All-order calculations of the spectra of Ba II, Ra II, Fr I and superheavy elements 
E119 I and E120 II.

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A technique based on summation of dominating classes of correlation diagrams to all orders in 
Coulomb interaction is used to calculate the energies of the lowest \(s, p\) and \(d\) states of Ba II, Ra II, Fr 
I, E119 I and E120 II. Breit and quantum electrodynamic corrections are also included. Comparison 
with experiment for Ba II, Ra II and Fr I demonstrates that the accuracy of the calculations is on 
the level of 0.1\%. The technique has been applied to predict the spectra of superheavy elements 
E119 and E120\(^+\). The role of the ladder diagrams (V. A. Dzuba, Phys. Rev. A 78, 042502 (2008)) 
which is the most recent addition to the method has been emphasised. Their inclusion significantly 
raises the accuracy of the calculations and expands the applicability of the method.

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I. INTRODUCTION

Accurate atomic calculations are very important for a 
number of applications, such as search for new physics be-
yond standard model in the measurements of the parity 
and time invariance violation in atoms \[1, 2\], search for 
space-time variation of fundamental constants \[3\], pre-
diction of the properties of atoms and ions were experi-
mental data is poor or absent, etc. The latter include in 
particular highly charge ions \[4\] and superheavy elements 
(\(Z > 100\)) \[5, 6\].

Atoms with one valence electron above closed shells 
play a special role in these studies. Their relatively sim-
ple electron structure allows high accuracy of the calcula-
tions leading to very accurate interpretation of experi-
mental data. For example, current best low-energy test of 
the standard model is based on the measurements of par-
ity non-conservation in cesium \[7\] which has one valence 
electron above closed-shells of Xe-like core. Interpreta-
tion of the measurements is based on accurate calcula-
tions of Ref. \[8\]. Further progress for the PNC measure-
ments is considered for atoms and ions which have electron 
structure similar to those of cesium. This includes 
Rb \[9\], Ba\(^+\) \[10\], Ra\(^+\) \[11\], Fr \[12\], and Fr-like ions \[13\]. 
Accurate predictions of the spectra and other prop-
erties of the superheavy elements were done for E119, and 
E120\(^+\) \[14, 15\] which are also analogous of cesium.

The most popular method currently used for accurate 
calculations for atoms with one valence electron is the 
coupled cluster (CC) method. Its accuracy depends on 
the number of terms included in the expansion of the 
wave function. Its simplest version, which includes only 
terms with single and double excitations (SD) from the 
reference ground state configuration, gives good accuracy 
only for limited number of systems. In particular, the 
accuracy is poor for cesium, and missed third-order dia-
grams need to be included for better accuracy \[16\]. The 
accuracy is significantly better if also valence triple exi-
tations are included (the CCSDvT approximation) \[17\]. 
However, the method becomes very demanding for com-
puter power.

An alternative approach was developed in our group 
about 25 years ago. It is based on summations of se-
lected classes of higher-order correlation diagrams to all 
orders in Coulomb interactions \[18\]. Further in the paper 
we will call it the correlation potential method (CPM) 
for convenience of references. The following classes of 
the correlations were included in CPM in all orders: (a) 
screening of Coulomb interaction of the valence electron 
with electrons in the core by other core electrons, (b) in-
teraction between an electron excited from atomic core 
with the hole in the core caused by this excitation, and 
(c) iterations of the correlation operator \(\hat{\Sigma}\). This turned 
out to be very powerful method which gives a fraction of a per 
cent accuracy for the energies of \(s, p\) states of alkali 
atoms. The computer power needed for the calculations 
is small even compared to simple SD approximation. On 
the other hand, accuracy for \(d\) states and accuracy for 
atoms other than alkali was not high. For example, the 
accuracy for Ba\(^+\) is almost the same as for Cs. This is 
contrary to what is expected since the relative value of 
the correlation corrections are smaller for Ba\(^+\) than for 
Cs due to two times stronger central potential. The rea-
son for lower accuracy was explained in Ref. \[20\] for the 
case of cesium and thallium. The fact of high accuracy 
for \(s, p\) states of alkali atoms and lower accuracy for 
other atomic systems is related to a particular choice of 
higher-order diagrams included in CPM method. The 
three classes of higher-order diagrams listed above dom-
inate in systems where valence electron is on large dis-
tances from the core. When valence electron is closer to 
the core another class of higher-order diagrams becomes 
important. These diagrams describe residual Coulomb 
interaction of the valence electron with the core. When 
valence electron is close to the core this interaction be-
comes strong and needs to be included in all orders. In 
the CPM method this interaction is included in second 
order only. This limits the accuracy of the calculations 
for systems where external electron is close to the core. 
The most pronounced example is probably thallium atom 
where external \(6p\) electron is very close to the \(6s\) electrons 
and strongly interacts with them \[21\].
A method to include the core-valence residual interaction to all-orders was developed in Ref. [22]. It is based on iterations of the equations similar to the CC SD equations. The terms arising from the iterations of these equations were described by diagrams which were called ladder diagrams. When the contribution of the ladder diagrams was added to the result of the CPM calculations it lead to significant improvement of the accuracy of the calculations for $s$, $p$ and $d$ states of Cs and Tl.

In present paper we further extend the application of the method by performing calculations for Ba$^+$ and Ra$^+$. Calculations for francium are also included as another test of the method which helps to estimate the accuracy for the E119 superheavy element. Breit and QED corrections are included for higher accuracy. The spectra of E119 and E120$^+$ were considered before [15, 16]. However, present paper presents more complete and accurate results.

II. METHOD OF CALCULATIONS

Accurate calculations for heavy and superheavy many-electron atoms need accurate treatment of correlations and relativistic effects. We use the all-order correlation potential method [21] supplemented by inclusion of ladder diagrams [22] to include dominating correlation effects to all orders in residual Coulomb interaction. For accurate treatment of relativistic effects we start the calculations with the relativistic Hartree-Fock (RHF) method based on solving Dirac-like equations and then we include Breit interaction and quantum electrodynamic (QED) corrections.

A. Correlations

Calculations start from the relativistic Hartree-Fock method (RHF) in the $V^{N-1}$ approximation. States of valence electron are calculated with the use of the correlation potential $\hat{\Sigma}$:

$$\hat{H}_0 + \hat{\Sigma} - \epsilon_v \psi_v = 0. \quad (1)$$

Here $\hat{H}_0$ is the RHF Hamiltonian, $\psi_v$ and $\epsilon_v$ are the wave function and removal energy of the valence electron. Correlation potential $\Sigma$ is defined in such a way that its average value over the wave function of valence electron in state $v$ is the correlation correction to the energy of this state

$$\delta\epsilon_v = \int \psi_v(r) \Sigma(r) \psi_v(r) dr_1 dr_2. \quad (2)$$

$\Sigma$ is a non-local operator similar to Hartree-Fock exchange potential. Many-body perturbation theory expansion for $\Sigma$ starts from second order. The second-order correlation operator $\hat{\Sigma}^{(2)}$ has been described in our previous works [22, 23]. For most of atomic systems inclusion of just second-order $\Sigma$ leads to significant improvements of the accuracy of the calculations. Further improvement is achieved when higher-order correlations are also included. Beyond second order we include four dominating classes of higher order correlations: (a) screening of Coulomb interaction, (b) hole-particle interaction, (c) iterations of $\Sigma$, and (d) ladder diagrams. All these higher-order correlations are included in all orders of residual Coulomb interaction.

Two of these classes of higher-order correlations are included in the calculations of $\Sigma$ [21], the screening of Coulomb interaction between valence and core electrons by other core electrons, and hole-particle interaction between a hole left in the core by electron excitation and the excited electron. Third chain of all-order diagrams, the iteration of the correlation potential, is included by iterating the equations [11]. Note that the single-electron wave functions for the states of valence electron found by solving equations [11] are often called Brueckner orbitals (BO).

Another chain of all-order diagrams describes residual Coulomb interaction of external electron with the core. It is included by solving coupled-cluster-like equations for ladder diagrams [22]. The equations are obtained by taking single-double (SD) approximation for the coupled-cluster (CC) method and removing terms which otherwise would lead to double counting of the effects which are already included in the correlation potential $\Sigma$. We stress once more that the most important all-order effect, the screening of Coulomb interaction, is better treated in the calculation of the all-order correlation potential $\Sigma$ than in solving of the CC equations. This is because of the use of the relativistic Fynman diagram technique while calculating $\Sigma$. Relativistic technique includes all possible time ordering of the hole-particle loops which in terms of the CC expansion means inclusion of selected triple and higher excitations.

The equations for ladder diagrams can be written as two sets of equations [22]. The first is for atomic core:

$$\left(\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n\right) \rho_{mnab} = g_{mnab} +$$

$$\sum_{rs} \sum_{rscar} \sum_{rcb} \left(g_{cnbr}^1 + g_{cnar}^2 + g_{embr}^3 + g_{emar}^4\right).$$

And another is for a specific state $v$ of an external electron:

$$\left(\epsilon_v + \epsilon_b - \epsilon_m - \epsilon_n\right) \rho_{mnvb} = g_{mnvb} +$$

$$\sum_{rs} \sum_{rscar} \sum_{rcb} \left(g_{cnbr}^1 + g_{cnar}^2 + g_{embr}^3 + g_{emar}^4\right).$$

Here parameters $g$ are Coulomb integrals

$$g_{mnab} = \int \int \psi^*_m(r_1) \psi^*_n(r_2) \psi_a(r_1) \psi_b(r_2) dr_1 dr_2,$$

variables $\rho$ are the coefficients representing expansion of the atomic wave function over double excitations from
the zero-order Hartree-Fock reference wave function; parameters \( \epsilon \) are the single-electron Hartree-Fock energies. Coefficients \( \rho \) are to be found by solving the equations iteratively starting from

\[
\rho_{mnij} = \frac{g_{mnij}}{\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n}.
\]

Indexes \( a, b, c \) numerate states in atomic core, indexes \( m, n, r, s \) numerate states above the core, indexes \( i, j \) numerate any states.

The equations for the core \( \Sigma \) do not depend on the valence state \( v \) and are iterated first. The convergence is controlled by the correction to the core energy

\[
\delta E_C = \frac{1}{2} \sum_{abmn} g_{abmn} \tilde{\rho}_{mnab},
\]

where

\[
\tilde{\rho}_{mnab} = \rho_{mnab} - \rho_{mnba}.
\]

When iterations for the core are finished the equations \( \delta \epsilon_v \) are iterated for as many valence states \( v \) as needed. Correction to the energy of the valence state \( v \) arising from the iterations of equations \( \delta \epsilon_v \) is given by

\[
\delta \epsilon_v = \sum_{mnb} g_{abmn} \tilde{\rho}_{mvab} + \sum_{mnab} g_{abmn} \tilde{\rho}_{mnwb}.
\]

Since Brueckner energy \( \epsilon_v \), in the equation \( \epsilon_v \) and the correction \( \delta \epsilon_v \), in the equation \( \delta \epsilon_v \) both include the second-order correlation correction, it is convenient to define the correction associated with the ladder diagrams as a difference

\[
\delta \epsilon_v^{(l)} = \delta \epsilon_v - \langle v | \hat{\Sigma}^{(2)} | v \rangle.
\]

Here \( \hat{\Sigma}^{(2)} \) is the second-order correlation potential.

B. Breit interaction

We treat Breit interaction in zero energy transfer approximation. The Breit Hamiltonian includes magnetic interaction between moving electrons and retardation:

\[
\hat{H}^B = -\frac{\alpha_1 \cdot \alpha_2 + (\alpha_1 \cdot \hat{n})(\alpha_2 \cdot \hat{n})}{2r}.
\]

Here \( \hat{n} = nr \), \( r \) is the distance between electrons, and \( \alpha \) is the Dirac matrix.

Similar to the way Coulomb interaction is used to form self-consistent Coulomb potential, Breit interaction is used to form self-consistent Breit potential. Other words, Breit interaction is included into self-consistent Hartree-Fock procedure. Thus the important relaxation effect is included. The resulting inter-electron potential in \( \hat{V} \) consist of two terms

\[
\hat{V} = V^C + V^B,
\]

\( V^C \) is the Coulomb potential, \( V^B \) is the Breit potential. Coulomb interaction in the second-order correlation potential \( \hat{\Sigma}^{(2)} \) is also modified to include Breit operator \( \hat{B} \). The Breit correction to the energy of external electron is found by comparing the second-order Brueckner energies (Eq. \( \hat{\Sigma}^{(2)} \)) calculated with and without Breit interaction.

C. QED corrections

We use the radiative potential method developed in Ref. \[24\] to include quantum radiative corrections. This potential has the form

\[
V_{\text{rad}}(r) = V_U(r) + V_g(r) + V_e(r),
\]

where \( V_U \) is the Uehling potential, \( V_g \) is the potential arising from the magnetic formfactor, and \( V_e \) is the potential arising from the electric formfactor. The \( V_U \) and \( V_e \) terms can be considered as additions to nuclear potential while inclusion of \( V_g \) leads to some modification of the Dirac equation (see Ref. \[24\] for details). As for the case of Breit interaction, the QED corrections to the energies of external electron are found by solving equations \( \hat{\Sigma}^{(2)} \) with and without radiative potential.

III. RESULTS AND DISCUSSION

Results of calculations of the energies of the lowest \( s \), \( p \) and \( d \) states of \( \text{Ba}^+ \), \( \text{Ra}^+ \), \( \text{Eu}^{120^+} \), \( \text{Fr} \) and \( \text{E}^{119} \) in different approximations are presented in Table I. The RHF column presents Hartree-Fock energies obtained by solving Eq. \( \hat{\Sigma} \) without \( \Sigma \), the \( \hat{\Sigma}^{(2)} \) column presents Brueckner energies obtained by solving Eq. \( \hat{\Sigma}^{(2)} \) with the second order correlation potential \( \hat{\Sigma}^{(2)} \). Note that since these energies are obtained by solving the equations \( \hat{\Sigma}^{(2)} \) rather than by calculating average value of the correlation potential \( \hat{\Sigma}^{(2)} \) as in \( \hat{\Sigma} \), they already include one all-order effect, the iterations of \( \hat{\Sigma}^{(2)} \). The \( \hat{\Sigma}^{\infty} \) column presents Brueckner energies obtained by solving Eq. \( \hat{\Sigma}^{(2)} \) with all-order \( \hat{\Sigma}^{\infty} \). The difference between this and previous columns illustrate the importance of higher-order correlation effects in \( \Sigma \), the screening of Coulomb interaction and hole-particle interaction.

The Ladder column presents contributions from ladder diagrams given by \( \hat{l} \). We present these contributions separately for the convenience of the discussion. We would like to emphasise the role of ladder diagrams since it is the latest addition to our all-order technique which has been tested before only for cesium and thallium atoms \[22\]. If ladder diagrams are not included the all-order correlation potential method developed in Ref. \[21\] gives good accuracy for \( s \) and \( p \) states of alkali atoms and their isoelectronic sequences. As it was demonstrated in Ref. \[22\] adding ladder diagrams widens the range of atomic systems for which the technique gives good accuracy. The ladder diagram contributions do not affect
TABLE I: Removal energies (cm$^{-1}$) of the lowest $s, p, d$ states of Ba$^+$, Ra$^+$, E120$^+$, Fr and E119 in different approximations together with ladder diagram, Breit and QED corrections and experimental data. $\Delta = \frac{|E_{\text{final}} - E_{\text{expt}}|}{E_{\text{expt}}}$.

| Ion/Atom | State | RHF | $\Sigma^{(2)}$ | $\Sigma^{\infty}$ | Ladder | Breit | QED | Final | $\Delta(\%)$ | Expt. a |
|----------|-------|-----|---------------|----------------|---------|-------|-----|-------|------------|---------|
| Ba$^+$   | 6$s_{1/2}$ | 75339 | 82379 | 80780 | -156 | -4 | -45 | 80575 | -0.14 | 80687 |
|          | 6$p_{1/2}$ | 57265 | 61216 | 60571 | -128 | -27 | 3 | 60419 | -0.01 | 60425 |
|          | 6$p_{3/2}$ | 55873 | 59424 | 58847 | -118 | -7 | 0 | 58722 | -0.02 | 58735 |
|          | 5$d_{3/2}$ | 68138 | 77444 | 76377 | -763 | 58 | 22 | 75694 | -0.16 | 75813 |
|          | 5$d_{5/2}$ | 67664 | 76500 | 75536 | -765 | 84 | 18 | 74873 | -0.19 | 75012 |
| Ra$^+$   | 7$s_{1/2}$ | 75898 | 83864 | 82035 | -219 | -12 | -90 | 81714 | 0.16 | 81842 |
|          | 7$p_{1/2}$ | 56878 | 61432 | 60744 | -182 | -51 | 0 | 60511 | 0.03 | 60491 |
|          | 7$p_{3/2}$ | 52905 | 56278 | 55776 | -140 | -11 | -3 | 55625 | -0.01 | 55633 |
|          | 6$d_{3/2}$ | 62355 | 71364 | 70294 | -620 | 72 | 42 | 69788 | 0.04 | 69758 |
|          | 6$d_{5/2}$ | 61592 | 69313 | 68563 | -643 | 92 | 33 | 68045 | -0.08 | 68099 |
| E120$^+$ | 8$s_{1/2}$ | 83262 | 92195 | 90241 | -518 | -68 | -132 | 89523 |
|          | 8$p_{1/2}$ | 60040 | 66792 | 65448 | -378 | -125 | -16 | 64929 |
|          | 8$p_{3/2}$ | 49290 | 52744 | 52006 | -178 | -12 | -11 | 51805 |
|          | 7$d_{3/2}$ | 56610 | 66765 | 64815 | -590 | 68 | 61 | 64354 |
|          | 7$d_{5/2}$ | 56408 | 63526 | 62678 | -623 | 82 | 46 | 62183 |
| Fr       | 7$s_{1/2}$ | 28767 | 34136 | 32924 | -136 | 5 | -47 | 32746 | -0.3 | 32849 |
|          | 7$p_{1/2}$ | 18855 | 21004 | 20707 | -76 | -14 | 0 | 20617 | 0 | 20612 |
|          | 7$p_{3/2}$ | 17655 | 19179 | 18971 | -57 | 0 | -1 | 18913 | -0.06 | 18925 |
|          | 6$d_{3/2}$ | 13825 | 17190 | 16724 | -139 | 34 | 11 | 16630 | 0.07 | 16619 |
|          | 6$d_{5/2}$ | 13924 | 16849 | 16512 | -153 | 37 | 9 | 16405 | -0.09 | 16419 |
| E119     | 8$s_{1/2}$ | 33608 | 40489 | 39040 | -403 | -24 | -77 | 38536 |
|          | 8$p_{1/2}$ | 20130 | 23905 | 23473 | -184 | -47 | 6 | 23236 |
|          | 8$p_{3/2}$ | 16672 | 18335 | 18114 | -74 | -1 | -3 | 18036 |
|          | 7$d_{3/2}$ | 13477 | 17495 | 16807 | -149 | 34 | 19 | 16711 |
|          | 7$d_{5/2}$ | 13827 | 16809 | 16567 | -181 | 34 | 15 | 16435 |

aBa$^+$ and Ra$^+$ data from Ref. [22], Fr data from Ref. [26].

much the $s$ and $p$ states of alkali atoms while improve significantly the accuracy for $d$ states. They also significantly improve the accuracy for such complicated system as thallium atom [22]. As one can see from the Table I ladder diagrams are important for all systems considered in present paper leading to significant improvements of the results. Breit and QED corrections are relatively small. However, adding them generally leads to better agreement with experiment. The data for Breit and QED corrections for Fr and E119 is in good agreement with recent calculations by Thierfelder and Schwerdtfeger [27]. Detailed discussion of the QED corrections and comparison with other calculations presented in our previous work [16]. Our final results for Ba$^+$, Ra$^+$ and Fr (see Table I) differ from the experimental data by small fraction of per cent only.

Final results for Fr and superheavy elements E119 and E120$^+$ are presented in Table II together with the results of our previous calculations for Cs [22], E119 and E120$^+$ [16], the results of the coupled cluster calculations by Eliav et al for Cs, Fr and E119 and experimental data for Cs and Fr. Judging by the data in the tables table we believe that the accuracy of the calculated energies is on the level of 0.2%.

There are two important differences between present calculations and those of Ref. [16]. Ladder diagrams were not included in [16]. On the other hand the ab initio results for superheavy elements were corrected in [16] by extrapolating of the theoretical error from lighter elements. This extrapolation assumes similar electron structure of the elements. In contrast, present calculations are pure ab initio calculations with no fitting or extrapolating. Calculation of ladder diagrams reveal some small differences in electron structure of superheavy elements and their lighter analogs. Indeed, the contribution of ladder diagrams tends to be larger for superheavy elements. This is consistent with larger removal energies. Larger removal energies means that valence electron is closer to the core, therefore its residual Coulomb interaction with the core described by ladder diagrams should be larger as well. Note that the difference between our present and previous [16] results is sometimes larger than 0.2% (the accuracy of present calculations). This is particularly true for the ground state energies. We believe that the accuracy of present calculations is better that in Ref. [16] since they are pure ab initio calculations with no fitting and no extrapolation and they do take into account small differences in electron structure between superheavy elements and their lighter analogs.

Table II shows very good agreement between present results and the results of the coupled cluster calculations of Ref. [15]. The agreement is better than with our previous calculation [16]. In the end, both methods, the method of present work and the CCSD method used in
The result of this paper is twofold. First, we demonstrate that supplementing previously developed all-order correlation potential method with ladder diagrams leads to significant improvement in accuracy of calculations not only for alkali atoms but also for their isoelectronic ions. Second, we apply the developed technique to perform very accurate calculations of the spectra of superheavy elements E119 and E120$^+$. 

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Ref. [15] demonstrate very similar levels of accuracy.

Table II presents also the energies of $d$ states of E119 and E120$^+$. Correlations for $d$ states are usually larger than for $s$ and $p$ states and accuracy of calculations is lower. That was part of the reason why these states were not considered before. However, as it is evident from the data in Table II, the inclusion of ladder diagrams leads to practically the same accuracy for $d$ states as for $s$ and $p$ states. Therefore, we include the results for the energies of $d$ states of superheavy elements in Table II.

### IV. CONCLUSION

The result of this paper is twofold. First, we demonstrate that supplementing previously developed all-order correlation potential method with ladder diagrams leads to significant improvement in accuracy of calculations not only for alkali atoms but also for their isoelectronic ions. Second, we apply the developed technique to perform very accurate calculations of the spectra of superheavy elements E119 and E120$^+$. 

### TABLE II: Removal energies (cm$^{-1}$) of Cs, Fr, E119 and E120$^+$; comparison with experiment [23, 24], our earlier calculations [16, 22] and the coupled cluster with single and double excitations (CCSD) calculations by Eliav et al [15].

| Atom/Ion State | This work | CCSD [15] | Expt. | Atom/Ion State | This work | Ref. [16] | CCSD [15] |
|----------------|-----------|-----------|-------|----------------|-----------|-----------|-----------|
| Cs 6$s_{1/2}$ | 31384 | 31455 | 31400 | E119 8$s_{1/2}$ | 38536 | 38582 | 38377 |
| 6$p_{1/2}$ | 20185 | 20233 | 20229 | 8$p_{1/2}$ | 23236 | 23272 | 22079 |
| 6$p_{3/2}$ | 19632 | 19681 | 19675 | 8$p_{3/2}$ | 18036 | 18053 | 18007 |
| 5$d_{5/2}$ | 16932 | 19009 | 16908 | 7$d_{5/2}$ | 16711 | 16505 |
| 5$d_{3/2}$ | 16849 | 16800 | 16810 | 7$d_{3/2}$ | 16435 | 16297 |
| 7$s_{1/2}$ | 12886 | 12872 | 12872 | 9$s_{1/2}$ | 14061 | 14079 | 14050 |
| 7$p_{1/2}$ | 9462 | 9641 | 9641 | 9$p_{1/2}$ | 10439 | 10415 | 10365 |
| 7$p_{3/2}$ | 9462 | 9459 | 9459 | 9$p_{3/2}$ | 8882 | 8866 | 8855 |
| 6$d_{5/2}$ | 8815 | 8818 | 8818 | 8$d_{5/2}$ | 8513 | 8455 |
| 6$d_{3/2}$ | 8772 | 8775 | 8775 | 8$d_{3/2}$ | 8399 | 8338 |
| 8$s_{1/2}$ | 7082 | 7090 | 7090 | 10$s_{1/2}$ | 7521 | 7536 | 7519 |
| 8$p_{1/2}$ | 5689 | 5698 | 5698 | 10$p_{1/2}$ | 6024 | 6018 | 5997 |
| 8$p_{3/2}$ | 5606 | 5615 | 5615 | 10$p_{3/2}$ | 5334 | 5328 | 5320 |
| 7$d_{3/2}$ | 5354 | 5359 | 5359 | 9$d_{3/2}$ | 5177 | 5154 |
| 7$d_{5/2}$ | 5333 | 5338 | 5338 | 9$d_{5/2}$ | 5118 | 5092 |
| Fr 7$s_{1/2}$ | 32746 | 32930 | 32849 | E120$^+$ 8$s_{1/2}$ | 89523 | 89931 |
| 7$p_{1/2}$ | 20617 | 20597 | 20612 | 8$p_{1/2}$ | 64929 | 65080 |
| 7$p_{3/2}$ | 18913 | 18918 | 18925 | 8$p_{3/2}$ | 51805 | 51874 |
| 6$d_{5/2}$ | 16630 | 16527 | 16619 | 7$d_{5/2}$ | 64354 | 62183 |
| 6$d_{3/2}$ | 16405 | 16339 | 16419 | 7$d_{3/2}$ | 62183 |
| 8$s_{1/2}$ | 13075 | 13131 | 13116 | 9$s_{1/2}$ | 40085 | 40110 |
| 8$p_{1/2}$ | 9730 | 9732 | 9736 | 9$p_{1/2}$ | 32618 | 32604 |
| 8$p_{3/2}$ | 9184 | 9190 | 9191 | 9$p_{3/2}$ | 27978 | 27951 |
| 7$d_{3/2}$ | 8584 | 8597 | 8604 | 8$d_{3/2}$ | 31489 |
| 7$d_{5/2}$ | 8490 | 8507 | 8516 | 8$d_{5/2}$ | 30727 |
| 9$s_{1/2}$ | 7160 | 7184 | 7178 | 10$s_{1/2}$ | 23307 | 23357 |
| 9$p_{1/2}$ | 5726 | 5738 | 5738 | 10$p_{1/2}$ | 19887 | 19926 |
| 9$p_{3/2}$ | 5477 | 5493 | 5493 | 10$p_{3/2}$ | 17664 | 17678 |
| 8$d_{5/2}$ | 5209 | 5243 | 5248 | 9$d_{3/2}$ | 19293 |
| 8$d_{3/2}$ | 5162 | 5198 | 5203 | 9$d_{3/2}$ | 18921 |

*Results for Cs are taken from Ref. [22].

*Cs data from Ref. [29]; Fr data from Ref. [20].
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