RELATIVISTIC DIRAC-FOCK ATOM PROPERTIES FOR $Z = 121$ TO $Z = 138$

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Abstract

We present relativistic Dirac-Fock calculations of atomic properties for atomic numbers $Z=121$ to 138, extending a previous tabulation of Desclaux. The calculations assume a single LS ground state configuration and include a correction for finite nuclear size, with an approximation for the mean nuclear mass $A(Z)$ based on the liquid-drop model.

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Contents

1. Introduction.....	2
1.1. Nuclear Model	3
1.2. Extension of Occupation and Angular Quantum Numbers	4
1.3. Dirac-Fock Expectation Values	6
Explanation of Tables	7
References	21
Tables	
1. Orbital Binding Energies from $Z = 121$ to $Z = 138$. See page 7 for Explanation of Tables	8
2. Dirac-Fock Radial Expectation Values from $Z = 121$ to $Z = 138$. See page 7 for Explanation of Tables.....	10

1. Introduction

Relativistic Dirac-Fock calculations of atomic properties are of considerable interest in many fields. For example, the multi-configuration Dirac-Fock atomic code of Desclaux has been used to calculate spinors, energy levels and various expectation values of atoms for $Z=1$ to $Z=120$ [1]. A semi-automated single-configuration extension based on LS-ground state electronic configurations [2] is now implemented as a starting point for self-consistent field calculations throughout the periodic table in the widely used real-space multiple-scattering code FEFF [3]. However, the mixing of g - f - d orbitals may be problematic for a single-configuration model, and the validity of Hund's rules for super-heavy atoms has been questioned [4]. Nevertheless, single-configuration calculations are of considerable value. For example, numerical Dirac-Fock spinors of the form calculated by FEFF have been used to derive relativistic effective core-potentials (RECPs) for the elements $Z=3$ -118; these spinors are then used in spin-orbit configuration interaction calculations of atomic and molecular spectra and other properties [5]. There has also been considerable interest in the physical properties and stability of super-heavy atoms [6]. For example, an island of stability is predicted for heavy isotopes of atomic mass $A = Z + N \approx 300$ with near magic numbers of protons Z and neutrons N [7]. Also an extension of the periodic table up to $Z = 172$ has recently been proposed [8]. Nevertheless, the experimental relevance of these predictions remains unclear at present.

In this work we extend the single-configuration code of Ref. [2] for high atomic numbers $Z=121$ to 138, corresponding to the $5g$ series of the transactinide row 8. Further extensions to higher Z or alternative electron-configurations are straightforward, but the results presented here are illustrative. Our calculations closely follow the formalism of Ref. [1, 2], and are only briefly summarized here. Specific quantities of interest include orbital binding energies and radial expectation values, which are tabulated in Tables 1 and 2. Other properties, such as the spinor-wave functions on an exponential radial grid are available as ASCII output files from the code. These quantities are calculated in terms of the occupied spinor states and energies obtained by solving the Dirac-Fock equations $H_0\Psi = E\Psi$ for the many-electron

ground state Ψ , where

$$H_0 = \sum_{i=1}^Z H_D(i) + \frac{1}{2} \sum_{i \neq j} \frac{1}{r_{ij}}, \quad (1)$$

H_D is the one-electron Dirac Hamiltonian

$$H_D = ic\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta c^2 + V_N(r), \quad (2)$$

$V_N(r)$ is the nuclear potential, and

$$\boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix}, \quad (3)$$

are the Dirac matrices in terms of the 2×2 Pauli matrices $\boldsymbol{\sigma}$ and the identity matrix $\mathbf{I}$. The Hamiltonian H_0 ignores the Breit interaction which is subsequently treated as a perturbation in the calculation of the total energy. Here and elsewhere we use atomic units with $e = \hbar = m = 1$ and $c=137.037$, except that energies are reported in $\text{Ry} = 13.605693$ eV. As the details for the self-consistent solution of the Dirac equation are well documented in Ref. [1], we only summarize the modifications to the code made for the calculations presented here.

1.1. Nuclear Model

For simplicity, the nuclear model used here assumes a uniform charge distribution with a Coulomb potential given by

$$V_N(r) = -\frac{Z}{2R} \left(3 - \frac{r^2}{R^2} \right), \quad (r < R), \quad (4)$$

$$= -\frac{Z}{R}, \quad (r > R). \quad (5)$$

This potential becomes significant only for atoms of high $Z > 100$ when the inner orbitals overlap significantly with the atomic nucleus. For the radial grid used in our work, only the first few points are affected. Here $R = 2.27 \times 10^{-5} A^{1/3}$ is the mean nuclear radius, and $A = Z + N$ is the nuclear mass number. Other nuclear models have also been considered, [9] but the numerical differences are essentially negligible. For large $Z > 121$, the nuclear masses A of the most stable nuclei are not yet available experimentally. However, approximate values can be obtained by maximizing the binding energy E_B with respect to Z for a given number A using a modern parameterization of the liquid-drop model [10]

$$E_B = a_V A - a_S A^{2/3} - \frac{a_C Z^2}{A^{1/3}} - a_A \frac{(A - 2Z)^2}{A} \pm \delta(A, Z), \quad (6)$$

where the parameters a_V, a_S, a_C , and a_A correspond to the volume term, surface term, coulomb term and asymmetry term, respectively. At the maximum E_B , one obtains a simple expression for the relation between Z and A ,

$$Z(A) = \frac{A}{2 + (a_C/2a_A)A^{2/3}}. \quad (7)$$

This expression only involves the Coulomb and asymmetry terms $a_C = 0.715$ and $a_A = 23.4$, which are obtained by linear regression from existing nuclear data from $Z = 1$ to $Z = 120$ [10]. The closest integer values of Z for a given A are given in Table A. We also checked that these isotopes (Z, A) are usually the most stable with respect to β -decay. However, slight changes in A only affect the nuclear radius by a factor of order $R/3A$, with generally negligible effects on the calculations.

1.2. Extension of Occupation and Angular Quantum Numbers

In order to extend the original code for atomic numbers Z beyond 120, an extension to the atomic configuration data and dimensions used in the code must be made. Although the ground states of the open g -subshell configurations are best defined in terms of multi-configuration representations, with J as the only good quantum number, the single-configuration results are of interest in themselves. For the $5g$ series $Z = 121$ to 138 of this work, the electron configurations used are chosen similar to those of Desclaux in Ref. [4], following Hund rules and the Madelung prescription, together with data in Ref. [6] and atomic masses $A = N + Z$ estimated from Eq. (7) for the predicted most stable nuclei. These configurations as listed in Table A represent our best estimates of the ground states of these elements based on the Pyykko predictions [8] and those based on the liquid drop model. They can also be regarded as anchors in that their average energy is useful for determining spinor wavefunctions. Alternative electron configurations, e.g. for deviations from Hund rules and configuration interaction calculations [12, 13, 14] are also possible. In any case, the wave functions for each of these elements are appropriate for the generation of relativistic effective core potentials (RECP) that can be used for the calculation of their electronic spectra using the parallel spin-orbit configuration-interaction (PSOCI) code. The process of generating RECPs for the purpose of doing calculations of their electronic states using spin-orbit configuration interaction is in progress, and a full discussion is reserved for future publication. This work is expected to reveal all of the states for a given total angular momentum J and will include intermediate angular momentum coupling of the electrons of each configuration, including comparisons with single configuration jj -coupled DFT ones [6, 12]. This has previously been done for Am, Eu, Ru and other elements,[13, 14] and we have found that the ground states are mixtures of determinantal wave functions that couple to a pure J state.

The relativistic total angular momentum quantum number κ is needed to define the eigenstates of a spherical Dirac equation. For various spin s with constant l , the values of κ are defined as[1]

$$\kappa = \begin{cases} l & \text{if } j = l - \frac{1}{2} \\ -(l+1) & \text{if } j = l + \frac{1}{2} \end{cases}, \quad (8)$$

and is positive if $j < l$ and negative if $j > l$. This gives the following relationship between the new orbitals added to the code and their corresponding κ values:

Orbital	κ	Orbital	κ
$8p_{\frac{1}{2}}$	1	$8p_{\frac{3}{2}}$	-2
$7d_{\frac{3}{2}}$	2	$7d_{\frac{5}{2}}$	-3
$6f_{\frac{5}{2}}$	3	$6f_{\frac{7}{2}}$	-4
$5g_{\frac{7}{2}}$	4	$5g_{\frac{9}{2}}$	-5

With the above changes, the modified single-configuration code can readily yield results for super-heavy elements beyond $Z = 120$. We have checked that the revised code reproduces the results for the orbital energies presented in Ref. [1] to at least six digits.

Table A

Atomic number Z and the closest integral atomic mass number $A = Z + N$ from Eq. (7), together with the default electron configurations used in the calculations reported here (see text).

Z	$A(Z)$	Uuo($Z=118$): $[Rn]5f^{14}6d^{10}7s^27p^6$
121	330	[Ubu] $8s^28p^1$
122	334	[Ubb] $7d^18s^28p^1$
123	337	[Ubt] $6f^17d^18s^28p^1$
124	340	[Ubq] $6f^38s^28p^1$
125	344	[Ubp] $5g^16f^38s^28p^1$
126	347	[Ubh] $5g^26f^27d^18s^28p^1$
127	350	[Ubs] $5g^36f^28s^28p^2$
128	354	[Ubo] $5g^46f^28s^28p^2$
129	357	[Ube] $5g^56f^28s^28p^2$
130	361	[Utn] $5g^66f^28s^28p^2$
131	364	[Utu] $5g^76f^28s^28p^2$
132	367	[Utb] $5g^86f^28s^28p^2$
133	371	[Utt] $5g^86f^38s^28p^2$
134	374	[Utg] $5g^86f^48s^28p^2$
135	378	[Utp] $5g^96f^48s^28p^2$
136	381	[Uth] $5g^{10}6f^48s^28p^2$
137	385	[Uts] $5g^{11}6f^37d^18s^28p^2$
138	388	[Uto] $5g^{12}6f^37d^18s^28p^2$

1.3. Dirac-Fock Expectation Values

The modified atomic code is now incorporated in the *ATOM* module of FEFF, which automatically carries out Dirac-Fock calculations of both the orbital binding energies and radial expectation values $\langle r^n \rangle$ as well as other atomic data. For example the radial expectation values are calculated from the spinor orbitals in terms of the radial density distributions,

$$\langle r^n \rangle = \int_0^\infty dr r^n [P^2(r) + Q^2(r)], \quad (9)$$

where $P(r)$ and $Q(r)$ represent the upper and lower components of the normalized Dirac spinors respectively. These results are presented in Tables 1 and 2. below, and closely follow the format of Desclaux [1]. In particular we present orbital energies (multiplied by -1) and the radial expectation values $\langle r^n \rangle$ with $n = -3, -2, -1, 1, 2, 4$, and 6. In the tables the $j = l - 1/2$ component of the orbital is labelled with an asterisk (*), and the absence of an asterisk indicates the $l + 1/2$ component. Additional data, such as the spinor states on an exponential radial grid are stored as ASCII files, or can be readily re-computed as desired. Extensions of our approach beyond $Z = 138$ are relatively straightforward, but may involve corrections to the nuclear model that are beyond the scope of the present theory. In addition to the Darwin, mass-velocity and spin-orbit coupling relativistic effects, the inclusion of intermediate angular momentum coupling and interelectron correlation are important for a proper description of electronic states of molecules comprised of heavy and super-heavy elements [5]. Relativistic effective core-potentials (RECPs) have been used extensively in calculations of structures and spectra of such molecules; for example for OsO^{2+} [11] and for UusH [15]. Related quantities such as relativistic phase shifts can also be computed using extensions of the FEFF codes [3].

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Explanation of Tables

Table 1. Orbital Binding Energies from $Z = 121$ to $Z = 138$.

Z	Atomic number
$2p, 2p^*, \text{ etc.}$	Absence of $*$ indicates $j = l + \frac{1}{2}$; $*$ indicates $j = l - \frac{1}{2}$

Table 2. Dirac-Fock Radial Expectation Values from $Z=121$ to $Z=138$

Z	Atomic number
n	Moment index n of expectation values $\langle r^n \rangle$ for $n= 6, 4, 2, 1, -1, -2, -3$
$2p, 2p^*, \text{ etc.}$	Absence of $*$ indicates $j = l + \frac{1}{2}$; $*$ indicates $j = l - \frac{1}{2}$

Table 1Orbital Binding Energies from $Z = 121$ to $Z = 138$. See page 7 for Explanation of Tables

Orbital	Z=121	122	123	124	125	126	127	128	129
1s	8804.338	9023.141	9247.773	9478.49	9715.518	9959.318	10210.36	10468.65	10734.68
2s	1875.459	1931.457	1989.199	2048.768	2110.207	2173.798	2239.817	2308.034	2378.739
2p*	1843.284	1901.409	1961.744	2024.448	2089.654	2157.739	2229.093	2303.626	2381.781
2p	1208.019	1231.626	1255.331	1279.126	1302.957	1327.008	1351.448	1375.934	1400.64
3s	517.3348	533.7441	550.5264	567.6968	585.204	603.2835	622.1373	641.4387	661.3954
3p*	498.4093	515.0997	532.2647	549.9353	568.0803	586.9521	606.7746	627.2494	648.6126
3p	341.8357	349.8449	357.8057	365.7106	373.4706	381.31	389.4055	397.4027	405.4818
3d*	308.8186	316.378	323.8882	331.342	338.6557	346.0464	353.6885	361.2316	368.8539
3d	285.2747	291.9256	298.4981	304.9842	311.3018	317.6674	324.2572	330.7161	337.2236
4s	157.1163	162.8289	168.5694	174.3375	180.0007	185.8409	192.0421	198.2597	204.6824
4p*	147.0155	152.7053	158.4506	164.2553	169.9972	175.9587	182.3305	188.7754	195.4901
4p	100.8938	103.9121	106.8246	109.6242	112.156	114.7076	117.4544	120.0451	122.6586
4d*	84.37944	87.14339	89.80033	92.343	94.62984	96.93586	99.4359	101.7793	104.1446
4d	77.65519	80.13088	82.49008	84.72544	86.68121	88.64531	90.79244	92.77168	94.76152
4f*	56.17113	58.33689	60.38692	62.31392	63.98303	65.66091	67.52132	69.21507	70.91962
4f	54.16836	56.24376	58.19829	60.02444	61.57296	63.12577	64.85798	66.41759	67.98356
5s	45.98289	48.12297	50.18098	52.15264	53.88578	55.67206	57.68932	59.58931	61.55388
5p*	41.07183	43.14898	45.15328	47.0819	48.79147	50.56698	52.58726	54.50841	56.51384
5p	27.1867	28.37077	29.42456	30.34157	30.9976	31.65364	32.4848	33.13964	33.79677
5d*	19.74437	20.77994	21.68679	22.45831	22.99976	23.54146	24.25677	24.79762	25.34068
5d	17.88379	18.82196	19.62576	20.2887	20.70299	21.11364	21.69555	22.09743	22.49754
5f*	8.726857	9.465997	10.07569	10.54979	10.84142	11.1308	11.58972	11.87285	12.15502
5f	8.278841	8.989399	9.564727	9.998428	10.20501	10.4067	10.77844	10.96862	11.15545
6s	11.33263	12.1331	12.80743	13.35126	13.76349	14.18908	14.80799	15.26101	15.73114
6p*	9.251268	9.997705	10.62196	11.12004	11.50596	11.90844	12.50672	12.94512	13.40587
6p	5.60206	6.043162	6.343349	6.498783	6.589683	6.679062	6.944	7.028584	7.112154
6d*	2.83914	3.1787	3.405815	3.518175	3.567042	3.614457	3.813202	3.856196	3.898113
6d	2.478358	2.782367	2.953408	2.988176	3.009118	3.028516	3.21671	3.231202	3.244317
7s	2.132357	2.385433	2.529562	2.563042	2.629777	2.699311	2.928381	3.002819	3.080479
7p*	1.427454	1.641348	1.76442	1.794119	1.848315	1.905634	2.10484	2.168484	2.236059
7p	0.709155	0.811252	0.838054	0.790041	0.789477	0.788702	0.897777	0.895108	0.892065
8s	0.264645	0.301832	0.310994	0.29267	0.298637	0.304922	0.378975	0.386205	0.393749
8p*	0.151759	0.182847	0.187425	0.165127	0.167392	0.169845	0.196975	0.199822	0.202879
7d*		0.191555	0.200802						
6f*			0.330996	0.281827	0.270651	0.258473	0.384684	0.368995	0.352321
5g*					0.524821	0.528228	0.699224	0.691446	0.68002

Table 1 (continued)

Orbital	Z=130	131	132	133	134	135	136	137	138
1s	11008.84	11291.5	11583.07	11884.26	12195.25	12516.25	12848.03	13191.12	13546.09
2s	2452.055	2528.108	2607.034	2689.261	2774.651	2863.061	2954.924	3050.397	3149.637
2p*	2463.859	2550.197	2641.166	2737.465	2839.278	2946.828	3060.959	3182.299	3311.545
2p	1425.565	1450.709	1476.072	1501.951	1528.06	1554.1	1580.36	1606.841	1633.544
3s	682.0371	703.3943	725.4986	748.705	772.7357	797.2992	822.7449	849.1076	876.4227
3p*	670.9272	694.2613	718.6882	744.6041	771.7878	800.0097	829.676	860.8882	893.7528
3p	413.6435	421.8882	430.2167	438.9689	447.8196	456.4244	465.1164	473.8964	482.7655
3d*	376.5559	384.338	392.2009	400.476	408.846	416.9742	425.1861	433.4825	441.8641
3d	343.7798	350.3846	357.038	364.0733	371.1703	377.9908	384.8608	391.7803	398.7494
4s	211.3196	218.1814	225.2778	232.999	240.9905	248.8736	257.0346	265.4844	274.2339
4p*	202.4933	209.8054	217.4477	225.8177	234.5798	243.3724	252.5964	262.2798	272.452
4p	125.2959	127.9574	130.6439	133.752	136.903	139.6932	142.5119	145.3598	148.2375
4d*	106.5326	108.9437	111.3787	114.2226	117.1073	119.6207	122.1605	124.7271	127.3214
4d	96.76249	98.77498	100.7994	103.2322	105.6944	107.789	109.8983	112.0225	114.1621
4f*	72.63541	74.36279	76.10215	78.23046	80.38692	82.15737	83.94097	85.73805	87.54897
4f	69.55632	71.1362	72.72358	74.70975	76.72062	78.37352	80.03668	81.71035	83.39482
5s	63.58676	65.69193	67.87329	70.53656	73.30039	75.75226	78.29739	80.94012	83.6846
5p*	58.61022	60.80484	63.10533	65.91502	68.86353	71.53097	74.34023	77.30118	80.42408
5p	34.45671	35.11998	35.78708	36.833	37.89636	38.60328	39.31658	40.03671	40.76414
5d*	25.8864	26.4352	26.98752	27.89096	28.80995	29.35039	29.89558	30.44598	31.002
5d	22.89633	23.29417	23.69144	24.44866	25.2173	25.65425	26.09289	26.53352	26.97647
5f*	12.43655	12.71773	12.99882	13.58094	14.17244	14.3968	14.62113	14.84573	15.07092
5f	11.3393	11.5205	11.69935	12.21876	12.74705	12.98693	13.22702	13.46755	13.70882
6s	16.21968	16.72794	17.2573	18.09835	18.97284	19.58924	20.23303	20.90573	21.60895
6p*	13.89114	14.4033	14.9448	15.79458	16.68972	17.33543	18.0222	18.75333	19.53234
6p	7.194887	7.276962	7.358549	7.632395	7.906343	8.000247	8.094716	8.189993	8.286354
6d*	3.939113	3.979335	4.018914	4.229443	4.442131	4.474742	4.507326	4.540066	4.573183
6d	3.256173	3.26688	3.276538	3.419447	3.559745	3.579439	3.598801	3.618009	3.637272
7s	3.161619	3.246508	3.335415	3.518523	3.707034	3.818162	3.935025	4.058018	4.187576
7p*	2.307968	2.384654	2.466589	2.642414	2.827475	2.934717	3.049849	3.173578	3.306676
7p	0.888673	0.88496	0.880958	0.897593	0.911576	0.908577	0.905564	0.90264	0.89994
8s	0.401627	0.409869	0.418498	0.431523	0.444475	0.455088	0.466338	0.478308	0.491103
8p*	0.206176	0.209745	0.213627	0.220193	0.226817	0.232216	0.238233	0.244974	0.25257
7d*									
6f*	0.334732	0.316287	0.297049	0.33206	0.365693	0.338685	0.311259	0.283515	0.255572
5g*	0.665213	0.647255	0.626388	0.900723	1.183872	1.142477	1.098866	1.053294	1.006049
5g						0.783858	0.751211	0.716835	0.681003

Table 2Dirac-Fock Radial Expectation Values from $Z = 121$ to $Z = 138$. See page 7 for Explanation of Tables

n =	6	4	2	1	-1	-2	-3
Z=121							
1s	2.73E-11	3.67E-08	1.05E-04	8.35E-03	2.32E+02	1.93E+05	
2s	1.88E-08	4.11E-06	1.46E-03	3.42E-02	6.41E+01	4.27E+04	
2p*	8.01E-09	1.98E-06	8.88E-04	2.56E-02	6.71E+01	1.89E+04	
2p	5.61E-08	8.24E-06	2.03E-03	4.07E-02	3.16E+01	1.39E+03	1.01E+05
3s	3.31E-06	1.53E-04	9.89E-03	9.21E-02	2.18E+01	1.05E+04	
3p*	2.43E-06	1.18E-04	8.44E-03	8.40E-02	2.23E+01	4.95E+03	
3p	1.05E-05	3.28E-04	1.44E-02	1.11E-01	1.30E+01	3.81E+02	2.85E+04
3d*	5.68E-06	1.94E-04	1.05E-02	9.43E-02	1.29E+01	2.14E+02	5.18E+03
3d	7.88E-06	2.46E-04	1.19E-02	1.01E-01	1.18E+01	1.71E+02	3.19E+03
4s	2.39E-04	2.85E-03	4.46E-02	1.98E-01	9.08E+00	3.10E+03	
4p*	2.21E-04	2.65E-03	4.25E-02	1.93E-01	9.15E+00	1.46E+03	
4p	7.77E-04	6.22E-03	6.56E-02	2.40E-01	6.07E+00	1.18E+02	8.75E+03
4d*	7.33E-04	5.72E-03	6.14E-02	2.31E-01	5.90E+00	6.52E+01	1.58E+03
4d	9.65E-04	6.90E-03	6.77E-02	2.43E-01	5.49E+00	5.23E+01	9.32E+02
4f*	7.57E-04	5.27E-03	5.64E-02	2.21E-01	5.28E+00	3.33E+01	2.59E+02
4f	8.55E-04	5.74E-03	5.90E-02	2.27E-01	5.13E+00	3.12E+01	2.30E+02
5s	1.19E-02	3.97E-02	1.69E-01	3.89E-01	4.17E+00	9.57E+02	
5p*	1.30E-02	4.16E-02	1.72E-01	3.91E-01	4.11E+00	4.40E+02	
5p	4.30E-02	9.24E-02	2.57E-01	4.79E-01	2.95E+00	3.64E+01	2.61E+03
5d*	6.14E-02	1.14E-01	2.81E-01	4.98E-01	2.75E+00	1.90E+01	4.36E+02
5d	8.07E-02	1.36E-01	3.08E-01	5.22E-01	2.59E+00	1.53E+01	2.53E+02
5f*	1.84E-01	2.16E-01	3.72E-01	5.69E-01	2.27E+00	8.42E+00	5.72E+01
5f	2.10E-01	2.36E-01	3.89E-01	5.82E-01	2.21E+00	7.87E+00	5.02E+01
6s	6.43E-01	5.64E-01	6.39E-01	7.58E-01	1.95E+00	2.74E+02	
6p*	8.66E-01	6.75E-01	6.94E-01	7.88E-01	1.86E+00	1.20E+02	
6p	3.39E+00	1.66E+00	1.09E+00	9.88E-01	1.35E+00	9.17E+00	6.24E+02
6d*	9.80E+00	3.19E+00	1.47E+00	1.14E+00	1.15E+00	4.07E+00	8.44E+01
6d	1.38E+01	3.99E+00	1.64E+00	1.21E+00	1.08E+00	3.21E+00	4.69E+01
7s	6.20E+01	1.14E+01	2.83E+00	1.59E+00	8.51E-01	6.09E+01	
7p*	1.15E+02	1.67E+01	3.40E+00	1.74E+00	7.72E-01	2.39E+01	
7p	8.15E+02	5.88E+01	6.24E+00	2.36E+00	5.42E-01	1.57E+00	9.92E+01
8s	2.21E+04	5.32E+02	1.87E+01	4.08E+00	3.11E-01	7.73E+00	
8p*	1.11E+05	1.52E+03	3.12E+01	5.25E+00	2.34E-01	1.71E+00	
Z=122							
1s	2.51E-11	3.46E-08	1.01E-04	8.19E-03	2.38E+02	2.05E+05	
2s	1.70E-08	3.84E-06	1.41E-03	3.35E-02	6.61E+01	4.58E+04	
2p*	7.15E-09	1.82E-06	8.49E-04	2.50E-02	6.95E+01	2.08E+04	
2p	5.30E-08	7.93E-06	1.99E-03	4.03E-02	3.19E+01	1.42E+03	1.04E+05
3s	3.01E-06	1.43E-04	9.57E-03	9.05E-02	2.24E+01	1.13E+04	
3p*	2.19E-06	1.10E-04	8.13E-03	8.25E-02	2.30E+01	5.45E+03	
3p	9.91E-06	3.15E-04	1.41E-02	1.10E-01	1.32E+01	3.91E+02	2.97E+04
3d*	5.33E-06	1.86E-04	1.03E-02	9.33E-02	1.31E+01	2.19E+02	5.38E+03
3d	7.43E-06	2.37E-04	1.17E-02	1.00E-01	1.19E+01	1.74E+02	3.28E+03
4s	2.17E-04	2.68E-03	4.32E-02	1.95E-01	9.30E+00	3.33E+03	
4p*	2.00E-04	2.48E-03	4.10E-02	1.89E-01	9.41E+00	1.61E+03	
4p	7.25E-04	5.94E-03	6.41E-02	2.37E-01	6.15E+00	1.22E+02	9.12E+03
4d*	6.81E-04	5.45E-03	5.99E-02	2.28E-01	5.97E+00	6.70E+01	1.65E+03
4d	9.00E-04	6.59E-03	6.62E-02	2.40E-01	5.56E+00	5.35E+01	9.65E+02
4f*	6.99E-04	5.01E-03	5.49E-02	2.19E-01	5.34E+00	3.41E+01	2.68E+02
4f	7.91E-04	5.46E-03	5.76E-02	2.24E-01	5.19E+00	3.19E+01	2.38E+02
5s	1.07E-02	3.70E-02	1.64E-01	3.82E-01	4.27E+00	1.04E+03	
5p*	1.16E-02	3.86E-02	1.66E-01	3.84E-01	4.22E+00	4.88E+02	
5p	3.94E-02	8.74E-02	2.50E-01	4.72E-01	2.99E+00	3.77E+01	2.74E+03
5d*	5.56E-02	1.07E-01	2.72E-01	4.90E-01	2.80E+00	1.97E+01	4.60E+02
5d	7.32E-02	1.28E-01	2.98E-01	5.14E-01	2.63E+00	1.58E+01	2.64E+02
5f*	1.60E-01	1.98E-01	3.57E-01	5.58E-01	2.31E+00	8.75E+00	6.04E+01
5f	1.83E-01	2.17E-01	3.73E-01	5.71E-01	2.25E+00	8.17E+00	5.29E+01
6s	5.57E-01	5.14E-01	6.11E-01	7.41E-01	2.00E+00	3.00E+02	
6p*	7.37E-01	6.09E-01	6.60E-01	7.69E-01	1.92E+00	1.35E+02	
6p	2.91E+00	1.51E+00	1.04E+00	9.67E-01	1.39E+00	9.68E+00	6.70E+02

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
6d*	7.89E+00	2.79E+00	1.38E+00	1.11E+00	1.19E+00	4.36E+00	9.25E+01
6d	1.10E+01	3.47E+00	1.54E+00	1.17E+00	1.11E+00	3.44E+00	5.10E+01
7s	4.79E+01	9.64E+00	2.62E+00	1.53E+00	8.90E-01	6.97E+01	
7p*	8.84E+01	1.40E+01	3.11E+00	1.67E+00	8.12E-01	2.83E+01	
7p	5.72E+02	4.71E+01	5.62E+00	2.24E+00	5.73E-01	1.78E+00	1.15E+02
8s	1.39E+04	3.93E+02	1.62E+01	3.79E+00	3.36E-01	9.76E+00	
8p*	5.70E+04	9.84E+02	2.52E+01	4.72E+00	2.64E-01	2.58E+00	
7d*	1.83E+04	4.10E+02	1.52E+01	3.62E+00	3.50E-01	3.86E-01	6.59E+00

Z=123

1s	2.31E-11	3.25E-08	9.76E-05	8.04E-03	2.44E+02	2.18E+05	
2s	1.53E-08	3.58E-06	1.36E-03	3.29E-02	6.82E+01	4.95E+04	
2p*	6.36E-09	1.68E-06	8.10E-04	2.43E-02	7.22E+01	2.30E+04	
2p	5.01E-08	7.64E-06	1.96E-03	4.00E-02	3.22E+01	1.45E+03	1.08E+05
3s	2.73E-06	1.34E-04	9.26E-03	8.90E-02	2.30E+01	1.22E+04	
3p*	1.97E-06	1.02E-04	7.84E-03	8.09E-02	2.38E+01	6.04E+03	
3p	9.32E-06	3.02E-04	1.38E-02	1.09E-01	1.33E+01	4.00E+02	3.08E+04
3d*	4.99E-06	1.78E-04	1.00E-02	9.23E-02	1.32E+01	2.24E+02	5.59E+03
3d	7.01E-06	2.28E-04	1.15E-02	9.93E-02	1.20E+01	1.77E+02	3.38E+03
4s	1.97E-04	2.51E-03	4.18E-02	1.92E-01	9.54E+00	3.61E+03	
4p*	1.80E-04	2.31E-03	3.96E-02	1.86E-01	9.67E+00	1.79E+03	
4p	6.77E-04	5.67E-03	6.27E-02	2.35E-01	6.23E+00	1.25E+02	9.51E+03
4d*	6.33E-04	5.19E-03	5.85E-02	2.25E-01	6.05E+00	6.89E+01	1.72E+03
4d	8.40E-04	6.30E-03	6.47E-02	2.37E-01	5.62E+00	5.48E+01	9.98E+02
4f*	6.46E-04	4.76E-03	5.36E-02	2.16E-01	5.41E+00	3.49E+01	2.78E+02
4f	7.32E-04	5.20E-03	5.62E-02	2.22E-01	5.25E+00	3.27E+01	2.47E+02
5s	9.60E-03	3.45E-02	1.58E-01	3.75E-01	4.38E+00	1.13E+03	
5p*	1.03E-02	3.57E-02	1.60E-01	3.77E-01	4.34E+00	5.44E+02	
5p	3.62E-02	8.26E-02	2.44E-01	4.66E-01	3.04E+00	3.90E+01	2.88E+03
5d*	5.04E-02	9.99E-02	2.64E-01	4.83E-01	2.84E+00	2.04E+01	4.86E+02
5d	6.66E-02	1.20E-01	2.90E-01	5.06E-01	2.67E+00	1.63E+01	2.76E+02
5f*	1.40E-01	1.82E-01	3.43E-01	5.47E-01	2.36E+00	9.09E+00	6.37E+01
5f	1.60E-01	1.99E-01	3.59E-01	5.60E-01	2.30E+00	8.48E+00	5.57E+01
6s	4.86E-01	4.70E-01	5.84E-01	7.24E-01	2.06E+00	3.31E+02	
6p*	6.34E-01	5.52E-01	6.29E-01	7.50E-01	1.98E+00	1.53E+02	
6p	2.56E+00	1.39E+00	1.00E+00	9.47E-01	1.42E+00	1.02E+01	7.16E+02
6d*	6.83E+00	2.54E+00	1.32E+00	1.08E+00	1.22E+00	4.61E+00	9.98E+01
6d	9.36E+00	3.13E+00	1.46E+00	1.14E+00	1.14E+00	3.63E+00	5.49E+01
7s	3.98E+01	8.54E+00	2.46E+00	1.49E+00	9.22E-01	7.85E+01	
7p*	7.18E+01	1.22E+01	2.91E+00	1.61E+00	8.45E-01	3.29E+01	
7p	4.97E+02	4.28E+01	5.36E+00	2.19E+00	5.87E-01	1.89E+00	1.24E+02
8s	1.20E+04	3.56E+02	1.53E+01	3.69E+00	3.46E-01	1.08E+01	
8p*	4.95E+04	8.91E+02	2.39E+01	4.60E+00	2.72E-01	2.92E+00	
7d*	1.48E+04	3.54E+02	1.41E+01	3.48E+00	3.65E-01	4.29E-01	7.56E+00
6f*	4.48E+02	3.00E+01	3.90E+00	1.81E+00	7.20E-01	1.08E+00	5.72E+00

Z=124

1s	2.12E-11	3.06E-08	9.42E-05	7.88E-03	2.51E+02	2.32E+05	
2s	1.39E-08	3.34E-06	1.31E-03	3.22E-02	7.03E+01	5.32E+04	
2p*	5.65E-09	1.54E-06	7.73E-04	2.37E-02	7.50E+01	2.55E+04	
2p	4.74E-08	7.35E-06	1.92E-03	3.96E-02	3.26E+01	1.48E+03	1.11E+05
3s	2.48E-06	1.26E-04	8.95E-03	8.75E-02	2.36E+01	1.31E+04	
3p*	1.77E-06	9.52E-05	7.55E-03	7.94E-02	2.45E+01	6.67E+03	
3p	8.77E-06	2.90E-04	1.36E-02	1.08E-01	1.35E+01	4.10E+02	3.20E+04
3d*	4.69E-06	1.71E-04	9.82E-03	9.13E-02	1.33E+01	2.30E+02	5.81E+03
3d	6.61E-06	2.19E-04	1.13E-02	9.84E-02	1.21E+01	1.81E+02	3.48E+03
4s	1.79E-04	2.35E-03	4.05E-02	1.89E-01	9.77E+00	3.88E+03	
4p*	1.62E-04	2.15E-03	3.82E-02	1.82E-01	9.95E+00	1.98E+03	
4p	6.33E-04	5.43E-03	6.13E-02	2.32E-01	6.31E+00	1.29E+02	9.92E+03
4d*	5.88E-04	4.95E-03	5.71E-02	2.23E-01	6.13E+00	7.08E+01	1.80E+03

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
4d	7.85E-04	6.02E-03	6.33E-02	2.35E-01	5.68E+00	5.60E+01	1.03E+03
4f*	5.98E-04	4.52E-03	5.23E-02	2.13E-01	5.47E+00	3.58E+01	2.88E+02
4f	6.79E-04	4.95E-03	5.49E-02	2.19E-01	5.31E+00	3.34E+01	2.55E+02
5s	8.64E-03	3.21E-02	1.52E-01	3.69E-01	4.48E+00	1.22E+03	
5p*	9.22E-03	3.31E-02	1.54E-01	3.69E-01	4.46E+00	6.05E+02	
5p	3.33E-02	7.82E-02	2.37E-01	4.60E-01	3.08E+00	4.03E+01	3.02E+03
5d*	4.58E-02	9.39E-02	2.56E-01	4.75E-01	2.89E+00	2.11E+01	5.12E+02
5d	6.07E-02	1.13E-01	2.81E-01	4.99E-01	2.71E+00	1.68E+01	2.88E+02
5f*	1.24E-01	1.68E-01	3.30E-01	5.37E-01	2.41E+00	9.44E+00	6.72E+01
5f	1.41E-01	1.84E-01	3.46E-01	5.49E-01	2.34E+00	8.79E+00	5.85E+01
6s	4.26E-01	4.31E-01	5.60E-01	7.09E-01	2.12E+00	3.63E+02	
6p*	5.53E-01	5.03E-01	6.01E-01	7.33E-01	2.04E+00	1.72E+02	
6p	2.30E+00	1.30E+00	9.64E-01	9.30E-01	1.45E+00	1.06E+01	7.62E+02
6d*	6.29E+00	2.39E+00	1.28E+00	1.07E+00	1.24E+00	4.80E+00	1.06E+02
6d	8.35E+00	2.89E+00	1.41E+00	1.12E+00	1.17E+00	3.81E+00	5.83E+01
7s	3.54E+01	7.86E+00	2.36E+00	1.46E+00	9.46E-01	8.63E+01	
7p*	6.11E+01	1.10E+01	2.77E+00	1.57E+00	8.72E-01	3.75E+01	
7p	5.24E+02	4.37E+01	5.38E+00	2.19E+00	5.87E-01	1.89E+00	1.26E+02
8s	1.39E+04	3.87E+02	1.59E+01	3.75E+00	3.39E-01	1.05E+01	
8p*	7.07E+04	1.11E+03	2.64E+01	4.82E+00	2.57E-01	2.52E+00	
6f*	4.78E+02	3.01E+01	3.83E+00	1.79E+00	7.35E-01	1.13E+00	6.11E+00
Z=125							
1s	1.95E-11	2.87E-08	9.09E-05	7.73E-03	2.58E+02	2.47E+05	
2s	1.25E-08	3.11E-06	1.26E-03	3.16E-02	7.26E+01	5.75E+04	
2p*	5.01E-09	1.42E-06	7.37E-04	2.31E-02	7.80E+01	2.83E+04	
2p	4.48E-08	7.08E-06	1.88E-03	3.92E-02	3.29E+01	1.51E+03	1.15E+05
3s	2.25E-06	1.18E-04	8.66E-03	8.60E-02	2.43E+01	1.41E+04	
3p*	1.59E-06	8.84E-05	7.26E-03	7.78E-02	2.54E+01	7.41E+03	
3p	8.25E-06	2.78E-04	1.33E-02	1.07E-01	1.36E+01	4.20E+02	3.32E+04
3d*	4.40E-06	1.64E-04	9.61E-03	9.03E-02	1.35E+01	2.35E+02	6.04E+03
3d	6.24E-06	2.11E-04	1.11E-02	9.74E-02	1.22E+01	1.84E+02	3.58E+03
4s	1.62E-04	2.20E-03	3.91E-02	1.86E-01	1.00E+01	4.20E+03	
4p*	1.46E-04	2.01E-03	3.69E-02	1.79E-01	1.02E+01	2.20E+03	
4p	5.91E-04	5.19E-03	5.99E-02	2.29E-01	6.39E+00	1.32E+02	1.03E+04
4d*	5.48E-04	4.72E-03	5.58E-02	2.20E-01	6.21E+00	7.27E+01	1.88E+03
4d	7.34E-04	5.76E-03	6.19E-02	2.32E-01	5.75E+00	5.73E+01	1.07E+03
4f*	5.56E-04	4.31E-03	5.10E-02	2.11E-01	5.54E+00	3.66E+01	2.99E+02
4f	6.30E-04	4.71E-03	5.36E-02	2.16E-01	5.37E+00	3.42E+01	2.64E+02
5s	7.81E-03	3.00E-02	1.47E-01	3.63E-01	4.59E+00	1.32E+03	
5p*	8.26E-03	3.08E-02	1.48E-01	3.63E-01	4.58E+00	6.75E+02	
5p	3.10E-02	7.46E-02	2.31E-01	4.54E-01	3.13E+00	4.15E+01	3.16E+03
5d*	4.25E-02	8.93E-02	2.49E-01	4.69E-01	2.93E+00	2.18E+01	5.37E+02
5d	5.65E-02	1.08E-01	2.75E-01	4.93E-01	2.74E+00	1.72E+01	2.99E+02
5f*	1.15E-01	1.59E-01	3.21E-01	5.29E-01	2.44E+00	9.71E+00	7.00E+01
5f	1.30E-01	1.74E-01	3.36E-01	5.42E-01	2.37E+00	9.03E+00	6.08E+01
6s	3.85E-01	4.03E-01	5.41E-01	6.97E-01	2.17E+00	3.94E+02	
6p*	4.94E-01	4.67E-01	5.78E-01	7.19E-01	2.10E+00	1.93E+02	
6p	2.16E+00	1.24E+00	9.44E-01	9.21E-01	1.46E+00	1.09E+01	7.94E+02
6d*	5.91E+00	2.29E+00	1.25E+00	1.05E+00	1.26E+00	4.93E+00	1.11E+02
6d	7.95E+00	2.79E+00	1.38E+00	1.11E+00	1.18E+00	3.88E+00	6.00E+01
7s	3.22E+01	7.38E+00	2.29E+00	1.43E+00	9.64E-01	9.35E+01	
7p*	5.51E+01	1.03E+01	2.67E+00	1.55E+00	8.89E-01	4.17E+01	
7p	5.11E+02	4.29E+01	5.32E+00	2.17E+00	5.90E-01	1.91E+00	1.29E+02
8s	1.27E+04	3.65E+02	1.54E+01	3.70E+00	3.44E-01	1.13E+01	
8p*	6.57E+04	1.05E+03	2.57E+01	4.76E+00	2.61E-01	2.79E+00	
6f*	4.99E+02	3.04E+01	3.82E+00	1.78E+00	7.39E-01	1.14E+00	6.25E+00
5g*	4.66E+00	1.10E+00	6.55E-01	7.21E-01	1.74E+00	3.81E+00	1.05E+01

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
Z=126							
1s	1.79E-11	2.70E-08	8.77E-05	7.57E-03	2.65E+02	2.64E+05	
2s	1.13E-08	2.90E-06	1.21E-03	3.10E-02	7.50E+01	6.21E+04	
2p*	4.43E-09	1.30E-06	7.02E-04	2.25E-02	8.12E+01	3.16E+04	
2p	4.24E-08	6.82E-06	1.85E-03	3.88E-02	3.32E+01	1.55E+03	1.19E+05
3s	2.04E-06	1.10E-04	8.37E-03	8.45E-02	2.50E+01	1.53E+04	
3p*	1.42E-06	8.20E-05	6.99E-03	7.63E-02	2.62E+01	8.24E+03	
3p	7.76E-06	2.67E-04	1.30E-02	1.05E-01	1.38E+01	4.30E+02	3.45E+04
3d*	4.13E-06	1.57E-04	9.40E-03	8.93E-02	1.37E+01	2.41E+02	6.27E+03
3d	5.89E-06	2.03E-04	1.09E-02	9.65E-02	1.24E+01	1.88E+02	3.69E+03
4s	1.47E-04	2.06E-03	3.79E-02	1.82E-01	1.03E+01	4.54E+03	
4p*	1.31E-04	1.87E-03	3.56E-02	1.76E-01	1.06E+01	2.45E+03	
4p	5.53E-04	4.96E-03	5.86E-02	2.27E-01	6.46E+00	1.36E+02	1.08E+04
4d*	5.11E-04	4.51E-03	5.45E-02	2.17E-01	6.29E+00	7.47E+01	1.96E+03
4d	6.86E-04	5.51E-03	6.05E-02	2.29E-01	5.81E+00	5.86E+01	1.10E+03
4f*	5.17E-04	4.11E-03	4.98E-02	2.08E-01	5.60E+00	3.75E+01	3.09E+02
4f	5.86E-04	4.49E-03	5.23E-02	2.14E-01	5.43E+00	3.50E+01	2.73E+02
5s	7.05E-03	2.81E-02	1.42E-01	3.56E-01	4.71E+00	1.43E+03	
5p*	7.40E-03	2.86E-02	1.43E-01	3.56E-01	4.71E+00	7.54E+02	
5p	2.89E-02	7.12E-02	2.26E-01	4.49E-01	3.17E+00	4.27E+01	3.30E+03
5d*	3.95E-02	8.50E-02	2.43E-01	4.64E-01	2.97E+00	2.24E+01	5.64E+02
5d	5.27E-02	1.03E-01	2.68E-01	4.87E-01	2.78E+00	1.77E+01	3.10E+02
5f*	1.06E-01	1.51E-01	3.13E-01	5.22E-01	2.47E+00	9.98E+00	7.29E+01
5f	1.21E-01	1.66E-01	3.28E-01	5.35E-01	2.40E+00	9.26E+00	6.31E+01
6s	3.48E-01	3.76E-01	5.23E-01	6.85E-01	2.22E+00	4.29E+02	
6p*	4.42E-01	4.33E-01	5.57E-01	7.06E-01	2.15E+00	2.16E+02	
6p	2.04E+00	1.20E+00	9.25E-01	9.11E-01	1.48E+00	1.12E+01	8.26E+02
6d*	5.56E+00	2.19E+00	1.22E+00	1.04E+00	1.27E+00	5.05E+00	1.16E+02
6d	7.58E+00	2.70E+00	1.36E+00	1.10E+00	1.19E+00	3.94E+00	6.16E+01
7s	2.93E+01	6.92E+00	2.21E+00	1.41E+00	9.82E-01	1.01E+02	
7p*	4.97E+01	9.59E+00	2.58E+00	1.52E+00	9.08E-01	4.65E+01	
7p	5.00E+02	4.22E+01	5.27E+00	2.16E+00	5.93E-01	1.94E+00	1.33E+02
8s	1.17E+04	3.44E+02	1.50E+01	3.64E+00	3.50E-01	1.22E+01	
8p*	6.08E+04	9.98E+02	2.50E+01	4.69E+00	2.65E-01	3.10E+00	
6f*	5.28E+02	3.10E+01	3.82E+00	1.78E+00	7.42E-01	1.16E+00	6.38E+00
5g*	4.27E+00	1.03E+00	6.33E-01	7.09E-01	1.77E+00	3.94E+00	1.11E+01
Z=127							
1s	1.64E-11	2.53E-08	8.45E-05	7.42E-03	2.73E+02	2.81E+05	
2s	1.02E-08	2.70E-06	1.17E-03	3.04E-02	7.75E+01	6.69E+04	
2p*	3.91E-09	1.19E-06	6.67E-04	2.19E-02	8.47E+01	3.51E+04	
2p	4.02E-08	6.58E-06	1.81E-03	3.84E-02	3.35E+01	1.58E+03	1.23E+05
3s	1.85E-06	1.03E-04	8.08E-03	8.31E-02	2.57E+01	1.65E+04	
3p*	1.27E-06	7.60E-05	6.72E-03	7.47E-02	2.72E+01	9.15E+03	
3p	7.31E-06	2.57E-04	1.28E-02	1.04E-01	1.39E+01	4.40E+02	3.58E+04
3d*	3.87E-06	1.51E-04	9.21E-03	8.84E-02	1.38E+01	2.46E+02	6.52E+03
3d	5.57E-06	1.95E-04	1.07E-02	9.56E-02	1.25E+01	1.91E+02	3.79E+03
4s	1.34E-04	1.93E-03	3.66E-02	1.79E-01	1.06E+01	4.90E+03	
4p*	1.18E-04	1.74E-03	3.43E-02	1.73E-01	1.09E+01	2.72E+03	
4p	5.18E-04	4.75E-03	5.73E-02	2.24E-01	6.54E+00	1.39E+02	1.12E+04
4d*	4.77E-04	4.30E-03	5.33E-02	2.15E-01	6.37E+00	7.67E+01	2.05E+03
4d	6.43E-04	5.28E-03	5.92E-02	2.27E-01	5.88E+00	6.00E+01	1.14E+03
4f*	4.82E-04	3.92E-03	4.87E-02	2.06E-01	5.67E+00	3.84E+01	3.20E+02
4f	5.45E-04	4.28E-03	5.11E-02	2.11E-01	5.50E+00	3.57E+01	2.82E+02
5s	6.38E-03	2.62E-02	1.38E-01	3.50E-01	4.82E+00	1.55E+03	
5p*	6.63E-03	2.66E-02	1.38E-01	3.49E-01	4.85E+00	8.42E+02	
5p	2.69E-02	6.79E-02	2.21E-01	4.44E-01	3.21E+00	4.40E+01	3.45E+03
5d*	3.67E-02	8.09E-02	2.37E-01	4.58E-01	3.01E+00	2.31E+01	5.91E+02
5d	4.92E-02	9.85E-02	2.62E-01	4.82E-01	2.81E+00	1.81E+01	3.21E+02
5f*	9.84E-02	1.44E-01	3.05E-01	5.16E-01	2.51E+00	1.03E+01	7.59E+01
5f	1.12E-01	1.58E-01	3.20E-01	5.28E-01	2.43E+00	9.50E+00	6.55E+01
6s	3.14E-01	3.51E-01	5.05E-01	6.73E-01	2.27E+00	4.65E+02	
6p*	3.93E-01	4.01E-01	5.36E-01	6.92E-01	2.21E+00	2.42E+02	

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
6p	1.90E+00	1.14E+00	9.05E-01	9.01E-01	1.50E+00	1.15E+01	8.61E+02
6d*	4.95E+00	2.05E+00	1.19E+00	1.03E+00	1.29E+00	5.22E+00	1.22E+02
6d	6.97E+00	2.56E+00	1.32E+00	1.09E+00	1.20E+00	4.03E+00	6.37E+01
7s	2.50E+01	6.27E+00	2.11E+00	1.38E+00	1.01E+00	1.11E+02	
7p*	4.01E+01	8.44E+00	2.43E+00	1.48E+00	9.38E-01	5.31E+01	
7p	3.91E+02	3.64E+01	4.93E+00	2.10E+00	6.12E-01	2.09E+00	1.46E+02
8s	7.23E+03	2.54E+02	1.30E+01	3.40E+00	3.76E-01	1.52E+01	
8p*	3.31E+04	6.69E+02	2.05E+01	4.26E+00	2.94E-01	4.36E+00	
6f*	2.54E+02	2.10E+01	3.30E+00	1.67E+00	7.80E-01	1.27E+00	7.18E+00
5g*	2.99E+00	8.72E-01	5.97E-01	6.91E-01	1.81E+00	4.10E+00	1.17E+01

Z=128

1s	1.50E-11	2.38E-08	8.15E-05	7.27E-03	2.81E+02	3.00E+05	
2s	9.16E-09	2.51E-06	1.12E-03	2.98E-02	8.01E+01	7.22E+04	
2p*	3.44E-09	1.08E-06	6.34E-04	2.13E-02	8.85E+01	3.92E+04	
2p	3.80E-08	6.34E-06	1.78E-03	3.81E-02	3.39E+01	1.61E+03	1.27E+05
3s	1.67E-06	9.62E-05	7.81E-03	8.16E-02	2.64E+01	1.77E+04	
3p*	1.14E-06	7.04E-05	6.45E-03	7.32E-02	2.81E+01	1.02E+04	
3p	6.89E-06	2.47E-04	1.25E-02	1.03E-01	1.41E+01	4.51E+02	3.72E+04
3d*	3.64E-06	1.44E-04	9.01E-03	8.74E-02	1.40E+01	2.52E+02	6.77E+03
3d	5.26E-06	1.88E-04	1.05E-02	9.47E-02	1.26E+01	1.95E+02	3.90E+03
4s	1.21E-04	1.81E-03	3.54E-02	1.76E-01	1.08E+01	5.29E+03	
4p*	1.06E-04	1.61E-03	3.30E-02	1.69E-01	1.12E+01	3.03E+03	
4p	4.85E-04	4.55E-03	5.61E-02	2.22E-01	6.62E+00	1.43E+02	1.17E+04
4d*	4.45E-04	4.11E-03	5.21E-02	2.12E-01	6.44E+00	7.88E+01	2.14E+03
4d	6.02E-04	5.06E-03	5.80E-02	2.25E-01	5.94E+00	6.13E+01	1.18E+03
4f*	4.50E-04	3.74E-03	4.76E-02	2.04E-01	5.74E+00	3.93E+01	3.31E+02
4f	5.08E-04	4.09E-03	5.00E-02	2.09E-01	5.56E+00	3.65E+01	2.91E+02
5s	5.77E-03	2.45E-02	1.33E-01	3.44E-01	4.94E+00	1.68E+03	
5p*	5.94E-03	2.47E-02	1.33E-01	3.43E-01	4.99E+00	9.40E+02	
5p	2.51E-02	6.49E-02	2.16E-01	4.38E-01	3.25E+00	4.52E+01	3.60E+03
5d*	3.42E-02	7.71E-02	2.32E-01	4.52E-01	3.05E+00	2.38E+01	6.19E+02
5d	4.60E-02	9.41E-02	2.56E-01	4.76E-01	2.85E+00	1.85E+01	3.32E+02
5f*	9.15E-02	1.37E-01	2.97E-01	5.09E-01	2.54E+00	1.05E+01	7.89E+01
5f	1.04E-01	1.50E-01	3.12E-01	5.22E-01	2.46E+00	9.73E+00	6.78E+01
6s	2.83E-01	3.28E-01	4.88E-01	6.62E-01	2.32E+00	5.04E+02	
6p*	3.51E-01	3.72E-01	5.16E-01	6.79E-01	2.27E+00	2.71E+02	
6p	1.80E+00	1.10E+00	8.87E-01	8.92E-01	1.51E+00	1.18E+01	8.95E+02
6d*	4.67E+00	1.97E+00	1.16E+00	1.02E+00	1.30E+00	5.35E+00	1.27E+02
6d	6.67E+00	2.48E+00	1.30E+00	1.08E+00	1.21E+00	4.09E+00	6.53E+01
7s	2.28E+01	5.89E+00	2.05E+00	1.36E+00	1.03E+00	1.20E+02	
7p*	3.61E+01	7.87E+00	2.35E+00	1.45E+00	9.58E-01	5.92E+01	
7p	3.83E+02	3.59E+01	4.89E+00	2.09E+00	6.15E-01	2.11E+00	1.50E+02
8s	6.68E+03	2.41E+02	1.26E+01	3.35E+00	3.82E-01	1.63E+01	
8p*	3.08E+04	6.35E+02	2.00E+01	4.20E+00	2.98E-01	4.82E+00	
6f*	2.64E+02	2.13E+01	3.30E+00	1.67E+00	7.83E-01	1.28E+00	7.32E+00
5g*	2.81E+00	8.28E-01	5.80E-01	6.80E-01	1.84E+00	4.24E+00	1.23E+01

Z=129

1s	1.38E-11	2.23E-08	7.84E-05	7.12E-03	2.89E+02	3.21E+05	
2s	8.24E-09	2.33E-06	1.08E-03	2.92E-02	8.29E+01	7.80E+04	
2p*	3.02E-09	9.87E-07	6.01E-04	2.06E-02	9.25E+01	4.39E+04	
2p	3.60E-08	6.11E-06	1.75E-03	3.77E-02	3.42E+01	1.64E+03	1.31E+05
3s	1.51E-06	8.98E-05	7.54E-03	8.02E-02	2.72E+01	1.92E+04	
3p*	1.01E-06	6.51E-05	6.20E-03	7.17E-02	2.92E+01	1.14E+04	
3p	6.49E-06	2.37E-04	1.23E-02	1.02E-01	1.43E+01	4.62E+02	3.86E+04
3d*	3.42E-06	1.39E-04	8.83E-03	8.65E-02	1.41E+01	2.58E+02	7.03E+03
3d	4.98E-06	1.81E-04	1.03E-02	9.39E-02	1.27E+01	1.99E+02	4.01E+03
4s	1.10E-04	1.69E-03	3.43E-02	1.73E-01	1.11E+01	5.72E+03	
4p*	9.45E-05	1.50E-03	3.18E-02	1.66E-01	1.16E+01	3.38E+03	

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
4p	4.54E-04	4.36E-03	5.49E-02	2.19E-01	6.70E+00	1.47E+02	1.22E+04
4d*	4.16E-04	3.93E-03	5.09E-02	2.10E-01	6.52E+00	8.09E+01	2.24E+03
4d	5.65E-04	4.85E-03	5.68E-02	2.22E-01	6.01E+00	6.26E+01	1.22E+03
4f*	4.20E-04	3.57E-03	4.65E-02	2.01E-01	5.80E+00	4.02E+01	3.43E+02
4f	4.73E-04	3.90E-03	4.88E-02	2.07E-01	5.62E+00	3.73E+01	3.01E+02
5s	5.21E-03	2.29E-02	1.29E-01	3.39E-01	5.07E+00	1.82E+03	
5p*	5.31E-03	2.29E-02	1.28E-01	3.36E-01	5.14E+00	1.05E+03	
5p	2.35E-02	6.20E-02	2.11E-01	4.33E-01	3.29E+00	4.65E+01	3.76E+03
5d*	3.18E-02	7.35E-02	2.26E-01	4.47E-01	3.09E+00	2.45E+01	6.48E+02
5d	4.31E-02	9.00E-02	2.51E-01	4.71E-01	2.88E+00	1.90E+01	3.44E+02
5f*	8.52E-02	1.30E-01	2.90E-01	5.03E-01	2.57E+00	1.08E+01	8.20E+01
5f	9.73E-02	1.43E-01	3.04E-01	5.15E-01	2.49E+00	9.97E+00	7.03E+01
6s	2.56E-01	3.06E-01	4.71E-01	6.50E-01	2.37E+00	5.48E+02	
6p*	3.13E-01	3.44E-01	4.96E-01	6.66E-01	2.33E+00	3.04E+02	
6p	1.70E+00	1.06E+00	8.70E-01	8.84E-01	1.53E+00	1.21E+01	9.31E+02
6d*	4.42E+00	1.90E+00	1.14E+00	1.01E+00	1.32E+00	5.48E+00	1.32E+02
6d	6.39E+00	2.41E+00	1.28E+00	1.07E+00	1.22E+00	4.16E+00	6.70E+01
7s	2.08E+01	5.53E+00	1.98E+00	1.33E+00	1.05E+00	1.30E+02	
7p*	3.25E+01	7.33E+00	2.26E+00	1.42E+00	9.79E-01	6.62E+01	
7p	3.77E+02	3.53E+01	4.85E+00	2.08E+00	6.18E-01	2.13E+00	1.53E+02
8s	6.15E+03	2.28E+02	1.23E+01	3.31E+00	3.88E-01	1.76E+01	
8p*	2.85E+04	6.01E+02	1.94E+01	4.13E+00	3.03E-01	5.35E+00	
6f*	2.78E+02	2.17E+01	3.30E+00	1.66E+00	7.85E-01	1.29E+00	7.44E+00
5g*	2.66E+00	7.90E-01	5.64E-01	6.70E-01	1.87E+00	4.37E+00	1.29E+01
Z=130							
1s	1.26E-11	2.09E-08	7.55E-05	6.97E-03	2.98E+02	3.42E+05	
2s	7.41E-09	2.16E-06	1.04E-03	2.86E-02	8.57E+01	8.42E+04	
2p*	2.65E-09	8.97E-07	5.69E-04	2.00E-02	9.69E+01	4.92E+04	
2p	3.41E-08	5.90E-06	1.72E-03	3.74E-02	3.45E+01	1.68E+03	1.36E+05
3s	1.37E-06	8.39E-05	7.28E-03	7.87E-02	2.80E+01	2.07E+04	
3p*	9.02E-07	6.01E-05	5.94E-03	7.02E-02	3.03E+01	1.27E+04	
3p	6.12E-06	2.28E-04	1.20E-02	1.01E-01	1.44E+01	4.73E+02	4.01E+04
3d*	3.22E-06	1.33E-04	8.64E-03	8.56E-02	1.43E+01	2.64E+02	7.30E+03
3d	4.71E-06	1.75E-04	1.01E-02	9.30E-02	1.28E+01	2.02E+02	4.12E+03
4s	9.94E-05	1.58E-03	3.31E-02	1.71E-01	1.14E+01	6.17E+03	
4p*	8.46E-05	1.39E-03	3.06E-02	1.63E-01	1.20E+01	3.77E+03	
4p	4.26E-04	4.17E-03	5.37E-02	2.17E-01	6.79E+00	1.51E+02	1.27E+04
4d*	3.89E-04	3.75E-03	4.98E-02	2.08E-01	6.60E+00	8.30E+01	2.33E+03
4d	5.30E-04	4.65E-03	5.56E-02	2.20E-01	6.08E+00	6.40E+01	1.26E+03
4f*	3.93E-04	3.41E-03	4.55E-02	1.99E-01	5.87E+00	4.11E+01	3.54E+02
4f	4.42E-04	3.73E-03	4.78E-02	2.04E-01	5.68E+00	3.81E+01	3.10E+02
5s	4.71E-03	2.14E-02	1.24E-01	3.33E-01	5.19E+00	1.97E+03	
5p*	4.75E-03	2.12E-02	1.23E-01	3.30E-01	5.29E+00	1.18E+03	
5p	2.20E-02	5.93E-02	2.06E-01	4.29E-01	3.33E+00	4.78E+01	3.92E+03
5d*	2.97E-02	7.02E-02	2.21E-01	4.42E-01	3.13E+00	2.52E+01	6.79E+02
5d	4.03E-02	8.62E-02	2.45E-01	4.66E-01	2.91E+00	1.94E+01	3.56E+02
5f*	7.94E-02	1.24E-01	2.83E-01	4.97E-01	2.61E+00	1.11E+01	8.52E+01
5f	9.08E-02	1.37E-01	2.97E-01	5.09E-01	2.53E+00	1.02E+01	7.27E+01
6s	2.31E-01	2.86E-01	4.56E-01	6.39E-01	2.43E+00	5.95E+02	
6p*	2.79E-01	3.19E-01	4.77E-01	6.53E-01	2.39E+00	3.41E+02	
6p	1.61E+00	1.02E+00	8.54E-01	8.75E-01	1.54E+00	1.23E+01	9.67E+02
6d*	4.18E+00	1.82E+00	1.12E+00	9.96E-01	1.33E+00	5.61E+00	1.38E+02
6d	6.13E+00	2.34E+00	1.26E+00	1.06E+00	1.23E+00	4.22E+00	6.87E+01
7s	1.89E+01	5.19E+00	1.92E+00	1.31E+00	1.07E+00	1.40E+02	
7p*	2.92E+01	6.82E+00	2.18E+00	1.40E+00	1.00E+00	7.39E+01	
7p	3.70E+02	3.49E+01	4.81E+00	2.07E+00	6.20E-01	2.16E+00	1.57E+02
8s	5.66E+03	2.15E+02	1.19E+01	3.26E+00	3.93E-01	1.89E+01	
8p*	2.63E+04	5.68E+02	1.89E+01	4.07E+00	3.08E-01	5.93E+00	
6f*	2.96E+02	2.22E+01	3.31E+00	1.66E+00	7.87E-01	1.30E+00	7.56E+00
5g*	2.54E+00	7.57E-01	5.49E-01	6.61E-01	1.90E+00	4.51E+00	1.35E+01

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
Z=131							
1s	1.16E-11	1.96E-08	7.27E-05	6.82E-03	3.07E+02	3.66E+05	
2s	6.65E-09	2.01E-06	9.98E-04	2.80E-02	8.87E+01	9.11E+04	
2p*	2.31E-09	8.13E-07	5.38E-04	1.94E-02	1.02E+02	5.53E+04	
2p	3.24E-08	5.69E-06	1.68E-03	3.70E-02	3.49E+01	1.71E+03	1.40E+05
3s	1.24E-06	7.83E-05	7.03E-03	7.73E-02	2.89E+01	2.23E+04	
3p*	8.01E-07	5.54E-05	5.70E-03	6.87E-02	3.15E+01	1.42E+04	
3p	5.77E-06	2.20E-04	1.18E-02	1.00E-01	1.46E+01	4.84E+02	4.16E+04
3d*	3.03E-06	1.28E-04	8.47E-03	8.47E-02	1.44E+01	2.70E+02	7.58E+03
3d	4.46E-06	1.69E-04	9.90E-03	9.22E-02	1.29E+01	2.06E+02	4.24E+03
4s	9.00E-05	1.48E-03	3.20E-02	1.68E-01	1.17E+01	6.67E+03	
4p*	7.56E-05	1.29E-03	2.95E-02	1.60E-01	1.24E+01	4.22E+03	
4p	4.00E-04	4.00E-03	5.26E-02	2.15E-01	6.87E+00	1.55E+02	1.32E+04
4d*	3.64E-04	3.59E-03	4.87E-02	2.05E-01	6.68E+00	8.52E+01	2.44E+03
4d	4.98E-04	4.46E-03	5.45E-02	2.18E-01	6.14E+00	6.54E+01	1.30E+03
4f*	3.68E-04	3.27E-03	4.44E-02	1.97E-01	5.93E+00	4.20E+01	3.66E+02
4f	4.13E-04	3.56E-03	4.67E-02	2.02E-01	5.74E+00	3.90E+01	3.20E+02
5s	4.26E-03	2.00E-02	1.20E-01	3.27E-01	5.33E+00	2.14E+03	
5p*	4.24E-03	1.97E-02	1.18E-01	3.24E-01	5.46E+00	1.32E+03	
5p	2.06E-02	5.68E-02	2.02E-01	4.24E-01	3.37E+00	4.92E+01	4.10E+03
5d*	2.77E-02	6.70E-02	2.16E-01	4.36E-01	3.17E+00	2.59E+01	7.10E+02
5d	3.78E-02	8.26E-02	2.40E-01	4.61E-01	2.95E+00	1.99E+01	3.68E+02
5f*	7.42E-02	1.19E-01	2.76E-01	4.91E-01	2.64E+00	1.14E+01	8.85E+01
5f	8.49E-02	1.30E-01	2.90E-01	5.03E-01	2.55E+00	1.05E+01	7.52E+01
6s	2.09E-01	2.67E-01	4.40E-01	6.28E-01	2.48E+00	6.46E+02	
6p*	2.48E-01	2.95E-01	4.59E-01	6.40E-01	2.46E+00	3.84E+02	
6p	1.53E+00	9.83E-01	8.38E-01	8.67E-01	1.56E+00	1.26E+01	1.01E+03
6d*	3.96E+00	1.76E+00	1.10E+00	9.87E-01	1.34E+00	5.74E+00	1.44E+02
6d	5.89E+00	2.27E+00	1.24E+00	1.05E+00	1.24E+00	4.28E+00	7.04E+01
7s	1.72E+01	4.86E+00	1.86E+00	1.29E+00	1.09E+00	1.52E+02	
7p*	2.61E+01	6.33E+00	2.10E+00	1.37E+00	1.02E+00	8.29E+01	
7p	3.64E+02	3.44E+01	4.78E+00	2.06E+00	6.22E-01	2.18E+00	1.61E+02
8s	5.20E+03	2.03E+02	1.16E+01	3.21E+00	4.00E-01	2.04E+01	
8p*	2.41E+04	5.35E+02	1.83E+01	4.01E+00	3.13E-01	6.61E+00	
6f*	3.19E+02	2.29E+01	3.33E+00	1.67E+00	7.89E-01	1.31E+00	7.66E+00
5g*	2.44E+00	7.27E-01	5.36E-01	6.52E-01	1.92E+00	4.64E+00	1.41E+01

Z=132

1s	1.06E-11	1.83E-08	6.99E-05	6.67E-03	3.17E+02	3.91E+05	
2s	5.96E-09	1.86E-06	9.58E-04	2.74E-02	9.19E+01	9.83E+04	
2p*	2.01E-09	7.35E-07	5.08E-04	1.88E-02	1.07E+02	6.22E+04	
2p	3.07E-08	5.49E-06	1.65E-03	3.67E-02	3.52E+01	1.75E+03	1.45E+05
3s	1.12E-06	7.31E-05	6.78E-03	7.59E-02	2.97E+01	2.41E+04	
3p*	7.10E-07	5.10E-05	5.46E-03	6.72E-02	3.28E+01	1.59E+04	
3p	5.45E-06	2.11E-04	1.16E-02	9.93E-02	1.47E+01	4.95E+02	4.32E+04
3d*	2.85E-06	1.23E-04	8.30E-03	8.38E-02	1.46E+01	2.76E+02	7.87E+03
3d	4.22E-06	1.63E-04	9.72E-02	9.14E-02	1.31E+01	2.10E+02	4.35E+03
4s	8.15E-05	1.39E-03	3.10E-02	1.65E-01	1.20E+01	7.20E+03	
4p*	6.75E-05	1.20E-03	2.84E-02	1.57E-01	1.28E+01	4.71E+03	
4p	3.75E-04	3.84E-03	5.15E-02	2.13E-01	6.95E+00	1.59E+02	1.38E+04
4d*	3.40E-04	3.44E-03	4.76E-02	2.03E-01	6.77E+00	8.74E+01	2.54E+03
4d	4.68E-04	4.28E-03	5.34E-02	2.15E-01	6.21E+00	6.68E+01	1.34E+03
4f*	3.44E-04	3.12E-03	4.35E-02	1.95E-01	6.00E+00	4.29E+01	3.79E+02
4f	3.86E-04	3.41E-03	4.57E-02	2.00E-01	5.80E+00	3.98E+01	3.30E+02
5s	3.85E-03	1.87E-02	1.16E-01	3.21E-01	5.46E+00	2.32E+03	
5p*	3.78E-03	1.82E-02	1.14E-01	3.17E-01	5.63E+00	1.48E+03	
5p	1.93E-02	5.44E-02	1.97E-01	4.19E-01	3.41E+00	5.06E+01	4.27E+03
5d*	2.59E-02	6.40E-02	2.11E-01	4.31E-01	3.21E+00	2.66E+01	7.43E+02
5d	3.55E-02	7.91E-02	2.35E-01	4.56E-01	2.98E+00	2.03E+01	3.80E+02
5f*	6.94E-02	1.13E-01	2.70E-01	4.85E-01	2.67E+00	1.17E+01	9.18E+01
5f	7.95E-02	1.25E-01	2.84E-01	4.98E-01	2.58E+00	1.07E+01	7.78E+01
6s	1.89E-01	2.49E-01	4.25E-01	6.17E-01	2.54E+00	7.01E+02	

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
6p*	2.21E-01	2.72E-01	4.41E-01	6.28E-01	2.53E+00	4.32E+02	
6p	1.45E+00	9.48E-01	8.23E-01	8.59E-01	1.57E+00	1.29E+01	1.04E+03
6d*	3.76E+00	1.69E+00	1.07E+00	9.77E-01	1.36E+00	5.87E+00	1.50E+02
6d	5.67E+00	2.21E+00	1.23E+00	1.04E+00	1.25E+00	4.35E+00	7.21E+01
7s	1.56E+01	4.55E+00	1.80E+00	1.27E+00	1.11E+00	1.64E+02	
7p*	2.34E+01	5.87E+00	2.03E+00	1.35E+00	1.05E+00	9.28E+01	
7p	3.59E+02	3.40E+01	4.74E+00	2.05E+00	6.25E-01	2.20E+00	1.65E+02
8s	4.78E+03	1.92E+02	1.13E+01	3.17E+00	4.06E-01	2.19E+01	
8p*	2.21E+04	5.03E+02	1.77E+01	3.94E+00	3.19E-01	7.36E+00	
6f*	3.49E+02	2.38E+01	3.36E+00	1.67E+00	7.89E-01	1.31E+00	7.75E+00
5g*	2.37E+00	7.01E-01	5.23E-01	6.44E-01	1.95E+00	4.77E+00	1.47E+01

Z=133

1s	9.66E-12	1.71E-08	6.71E-05	6.52E-03	3.27E+02	4.19E+05	
2s	5.34E-09	1.72E-06	9.20E-04	2.68E-02	9.52E+01	1.06E+05	
2p*	1.74E-09	6.62E-07	4.79E-04	1.82E-02	1.12E+02	7.02E+04	
2p	2.91E-08	5.30E-06	1.62E-03	3.64E-02	3.56E+01	1.78E+03	1.49E+05
3s	1.01E-06	6.81E-05	6.54E-03	7.45E-02	3.06E+01	2.60E+04	
3p*	6.29E-07	4.69E-05	5.22E-03	6.57E-02	3.41E+01	1.78E+04	
3p	5.15E-06	2.03E-04	1.13E-02	9.83E-02	1.49E+01	5.07E+02	4.48E+04
3d*	2.68E-06	1.18E-04	8.13E-03	8.30E-02	1.47E+01	2.83E+02	8.17E+03
3d	4.00E-06	1.57E-04	9.55E-03	9.06E-02	1.32E+01	2.13E+02	4.47E+03
4s	7.37E-05	1.30E-03	2.99E-02	1.62E-01	1.24E+01	7.79E+03	
4p*	6.02E-05	1.11E-03	2.73E-02	1.54E-01	1.33E+01	5.28E+03	
4p	3.53E-04	3.68E-03	5.05E-02	2.10E-01	7.03E+00	1.63E+02	1.44E+04
4d*	3.19E-04	3.29E-03	4.66E-02	2.01E-01	6.85E+00	8.97E+01	2.65E+03
4d	4.41E-04	4.11E-03	5.23E-02	2.13E-01	6.27E+00	6.82E+01	1.38E+03
4f*	3.22E-04	2.99E-03	4.25E-02	1.93E-01	6.06E+00	4.38E+01	3.91E+02
4f	3.61E-04	3.27E-03	4.48E-02	1.98E-01	5.86E+00	4.06E+01	3.40E+02
5s	3.46E-03	1.75E-02	1.12E-01	3.16E-01	5.61E+00	2.52E+03	
5p*	3.36E-03	1.68E-02	1.09E-01	3.11E-01	5.82E+00	1.67E+03	
5p	1.79E-02	5.19E-02	1.93E-01	4.14E-01	3.45E+00	5.21E+01	4.47E+03
5d*	2.39E-02	6.07E-02	2.05E-01	4.26E-01	3.26E+00	2.74E+01	7.80E+02
5d	3.29E-02	7.53E-02	2.29E-01	4.50E-01	3.02E+00	2.08E+01	3.94E+02
5f*	6.27E-02	1.06E-01	2.62E-01	4.77E-01	2.71E+00	1.20E+01	9.59E+01
5f	7.21E-02	1.17E-01	2.76E-01	4.90E-01	2.62E+00	1.10E+01	8.09E+01
6s	1.66E-01	2.30E-01	4.08E-01	6.05E-01	2.61E+00	7.67E+02	
6p*	1.91E-01	2.48E-01	4.21E-01	6.13E-01	2.62E+00	4.91E+02	
6p	1.31E+00	8.88E-01	7.97E-01	8.46E-01	1.60E+00	1.35E+01	1.10E+03
6d*	3.37E+00	1.58E+00	1.04E+00	9.60E-01	1.38E+00	6.12E+00	1.59E+02
6d	5.01E+00	2.04E+00	1.18E+00	1.02E+00	1.28E+00	4.54E+00	7.63E+01
7s	1.33E+01	4.09E+00	1.71E+00	1.24E+00	1.14E+00	1.83E+02	
7p*	1.94E+01	5.19E+00	1.91E+00	1.31E+00	1.09E+00	1.08E+02	
7p	3.26E+02	3.18E+01	4.58E+00	2.02E+00	6.36E-01	2.29E+00	1.75E+02
8s	4.16E+03	1.75E+02	1.07E+01	3.09E+00	4.16E-01	2.41E+01	
8p*	1.90E+04	4.54E+02	1.68E+01	3.84E+00	3.29E-01	8.44E+00	
6f*	2.48E+02	1.93E+01	3.06E+00	1.60E+00	8.23E-01	1.42E+00	8.64E+00
5g*	1.44E+00	5.40E-01	4.74E-01	6.17E-01	2.02E+00	5.07E+00	1.59E+01

Z=134

1s	8.83E-12	1.60E-08	6.45E-05	6.38E-03	3.37E+02	4.47E+05	
2s	4.79E-09	1.60E-06	8.83E-04	2.62E-02	9.85E+01	1.15E+05	
2p*	1.50E-09	5.96E-07	4.51E-04	1.76E-02	1.18E+02	7.90E+04	
2p	2.77E-08	5.11E-06	1.60E-03	3.60E-02	3.59E+01	1.82E+03	1.54E+05
3s	9.10E-07	6.35E-05	6.31E-03	7.32E-02	3.16E+01	2.80E+04	
3p*	5.55E-07	4.31E-05	5.00E-03	6.42E-02	3.55E+01	1.99E+04	
3p	4.86E-06	1.96E-04	1.11E-02	9.73E-02	1.51E+01	5.19E+02	4.65E+04
3d*	2.53E-06	1.13E-04	7.97E-03	8.21E-02	1.49E+01	2.89E+02	8.48E+03
3d	3.80E-06	1.52E-04	9.39E-03	8.98E-02	1.33E+01	2.17E+02	4.59E+03
4s	6.68E-05	1.21E-03	2.90E-02	1.59E-01	1.27E+01	8.37E+03	

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
4p*	5.36E-05	1.02E-03	2.62E-02	1.51E-01	1.37E+01	5.89E+03	
4p	3.31E-04	3.53E-03	4.94E-02	2.08E-01	7.11E+00	1.67E+02	1.49E+04
4d*	2.99E-04	3.15E-03	4.56E-02	1.99E-01	6.93E+00	9.20E+01	2.77E+03
4d	4.15E-04	3.95E-03	5.13E-02	2.11E-01	6.33E+00	6.96E+01	1.42E+03
4f*	3.01E-04	2.86E-03	4.16E-02	1.91E-01	6.13E+00	4.48E+01	4.04E+02
4f	3.39E-04	3.13E-03	4.38E-02	1.96E-01	5.92E+00	4.14E+01	3.51E+02
5s	3.12E-03	1.63E-02	1.08E-01	3.10E-01	5.75E+00	2.71E+03	
5p*	2.98E-03	1.56E-02	1.05E-01	3.05E-01	6.01E+00	1.87E+03	
5p	1.67E-02	4.95E-02	1.88E-01	4.10E-01	3.50E+00	5.36E+01	4.67E+03
5d*	2.20E-02	5.76E-02	2.00E-01	4.20E-01	3.30E+00	2.83E+01	8.19E+02
5d	3.05E-02	7.17E-02	2.24E-01	4.45E-01	3.05E+00	2.14E+01	4.09E+02
5f*	5.67E-02	9.96E-02	2.54E-01	4.70E-01	2.76E+00	1.24E+01	1.00E+02
5f	6.54E-02	1.10E-01	2.68E-01	4.83E-01	2.66E+00	1.13E+01	8.42E+01
6s	1.47E-01	2.12E-01	3.92E-01	5.93E-01	2.68E+00	8.35E+02	
6p*	1.66E-01	2.26E-01	4.02E-01	5.99E-01	2.71E+00	5.55E+02	
6p	1.19E+00	8.33E-01	7.72E-01	8.33E-01	1.63E+00	1.40E+01	1.17E+03
6d*	3.02E+00	1.47E+00	1.00E+00	9.43E-01	1.41E+00	6.38E+00	1.69E+02
6d	4.44E+00	1.89E+00	1.14E+00	1.01E+00	1.30E+00	4.73E+00	8.06E+01
7s	1.13E+01	3.69E+00	1.62E+00	1.21E+00	1.18E+00	2.02E+02	
7p*	1.61E+01	4.60E+00	1.80E+00	1.27E+00	1.13E+00	1.24E+02	
7p	2.98E+02	2.99E+01	4.44E+00	1.99E+00	6.47E-01	2.39E+00	1.85E+02
8s	3.65E+03	1.60E+02	1.03E+01	3.02E+00	4.26E-01	2.62E+01	
8p*	1.65E+04	4.11E+02	1.59E+01	3.74E+00	3.38E-01	9.61E+00	
6f*	1.84E+02	1.61E+01	2.82E+00	1.54E+00	8.55E-01	1.54E+00	9.54E+00
5g*	9.71E-01	4.35E-01	4.35E-01	5.94E-01	2.08E+00	5.35E+00	1.72E+01

Z=135

1s	8.06E-12	1.49E-08	6.19E-05	6.23E-03	3.49E+02	4.79E+05	
2s	4.28E-09	1.48E-06	8.47E-04	2.56E-02	1.02E+02	1.24E+05	
2p*	1.29E-09	5.34E-07	4.23E-04	1.70E-02	1.25E+02	8.94E+04	
2p	2.63E-08	4.94E-06	1.57E-03	3.57E-02	3.62E+01	1.85E+03	1.59E+05
3s	8.19E-07	5.92E-05	6.08E-03	7.18E-02	3.26E+01	3.02E+04	
3p*	4.89E-07	3.95E-05	4.77E-03	6.27E-02	3.71E+01	2.23E+04	
3p	4.59E-06	1.88E-04	1.09E-02	9.64E-02	1.52E+01	5.31E+02	4.83E+04
3d*	2.38E-06	1.09E-04	7.81E-03	8.13E-02	1.51E+01	2.96E+02	8.81E+03
3d	3.60E-06	1.46E-04	9.22E-03	8.90E-02	1.34E+01	2.21E+02	4.71E+03
4s	6.04E-05	1.13E-03	2.80E-02	1.57E-01	1.31E+01	9.05E+03	
4p*	4.76E-05	9.44E-04	2.52E-02	1.48E-01	1.43E+01	6.60E+03	
4p	3.12E-04	3.39E-03	4.84E-02	2.06E-01	7.19E+00	1.72E+02	1.56E+04
4d*	2.80E-04	3.02E-03	4.46E-02	1.96E-01	7.01E+00	9.44E+01	2.89E+03
4d	3.91E-04	3.80E-03	5.03E-02	2.09E-01	6.40E+00	7.11E+01	1.47E+03
4f*	2.81E-04	2.74E-03	4.07E-02	1.88E-01	6.19E+00	4.58E+01	4.17E+02
4f	3.18E-04	3.00E-03	4.29E-02	1.94E-01	5.98E+00	4.23E+01	3.61E+02
5s	2.82E-03	1.52E-02	1.05E-01	3.05E-01	5.90E+00	2.94E+03	
5p*	2.64E-03	1.44E-02	1.01E-01	2.99E-01	6.21E+00	2.10E+03	
5p	1.57E-02	4.74E-02	1.85E-01	4.05E-01	3.54E+00	5.51E+01	4.87E+03
5d*	2.06E-02	5.51E-02	1.96E-01	4.16E-01	3.34E+00	2.91E+01	8.57E+02
5d	2.88E-02	6.89E-02	2.19E-01	4.40E-01	3.09E+00	2.19E+01	4.22E+02
5f*	5.31E-02	9.52E-02	2.48E-01	4.65E-01	2.79E+00	1.27E+01	1.04E+02
5f	6.15E-02	1.06E-01	2.62E-01	4.78E-01	2.69E+00	1.16E+01	8.70E+01
6s	1.33E-01	1.98E-01	3.79E-01	5.82E-01	2.75E+00	9.06E+02	
6p*	1.47E-01	2.08E-01	3.86E-01	5.87E-01	2.79E+00	6.25E+02	
6p	1.13E+00	8.04E-01	7.59E-01	8.25E-01	1.64E+00	1.43E+01	1.21E+03
6d*	2.88E+00	1.42E+00	9.83E-01	9.35E-01	1.42E+00	6.51E+00	1.76E+02
6d	4.26E+00	1.83E+00	1.12E+00	9.97E-01	1.31E+00	4.80E+00	8.27E+01
7s	1.02E+01	3.45E+00	1.57E+00	1.19E+00	1.20E+00	2.19E+02	
7p*	1.43E+01	4.25E+00	1.73E+00	1.24E+00	1.16E+00	1.39E+02	
7p	2.92E+02	2.94E+01	4.40E+00	1.98E+00	6.50E-01	2.41E+00	1.90E+02
8s	3.32E+03	1.50E+02	9.93E+00	2.97E+00	4.34E-01	2.83E+01	
8p*	1.48E+04	3.82E+02	1.53E+01	3.67E+00	3.45E-01	1.08E+01	
6f*	2.06E+02	1.69E+01	2.86E+00	1.54E+00	8.53E-01	1.53E+00	9.56E+00
5g*	9.55E-01	4.24E-01	4.27E-01	5.88E-01	2.10E+00	5.48E+00	1.78E+01
5g	1.21E+00	4.85E-01	4.52E-01	6.04E-01	2.05E+00	5.23E+00	1.66E+01

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
Z=136							
1s	7.36E-12	1.40E-08	5.94E-05	6.09E-03	3.60E+02	5.13E+05	
2s	3.82E-09	1.36E-06	8.12E-04	2.51E-02	1.06E+02	1.34E+05	
2p*	1.11E-09	4.77E-07	3.97E-04	1.64E-02	1.32E+02	1.01E+05	
2p	2.49E-08	4.77E-06	1.54E-03	3.54E-02	3.66E+01	1.89E+03	1.65E+05
3s	7.38E-07	5.51E-05	5.87E-03	7.05E-02	3.36E+01	3.25E+04	
3p*	4.30E-07	3.61E-05	4.56E-03	6.12E-02	3.87E+01	2.50E+04	
3p	4.34E-06	1.81E-04	1.07E-02	9.55E-02	1.54E+01	5.44E+02	5.01E+04
3d*	2.25E-06	1.05E-04	7.65E-03	8.05E-02	1.52E+01	3.03E+02	9.14E+03
3d	3.42E-06	1.41E-04	9.06E-03	8.82E-02	1.35E+01	2.25E+02	4.84E+03
4s	5.46E-05	1.06E-03	2.70E-02	1.54E-01	1.34E+01	9.75E+03	
4p*	4.23E-05	8.71E-04	2.41E-02	1.45E-01	1.48E+01	7.38E+03	
4p	2.93E-04	3.26E-03	4.75E-02	2.04E-01	7.28E+00	1.76E+02	1.62E+04
4d*	2.62E-04	2.89E-03	4.36E-02	1.94E-01	7.09E+00	9.68E+01	3.01E+03
4d	3.69E-04	3.65E-03	4.93E-02	2.07E-01	6.46E+00	7.25E+01	1.51E+03
4f*	2.63E-04	2.62E-03	3.99E-02	1.86E-01	6.26E+00	4.67E+01	4.31E+02
4f	3.00E-04	2.88E-03	4.21E-02	1.92E-01	6.04E+00	4.31E+01	3.72E+02
5s	2.55E-03	1.42E-02	1.01E-01	3.00E-01	6.06E+00	3.17E+03	
5p*	2.35E-03	1.33E-02	9.68E-02	2.93E-01	6.42E+00	2.35E+03	
5p	1.47E-02	4.55E-02	1.81E-01	4.01E-01	3.58E+00	5.66E+01	5.08E+03
5d*	1.93E-02	5.27E-02	1.91E-01	4.11E-01	3.38E+00	2.99E+01	8.95E+02
5d	2.71E-02	6.62E-02	2.15E-01	4.36E-01	3.12E+00	2.23E+01	4.36E+02
5f*	4.97E-02	9.11E-02	2.43E-01	4.60E-01	2.82E+00	1.30E+01	1.07E+02
5f	5.80E-02	1.01E-01	2.56E-01	4.73E-01	2.72E+00	1.18E+01	8.98E+01
6s	1.20E-01	1.84E-01	3.66E-01	5.72E-01	2.81E+00	9.81E+02	
6p*	1.30E-01	1.92E-01	3.70E-01	5.75E-01	2.87E+00	7.03E+02	
6p	1.07E+00	7.76E-01	7.45E-01	8.18E-01	1.66E+00	1.46E+01	1.26E+03
6d*	2.75E+00	1.37E+00	9.67E-01	9.27E-01	1.43E+00	6.64E+00	1.82E+02
6d	4.09E+00	1.78E+00	1.10E+00	9.90E-01	1.32E+00	4.88E+00	8.48E+01
7s	9.26E+00	3.23E+00	1.51E+00	1.17E+00	1.23E+00	2.36E+02	
7p*	1.27E+01	3.93E+00	1.66E+00	1.22E+00	1.18E+00	1.55E+02	
7p	2.86E+02	2.90E+01	4.36E+00	1.97E+00	6.52E-01	2.44E+00	1.95E+02
8s	3.01E+03	1.40E+02	9.61E+00	2.92E+00	4.41E-01	3.04E+01	
8p*	1.33E+04	3.54E+02	1.47E+01	3.59E+00	3.53E-01	1.21E+01	
8f*	2.34E+02	1.79E+01	2.90E+00	1.55E+00	8.51E-01	1.52E+00	9.57E+00
5g*	9.42E-01	4.14E-01	4.19E-01	5.82E-01	2.13E+00	5.62E+00	1.85E+01
5g	1.18E+00	4.73E-01	4.44E-01	5.97E-01	2.08E+00	5.36E+00	1.72E+01

Z=137

1s	6.71E-12	1.30E-08	5.70E-05	5.94E-03	3.72E+02	5.50E+05	
2s	3.41E-09	1.26E-06	7.78E-04	2.45E-02	1.10E+02	1.45E+05	
2p*	9.41E-10	4.24E-07	3.71E-04	1.58E-02	1.40E+02	1.15E+05	
2p	2.37E-08	4.61E-06	1.51E-03	3.51E-02	3.69E+01	1.93E+03	1.70E+05
3s	6.64E-07	5.13E-05	5.65E-03	6.91E-02	3.46E+01	3.51E+04	
3p*	3.77E-07	3.30E-05	4.34E-03	5.97E-02	4.05E+01	2.80E+04	
3p	4.11E-06	1.75E-04	1.05E-02	9.46E-02	1.55E+01	5.56E+02	5.20E+04
3d*	2.12E-06	1.00E-04	7.50E-03	7.97E-02	1.54E+01	3.09E+02	9.49E+03
3d	3.24E-06	1.37E-04	8.91E-03	8.75E-02	1.36E+01	2.29E+02	4.97E+03
4s	4.93E-05	9.88E-04	2.61E-02	1.51E-01	1.38E+01	1.05E+04	
4p*	3.74E-05	8.02E-04	2.32E-02	1.41E-01	1.54E+01	8.28E+03	
4p	2.76E-04	3.13E-03	4.65E-02	2.02E-01	7.36E+00	1.81E+02	1.68E+04
4d*	2.46E-04	2.77E-03	4.27E-02	1.92E-01	7.18E+00	9.93E+01	3.14E+03
4d	3.48E-04	3.52E-03	4.84E-02	2.05E-01	6.53E+00	7.40E+01	1.56E+03
4f*	2.47E-04	2.51E-03	3.90E-02	1.84E-01	6.33E+00	4.77E+01	4.45E+02
4f	2.82E-04	2.77E-03	4.13E-02	1.90E-01	6.10E+00	4.39E+01	3.83E+02
5s	2.30E-03	1.33E-02	9.76E-02	2.95E-01	6.22E+00	3.44E+03	
5p*	2.08E-03	1.22E-02	9.29E-02	2.87E-01	6.65E+00	2.64E+03	
5p	1.39E-02	4.37E-02	1.77E-01	3.97E-01	3.62E+00	5.81E+01	5.29E+03
5d*	1.80E-02	5.04E-02	1.87E-01	4.06E-01	3.43E+00	3.07E+01	9.36E+02
5d	2.56E-02	6.36E-02	2.11E-01	4.31E-01	3.15E+00	2.28E+01	4.50E+02

Table 2 (continued)

n=	6	4	2	1	-1	-2	-3
5f*	4.66E-02	8.72E-02	2.37E-01	4.54E-01	2.85E+00	1.33E+01	1.11E+02
5f	5.46E-02	9.74E-02	2.51E-01	4.68E-01	2.75E+00	1.21E+01	9.27E+01
6s	1.08E-01	1.72E-01	3.53E-01	5.62E-01	2.88E+00	1.06E+03	
6p*	1.15E-01	1.76E-01	3.55E-01	5.63E-01	2.97E+00	7.92E+02	
6p	1.02E+00	7.49E-01	7.32E-01	8.10E-01	1.67E+00	1.50E+01	1.31E+03
6d*	2.62E+00	1.33E+00	9.50E-01	9.19E-01	1.45E+00	6.77E+00	1.89E+02
6d	3.93E+00	1.73E+00	1.09E+00	9.82E-01	1.33E+00	4.96E+00	8.69E+01
7s	8.35E+00	3.01E+00	1.46E+00	1.15E+00	1.25E+00	2.55E+02	
7p*	1.13E+01	3.62E+00	1.59E+00	1.19E+00	1.21E+00	1.74E+02	
7p	2.81E+02	2.86E+01	4.33E+00	1.96E+00	6.55E-01	2.47E+00	2.00E+02
8s	2.72E+03	1.31E+02	9.29E+00	2.87E+00	4.49E-01	3.28E+01	
8p*	1.18E+04	3.26E+02	1.41E+01	3.52E+00	3.61E-01	1.37E+01	
6f*	2.72E+02	1.92E+01	2.96E+00	1.56E+00	8.48E-01	1.51E+00	9.56E+00
5g*	9.34E-01	4.05E-01	4.12E-01	5.76E-01	2.15E+00	5.75E+00	1.92E+01
5g	1.17E+00	4.61E-01	4.36E-01	5.92E-01	2.10E+00	5.49E+00	1.79E+01

Z=138

1s	6.12E-12	1.21E-08	5.47E-05	5.80E-03	3.85E+02	5.87E+05	
2s	3.04E-09	1.16E-06	7.46E-04	2.40E-02	1.14E+02	1.55E+05	
2p*	7.99E-10	3.77E-07	3.46E-04	1.52E-02	1.49E+02	1.30E+05	
2p	2.25E-08	4.45E-06	1.49E-03	3.48E-02	3.73E+01	1.97E+03	1.76E+05
3s	5.98E-07	4.77E-05	5.45E-03	6.79E-02	3.57E+01	3.76E+04	
3p*	3.30E-07	3.01E-05	4.14E-03	5.82E-02	4.23E+01	3.13E+04	
3p	3.88E-06	1.68E-04	1.03E-02	9.37E-02	1.57E+01	5.69E+02	5.39E+04
3d*	2.00E-06	9.66E-05	7.35E-03	7.89E-02	1.56E+01	3.16E+02	9.85E+03
3d	3.08E-06	1.32E-04	8.76E-03	8.67E-02	1.38E+01	2.33E+02	5.10E+03
4s	4.46E-05	9.24E-04	2.52E-02	1.49E-01	1.42E+01	1.13E+04	
4p*	3.31E-05	7.38E-04	2.22E-02	1.38E-01	1.59E+01	9.22E+03	
4p	2.60E-04	3.01E-03	4.56E-02	2.00E-01	7.44E+00	1.85E+02	1.75E+04
4d*	2.31E-04	2.65E-03	4.18E-02	1.90E-01	7.26E+00	1.02E+02	3.27E+03
4d	3.29E-04	3.38E-03	4.74E-02	2.03E-01	6.59E+00	7.55E+01	1.60E+03
4f*	2.31E-04	2.40E-03	3.82E-02	1.83E-01	6.39E+00	4.87E+01	4.59E+02
4f	2.66E-04	2.66E-03	4.04E-02	1.88E-01	6.16E+00	4.48E+01	3.94E+02
5s	2.08E-03	1.24E-02	9.43E-02	2.89E-01	6.38E+00	3.69E+03	
5p*	1.84E-03	1.13E-02	8.92E-02	2.81E-01	6.88E+00	2.95E+03	
5p	1.30E-02	4.19E-02	1.73E-01	3.93E-01	3.66E+00	5.96E+01	5.52E+03
5d*	1.69E-02	4.83E-02	1.83E-01	4.02E-01	3.47E+00	3.15E+01	9.78E+02
5d	2.41E-02	6.12E-02	2.07E-01	4.27E-01	3.19E+00	2.33E+01	4.64E+02
5f*	4.38E-02	8.35E-02	2.32E-01	4.49E-01	2.88E+00	1.36E+01	1.15E+02
5f	5.15E-02	9.36E-02	2.46E-01	4.63E-01	2.78E+00	1.23E+01	9.57E+01
6s	9.71E-02	1.60E-01	3.41E-01	5.52E-01	2.95E+00	1.15E+03	
6p*	1.01E-01	1.62E-01	3.40E-01	5.51E-01	3.06E+00	8.87E+02	
6p	9.64E-01	7.24E-01	7.19E-01	8.03E-01	1.69E+00	1.53E+01	1.36E+03
6d*	2.50E+00	1.28E+00	9.34E-01	9.11E-01	1.46E+00	6.91E+00	1.96E+02
6d	3.77E+00	1.68E+00	1.07E+00	9.75E-01	1.34E+00	5.03E+00	8.91E+01
7s	7.54E+00	2.81E+00	1.41E+00	1.13E+00	1.28E+00	2.74E+02	
7p*	9.94E+00	3.33E+00	1.53E+00	1.17E+00	1.25E+00	1.94E+02	
7p	2.75E+02	2.81E+01	4.29E+00	1.95E+00	6.58E-01	2.49E+00	2.05E+02
8s	2.47E+03	1.23E+02	8.98E+00	2.83E+00	4.57E-01	3.52E+01	
8p*	1.04E+04	2.99E+02	1.35E+01	3.44E+00	3.70E-01	1.54E+01	
6f*	3.24E+02	2.09E+01	3.03E+00	1.57E+00	8.44E-01	1.50E+00	9.54E+00
5g*	9.31E-01	3.97E-01	4.05E-01	5.71E-01	2.18E+00	5.89E+00	1.99E+01
5g	1.15E+00	4.51E-01	4.28E-01	5.86E-01	2.13E+00	5.62E+00	1.85E+01

References

- [1] J. P. Desclaux *Relativistic Dirac-Fock Expectation Values for Atoms with $Z=1$ to $Z=120$* , At. Data. Nuc. Data. Tab. **12**, 311 (1973).
- [2] A.L. Ankudinov, S.I. Zabinsky and J.J. Rehr, *Single configuration Dirac-Fock atom code*, Computer Physics Comm. **98**, 359 (1996).
- [3] John J. Rehr, Joshua J. Kas, Micah P. Prange, Adam P. Sorini, Yoshinari Takimoto, Fernando Vila, *Ab initio theory and calculations of X-ray spectra*, Comptes Rendus Physique **10**, 548 (2009).
- [4] Brian G. Wybourne, *Hunds rules, jj-coupling and the g^n electron configurations*, Mol. Phys. **98**, 1243 (2000).
- [5] Jeffrey L. Tilson and Walter C. Ermler, *Massively parallel spin-orbit configuration interaction*, Theor. Chem. Acc. **133**, 1564 (2014).
- [6] Berkhard Fricke, *Superheavy Elements: A Prediction of Their Chemical and Physical Properties*, Recent Impact of Phys. Inorg. Chem. **21**, 89 (2007).
- [7] Yu. Ts. Oganessian, F. Sh. Abdullin, P. D. Bailey, D. E. Benker, M. E. Bennett, S. N. Dmitriev, J. G. Ezold, J. H. Hamilton, R. A. Henderson, M. G. Itkis, Yu. V. Lobanov, A. N. Mezentsev, K. J. Moody, S. L. Nelson, A. N. Polyakov, C. E. Porter, A. V. Ramayya, F. D. Riley, J. B. Roberto, M. A. Ryabinin, K. P. Rykaczewski, R. N. Sagaidak, D. A. Shaughnessy, I. V. Shirokovsky, M. A. Stoyer, V. G. Subbotin, R. Sudowe, A. M. Sukhov, Yu. S. Tsyganov, V. K. Utyonkov, A. A. Voinov, G. K. Vostokin, and P. A. Wilk *Synthesis of a New Element with Atomic Number $Z = 117$* , Phys. Rev. Lett. **104**, 142502 (2010).
- [8] Pekka Pyykko, *A suggested periodic table up to $Z \leq 172$, based on DiracFock calculations on atoms and ions*, Phys. Chem. Chem. Phys. **13**, 161 (2011).
- [9] L. Visscher and K.G. Dyall *Dirac-Fock atomic electronic structure calculations using different nuclear charge distributions*, Atom. Data Nucl. Data Tabl. **67**, 207 (1997).
- [10] G. F. Bertsch, B. Sabbey, and M. Uusnakki, *Fitting theories of nuclear binding energies*, Phys. Rev. C **71**, 054311 (2005).
- [11] W. C. Ermler and J. L. Tilson, *Generally contracted valence-core/valence basis sets for use with relativistic effective core potentials and spin-orbit coupling operators*, Comp. Theor. Them. **24**, 1002 (2012).
- [12] B. Fricke, W. Greiner and J.T. Waber, *Continuation of Periodic Table up to $Z[172]$ - Chemistry of Superheavy Elements*, Theor. Chim. Acta **21** 235260 (1973).
- [13] Jeffrey L. Tilson, Conrad Naleway, Michael Seth, Ron Shepard, Albert F. Wagner, and Walter C. Ermler, *An ab initio study of the ff spectroscopy of americium +3*, J. Chem. Phys. **116**, 5494 (2002).
- [14] Conrad Naleway, Michael Seth, Ron Shepard, Albert F. Wagner, Jeffrey L. Tilson, Walter C. Ermler, and Scott R. Brozell, *An ab initio study of the ionization potentials and ff spectroscopy of europium atoms and ions*, J. Chem. Phys. **116**, 5481 (2002).
- [15] C. S. Nash and B. E. Bursten, *Spin-orbit effects on the electronic structure of heavy and super-heavy halides: Prediction of an anomalously strong bond in $H[117]$* , J. Phys. Chem. A **103**, 164 (1999).