ATOMIC DATA AND NUCLEAR DATA TABLES **19**, 83–95 (1977)

DIRAC-FOCK-SLATER CALCULATIONS FOR THE ELEMENTS $Z = 100$, FERMIUM, TO $Z = 173$*

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Listed here for the elements $Z = 100$, fermium, to $Z = 173$ are energy eigenvalues and total energies found from relativistic Dirac-Fock-Slater calculations. The effect of high ionization on the energy eigenvalues is presented for two examples. The use of these tables in connection with the energy levels of superheavy elements and molecular orbital (MO) x-ray transitions in superheavy quasiatoms, is discussed. In addition, a brief comparison between the results of the Dirac-Fock-Slater and Dirac-Fock calculations is given.

* Work supported by Gesellschaft für Schwerionenforschung (GSI), Germany, and partially (G.S.) by the Bundesministerium für Forschung und Technologie (BMFT)

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INTRODUCTION

Within the last fifteen years several tables with the results of self-consistent-field (SCF) atomic calculations have been published. Such calculations can be nonrelativistic or relativistic and can make use either of Slater's exchange approximation or exact exchange. Thus there are four major ways to perform the calculations. In the following we give for each of the four possible methods the best known reference, a short description of the listed results, and the elements covered.

Nonrelativistic Hartree-Fock-Slater (HFS) calculations by F. Herman and S. Skillman[1] with energy eigenvalues, potentials, wavefunctions, and relativistic corrections to the energy eigenvalues, for all elements up to $Z = 103$.

Nonrelativistic Hartree-Fock (HF) calculations by J. B. Mann[2] with energy eigenvalues, total energies, radii, two-electron integrals, and wavefunctions for all elements up to $Z = 103$. See also Refs. 3 and 4.

Relativistic Hartree-Fock-Slater (rel. HFS) or *Dirac-Fock-Slater* (DFS) calculations by C. Lu et al.[5] with energy eigenvalues, total energies, radii, and potentials for all elements up to $Z = 126$.

Relativistic Hartree-Fock (rel. HF) or *Dirac-Fock* (DF) calculations by J. P. Desclaux[6] with energy eigenvalues, radii, wavefunctions, and radial expectation values for all elements up to $Z = 126$.

The tables of Refs. 5 and 6 present results for elements up to $Z = 126$. This number was chosen because several years ago $Z = 126$ was assumed to be the center of an island of nuclear stability. Later calculations of the late sixties shifted this island to $Z = 114$, but 126 was kept as a good endpoint in the tables of Refs. 5 and 6.

The discussion of the existence of elements near $Z = 126$ has been brought up again by recent experimental results.[7] Also, new theoretical Hartree-Fock calculations[8] indicate that stability around $Z = 126$ is more probable than at $Z = 114$.

Atomic Physics of Superheavy Elements

Two groups[9,10] extended SCF atomic calculations to even higher elements mainly to get results for the ground-state configurations, the first ionization potentials, and the principal maxima and radii of the outer-electron wavefunctions. The data, together with extrapolations from the known elements, were used to get an idea of the chemical behavior[11] of the superheavy elements up to $Z = 172$. A model calculation[12] including quantum electrodynamical effects was used to go even to $Z = 184$.

From an atomic-physics point of view, elements with very large proton numbers are especially interesting because many of the corrections, which have to be added to the SCF calculations, are known only in perturbation theory, where the expansion parameter is $Z\alpha(\alpha = 1/137)$.

These corrections take account of the quantum electrodynamical effects, vacuum polarization and vacuum fluctuation, and the so-called Breit interaction which includes magnetic effects and retardation.

The accuracy of the experimental binding energies for elements like uranium and plutonium is now better than 1 eV.[15] A theoretical calculation with such a small error must include the correlation energy as well as SCF effects of the contributions just mentioned. Comparisons between experiment and calculation of the binding energies of the innermost levels of fermium, which yield a

good agreement,[13,14] show that at $Z = 100$ the corrections already are of the order of percent. In the region of the superheavy elements they would be even larger.

Even if no superheavy elements are found near $Z = 114$ or $Z = 126$ at least the atomic clouds of superheavy elements can be produced for a very short time. The method is that of heavy-ion collision, where the energy is large enough so that two nuclei approach each other so closely that the electron clouds of both ions combine and the electrons feel a nuclear charge $Z_1 + Z_2$ in their center. Brief combination is possible because the velocity, at least for the inner electrons, is much larger than the velocity of the two nuclei approaching each other. If, by some process, an electron hole can be created in the inner level of either atom and thus of the combined atomic cloud, it is possible to observe an x-ray transition during the time of collision. The change of the electrons from the levels of the separated atoms to the levels of the combined system, is shown in the so-called correlation diagram, which has been discussed qualitatively in some detail by Lichten[16] as well as by Barat and Lichten.[17] *Ab initio* calculations within the adiabatic approximation, based on the Roothaan-Hartree-Fock method, have been made for small-Z systems.[18] For systems with $Z \gtrsim 40$ only relativistic many-electron molecular calculations lead to good results, which are given by Rosén et al.[19] For the innermost $1s$ electrons one-electron calculations by Müller et al.[20] may give a good first approximation. Explanation of the experimentally observed molecular orbital (MO) M-x-ray spectrum by taking into account all possible transitions of the molecular system I-Au, with a combined $Z = 132$, provides the first evidence of the quasiatomic levels of superheavy elements.[21]

As already mentioned the behavior of the energy levels as function of the distance between the two nuclei is given in the correlation diagrams, in which the levels of the separated systems are linked with the levels of the combined system. Thus the knowledge of the levels of the atomic systems involved is the first step in the construction of the diagrams.

The main purpose of this paper is to give the energy levels of the atoms with $Z > 100$ (the energy levels of the atoms with $Z < 100$ may be taken from any of the other tables). A secondary purpose is to give a first orientation for the expected transition energies for the x-ray spectra of possible superheavy elements since these offer the best means of detecting such elements in small quantities.

Method of Calculation

The Hamiltonian of the atomic problem is given as follows:

$$H = \sum_i T_i - \sum_i \frac{Ze^2}{\mathbf{r_i}} + \sum_{i<j} \frac{e^2}{|\mathbf{r_i} - \mathbf{r_j}|}$$
$$= H_0 + H_{\text{int}}. \tag{1}$$

Using a fully antisymmetrized determinantal wavefunction, one obtains, after the variation of the total energy, the Hartree-Fock equation, which can be written in the form

$$T_i\psi_i(\mathbf{r}) - \frac{Ze^2}{r_i}\psi_i(\mathbf{r})$$
$$+ \left[\sum_k \int \psi_k^*(\mathbf{r}')\psi_k(\mathbf{r}')\frac{e^2}{|\mathbf{r} - \mathbf{r}'|}d\tau'\right]\psi_i(\mathbf{r})$$
$$- \left[\sum_k \int \frac{\psi_i^*(\mathbf{r})\psi_k^*(\mathbf{r}')\psi_k(\mathbf{r})\psi_i(\mathbf{r}')}{\psi_i^*(\mathbf{r})\psi_i(\mathbf{r})}\frac{e^2}{|\mathbf{r} - \mathbf{r}'|}d\tau'\right]\psi_i(\mathbf{r})$$
$$= E_i\psi_i(\mathbf{r}). \tag{2}$$

The total energy is given by the expression

$$E_T = \sum_i \int \psi_i^*(\mathbf{r})H_0\psi_i(\mathbf{r})d\tau$$
$$+ \frac{1}{2}\sum_{i,k} \int\int d\tau\, d\tau' \psi_i^*(\mathbf{r})\psi_k^*(\mathbf{r}')\frac{e^2}{|\mathbf{r} - \mathbf{r}'|}$$
$$\times [\psi_i(\mathbf{r})\psi_k(\mathbf{r}') - \psi_i(\mathbf{r}')\psi_k(\mathbf{r})]. \tag{3}$$

We have used in this calculation the relativistic Hartree-Fock-Slater approximation [usually called Dirac-Fock-Slater (DFS) calculation] in which the last term on the left side of Eq. (2), the exchange term, is approximated by[22]

$$V_{\text{exch}}(r) = -\frac{3\alpha_s}{2\pi}[3\pi^2\rho(r)]^{1/3}. \tag{4}$$

This is a very good description as long as the total electron density $\rho(r)$ is not too small. For very large radii the total potential $1/r$ is used. This procedure results in the so-called Latter correction.[23] We have used here $\alpha_s = 2/3$.

Since we are interested in very heavy elements the wavefunctions have to be found by using the relativistic Dirac operator $T = c\boldsymbol{\alpha}\mathbf{p} + \beta mc^2$ in Eq. (2). Because $\boldsymbol{\alpha}$ and β are four component matrices this leads to the set of coupled differential equations

$$\frac{d}{dr}\begin{pmatrix} F_i(r) \\ G_i(r) \end{pmatrix}$$
$$= \begin{pmatrix} -\kappa_i/r & \alpha[\epsilon_i - V(r)] \\ -\alpha[\epsilon_i - V(r)] + \dfrac{2}{\alpha} & \kappa_i/r \end{pmatrix} \cdot \begin{pmatrix} F_i(r) \\ G_i(r) \end{pmatrix} \tag{5}$$

where α is the fine-structure constant, κ_i the Dirac

quantum number, and F_i and G_i the small and large components of the wavefunction i, respectively. The quantity ϵ_i in Eq. (5) represents the energy required to remove an electron from shell i if all other electrons remain unchanged. Therefore, usually it is called the "binding energy" in the sense of Koopmans' theorem. Because the Dirac equation for a point nucleus leads to a singularity for the $1s$ level at $Z = 137$ we have used an extended nucleus with a Fermi-type nuclear charge distribution

$$\rho(r) = \rho_0\{1 + \exp[4 \ln 3(r - c)/t]\}^{-1} \qquad (6)$$

with the surface thickness $t = 2.2$ fm and the number of nucleons $A = 0.0073\ Z^2 + 1.3\ Z + 63.6$. For the equivalent radius we required $R_{eq} = 1.2\ A^{1/3}$ fm, which determines the half-density radius c.

For further details of the actual calculations and numerical procedures we refer to Refs. 1–6 and 24.

Comments on the Results

Listed in Table I are the electron occupation numbers of the elements $Z = 100$ to $Z = 173$ found from the present DFS calculations. Given are the configurations with the smallest total energies. These are expected to be the ground-state configurations of the free atoms.

There are only a few minor discrepancies between the results of the Dirac-Fock[10] and the Dirac-Fock-Slater calculations for the differences of the total energies of the lowest states. Of course, the first method is more exact but it needs about an order-of-magnitude more computer time and the differences in the results are negligible for many purposes. For only four elements the lowest configurations came out differently in the two calculations but the difference between the total energies of the two lowest configurations is very small, of the order of 0.1 eV.

In the case of the inner levels the additional corrections already noted in the text have to be added. They are small for small Z and of the order of a percent at $Z \approx 100$. First estimates of the quantum electrodynamical corrections for elements near $Z \approx 170$ show[25] that their influence remains below a few percent of the binding energies. The uncertainty due to the unknown nuclear-charge distribution in this region also is of the same order of magnitude.[9]

In spite of the uncertainties in the DFS results, the listed energy eigenvalues of the elements in Table II are expected to give good approximations to the binding energies in the region where one does not know the appropriate corrections. They may be used to construct correlation diagrams and to get a first idea of the ex-

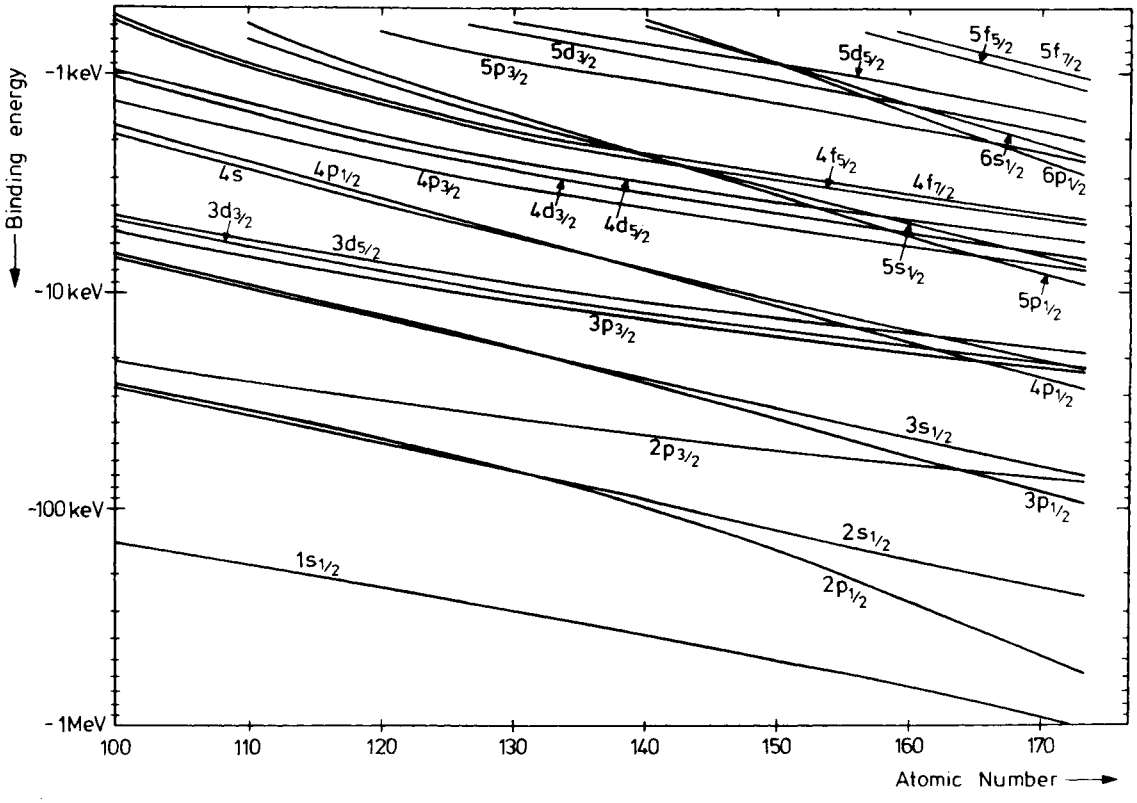

Fig. 1. Energy eigenvalues for the inner electrons of the elements $Z = 100$, fermium, to $Z = 173$

pected x-ray transition energies in the combined system during a heavy-ion collision or in a superheavy element which may be found in nature or a physics laboratory.

In the DFS calculations there is one parameter in front of Slater's exchange approximation in Eq. (4) which can be chosen within some narrow limits to yield an optimal agreement with those values one is looking for. Lu et al.[5] have chosen the original value used by Slater namely $\alpha_s = 1$. This leads to energy eigenvalues which are good approximations for the ionization energies for the outer electrons. The more correct value $\alpha_s = 2/3$ is used by most other authors, but this value has the disadvantage that the ionization energies for the outer electrons have to be calculated with the various corrections. Nearly independent of the value of α_s are the energy eigenvalues of the inner electrons calculated with the DFS approximation which by chance lead to a better agreement with the experimental results than do the exact DF calculations. The differences can be seen in Table III, where we have listed the energy eigenvalues for DF and the DFS calculations for the inner electrons of fermium together with the known experimental results.[13,14] The DFS results seem to be closer to the experimental results. But if all known corrections to the DF calculations are added they, of course, come out to be much more superior.

In order to obtain a general view we give the position of the energy eigenvalues in Fig. 1. The sequence of the levels, which is still normal at $Z = 100$, changes considerably with the higher elements. We see particularly the strong binding of the s and $p_{1/2}$ levels with the same principal quantum number. The reason for this is twofold. The wavefunctions of the electrons with a total angular momentum 1/2 are drawn nearer to the nucleus. This is the so-called direct relativistic effect. In response to this the other electrons are more strongly shielded and thus pushed away from the nucleus. This is the so-called indirect relativistic effect. The two effects together lead to a very unusual ordering of the levels. Figure 2 shows the energy eigenvalues of the outer electrons of the same elements. The behavior of the levels looks very normal for the elements up to $Z \approx 120$ and above $Z \approx 160$. In the intermediate region the onset of the filling of the shells, as well as their behavior with increasing Z, is very complicated.

The total energies in Table II provide an idea of how much energy may be gained from the electron cloud when the two atoms combine during a heavy-ion collision. To give an example we assume that Hg combines with Th to form the superheavy quasi atom $Z = 170$:

$$E_T(170) - E_T(90) - E_T(80) = (5.878 - 0.721 - 0.534)\,\text{MeV} = 4.623\,\text{MeV}.$$

This gain in energy is found for the most optimistic case that all electrons are present and contribute to the binding here amounting to more than 4.6 MeV. The total energies also are shown in Fig. 3 where the sharp rise for large Z can be seen even better.

In heavy-ion collisions the incoming projectile ion

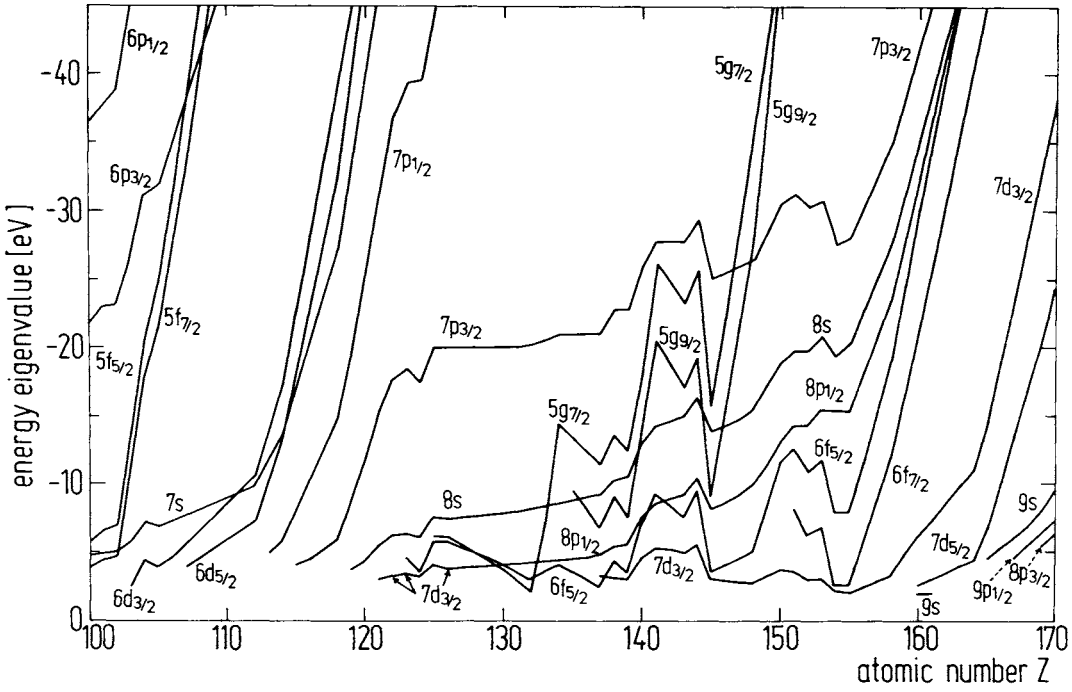

Fig. 2. Energy eigenvalues for the outer electrons of the elements $Z = 100$, fermium, to $Z = 173$

is highly ionized and, because of strong ionization processes during the collision, an even higher ionization of the combined system is expected. To give an idea of the effect of this ionization on the energy levels, we have listed in Table IV the energy eigenvalues of elements $Z = 139$ and $Z = 170$ in various highly ionized states. The table shows that the medium and outer electrons are very strongly affected whereas the innermost electrons are shifted by a considerable amount only for very large ionizations or for ionization of the inner electron shells.

Acknowledgment

We thank Profs. W. Greiner and J. T. Waber for their continuous interest and support.

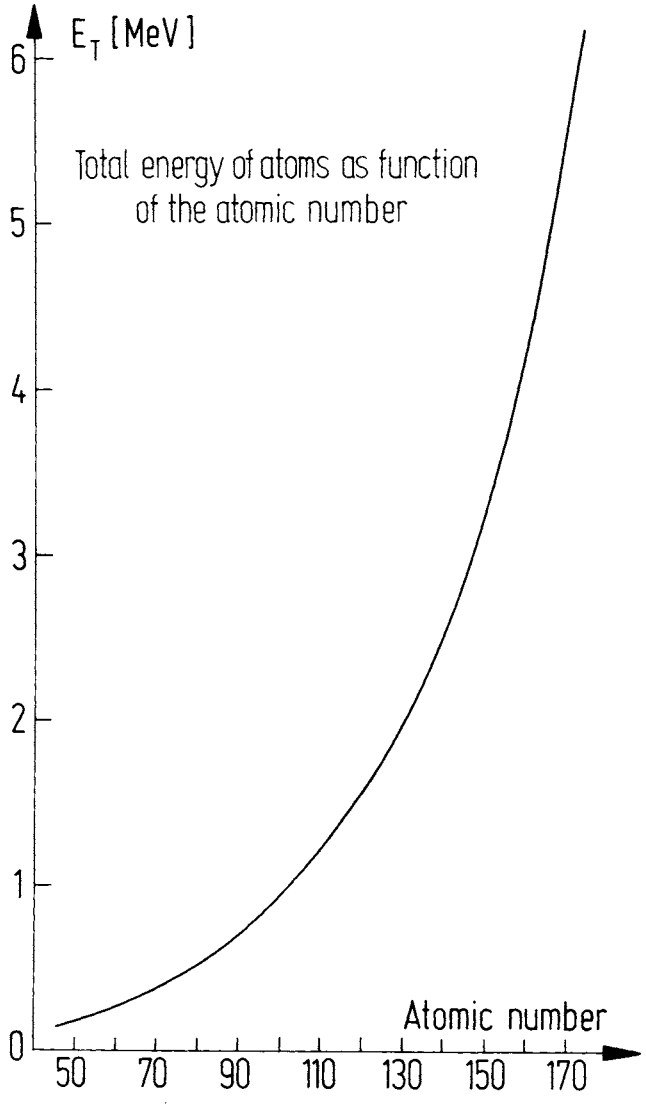

Fig. 3. Total energies of the atoms up to $Z = 173$

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EXPLANATION OF TABLES

TABLE I. Electron Occupation Numbers for the Elements $Z = 100$ to $Z = 173$

Values from present DFS (Dirac-Fock-Slater) calculations

TABLE II. Energy Eigenvalues and Total Energies, $Z = 100$ to $Z = 173$ (in eV)

Values from present DFS (Dirac-Fock-Slater) calculations

c,t	Nuclear-change density parameters c and t in Eq. (6) in fm (10^{-13} cm)
E_T	Total energy

TABLE III. Energy Eigenvalues (in eV) for $Z = 100$ from DF and DFS Calculations and Binding Energies from Experiment

DF	Dirac-Fock results of present authors
Corrections	Magnetic contribution, retardation, vacuum fluctuation, vacuum polarization, and rearrangement effect including rearrangement in the magnetic contribution
Experiment	From conversion electron energies in the beta decay of ^{254m}Es from F. T. Porter and M. S. Freedman, Phys. Rev. Lett. **27,** 293 (1971). The experimental error bars are between 7 and 14 eV
DFS RESULT	Dirac-Fock-Slater values of present authors

TABLE IV. Energy Eigenvalues (in eV) for $Z = 139$ and $Z = 170$ in Various States of Ionization

C,T	Same as c,t in TABLE II

TABLE I. Electron Occupation Numbers for the Elements $Z = 100$ to $Z = 173$
(Rn core plus $7S^2$ and $5F5/2^6$)

Z	5F7/2	6D3/2	6D5/2	7P1/2	7P3/2
100	6				
101	7				
102	8				
103	8	1			
104	8	2			
105	8	3			
106	8	4			
107	8	4	1		
108	8	4	2		
109	8	4	3		
110	8	4	4		
111	8	4	5		
112	8	4	6	1	
113	8	4	6	2	
114	8	4	6	2	
115	8	4	6	2	1
116	8	4	6	2	2
117	8	4	6	2	3
118	8	4	6	2	4

Z	5F7/2	6D3/2	6D5/2	7P1/2	7P3/2	8S1/2	8P1/2	7D3/2	6F5/2	5G7/2
119	8	4	6	2	4	1				
120	8	4	6	2	4	2				
121	8	4	6	2	4	2	1			
122	8	4	6	2	4	2	1	1		
123	8	4	6	2	4	2	1	1	1	
124	8	4	6	2	4	2	1	-	3	
125	8	4	6	2	4	2	1	-	3	1
126	8	4	6	2	4	2	1	1	2	2
127	8	4	6	2	4	2	2	-	2	3
128	8	4	6	2	4	2	2	-	2	4
129	8	4	6	2	4	2	2	-	2	5
130	8	4	6	2	4	2	2	-	2	6
131	8	4	6	2	4	2	2	-	2	7
132	8	4	6	2	4	2	2	-	2	8
133	8	4	6	2	4	2	2	-	3	8
134	8	4	6	2	4	2	2	-	4	8

Z	5G9/2	6F5/2	7D3/2	6F7/2
135	1	4		
136	2	4		
137	3	3	1	
138	4	3	1	
139	5	2	2	
140	6	3	1	
141	7	2	2	
142	8	2	2	
143	9	2	2	
144	10	1	3	
145	10	3	2	
146	10	4	2	
147	10	5	2	
148	10	6	2	
149	10	6	3	
150	10	6	4	
151	10	6	3	2
152	10	6	3	3
153	10	6	2	5

Z	5G9/2	6F5/2	7D3/2	6F7/2	7D5/2	8P3/2	9S1/2	9P1/2	6G7/2
154	10	6	2	6					
155	10	6	2	7					
156	10	6	2	8					
157	10	6	3	8					
158	10	6	4	8					
159	10	6	4	8	-	-	1		
160	10	6	4	8	1	-	1		
161	10	6	4	8	2	-	1		
162	10	6	4	8	4	-	-		
163	10	6	4	8	5	-	-		
164	10	6	4	8	6	-	-		
165	10	6	4	8	6	-	1		
166	10	6	4	8	6	-	2		
167	10	6	4	8	6	-	2	1	
168	10	6	4	8	6	-	2	2	
169	10	6	4	8	6	1	2	2	
170	10	6	4	8	6	2	2	2	
171	10	6	4	8	6	3	2	2	
172	10	6	4	8	6	4	2	2	
173	10	6	4	8	6	4	2	2	1

See page 89 for Explanation of Tables

TABLE II. Energy Eigenvalues and Total Energies, $Z = 100$ to $Z = 173$ (in eV)

	Z=100	Z=101	Z=102	Z=103	Z=104
	C=7.000 T=2.2	C=7.252 T=2.2	C=7.399 T=2.2	C=7.427 T=2.2	C=7.455 T=2.2
1S1/2	142049.7	145656.9	149346.1	153129.4	156995.1
2S1/2	27409.6	28220.2	29052.9	29915.6	30802.8
2P1/2	26555.4	27355.9	28177.9	29029.1	29905.2
2P3/2	20715.1	21204.2	21699.3	22206.7	22721.8
3S1/2	7095.7	7325.6	7561.8	7811.3	8068.9
3P1/2	6694.6	6918.1	7147.5	7389.9	7640.7
3P3/2	5320.0	5466.6	5615.2	5772.6	5933.9
3D3/2	4685.2	4821.6	4959.9	5106.9	5257.7
3D5/2	4420.9	4544.7	4670.0	4803.5	4940.3
4S1/2	1889.3	1959.8	2032.2	2113.3	2198.2
4P1/2	1701.9	1768.5	1836.9	1914.0	1994.8
4P3/2	1328.5	1372.5	1417.0	1468.9	1523.1
4D3/2	1031.5	1069.6	1108.2	1154.1	1202.3
4D5/2	965.2	999.7	1034.6	1076.5	1120.7
4F5/2	573.4	600.1	627.2	661.3	697.6
4F7/2	555.0	580.6	606.4	639.3	674.4
5S1/2	433.2	451.0	469.1	494.5	522.0
5P1/2	355.5	371.0	387.0	410.1	435.3
5P3/2	258.1	266.9	275.7	291.1	308.1
5D3/2	144.1	149.7	155.4	167.5	181.2
5D5/2	129.8	134.4	139.1	150.1	162.7
5F5/2	5.9	6.4	7.0	13.1	20.7
5F7/2	3.9	4.3	4.6	10.4	17.7
6S1/2	59.5	61.4	63.4	70.4	78.6
6P1/2	36.4	37.6	38.8	44.6	51.6
6P3/2	21.8	22.0	22.3	26.2	31.1
6D3/2				2.5	4.3
7S1/2	4.9	5.0	5.1	5.9	7.1
7P1/2					3.5
ET	948461	973705	999468	1025766	1052586

	Z=105	Z=106	Z=107	Z=108	Z=109
	C=7.483 T=2.2	C=7.511 T=2.2	C=7.538 T=2.2	C=7.566 T=2.2	C=7.594 T=2.2
1S1/2	160940.5	164974.2	169097.2	173312.1	177621.7
2S1/2	31709.8	32643.6	33503.7	34590.4	35604.9
2P1/2	30801.8	31726.3	32678.1	33658.0	34667.1
2P3/2	23239.2	23765.0	24297.8	24837.0	25382.6
3S1/2	8329.7	8597.8	8877.9	9163.9	9458.0
3P1/2	7894.7	8158.2	8429.9	8709.7	8997.9
3P3/2	6093.7	6258.1	6425.4	6595.4	6767.9
3D3/2	5406.9	5560.6	5717.3	5876.3	6037.9
3D5/2	5075.1	5213.9	5355.1	5498.2	5643.3
4S1/2	2281.6	2368.5	2460.6	2554.5	2651.2
4P1/2	2074.1	2157.9	2244.0	2334.9	2427.5
4P3/2	1574.4	1628.6	1684.5	1741.3	1799.2
4D3/2	1247.4	1295.6	1345.3	1396.0	1447.6
4D5/2	1161.6	1205.4	1250.5	1296.4	1343.2
4F5/2	730.6	766.5	803.7	841.7	880.5
4F7/2	706.1	740.6	776.4	812.9	850.1
5S1/2	546.5	573.9	602.8	632.6	663.4
5P1/2	457.4	482.5	509.0	536.5	564.9
5P3/2	321.5	337.3	354.0	371.0	388.4
5D3/2	191.2	203.6	216.8	230.4	244.2
5D5/2	171.4	182.5	194.4	206.5	218.9
5F5/2	24.4	30.5	37.3	44.4	51.7
5F7/2	21.1	26.8	33.3	39.9	46.8
6S1/2	82.9	89.3	96.3	103.6	111.1
6P1/2	54.6	59.7	65.4	71.3	77.3
6P3/2	31.9	34.6	37.7	40.8	43.8
6D3/2	3.8	4.5	5.5	6.5	7.4
7S1/2	6.8	7.2	4.0	4.6	5.3
6D5/2			7.6	8.1	8.5
ET	1079942	1107844	1136306	1165342	1194968

	Z=110	Z=111	Z=112	Z=113	Z=114
	C=7.621 T=2.2	C=7.649 T=2.2	C=7.676 T=2.2	C=7.704 T=2.2	C=7.731 T=2.2
1S1/2	182029.4	186538.3	191151.8	195276.6	200713.8
2S1/2	36648.2	37721.4	38825.9	39965.7	41139.6
2P1/2	35706.9	36778.9	37884.6	39028.6	40210.3
2P3/2	25934.7	26493.2	27058.2	27632.5	28213.5
3S1/2	9760.4	10071.6	10391.7	10724.1	11066.4
3P1/2	9294.9	9600.9	9916.6	10245.1	10584.3
3P3/2	6943.0	7120.7	7301.0	7486.8	7675.4
3D3/2	6202.1	6368.6	6537.9	6712.3	6889.6
3D5/2	5790.4	5939.3	6090.3	6245.9	6403.9
4S1/2	2750.7	2853.3	2959.0	3070.8	3186.2
4P1/2	2523.2	2622.0	2724.0	2832.3	2944.3
4P3/2	1858.2	1918.2	1979.3	2044.3	2110.6
4D3/2	1500.4	1554.0	1608.7	1667.3	1727.2
4D5/2	1390.8	1439.1	1488.4	1541.3	1595.3
4F5/2	920.1	960.4	1001.6	1046.4	1092.3
4F7/2	888.1	926.7	966.2	1009.2	1053.3
5S1/2	695.4	728.3	762.4	800.6	840.9
5P1/2	594.5	625.1	656.8	692.7	730.0
5P3/2	406.2	424.4	442.9	464.7	487.2
5D3/2	258.5	273.0	287.9	306.1	324.9
5D5/2	231.6	244.5	257.7	274.0	291.0
5F5/2	59.3	67.1	75.3	86.6	98.4
5F7/2	54.0	61.4	69.0	79.8	91.1
6S1/2	118.7	126.7	134.9	146.4	158.3
6P1/2	83.6	90.1	96.9	106.9	117.4
6P3/2	46.8	49.8	52.8	58.6	64.6
6D3/2	8.4	9.4	10.4	13.8	17.3
6D5/2	5.9	6.6	7.3	10.1	13.0
7S1/2	8.9	9.4	9.8	11.6	13.5
7P1/2				4.9	5.7
ET	1225199	1256051	1287542	1319687	1352505

	Z=115	Z=116	Z=117	Z=118	Z=119
	C=7.758 T=2.2	C=7.786 T=2.2	C=7.813 T=2.2	C=7.840 T=2.2	C=7.867 T=2.2
1S1/2	205669.4	210745.9	215947.7	221279.4	226748.8
2S1/2	42350.7	43598.9	44885.5	46212.4	47583.6
2P1/2	41433.2	42697.9	44006.6	45362.0	46769.2
2P3/2	28803.0	29399.2	30002.0	30611.4	31229.9
3S1/2	11420.8	11786.0	12162.1	12549.6	12951.5
3P1/2	10936.4	11300.2	11676.2	12065.1	12470.0
3P3/2	7868.7	8064.8	8263.7	8465.3	8672.2
3D3/2	7071.5	7256.1	7443.4	7633.4	7828.5
3D5/2	6565.8	6729.8	6895.8	7063.8	7236.4
4S1/2	3307.1	3431.7	3560.2	3692.7	3831.8
4P1/2	3062.0	3183.8	3309.7	3439.9	3577.2
4P3/2	2180.0	2250.7	2322.5	2395.6	2472.3
4D3/2	1790.1	1854.2	1919.5	1985.9	2056.0
4D5/2	1652.0	1709.9	1768.6	1828.3	1891.3
4F5/2	1141.0	1190.7	1241.3	1292.8	1347.6
4F7/2	1100.0	1147.7	1196.2	1245.5	1298.2
5S1/2	883.1	927.5	973.3	1020.5	1072.0
5P1/2	770.6	812.7	856.4	901.7	951.2
5P3/2	511.9	537.3	563.2	589.5	618.9
5D3/2	345.9	367.6	389.6	412.2	437.7
5D5/2	310.0	329.6	349.6	369.9	393.1
5F5/2	112.4	126.9	141.7	157.0	175.1
5F7/2	104.5	118.4	132.7	147.2	164.6
6S1/2	172.6	187.4	202.6	218.3	237.1
6P1/2	130.1	143.4	157.1	171.4	188.7
6P3/2	72.4	80.5	88.6	96.8	107.5
6D3/2	22.7	28.2	33.7	39.4	47.6
6D5/2	17.7	22.6	27.5	32.4	39.9
7S1/2	16.9	20.3	23.7	27.2	33.1
7P1/2	7.8	10.1	12.4	14.9	19.7
7P3/2	3.8	4.4	5.2	6.0	8.4
8S1/2					3.6
ET	1386015	1420239	1455201	1490925	1527433

See page 89 for Explanation of Tables

TABLE II. Energy Eigenvalues and Total Energies, $Z = 100$ to $Z = 173$ (in eV)

	Z=120	Z=121	Z=122	Z=123	Z=124
	C=7.894	C=7.921	C=7.948	C=7.975	C=8.002
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	232359.0	238116.4	244024.3	250086.7	256309.9
2S1/2	48999.4	50462.0	51971.2	53526.8	55130.9
2P1/2	48229.4	49746.5	51321.9	52957.0	54656.2
2P3/2	31855.6	32488.9	33127.6	33770.0	34413.2
3S1/2	13366.4	13795.2	14236.2	14687.1	15148.6
3P1/2	12889.7	13325.5	13775.9	14239.2	14716.4
3P3/2	8882.5	9096.6	9312.2	9526.7	9739.9
3D3/2	8027.0	8229.2	8432.8	8635.2	8836.3
3D5/2	7411.6	7589.7	7766.7	7945.6	8120.5
4S1/2	3975.8	4125.2	4278.0	4431.6	4586.1
4P1/2	3719.9	3868.6	4021.3	4175.7	4331.9
4P3/2	2550.9	2631.7	2712.4	2790.5	2865.7
4D3/2	2127.9	2201.9	2275.9	2347.1	2415.4
4D5/2	1955.9	2022.5	2088.7	2151.9	2212.0
4F5/2	1404.0	1462.4	1520.3	1575.2	1626.9
4F7/2	1352.3	1408.2	1463.7	1516.1	1565.2
5S1/2	1125.6	1181.9	1238.7	1293.4	1346.1
5P1/2	1003.0	1057.7	1113.0	1166.5	1218.2
5P3/2	649.3	681.2	712.4	740.2	764.6
5D3/2	464.2	492.3	519.6	543.5	563.9
5D5/2	417.3	442.9	467.6	488.7	506.4
5F5/2	194.1	214.5	234.1	250.1	262.6
5F7/2	183.0	202.7	221.5	236.7	248.4
6S1/2	257.0	278.4	299.2	316.9	331.3
6P1/2	207.1	227.2	246.7	263.0	276.2
6P3/2	119.0	131.5	142.9	150.7	154.9
6D3/2	56.5	66.5	75.3	80.6	82.5
6D5/2	47.9	57.0	64.9	69.4	70.5
7S1/2	39.6	47.1	53.4	56.9	57.6
7P1/2	25.1	31.4	36.7	39.4	39.7
7P3/2	11.3	15.1	17.7	18.4	17.4
8S1/2	4.2	5.4	6.2	6.4	6.1
8P1/2		3.0	3.3	3.4	3.3
7D3/2			3.3	3.4	
6F5/2				4.7	3.4
ET	1564753	1602913	1642191	1681888	1722777

	Z=125	Z=126	Z=127	Z=128	Z=129
	C=8.029	C=8.056	C=8.082	C=8.109	C=8.136
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	262678.4	269270.9	276024.4	282971.4	290120.5
2S1/2	56777.2	58499.0	60268.7	62100.6	63997.7
2P1/2	56413.2	58271.0	60198.3	62215.4	64329.5
2P3/2	35053.6	35714.0	36371.2	37034.5	37703.7
3S1/2	15618.1	16108.6	16609.8	17127.5	17662.5
3P1/2	15205.1	15720.4	16250.7	16803.3	17379.7
3P3/2	9950.0	10165.2	10378.9	10594.9	10813.1
3D3/2	9033.9	9237.7	9439.3	9643.1	9849.1
3D5/2	8291.4	8467.0	8639.9	8814.3	8989.9
4S1/2	4741.2	4898.6	5059.8	5226.2	5398.0
4P1/2	4489.6	4651.3	4818.0	4991.5	5172.2
4P3/2	2938.1	3006.7	3075.9	3145.6	3216.0
4D3/2	2480.9	2542.8	2605.0	2667.8	2731.2
4D5/2	2269.1	2321.9	2374.9	2428.3	2481.9
4F5/2	1675.6	1720.4	1765.3	1810.4	1855.8
4F7/2	1611.3	1653.2	1695.1	1737.2	1779.5
5S1/2	1398.1	1444.3	1493.4	1544.1	1596.5
5P1/2	1269.6	1315.6	1364.9	1416.2	1469.8
5P3/2	788.3	803.9	821.4	838.9	856.4
5D3/2	583.8	595.6	609.2	622.9	636.6
5D5/2	523.8	532.8	543.7	554.5	565.2
5F5/2	275.4	279.7	285.8	291.9	297.8
5F7/2	260.5	264.0	269.4	274.7	279.9
5G7/2	8.6	6.1	5.6	5.0	4.3
6S1/2	348.6	357.6	369.0	380.9	393.1
6P1/2	292.6	300.9	311.6	322.9	334.7
6P3/2	163.9	164.3	166.7	169.1	171.5
6D3/2	90.1	89.1	90.1	91.1	92.1
6D5/2	77.5	76.1	76.6	77.2	77.6
6F5/2	8.9	5.9	5.4	4.9	4.4
7S1/2	65.4	64.8	66.5	68.4	70.2
7P1/2	47.0	45.9	47.3	48.8	50.3
7P3/2	23.1	20.2	20.2	20.2	20.2
8S1/2	10.6	7.4	7.5	7.6	7.7
8P1/2	6.8	3.9	3.9	4.0	4.0
7D3/2		3.6			
ET	1764622	1807556	1851536	1896636	1942905

	Z=130	Z=131	Z=132	Z=133	Z=134
	C=8.162	C=8.189	C=8.215	C=8.242	C=8.268
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	297480.6	305061.0	312871.4	320928.7	329237.0
2S1/2	65962.9	67999.3	70110.1	72305.8	74583.0
2P1/2	66548.2	68880.4	71335.6	73931.2	76672.4
2P3/2	38379.1	39060.5	39748.0	40448.8	41156.1
3S1/2	18215.4	18787.1	19378.3	19997.6	20638.3
3P1/2	17981.5	18610.6	19268.6	19965.5	20695.9
3P3/2	11033.6	11256.5	11481.7	11717.5	11956.2
3D3/2	10057.4	10267.9	10480.6	10703.7	10929.5
3D5/2	9167.0	9345.5	9525.4	9714.7	9906.0
4S1/2	5575.5	5758.9	5948.6	6153.7	6366.2
4P1/2	5360.7	5557.5	5763.1	5987.2	6221.8
4P3/2	3287.1	3359.0	3431.6	3514.5	3598.8
4D3/2	2795.2	2860.0	2925.5	3001.1	3078.1
4D5/2	2536.0	2590.4	2645.2	2710.0	2775.8
4F5/2	1901.5	1947.6	1994.1	2050.4	2107.6
4F7/2	1822.0	1864.8	1908.0	1960.7	2014.5
5S1/2	1650.7	1706.9	1765.1	1835.0	1907.8
5P1/2	1525.9	1584.6	1646.3	1720.4	1798.6
5P3/2	874.2	892.0	910.1	937.3	965.1
5D3/2	650.4	664.3	678.5	701.4	725.2
5D5/2	576.0	586.9	597.8	617.2	637.3
5F5/2	303.8	309.8	315.9	330.2	345.1
5F7/2	285.1	290.3	295.5	308.8	322.6
5G7/2	3.6	2.8	2.0	8.0	14.5
6S1/2	405.9	419.1	433.0	454.3	476.6
6P1/2	347.2	360.3	374.3	395.9	418.8
6P3/2	173.9	176.3	178.8	185.6	192.7
6D3/2	93.1	94.1	95.2	99.7	104.4
6D5/2	78.1	78.4	79.1	82.7	86.3
6F5/2	3.9	3.5	3.0	3.6	4.1
7S1/2	72.2	74.3	76.5	80.7	85.1
7P1/2	52.0	53.8	55.8	59.5	63.5
7P3/2	20.2	20.2	20.2	20.6	21.1
8S1/2	7.9	8.0	8.2	8.4	8.6
8P1/2	4.1	4.1	4.3	4.3	4.4
ET	1990396	2039193	2089267	2140769	2193732

	Z=135	Z=136	Z=137	Z=138	Z=139
	C=8.295	C=8.321	C=8.347	C=8.374	C=8.400
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	337800.4	346637.3	355762.4	365183.9	374916.4
2S1/2	76937.4	79379.8	81917.7	84546.2	87274.1
2P1/2	79564.3	82628.4	85883.6	89339.3	93019.0
2P3/2	41862.0	42574.1	43296.1	44019.8	44750.4
3S1/2	21292.7	21969.9	22674.4	23398.7	24148.5
3P1/2	21453.7	22249.5	23089.4	23967.5	24891.8
3P3/2	12188.7	12423.7	12665.0	12904.3	13146.7
3D3/2	11149.2	11371.4	11599.9	11826.2	12055.4
3D5/2	10090.1	10275.7	10466.6	10654.4	10844.2
4S1/2	6575.8	6792.6	7020.7	7252.1	7491.8
4P1/2	6457.5	6704.6	6967.5	7238.7	7523.8
4P3/2	3673.7	3749.5	3829.8	3906.7	3984.9
4D3/2	3145.7	3214.2	3287.2	3356.6	3427.4
4D5/2	2831.8	2888.3	2948.9	3005.8	3063.5
4F5/2	2155.2	2203.3	2255.5	2303.9	2353.1
4F7/2	2058.4	2102.6	2151.0	2195.4	2240.5
5S1/2	1972.5	2039.7	2113.1	2184.8	2259.6
5P1/2	1869.8	1944.8	2027.4	2110.0	2197.4
5P3/2	983.6	1002.3	1024.9	1043.6	1062.8
5D3/2	739.6	754.2	772.6	787.1	802.2
5D5/2	648.2	659.2	673.9	684.6	695.7
5F5/2	351.1	357.1	366.9	372.6	378.7
5F7/2	327.7	332.8	341.6	346.3	351.4
5G7/2	13.5	12.5	15.1	13.7	12.5
5G9/2	9.4	8.2	10.6	9.0	7.6
6S1/2	492.3	508.7	529.4	546.8	565.3
6P1/2	435.4	453.1	475.5	495.1	516.2
6P3/2	195.1	197.7	203.9	206.2	208.7
6D3/2	105.4	106.5	111.1	111.9	113.0
6D5/2	86.8	87.2	91.1	91.3	91.7
6F5/2	3.6	3.0	4.9	4.2	3.6
7S1/2	87.8	90.5	96.6	99.5	102.6
7P1/2	66.0	68.8	74.8	77.7	81.1
7P3/2	21.1	21.1	22.9	22.8	22.8
7D3/2			3.3	3.1	3.0
8S1/2	8.8	9.0	10.1	10.3	10.5
8P1/2	4.6	4.7	5.3	5.4	5.6
ET	2248236	2304354	2362114	2421754	2483211

See page 89 for Explanation of Tables

TABLE II. Energy Eigenvalues and Total Energies, $Z = 100$ to $Z = 173$ (in eV)

	Z=140	Z=141	Z=142	Z=143	Z=144
	C=8.426 T=2.2	C=8.452 T=2.2	C=8.478 T=2.2	C=8.504 T=2.2	C=8.530 T=2.2
1S1/2	386752.9	397219.3	408040.0	419234.0	430821.0
2S1/2	90713.3	93673.4	96739.7	99919.4	103219.4
2P1/2	97819.9	102063.1	106597.1	111451.9	116659.4
2P3/2	45768.9	46518.1	47269.8	48028.1	48796.8
3S1/2	25147.5	25959.4	26794.9	27658.5	28555.1
3P1/2	26142.7	27180.4	28268.0	29412.1	30619.0
3P3/2	13515.2	13767.4	14018.1	14271.5	14531.7
3D3/2	12416.8	12655.8	12893.2	13133.3	13379.9
3D5/2	11150.1	11347.1	11541.5	11737.4	11938.8
4S1/2	7833.0	8095.0	8361.6	8637.1	8925.6
4P1/2	7932.1	8253.1	8585.6	8934.3	9303.6
4P3/2	4118.0	4201.9	4282.7	4364.5	4451.2
4D3/2	3553.7	3630.1	3703.3	3777.4	3856.4
4D5/2	3170.4	3232.8	3291.7	3351.1	3415.0
4F5/2	2451.4	2505.3	2555.7	2606.5	2661.7
4F7/2	2332.2	2381.7	2427.6	2473.8	2524.3
5S1/2	2374.8	2459.6	2543.3	2630.1	2723.9
5P1/2	2331.8	2433.6	2536.4	2644.6	2762.3
5P3/2	1106.4	1129.9	1149.7	1169.7	1193.9
5D3/2	840.3	859.6	875.0	890.7	910.6
5D5/2	727.9	743.0	754.1	765.3	780.6
5F5/2	403.2	413.2	419.2	425.3	435.4
5F7/2	374.1	383.0	387.9	392.8	401.7
5G7/2	23.6	26.2	24.7	23.2	25.7
5G9/2	18.1	20.5	18.8	17.0	19.3
6S1/2	601.7	625.9	646.9	668.8	695.7
6P1/2	557.0	585.1	610.7	637.8	670.6
6P3/2	221.1	227.6	230.1	232.6	239.3
6D3/2	122.4	127.2	128.2	129.2	134.1
6D5/2	99.7	103.7	103.9	104.2	108.2
6F5/2	7.3	9.2	8.5	7.8	9.7
7S1/2	112.8	119.8	123.4	127.3	134.9
7P1/2	91.5	98.8	103.1	107.6	116.0
7P3/2	26.0	27.7	27.7	27.6	29.4
7D3/2	4.6	5.3	5.1	4.9	5.5
8S1/2	13.0	14.2	14.6	15.0	16.4
8P1/2	7.6	8.5	8.9	9.2	10.4
ET	2546574	2612051	2679692	2749602	2821893

	Z=145	Z=146	Z=147	Z=148	Z=149
	C=8.556 T=2.2	C=8.582 T=2.2	C=8.608 T=2.2	C=8.634 T=2.2	C=8.660 T=2.2
1S1/2	440669.5	453003.5	465773.5	478997.2	492696.0
2S1/2	105918.2	109438.7	113083.8	116855.5	120759.7
2P1/2	121067.2	126990.7	133351.6	140183.9	147526.4
2P3/2	49278.6	50062.3	50853.3	51651.8	52461.6
3S1/2	29225.7	30178.8	31162.6	32177.6	33228.1
3P1/2	31548.7	32869.6	34254.7	35705.1	37225.3
3P3/2	14666.7	14936.0	15208.5	15484.3	15767.4
3D3/2	13494.5	13749.7	14007.9	14269.3	14537.8
3D5/2	12023.9	12232.1	12442.1	12654.0	12871.8
4S1/2	9120.6	9430.7	9750.7	10080.7	10424.6
4P1/2	9563.2	9967.9	10390.6	10831.3	11294.1
4P3/2	4485.5	4579.9	4675.8	4773.1	4875.7
4D3/2	3881.9	3968.3	4056.1	4145.2	4239.6
4D5/2	3431.9	3502.7	3574.4	3647.0	3724.4
4F5/2	2669.8	2731.6	2794.4	2858.0	2926.4
4F7/2	2530.3	2587.3	2645.1	2703.6	2766.7
5S1/2	2781.9	2887.5	2996.9	3109.9	3230.6
5P1/2	2838.8	2972.6	3112.7	3259.0	3415.5
5P3/2	1195.5	1225.8	1256.8	1288.5	1324.6
5D3/2	908.7	934.6	960.9	987.9	1019.3
5D5/2	776.0	796.7	817.9	839.4	865.3
5F5/2	427.9	443.1	458.7	474.7	495.0
5F7/2	393.6	407.5	421.7	436.2	454.9
5G7/2	15.7	22.1	28.9	35.9	47.1
5G9/2	9.2	15.1	21.4	28.0	38.7
6S1/2	704.7	737.4	771.5	806.9	847.5
6P1/2	684.2	724.4	766.9	811.5	862.3
6P3/2	232.8	240.4	248.1	255.9	267.6
6D3/2	126.7	131.8	136.9	142.1	151.2
6D5/2	100.6	104.2	107.9	111.6	118.9
6F5/2	3.5	4.1	4.6	5.2	8.3
7S1/2	130.9	138.1	145.6	153.4	165.1
7P1/2	112.8	121.2	130.0	139.5	153.1
7P3/2	25.0	25.5	26.0	26.4	28.6
7D3/2	3.0	2.9	2.9	2.8	3.3
8S1/2	13.7	14.3	14.9	15.5	17.2
8P1/2	8.1	8.7	9.3	9.9	11.5
ET	2896743	2974135	3054251	3137210	3223127

	Z=150	Z=151	Z=152	Z=153	Z=154
	C=8.686 T=2.2	C=8.711 T=2.2	C=8.737 T=2.2	C=8.763 T=2.2	C=8.788 T=2.2
1S1/2	506885.0	521579.0	536796.7	552562.7	568823.9
2S1/2	124794.6	128958.2	133251.6	137682.0	142223.2
2P1/2	155411.6	163872.1	172943.9	182669.0	193032.9
2P3/2	53279.6	54102.1	54929.4	55768.4	56606.4
3S1/2	34311.1	35422.8	36563.7	37741.0	38941.6
3P1/2	38812.3	40462.3	42174.8	43956.0	45789.1
3P3/2	16054.1	16340.8	16627.2	16920.9	17212.2
3D3/2	14809.8	15081.6	15353.0	15631.5	15907.2
3D5/2	13091.9	13310.3	13527.0	13749.4	13967.9
4S1/2	10779.1	11140.2	11507.9	11889.8	12276.2
4P1/2	11775.3	12270.8	12780.3	13310.8	13851.7
4P3/2	4980.1	5082.4	5182.5	5287.7	5390.1
4D3/2	4335.7	4429.7	4521.3	4618.1	4711.7
4D5/2	3803.0	3879.0	3952.2	4030.0	4104.3
4F5/2	2995.9	3062.8	3126.7	3195.2	3260.2
4F7/2	2831.0	2892.4	2950.7	3013.5	3072.6
5S1/2	3355.4	3480.5	3605.6	3738.3	3870.5
5P1/2	3578.6	3744.3	3912.4	4090.2	4269.3
5P3/2	1361.6	1395.7	1426.7	1461.9	1493.9
5D3/2	1051.6	1080.9	1107.0	1137.3	1164.4
5D5/2	891.8	915.1	935.1	959.1	979.6
5F5/2	515.9	533.5	547.8	566.0	580.8
5F7/2	474.2	490.2	502.7	519.2	532.2
5G7/2	58.9	67.5	72.6	81.6	87.2
5G9/2	50.0	58.0	62.5	70.9	75.9
6S1/2	889.9	930.1	968.0	1010.9	1051.5
6P1/2	915.6	967.7	1018.3	1074.8	1129.6
6P3/2	279.8	288.5	293.6	302.4	307.6
6D3/2	160.5	166.5	168.9	175.0	177.4
6D5/2	126.4	130.6	131.4	135.6	136.1
6F5/2	11.7	12.6	10.9	11.8	9.8
6F7/2		8.0	6.2	6.7	4.6
7S1/2	177.4	186.7	193.1	203.1	209.9
7P1/2	167.6	179.4	188.4	201.6	211.6
7P3/2	30.7	31.2	30.2	30.7	29.7
7D3/2	3.7	3.6	3.1	3.0	2.8
8S1/2	18.9	19.8	19.8	20.8	20.9
8P1/2	13.1	14.1	14.3	15.5	15.9
ET	3312120	3404311	3499814	3598731	3701115

	Z=155	Z=156	Z=157	Z=158	Z=159
	C=8.814 T=2.2	C=8.839 T=2.2	C=8.865 T=2.2	C=8.890 T=2.2	C=8.916 T=2.2
1S1/2	585797.1	603310.9	621441.6	640205.8	659621.6
2S1/2	146938.4	151773.6	156741.7	161841.7	167078.2
2P1/2	204200.2	216080.9	228740.9	242207.2	256513.7
2P3/2	57465.3	58333.8	59211.6	60098.8	61003.2
3S1/2	40188.0	41468.5	42782.6	44130.3	45519.4
3P1/2	47703.0	49676.4	51710.1	53802.7	55960.5
3P3/2	17512.2	17820.6	18133.3	18450.1	18778.6
3D3/2	16191.8	16484.5	16781.2	17081.9	17394.2
3D5/2	14193.1	14425.2	14659.7	14896.7	15143.6
4S1/2	12677.5	13094.3	13521.9	13960.3	14416.6
4P1/2	14415.2	14999.1	15599.0	16214.5	16852.6
4P3/2	5495.6	5609.0	5724.3	5841.6	5967.2
4D3/2	4808.6	4913.2	5019.6	5127.9	5244.4
4D5/2	4180.9	4265.0	4350.2	4436.7	4530.8
4F5/2	3327.5	3402.1	3477.9	3554.9	3639.6
4F7/2	3133.8	3202.2	3271.7	3342.2	3420.1
5S1/2	4007.8	4155.6	4307.5	4463.7	4630.2
5P1/2	4456.0	4654.6	4859.0	5069.1	5291.0
5P3/2	1526.9	1567.4	1608.8	1651.1	1700.3
5D3/2	1192.3	1227.8	1264.1	1301.1	1345.1
5D5/2	1000.7	1029.2	1058.3	1087.9	1124.2
5F5/2	596.0	618.7	641.9	665.6	695.8
5F7/2	545.5	566.3	587.5	609.1	637.3
5G7/2	93.0	106.2	119.9	134.1	154.6
5G9/2	81.1	93.8	106.8	120.3	140.1
6S1/2	1093.8	1144.6	1197.1	1251.2	1313.1
6P1/2	1187.0	1253.5	1322.3	1393.4	1472.8
6P3/2	313.2	325.9	338.9	352.2	371.6
6D3/2	180.3	190.1	200.1	210.4	226.6
6D5/2	137.0	144.6	152.3	160.2	173.9
6F5/2	7.9	11.5	15.2	19.1	28.5
6F7/2	2.5	5.6	8.6	11.9	20.5
7S1/2	217.5	232.2	247.5	263.4	285.6
7P1/2	222.7	241.3	260.7	281.1	308.0
7P3/2	28.1	30.5	32.8	35.0	42.3
7D3/2	2.0	2.4	2.9	3.3	7.9
8S1/2	20.2	22.8	25.1	27.5	34.9
8P1/2	15.4	18.1	20.8	23.7	31.7
9S1/2					4.0
ET	3807237	3917011	4030583	4148031	4269367

See page 89 for Explanation of Tables

TABLE II. Energy Eigenvalues and Total Energies, $Z = 100$ to $Z = 173$ (in eV)

	Z=160	Z=161	Z=162	Z=163	Z=164
	C=8.941	C=8.966	C=8.992	C=9.017	C=9.042
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	679704.4	700462.9	721909.6	744064.2	766933.7
2S1/2	172439.7	177927.3	183529.8	189261.7	195112.3
2P1/2	271668.2	287696.7	304608.6	322430.9	341169.2
2P3/2	61912.4	62830.2	63750.0	64687.6	65635.4
3S1/2	46936.8	48386.5	49862.2	51378.6	52928.2
3P1/2	58169.4	60431.9	62740.3	65110.3	67533.5
3P3/2	19105.9	19437.1	19766.2	20106.2	20450.9
3D3/2	17705.1	18019.4	18331.3	18654.2	18981.4
3D5/2	15387.2	15632.7	15874.2	16124.6	16377.5
4S1/2	14878.4	15350.4	15827.0	16320.4	16824.6
4P1/2	17500.1	18161.7	18831.1	19521.1	20225.2
4P3/2	6090.0	6214.1	6334.7	6462.8	6592.9
4D3/2	5358.0	5472.9	5584.1	5702.6	5823.1
4D5/2	4621.4	4712.6	4799.5	4893.1	4987.9
4F5/2	3720.4	3802.0	3879.1	3962.9	4047.8
4F7/2	3494.1	3568.7	3638.7	3715.2	3792.6
5S1/2	4796.3	4966.1	5134.7	5312.6	5494.8
5P1/2	5513.7	5741.1	5968.2	6205.9	6448.8
5P3/2	1745.9	1791.9	1834.1	1881.9	1930.5
5D3/2	1385.4	1426.1	1462.9	1505.2	1548.3
5D5/2	1156.5	1189.1	1217.4	1251.1	1285.2
5F5/2	722.2	748.6	771.0	798.5	826.5
5F7/2	661.4	685.6	705.7	730.8	756.4
5G7/2	171.3	188.0	200.6	218.1	236.1
5G9/2	156.0	171.9	183.8	200.5	217.7
6S1/2	1372.3	1432.8	1490.4	1554.4	1620.0
6P1/2	1550.1	1629.1	1705.6	1788.9	1874.4
6P3/2	387.0	402.5	414.1	430.2	446.7
6D3/2	239.0	251.3	259.8	272.7	285.9
6D5/2	183.6	193.2	198.9	208.9	219.0
6F5/2	34.0	39.5	41.1	46.9	52.8
6F7/2	25.4	30.1	31.1	36.1	41.2
7S1/2	304.3	323.4	338.9	359.3	380.3
7P1/2	331.6	355.8	376.7	402.7	429.6
7P3/2	45.7	49.0	48.5	51.7	54.9
7D3/2	9.3	10.6	8.6	9.8	11.1
7D5/2	5.0	5.6	3.5	3.9	4.4
8S1/2	38.6	42.3	42.4	46.3	50.3
8P1/2	36.0	40.5	41.5	46.3	51.4
9S1/2	4.1	4.3			
ET	4394763	4524233	4657879	4795618	4937547

	Z=165	Z=166	Z=167	Z=168	Z=169
	C=9.068	C=9.093	C=9.118	C=9.143	C=9.168
	T=2.2	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	790530.3	814861.0	839932.1	865749.2	892316.7
2S1/2	201081.6	207165.0	213359.4	219661.4	226068.5
2P1/2	360834.6	381431.9	402964.8	425434.8	448842.2
2P3/2	66596.1	67568.2	68551.3	69545.0	70549.7
3S1/2	54513.6	56132.9	57785.9	59471.6	61190.7
3P1/2	70012.3	72545.2	75132.2	77773.5	80470.1
3P3/2	20802.7	21160.2	21522.9	21890.4	22262.9
3D3/2	19315.5	19655.1	19999.8	20348.9	20702.8
3D5/2	16635.4	16896.8	17161.2	17428.0	17697.6
4S1/2	17342.1	17871.3	18411.7	18962.9	19525.0
4P1/2	20945.9	21681.5	22431.8	23196.2	23975.2
4P3/2	6727.5	6865.2	7005.4	7147.6	7292.2
4D3/2	5948.0	6075.8	6206.1	6338.2	6472.6
4D5/2	5086.3	5187.0	5289.4	5392.8	5497.7
4F5/2	4136.3	4227.0	4319.3	4412.7	4507.4
4F7/2	3873.4	3956.2	4040.5	4125.6	4211.9
5S1/2	5683.6	5877.5	6076.1	6278.7	6485.7
5P1/2	6699.3	6955.9	7218.1	7485.4	7758.1
5P3/2	1982.6	2036.5	2091.8	2148.0	2205.3
5D3/2	1594.8	1643.1	1692.7	1743.0	1794.5
5D5/2	1322.4	1361.2	1400.9	1441.1	1482.1
5F5/2	857.5	890.0	923.5	957.4	992.0
5F7/2	784.9	814.8	845.6	876.8	908.6
5G7/2	257.0	279.3	302.5	326.0	350.2
5G9/2	237.7	259.1	281.5	304.0	327.2
6S1/2	1689.9	1762.5	1837.4	1913.8	1992.3
6P1/2	1964.6	2057.8	2153.8	2251.7	2352.1
6P3/2	466.0	486.6	507.9	529.6	551.7
6D3/2	301.9	319.1	337.1	355.3	374.1
6D5/2	231.8	245.8	260.4	275.0	290.0
6F5/2	61.4	71.1	81.4	91.8	102.5
6F7/2	49.0	57.8	67.3	76.7	86.5
7S1/2	404.6	430.5	457.6	485.2	513.8
7P1/2	459.8	492.0	525.5	559.8	595.2
7P3/2	60.6	67.3	74.4	81.4	88.6
7D3/2	14.6	19.0	23.8	28.4	33.2
7D5/2	6.8	10.0	13.5	16.8	20.2
8S1/2	56.9	64.6	72.8	81.1	89.8
8P1/2	59.3	68.4	78.2	88.1	98.6
9S1/2	4.5	5.2	6.1	7.0	8.0
9P1/2			4.5	5.4	6.5
8P3/2					5.6
ET	5083690	5234064	5388684	5547557	5710683

	Z=170	Z=171	Z=172	Z=173
	C=9.193	C=9.463	C=9.243	C=9.268
	T=2.2	T=2.2	T=2.2	T=2.2
1S1/2	919638.3	938807.3	967112.1	1006175.0
2S1/2	232578.3	237306.9	243942.1	252712.6
2P1/2	473186.8	490782.6	516427.1	551833.0
2P3/2	71566.0	72617.0	73655.4	74685.2
3S1/2	62943.6	64299.3	66100.2	68406.9
3P1/2	83223.8	85410.8	88252.7	91842.9
3P3/2	22641.4	23032.7	23420.9	23810.7
3D3/2	21062.4	21434.1	21802.9	22173.5
3D5/2	17970.5	18251.3	18528.9	18808.5
4S1/2	20098.8	20558.9	21149.0	21890.2
4P1/2	24769.6	25420.1	26237.5	27247.8
4P3/2	7439.9	7591.9	7743.5	7899.8
4D3/2	6609.9	6751.3	6892.3	7038.2
4D5/2	5604.7	5714.2	5823.2	5937.0
4F5/2	4604.2	4703.1	4801.8	4905.5
4F7/2	4300.1	4389.9	4479.5	4574.1
5S1/2	6697.9	6871.6	7090.0	7363.8
5P1/2	8037.0	8269.6	8556.7	8910.2
5P3/2	2264.4	2324.5	2385.0	2451.4

	Z=170	Z=171	Z=172	Z=173
	C=9.193	C=9.463	C=9.243	C=9.268
	T=2.2	T=2.2	T=2.2	T=2.2
5D3/2	1847.7	1901.7	1956.2	2016.5
5D5/2	1524.5	1567.1	1610.1	1658.9
5F5/2	1028.0	1064.0	1100.5	1143.0
5F7/2	941.7	974.6	1008.1	1047.5
5G7/2	375.6	400.7	426.5	458.4
5G9/2	351.7	375.7	400.5	431.3
6S1/2	2073.4	2140.9	2224.4	2331.4
6P1/2	2455.6	2543.0	2649.8	2783.6
6P3/2	575.2	598.0	621.6	651.4
6D3/2	394.0	413.2	433.2	459.4
6D5/2	306.1	321.3	337.2	359.2
6F5/2	114.3	125.1	136.6	154.4
6F7/2	97.3	107.0	117.5	134.2
7S1/2	544.0	569.1	600.0	642.8
7P1/2	632.5	664.2	702.5	753.9
7P3/2	96.7	103.5	111.1	124.9
7D3/2	38.9	43.3	48.5	60.0
7D5/2	24.5	27.4	31.1	41.1
8S1/2	99.5	106.9	116.4	133.7
8P1/2	110.2	119.5	131.2	151.0
8P3/2	6.6	6.9	7.6	13.9
9S1/2	9.4	10.0	11.2	18.4
9P1/2		8.7	10.1	17.7
6G7/2				0.5
ET	5878055	6006887	6180167	6405743

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TABLE III. Energy Eigenvalues (in eV) for $Z = 100$ from DF and DFS Calculations and Binding Energies from Experiment

	DF Result	Corrections					Sum	Experiment	DFS Result
1S1/2	143028	-715	+41	-457	+155	-99	141953	141963	142050
2S1/2	27803	-91	+8	-96	+26	-69	27581	27573	27410
2P1/2	26868	-153	+13	-9	+4	-77	26646	26664	26555
2P3/2	21017	-92	+11	+3	0	-70	20869	20868	20715
3S1/2	7292	-19	+1	-25	+6	-42	7213	7200	7096
3P1/2	6864	-33	+3	-3	+1	-49	6783	6779	6695
3P3/2	5474	-20	+2	+1	0	-46	5411	5408	5320
3D3/2	4814							4746	4685
3D5/2	4548							4484	4421
4S1/2	1993							1940	1889
4P1/2	1793							1743	1702
4P3/2	1411							1371	1328
4D3/2	1099							1059	1031
4D5/2	1031							989	965

TABLE IV. Energy Eigenvalues (in eV) for $Z = 139$ and $Z = 170$ in Various States of Ionization

	Z=139	C=8.4		T=2.2		Z=170	C=9.193		T=2.2	
	NEUTRAL	8+	17+	29+	35+	NEUTRAL	36+	70+	108+	148+
1S1/2	374916.4	375016.1	375254.5	375734.0	375974.5	919638.3	920676.6	923114.4	927970.4	940986.6
2S1/2	87274.2	87373.9	87614.7	88093.7	88335.3	232578.8	233594.2	235966.5	240711.2	253012.2
2P1/2	93019.1	93118.7	93350.6	93837.0	94078.4	473186.0	474222.2	476654.1	481500.8	494454.2
2P3/2	44750.4	44850.3	45092.3	45572.7	45813.8	71566.1	72568.5	74896.4	79535.7	91190.1
3S1/2	24148.5	24248.6	24494.1	24982.2	25219.1	62943.6	63943.1	66257.1	70846.5	82149.7
3P1/2	24891.8	24991.8	25236.2	25722.0	25960.1	83223.8	84229.3	86367.8	91232.4	103050.0
3P3/2	13146.7	13246.6	13494.9	13989.0	14223.3	22641.4	23630.1	25903.7	30311.4	40218.8
3D3/2	12055.4	12155.4	12402.2	12892.6	13128.6	21062.4	22053.8	24337.1	28806.0	39230.0
3D5/2	10844.2	10944.2	11191.7	11684.0	11919.2	17970.5	18959.3	21232.4	25650.7	
4S1/2	7491.8	7591.3	7844.1	8348.0	8578.5	20098.9	21084.2	23346.7	27683.7	
4P1/2	7523.8	7623.4	7875.4	8377.6	8608.8	24769.7	25759.8	28037.5	32466.9	
4P3/2	3984.9	4084.2	4339.3	4845.5	5072.6	7439.9	8412.2	10620.4	14632.8	
4D3/2	3427.4	3526.7	3781.3	4287.0	4514.9	6609.9	7583.9	9800.4	13863.5	
4D5/2	3063.5	3162.7	3417.7	3923.4	4150.3	5604.8	6576.1	8776.8	12761.5	
4F5/2	2353.1	2452.5	2706.9	3212.4	3440.4	4604.3	5578.4	7794.9	11877.6	
4F7/2	2240.5	2339.9	2594.5	3100.3	3327.9	4300.1	5272.9	7453.2	11531.5	
5S1/2	2259.6	2358.7	2613.1	3110.0	3331.9	6697.9	7667.4	9855.9	13770.0	
5P1/2	2197.4	2296.5	2551.1	3049.5	3272.0	8037.0	9010.5	11225.0		
5P3/2	1062.8	1161.9	1409.9	1882.3	2098.0	2264.4	3219.1	5245.6		
5D3/2	802.2	901.3	1148.4	1618.5	1833.9	1847.7	2802.3	4830.0		
5D5/2	695.7	794.9	1039.8	1503.1	1717.0	1524.5	2475.1	4458.3		
5F5/2	378.7	477.8	720.9	1180.6	1393.8	1028.0	1978.2	3967.2		
5F7/2	351.4	450.5	692.5	1148.9	1361.4	941.7	1889.9	3319.0		
5G7/2	12.5	111.3	317.0			375.6	1322.4			
5G9/2	7.6	106.4				351.7	1297.2			
6S1/2	565.3	664.5	898.4	1281.9	1535.5	2073.4	3024.5			
6P1/2	516.2	615.4	849.6	893.8	1488.7	2455.6	3411.7			
6P3/2	208.7	307.4	517.9	777.2	1084.2	575.2	1481.4			
6D3/2	113.0	211.0	414.0	739.9	963.8	394.0	1291.6			
6D5/2	91.7	189.1	387.0			306.1	1187.9			
6F5/2	3.6					114.3	972.9			
7S1/2	102.6	198.6	385.1			97.3				
7P1/2	81.1	176.5	361.1			544.0				
7P3/2	22.8	109.5				632.5				
7D3/2	3.0					96.7				
8S1/2	10.5					38.9				
8P1/2	5.6					24.5				
						99.5				
						110.2				
						6.6				
						9.4				

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