$\mathbf{P} = \mathcal{P}\mathbf{D_T}$$

$$\mathbf{Q} = \mathcal{Q}\mathbf{D_O}$$

$$\mathbf{s}_{i\lambda} = \mathbf{S}_\lambda \mathbf{c}_{i\lambda}$$

$$\mathbf{q}_{i\lambda} = \mathbf{Q}_\lambda \mathbf{c}_{i\lambda}$$

$$\mathbf{R_{C\lambda}} = [N_{C\lambda}/(N_{C\lambda} - N_{O\lambda})]\Sigma_{i \subset closed}[\mathbf{s}_{i\lambda}\mathbf{q}_{i\lambda}^\dagger + \mathbf{q}_{i\lambda}\mathbf{s}_{i\lambda}^\dagger]$$

$$\mathbf{R_{O\lambda}} = [N_{O\lambda}/(N_{C\lambda} - N_{O\lambda})]\Sigma_{i \subset open}[\mathbf{s}_{i\lambda}\mathbf{q}_{i\lambda}^\dagger + \mathbf{q}_{i\lambda}\mathbf{s}_{i\lambda}^\dagger]$$

The closed- and open-shell vectors $\mathbf{c}_{i\lambda}$ then satisfy the respective equations

$$\mathbf{F_{C\lambda}}\mathbf{c}_{i\lambda} = \epsilon_{i\lambda}\mathbf{S}_\lambda \mathbf{c}_{i\lambda}$$

$$\mathbf{F_{O\lambda}}\mathbf{c}_{i\lambda} = \epsilon_{i\lambda}\mathbf{S}_\lambda \mathbf{c}_{i\lambda}$$

The two-Hamiltonian form [1] of the equations, used here, is probably somewhat less efficient, particularly in poorly convergent cases, than a one-Hamiltonian form [12], but the difference has not been significant enough to justify revision of the program.

III   Calculation of Integrals

The one-electron integral formulas, except for core potential integrals, are taken from ref. [1, 2, 13]. The two-electron integral formulas are taken from ref. [14]. Some notation changes have been made for both types of integrals, so all the integral formulas are summarized here.

Expressions used for both STO and GTO integrals are

$$V_n(x) = \frac{n!}{x^{n+1}} \qquad\qquad W_n(x) = \frac{n-1}{x}$$

$$n_{\lambda pq} = n_{\lambda p} + n_{\lambda q} \qquad\qquad \zeta_{\lambda pq} = \zeta_{\lambda p} + \zeta_{\lambda q}$$

$$E_k^n(x) = \left[\sum_{j=0}^{k-1} \binom{n}{j} x^j \right] / \left[\binom{n}{k} x^k \right]$$

The E_k^n are calculated with the recursion relation

$$E_k^n(x) = k[1 + E_{k-1}^n(x)]/[(n-k+1)x]$$

and the starting value

$$E_0^n(x) = 0$$

Both STO and GTO radial functions share the property that the product of two of them is a radial function of the same type. Accordingly, the basic radial electron repulsion integrals defined below, $R_{mn\nu}(x,y)$, need only three indices.

Formulas for STO integrals are

$$\begin{aligned}
N_{\lambda pq} &= [V_{n_{\lambda pp}}(\zeta_{\lambda pp})V_{n_{\lambda qq}}(\zeta_{\lambda qq})]^{-\frac{1}{2}} \\
S_{\lambda pq} &= N_{\lambda pq}V_{n_{\lambda pq}}(\zeta_{\lambda pq}) \\
U_{\lambda pq} &= N_{\lambda pq}V_{n_{\lambda pq}-1}(\zeta_{\lambda pq}) \\
T_{\lambda pq} &= \frac{1}{2}\zeta_{\lambda p}\zeta_{\lambda q}N_{\lambda pq}\{W_{n_{\lambda p}-\lambda}(\zeta_{\lambda p})W_{n_{\lambda q}-\lambda}(\zeta_{\lambda q})V_{n_{\lambda pq}-2}(\zeta_{\lambda pq}) \\
&\quad - [W_{n_{\lambda p}-\lambda}(\zeta_{\lambda p}) + W_{n_{\lambda q}-\lambda}(\zeta_{\lambda q})]V_{n_{\lambda pq}-1}(\zeta_{\lambda pq}) + V_{n_{\lambda pq}}(\zeta_{\lambda pq})\}
\end{aligned}$$

With a core potential of the form

$$\mathbf{U}_\lambda^{\mathbf{ECP}} = \sum_k d_{\lambda k}r^{n_{\lambda k}-2}e^{-\omega_{\lambda k}r}$$

the core-potential integrals are given by

$$U_{\lambda pq}^{ECP} = N_{\lambda pq}\sum_k d_{\lambda k}V_{n_{\lambda pq}+n_{\lambda k}-2}(\zeta_{\lambda pq} + \omega_{\lambda k})$$

The radial electron-repulsion integrals are given by

$$R_{mn\nu}(x,y) = \int_0^\infty \int_0^\infty r_1^m e^{-xr_1}(r_<^\nu/r_>^{\nu+1})r_2^n e^{-yr_2}\,dr_1 dr_2$$

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$$= \frac{(m+n-1)!}{xy(x+y)^{m+n-1}}[1 + E^{m+n-1}_{n-\nu-1}(y/x) + E^{m+n-1}_{m-\nu-1}(x/y)]$$

Formulas for GTO integrals are

$$
\begin{aligned}
N_{\lambda pq} &= [V_{\frac{1}{2}(n_{\lambda pp}-1)}(\zeta_{\lambda pp})V_{\frac{1}{2}(n_{\lambda qq}-1)}(\zeta_{\lambda qq})]^{-\frac{1}{2}} \\
S_{\lambda pq} &= N_{\lambda pq}V_{\frac{1}{2}(n_{\lambda pq}-1)}(\zeta_{\lambda pq}) \\
U_{\lambda pq} &= N_{\lambda pq}V_{\frac{1}{2}(n_{\lambda pq}-2)}(\zeta_{\lambda pq}) \\
T_{\lambda pq} &= 2\zeta_{\lambda p}\zeta_{\lambda q}N_{\lambda pq}\{W_{n_{\lambda p}-\lambda}(2\zeta_{\lambda p})W_{n_{\lambda q}-\lambda}(2\zeta_{\lambda q})V_{\frac{1}{2}(n_{\lambda pq}-3)}(\zeta_{\lambda pq}) \\
&\quad - [W_{n_{\lambda p}-\lambda}(2\zeta_{\lambda p}) + W_{n_{\lambda q}-\lambda}(2\zeta_{\lambda q})]V_{\frac{1}{2}(n_{\lambda pq}-1)}(\zeta_{\lambda pq}) + V_{\frac{1}{2}(n_{\lambda pq}+1)}(\zeta_{\lambda pq})\}
\end{aligned}
$$

With a core potential of the form

$$\mathbf{U}^{\mathbf{ECP}}_\lambda = \sum_k d_{\lambda k} r^{n_{\lambda k}-2}e^{-\omega_{\lambda k}r^2}$$

the core-potential integrals are given by

$$U^{ECP}_{\lambda pq} = N_{\lambda pq}\sum_k d_{\lambda k}V_{\frac{1}{2}(n_{\lambda pq}+n_{\lambda k}-3)}(\zeta_{\lambda pq} + \omega_{\lambda k})$$

The radial electron-repulsion integrals are given by

$$R_{mn\nu}(x,y) = \int_0^\infty \int_0^\infty r_1^m e^{-xr_1^2}(r_<^\nu/r_>^{\nu+1})r_2^n e^{-yr_2^2}dr_1 dr_2$$

$$= \frac{[\frac{1}{2}(m+n-3)]!}{xy(x+y)^{\frac{1}{2}(m+n-3)}}[1 + E^{\frac{1}{2}(m+n-3)}_{\frac{1}{2}(n-\nu-2)}(y/x) + E^{\frac{1}{2}(m+n-3)}_{\frac{1}{2}(m-\nu-2)}(x/y)]$$

For both STOs and GTOs, the coulomb and exchange supermatrices are given by

$$\mathcal{J}_{\lambda pq,\mu rs,\nu} = N_{\lambda pq}N_{\mu rs}R_{n_{\lambda pq},n_{\mu rs},\nu}(\zeta_{\lambda pq},\zeta_{\mu rs})$$

$$\mathcal{K}_{\lambda pq,\mu rs,\nu} = \frac{1}{2}N_{\lambda pq}N_{\mu rs}[R_{n_{\lambda p}+n_{\mu r},n_{\lambda q}+n_{\mu s},\nu}(\zeta_{\lambda p}+\zeta_{\mu r},\zeta_{\lambda q}+\zeta_{\mu s})$$

$$+R_{n_{\lambda p}+n_{\mu s},n_{\lambda q}+n_{\mu r},\nu}(\zeta_{\lambda p}+\zeta_{\mu s},\zeta_{\lambda q}+\zeta_{\mu r})]$$

The one-electron integrals are calculated together in the subroutine OEIP and the coulomb and exchange integrals are assembled in the subroutine TEIP, with the subroutine RDNT providing blocks of the $R_{mn\nu}$ integrals computed for the range of ν values needed.

IV   Eigenvectors and Eigenvalues

As given above, the basic eigenvalue-eigenvector problem to be solved has the form

$$\mathbf{Fc} = \epsilon \mathbf{Sc}$$

Roothaan and Bagus [1] gave a detailed derivation of a method of computing the eigenvalues ϵ and eigenvectors $\mathbf{c}$, in the presence of the overlap matrix $\mathbf{S}$, one at a time. They chose this method, rather than a method that involved transforming $\mathbf{S}$ to a unit matrix and then diagonalizing, due to arguments concerning stability, accuracy, and simplicity. Some of these constraints are less limiting using today's 64-bit floating-point words compared to the 36-bit words used then. Their method is summarized here.

Let $\mathbf{c_0}$ be an approximate eigenvector. Then

$$\mathbf{c_0^\dagger S c_0} = 1$$

$$\epsilon_0 = \mathbf{c_0^\dagger F c_0}$$

The first-order improvement to $\mathbf{c_0}$ is defined by

$$\mathbf{c} = \mathbf{c_0} + \delta\mathbf{c}$$

Without loss of generality, $\delta\mathbf{c}$ can be required to be orthogonal to $\mathbf{c_0}$. Next, define

$$\mathbf{s_0} = \mathbf{S c_0}$$

$$\mathbf{g_0} = (\mathbf{F} - \epsilon_0 \mathbf{S})\mathbf{c_0}$$

$$\mathbf{G_0} = \mathbf{F} - \epsilon_0 \mathbf{S} - \mathbf{s_0 g_0^\dagger} - \mathbf{g_0 s_0^\dagger}$$

Note that $\mathbf{G_0}$ is a symmetric matrix. It is shown that $\delta\mathbf{c}$ is determined by

$$\mathbf{G_0}\delta\mathbf{c} = -\mathbf{g_0}$$

This equation is solved by the method of Gaussian elimination, yielding

$$\mathbf{T}\delta\mathbf{c}' = -\mathbf{t}$$

where $\mathbf{T}$ is a lower-triangle matrix and $\delta\mathbf{c}'$ is not necessarily orthogonal to $\mathbf{c_0}$, but care must be taken because $\mathbf{G_0}$ is singular. The algorithm used is to

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store $\mathbf{G_0}$ in lower-triangle form, replace the first column of $\mathbf{G_0}$ (shown to be superfluous) by $\mathbf{g_0}$, and then use

$$T_{pq} = G_{pq} - \sum_{r=p+1}^{n} T_{rp}T_{rq}/T_{rr}$$

for $q \leq p$ and p starting at n and decreasing to 1 and noting that the sum does not exist for $p = n$. The first column of $\mathbf{T}$ will then contain $\mathbf{t}$ from which $\delta\mathbf{c}'$ can be obtained directly. Orthogonalization of $\delta\mathbf{c}'$ to $\mathbf{c_0}$ yields $\delta\mathbf{c}$:

$$\delta\mathbf{c} = \delta\mathbf{c}' - (\mathbf{c_0^\dagger}\mathbf{S}\delta\mathbf{c}')\mathbf{c_0}$$

Since eigenvectors are found one at a time, inaccurate input can result in duplication of eigenvectors. Due to the program design, for a given symmetry, vectors for closed shells must precede vectors for open shells, irrespective of energy order. The eigenvectors and eigenvalues are computed in the subroutine EIGEA.

V   SCF Iterations and Extrapolations

Roothaan and Bagus [1, 2] described and implemented two different extrapolation methods based on the orbital coefficients from three successive SCF iterations. The Fortran versions of the program have only used the first of these methods, as implemented by Roos et al. [2]. To summarize this method, the notation for a particular orbital coefficient $C_{pi\lambda}$ for iterations k, $k - 1$, and $k - 2$ is C_k, C_{k-1}, and C_{k-2} where the $pi\lambda$ indices have been suppressed. The extrapolated value is C. First, the quantity

$$f = (C_k - C_{k-1})/(2C_{k-1} - C_k - C_{k-2})$$

is computed. If $|f| \geq 2$, no extrapolation occurs and $C = C_k$. If $|f| < 2$, then

$$C = C_k + f(C_k - C_{k-1})$$

which is equivalent to

$$C = (C_{k-1}^2 - C_kC_{k-2})/(2C_{k-1} - C_k - C_{k-2})$$

The extrapolations are carried out in the subroutine EXTRAP.

VI   Convergence Control

The convergence of both diagonalization and SCF iterations is measured by the largest absolute differences in orbital coefficients in successive iterations. Roothaan and Bagus [1] designed a flexible way of controlling both types of iterations within acceptable ranges. Thus the minimum acceptable accuracy is set by the input, but higher accuracy is attempted by the program and used where possible. This algorithm is used in the present version of the program, with some control options omitted. The diagonalization control parameters are the initial diagonalization threshold (set at $2^{-23} = 1.19 \times 10^{-7}$), the maximum number of diagonalization iterations, NDIAG (default value is 25), and the diagonalization divergence limit, DGATH (default value is 10^{-5}).

Diagonalization iterations take place for an orbital until convergence is obtained or NDIAG iterations have occurred. In the latter case, the diagonalization threshold for the orbital is increased by a factor of two and up to NDIAG additional iterations occur. This process is continued until convergence is obtained or until the diagonalization threshold exceeds DGATH, causing the calculation to terminate. If convergence is obtained, the resulting diagonalization threshold is stored and the same procedure is applied to the next orbital. Once all the orbitals have been computed, the SCF iteration is complete. In subsequent SCF iterations, all the previous diagonalization thresholds larger than the minimum value are initially decreased by a factor of two to try to increase the accuracy.

The SCF threshold is set at 2^{BIAS} times the maximum diagonalization threshold where BIAS (default value is 1) is read in along with the SCF divergence limit, SCFAT (default value is 10^{-3}), the maximum number of SCF extrapolations, NXTRP (default value is 25), and the maximum total number of SCF extrapolations, MXXTRP (default value is 50).

SCF iterations and extrapolations are performed until convergence is obtained or NXTRP extrapolations have occurred. In the latter case, BIAS is increased by one and up to NXTRP additional extrapolations occur. This process is continued until convergence is obtained except that either the SCF threshold exceeding SCFAT or the number of extrapolations exceeding MXXTRP cause the calculation to terminate.

All of the convergence controls could probably be tightened in most cases if additional accuracy is desired. The default values for the convergence control parameters are given in the next two tables.

INTEGERS FOR CONVERGENCE CONTROL

Symbol	Explanation	Default Value
BIAS	Diagonalization-SCF threshold bias	2
NXTRP	Number of extrapolations	25
NDIAG	Number of diagonalization iterations	25
MXXTRP	Maximum number of extrapolations	50

VII   Exponent Variation

A specified number (NVAR) of orbital exponents may be varied either individually (ISCALE=0) or as a group (ISCALE=1) [2]. The intervals are set at ZSCALE times the initial exponent values. Energies are calculated until three adjacent values have the middle one lowest. Then a parabolic fit is used to approximate the minimum. Selected exponents can be constrained to be the same by setting NZET to the number of independent values.

Various situations in which exponent optimization and other procedures can go wrong are controlled by:

ALARM THRESHOLDS

Symbol	Explanation	Default (Slater)	Default (Gaussian)
DGATH	Diagonalization divergence	10^{-4}	10^{-4}
SCFAT	SCF divergence	10^{-3}	10^{-3}
EXPMN	Minimum exponent	10^{-2}	10^{-5}
DMNXP	Minimum exponent difference	10^{-2}	10^{-7}
RMNED	Relative minimum energy difference	10^{-11}	10^{-11}
RMXED	Relative maximum energy difference	10^{-1}	10^{-1}

These thresholds can usually be loosened somewhat without causing difficulties.

A fairly common problem in exponent optimization is exponent collapse, where two exponents approach each other very closely and their corresponding coefficients become very large in magnitude with opposite signs. A way of managing this problem is to express the natural logarithms of all the exponents for each l value as a series of Legendre polynomials and then constrain the number of independent coefficients[15].

$$\ln \zeta_p = \sum_{k=0}^{k_{max}} A_k P_k \left(\frac{2p-2}{N_{prim}-1} - 1 \right)$$

where N_{prim} is the number of primitive functions, p varies from 1 to N_{prim}, and $k_{max} = N_{prim} - 1$ means no constraints. For smaller values of k_{max} there are $N_{prim} - 1 - k_{max}$ constraints. If only two coefficients are retained then the exponents form an even-tempered set. To use this Legendre expansion, set ILEG=1 and then the coefficients are read in instead of the exponents and they are varied by a constant amount of ZSCALE.

VIII   Output Format and Options

The only output options are with respect to printing the integrals over basis functions (NPRINT) and to writing out optimized orbital exponents and orbital coefficients (IPNCH) to a separate file.

IX   Input Format and Conventions

The input directions principally follow the form established in ref. [2] and are given in detail in Appendix B. Free-format input is used.

X   Limitations of the Program

The program is written in Fortran 90 with all floating-point quantities designated as REAL*8, etc. On machines with 64-bit words, the compiler option to turn off all double precision should be used. Arrays are allocated dynamically. Most of the computer time is usually spent evaluating integrals and multiplying the supermatrices by supervectors. The latter code is written so that moderate vectorization can be achieved.

Simplicity in programming was a general goal. No calls are made to special libraries. All communication is by subroutine arguments. Variable names are kept the same wherever possible. All formulas are general except for the open-shell energy expressions, which are part of the input.

Files are defined by unit numbers: 5 (input), 6 (output), IPNCH (optional optimization output).

The largest angular momentum quantum number allowed is 24. These numbers are represented by their spectroscopic symbols [16], $s, p, d, f - i, k - o, q, r, t - z$ for 0-20, supplemented by $a - c, e$ for 21-24.

More than one open shell of a symmetry is permitted only if (1) the occupation numbers are the same and (2) the intra- and intershell open-shell energy coefficients are the same. Thus $1s2s\ ^3S$ can be done, but not the corresponding ^1S.

Acknowledgements

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A Open-Shell Energy Coefficients

Most of these coefficients are taken from ref. [1, 7]. Additional coefficients involving f and g orbitals have been derived and included, in some cases using energy expressions from Ref. [8, 9, 17]. The tables have been shortened by (1) listing intrashell and intershell coefficients separately, and (2) omitting almost all states where the electron configuration gives more than one wave function of that symmetry (such as d^3 ^2D). Ref. [7] listed coefficients for the average energy of such wave functions.

For some of the high-spin $d^m p^1$ cases, where the lowest energy wave function can be for a duplicated symmetry, the coefficients are provided for both wave functions.

For half-filled shells (d^5, f^7) in some cases where more than one wave function of a certain symmetry exists, the seniority number can be used to choose these wave functions so that they have no matrix element of the Hamiltonian between them[9]. Such cases are included in the tables with the addition of the seniority number as a left subscript (such as d^5 ^2_5G).

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Thus the states included are generally those with high S (low energy) and lower S, high L (higher energy) as well as some intermediate cases.

A few states are degenerate at the Hartree-Fock level [8]. Examples in these tables are

$$(d^3, d^7)\ {}^2H,\ {}^2P; \quad (d^3, d^7({}^2H,\ {}^2P))s^1\ {}^3H,\ {}^3P;\ {}^1H,\ {}^1P$$

$$(f^3, f^{11})\ {}^4F,\ {}^4S; \quad (f^3, f^{11}({}^4F,\ {}^4S))s^1\ {}^5F,\ {}^5S;\ {}^3F,\ {}^3S$$

$$(f^4, f^{10})\ {}^5F,\ {}^5S; \quad (f^4, f^{10}({}^5F,\ {}^5S))s^1\ {}^6F,\ {}^6S;\ {}^4F,\ {}^4S$$

Still more compact tables were obtained by redefining the open-shell energy coefficients by multiplying them by a factor of

$$N_{O\lambda}N_{O\mu}(2\nu + 1)$$

The occupation numbers make the hole-particle relationship apply to the tables. The factor of $(2\nu + 1)$ simplifies the expression for exchange integrals involving s orbitals and simplifies other relationships as well. These changes also generally reduce the size of the integers in the fractions. The original definitions of the coefficients are the form used for actual computation in the program. The revised form is more convenient for reference purposes; the program changes them back to their original form for computational use.

Intrashell coefficients are not unique; thus intrashell J coefficients can be set to zero except when they also serve as intershell coefficients. Some simple, general relationships are

$$J_{\lambda\mu 0} = 0$$

$$K_{\lambda\lambda 0} = N_{O\lambda}^2/(2\lambda + 1) - 2N_{O\lambda}$$

A state with open shells of more than one symmetry requires coefficients from more than one table. Thus $s^1 p^3\ {}^5S$ appears in the intershell table as $p^3({}^4S)s^1({}^2S)^5S$ and K_{101} is provided there; looking under $p^3({}^4S)$ in the intrashell table provides K_{110} and K_{112}; looking under $s^1({}^2S)$ in the intrashell table provides K_{000}.

Some simple general formulas, in terms of the $A_{\lambda\mu\nu}$, exist for a few groups of states [11]:

1. $\lambda^{N_{O\lambda}}\ {}^1S$ states with seniority 0. These are usually the highest-energy states from this electron configuration.

$$K_{\lambda\lambda\nu} = [N_{O\lambda}(4\lambda + 2 - N_{O\lambda})(\lambda + 1)/\lambda](2\nu + 1)A_{\lambda\lambda\nu} \qquad (\nu = 2, 2\lambda, 2)$$

2. $\lambda^{N_{O\lambda}}\ ^2\Lambda$ states with seniority 1. These are the only states for $N_{O\lambda} = 1$ or $4\lambda + 1$. For intermediate values of $N_{O\lambda}$, they are usually the highest-energy states from this electron configuration.

$$K_{\lambda\lambda\nu} = \{[N_{O\lambda}(4\lambda+2-N_{O\lambda})(\lambda+1)-(2\lambda+1)^2]/\lambda\}(2\nu+1)A_{\lambda\lambda\nu} \qquad (\nu = 2, 2\lambda, 2)$$

3. $\lambda^{N_{O\lambda}}\ ^{2\lambda+1}\Lambda$ states with seniority 2λ. These are the only high-spin states from this electron configuration and therefore the lowest-energy states.

$$K_{\lambda\lambda\nu} = -2(2\lambda^2 - 1)(2\nu + 1)A_{\lambda\lambda\nu} \qquad (\nu = 2, 2\lambda, 2)$$

4. $\lambda^{2\lambda+1}\ ^{2\lambda+2}S$ states with seniority $2\lambda + 1$. These are the high-spin states from this half-filled electron configuration and therefore the lowest-energy states.

$$K_{\lambda\lambda\nu} = -(2\lambda + 1)^2(2\nu + 1)A_{\lambda\lambda\nu} \qquad (\nu = 0, 2\lambda, 2)$$

General formulas for averages of states are (using $d_\lambda = 2\lambda + 1$):
1. For an intrashell average of states, the additional coefficients are

$$K_{\lambda\lambda\nu} = [N_{O\lambda}(2d_\lambda - N_{O\lambda})/(2d_\lambda - 1)]d_\nu A_{\lambda\lambda\nu} \qquad (\nu = 2, 2\lambda, 2)$$

2. For an intrashell average of high-spin states, the additional coefficients are

$$K_{\lambda\lambda\nu} = \{[N_{O\lambda}(2d_\lambda - N_{O\lambda}) - d_\lambda(d_\lambda - |d_\lambda - N_{O\lambda}|)^2]/(d_\lambda - 1)\}d_\nu A_{\lambda\lambda\nu}$$

$$(\nu = 2, 2\lambda, 2)$$

3. For an intershell average of states,

$$K_{\lambda\mu\nu} = 0$$

4. For an intershell average of high-spin states,

$$K_{\lambda\mu\nu} = -(d_\lambda - |d_\lambda - N_{O\lambda}|)(d_\mu - |d_\mu - N_{O\mu}|)d_\nu A_{\lambda\mu\nu}$$

$$(\nu = |\lambda - \mu|, \lambda + \mu, 2)$$

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Intrashell Coefficients

El. Config.	State	K_{000}			
s^1	^2S	-1			

El. Config.	State	K_{110}	K_{112}	α_1	
p^1, p^5	^2P	-5/3	2/3	± 1	
p^2, p^4	^3P	-8/3	-4/3	$\pm 1/2$	
p^2, p^4	^1D	-8/3	52/15		
p^2, p^4	^1S	-8/3	32/3		
p^3	^4S	-3	-6		
p^3	^2D	-3	6/5	0	
p^3	^2P	-3	6	0	

El. Config.	State	K_{220}	K_{222}	K_{224}	α_2
d^1, d^9	^2D	-9/5	2/7	18/35	± 1
d^2, d^8	^3F	-16/5	-104/49	324/245	$\pm 1/2$
d^2, d^8	^3P	-16/5	4	-24/5	$\pm 1/2$
d^2, d^8	^1G	-16/5	136/49	524/245	
d^2, d^8	^1D	-16/5	-4/49	1224/245	
d^2, d^8	^1S	-16/5	48/7	432/35	
d^3, d^7	^4F	-21/5	-174/49	-306/245	$\pm 1/3$
d^3, d^7	^4P	-21/5	18/7	-258/35	$\pm 1/3$
d^3, d^7	^2H	-21/5	6/49	894/245	$\pm 1/5$
d^3, d^7	^2G	-21/5	-94/49	1394/245	$\pm 3/10$
d^3, d^7	^2F	-21/5	306/49	-606/245	$\mp 1/6$
d^3, d^7	^2P	-21/5	6/49	894/245	$\pm 2/3$
d^4, d^6	^5D	-24/5	-4	-36/5	$\pm 1/4$
d^4, d^6	^3H	-24/5	-116/49	636/245	$\pm 1/10$
d^4, d^6	^3G	-24/5	-16/49	136/245	$\pm 3/20$
d^4, d^6	^3D	-24/5	124/49	-564/245	$\mp 1/12$
d^4, d^6	^1I	-24/5	-76/49	1836/245	
d^4, d^6	^1F	-24/5	32/7	48/35	

		K_{220}	K_{222}	K_{224}	α_2
d^5	^6S	-5	-50/7	-90/7	
d^5	^4G	-5	-150/49	-130/49	0
d^5	^4F	-5	90/49	-90/49	0
d^5	^4D	-5	-10/49	-270/49	0
d^5	^4P	-5	-30/7	30/7	0
d^5	^2I	-5	-130/49	270/49	0
d^5	^2H	-5	-90/49	510/49	0
d^5	^2_5G	-5	90/49	50/49	0
d^5	^2_3G	-5	410/49	10/49	0
d^5	^2_5F	-5	170/49	-30/49	0
d^5	^2_3F	-5	-150/49	570/49	0
d^5	^2_3D	-5	270/49	150/49	0
d^5	^2P	-5	750/49	-330/49	0
d^5	^2S	-5	290/49	-150/49	

		K_{330}	K_{332}	K_{334}	K_{336}	α_3
f^1, f^{13}	^2F	-13/7	4/21	18/77	100/231	± 1
f^2, f^{12}	^3H	-24/7	-92/63	-636/847	12500/7623	$\pm 1/2$
f^2, f^{12}	^3F	-24/7	-8/63	-12/77	-200/693	$\pm 1/2$
f^2, f^{12}	^3P	-24/7	100/21	156/77	-1700/231	$\pm 1/2$
f^2, f^{12}	^1I	-24/7	188/63	1044/847	172300/99099	
f^2, f^{12}	^1G	-24/7	-40/21	3508/847	5800/2541	
f^2, f^{12}	^1D	-24/7	772/315	-180/77	4700/693	
f^2, f^{12}	^1S	-24/7	128/21	576/77	3200/231	
f^3, f^{11}	^4I	-33/7	-256/63	-2166/847	17800/7623	$\pm 1/3$
f^3, f^{11}	^4G	-33/7	52/63	-318/847	-36100/7623	$\pm 1/3$
f^3, f^{11}	^4F	-33/7	-20/21	-90/77	-500/231	$\pm 1/3$
f^3, f^{11}	^4D	-33/7	248/63	78/77	-6400/693	$\pm 1/3$
f^3, f^{11}	^4S	-33/7	-20/21	-90/77	-500/231	
f^3, f^{11}	^2L	-33/7	12/7	18/847	41500/11011	$\pm 1/4$
f^3, f^{11}	^2K	-33/7	-116/63	1810/847	412700/99099	$\pm 9/28$
f^3, f^{11}	^2I	-33/7	80/63	1614/847	172600/99099	$\pm 2/21$
f^3, f^{11}	^2P	-33/7	-32/63	50/77	3400/693	0

		K_{330}	K_{332}	K_{334}	K_{336}	α_3
f^4, f^{10}	^5I	-40/7	-340/63	-3552/847	-5300/7623	$\pm 1/4$
f^4, f^{10}	^5G	-40/7	-32/63	-1704/847	-59200/7623	$\pm 1/4$
f^4, f^{10}	^5F	-40/7	-16/7	-216/77	-400/77	$\pm 1/4$
f^4, f^{10}	^5D	-40/7	164/63	-48/77	-8500/693	$\pm 1/4$
f^4, f^{10}	^5S	-40/7	-16/7	-216/77	-400/77	
f^4, f^{10}	^3M	-40/7	-116/63	-1032/847	538700/99099	$\pm 1/6$
f^4, f^{10}	^3L	-40/7	-200/63	228/847	465200/99099	$\pm 5/24$
f^4, f^{10}	^1N	-40/7	52/63	760/847	685700/99099	
f^4, f^{10}	^1K	-40/7	-328/315	2524/847	582800/99099	
f^4, f^{10}	^1F	-40/7	304/63	5604/847	-29800/7623	
f^5, f^9	^6H	-45/7	-344/63	-4794/847	-56800/7623	$\pm 1/5$
f^5, f^9	^6F	-45/7	-260/63	-390/77	-6500/693	$\pm 1/5$
f^5, f^9	^6P	-45/7	16/21	-222/77	-3800/231	$\pm 1/5$
f^5, f^9	^4M	-45/7	-32/7	-138/77	9400/3003	$\pm 1/9$
f^5, f^9	^4L	-45/7	-68/21	-2778/847	127900/33033	$\pm 5/36$
f^5, f^9	^4S	-45/7	44/21	18/7	100/21	
f^5, f^9	^2O	-45/7	-148/63	-90/847	873700/99099	$\pm 1/11$
f^5, f^9	^2N	-45/7	-1048/315	-1322/847	1143200/99099	$\pm 6/55$
f^6, f^8	^7F	-48/7	-136/21	-612/77	-3400/231	$\pm 1/6$
f^6, f^8	^5L	-48/7	-352/63	-2280/847	-263000/99099	$\pm 1/16$
f^6, f^8	^5K	-48/7	-128/63	-4072/847	-302200/99099	$\pm 9/112$
f^6, f^8	^5P	-48/7	-44/63	-164/77	-5300/693	0
f^6, f^8	^5S	-48/7	-16/63	-24/77	-400/693	
f^6, f^8	^3O	-48/7	-296/63	-1356/847	815000/99099	$\pm 1/22$
f^6, f^8	^3N	-48/7	-1172/315	-124/847	545500/99099	$\pm 3/55$
f^6, f^8	^1Q	-48/7	-152/35	-516/847	145000/11011	
f^6, f^8	^1P	-48/7	2132/315	1724/847	500/7623	

		K_{330}	K_{332}	K_{334}	K_{336}	α_3
f^7	^8S	-7	-28/3	-126/11	-700/33	
f^7	^6I	-7	-56/9	-630/121	-128800/14157	0
f^7	^6H	-7	-16/9	-390/121	-9800/1089	0
f^7	^6G	-7	-4/3	-982/121	-3500/363	0
f^7	^6F	-7	-28/9	-42/11	-700/99	0
f^7	^6D	-7	-256/45	-18/11	-1400/99	0
f^7	^6P	-7	-8	-6	0	0
f^7	^4N	-7	-16/3	-274/121	4200/1573	0
f^7	^4M	-7	-8/3	-18/121	19600/4719	0
f^7	^4_5L	-7	4/3	-54/121	4900/4719	0
f^7	^4_7K	-7	-4/5	-382/121	-700/4719	0
f^7	^2Q	-7	-236/45	-174/121	160300/14157	0
f^7	^2O	-7	-44/9	-54/121	230300/14157	0
f^7	^2_7N	-7	-16/5	194/121	26600/4719	0
f^7	^2_5N	-7	176/45	298/121	68600/14157	0

		K_{440}	K_{442}	K_{444}	K_{446}	K_{448}	α_4
g^1, g^{17}	^2G	-17/9	100/693	162/1001	20/99	490/1287	± 1
g^8, g^{10}	^9G	-80/9	-6200/693	-10044/1001	-1240/99	-30380/1287	$\pm 1/8$
g^9	^{10}S	-9	-900/77	-13122/1001	-180/11	-4410/143	

Intershell Coefficients for States with Open Shells of Different Symmetry

El. Config.	State	Coefficients	
		K_{101}	α_1
$p^1, p^5(^2P)\ s^1(^2S)$	^3P	-1	$\pm 1/2$
$p^1, p^5(^2P)\ s^1(^2S)$	^1P	3	
$p^2, p^4(^3P)\ s^1(^2S)$	^4P	-2	$\pm 1/3$
$p^2, p^4(^1D)\ s^1(^2S)$	^2D	0	0
$p^2, p^4(^3P)\ s^1(^2S)$	^2P	4	$\pm 2/3$
$p^2, p^4(^1S)\ s^1(^2S)$	^2S	0	
$p^3(^4S)\ s^1(^2S)$	^5S	-3	
$p^3(^2D)\ s^1(^2S)$	^3D	-1	0
$p^3(^2P)\ s^1(^2S)$	^3P	-1	0
$p^3(^4S)\ s^1(^2S)$	^3S	5	
$p^3(^2D)\ s^1(^2S)$	^1D	3	
$p^3(^2P)\ s^1(^2S)$	^1P	3	
		K_{202}	α_2
$d^1, d^9(^2D)\ s^1(^2S)$	^3D	-1	$\pm 1/2$
$d^1, d^9(^2D)\ s^1(^2S)$	^1D	3	
$d^2, d^8(^3F)\ s^1(^2S)$	^4F	-2	$\pm 1/3$
$d^2, d^8(^3P)\ s^1(^2S)$	^4P	-2	$\pm 1/3$
$d^2, d^8(^1G)\ s^1(^2S)$	^2G	0	0
$d^2, d^8(^3F)\ s^1(^2S)$	^2F	4	$\pm 2/3$
$d^2, d^8(^1D)\ s^1(^2S)$	^2D	0	0
$d^2, d^8(^3P)\ s^1(^2S)$	^2P	4	$\pm 2/3$
$d^2, d^8(^1S)\ s^1(^2S)$	^2S	0	
$d^3, d^7(^4F)\ s^1(^2S)$	^5F	-3	$\pm 1/4$
$d^3, d^7(^4P)\ s^1(^2S)$	^5P	-3	$\pm 1/4$
$d^3, d^7(^2H)\ s^1(^2S)$	^3H	-1	$\pm 1/10$
$d^3, d^7(^2G)\ s^1(^2S)$	^3G	-1	$\pm 3/20$
$d^3, d^7(^4F)\ s^1(^2S)$	^3F	5	$\pm 5/12$
$d^3, d^7(^2F)\ s^1(^2S)$	^3F	-1	$\mp 1/12$
$d^3, d^7(^4P)\ s^1(^2S)$	^3P	5	$\pm 5/12$
$d^3, d^7(^2P)\ s^1(^2S)$	^3P	-1	$\pm 1/3$
$d^3, d^7(^2H)\ s^1(^2S)$	^1H	3	
$d^3, d^7(^2G)\ s^1(^2S)$	^1G	3	
$d^3, d^7(^2F)\ s^1(^2S)$	^1F	3	

		K_{202}	α_2
$d^3, d^7(^2P)\ s^1(^2S)$	^1P	3	
$d^4, d^6(^5D)\ s^1(^2S)$	^6D	-4	$\pm 1/5$
$d^4, d^6(^3H)\ s^1(^2S)$	^4H	-2	$\pm 1/15$
$d^4, d^6(^3G)\ s^1(^2S)$	^4G	-2	$\pm 1/10$
$d^4, d^6(^5D)\ s^1(^2S)$	^4D	6	$\pm 3/10$
$d^4, d^6(^3D)\ s^1(^2S)$	^4D	-2	$\mp 1/18$
$d^4, d^6(^1I)\ s^1(^2S)$	^2I	0	0
$d^4, d^6(^3H)\ s^1(^2S)$	^2H	4	$\pm 2/15$
$d^4, d^6(^3G)\ s^1(^2S)$	^2G	4	$\pm 1/5$
$d^4, d^6(^1F)\ s^1(^2S)$	^2F	0	0
$d^4, d^6(^3D)\ s^1(^2S)$	^2D	4	$\mp 1/9$
$d^5(^6S)\ s^1(^2S)$	^7S	-5	
$d^5(^4G)\ s^1(^2S)$	^5G	-3	0
$d^5(^4F)\ s^1(^2S)$	^5F	-3	0
$d^5(^4D)\ s^1(^2S)$	^5D	-3	0
$d^5(^4P)\ s^1(^2S)$	^5P	-3	0
$d^5(^6S)\ s^1(^2S)$	^5S	7	
$d^5(^2I)\ s^1(^2S)$	^3I	-1	0
$d^5(^2H)\ s^1(^2S)$	^3H	-1	0
$d^5(^4G)\ s^1(^2S)$	^3G	5	0
$d^5(^2_5G)\ s^1(^2S)$	^3_5G	-1	0
$d^5(^2_3G)\ s^1(^2S)$	^3_3G	-1	0
$d^5(^4F)\ s^1(^2S)$	^3F	5	0
$d^5(^2_5F)\ s^1(^2S)$	^3_5F	-1	0
$d^5(^2_3F)\ s^1(^2S)$	^3_3F	-1	0
$d^5(^4D)\ s^1(^2S)$	^3D	5	0
$d^5(^2_3D)\ s^1(^2S)$	^3_3D	-1	0
$d^5(^4P)\ s^1(^2S)$	^3P	5	0
$d^5(^2P)\ s^1(^2S)$	^3P	-1	0
$d^5(^2S)\ s^1(^2S)$	^3S	-1	
$d^5(^2I)\ s^1(^2S)$	^1I	3	
$d^5(^2H)\ s^1(^2S)$	^1H	3	
$d^5(^2_5G)\ s^1(^2S)$	^1_5G	3	
$d^5(^2_3G)\ s^1(^2S)$	^1_3G	3	
$d^5(^2_5F)\ s^1(^2S)$	^1_5F	3	

		K_{202}	α_2
$d^5(^2_3F)\ s^1(^2S)$	^1_3F	3	
$d^5(^2_3D)\ s^1(^2S)$	^1_3D	3	
$d^5(^2P)\ s^1(^2S)$	^1P	3	
$d^5(^2S)\ s^1(^2S)$	^1S	3	

		K_{303}	α_3
$f^1, f^{13}(^2F)\ s^1(^2S)$	^3F	-1	$\pm 1/2$
$f^1, f^{13}(^2F)\ s^1(^2S)$	^1F	3	
$f^2, f^{12}(^3H)\ s^1(^2S)$	^4H	-2	$\pm 1/3$
$f^2, f^{12}(^3F)\ s^1(^2S)$	^4F	-2	$\pm 1/3$
$f^2, f^{12}(^3P)\ s^1(^2S)$	^4P	-2	$\pm 1/3$
$f^2, f^{12}(^1I)\ s^1(^2S)$	^2I	0	0
$f^2, f^{12}(^3H)\ s^1(^2S)$	^2H	4	$\pm 2/3$
$f^2, f^{12}(^1G)\ s^1(^2S)$	^2G	0	0
$f^2, f^{12}(^3F)\ s^1(^2S)$	^2F	4	$\pm 2/3$
$f^2, f^{12}(^1D)\ s^1(^2S)$	^2D	0	0
$f^2, f^{12}(^3P)\ s^1(^2S)$	^2P	4	$\pm 2/3$
$f^2, f^{12}(^1S)\ s^1(^2S)$	^2S	0	
$f^3, f^{11}(^4I)\ s^1(^2S)$	^5I	-3	$\pm 1/4$
$f^3, f^{11}(^4G)\ s^1(^2S)$	^5G	-3	$\pm 1/4$
$f^3, f^{11}(^4F)\ s^1(^2S)$	^5F	-3	$\pm 1/4$
$f^3, f^{11}(^4D)\ s^1(^2S)$	^5D	-3	$\pm 1/4$
$f^3, f^{11}(^4S)\ s^1(^2S)$	^5S	-3	
$f^3, f^{11}(^2L)\ s^1(^2S)$	^3L	-1	$\pm 1/8$
$f^3, f^{11}(^2K)\ s^1(^2S)$	^3K	-1	$\pm 9/56$
$f^3, f^{11}(^4I)\ s^1(^2S)$	^3I	5	$\pm 5/12$
$f^3, f^{11}(^2I)\ s^1(^2S)$	^3I	-1	$\pm 1/21$
$f^3, f^{11}(^4G)\ s^1(^2S)$	^3G	5	$\pm 5/12$
$f^3, f^{11}(^4F)\ s^1(^2S)$	^3F	5	$\pm 5/12$
$f^3, f^{11}(^4D)\ s^1(^2S)$	^3D	5	$\pm 5/12$
$f^3, f^{11}(^2P)\ s^1(^2S)$	^3P	-1	0
$f^3, f^{11}(^4S)\ s^1(^2S)$	^3S	5	
$f^3, f^{11}(^2L)\ s^1(^2S)$	^1L	3	
$f^3, f^{11}(^2K)\ s^1(^2S)$	^1K	3	
$f^3, f^{11}(^2I)\ s^1(^2S)$	^1I	3	
$f^3, f^{11}(^2P)\ s^1(^2S)$	^1P	3	

			K_{303}	α_3
$f^4, f^{10}(^5I)\ s^1(^2S)$		^6I	-4	$\pm1/5$
$f^4, f^{10}(^5G)\ s^1(^2S)$		^6G	-4	$\pm1/5$
$f^4, f^{10}(^5F)\ s^1(^2S)$		^6F	-4	$\pm1/5$
$f^4, f^{10}(^5D)\ s^1(^2S)$		^6D	-4	$\pm1/5$
$f^4, f^{10}(^5S)\ s^1(^2S)$		^6S	-4	
$f^4, f^{10}(^3M)\ s^1(^2S)$		^4M	-2	$\pm1/9$
$f^4, f^{10}(^3L)\ s^1(^2S)$		^4L	-2	$\pm5/36$
$f^4, f^{10}(^5I)\ s^1(^2S)$		^4I	6	$\pm3/10$
$f^4, f^{10}(^5G)\ s^1(^2S)$		^4G	6	$\pm3/10$
$f^4, f^{10}(^5F)\ s^1(^2S)$		^4F	6	$\pm3/10$
$f^4, f^{10}(^5D)\ s^1(^2S)$		^4D	6	$\pm3/10$
$f^4, f^{10}(^5S)\ s^1(^2S)$		^4S	6	
$f^4, f^{10}(^1N)\ s^1(^2S)$		^2N	0	0
$f^4, f^{10}(^3M)\ s^1(^2S)$		^2M	4	$\pm2/9$
$f^4, f^{10}(^3L)\ s^1(^2S)$		^2L	4	$\pm5/18$
$f^4, f^{10}(^1K)\ s^1(^2S)$		^2K	0	0
$f^4, f^{10}(^1F)\ s^1(^2S)$		^2F	0	0
$f^5, f^9(^6H)\ s^1(^2S)$		^7H	-5	$\pm1/6$
$f^5, f^9(^6F)\ s^1(^2S)$		^7F	-5	$\pm1/6$
$f^5, f^9(^6P)\ s^1(^2S)$		^7P	-5	$\pm1/6$
$f^5, f^9(^4M)\ s^1(^2S)$		^5M	-3	$\pm1/12$
$f^5, f^9(^4L)\ s^1(^2S)$		^5L	-3	$\pm5/48$
$f^5, f^9(^6H)\ s^1(^2S)$		^5H	7	$\pm7/30$
$f^5, f^9(^6F)\ s^1(^2S)$		^5F	7	$\pm7/30$
$f^5, f^9(^6P)\ s^1(^2S)$		^5P	7	$\pm7/30$
$f^5, f^9(^4S)\ s^1(^2S)$		^5S	-3	
$f^5, f^9(^2O)\ s^1(^2S)$		^3O	-1	$\pm1/22$
$f^5, f^9(^2N)\ s^1(^2S)$		^3N	-1	$\pm3/55$
$f^5, f^9(^4M)\ s^1(^2S)$		^3M	5	$\pm5/36$
$f^5, f^9(^4L)\ s^1(^2S)$		^3L	5	$\pm25/144$
$f^5, f^9(^4S)\ s^1(^2S)$		^3S	5	
$f^5, f^9(^2O)\ s^1(^2S)$		^1O	3	
$f^5, f^9(^2N)\ s^1(^2S)$		^1N	3	
$f^6, f^8(^7F)\ s^1(^2S)$		^8F	-6	$\pm1/7$
$f^6, f^8(^5L)\ s^1(^2S)$		^6L	-4	$\pm1/20$

		K_{303}	α_3
$f^6, f^8(^5K)\ s^1(^2S)$	^6K	-4	$\pm 9/140$
$f^6, f^8(^7F)\ s^1(^2S)$	^6F	8	$\pm 4/21$
$f^6, f^8(^5P)\ s^1(^2S)$	^6P	-4	0
$f^6, f^8(^5S)\ s^1(^2S)$	^6S	-4	
$f^6, f^8(^3O)\ s^1(^2S)$	^4O	-2	$\pm 1/33$
$f^6, f^8(^3N)\ s^1(^2S)$	^4N	-2	$\pm 2/55$
$f^6, f^8(^5L)\ s^1(^2S)$	^4L	6	$\pm 3/40$
$f^6, f^8(^5K)\ s^1(^2S)$	^4K	6	$\pm 27/280$
$f^6, f^8(^5P)\ s^1(^2S)$	^4P	6	0
$f^6, f^8(^5S)\ s^1(^2S)$	^4S	6	
$f^6, f^8(^1Q)\ s^1(^2S)$	^2Q	0	0
$f^6, f^8(^3O)\ s^1(^2S)$	^2O	4	$\pm 2/33$
$f^6, f^8(^3N)\ s^1(^2S)$	^2N	4	$\pm 4/55$
$f^6, f^8(^1P)\ s^1(^2S)$	^2P	0	0
$f^7(^8S)\ s^1(^2S)$	^9S	-7	
$f^7(^6I)\ s^1(^2S)$	^7I	-5	0
$f^7(^6H)\ s^1(^2S)$	^7H	-5	0
$f^7(^6G)\ s^1(^2S)$	^7G	-5	0
$f^7(^6F)\ s^1(^2S)$	^7F	-5	0
$f^7(^6D)\ s^1(^2S)$	^7D	-5	0
$f^7(^6P)\ s^1(^2S)$	^7P	-5	0
$f^7(^8S)\ s^1(^2S)$	^7S	9	
$f^7(^4N)\ s^1(^2S)$	^5N	-3	0
$f^7(^4M)\ s^1(^2S)$	^5M	-3	0
$f^7(^4_5L)\ s^1(^2S)$	^5_5L	-3	0
$f^7(^4_7K)\ s^1(^2S)$	^5_7K	-3	0
$f^7(^6I)\ s^1(^2S)$	^5I	7	0
$f^7(^6H)\ s^1(^2S)$	^5H	7	0
$f^7(^6G)\ s^1(^2S)$	^5G	7	0
$f^7(^6F)\ s^1(^2S)$	^5F	7	0
$f^7(^6D)\ s^1(^2S)$	^5D	7	0
$f^7(^6P)\ s^1(^2S)$	^5P	7	0
$f^7(^2Q)\ s^1(^2S)$	^3Q	-1	0
$f^7(^2O)\ s^1(^2S)$	^3O	-1	0
$f^7(^4N)\ s^1(^2S)$	^3N	5	0

		K_{303}	α_3
$f^7(^2_7N)\ s^1(^2S)$	^3_7N	-1	0
$f^7(^2_5N)\ s^1(^2S)$	^3_5N	-1	0
$f^7(^4M)\ s^1(^2S)$	^3M	5	0
$f^7(^4_5L)\ s^1(^2S)$	^3_5L	5	0
$f^7(^4_7K)\ s^1(^2S)$	^3_7K	5	0
$f^7(^2Q)\ s^1(^2S)$	^1Q	3	
$f^7(^2O)\ s^1(^2S)$	^1O	3	
$f^7(^2_7N)\ s^1(^2S)$	^1_7N	3	
$f^7(^2_5N)\ s^1(^2S)$	^1_5N	3	

		K_{404}	α_4
$g^1, g^{17}(^2G)\ s^1(^2S)$	^3G	-1	$\pm 1/2$
$g^1, g^{17}(^2G)\ s^1(^2S)$	^1G	3	
$g^8, g^{10}(^9G)\ s^1(^2S)$	^{10}G	-8	$\pm 1/9$
$g^9(^{10}S)\ s^1(^2S)$	^{11}S	-9	
$g^9(^{10}S)\ s^1(^2S)$	^9S	11	

		J_{212}	K_{211}	K_{213}	α_1	α_2
—— 2 or 14 d, p electrons ——						
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^3F	-2/7	-2	3/7	$\pm 1/6$	$\pm 1/3$
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^3D	1	8/5	-3/5	$\pm 1/12$	$\pm 5/12$
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^3P	-1	0	-3	$\mp 1/4$	$\pm 3/4$
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^1F	-2/7	14/5	27/35		
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^1D	1	-4/5	9/5		
$d^1p^1, d^9p^5(^2D,\ ^2P)$	^1P	-1	4/5	21/5		
—— 3 or 13 d, p electrons ——						
$d^1p^2, d^9p^4(^2D,\ ^3P)$	^4F	2/7	-8/5	6/35	$\pm 1/9$	$\pm 2/9$
$d^1p^2, d^9p^4(^2D,\ ^3P)$	^4D	-1	-8/5	-12/5	$\pm 1/18$	$\pm 5/18$
$d^1p^2, d^9p^4(^2D,\ ^3P)$	^4P	1	12/5	-12/5	$\mp 1/6$	$\pm 1/2$
$d^1p^2, d^9p^4(^2D,\ ^1D)$	^2G	-4/7	-8/5	36/35	0	$\pm 1/2$
$d^1p^2, d^9p^4(^2D,\ ^1D)$	^2S	-2	2/5	-12/5		
$d^2p^1, d^8p^5(^3F,\ ^2P)$	^4G	-1/7	-14/5	18/35	$\pm 1/12$	$\pm 1/4$
$d^2p^1, d^8p^5(^3F,\ ^2P)$	^4F	3/7	2/5	-54/35	$\pm 1/36$	$\pm 11/36$
$d^2p^1, d^8p^5(^3F,\ ^2P)$	^4D	-12/35	28/25	-666/175	$\mp 1/9$	$\pm 4/9$
$d^2p^1, d^8p^5(^3P,\ ^2P)$	^4D	1/5	-28/25	-12/25	$\pm 1/6$	$\pm 1/6$
$d^2p^1, d^8p^5(^3P,\ ^2P)$	^4P	-1	-8/5	-12/5	$\pm 1/6$	$\pm 1/6$
$d^2p^1, d^8p^5(^3P,\ ^2P)$	^4S	2	16/5	-6/5		

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^2p^1, d^8p^5(^1G,\ ^2P)$	^2H	-4/7	-8/5	36/35	$\pm1/5$	0
$d^2p^1, d^8p^5(^3P,\ ^2P)$	^2S	2	-2/5	12/5		

—— 4 or 12 d, p electrons ——

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^1p^3, d^9p^3(^2D,\ ^4S)$	^5D	0	-6/5	-9/5	0	$\pm1/4$
$d^1p^3, d^9p^3(^2D,\ ^2D)$	^3G	0	-6/5	27/35	0	$\pm1/4$
$d^1p^3, d^9p^3(^2D,\ ^2D)$	^3S	0	14/5	-9/5		
$d^1p^3, d^9p^3(^2D,\ ^2D)$	^1G	0	-6/5	87/35		
$d^1p^3, d^9p^3(^2D,\ ^2D)$	^1S	0	-6/5	-9/5		
$d^2p^2, d^8p^4(^3F,\ ^3P)$	^5G	1/7	-16/5	-18/35	$\pm1/16$	$\pm3/16$
$d^2p^2, d^8p^4(^3F,\ ^3P)$	^5F	-3/7	-8/5	-114/35	$\pm1/48$	$\pm11/48$
$d^2p^2, d^8p^4(^3F,\ ^3P)$	^5D	12/35	32/25	-804/175	$\mp1/12$	$\pm1/3$
$d^2p^2, d^8p^4(^3P,\ ^3P)$	^5D	-1/5	-62/25	-48/25	$\pm1/8$	$\pm1/8$
$d^2p^2, d^8p^4(^3P,\ ^3P)$	^5P	1	2/5	-12/5	$\pm1/8$	$\pm1/8$
$d^2p^2, d^8p^4(^3P,\ ^3P)$	^5S	-2	-16/5	-24/5		
$d^2p^2, d^8p^4(^3P,\ ^3P)$	^3S	-2	8/5	12/5		
$d^2p^2, d^8p^4(^1G,\ ^1D)$	^1I	-8/7	-16/5	72/35		
$d^2p^2, d^8p^4(^1G,\ ^1D)$	^1H	10/7	2/5	36/35		
$d^3p^1, d^7p^5(^4F,\ ^2P)$	^5G	1/7	-14/5	3/35	$\pm1/16$	$\pm3/16$
$d^3p^1, d^7p^5(^4F,\ ^2P)$	^5F	-3/7	-6/5	-93/35	$\pm1/48$	$\pm11/48$
$d^3p^1, d^7p^5(^4F,\ ^2P)$	^5D	12/35	42/25	-699/175	$\mp1/12$	$\pm1/3$
$d^3p^1, d^7p^5(^4P,\ ^2P)$	^5D	-1/5	-52/25	-33/25	$\pm1/8$	$\pm1/8$
$d^3p^1, d^7p^5(^4P,\ ^2P)$	^5P	1	4/5	-9/5	$\pm1/8$	$\pm1/8$
$d^3p^1, d^7p^5(^4P,\ ^2P)$	^5S	-2	-14/5	-21/5		
$d^3p^1, d^7p^5(^2H,\ ^2P)$	^3I	-3/7	-12/5	39/35	$\pm1/12$	$\pm1/12$
$d^3p^1, d^7p^5(^2H,\ ^2P)$	^1I	-3/7	0	15/7		
$d^3p^1, d^7p^5(^2P,\ ^2P)$	^1S	4/7	-14/5	33/35		

—— 5 or 11 d, p electrons ——

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^1p^4, d^9p^2(^2D,\ ^3P)$	^4F	-2/7	-4/5	-6/5	$\mp1/9$	$\pm2/9$
$d^1p^4, d^9p^2(^2D,\ ^3P)$	^4D	1	-4/5	-6/5	$\mp1/18$	$\pm5/18$
$d^1p^4, d^9p^2(^2D,\ ^3P)$	^4P	-1	-4/5	-6/5	$\pm1/6$	$\pm1/2$
$d^1p^4, d^9p^2(^2D,\ ^1D)$	^2G	4/7	-4/5	48/35	0	$\pm1/2$
$d^1p^4, d^9p^2(^2D,\ ^1D)$	^2S	2	16/5	-6/5		
$d^2p^3, d^8p^3(^3F,\ ^4S)$	^6F	0	-12/5	-18/5	0	$\pm1/5$
$d^2p^3, d^8p^3(^3P,\ ^4S)$	^6P	0	-12/5	-18/5	0	$\pm1/5$
$d^2p^3, d^8p^3(^3F,\ ^2D)$	^4H	0	-12/5	24/35	0	$\pm1/5$

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^2p^3, d^8p^3(^1G,\ ^2D)$	^2I	0	-12/5	12/5	0	0
$d^3p^2, d^7p^4(^4F,\ ^3P)$	^6G	-1/7	-22/5	-66/35	$\pm1/20$	$\pm3/20$
$d^3p^2, d^7p^4(^4F,\ ^3P)$	^6F	3/7	-18/5	-138/35	$\pm1/60$	$\pm11/60$
$d^3p^2, d^7p^4(^4F,\ ^3P)$	^6D	-12/35	-12/5	-1086/175	$\mp1/15$	$\pm4/15$
$d^3p^2, d^7p^4(^4P,\ ^3P)$	^6D	1/5	-68/25	-72/25	$\pm1/10$	$\pm1/10$
$d^3p^2, d^7p^4(^4P,\ ^3P)$	^6P	-1	-16/5	-24/5	$\pm1/10$	$\pm1/10$
$d^3p^2, d^7p^4(^4P,\ ^3P)$	^6S	2	8/5	-18/5		
$d^3p^2, d^7p^4(^2H,\ ^3P)$	^4I	3/7	-12/5	24/35	$\pm1/18$	$\pm1/18$
$d^3p^2, d^7p^4(^2H,\ ^1D)$	^2K	-6/7	-18/5	96/35	0	$\pm1/7$
$d^4p^1, d^6p^5(^5D,\ ^2P)$	^6F	2/7	-12/5	-36/35	$\pm1/15$	$\pm2/15$
$d^4p^1, d^6p^5(^5D,\ ^2P)$	^6D	-1	-12/5	-18/5	$\pm1/30$	$\pm1/6$
$d^4p^1, d^6p^5(^5D,\ ^2P)$	^6P	1	8/5	-18/5	$\mp1/10$	$\pm3/10$
$d^4p^1, d^6p^5(^3H,\ ^2P)$	^4I	-1/7	-12/5	24/35	$\pm1/18$	$\pm1/18$
$d^4p^1, d^6p^5(^1I,\ ^2P)$	^2K	-2/7	-2	12/7	$\pm1/7$	0
—— 6 or 10 d, p electrons ——						
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^3F	2/7	-2/5	-3/5	$\mp1/6$	$\pm1/3$
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^3D	-1	-2/5	-3/5	$\mp1/12$	$\pm5/12$
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^3P	1	-2/5	-3/5	$\pm1/4$	$\pm3/4$
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^1F	2/7	-2/5	159/35		
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^1D	-1	-2/5	-3/5		
$d^1p^5, d^9p^1(^2D,\ ^2P)$	^1P	1	38/5	-3/5		
$d^2p^4, d^8p^2(^3F,\ ^3P)$	^5G	-1/7	-8/5	-12/5	$\mp1/16$	$\pm3/16$
$d^2p^4, d^8p^2(^3F,\ ^3P)$	^5F	3/7	-8/5	-12/5	$\mp1/48$	$\pm11/48$
$d^2p^4, d^8p^2(^3F,\ ^3P)$	^5D	-12/35	-8/5	-12/5	$\pm1/12$	$\pm1/3$
$d^2p^4, d^8p^2(^3P,\ ^3P)$	^5D	1/5	-8/5	-12/5	$\mp1/8$	$\pm1/8$
$d^2p^4, d^8p^2(^3P,\ ^3P)$	^5P	-1	-8/5	-12/5	$\mp1/8$	$\pm1/8$
$d^2p^4, d^8p^2(^3P,\ ^3P)$	^5S	2	-8/5	-12/5		
$d^2p^4, d^8p^2(^3P,\ ^3P)$	^3S	2	28/5	12/5		
$d^2p^4, d^8p^2(^1G,\ ^1D)$	^1I	8/7	-8/5	96/35		
$d^2p^4, d^8p^2(^1G,\ ^1D)$	^1H	-10/7	-8/5	6/35		
$d^3p^3, d^7p^3(^4F,\ ^4S)$	^7F	0	-18/5	-27/5	0	$\pm1/6$
$d^3p^3, d^7p^3(^4P,\ ^4S)$	^7P	0	-18/5	-27/5	0	$\pm1/6$
$d^3p^3, d^7p^3(^4P,\ ^2P)$	^5S	0	-2	-3		
$d^3p^3, d^7p^3(^2H,\ ^2D)$	^3K	0	-18/5	81/35	0	$\pm1/7$
$d^3p^3, d^7p^3(^2H,\ ^2D)$	^1K	0	-6/5	177/35		

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^4p^2, d^6p^4(^5D,\ ^3P)$	^7F	-2/7	-24/5	-132/35	±1/18	±1/9
$d^4p^2, d^6p^4(^5D,\ ^3P)$	^7D	1	-6/5	-24/5	±1/36	±5/36
$d^4p^2, d^6p^4(^5D,\ ^3P)$	^7P	-1	-14/5	-36/5	∓1/12	±1/4
$d^4p^2, d^6p^4(^3H,\ ^3P)$	^5I	1/7	-18/5	-24/35	±1/24	±1/24
$d^4p^2, d^6p^4(^1I,\ ^1D)$	^1L	-4/7	-4	24/7		
$d^4p^2, d^6p^4(^1I,\ ^1D)$	^1K	4/7	-4/5	48/35		
$d^5p^1, d^5p^5(^6S,\ ^2P)$	^7P	0	-2	-3	±1/6	0
$d^5p^1, d^5p^5(^4G,\ ^2P)$	^5H	0	-2	-3/7	±1/20	0
$d^5p^1, d^5p^5(^4P,\ ^2P)$	^5S	0	-2	-3		
$d^5p^1, d^5p^5(^2I,\ ^2P)$	^3K	0	-2	9/7	±1/14	0
$d^5p^1, d^5p^5(^2I,\ ^2P)$	^1K	0	-6/5	117/35		
$d^5p^1, d^5p^5(^2P,\ ^2P)$	^1S	0	-2	-3/7		

—— 7 or 9 d, p electrons ——

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^2p^5, d^8p^1(^3F,\ ^2P)$	^4G	1/7	-4/5	-6/5	∓1/12	±1/4
$d^2p^5, d^8p^1(^3F,\ ^2P)$	^4F	-3/7	-4/5	-6/5	∓1/36	±11/36
$d^2p^5, d^8p^1(^3F,\ ^2P)$	^4D	12/35	-4/5	-6/5	±1/9	±4/9
$d^2p^5, d^8p^1(^3P,\ ^2P)$	^4D	-1/5	-4/5	-6/5	∓1/6	±1/6
$d^2p^5, d^8p^1(^3P,\ ^2P)$	^4P	1	-4/5	-6/5	∓1/6	±1/6
$d^2p^5, d^8p^1(^3P,\ ^2P)$	^4S	-2	-4/5	-6/5		
$d^2p^5, d^8p^1(^1G,\ ^2P)$	^2H	4/7	-4/5	48/35	∓1/5	0
$d^2p^5, d^8p^1(^3P,\ ^2P)$	^2S	-2	-4/5	-6/5		
$d^3p^4, d^7p^2(^4F,\ ^3P)$	^6G	1/7	-12/5	-18/5	∓1/20	±3/20
$d^3p^4, d^7p^2(^4F,\ ^3P)$	^6F	-3/7	-12/5	-18/5	∓1/60	±11/60
$d^3p^4, d^7p^2(^4F,\ ^3P)$	^6D	12/35	-12/5	-18/5	±1/15	±4/15
$d^3p^4, d^7p^2(^4P,\ ^3P)$	^6D	-1/5	-12/5	-18/5	∓1/10	±1/10
$d^3p^4, d^7p^2(^4P,\ ^3P)$	^6P	1	-12/5	-18/5	∓1/10	±1/10
$d^3p^4, d^7p^2(^4P,\ ^3P)$	^6S	-2	-12/5	-18/5		
$d^3p^4, d^7p^2(^2H,\ ^3P)$	^4I	-3/7	-12/5	-6/35	∓1/18	±1/18
$d^3p^4, d^7p^2(^2H,\ ^1D)$	^2K	6/7	-12/5	114/35	0	±1/7
$d^4p^3, d^6p^3(^5D,\ ^4S)$	^8D	0	-24/5	-36/5	0	±1/7
$d^4p^3, d^6p^3(^3H,\ ^4S)$	^6H	0	-12/5	-18/5	0	±1/25
$d^4p^3, d^6p^3(^5D,\ ^2D)$	^6S	0	-6/5	-24/5		
$d^4p^3, d^6p^3(^3H,\ ^2D)$	^4K	0	-22/5	54/35	0	±1/21
$d^4p^3, d^6p^3(^1I,\ ^2D)$	^2L	0	-18/5	18/5	0	0
$d^5p^2, d^5p^4(^6S,\ ^3P)$	^8P	0	-4	-6	±1/7	0

		J_{212}	K_{211}	K_{213}	α_1	α_2
$d^5p^2, d^5p^4(^4G,\ ^3P)$	^6H	0	-4	-18/7	$\pm 1/25$	0
$d^5p^2, d^5p^4(^2I,\ ^3P)$	^4K	0	-14/5	18/35	$\pm 1/21$	0
$d^5p^2, d^5p^4(^2I,\ ^1D)$	^2L	0	-18/5	18/5	0	0
$d^6p^1, d^4p^5(^5D,\ ^2P)$	^6F	-2/7	-8/5	-12/5	$\pm 1/15$	$\mp 2/15$
$d^6p^1, d^4p^5(^5D,\ ^2P)$	^6D	1	-8/5	-12/5	$\pm 1/30$	$\mp 1/6$
$d^6p^1, d^4p^5(^5D,\ ^2P)$	^6P	-1	-8/5	-12/5	$\mp 1/10$	$\mp 3/10$
$d^6p^1, d^4p^5(^3H,\ ^2P)$	^4I	1/7	-8/5	6/35	$\pm 1/18$	$\mp 1/18$
$d^6p^1, d^4p^5(^1I,\ ^2P)$	^2K	2/7	-8/5	66/35	$\pm 1/7$	0
—— 8 d, p electrons ——						
$d^3p^5, d^7p^1(^4F,\ ^2P)$	^5G	-1/7	-6/5	-9/5	$\mp 1/16$	$\pm 3/16$
$d^3p^5, d^7p^1(^4F,\ ^2P)$	^5F	3/7	-6/5	-9/5	$\mp 1/48$	$\pm 11/48$
$d^3p^5, d^7p^1(^4F,\ ^2P)$	^5D	-12/35	-6/5	-9/5	$\pm 1/12$	$\pm 1/3$
$d^3p^5, d^7p^1(^4P,\ ^2P)$	^5D	1/5	-6/5	-9/5	$\mp 1/8$	$\pm 1/8$
$d^3p^5, d^7p^1(^4P,\ ^2P)$	^5P	-1	-6/5	-9/5	$\mp 1/8$	$\pm 1/8$
$d^3p^5, d^7p^1(^4P,\ ^2P)$	^5S	2	-6/5	-9/5		
$d^3p^5, d^7p^1(^2H,\ ^2P)$	^3I	3/7	-6/5	27/35	$\mp 1/12$	$\pm 1/12$
$d^3p^5, d^7p^1(^2H,\ ^2P)$	^1I	3/7	-6/5	21/5		
$d^3p^5, d^7p^1(^2P,\ ^2P)$	^1S	-4/7	-6/5	-9/5		
$d^4p^4, d^6p^2(^5D,\ ^3P)$	^7F	2/7	-16/5	-24/5	$\mp 1/18$	$\pm 1/9$
$d^4p^4, d^6p^2(^5D,\ ^3P)$	^7D	-1	-16/5	-24/5	$\mp 1/36$	$\pm 5/36$
$d^4p^4, d^6p^2(^5D,\ ^3P)$	^7P	1	-16/5	-24/5	$\pm 1/12$	$\pm 1/4$
$d^4p^4, d^6p^2(^3H,\ ^3P)$	^5I	-1/7	-16/5	-48/35	$\mp 1/24$	$\pm 1/24$
$d^4p^4, d^6p^2(^1I,\ ^1D)$	^1L	4/7	-16/5	132/35		
$d^4p^4, d^6p^2(^1I,\ ^1D)$	^1K	-4/7	-8/5	36/35		
$d^5p^3(^6S,\ ^4S)$	^9S	0	-6	-9		
$d^5p^3(^4G,\ ^4S)$	^7G	0	-18/5	-27/5	0	0
$d^5p^3(^4F,\ ^4S)$	^7F	0	-18/5	-27/5	0	0
$d^5p^3(^6S,\ ^4S)$	^7S	0	2/5	3/5		
$d^5p^3(^2I,\ ^2D)$	^3L	0	-22/5	99/35	0	0
$d^5p^3(^2I,\ ^2D)$	^1L	0	-6/5	207/35		

		J_{312}	K_{312}	K_{314}	α_1	α_3
$f^1(^2F)\,p^1(^2P)$	^3G	-1/3	-15/7	10/21	1/8	3/8
$f^1(^2F)\,p^1(^2P)$	^3F	1	9/7	-2/7	1/24	11/24
$f^1(^2F)\,p^1(^2P)$	^3D	-4/5	9/35	-20/7	-1/6	2/3
$f^1(^2F)\,p^1(^2P)$	^1G	-1/3	3	2/3		
$f^1(^2F)\,p^1(^2P)$	^1F	1	-3/7	10/7		
$f^1(^2F)\,p^1(^2P)$	^1D	-4/5	3/5	4		
$f^2(^3H)\,p^1(^2P)$	^4I	-1/3	-24/7	16/21	1/18	5/18
$f^2(^3H)\,p^1(^2P)$	^4H	13/15	24/35	-20/21	1/90	29/90
$f^3(^4I)\,p^1(^2P)$	^5K	-2/15	-141/35	16/21	1/28	3/14
$f^3(^4I)\,p^1(^2P)$	^5I	1/3	-3/7	-40/21	1/168	41/168
$f^4(^5I)\,p^1(^2P)$	^6K	2/15	-144/35	8/21	1/35	6/35
$f^4(^5I)\,p^1(^2P)$	^6I	-1/3	-12/7	-62/21	1/210	41/210
$f^5(^6H)\,p^1(^2P)$	^7I	1/3	-27/7	-10/21	1/36	5/36
$f^5(^6H)\,p^1(^2P)$	^7H	-13/15	-99/35	-82/21	1/180	29/180
$f^6(^7F)\,p^1(^2P)$	^8G	1/3	-24/7	-40/21	1/28	3/28
$f^6(^7F)\,p^1(^2P)$	^8F	-1	-24/7	-32/7	1/84	11/84
$f^6(^7F)\,p^1(^2P)$	^8D	4/5	6/35	-32/7	-1/21	4/21
$f^7(^8S)\,p^1(^2P)$	^9P	0	-3	-4	0	1/8
$f^1(^2F)\,p^2(^3P)$	^4G	1/3	-12/7	8/21	1/12	1/4
$f^1(^2F)\,p^2(^3P)$	^4F	-1	-12/7	-16/7	1/36	11/36
$f^1(^2F)\,p^2(^3P)$	^4D	4/5	66/35	-16/7	-1/9	4/9
$f^1(^2F)\,p^3(^4S)$	^5F	0	-9/7	-12/7	0	1/4

			J_{322}	J_{324}	K_{321}	K_{323}	K_{325}	α_2	α_3
$f^1(^2F)$	$d^1(^2D)$	^3H	-10/21	-3/77	-81/35	-8/45	320/693	1/5	3/10
$f^1(^2F)$	$d^1(^2D)$	^3G	5/7	2/7	69/35	-58/45	20/63	7/40	13/40
$f^1(^2F)$	$d^1(^2D)$	^3F	11/21	-6/7	-27/35	-26/45	-20/63	1/8	3/8
$f^1(^2F)$	$d^1(^2D)$	^3D	-2/7	9/7	27/35	32/15	-40/21	0	1/2
$f^1(^2F)$	$d^1(^2D)$	^3P	-8/7	-6/7	3/35	-4/5	-30/7	-1/2	1
$f^1(^2F)$	$d^1(^2D)$	^1H	-10/21	-3/77	99/35	32/45	340/693		
$f^1(^2F)$	$d^1(^2D)$	^1G	5/7	2/7	-51/35	82/45	40/63		
$f^1(^2F)$	$d^1(^2D)$	^1F	11/21	-6/7	9/7	10/9	80/63		
$f^1(^2F)$	$d^1(^2D)$	^1D	-2/7	9/7	-9/35	-8/5	20/7		
$f^1(^2F)$	$d^1(^2D)$	^1P	-8/7	-6/7	3/7	4/3	110/21		
$f^2(^3H)$	$d^1(^2D)$	^4K	-10/21	4/77	-102/35	-4/5	200/231	2/21	5/21
$f^2(^3H)$	$d^1(^2D)$	^4I	11/21	-24/77	-18/35	-64/45	250/693	1/14	11/42
$f^3(^4I)$	$d^1(^2D)$	^5L	-4/21	3/77	-99/35	-8/5	260/231	1/16	3/16
$f^3(^4I)$	$d^1(^2D)$	^5K	4/21	-17/77	-45/7	-8/9	-20/693	5/112	23/112
$f^4(^5I)$	$d^1(^2D)$	^6L	4/21	-3/77	-18/7	-20/9	760/693	1/20	3/20
$f^4(^5I)$	$d^1(^2D)$	^6K	-4/21	17/77	-18/7	-4/9	-640/693	1/28	23/140
$f^5(^6H)$	$d^1(^2D)$	^7K	10/21	-4/77	-81/35	-12/5	130/231	1/21	5/42
$f^5(^6H)$	$d^1(^2D)$	^7I	-11/21	40/77	-81/35	-38/45	-1570/693	1/28	11/84
$f^6(^7F)$	$d^1(^2D)$	^8H	10/21	3/77	-72/35	-32/15	-60/77	2/35	3/35
$f^6(^7F)$	$d^1(^2D)$	^8G	-5/7	-2/7	-72/35	-32/15	-80/21	1/20	13/140
$f^6(^7F)$	$d^1(^2D)$	^8F	-11/21	6/7	-72/35	8/15	-80/21	1/28	3/28
$f^6(^7F)$	$d^1(^2D)$	^8D	2/7	-9/7	-72/35	-32/15	-80/21	0	1/7
$f^6(^7F)$	$d^1(^2D)$	^8P	8/7	6/7	138/35	-32/15	-80/21	-1/7	2/7
$f^7(^8S)$	$d^1(^2D)$	^9D	0	0	-9/5	-28/15	-10/3	1/8	0
$f^1(^2F)$	$d^2(^3F)$	^4I	-5/21	9/77	-72/35	-46/45	580/693	1/6	1/6
$f^1(^2F)$	$d^2(^3F)$	^4H	5/21	-51/77	-72/35	-46/45	160/693	1/6	1/6
$f^1(^2F)$	$d^3(^4F)$	^5I	5/21	-9/77	-9/5	-44/45	40/77	1/8	1/8
$f^1(^2F)$	$d^3(^4F)$	^5H	-5/21	51/77	-9/5	16/45	-70/99	1/8	1/8
$f^1(^2F)$	$d^4(^5D)$	^6H	10/21	3/77	-54/35	-8/5	40/231	2/25	3/25
$f^1(^2F)$	$d^4(^5D)$	^6G	-5/7	-2/7	-54/35	-8/5	-20/7	7/100	13/100
$f^1(^2F)$	$d^4(^5D)$	^6F	-11/21	6/7	-54/35	16/15	-20/7	1/20	3/20
$f^1(^2F)$	$d^4(^5D)$	^6D	2/7	-9/7	-54/35	-8/5	-20/7	0	1/5
$f^1(^2F)$	$d^4(^5D)$	^6P	8/7	6/7	156/35	-8/5	-20/7	-1/5	2/5
$f^1(^2F)$	$d^5(^6S)$	^7F	0	0	-9/7	-4/3	-50/21	0	1/6

Inter- and Intrashell Coefficients for States with Two Open Shells of the Same Symmetry

El. Config.	State	Coefficients			

		K_{000}
$s^1 s'^1({}^2S)$	${}^3S$	-1

El. Config.	State	J_{112}	K_{110}	K_{112}	α_1
$p^1 p'^1({}^2P)$	${}^3D$	-1/5	-5/3	4/15	1/4
$p^1 p'^1({}^2P)$	${}^3S$	-2	-5/3	-10/3	
$p^1 p'^1({}^2P)$	${}^1P$	1	-5/3	8/3	
$p^2 p'^2({}^3P)$	${}^5D$	-1/5	-8/3	-26/15	1/8
$p^2 p'^2({}^3P)$	${}^5S$	-2	-8/3	-16/3	
$p^2 p'^2({}^1D)$	${}^1G$	-4/5	-8/3	28/15	
$p^3 p'^3({}^4S)$	${}^7S$	0	-3	-6	
$p^3 p'^3({}^2D)$	${}^3G$	0	-3	-6/5	0

El. Config.	State	J_{222}	J_{224}	K_{220}	K_{222}	K_{224}	α_2
$d^1 d'^1({}^2D)$	${}^3G$	-20/49	-1/49	-9/5	-26/49	116/245	1/4
$d^1 d'^1({}^2D)$	${}^3D$	15/49	-36/49	-9/5	44/49	-234/245	1/4
$d^1 d'^1({}^2D)$	${}^3S$	-10/7	-18/7	-9/5	-18/7	-162/35	
$d^1 d'^1(2D)$	${}^1F$	40/49	9/49	-9/5	94/49	216/245	
$d^1 d'^1(2D)$	${}^1P$	-5/7	12/7	-9/5	-8/7	138/35	
$d^2 d'^2({}^3F)$	${}^5I$	-5/49	-9/49	-16/5	-114/49	234/245	1/8
$d^2 d'^2({}^1G)$	${}^1L$	-80/49	-4/49	-16/5	-24/49	484/245	
$d^3 d'^3({}^4F)$	${}^7I$	-5/49	-9/49	-21/5	-184/49	-396/245	1/12
$d^3 d'^3({}^2H)$	${}^3N$	-45/49	-4/49	-21/5	-12/7	122/35	1/20
$d^4 d'^4({}^5D)$	${}^9G$	-20/49	-1/49	-24/5	-236/49	-1774/245	1/16
$d^4 d'^4({}^5D)$	${}^9D$	-15/49	-36/49	-24/5	-166/49	-2124/245	1/16
$d^4 d'^4({}^5D)$	${}^9S$	-10/7	-18/7	-24/5	-48/7	-432/35	
$d^4 d'^4({}^3H)$	${}^5N$	-5/49	-16/49	-24/5	-18/7	68/35	1/80
$d^4 d'^4({}^1I)$	${}^1Q$	-20/49	-20/49	-24/5	-58/7	1476/245	
$d^5 d'^5({}^6S)$	${}^{11}S$	0	0	-5	-50/7	-90/7	
$d^5 d'^5({}^4G)$	${}^7L$	0	0	-5	-150/49	-130/49	0
$d^5 d'^5({}^2I)$	${}^3Q$	0	0	-5	-130/49	270/49	0

$f^1 f'^1$ two lines of coefficients each

		J_{332}	J_{334}	J_{336}	K_{330}
$f^1 f'^1(^2F)$	^3I	-5/9	-9/121	-25/14157	-13/7
$f^1 f'^1(^2F)$	^3G	2/3	-97/121	-50/363	-13/7
$f^1 f'^1(^2F)$	^3D	-19/45	9/11	-125/99	-13/7
$f^1 f'^1(^2F)$	^3S	-4/3	-18/11	-100/33	-13/7
$f^1 f'^1(^2F)$	^1H	5/9	51/121	25/1089	-13/7
$f^1 f'^1(^2F)$	^1F	2/9	3/11	50/99	-13/7
$f^1 f'^1(^2F)$	^1P	-1	-3/11	25/11	-13/7
		K_{332}	K_{334}	K_{336}	α_3
$f^1 f'^1(^2F)$	^3I	-58/63	72/847	42550/99099	1/4
$f^1 f'^1(^2F)$	^3G	32/21	-1160/847	400/2541	1/4
$f^1 f'^1(^2F)$	^3D	-206/315	144/77	-1450/693	1/4
$f^1 f'^1(^2F)$	^3S	-52/21	-234/77	-1300/231	
$f^1 f'^1(^2F)$	^1H	82/63	912/847	3650/7623	
$f^1 f'^1(^2F)$	^1F	40/63	60/77	1000/693	
$f^1 f'^1(^2F)$	^1P	-38/21	-24/77	1150/231	

B   Input for Atomic SCF Program, Columbus Version

Free-Format input for integers and floating-point numbers (ending a line with a / provides the default values for any remaining input variables).

LIM No. of data sets to be run. This line appears only once no matter how many data sets are included.

ANAME (A80) Title for data set.

NFLAG1,NPRINT,NSYM,NVAR,MXVAR,NEXTRA,ISCALE,IAMP,IRD,
NZET,NJ,NK,IPNCH,NLAB,LCPU,ILEG

> NFLAG1=0 : Slater basis.
>
> =1 : Gaussian basis.
>
> NPRINT=0 : Do not print integrals.
>
> =1 : Print integrals.
>
> NSYM : Maximum $(\ell+1)$ value. (=2 means s,p)
>
> (=25 is maximum)
>
> NVAR : No. of exponents to be varied.
>
> MXVAR,NEXTRA,ISCALE : See later notes on exponent optimization.
>
> IAMP=0 : Do not print radial functions.
>
> =1 : Print radial functions (additional input needed later).
>
> IRD=0 : Use default convergence parameters.
>
> =1 : Read in convergence parameters (additional input needed later).
>
> NZET=0 : Normal default.
>
> ≥ 1 : No. of orbital exponents, if less than no. of basis functions (some basis functions constrained to have the same exponents, additional input needed later to specify).
>
> NJ : No. of J-type open-shell energy coefficients to be read in.
>
> NK : No. of K-type open-shell energy coefficients to be read in.
>
> IPNCH : If non-zero, unit no. for writing out orbital exponents and orbital coefficients.
>
> NLAB=0 : n-labels for occupied orbitals will not be read in.
>
> =1 : Read in n-labels for occupied orbitals (to be used when the order is not $\ell+1,\ell+2,...$ for each ℓ).
>
> LCPU=0 : No core potentials used.
>
> ≥ 1 : Maximum $(\ell+1)$ value for which a core potential is used.
>
> ILEG=0 : Normal default.
>
> ≥ 1 : Use Legendre expansion of natural logarithms of exponents.

Requires that expansion coefficients be input in place of
exponent values.

(NBAS(I), I=1,NSYM) No. of basis functions of each symmetry.

(NCSH(I), I=1,NSYM) No. of closed shells of each symmetry.

(NOSH(I), I=1,NSYM) No. of open shells of each symmetry.

(NCCUP(I), I=1,NSYM) Open-shell occupation no. for each symmetry.

(Omit if NLAB is zero): (NLBL(I), I=1,NSHT) n-labels of occupied orbitals.
NSHT=Total no. of shells.

(Omit if NVAR is zero): (NBVAR(I), I=1,NVAR) Indices of exponents to be
varied.

(IPQN(I), I=1,NBAST) Principal quantum numbers of basis functions.
NBAST=Total no. of basis functions=NBAS(1)+NBAS(2)+...

ZN,ZSCALE
ZN : Nuclear Charge.
ZSCALE : Fractional change of exponents during optimization if
ILEG=0. Absolute change of coefficients if ILEG=1.

(Omit if NZET was read in as zero): (NXZET(I), I=1,NBAST)
Orbital exponent index for basis functions.

(ZETA(I), I=1,NZET) Orbital exponents for basis functions.
NZET=NBAST unless a different non-zero value was read in.
If ILEG=1, coefficients of Legendre expansion of natural logarithms of
exponent values.

L1,L2,L3,NUM,NDEN For I=1,NJ. One such line for each non-zero
J-type open-shell energy coefficient.
L1 : lambda (=0 is minimum)
L2 : mu (=0 is minimum; =L1 is maximum)
L3 : nu (=0 is minimum; =2*L2 is maximum)
NUM : numerator of fraction.
NDEN : denominator of fraction (default is 1).

L1,L2,L3,NUM,NDEN For I=1,NK. One such line for each non-zero
K-type open-shell energy coefficient.
L1 : lambda (=0 is minimum)
L2 : mu (=0 is minimum; =L1 is maximum)
L3 : nu (=L1-L2 is minimum; =L1+L2 is maximum)
NUM : numerator of fraction.
NDEN : denominator of fraction (default is 1).

(C(IJM+M), M=1,NBAS(I)) For each shell, read in the initial approximation
to the orbital coefficients, where I designates the symmetry.

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NDIAG,NXTRP,MXXTRP

    NDIAG : No. of diagonalization iterations before diagonalization
            threshold is increased (default is 25).

    NXTRP :No. of SCF iterations before SCF threshold is increased
            (default is 25).

    MXXTRP : No. of SCF iterations allowed (default is 50).

(Omit if IRD=0): BIAS,DGATH,SCFAT,EXPMN,DMNXP,RMNED,
    RMXED

    BIAS : The SCF threshold is 2.0^{BIAS} times the diagonalization
            threshold (default is 1).

    DGATH : Diagonalization threshold maximum (default is 10^{-4}).

    SCFAT : SCF threshold maximum (default is 10^{-3}).

    EXPMN : Minimum exponent value permitted (default is 10^{-2} for
            Slaters, and 10^{-5} for Gaussians).

    DMNXP : Smallest exponent difference permitted (default is 10^{-2} for
            Slaters, and 10^{-7} for Gaussians).

    RMNED : Minimum relative energy change permitted (default is 10^{-11}).

    RMXED : Maximum relative energy change permitted (default is 10^{-1}).

(Omit if LCPU=0): CNAME (A80) Title for core potential.

(Omit if LCPU=0): NZCOR No. of electrons to be replaced by core
    potential.

(Omit if LCPU=0): Groups of lines for the first LCPU symmetries,

    ICPU : No. of functions in potential expansion,

    (Omit if ICPU=0) (NCP(ICP),ZCP(ICP),DCP(ICP), ICP=1,ICPU)
    ICPU such lines.

    NCP(ICP) : Power (+2) of r.

    ZCP(ICP) : Exponential parameter.

    DCP(ICP) : Coefficient.

(Omit if IAMP=0): NGRPS No. of groups of points at which to evaluate
    the radial functions.

(Omit if IAMP=0): (NPTS(I),DEL(I), I=1,NGRPS)

    NPTS(I) : No. of points in this group.

    DEL(I) : Distance between points for this group.

Exponent Optimization

    NVAR : No. of exponents to be varied.

    (NBVAR(I), I=1,NVAR) : Exponents to be varied, in order.

    MXVAR : No. of times this set of optimizations is to be carried out

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(default is 1 if NVAR.gt.0).

NEXTRA : No longer used.

ISCALE=0 : Fractional exponent change = ZSCALE if ILEG=0. Absolute coefficient change if ILEG=1.

=1 : All designated exponents simultaneously changed with fractional increment ZSCALE if ILEG=0. All designated coefficients changed with absolute increment ZSCALE if ILEG=1.

C   Sample Input

Example 1

The orbital exponent of the Gaussian function added to describe the $3p$ orbital of the C atom is optimized. This value could previously only be estimated to be 0.021 (T. H. Dunning and P. J. Hay in Methods of Electronic Structure Theory, H. F. Schaefer, ed., Plenum Press, New York, 1977) because the version of the program available at that time could not do the calculation. The results obtained here are an exponent value of 0.022441 and a total energy of -37.38334669. In doing the corresponding $2p^14p^1$ calculation, a very careful choice of the initial $4p$ vector was required to keep it from collapsing to $3p$.

```
1
CARBON  (1S)2 (2S)2 (2P)1 (3P)1  1P STATE (z=0.022441; e=-37.38334669)
1 0 2 1 1 0 0 0 0 0 1 2 /
9 6
2 0
0 2
0 1
15
1 1 1 1 1 1 1 1 1 2 2 2 2 2 2
6.0 0.01
4233.0 634.9  146.1  42.50  14.19  5.148  1.967 0.4962 0.1533
 18.16 3.986  1.143  0.3594 0.1146 0.021
1 1 2  1  1
1 1 0 -5  3
1 1 2  8  3
 0.0012  0.0093  0.0454  0.1546  0.3587  0.4381  0.1458  0.0020  0.0004
-0.0003 -0.0020 -0.0097 -0.0361 -0.0894 -0.1770 -0.0527  0.5741  0.5476
 0.0147  0.0915  0.3061  0.5074  0.3173  0.0000
-0.0029 -0.0183 -0.0612 -0.1015 -0.0635  1.0000
```

Example 2

The s and p primitives for a cc-pVTZ (correlation-consistent polarized valence triple-zeta) basis set, $(5s5p2d1f)/[4s3p2d1f]/[3s3p2d1f]$, have been optimized for use with the O core potential of L. F. Pacios and P. C. Christiansen, J. Chem. Phys. 82, 2664, 1985. The d and f functions are added later.

```
 1
O  (2s)2 (2p)4 3P, cc-pVTZ, Christiansen RECP (e=-15.67084530)
 1 0 2 0 0 0 0 0 0 0 0 0 2 0 1 2 0
 5 5
 1 0
 0 1
 0 4
 2 2
 1 1 1 1 1 2 2 2 2 2
 8.0 0.002
 37.70  6.840  1.053  0.4163  0.1706
 34.57  7.760  2.282  0.7160  0.2140
 1 1 0 -8  3
 1 1 2 -4  3
 -0.02 -0.14  0.38  0.54  0.21
  0.02  0.10  0.31  0.49  0.34
O core potential
 2
 7
 0    2.1892    2.193891
 1    4.3740    1.042944
 2    2.4049 -16.344477
 2    2.2479  11.216304
 1 100.0039  -1.486456
 2  34.1980  -5.766847
 2  10.0286  -0.798420
 3
 1 100.0039  -1.486456
 2  34.1980  -5.766847
 2  10.0286  -0.798420
```

Example 3

The s, p, and d primitives for a cc-pVDZ (correlation-consistent polarized valence double-zeta) basis set, $(6s6p4d1f)/[4s3p2d1f]/[3s3p2d1f]$, were optimized in other calculations for use with the 10-electron Ni core potential of M. M. Hurley, L. F. Pacios, P. C. Christiansen, R. B. Ross, and W. C. Ermler, J. Chem. Phys. 84, 6840, 1986. The present calculation was used to obtain the s, p, and d contractions together. The f functions were added later. This basis set was developed as perhaps the smallest set to get the lower electronic states in the right order. This type of basis gets the spin-orbit coupling 15% to 20% too small. A $6d$ basis set is needed for reasonably accurate spin-orbit coupling. For this electron configuration, there are two $3d^84s^14p^1$ ^5D wave functions, usually written so that one has the d shell coupled to ^3F and the other to ^3P. Presumably an MCSCF calculation would result in the ^3F term being predominant, so it is used here. Since there are three open shells, open-shell energy coefficients need to be taken from $3(3+1)/2=6$ places in tables: s^1 for K_{000}; p^1 for K_{110}, K_{112}; $d^8(^3F)$ for $K_{220}, K_{222}, K_{224}$; $p^1s^1(^3P)$ for K_{101}; $d^8(^3F)s^1(^4F)$ for K_{202}; $d^8(^3F)p^1(^4D)$ for $J_{212}, K_{211}, K_{213}$.

```
 1
Ni  (4s)1 (3d)8(3F) (4p)1 5D, cc-pVDZ Christiansen RECP (e=-168.27973327)
 1 0 3 0 0 0 0 0 0 0 0 1 10 0 1 3 0
 6 6 4
 1 1 0
 1 1 1
 1 1 8
 3 4 3 4 3
 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3
28.0 0.0007
 124.9 6.941 2.575 0.8926 0.1069 0.03769
 65.66 16.88 2.886 0.9170 0.1326 0.03337
 23.40 6.129 1.741 0.3993
 2 1 2   12 35
 0 0 0   -1   1
 1 0 1   -1   1
 1 1 0   -5   3
 1 1 2    2   3
 2 0 2   -2   1
 2 1 1   -4   5
 2 1 3   -6   5
 2 2 0  -16   5
```

```
2 2 2 -104  49
2 2 4  324 245
-0.00 -0.48  0.79  0.56  0.00  0.00
 0.00  0.13 -0.27 -0.26  0.94  0.18
-0.01 -0.03  0.64  0.45  0.01 -0.00
 0.00  0.00 -0.14 -0.07  0.67  0.47
 0.09  0.35  0.56  0.35
Ni core potential
10
10 / !No. expansion fns (Ni s potential)
0  31.8744    3.171606
1   2.4875    7.880363
2   8.6773  218.644477
2   6.1502 -202.672719
2   4.3453  106.501105
2   3.3950  -48.543110
1 571.4202   -9.794457
2 155.5959  -84.096072
2  45.5220  -32.098072
2  14.8828   -4.438070
10 / !No. expansion fns (Ni p potential)
0  30.3227    5.445407
1   2.2244   -6.764236
2   7.9169  154.697624
2   5.5321 -121.264700
2   4.0426   54.267602
2   1.7805    1.342317
1 571.4202   -9.794457
2 155.5959  -84.096072
2  45.5220  -32.098072
2  14.8828   -4.438070
 4 / !No. expansion fns (Ni d potential)
1 571.4202   -9.794457
2 155.5959  -84.096072
2  45.5220  -32.098072
2  14.8828   -4.438070
```

Example 4

Optimize the exponents for a minimal Slater basis set for C, starting with exponent values from Slater's Rules. See E. Clementi and D. L. Raimondi, J. Chem. Phys. 38, 2686, 1963.

```
1
C  (2s)2 (2p)2 3P, minimal Slater (z=5.6727,1.6083,1.5679; e=-37.622389)
 0 0 2 3 3 0 0 0 0 0 0 2 /
 2 1
 2 0
 0 1
 0 2
 1 2 3
 1 2 2
 6.0 -0.005
 5.7    1.625
 1.625
 1 1 0 -8  3
 1 1 2 -4  3
  1.0 0.0
 -0.2 1.0
  1.0
```

Example 5

For a pvtz S basis set, optimize the (s, p)-exponents in Hartree-Fock calculations on the ground, ^3P, state, using a 10-electron core potential. One s Legendre constraint is used to prevent the 2nd and 3rd s exponents from collapsing. The core potential is from L. F. Pacios and P. A. Christiansen, J. Chem. Phys. 82, 2664, 1985. Two d and one f functions were added later. The d potential could have been omitted in this case.

```
1
S  (3s)2 (3p)4 3P, Christiansen core potential (e=-9.93127973)
 1 0 2 9 32 0 0 0 0 0 0 2 0 1 3 1
 5 5
 1 0
 0 1
 0 4
 3 3
 1 2 3 4 6 7 8 9 10
 1 1 1 1 1 2 2 2 2 2
```

```
16.0     0.0002
 -0.193608 -2.052666  0.848376 -0.530008  0.000
 -0.243022 -2.326330  0.329400 -0.031719 -0.118918
 1 1 0      -8      3
 1 1 2      -4      3
 -0.00 -0.34  0.38  0.39  0.47
 -0.01 -0.03  0.35  0.53  0.26
 S core potential
 10
  9 / !No. expansion fns (S s potential)
 0   4.2705    2.956192
 1   6.4145    5.373976
 2   3.9961 -115.523128
 2   3.2682  182.122366
 2   2.7904  -59.912218
 1  70.1180   -6.839463
 2  22.8283  -26.413399
 2   7.7010   -9.881822
 2   2.6916   -1.090965
  9 / !No. expansion fns (S p potential)
 0   3.3434    4.771437
 1   5.2359    4.199833
 2   3.1484 -100.904171
 2   2.6019  140.849325
 2   2.2363  -48.719188
 1  70.1180   -6.839463
 2  22.8283  -26.413399
 2   7.7010   -9.881822
 2   2.6916   -1.090965
  4 / !No. expansion fns (S d potential)
 1  70.1180   -6.839463
 2  22.8283  -26.413399
 2   7.7010   -9.881822
 2   2.6916   -1.090965
```