Which one of the two atomic potential is better – the newest or the “ancient” one?

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Abstract

Recently, there appeared the tables of atomic potential by Maldonado et al. We show that this potential, when used to calculate some quantities which can be compared with experiment, gives worse results than the more than 40 years old tables by Lu et al.

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Introduction

In principle, the atom is a very simple system. The nucleus in the center and from one (for hydrogen) to ∼100 (for transuranic elements) electrons “orbiting” around. However, except the hydrogen atom – i.e. system of one proton and one electron – it cannot be exactly described. It is well known that the problem of three or more bodies is not analytically solvable in classical mechanics, not to mention the quantum one.

Therefore a concept of atomic potential was introduced. Such potential is an environment in which the electrons are moving as well as which they simultaneously help to create. And it then enables one to calculate various atomic characteristics needed (atomic energy levels, transition probabilities etc.) or some nuclear-atomic quantities (e.g. internal conversion coefficients) as well as other quantities such as, e.g., Fermi function required in the β-decay studies. That is why the correctness of the atomic potential, i.e. its ability to describe the reality as well as possible, is extremely important.

From the first decade of the last century, when Rutherford introduced the first realistic atomic model [1], it is clear that the atomic potential must be composed from a Coulombic one, \( V_C \sim 1/r \), and an ‘electronic’ part originated from the electronic cloud. However, as stated above, to calculate this electronic part (the ‘screening’) is a difficult task. One way to manage the screening is to use the so called screening constants, i.e. to replace the atomic number \( Z \) by an “effective” \( Z_{\text{eff}} = Z - \sigma \) where \( \sigma \) is calculated under various assumption and tabulated – see e.g. [2, 3]. This approach, however, does not supply a uniform potential for atom since the screening constants are not characteristics of the atom but of the particular atomic shells.

In the twenties of the last century, the statistical Thomas-Fermi model (potential) [4] and its relativistic improvement, Thomas-Fermi-Dirac model [5], were suggested. Approximately at the same time the Hartree-Fock model [6] was developed. This approach
does not use the conception of a potential and contains non-local terms. Finally the Hartree-Fock-Slater (HFS) model \[7\], where those non-local terms are replaced by an averaged potential was created. This one became the most popular approach and the HFS potential was often evaluated and tabulated for broad range of atomic numbers.

Another approach is the so called ROEP (relativistic, optimized, effective potential) approximation (see, e.g. \[8, 9\]) and its generalization RNPOEP (relativistic, numerically parametrized, optimized, effective potential) \[10\].

In this work we would like to show that the very recent tables \[11\] of the potential based on the RNPOEP method, when used to calculate some quantities, give surprisingly worse results than the more than 40 years old HFS tables \[12\].

2 Comparison

The potential \[12\] is obtained by self-consistent solution of the Dirac equation \[13\] and the detailed description of the method utilized is given in \[14\]. Moreover the effect of finite nucleus described by the Fermi distribution of the nuclear charge is taken into account. The potential is tabulated for all atoms (with \(Z=2\) to 126) in an exponentially equidistant mesh.

In the tables \[11\], the finite nucleus is described by a homogeneously charged sphere. The resulting potential, however, is not tabulated but is given in terms of Yukawan functions times a power of \(r\). In particular, \(V(r) = -\frac{Z}{2R}(3-r^2/R^2)\) for \(r < R\), \(V(r) = -\frac{1}{r}\left[Z - N + 1 + (N-1)f(r)\right]\) for \(r \geq R\). Here, \(Z\) is the atomic number, \(N\) is the number of electrons in the atom, \(R\) is the atomic radius and \(f(r) = \sum_{k=1}^{nC} c_k n_k e^{-\beta_k r}\). Usually, \(n_C=6\) and the parameters \(c_k, n_k,\) and \(\beta_k\) are results of the calculations and are tabulated in \[11\].

When we draw the shapes of the two potentials \[11, 12\] for the lightest (except hydrogen) element \(^2\text{He}\), which is presented in Fig.1, we see a strange behaviour of the potential \[11\]. For higher \(r\), the atomic potential for the neutral atom should behave as \(\sim 1/r\). The potential \[11\], however, shows an unexpected “wave” for \(r\) between 1 and \(\sim 20\).

![Figure 1: Comparison of the shapes of the potentials of Refs. (a) HFS [12], (b) RNPOEP [11] for neutral atom \(^2\text{He}\).](image-url)
Bohr radii. The reason of this behaviour is not clear. One possible reason may be the fact, that the potential [11] is a combination of analytical function. The effect may be similar to known oscillation of a function interpolated by polynomials when the interpolation is done improperly.

The above fact is only indirect and too weak argument against the potential [11]. To decide which of the two potentials is better, we do two studies. First, we evaluate the electron binding energies for several atoms with various Z. Comparing them with experimental values indicates the quality of the particular potentials. Second, we evaluate some internal conversion coefficients (ICC) for several transitions where the experimental values are known. And again, we may compare the calculated and experimental values and decide.

2.1 Binding energies

We have calculated electron energy eigenvalues using the both potentials [11, 12], respectively. To this aim the proper subroutine of the internal conversion coefficients evaluating program [15] was used. The calculations were performed for a broad range of atomic numbers, in particular for 17Cl, 29Cu, 36Kr, 37Rb, 45Tc, 62Sm, 74W, 76Os, and 88Ra. These eigenvalues were compared with the experimental electron binding energies [16]. As an example, the results for the 29Cu and 88Ra are given in Tables 1 and 2, respectively.

The 8 elements studied contain altogether 136 atomic subshells, this means that we have 136 energy eigenvalues. From these, in 79 cases the values calculated with the potential [12] are closer to the experimental binding energies than those calculated with [11]. This is about 58% of cases. However, all the cases of better agreement are those on the inner atomic shells as seen from Table 3. This is important since the binding energies of the outermost electrons are affected by chemical environment of the atom. Our calculations assume free isolated atom which need not be (and probably is not) true for the experimental values [16]. Therefore the disagreement of energies at the outer atomic subshells is not too significant.

As a quantitative measure of the agreement we have evaluated the quantity

\[ \Delta^2 = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\text{theor} - \text{exp}}{\text{exp}} \times 100 \right)^2, \]  

where theor and exp are theoretical and experimental, respectively, binding energies and i runs over the atomic subshells taken into consideration. (The scaling factor 100 has no physical meaning; it is there to ensure that the resulting \( \Delta^2 \)'s are in a “readable” range.) Following the above argumentations we took the inner subshells only which are enumerated in Table 3. Note that the expression \( \Delta^2 \) in (1) formally resembles the known quantity \( \chi^2 \) but it is not – it does not bear the statistical contents of the \( \chi^2 \). Nevertheless, it may be a measure of agreement – the larger \( \Delta^2 \), the poorer agreement. The values of \( \Delta^2 \) are presented in Table 3 too.
2.2 Conversion coefficients

For the calculations of the internal conversion coefficients, the good description of the atom – i.e. a good atomic potential – is needed, too. Therefore, we have evaluated some ICC (for which experimental data are available) using, respectively, both atomic potentials [11, 12]. The comparison with the mentioned experimental values may supply further arguments which of the two potentials is “better”.

For this aim we have chosen the ICC of the transitions of pure E2 multipolarity, in particular of the transitions \(2^+ \rightarrow 0^+\). These were chosen since their multipolarity is unambiguously determined and the comparison may not be disturbed by an effect of multipolarity mixing.

The following data were taken into account (the values of the transition energies are from [16]):

\( ^{152}\text{Sm} \) transition 121.78 keV

\[
\begin{align*}
K/L &= 1.74 \pm 0.06; \quad K/L_3 = 4.22 \pm 0.17 \quad [17] \\
M/L &= 0.250 \pm 0.015 \quad [18]
\end{align*}
\]

\( ^{162}\text{Dy} \) transition 86.788 keV

\[
\begin{align*}
K/L &= 0.62 \pm 0.03; \quad K/L_3 = 1.28 \pm 0.06 \quad [17] \\
M/L &= 0.242 \pm 0.015 \quad [18] \\
L_1/L_2 &= 0.136 \pm 0.004; \quad L_1/L_3 = 0.130 \pm 0.003; \quad L_2/L_3 = 0.962 \pm 0.014 \quad \text{weighted mean from} \ [19, 20, 21, 22]
\end{align*}
\]

\( ^{166}\text{Er} \) transition 80.557 keV

see Table 4

\( ^{182}\text{W} \) transition 100.107 keV

\[
\begin{align*}
K/L &= 0.375 \pm 0.027 \quad \text{w.m. from} \ [17, 23] \\
K/L_3 &= 0.850 \pm 0.026 \quad [17] \\
M/L &= 0.244 \pm 0.015 \quad [18] \\
\text{The next K to O are normalized to L}_3=10000: \quad [24] \\
K &= 7752 \pm 444; \quad L = 21789 \pm 203; \quad M = 5320 \pm 160; \quad N = 1138 \pm 62; \quad O = 199 \pm 30 \\
L_1/L_2 &= 0.091 \pm 0.015; \quad L_1/L_3 = 0.099 \pm 0.017; \quad L_2/L_3 = 1.087 \pm 0.014; \quad \text{w.m. from} \ [24, 19] \quad \text{and references therein} \\
M_1/M_2 &= 0.080 \pm 0.030; \quad M_1/M_3 = 0.082 \pm 0.038; \quad M_2/M_3 = 1.031 \pm 0.031 \quad \text{w.m. from} \ [24, 25] \\
L_3/M_3 &= 3.72 \pm 0.07; \quad M/NO = 3.59 \pm 0.09 \quad [23]
\end{align*}
\]

\( ^{188}\text{Os} \) transition 155.021 keV

\[
\begin{align*}
K/L &= 0.840 \pm 0.025; \quad K/L_3 = 2.24 \pm 0.07 \quad [17] \\
M/L &= 0.255 \pm 0.015 \quad [18]
\end{align*}
\]
\[ \frac{L_1}{L_3} = 0.266 \pm 0.005; \frac{L_2}{L_3} = 1.38 \pm 0.02 \] [22]

\(^{198}\text{Hg}\), transition 411.805 keV

\[ K/L = 2.69 \pm 0.06 \text{ w.m. from } [17, 26] \]

\[ K/L_3 = 15.15 \pm 0.60 \] [17]

\[ L:\text{M}:N:O = 1 : (0.252 \pm 0.004) : (0.077 \pm 0.004) : (0.018 \pm 0.002) \] [26]

\[ \frac{L_1}{L_2} = 0.969 \pm 0.027; \frac{L_1}{L_3} = 2.221 \pm 0.035; \frac{L_2}{L_3} = 2.294 \pm 0.067 \text{ w.m. from } [19, 26] \]

\[ K = 0.0308 \pm 0.0009 \] [27]

\(^{199}\text{Hg}\), transition 158.371 keV

All the next values are normalized to \(L_3=0.172\) [28]:

\[ K = 0.284 \pm 0.011; L_1 = 0.0387 \pm 0.0008; L_2 = 0.251 \pm 0.003; \]

\[ M_1 = 0.00943 \pm 0.00058; M_2 = 0.0645 \pm 0.0034; M_3 = 0.0457 \pm 0.0024; \]

\[ M_{45} = 0.00105 \pm 0.00010; N_1 = 0.00236 \pm 0.00017; N_2 = 0.0169 \pm 0.0010; \]

\[ N_3 = 0.0111 \pm 0.0006; OPN_{67} = .0051 \pm 0.0003; \]

Total ICC = 0.903 \pm 0.013.

Altogether 64 experimental data items were used.

To compare the agreement with experiment we chose the quantity similar to that in (1), in particular

\[ r = \left( \frac{\text{theor} - \text{exp}}{\sigma_{\text{exp}}} \right)^2 \] (2)

(where \(\sigma_{\text{exp}}\) is the experimental uncertainty), for the individual ICC or ICC ratios. Note that the \(r\) is, in fact, the square of the residual used in the quantity \(\chi^2\). Their sum, however, cannot be declared to be \(\chi^2\) since the particular data items are not independent. Nevertheless the claim “the higher \(r\), the worse agreement” is unquestionably true.

In Table 4, there are the experimental and theoretical data for the E2 transition 80.557 keV in \(^{166}\text{Er}\) together with the resulting values of \(r\). We see that the results with the potential [12] are better than those with [11] in 11 cases from 12. And the agreement in the remaining case (i.e. K/L) is almost the same.

The Table 5 shows the overview of the ICC comparison. For every transition studied, it includes the number of data items at disposal. In the last three columns are, respectively, the number of cases in favor (results [12] agree better), of cases ‘neutral’ (the agreement is practically the same), and ‘contra’ (results [11] agree better). We see that the absolute majority of cases (40 from 64) is ‘in favor’. In 16 cases (from 64), both sets of data agree with experiment similarly. And only in 8 cases the result with potential [11] agrees better than that with [12].

3 Conclusions

We have studied the quality of two atomic potentials. One of them, [12], was published more than 40 years ago (in tabular form), the other, [11], (given in form of several coefficients in analytical formulae) is quite new. We have checked their quality by the
comparison of the experimental data available with the theoretical results obtained by use of these two potentials. The data used were of two different areas – the electron binding energies and the internal conversion coefficients, respectively. In both these areas it turned out that – surprisingly – the older potential [12] describes the reality in general better than does the newest one [11].

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References

[1] E. Rutherford: *Phil. Mag.* 6(1911)21

[2] E. Clementi, D.L. Raimondi: *J. Chem. Phys.* 38(1963)2686; E. Clementi, D.L. Raimondi, W.P. Reinhardt: *J. Chem. Phys.* 47(1967)1300

[3] D. Thomas: http://www.chembio.uoguelph.ca/educmat/atomdata/shield/shield.htm

[4] L.H. Thomas: *Proc. Cambridge Phil. Soc.* 23(1927)542; E. Fermi: *Rend. Accad. Naz. Lincei* 1927 6(1927)602

[5] P.A.M. Dirac: *Proc. Cambridge Phil. Soc.* 26(1930)376

[6] D.R. Hartree: *Proc. Cambridge Phil. Soc.* 24(1928)89; D.R. Hartree: *Proc. Cambridge Phil. Soc.* 20(1924)189; V. Fock: *Z. Physik* 61(1930)126; *Z. Physik* 62(1930)795

[7] C. Slater: *Phys. Rev.* 81(1951)385

[8] R.T. Sharp, G.K. Horton: *Phys. Rev.* 90(53)317

[9] J.R. Talman, W.F. Shadwick: *Phys. Rev.* A14(1976)36

[10] E. Buendía, F.J. Gálvez, P. Maldonado, A. Sarsa: *J. Phys. B At. Mol. Opt. Phys.* 40(2007)3045

[11] P. Maldonado, A. Sarsa, E. Buendía, F.J. Gálvez: *At. Data Nucl. Data Tables* 97(2011)109

[12] C.C. Lu, T.T. Carlson, F.B. Malik, T.C. Tucker, C.W. Nestor Jr.: *At. Data* 3(1971)1
[13] I.P. Grant: *Proc. Roy. Soc. (London)* A262(1961)555; M.A. Coulthard: *Proc. Roy. Soc.* 91(1967)44

[14] T.C. Tucker, L.D. Roberts, C.W. Nestor Jr., T.A. Carlson, F.B. Malik: *Phys. Rev.* 178(1969)998, doi:10.1103/PhysRev.178.998

[15] M. Ryšavý, O. Dragoun, M. Vinduška: *Czech. J. Phys.* 27(1977)538, doi: 10.1007/BF01587131

[16] R.B. Firestone, V.S. Shirley: 1996 *Table of Isotopes, 8th Edition*, Vol. 1, (John Wiley & Sons)

[17] M. Bogdanović, M. Mladjenović, R. Stepić: *Z. Physik* 216(1968)267, doi: 10.1007/BF01392966

[18] M. Bogdanović, M. Mladjenović, R. Stepić: *Nucl. Phys.* A106(1968)209, doi: 10.1016/0375-9474(67)90839-1

[19] J.H. Hamilton: *Phys. Lett.* 20(1966)32, doi:10.1016/0031-9163(66)91036-5

[20] S.-E. Karlsson, I. Andersson, Ö. Nilsson, G. Malmsten, C. Nordling, K. Siegbahn: *Nucl. Phys.* 89(1966)513, doi:10.1016/0029-5582(66)90927-8

[21] W. Gelletly, J.S. Geiger, R.L. Graham: *Bull. Am. Phys. Soc.* 11(1966)352

[22] P. Erman, G.T. Emery, M.L. Perlman: *Phys. Rev.* 147(1966)858, doi: 10.1103/PhysRev.147.858

[23] Ö. Nilsson, I. Thorén, G. Malmsten, S. Högb erg: *Nucl. Phys.* A120(1968)561, doi: 10.1016/0375-9474(68)90464-8

[24] Ö. Nilsson, I. Thorén, G. Malmsten, S. Högb erg: *Nucl. Phys.* A100(1967)351, doi: 10.1016/0375-9474(67)90414-9

[25] S. Högb erg, J.-E. Bergmark, G. Malmsten, Ö. Nilsson: *Nucl. Phys.* A120(1968)569, doi:10.1016/0375-9474(68)90465-X

[26] V.M. Kel’man, R.Ya. Metzkhar’vishvili: *Zh. Eksp. Teor. Fiz.* 36(1959)691

[27] B.-G. Pettersson, L. Holmberg, T.R. Gerholm: *Nucl. Phys.* 65(1965)454, doi: 10.1016/0029-5582(65)90009-X

[28] O. Dragoun, V. Brabec, M. Ryšavý, A. Špalek: *Z. Physik* A281(1977)347, doi: 10.1007/BF01408182
Table 1: Comparison of binding energies for $^{65}$Cu.

| shell | energies [eV] | rel. diff. [%]$^{*)}$ |
|-------|---------------|------------------------|
|       | 12 | 11 | exp. | 16 | 12 | 11 |
| K     | 8945.79  | 8853.25  | 8978.9 | 0.37 | 1.40 |
| L₁    | 1086.66  | 1064.66  | 1096.1 | -0.86 | -2.87 |
| L₂    | 959.05   | 931.67   | 951.0  | 0.85  | -2.03 |
| L₃    | 937.89   | 911.20   | 931.1  | 0.73  | -2.14 |
| M₁    | 121.41   | 119.25   | 119.8  | 1.34  | -0.46 |
| M₂    | 80.63    | 78.03    | 73.6   | 9.55  | 6.02  |
| M₃    | 77.94    | 75.52    | 73.6   | 5.90  | 2.61  |
| M₄    | 10.15    | 8.58     | 1.6    | 534.37| 436.25 |
| M₅    | 9.84     | 8.31     | 1.6    | 515.00| 419.38 |

$^{*)}$ rel. diff. = $\frac{|x| - \text{exp}}{\text{exp}} \times 100$
Table 2: Comparison of binding energies for $^{88}$Ra.

| shell | energies [eV] | rel. diff. [%] |
|-------|---------------|----------------|
|       | [12] | [11] | exp. [16] | [12] | [11] |
| K     | 104470.20 | 103862.93 | 103915 | 0.53 | -0.05 |
| L₁    | 19255.93 | 19112.69 | 19232 | 0.12 | -0.62 |
| L₂    | 18571.80 | 18408.23 | 18484 | 0.48 | -0.41 |
| L₃    | 15460.97 | 15337.17 | 15444 | 0.11 | -0.69 |
| M₁    | 4801.88 | 4736.89 | 4822 | -0.42 | -1.77 |
| M₂    | 4486.08 | 4411.20 | 4483 | 0.07 | -1.60 |
| M₃    | 3775.30 | 3716.60 | 3785 | -0.26 | -1.81 |
| M₄    | 3260.29 | 3194.91 | 3248 | 0.38 | -1.63 |
| M₅    | 3112.27 | 3049.39 | 3105 | 0.23 | -1.79 |
| N₁    | 1192.01 | 1163.60 | 1208 | -1.32 | -3.68 |
| N₂    | 1050.11 | 1020.05 | 1055 | -0.46 | -3.31 |
| N₃    | 867.94 | 842.15 | 879 | -1.26 | -4.19 |
| N₄    | 637.33 | 612.57 | 636 | 0.21 | -3.68 |
| N₅    | 603.24 | 579.10 | 603 | 0.04 | -3.96 |
| N₆    | 299.86 | 278.77 | 287 | 4.48 | -2.87 |
| N₇    | 291.25 | 270.51 | 279 | 4.39 | -3.04 |
| O₁    | 255.99 | 242.95 | 251 | 1.99 | -3.21 |
| O₂    | 202.81 | 189.64 | 197 | 2.95 | -3.74 |
| O₃    | 162.87 | 150.54 | 153 | 6.45 | -1.61 |
| O₄    | 84.91 | 73.51 | 72 | 17.93 | 2.10 |
| O₅    | 79.13 | 67.88 | 66 | 19.89 | 2.85 |
| P₁    | 41.57 | 35.99 | 31 | 34.10 | 16.10 |
| P₂    | 26.19 | 22.19 | 20 | 30.95 | 10.95 |
| P₃    | 19.32 | 16.83 | 12 | 61.00 | 40.25 |

*) rel. diff. = \( \frac{|x|-\text{exp}}{\text{exp}} \times 100 \)
Table 3: List of atomic subshells where eigenenergies with potential \[12\] agree better with experiment.

| element | last | in favor*) | \(\Delta^2\) **) | n \[12\] | \[11\] |
|---------|------|------------|-----------------|--------|--------|
| 17Cl    | M\(_3\) | K,L\(_1\)  | 2               | 0.45   | 9.10   |
| 29Cu    | M\(_5\) | K,L\(_{1-3}\),M\(_1\) | 4    | 0.53   | 4.72   |
| 36Kr    | N\(_3\) | K,L\(_{1-3}\),M\(_{1-5}\),N\(_1\) | 10   | 2.67   | 20.92  |
| 37Rb    | O\(_1\) | K,L\(_{1-3}\),M\(_{1-3}\) | 7    | 1.17   | 21.39  |
| 43Tc    | N\(_5\) | K,L\(_{1-3}\),M\(_{1-3}\) | 7    | 0.39   | 5.13   |
| 62Sm    | N\(_6\) | K,L\(_{1-3}\),M\(_{1-5}\),N\(_{1,3}\) | 11   | 0.47   | 4.61   |
| 74W     | O\(_4\) | L\(_{1-3}\),M\(_{1-5}\),N\(_{1-5}\) | 13   | 0.31   | 7.63   |
| 76Os    | O\(_3\) | K,L\(_{1-3}\),M\(_{1-5}\),N\(_{1,3}\) | 12   | 0.19   | 3.69   |
| 88Ra    | P\(_3\) | K,L\(_{1-3}\),M\(_{1-5}\),N\(_{1-5}\),O\(_{1,2}\) | 16   | 1.08   | 6.96   |

*) the subshells where the results with \[12\] are closer to experiment

**) see Eq.(1)

Table 4: Comparison of ICC ratios for \(^{166}68\text{Er}\).

| shells | experiment | ref. | theory \[12\] | \[11\] | \[12\] | \[11\] | r\(^2\) *) |
|---------|------------|------|---------------|--------|--------|--------|-------------|
| K/L     | 0.416 ± 0.028 | \[17\] [23] | 0.4121 | 0.4123 | 0.019 | 0.017 |             |
| K/L\(_3\) | 0.805 ± 0.034 | \[17\] | 0.8466 | 0.8484 | 1.497 | 1.629 |             |
| L\(_3\)/M\(_3\) | 4.00 ± 0.05 | \[23\] | 4.0748 | 4.0831 | 2.238 | 2.762 |             |
| L\(_1\)/L\(_3\) | 0.0864 ± 0.0011 | \[20\] [21] [22] | 0.0812 | 0.0805 | 22.347 | 28.769 |             |
| L\(_2\)/L\(_3\) | 0.958 ± 0.010 | \[20\] [21] [22] | 0.9730 | 0.9771 | 2.250 | 3.648 |             |
| L\(_1\)/L\(_2\) | 0.0910 ± 0.0037 | \[20\] | 0.0835 | 0.0824 | 4.109 | 5.402 |             |
| M/L     | 0.250 ± 0.018 | \[18\] | 0.2440 | 0.2432 | 0.006 | 0.143 |             |
| M/NO    | 3.78 ± 0.09 | \[23\] | 3.798 | 3.861 | 0.040 | 0.810 |             |
| M\(_1\)**) | 7.90 ± 0.18 | \[25\] | 7.500 | 7.462 | 4.938 | 5.921 |             |
| M\(_2\)**) | 93.4 ± 0.8 | \[25\] | 94.75 | 94.96 | 2.848 | 3.803 |             |
| M\(_4\)**) | 1.05 ± 0.04 | \[25\] | 1.049 | 1.007 | 0.001 | 1.156 |             |
| M\(_5\)**) | 1.05 ± 0.05 | \[25\] | 0.974 | 0.936 | 2.310 | 5.198 |             |

*) see Eq.(2)

**) these subshells are normalized to M\(_3\)=100
Table 5: Overview of the agreement with experimental data for the two sets of the ICC – with potentials [12] and [11], respectively.

| element   | no. of data | pro*) | neu**) | con)***) |
|-----------|-------------|-------|--------|----------|
| $^{152}$Sm  | 3           | 2     | 1      | 0        |
| $^{162}$Dy  | 6           | 2     | 2      | 2        |
| $^{166}$Er  | 12          | 11    | 1      | 0        |
| $^{182}$W   | 16          | 7     | 7      | 2        |
| $^{188}$Os  | 5           | 4     | 0      | 1        |
| $^{198}$Hg  | 9           | 6     | 2      | 1        |
| $^{199}$Hg  | 13          | 8     | 3      | 2        |
| total      | 64          | 40    | 16     | 8        |

*) results ‘in favor’, for [12] are better
**) agreement comparable for both [12] and [11]
****) results for [11] are better