Relativistic Self-Consistent-Field Calculations of the Hyperfine Structure in the 4d-Shell Ions

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Abstract
Relativistic self-consistent-field calculations of the radial hyperfine integrals have been performed in the 4d-shell element ions. The comparison with available experimental results gives an estimate of configuration interaction effects in the hyperfine interaction in these ions. The results can also be used to derive nuclear moments from laser spectroscopic measurements of radioactive isotopes.

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1 Introduction
During the last three decades a great deal of experimental[1] and theoretical[2, 3] work has been done on the hyperfine structure (hfs) of the 4d-shell elements’ atoms, whereas relatively little is known about the hfs in the singly charged ions. In the past years, the application of the laser-rf-double-resonance (LRDR) technique[4, 5] as well as the use of saturation spectroscopy in hollow-cathodes[6], has given experimental data of the hfs in the Y and Zr ions. It is also expected that ion traps will open up a possibility to perform measurements in these ions. Of particular interest is it to perform systematic studies of the hfs in the 4d-shell atoms and ions since many-body effects are significant. In the atoms many of these effects are masked by the problem of obtaining accurate values of the eigenvectors used in the analysis. The ions on the other hand are closer to Russel-Saunders (LS)
coupling, yielding a way of obtaining more accurate eigenvectors. There is also an increased interest in spectroscopy of the 4d-shell elements as a way of extracting nuclear properties, such as nuclear moments and changes in the mean-squares charge radii, from radioactive isotopes[7]. In most cases these studies are performed using collinear laser spectroscopy on mass-separated ion-beams or using ion-traps. As there are very little known of the 4d-shell ions, it is important to have as much data available as possible. This becomes more important as some 4d-shell atoms only have one stable isotope and in some cases with I=1/2, thus only giving rise to magnetic dipole interaction. The best example is Y, which is expected to exhibit drastic changes in the nuclear radii, due to the shape transition at N=59. It is important to have high quality calculations in order to extract the nuclear electric quadrupole moment. In this article relativistic hyperfine integrals of the magnetic dipole and electric quadrupole interactions for the 4d-shell ions, within the configurations 4d^N, 4d^{N-1}s and 4d^{N-2}s^2, are presented. These integrals have been calculated using relativistic (SCF) wave functions of Hartree-Fock (HF) type and with a statistical exchange known as optimised Hartree-Fock-Slater (OHFS)[2].

2 Theoretical Approach

Hyperfine structure analysis of the magnetic dipole interaction is normally performed with the effective Hamiltonian taken as[1, 2]

\[ H_{1\text{eff}}^{\text{f}} = 2\frac{\mu_0}{4\pi} \mu_B \sum_{i=1}^{N} \left[ l_i \langle r^{-3} \rangle_{01} - \sqrt{10}(sC^2)_{i1} (r^{-3})_{12} + s_i \langle r^{-3} \rangle_{10} \right] \cdot M^1 \]  

where \( M^1 \) is a nuclear tensor operator of rank 1, \( l_i \), \( (sC^2)_{i1} \) and \( s_i \) are the orbital, spin-dipole and spin operators, respectively, of the open shell electrons, with the summation over all open shells in the model space. In the case of an unpaired s-electron only the spin operator term contributes to the hfs energy. The effective Hamiltonian for the quadrupole interaction is usually given as[1, 2]

\[ H_{2\text{eff}}^{\text{f}} = \frac{e}{4\pi\epsilon_0} \sum_{i=1}^{N} \left[ C_i^2 \langle r^{-3} \rangle_{02} + \sqrt{3} \frac{3}{10} U_{i}^{(11)^2} \langle r^{-3} \rangle_{11} + \sqrt{3} \frac{3}{10} U_{i}^{(13)^2} \langle r^{-3} \rangle_{13} \right] \cdot M^2 \]

where \( M^2 \) is a nuclear tensor-operator of rank 2, \( C_i^2 \) is a second-rank tensor-operator and \( U^{(\kappa\lambda)k} \) are double tensor operators of rank \( \kappa \) in spin space,
rank λ in orbital space and rank k in the combined spin-orbital space. The effective radial integrals \( \langle r^{-3}_{ij} \rangle_{nl} \) in (1) and (2) are linear combinations of relativistic one-electron radial integrals \( \langle r^{-3}_{ij} \rangle_{nl}^{M} \) and \( \langle r^{-3}_{ij} \rangle_{nl}^{E} \) [2]. In the non-relativistic limit the integrals \( \langle r^{-3}_{ij} \rangle_{nl}^{01} \), \( \langle r^{-3}_{ij} \rangle_{nl}^{12} \) and \( \langle r^{-3}_{ij} \rangle_{nl}^{02} \) will approach the non-relativistic value of \( r^{-3} \), i.e.

\[
\langle r^{-3} \rangle = \int P^{2}_{nl}(r)r^{-3}dr
\]  

For s-electrons the effective integral is defined by

\[
\langle r^{-3} \rangle_{ns}^{10} = \frac{2}{3} \langle r^{-3} \rangle_{ns}^{M}
\]  

which in the non-relativistic limit approaches the value

\[
\langle r^{-3} \rangle_{ns}^{10} \to \frac{2}{3} \left[ \frac{dP_{ns}(r)}{dr} \right]_{r=0}^{2}
\]  

The \( \langle r^{-3} \rangle_{nl}^{10} \), \( \langle r^{-3} \rangle_{nl}^{11} \) and \( \langle r^{-3} \rangle_{nl}^{12} \) integrals have no non-relativistic values and will approach zero. If we in addition to relativistic effects also include configuration interaction effects, the picture gets more complicated. However, it has been shown that the effective Hamiltonians in (1) and (2) also act as effective operators in the case of configuration interaction. The radial integrals should then be modified to take this into account. This is normally done by adding a configuration interaction contribution \( \Delta_{nl}^{ij} \) to the relativistic value.

\[
\langle r^{-3} \rangle_{nl,E}^{ij} = \langle r^{-3} \rangle_{nl,R}^{ij}(1 + \Delta_{nl}^{ij})
\]  

The indices E and R refer to experimental and relativistic Hartree-Fock values. In this way can configuration interaction effects of one-body type be included in the effective Hamiltonian. Configuration interaction effects of two-body type can be included in the \( \Delta_{nl}^{ij} \) corrections if they are allowed to be LS dependent. A discussion of these two-body operators can be found in \([8, 9]\). For the contact term \( \langle r^{-3} \rangle_{nl,E}^{10} \) and the pure relativistic terms \( \langle r^{-3} \rangle_{nl,E}^{11} \) and \( \langle r^{-3} \rangle_{nl,E}^{13} \), it is common to instead use.

\[
\langle r^{-3} \rangle_{nl,E}^{10} = \langle r^{-3} \rangle_{nl,R}^{10} + \langle r^{-3} \rangle_{nl,C}^{10}
\]

\[
\langle r^{-3} \rangle_{nl,E}^{11} = \langle r^{-3} \rangle_{nl,R}^{11}
\]

\[
\langle r^{-3} \rangle_{nl,E}^{13} = \langle r^{-3} \rangle_{nl,R}^{13}
\]  

Here the index C stands for core-polarisation. The reason to use (7) instead of (6) for the contact term \( \langle r^{-3} \rangle_{nl,E}^{10} \) is that the dominant contribution is
from configuration interaction (core-polarisation) and not from relativistic effects. The configuration interaction for the \( \langle r^{-3} \rangle_{nl,E}^{11} \) and \( \langle r^{-3} \rangle_{nl,E}^{13} \) terms is usually assumed to be small compared with the SCF-values and are therefore neglected. Normally one defines effective radial parameters \( a_{nl}^{ij} \) and \( b_{nl}^{ij} \) which are related to the nuclear moments \( \mu_I \) and \( Q \), respectively, and to the effective values of the radial integrals \( \langle r^{-3} \rangle \) as:

\[
\begin{align*}
    a_{nl}^{ij} &= \frac{2 \mu_B \mu_I}{\hbar} \langle r^{-3} \rangle_{nl}^{ij} l > 0, ij = 01, 12, 10 \\
    a_{ns}^{10} &= \frac{2 \mu_B \mu_I}{\hbar} \langle r^{-3} \rangle_{ns}^{10} \\
    b_{nl}^{ij} &= \frac{e^2}{\hbar} Q \langle r^{-3} \rangle_{nl}^{ij} l > 0, ij = 02, 11, 13
\end{align*}
\]

These parameters are treated as adjustable quantities to be fitted to the experimental data in order to take configuration interaction and relativistic effects into account. The experimentally determined hfs-constants for a particular \( |SLJ\rangle \) state are normally first evaluated assuming \( J \) to be a good quantum number. Knowing these first order values, it is possible to calculate the influence on the hfs from other \( J \) states. This is normally done using perturbation theory to the second order, why the corrections are referred to as second order corrections (SOC). In most cases these corrections are smaller than the experimental uncertainty and can be neglected, but in the case of high-precision measurements or when different \( J \) states are close energetically can the corrections be substantial. An indication of large second order hyperfine interaction is comparably large errors for the obtained experimental \( A \) and \( B \) constants. The corrected hfs-constants can then be expressed as,

\[
\begin{align*}
    A(J) &= \sum_{\text{all config.}} \sum_{nl,ij=01,12,10} k_{nl}^{ij} a_{nl}^{ij} \\
    B(J) &= \sum_{\text{all config.}} \sum_{nl,ij=02,11,13} k_{nl}^{ij} b_{nl}^{ij}
\end{align*}
\]

in terms of (effective) radial parameters and an angular term \( (k_{nl}^{ij}) \), that can be calculated using the eigenvectors of the states. In the 4d shell ions a mixing exists between the configurations \( 4d^N \), \( 4d^{N-1}5s \) and \( 4d^{N-2}5s^2 \). Due to this mixing will the magnetic dipole interaction constants be expressed in twelve different radial parameters, three from each configuration for the d-electrons, one from the unpaired s-electron and two cross-configuration
parameters. For the quadrupole interaction eleven parameters are needed, three for the d-electrons from each configuration and two cross-configuration terms. The cross-configuration radial parameters are normally assumed to be small and are therefore omitted from the analysis. For the determination of these hyperfine parameters the hfs-constants should be known in a sufficient number of atomic states in the three configurations. The parameters are determined in a least-squares fit procedure. In most cases are the hfs-constants only known in a few states. In order to reduce the number of free parameters’, assumptions have to be made to get experimental values of the hyperfine parameters. For example, ratios between the spin-dipole and orbital parameters, calculated with relativistic wavefunctions, can be used. However, even if the hfs is known in ten or more states, the parameters evaluated in the least-squares fit may be of rather unphysical magnitude. This is especially the case for the parameters which coefficients, in the parameterised expressions are small or sensitive to the intermediate coupling constants, namely the spin-dipole and the relativistic quadrupole operators $U^{(11)2}$ and $U^{(13)2}$. The quadrupole parameters $b_{n\ell}^{11}$ and $b_{n\ell}^{13}$ are in addition hard to extract due to their small values. Another problem in the extraction of the hyperfine parameters is that the expressions for the different hfs constants are linear dependent in pure LS-coupling. It is only the breakdown of LS-coupling that can resolve the linear dependence, which puts great demands on the eigenvectors used. The calculations performed in this work was done using relativistic wavefunctions of Hartree-Fock(HF) type, and wavefunctions obtained by the so called Optimised Hartree-Fock-Slater (OHFS) method [2]. Further description on the Self-Consistent-Field procedure, as well as the methods used can be found in the review by Lindgren and Rosen [2].

3 Results

Using the relativistic wavefunctions calculated by the HF and OHFS SCF procedures, hyperfine radial integrals have been obtained for the $4d^N$, $4d^{N-1}5s$ and $4d^{N-2}5s^2$ configurations in the 4d shell element ions. The wavefunctions has been evaluated for the average energy of the configurations. The results are presented in tables’ 1-3. As a general trend all the hyperfine integrals are increasing in magnitude with increasing occupation number. The integrals $\langle r^{-3}\rangle_{4d}^{01}$, $\langle r^{-3}\rangle_{4d}^{12}$ and $\langle r^{-3}\rangle_{4d}^{02}$ are found to increase when going from the configuration $4d^N$ to $4d^{N-2}5s^2$ for a certain element. The effective nuclear charge seen by the d-electrons is increased due to less screening when an
4d-electron is changed to an 5s-electron. The $\langle r^{-3}\rangle_{4d}^{10}$, $\langle r^{-3}\rangle_{4d}^{11}$ and $\langle r^{-3}\rangle_{4d}^{13}$ integrals are more sensitive to relativistic effects and the contraction of d-shells, and show a more irregular behaviour. From the calculated integrals one finds an interesting feature, the ratio $\langle r^{-3}\rangle_{nd}^{11}/\langle r^{-3}\rangle_{nd}^{13}$ seems to be fairly constant. In addition, the change compared with similar calculations in the 3d to 5d element atoms [3, 11] is very small, while the individual values change drastically. The reason for this is not known Experimental data exists only in Y and Zr, however, there might exist Fabry-Perot measurements but these have not been considered here. The quality of the experimental hyperfine integrals is depending on the number of states analysed and the quality of the eigenvectors used.

3.1 Y$^+$

An extended analysis has been done in Y [10], where the odd parity 4d5p configuration has also been analysed. The comparison between the experimental and calculated integrals show that the HF values describe the orbital operator better than the OHFS, following the trend found in the 4d-shell atoms [3]. It can also be seen that the agreement for the orbital part is good, while the spin-orbital integrals differ significantly. This result is by no means surprising, as the spin-orbital part is more sensitive to the quality of the eigenvectors as well as relativistic and configuration interaction effects. The bad agreement for the d-electron contact terms is due to core polarisation. However, the problem with linear dependence as discussed earlier, is a very severe problem, that also causes the contact terms to be linked to each other. This problem can be resolved by obtaining more experimental data. Yttrium is also a special case as it has only one stable isotope with I=1/2, so one can not compare the hyperfine interaction constants of radioactive isotopes with the stable isotope in order to deduce the nuclear quadrupole moment. In this case calculations of the radial hyperfine integrals, can be used to deduce the nuclear quadrupole moment.

3.2 Zr$^+$

The hyperfine structure in Zr$^+$ has been studied experimentally by Young et al. [4] and theoretically by Beck and Datta [13]. The ionic ground state was measured by Campbell et al. [12]. The 12 states measured arises from the 4d$^3$ and 4d$^2$5s configurations. In the first approximation is this enough for an analysis of the 7 radial hfs parameters of these configurations. However there are two complications, first the states are mixed within the 3 configu-
rations $4d^3$, $4d^25s$ and $4d5s^2$, leading to 10 radial hfs parameters, secondly while some states are heavily mixed, some are close to LS-coupling. This will lead to a linear dependence of some parameters and that other parameters will have a very small angular factor for some states. The equation-system to be solved will be very badly conditioned, and the least-squares fit will be very sensitive to small changes in the angular factors. This makes an analysis quite uncertain, unless more states are measured. The experimental values of the radial parameters presented in tables 2 and 3, are obtained from assuming pure LS-coupling and excluding the most heavily mixed states. The result is as expected quite bad.

4 Conclusion

The lack of experimental data makes it hard to draw any conclusions other than the obvious. The 4d-shell elements are quite difficult to perform experiments on, due to their refractoriness, and the short wavelength transitions in the ions. There have, however, been recent developments on different ion-sources as well as on lasers, so the available experimental data is expected to increase within a not too distant future. One reason for systematic studies is to find dependence of hfs effects depending on the degree of ionisation. If the studies could be done on singly as well as multiple charged ions, one could study the $\langle r^{-3}\rangle_{4d}^{10}$ integral that shows the extent of core-polarisation for non-s-electrons. It has been shown in studies of ErI, ErII and ErIII that $\langle r^{-3}\rangle_{4f}^{10}$ exhibits a near proportionality to the number of electrons in the open shell [14]. This is of importance as the available ab initio methods fail to reproduce these effects.
Table 1: Relativistic hyperfine integrals (in units of $a_0^{-3}$) for the magnetic dipole and electric quadrupole interaction in the $4d^{N-2}5s^2$ configurations.

| Z   | Ion  | Conf.  | Method | $\langle r^{-3}\rangle_{4d}^{01}$ | $\langle r^{-3}\rangle_{4d}^{12}$ | $\langle r^{-3}\rangle_{4d}^{10}$ | Magnetic dipole $\langle r^{-3}\rangle_{4d}$ | $\langle r^{-3}\rangle_{4d}^{02}$ | $\langle r^{-3}\rangle_{4d}^{13}$ | $\langle r^{-3}\rangle_{4d}^{11}$ | Electric quadrupole $\langle r^{-3}\rangle_{4d}$ |
|-----|------|--------|--------|-------------------------------|-------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|--------------------------------|
| 40  | Zr   | $4d5s^2$ | OHFS   | 3.014                         | 3.172                         | -0.070                        | 3.303                         | 0.358                         | -0.124                        |                                |                                |
|     |      |        |        | 2.782                         | 2.945                         | -0.073                        | 2.796                         | 0.349                         | -0.112                        |                                |                                |
| 41  | Nb   | $4d^25s^2$ | OHFS   | 3.804                         | 4.012                         | -0.091                        | 3.828                         | 0.478                         | -0.164                        |                                |                                |
|     |      |        |        | 3.502                         | 3.703                         | -0.089                        | 3.523                         | 0.447                         | -0.157                        |                                |                                |
| 42  | Mo   | $4d^35s^2$ | OHFS   | 4.647                         | 4.914                         | -0.117                        | 4.679                         | 0.620                         | -0.210                        |                                |                                |
|     |      |        |        | 4.309                         | 4.584                         | -0.123                        | 4.336                         | 0.604                         | -0.215                        |                                |                                |
| 43  | Tc   | $4d^45s^2$ | OHFS   | 5.551                         | 5.887                         | -0.147                        | 5.592                         | 0.785                         | -0.264                        |                                |                                |
|     |      |        |        | 5.143                         | 5.443                         | -0.131                        | 5.180                         | 0.707                         | -0.236                        |                                |                                |
| 44  | Ru   | $4d^55s^2$ | OHFS   | 6.523                         | 6.939                         | -0.181                        | 6.575                         | 0.977                         | -0.328                        |                                |                                |
|     |      |        |        | 6.073                         | 6.462                         | -0.171                        | 6.120                         | 0.904                         | -0.305                        |                                |                                |
| 45  | Rh   | $4d^65s^2$ | OHFS   | 7.570                         | 8.078                         | -0.221                        | 7.634                         | 1.200                         | -0.401                        |                                |                                |
|     |      |        |        | 7.075                         | 7.536                         | -0.201                        | 7.135                         | 1.095                         | -0.363                        |                                |                                |
| 46  | Pd   | $4d^75s^2$ | OHFS   | 8.690                         | 9.305                         | -0.267                        | 8.769                         | 1.457                         | -0.485                        |                                |                                |
|     |      |        |        | 8.145                         | 8.687                         | -0.235                        | 8.219                         | 1.314                         | -0.428                        |                                |                                |
| 47  | Ag   | $4d^85s^2$ | OHFS   | 9.891                         | 10.627                        | -0.320                        | 9.987                         | 1.752                         | -0.581                        |                                |                                |
|     |      |        |        | 9.346                         | 10.117                        | -0.342                        | 9.429                         | 1.741                         | -0.605                        |                                |                                |
Table 2: Relativistic hyperfine integrals (in units of $a_0^{-3}$) for the magnetic dipole and electric quadrupole interaction in the $4d^{N-1}s$ configurations.

| Z | Ion | Conf. | Method | $\langle r^{-3}\rangle_{4d}^{01}$ | $\langle r^{-3}\rangle_{4d}^{12}$ | $\langle r^{-3}\rangle_{4d}^{10}$ | $\langle r^{-3}\rangle_{5s}^{01}$ | $\langle r^{-3}\rangle_{4d}^{02}$ | $\langle r^{-3}\rangle_{4d}^{13}$ | $\langle r^{-3}\rangle_{4d}^{11}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | Y | 4d5s | OHFS | 1.841 | 1.950 | -0.049 | 69.59 | 1.850 | 0.226 | -0.084 |
|   |   |   | HF | 1.779 | 1.863 | -0.037 | 60.86 | 1.788 | 0.190 | -0.065 |
|   |   |   | Exp | 0.933 | 7.352 | 11.342 | 44.74 |        |        |        |
| 40 | Zr | 4d25s | OHFS | 2.588 | 2.741 | -0.068 | 81.93 | 2.602 | 0.329 | -0.120 |
|   |   |   | HF | 2.442 | 2.589 | -0.066 | 70.79 | 2.454 | 0.311 | -0.115 |
|   |   |   | Exp | 2.74 | 0.95 | 7.20 | 37.44 |        |        |        |
| 41 | Nb | 4d35s | OHFS | 3.359 | 3.564 | -0.091 | 93.68 | 3.379 | 0.448 | -0.160 |
|   |   |   | HF | 3.137 | 3.320 | -0.081 | 82.118 | 3.156 | 0.404 | -0.143 |
| 42 | Mo | 4d45s | OHFS | 4.179 | 4.444 | -0.117 | 105.06 | 4.206 | 0.587 | -0.207 |
|   |   |   | HF | 3.910 | 4.169 | -0.116 | 92.21 | 3.934 | 0.559 | -0.202 |
| 43 | Tc | 4d55s | OHFS | 5.056 | 3.390 | -0.148 | 116.48 | 5.091 | 0.749 | -0.262 |
|   |   |   | HF | 4.722 | 5.018 | -0.131 | 103.05 | 4.755 | 0.675 | -0.232 |
| 44 | Ru | 4d65s | OHFS | 5.998 | 6.412 | -0.183 | 127.90 | 6.043 | 0.938 | -0.325 |
|   |   |   | HF | 5.620 | 6.003 | -0.169 | 113.54 | 5.602 | 0.856 | -0.300 |
| 45 | Rh | 4d75s | OHFS | 7.012 | 7.520 | -0.224 | 139.33 | 7.069 | 1.158 | -0.399 |
|   |   |   | HF | 6.584 | 7.072 | -0.217 | 124.18 | 6.365 | 1.093 | -0.382 |
| 46 | Pd | 4d85s | OHFS | 8.102 | 8.717 | -0.270 | 150.87 | 8.173 | 1.411 | -0.484 |
|   |   |   | HF | 7.626 | 8.138 | -0.222 | 134.70 | 7.695 | 1.234 | -0.404 |
| 47 | Ag | 4d95s | OHFS | 9.268 | 10.006 | -0.342 | 162.93 | 9.355 | 1.702 | -0.580 |
|   |   |   | HF | 8.787 | 9.554 | -0.324 | 147.79 | 8.862 | 1.688 | -0.500 |
Table 3: Relativistic hyperfine integrals (in units of $a_0^{-3}$) for the magnetic dipole and electric quadrupole interaction in the 4$d^N$ configurations.

| Z | Ion | Conf. | Method | $\langle r^{-3}\rangle_{4d}^{01}$ | $\langle r^{-3}\rangle_{4d}^{12}$ | $\langle r^{-3}\rangle_{4d}^{10}$ | $\langle r^{-3}\rangle_{4d}^{02}$ | $\langle r^{-3}\rangle_{4d}^{13}$ | $\langle r^{-3}\rangle_{4d}^{11}$ |
|---|---|---|---|---|---|---|---|---|---|
| 39 | Y | 4$d^2$ | OHFS | 1.506 | 1.605 | -0.045 | 1.512 | 0.198 | -0.077 |
| | | | HF | 1.492 | 1.569 | -0.034 | 1.499 | 0.167 | -0.060 |
| | | | Exp | 1.466 | 1.562 | -3.455 | | | |
| 40 | Zr | 4$d^3$ | OHFS | 2.195 | 2.343 | -0.067 | 2.206 | 0.301 | -0.114 |
| | | | HF | 2.117 | 2.251 | -0.060 | 2.127 | 0.277 | -0.104 |
| | | | Exp | 2.09 | 1.27 | -4.38 | | | |
| 41 | Nb | 4$d^4$ | OHFS | 2.927 | 3.129 | -0.091 | 2.943 | 0.419 | -0.157 |
| | | | HF | 2.784 | 2.954 | -0.076 | 2.799 | 0.369 | -0.133 |
| | | | Exp | | | | | | |
| 42 | Mo | 4$d^5$ | OHFS | 3.711 | 3.975 | -0.118 | 3.733 | 0.557 | -0.205 |
| | | | HF | 3.521 | 3.769 | -0.112 | 3.542 | 0.521 | -0.193 |
| | | | Exp | | | | | | |
| 43 | Tc | 4$d^6$ | OHFS | 4.556 | 4.892 | -0.150 | 4.585 | 0.718 | -0.262 |
| | | | HF | 4.306 | 4.602 | -0.132 | 4.334 | 0.647 | -0.231 |
| | | | Exp | | | | | | |
| 44 | Ru | 4$d^7$ | OHFS | 5.464 | 5.883 | -0.187 | 5.503 | 0.906 | -0.327 |
| | | | HF | 5.170 | 5.554 | -0.172 | 5.207 | 0.835 | -0.300 |
| | | | Exp | | | | | | |
| 45 | Rh | 4$d^8$ | OHFS | 6.443 | 6.958 | -0.229 | 6.492 | 1.124 | -0.403 |
| | | | HF | 6.096 | 6.615 | -0.234 | 6.140 | 1.095 | -0.404 |
| | | | Exp | | | | | | |
| 46 | Pd | 4$d^9$ | OHFS | 7.497 | 8.122 | -0.278 | 7.559 | 1.375 | -0.489 |
| | | | HF | 7.109 | 7.605 | -0.217 | 7.172 | 1.172 | -0.391 |
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