Energy levels and lifetimes of Gd IV and enhancement of the electron dipole moment

V. A. Dzuba† and O. P. Sushkov‡
School of Physics, University of New South Wales, Sydney 2052, Australia

W. R. Johnson§ and U. I. Safronova¶
Department of Physics, 225 Nieuwland Science Hall
University of Notre Dame, Notre Dame, IN 46566
(Dated: November 16, 2018)

We have calculated energy levels and lifetimes of $4f^7$ and $4f^65d$ configurations of Gd IV using Hartree-Fock and configuration interaction methods. This allows us to reduce significantly the uncertainty of the theoretical determination of the electron electric dipole moment (EDM) enhancement factor in this ion and, correspondingly, in gadolinium-containing garnets for which such measurements were recently proposed. Our new value for the EDM enhancement factor of Gd$^{3+}$ is $-2.2 \pm 0.5$. Calculations of energy levels and lifetimes for Eu III are used to control the accuracy.

PACS numbers: PACS: 11.30.Er, 32.10.Dk, 31.15.Ne

I. INTRODUCTION

There have been recent suggestions by Lamoreaux \cite{1} and Hunter \cite{2} for searches of the electron electric dipole moment (EDM) in solid state experiments with the compounds Gadolinium Gallium Garnet Gd$_5$Ga$_5$O$_{12}$ and Gadolinium Iron Garnet Gd$_3$Fe$_5$O$_{12}$. It is known that an EDM of a system in a stationary quantum state violates both time-reversal (T) and space-reflection (P) symmetries. This is why searches for EDMs of elementary particles, atoms, and molecules are very important for studies of violations of fundamental symmetries \cite{3}. The best limit on the electron EDM comes from the Berkeley experiment of Regan et al. \cite{4} with an atomic Thallium beam, $d_e < 1.6 \times 10^{-27}$ cm. There are ideas on how to improve the sensitivity substantially working with PbO \cite{5} and YbF \cite{6} molecules. An alternative that can provide a real breakthrough is to use solids containing uncompensated electron spins. This idea was already suggested in \cite{7} by Shapiro \cite{8}. Application of a strong electric field to electrons bound within a solid would align the EDMs of the unpaired electrons. This should lead to a simultaneous alignment of the electron spins; the magnetic field arising from this alignment could be detected experimentally. Another possibility is to polarize electrons by the external magnetic field. This causes alignment of electron EDMs, and hence induces a voltage across the sample that could be detected. An experiment of this kind has been performed with nickel-zinc ferrite \cite{9}; however, due to experimental limitations, the result was not very impressive. Interest in this approach has been renewed recently owing to the suggestions by Lamoreaux \cite{1}, Hunter \cite{2} to perform similar experiments with Gadolinium Gallium Garnet and Gadolinium Iron Garnet, employing new experimental techniques. The estimates of sensitivity presented in \cite{1} look highly promising: an improvement by several orders of magnitude is feasible.

The first calculations of the expected effects have been performed in recent papers Buhmann et al. \cite{10}, Kuenzi et al. \cite{11}, using a semiempirical approach. The compounds under consideration contain Gd$^{3+}$ ions, see Ref. \cite{12}, that give the most important contributions to the effect owing to their large nuclear charge. Therefore, from the theoretical point of view, the problem can be split into two closely connected, but still distinct, parts. The first part is the evaluation of the EDM of a Gd$^{3+}$ ion induced by an assumed electron EDM, and the second part is an account of the combined electron-lattice dynamics of the solid. It has been shown by Buhmann et al. \cite{10} that the main contribution to the Gd$^{3+}$ EDM comes from mixing between $4f$ and $5d$ electrons. This mixing depends on the energy separation between $4f^7$ and $4f^65d$ configurations. There are experimental data on the relevant energy intervals \cite{13}. However, Ref. \cite{13} does not contain identification of all possible levels; therefore, one cannot rely completely on the data. It has been pointed out by \cite{14} that accurate calculations of the energy levels of the $4f^65d$ configuration of Gd$^{3+}$ ion are the needed to improve the accuracy of the EDM calculation.

There were recent measurements of lifetimes of some states of the $4f^65d$ configuration of Eu III \cite{15}, which has an electronic structure similar to Gd IV. Therefore, calculations of lifetimes in Eu III provide a good test of the accuracy of $E1$-transition amplitudes which determine both lifetimes and the EDM enhancement factor. In the present work we perform calculations of the energy levels and lifetimes of both Eu III and Gd IV.

---

*Electronic address: dzuba@newt.phys.unsw.edu.au
†Electronic address: sushkov@newt.phys.unsw.edu.au
‡Electronic address: johnson@nd.edu
§Electronic address: usafrono@nd.edu
¶Electronic address: safronova@nd.edu
II. CALCULATION OF ENERGIES

We use two different sets of computer codes to do our calculations. One is our own configuration interaction program and the second is a code written by Cowan [14] and freely available via the Internet. We use both codes to compute energy levels of Eu III and Gd IV. Calculations for the Eu III are mostly done to control the accuracy. These two ions have similar electronic structure, however, much of the reliable experimental data is available for Eu III while limited data are available for Gd IV. We restrict our study to the lowest odd configuration 4f7 and even configuration 4f65d; these are the configurations most relevant to the atomic EDM.

We will describe our approach in detail while restricting our comments on the Cowan code to fewer general remarks. Since our calculations are relativistic, we will use the abbreviation RCI (relativistic configuration interaction) to refer to them. We start our calculations using the relativistic Hartree-Fock (HF) method. Calculations of the self-consistent field are done for an ion in its ground state. This is an open-shell system with 7 out of 14 electrons in its outermost 4f subshell. Therefore, we apply 50% weighting to the contribution of the 4f subshell to the HF potential. This weighting is further reduced to \( \approx 46\% \) when the interaction of a 4f electron with other electrons of the same subshell is calculated (6/13 \( \approx 0.46 \)).

Note, that our calculations are relativistic and we apply the same weighting to both 4f subshells. RCI results for the 4f65d configuration are sensitive to how the 5d state is calculated. It is natural to calculate it in the field of the 4f6 subshell, which means that HF potential is modified by removing a contribution of one 4f electron. However, the 5d state obtained in this way is still not good enough to achieve accurate energy levels. This is probably because the self-consistent field is calculated for the configuration 4f7 and not for 4f65d. Therefore, we further modify the 5d state by introducing a correction to the HF potential in which this state is calculated:

\[
\delta V = -\frac{\alpha}{2(a^2 + r^2)}. \quad (1)
\]

Here \( \alpha \) is polarizability of an ion in the 4f6 configuration, \( a \) is a cut-off parameter introduced to remove the singularity in the origin. Potential \( \delta V \) describes the effect of core polarization by the field of external electron. We treat \( \alpha \) as a fitting parameter. Its value \( \alpha = 0.5a_B^2 \) has been chosen to obtain accurate energy levels for Eu III. The value of \( \alpha \) is not very important because the 5d wave function is small at short distances. We use \( a = a_B \). We use the same values of \( \alpha \) and \( a \) for both Eu III and Gd IV.

We now have four single-electron basis states, 4f5/2, 4f7/2, 5d3/2 and 5d5/2. Many-electron basis states for the RCI calculations are constructed by distributing seven electrons over these states in all possible ways. Then, many-electron states of definite parity and total angular momentum \( J \) are constructed. The actual matrix size depends on the configuration considered and the value of the total angular momentum \( J \); it varies between \( 1 \) (4f7, \( J = 25/2 \)) and 377 (4f65d, \( J = 9/2 \)).

Energy intervals in the RCI calculations are sensitive to the value of Slater integrals \( F_2(4f, 4f), F_2(4f, 5d) \), etc.). In the HF approximation, the value of these integrals, and consequently the energy intervals, are overestimated. This is because of screening of the Coulomb interaction between valence electrons by core electrons (see, e.g. [13]). In the present work we include this screening semi-empirically by introducing screening factor \( f_2 = 0.8 \). The value of this factor was chosen to fit energy intervals in Eu III. Thus, in the end, we have two fitting parameters, a core polarizability \( \alpha \) and a screening factor \( f_2 \). The values of both of these factors are chosen for Eu III and then the same values are used for Gd IV.

Calculations with the Cowan code are very similar to the RCI calculations. This is also a configuration interaction method, although in its non-relativistic realization. There are also two fitting procedures in the Cowan code. One is scaling of the Coulomb integrals by a factor of 0.85. This is very similar to our screening of Coulomb interaction. Another fitting which we use in the Cowan code is changing “by hand” the average energy of the ground state configuration. This is equivalent to shifting all energy intervals between the ground and excited configuration by the same value. A few more details about calculations with the Cowan code will be given in Section V.

III. CALCULATION OF LIFETIMES

Lifetimes of the three 4f65d \( ^8P_{5/2,7/2,9/2} \) states of Eu III have been recently measured by Zhiguo et al. [13]. Calculations using the Cowan code give values which are about three times smaller (see Table I). It is important to investigate the source of this discrepancy.

In a single-configuration approximation which we use in the present work, lifetimes of all states of the 4f65d configuration are determined by single radial integral

\[
R_{4f,5d} = \int_0^\infty R_{4f}(r)R_{5d}(r)r^3dr, \quad (2)
\]

and can be presented in a form

\[
\tau_i = A_i/R_{4f,5d}^2, \quad (3)
\]

where \( i \) denote a particular energy level. The parameter \( A_i \) is sensitive to the mixing of states (correlations between valence electrons) while there are also many-body corrections to \( R_{4f,5d} \) due to correlations between valence and core electrons. Since the ratio of experimental and calculated lifetimes is almost the same for all

---

1 ftp://aphysics.lanl.gov/pub/cowan
three $^8P$ states (see Table I), it is natural to assume that the most of discrepancy comes from many-body corrections to $R_{1f,5d}$. Note, that the ratio of the experimental and calculated lifetimes is even more stable in the work of Mashonkina et al. [16]. The ratio is 3.0 ± 0.3 and the corresponding lifetimes are presented in column four of Table I. Calculations in this work were also done with the Cowan code, however the mixing of states was more carefully considered.

In the HF approximation, $R_{1f,5d} = 0.77a_B$. Now we calculate a correction to this value due to core polarization by the dipole electric field of the emitted photon. We do this in the random-phase approximation (RPA) using the time-dependent Hartree-Fock method (TDHF) [17]. The TDHF equations can be written in a form

$$(H_0 - e_i)\delta \psi_i = -(\hat{f} + \delta V)\psi_i,$$  

(4)

where $H_0$ is HF Hamiltonian. The single-electron orbital $\psi_i$ satisfies HF equation

$$(H_0 - e_i)\psi_i = 0,$$  

$\hat{f}$ is the operator of the external electric field, $\delta \psi_i$ is a correction to the orbital $\psi_i$ due to external field $\hat{f}$, and $\delta V$ is the modification of the HF potential induced by corrections to the core states. Equations (4) are solved self-consistently for all core states. Note that since Eu III and Gd IV are open-shell systems, the same weighting procedure described in the previous section must be applied to left-hand-side and right-hand-side of Eq. (4). The transition amplitude between states $4f$ and $5d$ in the RPA is

$$\langle 4f | \hat{f} + \delta V | 5d \rangle$$  

(5)

(the HF approximation corresponds to $\delta V = 0$). Core polarization reduces the value of the $R_{1f,5d}$ radial integral bringing lifetimes into better agreement with experiment (see column “RPA” in Table I).

The remaining discrepancy should be attributed to correlations. A detailed investigation of correlations leads beyond the scope of the present work, but one note that correlations increase the density of the external electron at short distances. Therefore, owing to normalization, it must decrease the density at large distances, thereby decreasing the value of the radial integral. Calculated lifetimes are also sensitive to mixing of states. Analysis of the RCI and Cowan code calculations shows that the smallest mixing is for the $^8P_{3/2}$ state. Therefore, we can use this state to extract the value of $R_{1f,5d}$ that ensures the best fit of the experimental data. This value is $R_{1f,5d} = 0.41a_B$ for Eu$^{+2}$. To calculate lifetimes which correspond to the “best fit” value of $R_{1f,5d}$, one need only multiply the results from the Cowan code by a factor of 3.6. In summary, the values of $R_{1f,5d}$ for Eu III and Gd IV are:

|        | Eu III | Gd IV |
|---------|--------|-------|
| HF      | 0.77 $a_B$ | 0.63 $a_B$ |
| RPA     | 0.56 $a_B$ | 0.42 $a_B$ |
| Best fit | 0.41 $a_B$ | 0.34 $a_B$ |

### IV. RESULTS

In Table I, we list and compare energies of $4f^7$ and $4f^85d$ states in Eu III calculated using the RCI code and the Cowan code. Energies are given relative to the ground state $4f^7 S_{7/2}$. As mentioned above, both codes permit us to obtain results that are generally in good agreement with experimental energies by scaling the electrostatic Slater parameters to simulate correlation effects (Refs. [18] [19]). We use the scaling factor of 0.8 in RCI code and 0.85 in the Cowan code. Also the energies of the $4f^85d$ LSJ levels are shifted by 13500 cm$^{-1}$ in the Cowan code relative to the ground state $4f^7 S_{7/2}$. In the RCI code we don’t shift the energies but modify the $5d$ state as was described in Section I to improve the energy interval between the $4f^7$ and $4f^85d$ configurations.

In Table I, energies of the $4f^7 LSJ$, $4f^85d LSJ$, and $4f^86s LSJ$ levels in Eu III are compared with recommended data from the National Institute for Standards and Technology (NIST) by Martin et al. [20]. The 105 levels obtained from spectral analysis by Sugar and Spector [21] given in the NIST publication, classify about 300 of the observed lines. It should be noted that the spectral analysis in [21] was based on the Cowan code, probably, a simpler version than we use here.

It should be noted that we use different coupling schemes in RCI (jj coupling) and Cowan code (LS coupling) to build energy matrices. We use, for convenience, LS coupling labeling of states; however, neither jj nor LS coupling can describe the physical states properly. To combine together our results obtained with different coupling schemes, we calculated Landé $g$-factors for each level. For low-lying states, the $g$-factors are very close to their non-relativistic values and identification of levels is easy. However, higher in the spectrum, strong mixing between states makes level identification difficult. We restricted our calculations to levels which are reliably identified in both calculations.

As can be seen from Table I that results of both calculations for Eu III are in good agreement with one another and with experiment. This gives us confidence in similar calculations for Gd IV.

The RCI calculations for Gd IV are done in exactly the same way as for Eu III. All fitting parameters were chosen for Eu III and no a priori data on Gd IV was
used in the calculations. In a sense, we can say that the Gd IV calculations are predictive. They produce an energy spectrum of Gd IV regardless of what is known about it. In contrast, the calculations with the Cowan code are not exactly the same for both ions. While we use the same scaling factor for Coulomb integrals (0.85) the energy shift for the $4f^5d$ configuration is larger for Gd IV ($18000 \text{ cm}^{-1}$) than for Eu ($15500 \text{ cm}^{-1}$). A larger energy shift is needed to obtain good agreement with available experimental data.

In Table I, we compare energies of the $4f^7$ LSJ and $4f^5d$ LSJ levels with available experimental data and $E_\text{dd}$ predictions given by Kielkopf and Crosswhite [12]. It can be seen from Table I that for the $4f^7$ configuration the energies obtained by Cowan code $E_{\text{C}}$ are in better agreement with energies from [12] than are energies obtained by RCI code $E_{\text{R}}$. However, for the $4f^5d$ configuration, results of both calculations are in very good agreement with each other and with [12].

In Tables I and II, we present lifetimes of the $4f^5d$ LSJ levels calculated using the Cowan code with the HF value of the $R_{4f,5d}$ radial integral. To get more accurate predictions for the lifetimes one should multiply the values presented in tables by the factor of 3.6 (see section II).

V. CONCLUSION

In a recent work on calculation of the EDM enhancement factor ($K$) in Gd IV [13], the result was presented in a form of two different numbers: $K_\text{A} \approx -6.4$ and $K_\text{B} \approx -3.3$. These two numbers were based on different assumptions about the energy splitting between $4f$ and $5d$ states of Gd IV. The first number, ($K_\text{A}$) corresponds to $E_{5d} - E_{4f} \approx 40,000 \text{ cm}^{-1}$ which is a result of extrapolation from Eu III. The second number ($K_\text{B}$) corresponds to $E_{5d} - E_{4f} \approx 100,000 \text{ cm}^{-1}$ which is based on available experimental data for Gd IV (too incomplete at that time to be fully trusted).

The present work clearly indicates that the correct energy splitting is closer to $100,000 \text{ cm}^{-1}$ and consequently, the enhancement factor is rather -3.3.

Furthermore, an analysis of lifetimes of Eu III suggests that core polarization by the electric field of an external photon is an important effect for both ions, Eu III and Gd IV. It reduces the value of the $R_{4f,5d}$ radial integral by a factor of about 1.5. This effect was not included in the calculation of the EDM enhancement factor ($K_{\text{EDM}}$) [9]. Only contributions proportional to the $R_{4f,5d}$ radial integral were considered in that work. To include core polarization by the electric field, one should divide the final answer of Ref. [9] by the factor of 1.5. This leaves us with $K_{\text{EDM}} = -2.2(-3.3/1.5)$.

Acknowledgments

One of the authors (V.D.) is grateful to the Physics Department of the University of Notre Dame for the hospitality and support during his visit in May, 2002. The work of W.R.J. was supported in part by National Science Foundation Grant No. PHY-01-39928. U.I.S. acknowledges partial support by Grant No. B516165 from Lawrence Livermore National Laboratory.

[1] S. K. Lamoreaux, nucl-ex/0109014.
[2] L. R. Hunter, workshop on Tests of Fundamental Symmetries in Atoms and Molecules, Harvard, (2001) available online [http://itamp.harvard.edu/fundamentalworkshop.html].
[3] I. B. Khriplovich and S. K. Lamoreaux, CP Violation Without Strongness (Springer, Berlin, 1997).
[4] B. C. Regan, E. D. Commins, C. J. Schmidt, and D. DeMille, Phys. Rev. Lett. 88, 071805 (2002).
[5] D. DeMille, workshop on Tests of Fundamental Symmetries in Atoms and Molecules, Harvard, (2001) available online [http://itamp.harvard.edu/fundamentalworkshop.html].
[6] J. J. Hudson, B. E. Sauer, M. R. Tarbutt, and E. A. Hinds, hep-ex/0202014.
[7] F. L. Shapiro, Sov. Phys. Usp 11, 345 (1968).
[8] B. V. Vasil’ev and E. V. Kolycheva, Sov. Phys. JETP 47, 243 (1978).
[9] S. Ya. Buhmann, V. A. Dzuba, and O. P. Sushkov, physics/0204076.
[10] S. A. Kuenzi, O. P. Sushkov, V. A. Dzuba, and J. M. Cadogan, cond-mat/0205113.
[11] A. Paolletti, Physics of Magnetic Garnet (North-Holland, Amsterdam, 1978).
[12] J. F. Kielkopf and H. M. Crosswhite, J. Opt. Soc. Am. 60, 347 (1970).
[13] Z. Zhiguo, Z. S. Li, H. Lundberg, K. Y. Zhang, Z. W. Dai, J. Zhankui, and S. Svanberg, J. Phys. B 33, 521 (2000).
[14] R. D. Cowan, The Theory of Atomic Structure and Spectra (University of California Press, Berkeley, 1981).
[15] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 54, 3948 (1996).
[16] L. A. Mashonkina, A. N. Ryabtsev, and T. A. Ryabchikova, Astronomy Letters 28, 34 (2002).
[17] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, J. Phys. B 20, 1399 (1987).
[18] M. S. Pindzola, T. W. Gorczyca, N. R. Badnell, D. C. Griffin, M. Stenke, G. Hofmann, B. Weissbecker, K. Tischert, E. Salzborn, A. Müller, et al., Phys. Rev. A 49, 933 (1994).
[19] M. Satake, M. Imai, K. Kawatsura, K. Komaki, H. Kawara, A. Vasiliev, and U. I. Safronova, Phys. Rev. A 65, 052704 (2002).
[20] W. C. Martin, R. Zalubas, and L. Hagan, Atomic Energy Levels - The Rare-Earth Elements (U. S. Government Printing Office, Washington DC, 1978).
[21] J. Sugar and N. Spector, J. Opt. Soc. Am 64, 1484
| $LSJ$  | $E^M$ | $E^N$ | $\sigma^C$ | $E^M$ | $E^N$ | $\sigma^C$ | $E^M$ | $E^N$ | $\sigma^C$ | $LSJ$  | $E^M$ | $E^N$ | $\sigma^C$ |
|-------|-------|-------|----------|-------|-------|----------|-------|-------|----------|-------|-------|-------|----------|
| $^6P_{3/2}$ | 34182 | 30406 | 34103 | 3642 | 33856 | 1.503 | | | | | | | |
| $^6P_{3/2}$ | 33691 | 30001 | 34800 | 34160 | 34394 | 1.221 | | | | | | | |
| $^6P_{3/2}$ | 33139 | 29581 | 35722 | 34848 | 35109 | 1.496 | | | | | | | |
| $^6P_{3/2}$ | 34700 | 32295 | 38101 | 36634 | 36962 | 1.524 | | | | | | | |
| $^6P_{3/2}$ | 34972 | 32560 | 39512 | 37696 | 38067 | 1.472 | | | | | | | |
| $^6P_{3/2}$ | 35217 | 32783 | 41065 | 38865 | 38290 | 1.578 | | | | | | | |
| $^6P_{3/2}$ | 35396 | 32921 | 34784 | 40158 | 40659 | 1.429 | | | | | | | |
| $^6P_{3/2}$ | 35465 | 32926 | 32308 | | | | | | | | | | | |
| $^6P_{3/2}$ | 35352 | 32716 | 32073 | $^6D_{3/2}$ | 37444 | 35992 | 35627 | 9.567 | | | | | | |
| $^6P_{3/2}$ | 38726 | 37059 | 38786 | 37159 | 37569 | 1.455 | | | | | | | |
| $^6D_{1/2}$ | 40016 | 38129 | 38229 | 4.369 | | | | | | | | | | |
| $^6D_{1/2}$ | 40484 | 37342 | 41275 | 39101 | 39226 | 3.804 | | | | | | | |
| $^6D_{1/2}$ | 40295 | 37457 | 42482 | 40017 | 40133 | 3.052 | | | | | | | |
| $^6D_{1/2}$ | 40145 | 37275 | | | | | | | | | | | | |
| $^6D_{9/2}$ | 39231 | 36562 | $^6F_{1/2}$ | 40362 | 38832 | 2.978 | | | | | | | |
| $^6D_{9/2}$ | 40999 | 39334 | 39014 | 5.622 | | | | | | | | | | |
| $^6D_{9/2}$ | 40780 | 41816 | 42741 | 40692 | 40372 | 1.259 | | | | | | | |
| $^6D_{9/2}$ | 45839 | 46501 | 43751 | 41474 | 41150 | 3.811 | | | | | | | |
| $^6D_{9/2}$ | 48578 | 47555 | 44824 | 42294 | 41988 | 9.703 | | | | | | | |
| $^6D_{9/2}$ | 48743 | 47645 | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 50215 | 47912 | | | | | | | | | | | | |
| $^6G_{3/2}$ | 50416 | 47996 | 49636 | 7.318 | | | | | | | | | | |
| $^6G_{3/2}$ | 48780 | 47186 | $^6G_{7/2}$ | 42741 | 40692 | 40372 | 1.259 | | | | | | | |
| $^6G_{3/2}$ | 55764 | 47434 | 46108 | 1.865 | | | | | | | | | | |
| $^6G_{3/2}$ | 55764 | 47434 | 46108 | 1.865 | | | | | | | | | | |
| $^6G_{3/2}$ | 55764 | 47434 | 46108 | 1.865 | | | | | | | | | | |
| $^6G_{3/2}$ | 47685 | 48188 | 47685 | 48188 | 47685 | 1.495 | | | | | | | |
| $^6G_{3/2}$ | 56851 | 48188 | 47685 | 1.495 | | | | | | | | | | |
| $^6G_{3/2}$ | 57693 | 49130 | 47714 | 9.094 | | | | | | | | | | |
| $^6G_{3/2}$ | 59667 | 50735 | 49086 | 7.674 | | | | | | | | | | |
| $^6G_{3/2}$ | 59667 | 50735 | 49086 | 7.674 | | | | | | | | | | |
| $^6G_{3/2}$ | 49859 | 49110 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 50215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| $^6G_{3/2}$ | 49215 | 47912 | $^6D_{1/2}$ | 45957 | 43138 | 42850 | 4.903 | | | | | | | |
| LSJ     | \( E^M \) cm\(^{-1} \) | \( E^C \) | \( E^{\exp} \) | \( \tau^C \) sec | \( \tau^{5d} \) sec | \( E^{5d} \) cm\(^{-1} \) | \( E^{\exp} \) | \( \tau^{5d} \) sec |
|---------|-----------------|-------|----------|-------------|----------------|-------------------|---------|-------------|
| \( ^6P_{3/2} \) | 38308           | 34114 | 33262    | 3.364[-5]   | 103091         | 105613            | 104264  | 2.131[-8]  |
| \( ^6P_{5/2} \) | 37638           | 33577 | 32680    | 1.624[-5]   | 105108         | 106266            | 106493  | 1.969[-9]  |
| \( ^6P_{7/2} \) | 37103           | 33018 | 32084    | 9.024[-6]   | 107493         | 109547            | 109005  | 4.311[-9]  |
| \( ^6H_{5/2} \) | 38833           | 36109 | 35808    | 3.541[-6]   | 108974         | 110344            |         | 1.093[-8]  |
| \( ^6H_{9/2} \) | 39191           | 36468 | 36151    | 2.527[-6]   | 109790         | 110989            |         | 1.086[-8]  |
| \( ^6H_{11/2} \) | 39504           | 36766 | 36430    | 2.160[-6]   | 110760         | 111763            |         | 1.075[-8]  |
| \( ^6H_{13/2} \) | 39722           | 36950 | 36508    | 6.287[-6]   | 111838         | 112641            |         | 1.067[-8]  |
| \( ^6H_{15/2} \) | 39782           | 36957 | 36547    |         | 113003         | 113620            |         | 1.069[-8]  |
| \( ^6I_{17/2} \) | 39566           | 36677 | 36206    | 6.089[-8]   | 114270         | 114729            |         | 1.089[-8]  |
| \( ^6D_{3/2} \) | 44618           | 41738 | 40444    | 4.803[-7]   | 112718         | 115165            |         | 1.405[-8]  |
| \( ^6D_{5/2} \) | 45660           | 41983 | 40694    | 4.429[-7]   | 112551         | 115883            |         | 1.317[-8]  |
| \( ^6D_{7/2} \) | 45363           | 42131 | 40857    | 2.438[-6]   | 113476         | 114424            | 111745  | 1.068[-8]  |
| \( ^6D_{9/2} \) | 45120           | 41877 | 40599    | 2.167[-6]   | 114715         | 115140            | 113129  | 9.812[-9]  |
| \( ^6F_{1/2} \) | 43876           | 40934 | 39508    | 7.829[-7]   | 116120         | 116239            | 114214  | 9.076[-9]  |
| \( ^6F_{3/2} \) | 48999           | 53498 | 50633    | 8.558[-7]   | 118102         | 118166            |         | 1.166[-8]  |
| \( ^6G_{3/2} \) | 54398           | 52556 | 49825    | 1.884[-7]   | 114452         | 113648            |         | 1.207[-8]  |
| \( ^6G_{5/2} \) | 54061           | 51626 | 49526    | 7.487[-7]   | 115542         | 113646            |         | 1.196[-8]  |
| \( ^6G_{7/2} \) | 54132           | 53018 | 49652    | 2.167[-6]   | 116881         | 116786            |         | 1.229[-8]  |
| \( ^6G_{9/2} \) | 54277           | 53113 | 49652    | 4.888[-7]   | 118099         | 117691            | 116230  | 1.156[-8]  |
| \( ^6G_{11/2} \) | 55684           | 54908 | 51360    | 9.024[-6]   | 119010         | 118415            | 117229  | 1.059[-8]  |
| \( ^6F_{1/2} \) | 58661           | 55022 | 50825    | 2.167[-7]   | 116779         | 117952            |         | 1.700[-8]  |
| \( ^6F_{3/2} \) | 59353           | 58025 | 50825    | 8.230[-8]   | 118903         | 118862            | 118109  | 1.553[-8]  |
| \( ^6F_{5/2} \) | 59953           | 57566 | 50825    | 3.107[-7]   | 119962         | 119714            | 119292  | 1.528[-8]  |
| \( ^6F_{7/2} \) | 60303           | 57909 | 50825    | 5.352[-7]   | 120838         | 120449            | 120220  | 1.513[-8]  |
| \( ^6F_{9/2} \) | 60310           | 58200 | 50825    | 5.352[-7]   | 121510         | 121003            | 121063  | 1.496[-8]  |
| \( ^6F_{11/2} \) | 59774           | 57330 | 50825    | 2.946[-7]   | 122130         | 121368            | 121725  | 1.393[-8]  |
| \( ^4N_{1/2} \) | 60545           | 55382 | 50825    | 5.352[-7]   | 128024         | 129607            |         | 1.376[-7]  |
| \( ^4N_{3/2} \) | 61512           | 56379 | 50825    | 4.624[-9]   | 129323         |                   |         | 5.208[-9]  |

* TABLE III: Energies (cm\(^{-1}\)) and lifetimes \( \tau \) (sec) for in Gd IV calculated by RCI \( (E^M) \) and Cowan code \( (E^C) \). Energies are given relative to the ground states 4\( f^7 \) 8\( S_{7/2} \). Comparison with experimental data from Ref. [4] \( (E^{\exp}) \).