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Abstract

How to use recent symbolic programming language as $\textit{Mathematica}$\textsuperscript{\textregistered} to build good quality programmes that yield valuable data in a short computation time. It is shown how to build good wave functions for any couple of states (both having proper quantum defects) $a \equiv n_a l_a$ and $b \equiv n_b l_b$ for a transition $a \rightarrow b$. The correct normalization of these wave functions $|n_a l_a\rangle$ and $|n_b l_b\rangle$ once obtained, enables the production of atomic useful data: such as line strengths, or average quantities as $\langle a | \rho^\alpha | a \rangle$, $\langle b | \rho^\alpha | b \rangle$ and $\langle a | \rho^\alpha b \rangle$ with $\alpha$ values $\{-2,-1,0,1,2\}$.

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1First author footnote.
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1. Introduction

It is well known that structures of Alkaline atoms exist with the so-called optical electron. This electron is to be understood as suffering the polarization potential. (see M. Seaton (1958) [3] for theory and Theodosiou & al 1999 [6] for astrophysical interest):

$$V_p(r) = \frac{1}{2} \alpha \langle \frac{1}{r^2} \rangle$$

$$\alpha$$ being the static dipolar polarizability, whose existence gives rise to quantum defects that modify the coulombic wave function.

Aspect of the calculation

1.1. Using symbolic Mathematica

The purpose is to take into account the structure effect in alkaline atoms and related ion ions due to the polarization potential. Including this potential (same sign as to the Coulomb potential,) it can be taken into account as a modification to the quantum number \(|n, l, m>\) of the coulombic wave functions: giving a new set of observables: \(|n_s, l_s, m_s>\). These formulae are valid for Coulomb interaction for kets \(|n, l, m>\) with principal quantum number, \(l\) momentum number, and \(m\) the azimuthal number.

$$n \geq 1$$

$$0 \leq l \leq n - 1$$

$$-l \leq m \leq l$$

(2)

For what follows we shall use the Mathematica function

\(SphericalHarmonicY[l, m, \theta, \phi]\) that is extended to non integer quantum numbers.

That is:

$$Y^*_l^m(\theta, \phi) = (-1)^m Y_{l-m}(\theta, \phi)$$

(3)

For consistency with the the structural modification of \(|n, l, m>\) coulombic states with as usual \(|l, m> = Y_l(\theta, \phi)\) states we need to define a restriction of the basic ket \(|n_s, l_s, m_s>\)

\(|nlm> \rightarrow |n_s, l_s, m_s>\)

$$n_s = n - \delta_l$$

$$l_s = l - \delta_l$$

$$-l_s \leq m_s \leq l_s$$

1.2. isolated line problem

Two points of view:

If two experimental lines (transition \(a \rightarrow b\) and transition \(i \rightarrow f\)) let us say of MgI exist and imply the same angular momentum change and are reported in \(cm^{-1}\) or Å.
This becomes a simple system of two linear equations: two identified levels, can be solved (in a symbolic way Mathematica instruction Solve[]) to give experimental quantum defects:

Explicitly: for MgI \(3s \rightarrow 3p\) and MgI \(3s \rightarrow 4p\) with \(Z=1\).

\[
\Delta E_{3s3p} = 0.159715 au \\
\Delta E_{3s4p} = 0.224959 au
\]

\[
myapp = \text{Solve}[[Z^2 \times 0.5 \times (\frac{1}{(3-\delta_s)^2} - \frac{1}{(3-\delta_p)^2})] == 0.159715 \\
0.5 \times Z^2 \times Z \times (\frac{1}{(3-\delta_s)^2} - \frac{1}{(4-\delta_p)^2})] == 0.2249599; \{\delta_s, \delta_p\}]
\]

Two distinct energy levels for two different quantum defects.

\[
\delta_s \rightarrow 0.950211, \delta_s \rightarrow 4.33938, \delta_p \rightarrow 0.95211 \\
\delta_s \rightarrow 1.66062, \delta_p \rightarrow 3.49592, \delta_s \rightarrow 3.47752 \\
\delta_s \rightarrow 3.49592, \delta_s \rightarrow 2.52248, \delta_p \rightarrow 4.77693 - 2.09315 \times I \\
\delta_s \rightarrow 1.28434 + 0.360287 \times I, \delta_p \rightarrow 4.77693 + 2.09315 \times I \\
\delta_s \rightarrow 1.28434 - 0.360287 \times I, \delta_p \rightarrow 4.77693 - 2.09315 \times I \\
\delta_s \rightarrow 4.71566 - 0.360287 \times I, \delta_p \rightarrow 4.77693 + 2.09315 \times I, \\
\delta_s \rightarrow 4.71566 + 0.360287 \times I
\]

Two distinct energy levels are to be given to obtain two different quantum defects here \(\delta_s\) and \(\delta_p\). After inspection of the output one keeps from the list: \(\delta_s \approx 1.660\) and \(\delta_p \approx 0.9502\). Conversely another way is to use the quantum defect theory to give calculate the perturbed energy levels (non hydrogenic behavior). When the polarization potential is used, then the energy levels are obtained:

\[
\Delta E_{n,m_n} = 0.5 \times Z^2 \times (\frac{1}{(n-\delta_s)^2} - \frac{1}{(m-\delta_p)^2})
\]

Finally the energy interval \(\Delta E_{n,m_n}\) is:

\[
\Delta E_{n_n} = 0.5 \times Z^2 \times (\frac{1}{(n-\delta_s)^2}) \\
\Delta E_{m_m} = 0.5 \times Z^2 \times (\frac{1}{(m-\delta_p)^2}) \\
\Delta E_{n,m_n} = E_{n_n} - E_{m_m} \\
= 0.5 \times Z^2 \times (\frac{1}{(n-\delta_s)^2} - \frac{1}{(m-\delta_p)^2})
\]
1.3. Atomic quantum defects used as input quantities.

We will simply represent a term or an identified transition as: It is very easy (in fact easier that any calculations before the existence of symbolic software) to build \((a \equiv n_a l_a)\) down level wave function \(w_a(r)\) and a wave function \(w_b(r)\) for \((b \equiv n_b l_b)\) upper level \(w_a(r)\) and \(w_b(r)\) normalized as the following:

\[
\text{Norm}_a = \int_0^\infty |w_a(r)|^2 r^2 dr \quad w_a(r) = \frac{w_a(r)}{\sqrt{\text{Norm}_a}}
\]

\[
\text{Norm}_b = \int_0^\infty |w_b(r)|^2 r^2 dr \quad w_b(r) = \frac{w_b(r)}{\sqrt{\text{Norm}_b}}
\]

Once the quantum defects are defined (theoretical or experimental) it is easy to use the symbolic software to calculate relevant integrals \(S_{ab} = |<a|r|b>|^2\) giving quantities such oscillator line strengths, or Einstein coefficients \(A_{ab}\) and to produce a lot of data, that are in excellent agreement, with former calculations.

Making this substitution:

\[
n \rightarrow n_\star = n - \delta_n
\]

\[
l \rightarrow l_\star = l - \delta_l
\]

The radial part \(R_{n_\star l_\star}(r)\) of the wave function is given by the following formula:

\[
|n_\star l_\star m_\star \rangle = w_a(r) \times Y_{l_\star m_\star}(\Theta, \Phi)
\]

\[
w_a(r) = R_{n_\star l_\star}(r) = \frac{1}{\sqrt{\Gamma(n_\star + l_\star + 1) \Gamma(n_\star - l_\star)}} \frac{1}{2^{0.5}} \times \exp\left(-\frac{R}{\alpha_r}\right) \times \left(\frac{\beta_r}{\alpha_r}\right)^l
\]

\[
\times \text{LaguerreL}(n_\star - l_\star - 1, 2l_\star + 1, \frac{\beta_r}{\alpha_r})
\]

\[
\times |n_\star l_\star m_\star \rangle = \text{Norm}
\]

It is very important to have the normalization carefully performed, it has the radial part, with some non integer parameters \((n_a l_a)\). It is proved that the Mathematica function LaguerreL[a,b,x] can be extended to non integer arguments. The same applies to the spherical harmonics Mathematica function SphericalHarmonicY[l,m,\Theta,\Phi]. I need that the norm \(<n_\star l_\star m_\star |n_\star l_\star m_\star \rangle = \text{Norm} \times \text{NormAng} \) exists.

\[
\text{NormAng} = \int_0^{2\pi} d\Phi \int_0^\pi |Y_{l_\star m_\star}(\Theta, \Phi)|^2 \sin(\Theta) d\Theta
\]
\[ \text{Norm} = \int_0^\infty r^2 |wa(r)|^2 \, dr \] (15)

With the norm calculated further calculations the averaged quantities:

\[ I_{nlm}^\alpha = < n_{nlm} | r^\alpha | n_{nlm} > \] (16)

With the normalized ket \( |n_{nlm} >^N = \frac{|n_{nlm} >}{\sqrt{\text{Norm} \times \text{Norm}^\alpha}} \) In fact we are dealing with the restriction to this quantity to give: It is well known that for hydrogen and hydrogenic ions, average values of operators \( < nlm | r^\alpha | nlm > \) being the Bohr radius, \( Z = 1 \) for hydrogen \( \alpha \equiv \{-2, -1, 0, 1, 2\} \).

\[ a = \frac{a_0}{Z} \]
\[ < nlm | r^2 | nlm >= \frac{n^2 \times (5n^2 + 1 - 3l(l + 1))}{2} \]
\[ < nlm | r | nlm >= \frac{2n^2}{2l + 1} \]
\[ < nlm | \frac{1}{r} | nlm >= \frac{2n^2}{2l + 1} \]
\[ < nlm | 1 < \infty r^2 > nlm = \frac{2n^2}{(2l + 1) \alpha} \] (17)

Now we have to take advantage from a more recent way to deal with the task of evaluating the Bates & Damgaard integral [1].

It has been shown by Kostelecky & al that a Supersymmetry transformation [7], exits and enables a gratifying simplification of the evaluation of the integrals relevant to the oscillator strengths for alkaline structures or ions of heavier elements. That is:

\[ l_\ast = l - \delta_l + I(l) \]
\[ I(l) = \{0, 1, 2\} \] (18)

Depending on the quantum defect \( \delta_l \) the higher is \( \delta_l \) the higher is the parameter \( I(l) \), \( I(l) \) can not be negative.

Another interesting development of these symbolic programmes notebooks using Mathematica, is to use these good wave functions to get a clear and good insight on physical grandeurs such as the average radii of most ions through He to Fe when databases as TopBase [9] provide the quantum defects of these ions. For instance, using data from TopBase one has access to the different quantum numbers with their defects existing for Fe. Here the author wants to show how screening for these structures atoms can be explained through simple considerations:

Defining the suitable modified ket for atoms with known quantum defects:

\[ |n_{nlm} > = \frac{wa(r)}{\text{Norm}} \times Y_{l,m_s} (\theta, \phi) \]
\[ n_s = n - \delta_l \]
\[ l_\ast = l - \delta_l \] (19)

Once quantum defects are defined, it is possible to modify the average operators \( < ar^\alpha | a > \) values, whose expressions are shown in [6]. Using the above transformation that is:
\[ a = \frac{a_0}{Z} \]

\[
< n_l m_s | n_l m_s > = \text{Norm} \\
< n_l m_s | r^2 | n_l m_s > = n^2 \times \frac{2}{Z^2} (5n^2 + 1 - 3l(l+1)) \\
< n_l m_s | r | n_l m_s > = \frac{a_0}{Z^2} (3n^2 - l(l+1)) \\
< n_l m_s | \frac{1}{r} | n_l m_s > = \frac{2}{Z^2} \\
< n_l m_s | \frac{1}{r^2} | n_l m_s > = \frac{2}{Z^2} \frac{2}{l(l+1))} 
\]

These formulae produced with the \( < r^\alpha > \) extension of the hydrogenic values are shown to be in very good accordance, with the data produced with the numerical integration of LaguerreL polynomial extension, if a careful normalization on radial variable \( r \) is done, and \( \theta, \phi \) angular variables.

In fact \textit{Mathematica} function \( \text{LaguerreL}[a,b,x] \) \cite{9} can be extended to non integer arguments, while usual \textit{Mathematica} function \( \text{SphericalHarmonicY}[l,m,\theta,\phi] \) are changed by the transformation:

function \( \text{SphericalHarmonicY}[l,m,\theta,\phi] \rightarrow \text{SphericalHarmonicY}[l*,m*,\theta,\phi] \).

On the final integration of the angles : we perform the following angular average on \( (\theta,\phi) \) variables:

\[
|i| \equiv |n_{ls}| \\
|f| \equiv |n_{ls}| \\
|<i|cos(\theta)|f>|^2 = \left| \sum_{M=-m_s}^{m_s} \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\phi Y_{ls,m_s} Y_{l'M,m'_{ls}} \right|^2 \\
M = -(m_{ls} + m_{ls})
\]

About an extension of the average values of the diagonal operators existing for H and hydrogen ions to the atomic radii of atomic elements from He to Na elements. This extension will be hereafter written as:

with for each element heavier than H:

here is to be understood as the quantum defect QD of the particular atom or ion of the non hydrogen species. It is well known that the \( \delta \) are tabulated in a textbook such as: \textit{Mechanics of the Atom} by Max Born \cite{5}.

Another interesting development of these symbolic programmes notebooks in \textit{Mathematica}, is to use these good wave functions to get a clear and good insight on physical grandeurs such as the average radii of most ions through He to Fe when databases as TopBase provide the quantum defects on these ions. For instance, using data from TopBase one has access to the different quantum numbers with their defects existing for \( ^{16}O_{8} \), and \( ^{24}Mg_{12} \), neutral elements and their ionized species.

Here the author wants to show how screening for these structures atoms can be explained through simple considerations:
| $^6\text{Li}_3$ | Ionization Number $Z_i$ | $\delta_s$ | $\delta_p$ |
|---------|---------------------|--------|--------|
|         | 3                   | 0.3995 | 0.0438 |
|         | 2                   | 0.181  | 0.053  |
|         | 1                   | 0.0071 | −0.045 |

Table A: Here Quantum defects $\delta_s$ and $\delta_p$ are given for neutral Lithium and its ionized species.
Table B: Here Quantum defects $\delta_s$ and $\delta_p$ are given for neutral Oxygen and its ionized species.

| $^{16}\text{O}_8$ | Ionization Number $Z_i$ | $\delta_s$ | $\delta_p$ |
|------------------|------------------------|----------|----------|
| 8                | 1.141                  | 0.591    |          |
| 7                | 0.861                  | 0.564    |          |
| 6                | 0.539                  | 0.311    |          |
| 5                | 0.431                  | 0.121    |          |
| 4                | 0.227                  | 0.008    |          |
| 3                | 0.111                  | 0.002    |          |
| 2                | 0.307                  | −0.007$^3$|          |
| 1                | 0.0                    | 0.0      |          |
Table C: Here Quantum defects $\delta_s$ and $\delta_p$ are given for neutral Sodium Na and its ionized species.

| Ionization Number $Z_i$ | $\delta_s$ | $\delta_p$ |
|--------------------------|------------|------------|
| 11                       | 1.342      | 0.852      |
| 10                       | 0.989      | 0.5180     |
| 9                        | 0.812      | 0.498      |
| 8                        | 0.653      | 0.372      |
| 7                        | 0.415      | 0.289      |
| 6                        | 0.325      | 0.211      |
| 5                        | 0.283      | 0.087      |
| 4                        | 0.153      | $-0.012^3$ |
| 3                        | 0.078      | 0.021      |
| 2                        | 0.014      | $-0.005^3$ |
| 1                        | 0.000      | 0.000      |
2.2. Building wave function \( w_a(r) \) using Topbase quantum defect tables.

\[
\begin{array}{|c|c|c|c|}
\hline
\text{\(^{24}M_{G12}\)} & \text{Ionization Number } Z_j & \delta_s & \delta_p \\
\hline
12 & 1.544 & 0.982 \\
11 & 1.069 & 0.700 \\
10 & 0.829 & 0.417 \\
9 & 0.696 & 0.696 \\
8 & 0.517 & 0.426 \\
7 & 0.438 & 0.368 \\
6 & 0.307 & 0.233 \\
5 & 0.225 & 0.154 \\
4 & 0.138 & 0.071 \\
3 & 0.071 & 0.015 \\
2 & 0.071 & -0.004 \\
1 & 0 & 0 \\
\hline
\end{array}
\]

Table D: Here Quantum defects \( \delta_s \) and \( \delta_p \) are given for Mg and ions.

3. Summary

It is seen from the Tables: (two distincts for S states quantum defects \( \delta_s \)) and (two for P states quantum defects \( \delta_p \)), that for low states \((n \leq 4)\), with high \(\delta_s\), there is a breakdown of the extended Messiah quantities \(I_{n,s}^{\alpha}\), these giving non-physical results such as negative numbers for \(< r^{\alpha} >\) powers, while the wave function approach <
\(n_s l_s m_s^N|^{r^\alpha} n_s l_s m_s^N\) still gives plausible results. However the production of a properly normalized wave function such as \(w_a(r) = |\Psi_a(r, \theta, \phi)\rangle\) with \(a \equiv n_s l_s\) and the norm \(\text{Norm} = \int_0^\infty |\Psi_a(r, \theta, \phi)|^2 r^2 dr Sin(\theta) d\theta d\phi\) has to be carefully calculated. It is obvious that there is basic case of failure of the ket building \(|w_a(r) \times Y_{l m_s}(\theta, \phi)\rangle\) method when the calculation implies low \(n\) states with an high \(\delta\), that is a situation for which \(n_s \leq 1\). For high states \(n_s = n - \delta_l\) with \(n \geq 4\) and \(\delta_l \leq 1\) the two approaches merge and give the same results for all powers of \(<r^\alpha>\). As a matter of fact, others \(\alpha\) powers such as \(\alpha \equiv \{-6, -5, -4, -3, 3, 4, 5, 6\}\) are accessible.
4. Oscillator strengths for MgII $3s \rightarrow 3p$ and $3s \rightarrow 4p$.

It is well known that the Magnesium MgII element (one fold ionized) exists in most stars, it is very well studied through two transitions: $3s \rightarrow 3p$ and $3s \rightarrow 4p$. The number of protons is $N_p = 12$ the number of electrons is $N_e = 11$.

To illustrate the capability of these wave functions we compare our results with existing data
1) the NBS Atomic Transition Probabilities Sodium through Calcium (1969) [12]
2) The interesting paper from C.E. Theodosiou & S.R. Federman [10]
3) New data on line on NIST database (2005) [11]
4) New data from TopBase (1999) [9]

This conjecture can be proved as follows: It is a recent advantage to use Symbolic language as Mathematica, to perform the plain recovering radial integral: where Norm has to be evaluated independently to insure the correctness of the symbolic evaluation.

It is there the point to be fixed: how to build a wave function that contains the quantum defect appropriate to each species, and to register it. It is there necessary to recall the first significant work and universally reckoned in the matter of elements heavier than H (such as HeI and NaI or OII) D. Bates & A. Damgaard [1] with their $W_n^*l^*+$1/2(r)

These functions could be summed and their products converge and are proportional to the oscillator strengths as:

$$S_{if} = S(M)S(L)\left| \int_0^\infty R_i R_f r dr \right|^2 \over (4l^2 - 1) \tag{22}$$

In fact we are dealing with the restriction to this quantity to give:

$$R_i = R_f$$

$$<i|ri> = \int_0^\infty R^*_i R_f r dr \tag{23}$$

The quantity is $R_{if} = <i|ri>$ is now is the ionic radius when $|i> = |n_alasl>$, when data such as $\delta_l$ and $Z_i = N_Z - Z_E$ being the charge of the considered ion.

Now we have to take advantages from a more recent way to deal with the task of evaluating the Bates & Damgaard integral [1] our $wa(r)$ is to be identified with $R_{n_i}(r) = wa(r) \times r$ in their fundamental paper.

$$wa(r) = \frac{1}{n^2} \sqrt{\frac{\beta^3}{2\Gamma(n_a + l_a + 1)\Gamma(n - l)}} \times$$

$$\exp(-\frac{\beta r}{2n_a}, l_a + \frac{\beta r}{n_a} \times \text{LaguerreL}[n - l - 1, 2l + 1, \frac{\beta r}{n_a}]) \tag{24}$$

$$\text{LaguerreL}[n - l - 1, 2l + 1, \frac{\beta r}{n_a}]$$ is a function in the Mathematica that is: LaguerreL[a,b,x], that is conform with the generating function:

$$L_n^a = \sum_{s=0}^p (-1)^s \frac{(a + n)!}{(n - s)! (a + s)! s!} x^s \tag{26}$$
It is very important to perform with attention the calculation of the normalization integral, once \( n_*, l_* \) are defined:

\[
\text{Norm} = \int_0^\infty |w_a(r)|^2 r^2 dr
\]

It is very rewarding to use the Mathematica \texttt{NIntegrate}[\texttt{f[x], x, 0, }\infty] with:

\[
f_{\text{test}}(r, \alpha) = |w_a(r)|^2 \times \frac{r^2}{\text{Norm}} \times r^\alpha.
\]

\texttt{NIntegrate}[\texttt{f_{\text{test}}[r, \alpha], \{r, 0, }\infty\}] gives all quantities useful to shapes or spatial extension of atoms and ionic species existing when \( Z \) is given.

\[
< n_*, l_* | r | n_*, l_* > = \int_0^\infty |w_a(r)|^2 \times \text{Norm} \times r^\alpha dr
\]

At this stage, the oscillator strengths can be obtained using three different operators namely \( \vec{R} \) dipolar term, \( \vec{V} \) velocity operator, \( \vec{\gamma} \) giving in theory the same numbers when evaluating:

\[
S_{ij} = | \langle i | r | f \rangle |^2.
\]

In fact, it has never been verified that the following three operators, giving the same on theory until our days.

\[
g_{f12} = 2 \times \Delta E_{12} \left| \int d\Omega \int_0^\infty w_1(\vec{r}).r.w_2(\vec{r}).r^2 dr \right|^2
\]

\[
g_{f12} = \frac{2}{\Delta E_{12}} \left| \int d\Omega \int_0^\infty w_1(\vec{r}).\left( \frac{1}{r} + \frac{d}{dr} \right).w_2(\vec{r}).r^2 dr \right|^2
\]

\[
g_{f12} = \frac{2}{\Delta E_{12}} \left| Z \int d\Omega \int_0^\infty w_1(\vec{r}).w_2(\vec{r}).r^2 dr \right|^2
\]

It is very interesting to verify that the applying Mathematica Command (Messiah M´ecanique Quantique) \[12\] with the wave function \( w_a(r) \) hereafter described, it is necessary to perform the calculation of the norm.

Table E: Oscillator strengths for singly ionized Mg : MgII 3\( s \to 3p \).

| \( \text{MgII} 3s \to 3p \) | \( \lambda_{ik}(\text{Å}) \) | \( f_{ik}^a \) | \( f_{ik}^b \) | \( f_{ik}^c \) | \( f_{ik}^d \) | \( f_{ik}^e \) |
|----------------|----------------|-------------|-------------|-------------|-------------|-------------|
| \( \frac{1}{2} \to \frac{1}{2} \) | 2798.0 | 0.940 \( B^+ \) | 0.909 \( A^+ \) | 0.901 \( A^+ \) | 0.901 | 0.8543 |
| \( \frac{1}{2} \to \frac{3}{2} \) | \( R = 2.00 \) | 0.940 | 0.909 | 0.901 \( A^+ \) | 0.901 | 0.8543 |

\( a \) NBS National Bureau of Standards \[12\] (1966)

\[2 R \neq 2 \text{ that is } R = 1.78 \text{ failure of the rule for degenerated lines.} \]

That is failure of the simple rule for intensity ratio of \( R = \frac{\lambda_{1/2} - \lambda_{3/2}}{\lambda_{1/2}} = \frac{2}{\lambda_{1/2}} \).
Table F: Oscillator strengths for singly ionized Mg: MgII 3s → 4p.

| MgII 3s → 4p | $\lambda_{ik}(\text{Å})$ | $f_{ik}^a$ | $f_{ik}^b$ | $f_{ik}^c$ | $f_{ik}^d$ | $f_{ik}^e$ |
|--------------|----------------|-----------|-----------|-----------|-----------|-----------|
|              | NBS | NBS | NIST | Theodosiou | TopBase | de Kertanguy |
| $\frac{1}{2} \rightarrow \frac{1}{2}$ | 1240.1 | 0.23 $10^{-4}$ | 9.72 $10^{-4}$ | 9.88 $10^{-4}$ | 10.98 $10^{-4}$ | 0.00319 |
| $\frac{1}{2} \rightarrow \frac{3}{2}$ | $R = 1.78^2$ | 0.23 $10^{-4}$ | 9.72 $10^{-4}$ | 9.88 $10^{-4}$ | 10.98 $10^{-4}$ | 0.00319 |

$^b$ NIST former NBS [13]
$^c$ Theodosiou C.E. & al [4] [10]
$^d$ Topbase on line results [9] 1999
$^e$ de Kertanguy A. 2012 Mathematica notebook
5. Explanation of tables

Table A is made with Topbase data, the resulting output are quantum defects $\delta_s$ and $\delta_p$, for Lithium and Table B concerns the Oxygen element O, with all its ionization stages. Table C and Table D gives quantum defects $\delta_s$ and $\delta_p$ for Sodium Na element and Magnesium Mg element. Table E gives different estimates for the fundamental quantities : line strength factors for MgII $3s \rightarrow 3p$ and the same quantities in Table F, MgII transition $3s \rightarrow 4p$. These estimates give two Tables 1 & 2 results, the first calculation is performed (giving Table 1) with the wave functions $w_\alpha(r)$, that is to evaluate $l_{\alpha n l}^N$ and give a very good agreement when the same theoretical $\delta_s$ values are used in both calculations. Table 3 and 4 show results for the $\alpha$ powers of the r radial operator with another momentum $l=1$ value related to quantum defect $\delta_s$. For p states one requires $l=1$ and the existence of $\delta_p$, substituting $n \rightarrow n_\delta = n - \delta_p$ and $l \rightarrow l_\delta = 1 - \delta_p$. These estimates give 2 more Tables 3 & 4 results, with the wave functions $w_\alpha(r)$, that is to evaluate $l_{\alpha n l}^N$ and changing the value of give a very good agreement when the same theoretical $\delta_p$ values are used in both calculations. As done in upper tables two methods are used: first to calculate $<n,l,m_N^l | \alpha^* | n,l,m_N^l>$ & $\alpha$ values $\{-2,-1,0,1,2\}$, (Table 3) and second gives the Messiah formulae using the upward replacement (Table 4). Table 4 contains the extrapolated results obtained by using the analytic results for hydrogenic ions.

5.1. $<n,l,m_N^l | \alpha^* | n,l,m_N^l>$ expectation values $\delta_s$ -values from Topbase.

It contains $<r^\alpha>$ predictions for the $\alpha \equiv \{-2,-1,0,1,2\}$, when $\alpha = 0$, the average operator is just the norm of the wave function.

It is clear that there are no wave solutions when : $n_\delta < 1$, there is a breakdown of the theory of the quantum defect. This remark leads to the definition of the range of application of the full relativistic theory, when the corrected wave function $W_{n,l \frac{l}{2}}$ does not exist anymore.

Table 1: $<r^\alpha>$ values using Topbase l=0 $\delta_s$ values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| $^4$Z | M | Ze | n | $\delta_s$ | $<\frac{1}{r^2}>$ | $<\frac{1}{r}>$ | N | $<r>$ | $<r^2>$ |
|-------|---|----|---|---------|----------------|----------------|---|------|------|
| Li    | average Operators | $\delta_s$ |    |          |                |                |    |      |      |
| $^{63}$ | 3  | 2  | 0.399 | 2.5591 | 0.3925 | 1 | 3.9416 | 18.418 |
| $^{63}$ | 3  | 3  | id   | 0.5947 | 0.1483 | 1 | 10.230 | 119.36 |
| $^{63}$ | 3  | 4  | id   | 0.2237 | 0.0777 | 1 | 19.518 | 429.22 |
| $^{63}$ | 3  | 5  | id   | 0.1071 | 0.0473 | 1 | 31.806 | 1133.7 |
| $^{63}$ | 3  | 6  | id   | 0.0593 | 0.0319 | 1 | 47.094 | 2478.7 |
| $^{63}$ | 3  | 7  | id   | 0.0362 | 0.0229 | 1 | 65.383 | 4769.9 |

Table 1 Continued...
Table 1: $\langle r^\alpha \rangle$ values using Topbase $l=0$ $\delta_s$ values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| $^A_Z$M | $Z_e$ | $n$ | $\delta_s$ | $\langle \frac{1}{r^2} \rangle$ | $\langle \frac{1}{r} \rangle$ | $N$ | $<r>$ | $<r^2>$ |
|---|---|---|---|---|---|---|---|---|
| $^{63}$ | 2 | 2 | 0.181 | 1.3101 | 0.5387 | 1 | 2.8014 | 9.1731 |
| $^{63}$ | 2 | 3 | $id$ | 0.3738 | 0.2334 | 1 | 6.4411 | 47.151 |
| $^{63}$ | 2 | 4 | $id$ | 0.1547 | 0.1297 | 1 | 11.581 | 150.92 |
| $^{63}$ | 2 | 5 | $id$ | 0.0783 | 0.0823 | 1 | 18.221 | 371.90 |
| $^{63}$ | 2 | 6 | $id$ | 0.0450 | 0.0569 | 1 | 26.362 | 776.47 |
| $^{63}$ | 2 | 7 | $id$ | 0.0281 | 0.0416 | 1 | 36.002 | 1446.0 |
| $^O$ average Operators | | | | | | | | |
| $^{168}$ | 8 | 2 | 1.141 | 0.4335 | 0.2893 | 1 | 5.2443 | 32.213 |
| $^{168}$ | 8 | 3 | $id$ | 0.1191 | 0.1223 | 1 | 12.321 | 172.60 |
| $^{168}$ | 8 | 4 | $id$ | 0.0484 | 0.0671 | 1 | 22.398 | 564.57 |
| $^{168}$ | 8 | 5 | $id$ | 0.0242 | 0.0423 | 1 | 35.475 | 1409.6 |
| $^{168}$ | 8 | 6 | $id$ | 0.0138 | 0.0291 | 1 | 51.552 | 2969.4 |
| $^{168}$ | 8 | 7 | $id$ | 0.0086 | 0.0212 | 1 | 70.629 | 2963.4 |
| $^{168}$ | 7 | 2 | 0.861 | 0.5469 | 0.4157 | 1 | 7.5890 | 65.373 |
| $^{168}$ | 7 | 3 | $id$ | 0.2464 | 0.2570 | 1 | 5.7363 | 37.326 |
| $^{168}$ | 7 | 4 | $id$ | 0.0114 | 0.1538 | 1 | 9.6523 | 104.80 |
| $^{168}$ | 7 | 5 | $id$ | 0.0618 | 0.1022 | 1 | 14.568 | 237.75 |
| $^{168}$ | 7 | 6 | $id$ | 0.0372 | 0.0728 | 1 | 20.484 | 468.95 |
| $^{168}$ | 7 | 7 | $id$ | 0.0240 | 0.0545 | 1 | 27.404 | 837.84 |
| $^{168}$ | 6 | 2 | 0.539 | 0.6967 | 0.5139 | 1 | 2.8200 | 9.2150 |
| $^{168}$ | 6 | 3 | $id$ | 0.2464 | 0.2570 | 1 | 5.7365 | 37.326 |
| $^{168}$ | 6 | 4 | $id$ | 0.1140 | 0.1538 | 1 | 5.736 | 37.326 |
| $^{168}$ | 6 | 5 | $id$ | 0.0696 | 0.1022 | 1 | 14.568 | 237.58 |
| $^{168}$ | 6 | 6 | $id$ | 0.0372 | 0.0720 | 1 | 20.484 | 468.95 |
| $^{168}$ | 6 | 7 | $id$ | 0.0240 | 0.0545 | 1 | 27.404 | 837.84 |
| $^{168}$ | 5 | 2 | 0.431 | 16.439 | 1.5907 | 1 | 0.9605 | 1.0890 |
| $^{168}$ | 5 | 3 | $id$ | 13.676 | 0.6060 | 1 | 2.5055 | 7.1630 |
| $^{168}$ | 5 | 4 | $id$ | 5.1000 | 0.3140 | 1 | 4.8079 | 26.042 |
| $^{168}$ | 5 | 5 | $id$ | 2.4311 | 0.1916 | 1 | 7.8590 | 69.225 |
| $^{168}$ | 5 | 6 | $id$ | 1.3420 | 0.1289 | 1 | 11.680 | 151.97 |

Table 1 Continued...
Table 1: \( <r^\alpha> \) values using Topbase l=0 \( \delta_s \) values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| \( M \) | \( Z_e \) | \( n \) | \( \delta_s \) | \( <\frac{1}{r^2}> \) | \( <\frac{1}{r}> \) | \( N \) | \( <r> \) | \( <r^2> \) |
|------|------|------|---------|---------|---------|------|------|--------|
| 168  | 5    | 7    | id      | 0.8180  | 0.0926  | 1    | 16.212| 293.29 |
| 168  | 4    | 2    | 0.227   | 16.439  | 1.5900  | 1    | 0.9605| 1.0830 |
| 168  | 4    | 3    | id      | 4.2960  | 0.6505  | 1    | 2.3242| 6.1460 |
| 168  | 4    | 4    | id      | 1.7050  | 0.3512  | 1    | 4.2870| 20.697 |
| 168  | 4    | 5    | id      | 0.8425  | 0.2194  | 1    | 6.8517| 52.591 |
| 168  | 4    | 6    | id      | 0.4761  | 0.1500  | 1    | 10.010| 112.08 |
| 168  | 4    | 7    | id      | 0.2948  | 0.1089  | 1    | 13.779| 157.192|
| 168  | 3    | 2    | 0.111   | 13.775  | 1.6828  | 1    | 0.8996| 0.9470 |
| 168  | 3    | 3    | id      | 3.8490  | 0.7192  | 1    | 2.0937| 4.9825 |
| 168  | 3    | 4    | id      | 1.5776  | 0.3968  | 1    | 3.7878| 16.144 |
| 168  | 3    | 5    | id      | 0.7939  | 0.2511  | 1    | 5.9819| 40.079 |
| 168  | 3    | 6    | id      | 0.4542  | 0.1730  | 1    | 8.6760| 84.102 |
| 168  | 3    | 7    | id      | 0.2837  | 0.1264  | 1    | 11.870| 157.19 |
| 168  | 2    | 2    | 0.020   | 13.189  | 1.7870  | 1    | 0.8408| 0.8252 |
| 168  | 2    | 3    | id      | 3.8672  | 0.7886  | 1    | 1.9033| 4.1152 |
| 168  | 2    | 4    | id      | 1.6220  | 0.4420  | 1    | 3.9444| 12.926 |
| 168  | 2    | 5    | id      | 0.8283  | 0.2823  | 1    | 5.3140| 31.628 |
| 168  | 2    | 6    | id      | 0.4783  | 0.1958  | 1    | 7.6620| 65.596 |
| 168  | 2    | 7    | id      | 0.3008  | 0.1437  | 1    | 10.439| 121.57 |

| \( Na \) average Operators | \(\delta_s\) |
|-----------------------------|-------------|
| 2211 11                     | 2           | 1.34       | 1.3886   | 0.3637  | 1       | 4.2359  | 21.194  |
| 2211 11                     | 3           | id         | 0.3370   | 0.1415  | 1       | 10.710  | 130.70  |
| 2211 11                     | 4           | id         | 0.1293   | 0.0747  | 1       | 20.184  | 458.83  |
| 2211 11                     | 5           | id         | 0.0620   | 0.0460  | 1       | 32.658  | 1195.0  |
| 2211 11                     | 6           | id         | 0.0349   | 0.0312  | 1       | 48.132  | 2588.8  |
| 2211 11                     | 7           | id         | 0.0214   | 0.0225  | 1       | 66.606  | 4949.7  |
| 2211 10                     | 2           | 0.989      | 0.9654   | 0.4949  | 1       | 3.0270  | 10.693  |
| 2211 10                     | 3           | id         | 7.8237   | 2.1281  | 1       | 0.6677  | 0.5780  |
| 2211 10                     | 4           | id         | 0.0114   | 0.1538  | 1       | 9.6523  | 104.80  |
| 2211 10                     | 5           | id         | 0.0618   | 0.1022  | 1       | 14.568  | 237.75  |

Table 1 Continued…
Table 1: $<r^\alpha>$ values using Topbase $l=0$ $\delta$, values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| $^A Z$ | $M$ | $Z_e$ | $n$ | $\delta$ | $<\frac{1}{r^2}>$ | $<\frac{1}{r}>$ | $N$ | $<r>$ | $<r^2>$ |
|-------|-----|-------|-----|--------|-----------------|-----------------|-----|-------|-------|
| $^{22}11$ | 10  | 6     | id  | 0.0372 | 0.0728          | 1               | 20.484 | 468.95 |
| $^{22}11$ | 10  | 7     | id  | 0.0240 | 0.0545          | 1               | 27.404 | 837.84 |
| $^{22}11$ | 9    | 2     | 0.812 | 1.2513 | 0.6270          | 1               | 2.3550 | 6.4460 |
| $^{22}11$ | 9    | 3     | id  | 0.4044 | 0.2953          | 1               | 5.0423 | 28.855 |
| $^{22}11$ | 9    | 4     | id  | 0.1783 | 0.1114          | 1               | 13.417 | 85.719 |
| $^{22}11$ | 9    | 5     | id  | 0.0938 | 0.19161         | 1               | 2.4311 | 151.97 |
| $^{22}11$ | 9    | 6     | id  | 0.0552 | 0.0783          | 1               | 19.104 | 201.62 |
| $^{22}11$ | 9    | 7     | id  | 0.0352 | 0.0580          | 1               | 25.791 | 742.19 |
| $^{22}11$ | 8    | 2     | 0.653 | 7.7476 | 2.2068          | 1               | 0.6214 | 0.4907 |
| $^{22}11$ | 8    | 3     | id  | 1.4630 | 0.7265          | 1               | 2.006  | 4.6667 |
| $^{22}11$ | 8    | 4     | id  | 0.5045 | 0.3572          | 1               | 4.1408 | 319.45 |
| $^{22}11$ | 8    | 5     | id  | 0.2302 | 0.2117          | 1               | 7.0255 | 55.521 |
| $^{22}11$ | 8    | 6     | id  | 0.1237 | 0.1399          | 1               | 10.660 | 127.29 |
| $^{22}11$ | 8    | 7     | id  | 0.0739 | 0.0993          | 1               | 51.552 | 2969.4 |
| $^{22}11$ | 8    | 7     | id  | 0.0086 | 0.0212          | 1               | 15.045 | 252.95 |
| $^{22}11$ | 7    | 2     | 0.495 | 0.9654 | 0.4949          | 1               | 3.0278 | 10.693 |
| $^{22}11$ | 7    | 3     | id  | 0.2875 | 0.2207          | 1               | 6.7929 | 52.408 |
| $^{22}11$ | 7    | 4     | id  | 0.1216 | 0.1243          | 1               | 12.058 | 163.57 |
| $^{22}11$ | 7    | 5     | id  | 0.0623 | 0.0796          | 1               | 18.823 | 396.83 |
| $^{22}11$ | 7    | 6     | id  | 0.0361 | 0.0553          | 1               | 27.088 | 819.84 |
| $^{22}11$ | 7    | 7     | id  | 0.0227 | 0.0406          | 1               | 36.567 | 1515.2 |
| $^{22}11$ | 6    | 2     | 0.325 | 1.7919 | 2.2101          | 1               | 0.7036 | 0.5909 |
| $^{22}11$ | 6    | 3     | id  | 3.8833 | 0.7973          | 1               | 1.9061 | 4.1514 |
| $^{22}11$ | 6    | 4     | id  | 14.171 | 0.4072          | 1               | 3.7086 | 15.506 |
| $^{22}11$ | 6    | 5     | id  | 66.731 | 0.2464          | 1               | 6.1110 | 41.865 |
| $^{22}11$ | 6    | 6     | id  | 36.567 | 0.1650          | 1               | 9.1135 | 92.839 |
| $^{22}11$ | 6    | 7     | id  | 22.161 | 0.1181          | 1               | 12.716 | 180.43 |
| $^{22}11$ | 5    | 2     | 0.283 | 43.840 | 2.1390          | 1               | 0.7195 | 0.6109 |
| $^{22}11$ | 5    | 3     | id  | 10.761 | 0.8386          | 1               | 1.8069 | 3.7194 |
| $^{22}11$ | 5    | 4     | id  | 4.1501 | 0.4443          | 1               | 3.3943 | 12.975 |

Table 1 Continued...
Table 1: $< r^\alpha >$ values using Topbase $l=0$ $\delta_s$ values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

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| $M$ | $Z_e$ | $n$ | $\delta_s$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|-----|------|----|------------|-----------------|-----------------|----|--------|--------|
| $^{22}\text{Ne}$ | 5 | 5 | id | 2.0159 | 0.2745 | 1 | 5.4817 | 33.669 |
| $^{22}\text{Ne}$ | 5 | 6 | id | 1.1269 | 0.1863 | 1 | 8.0690 | 72.759 |
| $^{22}\text{Ne}$ | 7 | id | 0.6925 | 0.1346 | 1 | 11.156 | 138.87 |
| $^{22}\text{Ne}$ | 2 | 0.380 | 44.630 | 2.3747 | 1 | 0.6461 | 0.4917 |
| $^{22}\text{Ne}$ | 3 | 4 | id | 4.3994 | 0.5066 | 1 | 2.9749 | 9.9640 |
| $^{22}\text{Ne}$ | 4 | 5 | id | 2.1526 | 0.3146 | 1 | 4.7821 | 25.621 |
| $^{22}\text{Ne}$ | 6 | id | 1.2090 | 0.2141 | 1 | 7.0170 | 55.035 |
| $^{22}\text{Ne}$ | 7 | 7 | id | 0.7454 | 0.1551 | 1 | 9.6823 | 104.59 |
| $^{22}\text{Ne}$ | 3 | 2 | 0.153 | 37.181 | 2.6404 | 1 | 0.5753 | 0.3878 |
| $^{22}\text{Ne}$ | 3 | 3 | id | 10.147 | 1.1109 | 1 | 1.3573 | 2.0949 |
| $^{22}\text{Ne}$ | 4 | 4 | id | 4.1109 | 0.6038 | 1 | 2.4727 | 9.9647 |
| $^{22}\text{Ne}$ | 5 | id | 2.0556 | 0.3832 | 1 | 3.9210 | 17.225 |
| $^{22}\text{Ne}$ | 6 | id | 1.1709 | 0.2633 | 1 | 5.7030 | 36.347 |
| $^{22}\text{Ne}$ | 7 | id | 0.7291 | 0.1920 | 1 | 7.8180 | 68.206 |
| $^{24}\text{Mg}$ | 2 | 2 | 0.078 | 13.189 | 1.7870 | 1 | 0.8408 | 0.8252 |
| $^{24}\text{Mg}$ | 3 | id | 10.147 | 1.1100 | 1 | 1.3570 | 2.0940 |
| $^{24}\text{Mg}$ | 4 | id | 4.1120 | 0.6038 | 1 | 2.4727 | 6.8813 |
| $^{24}\text{Mg}$ | 5 | id | 2.0556 | 0.3832 | 1 | 3.9215 | 17.225 |
| $^{24}\text{Mg}$ | 6 | id | 1.1709 | 0.2633 | 1 | 5.7035 | 36.347 |
| $^{24}\text{Mg}$ | 7 | id | 0.7291 | 0.1920 | 1 | 7.8189 | 68.206 |

| $Mg$ | average Operators | $\delta_s$ |
|------|------------------|------------|
| $^{24}\text{Mg}$ | 2 | 1.545 | 0.0729 | 0.1673 | 1 | 8.6510 | 86.600 |
| $^{24}\text{Mg}$ | 3 | id | 0.0253 | 0.0837 | 1 | 17.579 | 350.53 |
| $^{24}\text{Mg}$ | 4 | id | 0.0118 | 0.0503 | 1 | 29.445 | 975.38 |
| $^{24}\text{Mg}$ | 5 | id | 0.0064 | 0.0335 | 1 | 4.2359 | 21.194 |
| $^{24}\text{Mg}$ | 6 | id | 0.0038 | 0.0239 | 1 | 62.178 | 4321.0 |
| $^{24}\text{Mg}$ | 7 | id | 0.0025 | 0.0179 | 1 | 4.2359 | 21.194 |
| $^{24}\text{Mg}$ | 11 | 2 | 1.069 | 0.1110 | 0.2328 | 1 | 5.9930 | 41.400 |
| $^{24}\text{Mg}$ | 11 | 3 | id | 0.0460 | 0.1294 | 1 | 11.140 | 140.75 |

*Table 1 Continued...*
Table 1: \( \langle r^\alpha \rangle \) values using Topbase l=0 \( \delta \), values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| \( M \) | \( Z_\text{c} \) | \( n \) | \( \delta \) | \( \langle \frac{1}{r} \rangle \) | \( \langle \frac{1}{r^2} \rangle \) | \( N \) | \( \langle r \rangle \) | \( \langle r^2 \rangle \) |
|------|----|----|-------|--------|--------|----|------|--------|
| 2412 | 11 | 4  | id    | 0.0233 | 0.0822 | 1   | 17.786 | 356.15 |
| 2412 | 11 | 5  | id    | 0.0133 | 0.0568 | 1   | 25.933 | 704.06 |
| 2412 | 11 | 6  | id    | 0.0083 | 0.0416 | 1   | 35.570 | 1415.9 |
| 2412 | 11 | 7  | id    | 0.0056 | 0.0317 | 1   | 46.726 | 2438.2 |
| 2412 | 10 | 2  | 0.829 | 1.3100 | 0.6366 | 1   | 2.3220 | 6.2720 |
| 2412 | 10 | 3  | id    | 0.4204 | 0.2984 | 1   | 4.9933 | 28.298 |
| 2412 | 10 | 4  | id    | 0.1849 | 0.1724 | 1   | 8.6640 | 84.436 |
| 2412 | 10 | 5  | id    | 0.0970 | 0.1122 | 1   | 13.333 | 199.15 |
| 2412 | 10 | 6  | id    | 0.0570 | 0.0728 | 1   | 19.005 | 403.59 |
| 2412 | 10 | 7  | id    | 0.0363 | 0.0583 | 1   | 25.676 | 735.56 |
| 2412 | 9  | 2  | 0.696 | 1.6269 | 0.7535 | 1   | 1.9400 | 4.3700 |
| 2412 | 9  | 3  | id    | 0.5516 | 0.3664 | 1   | 4.0430 | 18.550 |
| 2412 | 9  | 4  | id    | 0.2496 | 0.2159 | 1   | 6.8968 | 53.503 |
| 2412 | 9  | 5  | id    | 0.1333 | 0.1421 | 1   | 10.499 | 123.48 |
| 2412 | 9  | 6  | id    | 0.0794 | 0.1006 | 1   | 14.852 | 246.51 |
| 2412 | 9  | 7  | id    | 0.0510 | 0.0749 | 1   | 19.955 | 44.350 |
| 2412 | 8  | 2  | 0.517 | 1.6620 | 0.8111 | 1   | 1.7775 | 3.6578 |
| 2412 | 8  | 3  | id    | 0.6022 | 0.4122 | 1   | 3.5670 | 14.433 |
| 2412 | 8  | 4  | id    | 0.2824 | 0.2488 | 1   | 5.9560 | 39.918 |
| 2412 | 8  | 5  | id    | 0.1543 | 0.1662 | 1   | 8.9466 | 89.670 |
| 2412 | 8  | 6  | id    | 0.0933 | 0.1189 | 1   | 12.536 | 175.64 |
| 2412 | 8  | 7  | id    | 0.0739 | 0.0993 | 1   | 51.552 | 2969.4 |
| 2412 | 8  | 7  | id    | 0.0060 | 0.0893 | 1   | 16.725 | 312.21 |
| 2412 | 7  | 2  | 0.438 | 48.388 | 0.2444 | 1   | 0.6297 | 0.4712 |
| 2412 | 7  | 3  | id    | 10.987 | 0.9108 | 1   | 1.6600 | 3.1461 |
| 2412 | 7  | 4  | id    | 13.046 | 0.4731 | 1   | 3.1900 | 11.474 |
| 2412 | 7  | 5  | id    | 6.2094 | 0.2884 | 1   | 5.2210 | 30.557 |
| 2412 | 7  | 6  | id    | 3.4259 | 0.1940 | 1   | 7.7510 | 67.164 |
| 2412 | 7  | 7  | id    | 2.0860 | 0.1393 | 1   | 10.782 | 129.72 |
| 2412 | 6  | 2  | 0.307 | 37.566 | 2.4383 | 1   | 0.6288 | 0.4662 |

*Table 1 Continued...*
### Table 1: \( \langle r^\alpha \rangle \) values using Topbase \( l=0 \) \( \delta_s \) values Mathematica integration of LaguerreL\([a,b,x]\) with proper normalization.

| \( M \) | \( Z_e \) | \( n \) | \( \delta_s \) | \( \frac{1}{r^2} \) | \( \frac{1}{r} \) | \( N \) | \( <r> \) | \( <r^2> \) |
|--------|--------|------|--------|--------|--------|--------|--------|--------|
| \( ^{24}_{12} \) | 6 | 3 | \textit{id} | 9.3389 | 0.9642 | 1 | 1.5683 | 2.8014 |
| \( ^{24}_{12} \) | 6 | 4 | \textit{id} | 5.0650 | 0.5134 | 1 | 2.9364 | 25.099 |
| \( ^{24}_{12} \) | 6 | 5 | \textit{id} | 2.4678 | 0.3179 | 1 | 4.7330 | 25.099 |
| \( ^{24}_{12} \) | 6 | 6 | \textit{id} | 1.3823 | 0.2160 | 1 | 6.9583 | 54.104 |
| \( ^{24}_{12} \) | 6 | 7 | \textit{id} | 0.8506 | 0.1563 | 1 | 9.6121 | 103.08 |
| \( ^{24}_{12} \) | 5 | 2 | 0.254 | 34.938 | 2.5984 | 1 | 0.6013 | 0.4248 |
| \( ^{24}_{12} \) | 5 | 3 | \textit{id} | 9.1461 | 1.0382 | 1 | 1.4540 | 2.4060 |
| \( ^{24}_{12} \) | 5 | 4 | \textit{id} | 4.3370 | 0.5614 | 1 | 2.6823 | 8.0990 |
| \( ^{24}_{12} \) | 5 | 5 | \textit{id} | 2.1412 | 0.3509 | 1 | 4.2850 | 20.571 |
| \( ^{24}_{12} \) | 5 | 6 | \textit{id} | 1.2103 | 0.2399 | 1 | 6.2630 | 43.832 |
| \( ^{24}_{12} \) | 5 | 7 | \textit{id} | 0.7495 | 0.1743 | 1 | 8.6160 | 138.87 |
| \( ^{24}_{12} \) | 4 | 2 | 0.138 | 31.752 | 2.5965 | 1 | 0.5839 | 0.3993 |
| \( ^{24}_{12} \) | 4 | 3 | \textit{id} | 8.7414 | 0.9483 | 1 | 1.0984 | 2.1368 |
| \( ^{24}_{12} \) | 4 | 4 | \textit{id} | 3.8970 | 0.6037 | 1 | 2.4913 | 6.9845 |
| \( ^{24}_{12} \) | 4 | 5 | \textit{id} | 1.9528 | 0.3808 | 1 | 3.9450 | 17.432 |
| \( ^{24}_{12} \) | 4 | 6 | \textit{id} | 1.1141 | 0.2619 | 1 | 5.7324 | 36.710 |
| \( ^{24}_{12} \) | 4 | 7 | \textit{id} | 0.6945 | 0.1911 | 1 | 7.852 | 68.710 |
| \( ^{24}_{12} \) | 3 | 2 | 0.071 | 30.547 | 2.7850 | 1 | 0.5388 | 0.3388 |
| \( ^{24}_{12} \) | 3 | 3 | \textit{id} | 8.9910 | 1.2328 | 1 | 1.2170 | 1.6820 |
| \( ^{24}_{12} \) | 3 | 4 | \textit{id} | 3.9230 | 0.6920 | 1 | 2.1670 | 5.2877 |
| \( ^{24}_{12} \) | 3 | 5 | \textit{id} | 2.0045 | 0.4423 | 1 | 3.9210 | 12.883 |
| \( ^{24}_{12} \) | 3 | 6 | \textit{id} | 1.1585 | 0.3069 | 1 | 4.8800 | 26.695 |
| \( ^{24}_{12} \) | 3 | 7 | \textit{id} | 0.7288 | 0.2253 | 1 | 6.6570 | 49.442 |
| \( ^{24}_{12} \) | 2 | 2 | 0.013 | 30.547 | 2.7859 | 1 | 0.5388 | 0.3388 |
| \( ^{24}_{12} \) | 2 | 3 | \textit{id} | 8.9910 | 1.2328 | 1 | 1.2170 | 1.6820 |
| \( ^{24}_{12} \) | 2 | 4 | \textit{id} | 3.9230 | 0.6920 | 1 | 2.1679 | 5.2870 |
| \( ^{24}_{12} \) | 2 | 5 | \textit{id} | 2.0045 | 0.4423 | 1 | 3.9164 | 12.883 |
| \( ^{24}_{12} \) | 2 | 6 | \textit{id} | 1.1585 | 0.2633 | 1 | 5.7035 | 26.695 |
| \( ^{24}_{12} \) | 2 | 7 | \textit{id} | 0.7288 | 0.2253 | 1 | 6.6570 | 49.442 |

*Table 1 Continued.*
Table 1: \(< r^\alpha >\) values using Topbase \(l=0\) \(\delta_s\) values Mathematica integration of LaguerreL\([a,b,x]\) with proper normalization.

| \(M\) | \(Z_e\) | \(n\) | \(\delta_s\) | \(< \frac{1}{r^2} >\) | \(< \frac{1}{r} >\) | \(N\) | \(< r >\) | \(< r^2 >\) |
|------|------|------|---------|-----------------|-----------------|-----|--------|--------|
| 26   | 13   | 2    | 1.771   | 0.1474          | 0.2098          | 1   | 7.0670 | 58.100 |
| 26   | 13   | 3    | \(id\)  | 0.0407          | 0.0959          | 1   | 15.488 | 272.58 |
| 26   | 13   | 4    | \(id\)  | 0.0118          | 0.0559          | 1   | 26.685 | 801.02 |
| 26   | 13   | 5    | \(id\)  | 0.0095          | 0.0365          | 1   | 40.872 | 1871.1 |
| 26   | 13   | 6    | \(id\)  | 0.0056          | 0.0257          | 1   | 58.050 | 3766.7 |
| 26   | 13   | 7    | \(id\)  | 0.0036          | 0.0191          | 1   | 78.240 | 6831.4 |
| 26   | 12   | 2    | 1.209   | 0.1425          | 0.2567          | 1   | 5.4880 | 34.759 |
| 26   | 12   | 3    | \(id\)  | 0.0568          | 0.1391          | 1   | 10.424 | 123.50 |
| 26   | 12   | 4    | \(id\)  | 0.0281          | 0.0871          | 1   | 16.861 | 319.97 |
| 26   | 12   | 5    | \(id\)  | 0.0159          | 0.0596          | 1   | 24.797 | 689.20 |
| 26   | 12   | 6    | \(id\)  | 0.0098          | 0.0433          | 1   | 34.234 | 1310.5 |
| 26   | 12   | 7    | \(id\)  | 0.0065          | 0.0329          | 1   | 45.170 | 2278.1 |
| 26   | 11   | 2    | 0.899   | 1.6150          | 0.6797          | 1   | 2.1880 | 5.5740 |
| 26   | 11   | 3    | \(id\)  | 0.5024          | 0.3120          | 1   | 4.7880 | 26.036 |
| 26   | 11   | 4    | \(id\)  | 0.2172          | 0.1783          | 1   | 8.3890 | 79.170 |
| 26   | 11   | 5    | \(id\)  | 0.1128          | 0.1153          | 1   | 12.990 | 189.00 |
| 26   | 11   | 6    | \(id\)  | 0.0659          | 0.0800          | 1   | 18.591 | 386.18 |
| 26   | 11   | 7    | \(id\)  | 0.0418          | 0.0594          | 1   | 25.190 | 708.06 |
| 26   | 10   | 2    | 0.715   | 1.7090          | 0.7535          | 1   | 1.9400 | 4.3700 |
| 26   | 10   | 3    | \(id\)  | 0.5753          | 0.3707          | 1   | 4.0002 | 18.156 |
| 26   | 10   | 4    | \(id\)  | 0.2592          | 0.2178          | 1   | 6.8380 | 52.600 |
| 26   | 10   | 5    | \(id\)  | 0.1381          | 0.1432          | 1   | 10.427 | 121.78 |
| 26   | 10   | 6    | \(id\)  | 0.0821          | 0.1012          | 1   | 14.765 | 243.48 |
| 26   | 10   | 7    | \(id\)  | 0.0527          | 0.0755          | 1   | 19.854 | 439.85 |
| 26   | 9    | 2    | 0.610   | 2.0610          | 0.8759          | 1   | 3.3910 | 3.1860 |
| 26   | 9    | 3    | \(id\)  | 0.7223          | 0.4351          | 1   | 3.3910 | 13.053 |
| 26   | 9    | 4    | \(id\)  | 0.3320          | 0.2595          | 1   | 5.7250 | 36.870 |
| 26   | 9    | 5    | \(id\)  | 0.1796          | 0.1721          | 1   | 8.6586 | 83.980 |
| 26   | 9    | 6    | \(id\)  | 0.1078          | 0.1224          | 1   | 12.192 | 166.12 |

Table I Continued...
Table 1: $< r^\alpha >$ values using Topbase l=0 $\delta_s$ values Mathematica integration of LaguerreL[a,b,x] with proper normalization.

| $\delta_s$ | $\alpha$ | $< r^2 >$ |
|------------|----------|-----------|
| 1          | 16.325   | 297.42    |
| 2          | 0.6224   | 0.4606    |
| 3          | 1.6481   | 3.1000    |
| 4          | 3.1739   | 11.353    |
| 5          | 5.1990   | 30.303    |
| 6          | 7.7254   | 66.705    |
| 7          | 10.751   | 128.97    |
| 8          | 0.5600   | 0.3718    |
| 9          | 1.4563   | 2.4193    |
| 10         | 2.7813   | 8.7150    |
| 11         | 4.5348   | 23.046    |
| 12         | 6.7160   | 50.422    |
| 13         | 9.3270   | 97.076    |
| 14         | 0.4968   | 0.2925    |
| 15         | 1.2855   | 1.8840    |
| 16         | 2.4490   | 6.7580    |
| 17         | 5.9010   | 38.925    |
| 18         | 5.9016   | 38.952    |
| 19         | 8.1903   | 74.840    |
| 20         | 0.4924   | 0.2858    |
| 21         | 1.2250   | 1.7090    |
| 22         | 2.2914   | 5.9122    |
| 23         | 3.6900   | 15.262    |
| 24         | 5.4236   | 32.870    |
| 25         | 7.4898   | 62.580    |
| 26         | 0.4783   | 0.2689    |
| 27         | 1.1591   | 1.5289    |
| 28         | 2.1390   | 5.1547    |
| 29         | 3.4206   | 13.108    |
| 30         | 5.0010   | 27.950    |

Table 1 Continued...
Table 1: $< r^\alpha >$ values using Topbase $l=0$ $\delta_s$ values Mathematica integration of Laguerre$[a,b,x]$ with proper normalization.

| $^\Lambda Z$ | $M$ | $Z_e$ | $n$ | $\delta_s$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|---------|------|------|-----|-------------|----------------|----------------|-----|-------|-------|
| 2613    | 4    | 7    | $id$ | 1.1976      | 0.2182         | 1              | 6.8820 | 52.842 |
| 2613    | 3    | 2    | 0.065 | 49.285      | 3.1342         | 1              | 0.4836 | 0.2738 |
| 2613    | 3    | 3    | $id$ | 13.659      | 1.3323         | 1              | 1.1309 | 1.4538 |
| 2613    | 3    | 4    | $id$ | 5.5760      | 0.7331         | 1              | 2.0509 | 4.7333 |
| 2613    | 3    | 5    | $id$ | 2.7997      | 0.4631         | 1              | 3.2430 | 11.784 |
| 2613    | 3    | 6    | $id$ | 1.5993      | 0.3188         | 1              | 4.7090 | 24.777 |
| 2613    | 3    | 7    | $id$ | 0.9979      | 0.2328         | 1              | 6.4473 | 46.374 |
| 2613    | 2    | 2    | 0.065 | 45.727      | 3.2056         | 1              | 0.4704 | 0.2586 |
| 2613    | 2    | 3    | $id$ | 13.102      | 1.3932         | 1              | 1.0791 | 1.3232 |
| 2613    | 2    | 4    | $id$ | 5.4364      | 0.7750         | 1              | 1.9378 | 4.2252 |
| 2613    | 2    | 5    | $id$ | 2.7559      | 0.4927         | 1              | 3.0465 | 10.395 |
| 2613    | 2    | 6    | $id$ | 1.5844      | 0.3406         | 1              | 4.4052 | 21.682 |
| 2613    | 2    | 7    | $id$ | 0.9930      | 0.2495         | 1              | 6.0139 | 40.344 |

Table 1 Continued...

5.2. Theoretical values $< r^\alpha >$ using the Messiah formulae $[6]$. $I_{^\alpha}^{\text{rel}}$, Messiah formulae

Table 2: sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions (only until the changes obtained comparing both tables 1 are less than 1%).

$< r^\alpha >$ values using extended Messiah formulae.

| $^\Lambda Z$ | $M$ | $Z_e$ | $n$ | $\delta_s$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|---------|------|------|-----|-------------|----------------|----------------|-----|-------|-------|
| Li average Operators | $\delta_s$ | Same as Table 1 |
| 63      | 3    | 2    | 0.399 | 2.5591      | 0.3925         | 1              | 3.9416 | 18.418 |
| 63      | 3    | 3    | $id$ | 0.5947      | 0.1483         | 1              | 10.230 | 119.36 |
| 63      | 3    | 4    | $id$ | 0.2237      | 0.0777         | 1              | 19.518 | 429.22 |

Table 2 Continued...
Table 2: sketches the averaged operator values obtained by extrapolating
the Messiah formulae for hydrogenic ions (only until the changes
obtained comparing both tables 1 are less than 1%).

\(< r^\alpha >\) values using extended Messiah formulae.

| $^A Z$ | $M$ | $Z_e$ | $n$ | $\delta_n$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|-------|-----|------|-----|-------------|----------------|----------------|-----|--------|--------|
| 63    | 3   | 5    | id  | 0.1071      | 0.0473         | 1              | 31.806 | 1133.7 |
| 63    | 3   | 6    | id  | 0.0593      | 0.0319         | 1              | 47.094 | 2478.7 |
| 63    | 3   | 7    | id  | 0.0362      | 0.0229         | 1              | 65.383 | 4769.9 |
| 63    | 2   | 2    | 0.181| 1.3101      | 0.5387         | 1              | 2.8014 | 9.1731 |
| 63    | 2   | 3    | id  | 0.3738      | 0.2334         | 1              | 6.4411 | 47.151 |
| 63    | 2   | 4    | id  | 0.1547      | 0.1297         | 1              | 11.581 | 150.92 |
| 63    | 2   | 5    | id  | 0.0783      | 0.0823         | 1              | 18.221 | 371.90 |
| 63    | 2   | 6    | id  | 0.0450      | 0.0569         | 1              | 26.362 | 776.47 |
| 63    | 2   | 7    | id  | 0.0281      | 0.0416         | 1              | 36.002 | 1446.0 |

**O average Operators**

| $^A Z$ | $M$ | $Z_e$ | $n$ | $\delta_n$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|-------|-----|------|-----|-------------|----------------|----------------|-----|--------|--------|
| 168   | 8   | 2    | 1.141| 4.394$^1$  | 1.355$^1$      | 1              | 5.2443 | 32.213 |
| 168   | 8   | 3    | id  | 0.1191     | 0.433$^1$      | 1              | 12.321 | 172.60 |
| 168   | 8   | 4    | id  | 0.119$^1$  | 0.1223         | 1              | 22.398 | 564.57 |
| 168   | 8   | 5    | id  | 0.048$^1$  | 0.067$^1$      | 1              | 35.475 | 1409.6 |
| 168   | 8   | 6    | id  | 0.0242     | 0.042$^1$      | 1              | 51.552 | 2969.4 |
| 168   | 8   | 7    | id  | 0.0080     | 0.021$^1$      | 1              | 70.629 | 2963.4 |
| 168   | 7   | 2    | 0.861| 3.396$^1$  | 1.404$^1$      | 1              | 3.5490 | 14.646 |
| 168   | 7   | 3    | id  | 0.546$^1$  | 0.415$^1$      | 1              | 7.5890 | 65.375 |
| 168   | 7   | 4    | id  | 0.177$^1$  | 0.196$^1$      | 1              | 13.129 | 193.90 |
| 168   | 7   | 5    | id  | 0.078$^1$  | 0.113$^1$      | 1              | 20.484 | 455.6 |
| 168   | 7   | 6    | id  | 0.041$^1$  | 0.052$^1$      | 1              | 28.709 | 920.90 |
| 168   | 7   | 7    | id  | 0.0240     | 0.0545         | 1              | 38.749 | 1675.2 |
| 168   | 6   | 2    | 0.539| 3.460$^1$  | 1.492$^1$      | 1              | 2.8200 | 9.2150 |
| 168   | 6   | 3    | id  | 0.696$^1$  | 0.513$^1$      | 1              | 5.7360 | 37.320 |
| 168   | 6   | 4    | id  | 0.246$^1$  | 0.257$^1$      | 1              | 9.6520 | 104.80 |
| 168   | 6   | 5    | id  | 2.4311     | 0.1916         | 1              | 2.4311 | 151.97 |
| 168   | 6   | 6    | id  | 1.3425     | 0.1289         | 1              | 11.660 | 115.17 |
| 168   | 6   | 7    | 0.431| 0.8180     | 0.0926         | 1              | 16.212 | 293.29 |

*Table 2 Continued...*
A Z M Zn δn < 1/2 > < 1/r > N < r > < r^2 >  

| αZ  |   |   |   |   |   |
|------|---|---|---|---|---|
| 2211 | 11 | 2 | 1.342 | 22.211 | 2.3091 | 1 | 0.7611 | 0.8311 |
| 2211 | 11 | 3 | id  | 1.3881 | 0.3631 | 1 | 4.2351 | 21.194 |
| 2211 | 11 | 4 | id  | 0.3371 | 0.1451 | 1 | 10.71 | 130.70 |
| 2211 | 11 | 5 | id  | 0.1291 | 0.0741 | 1 | 20.181 | 458.31 |
| 2211 | 11 | 6 | id  | 0.0621 | 0.0461 | 1 | 32.651 | 1195.1 |
| 2211 | 11 | 7 | id  | 0.0391 | 0.0311 | 1 | 48.131 | 2588.1 |
| 2211 | 10 | 2 | 0.989 | 7.6081 | 1.9601 | 1 | 0.7621 | 0.7741 |
| 2211 | 10 | 3 | id  | 0.9651 | 0.4941 | 1 | 3.0271 | 10.691 |
| 2211 | 10 | 4 | id  | 0.2871 | 0.2201 | 1 | 6.7921 | 52.401 |
| 2211 | 10 | 5 | id  | 0.1216 | 0.1241 | 1 | 12.0581 | 163.57 |
| 2211 | 10 | 6 | id  | 0.0621 | 0.0791 | 1 | 18.821 | 396.83 |
| 2211 | 10 | 7 | id  | 0.0361 | 0.0553 | 1 | 27.0881 | 819.45 |
| 2211 | 9  | 2 | 0.812 | 0.9651 | 0.4941 | 1 | 3.0271 | 10.691 |
| 2211 | 9  | 3 | id  | 0.2871 | 0.22071 | 1 | 6.7921 | 52.401 |
| 2211 | 9  | 4 | id  | 0.1211 | 0.1241 | 1 | 12.051 | 163.51 |
| 2211 | 9  | 5 | id  | 0.0621 | 0.0791 | 1 | 18.823 | 396.83 |
| 2211 | 9  | 6 | id  | 0.0361 | 0.0551 | 1 | 27.081 | 819.81 |
| 2211 | 9  | 7 | id  | 0.0221 | 0.0401 | 1 | 36.851 | 1515.1 |
| 2211 | 8  | 2 | 0.653 | 7.7476 | 2.2068 | 1 | 0.6214 | 0.4907 |
| 2211 | 8  | 3 | id  | 1.4630 | 0.7265 | 1 | 2.0060 | 4.6667 |
| 2211 | 8  | 4 | id  | 0.5045 | 0.3572 | 1 | 4.1408 | 19.452 |
| 2211 | 8  | 5 | id  | 0.2302 | 0.2117 | 1 | 7.0255 | 55.521 |
| 2211 | 8  | 6 | id  | 0.1237 | 0.1399 | 1 | 10.661 | 127.29 |
| 2211 | 8  | 7 | id  | 0.0086 | 0.0212 | 1 | 15.045 | 252.95 |
| 2211 | 7  | 2 | 0.495 | 7.8231 | 2.1281 | 1 | 0.6671 | 0.5781 |
| 2211 | 7  | 3 | id  | 1.2511 | 0.6271 | 1 | 2.3551 | 6.4461 |
| 2211 | 7  | 4 | id  | 0.4041 | 0.2951 | 1 | 5.0421 | 28.851 |

Table 2 Continued...
Table 2: sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions (only until the changes obtained comparing both tables 1 are less than 1%). 

\(< r^2 >\) values using extended Messiah formulae.

| A  | Z   | M  | Z_e | n  | \( \delta_x \) | \( \frac{1}{r^2} \) | \( \frac{1}{r} \) | N   | \(< r >\) | \(< r^2 >\) |
|----|-----|----|-----|----|----------------|----------------|----------------|-----|----------|----------|
| 22 | 11  | 7  | 5   | id | 0.017\(^1\)  | 0.171\(^1\)  | 1  | 8.729\(^1\) | 85.71\(^1\) |
| 22 | 11  | 7  | 6   | id | 0.093\(^1\)  | 0.111\(^1\)  | 1  | 13.41\(^1\) | 201.6\(^1\) |
| 22 | 11  | 7  | 7   | id | 0.055\(^1\)  | 0.078\(^1\)  | 1  | 19.10\(^1\) | 407.8\(^1\) |
| 22 | 11  | 6  | 2   | 0.325 | 7.747\(^1\) | 2.206\(^1\)  | 1  | 2.355\(^1\) | 6.446\(^1\) |
| 22 | 11  | 6  | 3   | id | 1.463\(^1\)  | 0.726\(^1\)  | 1  | 2.006\(^1\) | 4.666\(^1\) |
| 22 | 11  | 6  | 4   | id | 0.504\(^1\)  | 0.357\(^1\)  | 1  | 4.140\(^1\) | 19.45\(^1\) |
| 22 | 11  | 6  | 5   | id | 0.230\(^1\)  | 0.211\(^1\)  | 1  | 7.025\(^1\) | 55.52\(^1\) |
| 22 | 11  | 6  | 6   | id | 0.123\(^1\)  | 0.139\(^1\)  | 1  | 10.66\(^1\) | 127.2\(^1\) |
| 22 | 11  | 6  | 7   | id | 0.073\(^1\)  | 0.099\(^1\)  | 1  | 15.04\(^1\) | 325.2\(^1\) |
| 22 | 11  | 5  | 2   | 0.283 | 0.965\(^1\) | 0.494\(^1\)  | 1  | 3.027\(^1\) | 10.69\(^1\) |
| 22 | 11  | 5  | 3   | id | 0.287\(^1\)  | 0.220\(^1\)  | 1  | 6.792\(^1\) | 52.40\(^1\) |
| 22 | 11  | 5  | 4   | id | 0.121\(^1\)  | 0.124\(^1\)  | 1  | 12.05\(^1\) | 163.5\(^1\) |
| 22 | 11  | 5  | 5   | id | 0.062\(^1\)  | 0.079\(^1\)  | 1  | 18.82\(^1\) | 396.8\(^1\) |
| 22 | 11  | 5  | 6   | id | 0.036\(^1\)  | 0.055\(^1\)  | 1  | 27.08\(^1\) | 819.8\(^1\) |
| 22 | 11  | 5  | 7   | id | 0.022\(^1\)  | 0.040\(^1\)  | 1  | 36.85\(^1\) | 1515.1\(^1\) |
| 22 | 11  | 4  | 2   | 0.380 | 44.630 | 2.3747 | 1  | 0.6461 | 0.4917 |
| 22 | 11  | 4  | 3   | id | 11.264 | 0.9483 | 1  | 1.5962 | 2.9011 |

Table 2 Continued…
Table 2: sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions (only until the changes obtained comparing both tables 1 are less than 1%).

\[ <r^a > \text{ values using extended Messiah formulae.} \]

| A Z        | 24 12 | 11  5 | id | 0.046 | 0.129 | 11.14 | 140.7 | 24 12 | 11  6 | id | 0.023 | 0.082 | 17.78 | 356.1 | 24 12 | 11  7 | id | 0.013 | 0.056 | 25.93 | 1145.1 | 24 12 | 10  2 | 0.829 | 8.363 | 2.188 | 1.651 | 0.552 | 24 12 | 10  3 | id | 1.311 | 0.636 | 2.322 | 6.272 | 24 12 | 10  4 | id | 0.420 | 0.298 | 4.993 | 28.29 | 24 12 | 10  5 | id | 0.184 | 0.172 | 8.664 | 84.43 | 24 12 | 10  6 | id | 0.097 | 0.112 | 13.33 | 199.1 | 24 12 | 10  7 | id | 0.057 | 0.071 | 19.00 | 403.5 | 24 12 | 9   2 | 0.696 | 8.978 | 2.352 | 0.588 | 0.441 | 24 12 | 9   3 | id | 1.627 | 0.753 | 1.940 | 4.370 | 24 12 | 9   4 | id | 0.551 | 0.366 | 4.043 | 18.55 | 24 12 | 9   5 | id | 0.249 | 0.215 | 6.896 | 53.50 | 24 12 | 9   6 | id | 0.133 | 0.142 | 10.49 | 123.4 | 24 12 | 9   7 | id | 0.079 | 0.100 | 14.85 | 246.5 | 24 12 | 8   2 | 0.517 | 7.800 | 2.274 | 0.587 | 0.432 | 24 12 | 8   3 | id | 1.662 | 0.811 | 1.777 | 3.657 | 24 12 | 8   4 | id | 0.602 | 0.412 | 3.567 | 14.43 | 24 12 | 8   5 | id | 0.282 | 0.249 | 5.955 | 39.91 | 24 12 | 8   6 | id | 0.154 | 0.166 | 8.946 | 89.67 | 24 12 | 8   7 | id | 0.093 | 0.118 | 12.53 | 175.6 | 24 12 | 7   2 | 0.438 | 154.8 | 2.462 | 0.629 | 0.4712 | 24 12 | 7   3 | id | 35.07 | 0.914 | 1.6603 | 3.1461 | 24 12 | 7   4 | id | 13.046 | 0.4731 | 3.1900 | 11.474 | 24 12 | 7   5 | id | 6.294 | 0.2884 | 5.2210 | 30.557 | 24 12 | 7   6 | id | 3.4259 | 0.1940 | 7.7510 | 67.164 | 24 12 | 7   7 | id | 2.0860 | 0.1393 | 10.78 | 129.72 | 24 12 | 6   2 | 0.3078 | 52.61 | 2.4383 | 0.6288 | 0.4662 |

*Table 2 Continued...*
Table 2: sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions (only until the changes obtained comparing both tables 1 are less than 1%).

\[ < r^\alpha > \] values using extended Messiah formulae.

| A Z | M | Z_e | n | \( \delta_s \) | \( \frac{1}{r^2} \) | \( \frac{1}{r} \) | N | \( r \) | \( r^2 \) |
|-----|---|-----|---|----------|----------|----------|---|----------|----------|
| 2412 | 6 | 3 | id | 13.06^1 | 0.9642 | 1 | 1.5683 | 2.8014 |
| 2412 | 5 | 2 | 0.254 | 41.70^1 | 2.5984 | 1 | 0.6013 | 0.4248 |
| Mg average Operators | \( \delta_s \) | Same as Table 1 |
| 2412 | 4 | 2 | 0.138 | 34.79^1 | 2.5965 | 1 | 0.5839 | 0.3993 |
| 2412 | 4 | 3 | id | 9.578^1 | 0.9483 | 1 | 1.0984 | 2.1368 |
| Mg average Operators | \( \delta_s \) | Same as Table 1 |
| 2412 | 3 | 2 | 0.071 | 32.49^1 | 2.785 | 1 | 0.5388 | 0.3388 |
| 2412 | 3 | 3 | id | 9.280^1 | 1.2328 | 1 | 1.2170 | 1.6820 |
| Mg average Operators | \( \delta_s \) | Same as Table 1 |
| 2412 | 2 | 2 | 0.0132 | 32.492 | 2.7859 | 1 | 0.5388 | 0.3388 |
| 2412 | 2 | 3 | id | 9.280^1 | 1.2328 | 1 | 1.2170 | 1.6820 |

Table 2 Continued...
Table 3 and 4 show results for the $\alpha$ powers of the $r$ radial operator with another angular momentum $l = 1$ value related to quantum defect $\delta_p$. For $p$ states one requires $l = 1$ and the existence of $\delta_p$, substituting $n \rightarrow n^* = n - \delta_p$ and $l \rightarrow l^* = 1 - \delta_p$. These estimates give 2 more Tables 3 & 4 results, with the wave functions $w_{n^*l^*}$ that is to evaluate $\alpha$ values, and changing the value of give a very good agreement when the same theoretical $\delta_p$ values are used in both calculations. As done in upper tables two methods are used: first to calculate $\langle n^*_l m^*_n | r^\alpha | n^*_l m^*_n \rangle$ & $\alpha$ values $\{-2, -1, 0, 1, 2\}$, (Table 3) and second gives the Messiah formulae using the upward replacement (Table 4). Table 4 contains the extrapolated results obtained by using the analytic results for hydrogenic ions.

5.3. $\langle n^*_l m^*_n | r^\alpha | n^*_l m^*_n \rangle$ expectation values $\delta_p$-values from Topbase. (that is $n_s = n - \delta_p$ with angular momentum $l = 1$).
Table 3: $< r^m >$ values l=1 P states using Topbase quantum defects $\delta_p$
obtained with integration of LaguerreL[a,b,x] with proper normalization.

| $^{\text{A}Z}$ | $M$ | $Z_e$ | $n$ | $\delta_p$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|----------------|-----|-------|-----|------------|----------------|----------------|----|--------|--------|
| **Li average Operators** | 63  | 3     | 2   | 0.399     | 2.5591         | 0.3925         | 1   | 3.9416 | 18.418 |
|                | 63  | 3     | 3   | $id$      | 0.5947         | 0.1483         | 1   | 10.230 | 119.36 |
|                | 63  | 3     | 4   | $id$      | 0.2237         | 0.0777         | 1   | 19.518 | 429.22 |
|                | 63  | 3     | 5   | $id$      | 0.1071         | 0.0473         | 1   | 31.806 | 1133.7 |
|                | 63  | 3     | 6   | $id$      | 0.0593         | 0.0319         | 1   | 47.094 | 2478.7 |
|                | 63  | 3     | 7   | $id$      | 0.0362         | 0.0229         | 1   | 65.383 | 4769.9 |
|                | 63  | 2     | 2   | 0.181     | 1.3101         | 0.5387         | 1   | 2.8014 | 9.1731 |
|                | 63  | 2     | 3   | $id$      | 0.3738         | 0.2334         | 1   | 6.4411 | 47.151 |
|                | 63  | 2     | 4   | $id$      | 0.1547         | 0.1297         | 1   | 11.581 | 150.92 |
|                | 63  | 2     | 5   | $id$      | 0.0783         | 0.0823         | 1   | 18.221 | 371.90 |
|                | 63  | 2     | 6   | $id$      | 0.0450         | 0.0569         | 1   | 26.362 | 776.47 |
|                | 63  | 2     | 7   | $id$      | 0.0281         | 0.0416         | 1   | 36.002 | 1446.0 |
| **O average Operators** | 168 | 8     | 2   | 1.141     | 0.0533         | 0.2032         | 1   | 6.0285 | 43.028 |
|                | 168 | 8     | 3   | $id$      | 0.0174         | 0.0965         | 1   | 14.182 | 231.30 |
|                | 168 | 8     | 4   | $id$      | 0.0077         | 0.0562         | 1   | 25.336 | 728.14 |
|                | 168 | 8     | 5   | $id$      | 0.0040         | 0.0367         | 1   | 39.490 | 1756.6 |
|                | 168 | 8     | 6   | $id$      | 0.0024         | 0.0258         | 1   | 56.644 | 3599.8 |
|                | 168 | 8     | 7   | $id$      | 0.0015         | 0.01919        | 1   | 76.798 | 6600.8 |
|                | 168 | 7     | 2   | 0.861     | 1.6510         | 0.8821         | 1   | 1.5099 | 2.8484 |
|                | 168 | 7     | 3   | $id$      | 0.2528         | 0.3185         | 1   | 4.5185 | 23.629 |
|                | 168 | 7     | 4   | $id$      | 0.0923         | 0.1627         | 1   | 9.027  | 92.428 |
|                | 168 | 7     | 5   | $id$      | 0.0434         | 0.0985         | 1   | 15.035 | 254.33 |
|                | 168 | 7     | 6   | $id$      | 0.0238         | 0.0659         | 1   | 22.544 | 569.42 |
|                | 168 | 7     | 7   | $id$      | 0.0144         | 0.0472         | 1   | 3.5520 | 1112.7 |
|                | 168 | 6     | 2   | 0.539     | 2.1265         | 1.2052         | 1   | 1.5099 | 1.4812 |
|                | 168 | 6     | 3   | $id$      | 0.4875         | 0.4514         | 1   | 3.1703 | 11.623 |
|                | 168 | 6     | 4   | $id$      | 0.1823         | 0.2347         | 1   | 6.2480 | 44.277 |

*Table 3 Continued...*
Table 3: $< r^{\alpha} >$ values $l=1$ P states using Topbase quantum defects $\delta_p$
obtained with integration of LaguerreL[a,b,x] with proper normalization.

| $A^Z$ | $M$ | $Z_e$ | $n$ | $\delta_p$ | $< \frac{1}{r^2} >$ | $< \frac{1}{r} >$ | $N$ | $< r >$ | $< r^2 >$ |
|-------|-----|------|-----|------------|----------------|----------------|-----|--------|--------|
| $^{16}\text{O}$ | 6   | 5    | $id$ | 0.0870     | 0.1431         | 1  | 10.325 | 119.96 |
| $^{16}\text{O}$ | 6   | 6    | $id$ | 0.0481     | 0.0964         | 1  | 15.403 | 265.85 |
| $^{16}\text{O}$ | 6   | 7    | $id$ | 0.0293     | 0.0690         | 1  | 21.481 | 910.36 |
| $^{16}\text{O}$ | 5   | 2    | $0.431$ | 3.8750     | 1.6248        | 1  | 0.8115 | 0.8178 |
| $^{16}\text{O}$ | 5   | 3    | $id$ | 0.8827     | 0.6060         | 1  | 2.3633 | 6.459  |
| $^{16}\text{O}$ | 5   | 4    | $id$ | 0.3292     | 0.3140         | 1  | 4.6650 | 24.998 |
| $^{16}\text{O}$ | 5   | 5    | $id$ | 2.4311     | 0.1916         | 1  | 7.7160 | 66.998 |
| $^{16}\text{O}$ | 5   | 6    | $id$ | 0.0866     | 0.1289         | 1  | 11.518 | 148.66 |
| $^{16}\text{O}$ | 5   | 7    | $id$ | 0.8180     | 0.0926         | 1  | 16.212 | 509.82 |
| $^{16}\text{O}$ | 4   | 2    | $0.227$ | 3.8193     | 1.6499        | 1  | 0.7801 | 0.7444 |
| $^{16}\text{O}$ | 4   | 3    | $id$ | 0.9786     | 0.6656         | 1  | 2.1246 | 5.2119 |
| $^{16}\text{O}$ | 4   | 4    | $id$ | 0.3846     | 0.3573         | 1  | 4.0691 | 18.779 |
| $^{16}\text{O}$ | 4   | 5    | $id$ | 0.1890     | 0.2224         | 1  | 6.6136 | 49.223 |
| $^{16}\text{O}$ | 4   | 6    | $id$ | 0.1064     | 0.1517         | 1  | 9.7581 | 106.72 |
| $^{16}\text{O}$ | 4   | 7    | $id$ | 0.0657     | 0.1100         | 1  | 13.502 | 203.85 |
| $^{16}\text{O}$ | 3   | 2    | $0.111$ | 3.0988     | 1.5226        | 1  | 0.8226 | 0.8120 |
| $^{16}\text{O}$ | 3   | 3    | $id$ | 0.9113     | 0.6733         | 1  | 2.0640 | 4.9117 |
| $^{16}\text{O}$ | 3   | 4    | $id$ | 0.3830     | 0.3778         | 1  | 3.8070 | 16.144 |
| $^{16}\text{O}$ | 3   | 5    | $id$ | 0.7939     | 0.2511         | 1  | 5.9819 | 40.079 |
| $^{16}\text{O}$ | 3   | 6    | $id$ | 0.1130     | 0.1674         | 1  | 8.7920 | 86.688 |
| $^{16}\text{O}$ | 3   | 7    | $id$ | 0.0711     | 0.1222         | 1  | 12.034 | 162.02 |
| $^{16}\text{O}$ | 2   | 2    | $0.020$ | 4.3502     | 1.8018        | 1  | 0.6957 | 0.5825 |
| $^{16}\text{O}$ | 2   | 3    | $id$ | 1.2701     | 0.7930         | 1  | 1.7547 | 3.5480 |
| $^{16}\text{O}$ | 2   | 4    | $id$ | 0.5319     | 0.4439         | 1  | 3.2420 | 11.923 |
| $^{16}\text{O}$ | 2   | 5    | $id$ | 0.2711     | 0.2823         | 1  | 5.1585 | 29.959 |
| $^{16}\text{O}$ | 2   | 6    | $id$ | 0.1564     | 0.1963         | 1  | 7.5032 | 63.128 |
| $^{16}\text{O}$ | 2   | 7    | $id$ | 0.0983     | 0.1440         | 1  | 10.276 | 118.13 |

$Na$ average Operators $\delta_p$

| $^{22}\text{Ne}$ | 11  | 2    | $1.342$ | $1.3886$ | $0.3637$ | 1  | 4.2359 | 21.194 |
| $^{22}\text{Ne}$ | 11  | 3    | $id$ | $0.3370$ | $0.1415$ | 1  | 10.710 | 130.70 |

Table 3 Continued...
Table 3: \( \langle r^\alpha \rangle \) values \( l=1 \) P states using Topbase quantum defects \( \delta_p \) obtained with integration of LaguerreL\([a,b,x]\) with proper normalization.

| A | Z | n | \( \delta_p \) | \( \langle \frac{1}{r} \rangle \) | \( \langle \frac{1}{r^2} \rangle \) | N | \( \langle r \rangle \) | \( \langle r^2 \rangle \) |
|---|---|---|---|---|---|---|---|---|
| 22 | 11 | 4 | id | 0.1293 | 0.0747 | 1 | 20.184 | 458.83 |
| 22 | 11 | 5 | id | 0.062 | 0.046 | 1 | 32.658 | 1195.0 |
| 22 | 11 | 6 | id | 0.0349 | 0.0312 | 1 | 48.132 | 2588.8 |
| 22 | 11 | 7 | id | 0.0214 | 0.0225 | 1 | 66.606 | 4949.7 |
| 22 | 11 | 10 | 2 | 0.989 | 0.9654 | 0.4949 | 1 | 3.072 | 10.693 |
| 22 | 11 | 10 | 3 | id | 7.8237 | 2.1281 | 1 | 0.6677 | 0.578 |
| 22 | 11 | 10 | 4 | id | 0.0114 | 0.1538 | 1 | 9.6523 | 104.8 |
| 22 | 11 | 10 | 5 | id | 0.0618 | 0.1022 | 1 | 14.568 | 237.75 |
| 22 | 11 | 10 | 6 | id | 0.0372 | 0.0728 | 1 | 20.484 | 468.95 |
| 22 | 11 | 10 | 7 | id | 0.0240 | 0.0545 | 1 | 27.404 | 837.84 |
| 22 | 11 | 9 | 2 | 0.812 | 1.2513 | 0.6270 | 1 | 2.355 | 6440 |
| 22 | 11 | 9 | 3 | id | 0.4044 | 0.2953 | 1 | 5.0423 | 28.855 |
| 22 | 11 | 9 | 4 | id | 0.1783 | 0.1114 | 1 | 13.417 | 85.719 |
| 22 | 11 | 9 | 5 | id | 0.0938 | 0.1916 | 1 | 2.4310 | 151.97 |
| 22 | 11 | 9 | 6 | id | 0.0552 | 0.0783 | 1 | 19.104 | 201.62 |
| 22 | 11 | 9 | 7 | id | 0.0352 | 0.0580 | 1 | 25.791 | 742.19 |
| 22 | 11 | 8 | 2 | 0.653 | 7.7476 | 2.2068 | 1 | 0.6214 | 0.4907 |
| 22 | 11 | 8 | 3 | id | 1.4630 | 0.7265 | 1 | 2.0060 | 4.6667 |
| 22 | 11 | 8 | 4 | id | 0.5045 | 0.3572 | 1 | 4.1408 | 319.452 |
| 22 | 11 | 8 | 5 | id | 0.2302 | 0.2117 | 1 | 7.0255 | 55.521 |
| 22 | 11 | 8 | 6 | id | 0.1237 | 0.1399 | 1 | 10.660 | 127.29 |
| 22 | 11 | 8 | 7 | id | 0.0739 | 0.0993 | 1 | 51.552 | 2969.4 |
| 22 | 11 | 8 | 7 | id | 0.0086 | 0.0212 | 1 | 15.045 | 252.95 |
| 22 | 11 | 7 | 2 | 0.495 | 0.9654 | 0.4949 | 1 | 3.0278 | 10.693 |
| 22 | 11 | 7 | 3 | id | 0.2875 | 0.2207 | 1 | 6.7929 | 52.408 |
| 22 | 11 | 7 | 4 | id | 0.1216 | 0.1243 | 1 | 12.058 | 163.57 |
| 22 | 11 | 7 | 5 | id | 0.0623 | 0.0796 | 1 | 18.823 | 396.83 |
| 22 | 11 | 7 | 6 | id | 0.0361 | 0.0553 | 1 | 27.088 | 819.84 |
| 22 | 11 | 7 | 7 | id | 0.0227 | 0.0406 | 1 | 36.567 | 1515.2 |
| 22 | 11 | 6 | 2 | 0.325 | 1791.9 | 2.2101 | 1 | 0.7036 | 0.5909 |

Table 3 Continued...
Table 3: \(< r^{\alpha} >\) values l=1 P states using Topbase quantum defects \(\delta_p\) obtained with integration of LaguerreL[a,b,x] with proper normalization.

| AZ | M  | Z_e | n  | \(\delta_p\) | \(< \frac{1}{r^2} >\) | \(< \frac{1}{r} >\) | N  | \(< r >\) | \(< r^2 >\) |
|----|----|-----|----|------------|----------------|----------------|----|---------|---------|
| 22 | 11 | 6   | 3  | id         | 388.33         | 0.7973         | 1  | 1.9061  | 4.1514  |
| 22 | 11 | 6   | 4  | id         | 141.71         | 0.4072         | 1  | 3.7086  | 15.506  |
| 22 | 11 | 6   | 5  | id         | 66.731         | 0.2464         | 1  | 6.1110  | 41.865  |
| 22 | 11 | 6   | 6  | id         | 36.567         | 0.1650         | 1  | 9.1135  | 92.839  |
| 22 | 11 | 6   | 7  | id         | 22.161         | 0.1181         | 1  | 12.716  | 180.43  |
| 22 | 11 | 5   | 2  | 0.283     | 43.840         | 2.1390         | 1  | 0.7195  | 0.6109  |
| 22 | 11 | 5   | 3  | id         | 10.761         | 0.8386         | 1  | 1.8069  | 3.7194  |
| 22 | 11 | 5   | 4  | id         | 4.1501         | 0.4443         | 1  | 3.3943  | 12.975  |
| 22 | 11 | 5   | 5  | id         | 2.0159         | 0.2745         | 1  | 5.4817  | 33.669  |
| 22 | 11 | 5   | 6  | id         | 1.1269         | 0.1863         | 1  | 8.069   | 72.759  |
| 22 | 11 | 5   | 7  | id         | 0.6925         | 0.1346         | 1  | 11.156  | 138.87  |
| 22 | 11 | 4   | 2  | 0.380     | 44.630         | 2.3747         | 1  | 0.6461  | 0.4917  |
| 22 | 11 | 4   | 3  | id         | 11.264         | 0.9483         | 1  | 1.5962  | 2.9011  |
| 22 | 11 | 4   | 4  | id         | 4.3994         | 0.5066         | 1  | 2.9749  | 9.9640  |
| 22 | 11 | 4   | 5  | id         | 2.1526         | 0.31461        | 1  | 4.7821  | 25.621  |
| 22 | 11 | 4   | 6  | id         | 1.2090         | 0.2141         | 1  | 7.0170  | 55.035  |
| 22 | 11 | 4   | 7  | id         | 0.7454         | 0.1551         | 1  | 9.6823  | 104.59  |
| 22 | 11 | 3   | 2  | 0.153     | 37.181         | 2.6404         | 1  | 0.5753  | 0.3878  |
| 22 | 11 | 3   | 3  | id         | 10.147         | 1.1109         | 1  | 1.3573  | 2.0949  |
| 22 | 11 | 3   | 4  | id         | 4.1109         | 0.6038         | 1  | 2.4727  | 9.9647  |
| 22 | 11 | 3   | 5  | id         | 2.0556         | 0.3832         | 1  | 3.9210  | 17.225  |
| 22 | 11 | 3   | 6  | id         | 1.1709         | 0.2633         | 1  | 5.7030  | 36.347  |
| 22 | 11 | 3   | 7  | id         | 0.7291         | 0.1920         | 1  | 7.8189  | 68.206  |
| 22 | 11 | 2   | 2  | 0.078     | 13.189         | 1.7870         | 1  | 0.8408  | 0.8252  |
| 22 | 11 | 2   | 3  | id         | 10.147         | 1.1100         | 1  | 1.3570  | 2.0940  |
| 22 | 11 | 2   | 4  | id         | 4.1120         | 0.6038         | 1  | 2.4727  | 6.8813  |
| 22 | 11 | 2   | 5  | id         | 2.0556         | 0.3832         | 1  | 3.9215  | 17.225  |
| 22 | 11 | 2   | 6  | id         | 1.1709         | 0.2633         | 1  | 5.7035  | 36.347  |
| 22 | 11 | 2   | 7  | id         | 0.7291         | 0.1920         | 1  | 7.8189  | 68.206  |

\(\delta_p\) Operators

Table 3 Continued...
Table 3: \(< r^{\alpha} >\) values \(l=1\) P states using Topbase quantum defects \(\delta_p\) obtained with integration of LaguerreL\([a,b,x]\) with proper normalization.

| \(^A Z\) | \(M\) | \(Z_e\) | \(n\) | \(\delta_p\) | \(< \frac{1}{r}\>\) | \(< \frac{1}{r^2}\>\) | \(N\) | \(< r >\) | \(< r^2 >\) |
|---------|-------|-------|------|-----------|----------|----------|---|---------|----------|
| 24\(12\) | 12    | 2     | 1.545| 0.0729    | 0.16731  | 1        | 8.6510 | 86.600  |
| 24\(12\) | 12    | 3     | id   | 0.0253    | 0.0837   | 1        | 17.579 | 350.53 |
| 24\(12\) | 12    | 4     | id   | 0.0118    | 0.0503   | 1        | 29.445 | 975.38 |
| 24\(12\) | 12    | 5     | id   | 0.0064    | 0.0335   | 1        | 4.2359 | 21.194 |
| 24\(12\) | 12    | 6     | id   | 0.0038    | 0.0239   | 1        | 62.178 | 4321.0 |
| 24\(12\) | 12    | 7     | id   | 0.0025    | 0.0179   | 1        | 4.2359 | 21.194 |
| 24\(12\) | 11    | 2     | 1.069| 0.1110    | 0.2328   | 1        | 5.9930 | 41.400 |
| 24\(12\) | 11    | 3     | id   | 0.0460    | 0.1294   | 1        | 11.140 | 140.75 |
| 24\(12\) | 11    | 4     | id   | 0.0233    | 0.0822   | 1        | 17.786 | 356.15 |
| 24\(12\) | 11    | 5     | id   | 0.0133    | 0.0568   | 1        | 25.933 | 704.06 |
| 24\(12\) | 11    | 6     | id   | 0.0083    | 0.0416   | 1        | 35.570 | 1415.9 |
| 24\(12\) | 11    | 7     | id   | 0.0056    | 0.0317   | 1        | 46.726 | 2438.2 |
| 24\(12\) | 10    | 2     | 0.829| 1.310     | 0.6366   | 1        | 2.3220 | 6.2720 |
| 24\(12\) | 10    | 3     | id   | 0.4204    | 0.2984   | 1        | 4.9933 | 28.298 |
| 24\(12\) | 10    | 4     | id   | 0.1849    | 0.1724   | 1        | 8.6640 | 84.436 |
| 24\(12\) | 10    | 5     | id   | 0.0970    | 0.1122   | 1        | 13.333 | 199.15 |
| 24\(12\) | 10    | 6     | id   | 0.0570    | 0.0728   | 1        | 19.005 | 403.59 |
| 24\(12\) | 10    | 7     | id   | 0.0363    | 0.0583   | 1        | 25.676 | 735.56 |
| 24\(12\) | 9     | 2     | 0.696| 1.6269    | 0.7535   | 1        | 1.9400 | 4.3700 |
| 24\(12\) | 9     | 3     | id   | 0.5516    | 0.3664   | 1        | 4.0430 | 18.550 |
| 24\(12\) | 9     | 4     | id   | 0.2496    | 0.2159   | 1        | 6.8968 | 53.503 |
| 24\(12\) | 9     | 5     | id   | 0.1333    | 0.1421   | 1        | 10.499 | 123.48 |
| 22\(11\) | 9     | 6     | id   | 0.0794    | 0.1006   | 1        | 14.852 | 246.51 |
| 24\(12\) | 9     | 7     | id   | 0.0510    | 0.0749   | 1        | 19.955 | 44.350 |
| 24\(12\) | 8     | 2     | 0.517| 1.6620    | 0.8111   | 1        | 1.7775 | 3.6578 |
| 24\(12\) | 8     | 3     | id   | 0.6022    | 0.4122   | 1        | 3.5670 | 14.433 |
| 24\(12\) | 8     | 4     | id   | 0.2824    | 0.2488   | 1        | 5.9560 | 39.918 |
| 24\(12\) | 8     | 5     | id   | 0.1543    | 0.1662   | 1        | 8.9466 | 89.670 |
| 24\(12\) | 8     | 6     | id   | 0.0933    | 0.1189   | 1        | 12.536 | 175.64 |
| 24\(12\) | 8     | 7     | id   | 0.0739    | 0.0993   | 1        | 51.552 | 2969.4 |

Table 3 Continued...
Table 3: \(<r^\alpha>\) values l=1 P states using Topbase quantum defects \(\delta_p\) obtained with integration of LaguerreL[a,b,x] with proper normalization.

| AZ | Z_e | n  | \(\delta_p\) | \(<\frac{1}{r^\alpha}>\) | \(<\frac{1}{r}>\) | N  | \(<r>\) | \(<r^2>\) |
|----|-----|----|-------------|----------------|----------------|----|-------|-------|
| 2412 | 8   | 7   | id          | 0.0060         | 0.0893         | 1  | 16.725 | 312.21 |
| 2412 | 7   | 2   | 0.438       | 48.388         | 0.2444         | 1  | 0.6297 | 0.4712 |
| 2412 | 7   | 3   | id          | 10.987         | 0.9108         | 1  | 1.6600 | 3.1461 |
| 2412 | 7   | 4   | id          | 13.046         | 0.4731         | 1  | 3.1900 | 11.474 |
| 2412 | 7   | 5   | id          | 6.2094         | 0.2884         | 1  | 5.2210 | 30.557 |
| 2211 | 7   | 6   | id          | 3.4259         | 0.19401        | 1  | 7.7510 | 67.164 |
| 2412 | 7   | 7   | id          | 2.0860         | 0.1393         | 1  | 10.782 | 129.72 |
| 2412 | 6   | 2   | 0.307       | 37.566         | 2.4383         | 1  | 0.6288 | 0.4662 |
| 2412 | 6   | 3   | id          | 9.3389         | 0.9642         | 1  | 1.5683 | 2.8014 |
| 2412 | 6   | 4   | id          | 5.0650         | 0.5134         | 1  | 2.9364 | 25.099 |
| 2412 | 6   | 5   | id          | 2.4678         | 0.3179         | 1  | 4.7330 | 25.099 |
| 2412 | 6   | 6   | id          | 1.3823         | 0.2160         | 1  | 6.9583 | 54.104 |
| 2412 | 6   | 7   | id          | 0.8506         | 0.1563         | 1  | 9.6121 | 103.08 |
| 2412 | 5   | 2   | 0.254       | 34.938         | 2.5984         | 1  | 0.6013 | 0.4248 |
| 2412 | 5   | 3   | id          | 9.1461         | 1.0382         | 1  | 1.4540 | 2.4060 |
| 2412 | 5   | 4   | id          | 4.3370         | 0.5614         | 1  | 2.6823 | 8.0990 |
| 2412 | 5   | 5   | id          | 2.1412         | 0.3509         | 1  | 4.2850 | 20.571 |
| 2412 | 5   | 6   | id          | 1.2103         | 0.2399         | 1  | 6.2630 | 43.832 |
| 2412 | 5   | 7   | id          | 0.7495         | 0.1743         | 1  | 8.6160 | 138.87 |
| 2412 | 4   | 2   | 0.138       | 31.752         | 2.5965         | 1  | 0.5839 | 0.3993 |
| 2412 | 4   | 3   | id          | 8.7414         | 0.9483         | 1  | 1.0984 | 2.1368 |
| 2412 | 4   | 4   | id          | 3.8970         | 0.6037         | 1  | 2.4913 | 6.9845 |
| 2412 | 4   | 5   | id          | 1.9528         | 0.3808         | 1  | 3.9450 | 17.432 |
| 2412 | 4   | 6   | id          | 1.1141         | 0.2619         | 1  | 5.7324 | 36.710 |
| 2412 | 4   | 7   | id          | 0.6945         | 0.1911         | 1  | 7.8520 | 68.710 |
| 2412 | 3   | 2   | 0.071       | 30.547         | 2.7850         | 1  | 0.5388 | 0.3388 |
| 2412 | 3   | 3   | id          | 8.9910         | 1.2328         | 1  | 1.2170 | 1.6820 |
| 2412 | 3   | 4   | id          | 3.9230         | 0.6920         | 1  | 2.1670 | 5.2877 |
| 2412 | 3   | 5   | id          | 2.0045         | 0.4423         | 1  | 3.9210 | 12.883 |
| 2412 | 3   | 6   | id          | 1.1585         | 0.3069         | 1  | 4.880 | 26.695 |

Table 3 Continued...
Table 3: $< r^{\alpha} >$ values l=1 P states using Topbase quantum defects $\delta_p$
 obtained with integration of LaguerreL[a,b,x] with proper normalization.

| $^{A}Z$ | $M$ | $Z_c$ | $n$ | $\delta_p$ | $\frac{1}{r^1}$ | $\frac{1}{r^2}$ | $N$ | $< r >$ | $< r^2 >$ |
|--------|-----|------|-----|-----------|----------------|----------------|-----|--------|--------|
| $^{24}12$ | 3 | 7 | id | 0.7288 | 0.2253 | 1.0 | 6.6570 | 49.442 |
| $^{24}12$ | 2 | 2 | 0.013 | 30.547 | 2.7859 | 1.0 | 0.5388 | 0.3388 |
| $^{24}12$ | 2 | 3 | id | 8.9910 | 1.2328 | 1.0 | 1.2170 | 1.6820 |
| $^{24}12$ | 2 | 4 | id | 3.9230 | 0.6920 | 1.0 | 2.1679 | 5.2870 |
| $^{24}12$ | 2 | 5 | id | 2.0045 | 0.4423 | 1.0 | 3.9164 | 12.883 |
| $^{24}12$ | 2 | 6 | id | 1.1585 | 0.2633 | 1.0 | 5.7035 | 26.695 |
| $^{24}12$ | 2 | 7 | id | 0.7288 | 0.2253 | 1.0 | 6.6570 | 49.442 |

Table 3 Continued...
5.4. Theoretical values using $\delta_p$ with angular momentum $l = 1$ and $l_\ast = l - \delta_p < r^\alpha >$ using the Messiah formulae [6].
Table 4: \(< r^α >\) l=1 P states values. Quantum defects same as in Table 3. The Table sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions only until the changes obtained in Table 1 are less than 1%. \(< r^α >\) values using extending the Messiah formulae.

| \(\Delta Z\) | \(M\) | \(Z_e\) | \(n\) | \(\delta_p\) | \(< \frac{1}{r^2}\>\) | \(< \frac{1}{r}\>\) | \(\langle r\rangle\) | \(< r^2\>\) |
|------------|--------|--------|-----|-----------|----------------|----------------|----------|--------|
| identical as upper | \(6^3\) | 2 | 3 | id | 0.3995 | 0.2230 | 0.3914 | 1 | 3.3537 | 13.927 |
| Table 3       | \(6^3\) | 3 | 3 | id | 0.0519 | 0.1481 | 1 | 9.6486 | 107.63 |
| identical as upper | \(6^3\) | 4 | 4 | id | 0.0019 | 0.0772 | 1 | 18.943 | 407.01 |
| \(O\) | \(16^8\) | 2 | 2 | id | 0.181 | 0.3919 | 0.5387 | 1 | 2.3380 | 6.5924 |
| average Operators | \(16^8\) | 3 | 3 | id | 0.1118 | 0.2334 | 1 | 5.9782 | 41.196 |
| \(16^8\) | 4 | 4 | id | 0.0462 | 0.1297 | 1 | 11.18 | 140.20 |
| \(16^8\) | 5 | 5 | id | 0.0234 | 0.0823 | 1 | 17.758 | 355.02 |
| \(16^8\) | 6 | 6 | id | 0.01346 | 0.0569 | 1 | 25.898 | 752.06 |
| \(16^8\) | 7 | 7 | id | 0.0084 | 0.0416 | 1 | 35.539 | 1412.71 |
| \(16^8\) | 8 | 2 | 1.141 | 0.3221 | 0.6740 | 1 | 6.0285 | 43.028 |
| \(16^8\) | 3 | 3 | id | 0.0533 | 0.2032 | 1 | 14.182 | 231.30 |
| \(16^8\) | 4 | 4 | id | 0.0174 | 0.0965 | 1 | 25.336 | 728.14 |
| \(16^8\) | 5 | 5 | id | 0.0077 | 0.0562 | 1 | 39.490 | 1756.6 |
| \(16^8\) | 6 | 6 | id | 0.0040 | 0.0562 | 1 | 56.644 | 3599.8 |
| \(16^8\) | 7 | 7 | id | 0.0024 | 0.0258 | 1 | 76.798 | 6600.8 |
| \(16^8\) | 8 | 2 | 0.861 | 1.1650 | 0.8821 | 1 | 1.5099 | 2.8484 |
| \(16^8\) | 3 | 3 | id | 0.2528 | 0.3185 | 1 | 4.5185 | 23.629 |
| \(16^8\) | 4 | 4 | id | 0.0923 | 0.1627 | 1 | 9.0270 | 92.428 |
| \(16^8\) | 5 | 5 | id | 0.0438 | 0.0985 | 1 | 15.035 | 254.33 |
| \(16^8\) | 6 | 6 | id | 0.0238 | 0.0659 | 1 | 22.544 | 569.42 |
| \(16^8\) | 7 | 7 | id | 0.0144 | 0.0472 | 1 | 31.552 | 1112.7 |
| \(16^8\) | 8 | 2 | 0.539 | 2.1265 | 1.2052 | 1 | 1.0926 | 1.4812 |
| \(16^8\) | 3 | 3 | id | 0.48754 | 0.4514 | 1 | 3.1703 | 11.623 |

Table 4 Continued...
Table 4: $< r^{\alpha} >$ l=1 P states values. Quantum defects same as in Table 3. The table sketches the averaged operator values obtained by extrapolating the Messiah formulae for hydrogenic ions only until the changes obtained in Table 1 are less than 1%. $< r^{\alpha} >$ values using extending the Messiah formulae.

$$\begin{array}{cccccccc}
\hline
^4Z & M & Z_e & n & \delta_p & \frac{1}{r^2} & \frac{1}{r^3} & N & < r > & < r^2 > \\
\hline
168 & 6 & 4 & id & 0.1823 & 0.2343 & 1 & 6.2480 & 44.277 \\
168 & 6 & 5 & id & 0.0870 & 0.1431 & 1 & 10.323 & 119.96 \\
168 & 6 & 6 & id & 0.0481 & 0.0964 & 1 & 15.403 & 265.85 \\
168 & 6 & 7 & id & 0.0094 & 0.0276 & 1 & 54.061 & 1974.5 \\
168 & 5 & 2 & 0.431 & 3.8750 & 1.6248 & 1 & 0.8115 & 0.8178 \\
168 & 5 & 3 & id & 0.9786 & 0.6665 & 1 & 2.1240 & 5.2119 \\
168 & 5 & 4 & id & 0.3848 & 0.3573 & 1 & 4.0691 & 18.779 \\
168 & 5 & 5 & id & 2.4311 & 0.1916 & 1 & 7.8590 & 69.225 \\
\hline
\textbf{Na} & average Operators & \delta_p & \\
2211 & 11 & 2 & 1.342 & 3.2900 & 1.5097 & 1 & 0.8658 & 0.9257 \\
2211 & 11 & 3 & id & 0.0613 & 0.2169 & 1 & 5.6835 & 38.404 \\
\hline
\textbf{Mg} & Operators & \delta_p & \\
2412 & 12 & 2 & 1.545 & 1.7846 & 0.9647 & 1 & 1.5450 & 3.1736 \\
2412 & 12 & 3 & id & 0.2290 & 0.2455 & 1 & 6.0987 & 43.376 \\
2412 & 12 & 4 & id & 0.0702 & 0.2455 & 1 & 13.652 & 211.68 \\
2412 & 12 & 5 & id & 0.0297 & 0.0619 & 1 & 24.206 & 659.16 \\
2412 & 12 & 6 & id & 0.0038 & 0.0619 & 1 & 62.178 & 1596.9 \\
2412 & 12 & 7 & id & 0.0025 & 0.0179 & 1 & 4.2359 & 21.194 \\
\hline
\end{array}$$

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* means that these low states quantum defects $\delta_s \geq n$ principal quantum number: no wave solution for $n_s \leq 1$.

** the upper footnote clearly indicates where relativistic theory of these highly stripped ions has to be considered $\delta_s \geq n$ principal quantum number: no wave solution for $n_s \leq 1$.

*** means that the data contained in the Tables are given correct to the third figure after the decimal point.
1 means that numerical Integral $\int_{0}^{\infty} r^2 |wa(r)|^2 \, dr$ differs from $< r^\alpha >$ from more than 1% Messiah quantities.

2 means that Messiah extrapolated quantities $< r^\alpha >$ are negative $\leq 0$ thus non-physical!

3 means that the polarization $V_p(r) = \frac{\alpha}{2r}$ change sign and acts as a repulsive potential!