Construction of the energy matrix for complex atoms

Part VIII: Hyperfine structure HPC calculations for terbium atom

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Abstract. A parametric analysis of the hyperfine structure (hfs) for the even parity configurations of atomic terbium (Tb I) is presented in this work. We introduce the complete set of $4f$ core states in our high-performance computing (HPC) calculations. For calculations of the huge hyperfine structure matrix, requiring approximately 5000 hours when run on a single CPU, we propose the methods utilizing a personal computer cluster or, alternatively a cluster of Microsoft Azure virtual machines (VM). These methods give a factor 12 performance boost, enabling the calculations to complete in an acceptable time.

1 Introduction

The present paper is the eighth one in the series of our methodological approach regarding the atomic structure calculations. Six previously published papers, under the common title Construction of the energy matrix for complex atoms, contain a description of our method for semi-empirical analysis of complex electronic systems in multiconfiguration approximation up to the second order of the perturbation theory [1–6]. The seventh paper [7] of the above-mentioned cycle was the application of our many-body parametrization method to analyze fine structure in 4f- and 5f-shell atoms.

The choice of the investigated element was caused by a new experimental data of the hyperfine structure splitting of the atomic terbium levels obtained by our experimental group [8–11]. Within the work [10] the fine- and hyperfine structure analysis of seven even-parity configurations of Tb I ($4f^85d^3$, $4f^85d^26s$, $4f^85d^26s^2$, $4f^86s6p$, $4f^86s7p$, $4f^86s8p$, $4f^95d6p$) was performed. The calculations were carried out in limited basis states, it means for $4f^8$-core to 13 terms and for $4f^9$-core to 3 terms.

After applying of novelty type of optimizing calculation procedures we were able to repeat the fine structure (fs) analysis for terbium atom in a full number of $4f$ and $4f^9$-core states and the results were described in the aforementioned paper [7]. The huge energy matrix of the configuration system under consideration contained 74418 possible energy levels. The size of the largest submatrix, for $J = 9/2$, was 9936. The results of the fine structure calculations obtained within paper [7] compared to those published earlier [10] conducted with the restricted $4f^8$-core, were definitely better. In the fine structure least-squares fit we achieved mean error for energy levels values of $\sigma(E) = 37$ cm$^{-1}$ (old value was $\sigma(E) = 56$ cm$^{-1}$). We used 99 known experimental even-parity energy levels and 26 fitted parameters. The description of the levels above 17000 cm$^{-1}$ based on comparison with experimental $g_j$-Landé factors seemed to be correctly determined. However, the confirmation of the obtained levels designation could be possible after the performing of the hyperfine structure parameterization in the same, complete basis states.

Therefore, in the current article we are reporting the results of the hyperfine structure analysis in the full number of $4f^8$ and $4f^9$-core states, abandoning the previous limitations. Such huge hyperfine structure calculations have not been presented in literature so far.
Fig. 1. Computation of each $J$ is assigned to a DS11v2 - 2 cores - Azure VM in a way to minimize the total execution time, now dominated by the $J = 9/2$ submatrix. Running the calculations on 6 VMs 2 cores each resulted in 12 times performance boost. In this version, the electronic configurations are statically assigned to two threads. One thread calculates $4f^8 5d^2 6s$, $4f^9 5d^5 6p$, the other one $4f^8 5d^3$, $4f^8 5d^6 5s^2$, $4f^6 6s 6p$, $4f^6 6s 7p$, $4f^6 6s 8p$.

The next section of this paper contains the details of computational procedures optimization. The results of fine- and hyperfine structure many-body parametrization method for the even configurations system of terbium atom are presented in sect. 3.

2 Computing hfs angular coefficients with Azure HPC infrastructure

At least two levels of parallel computation are possible and desired as the calculating angular coefficient is a time consuming process. One level is straightforward as the underlying Hamiltonian is block diagonal with respect to $J$. In consequence, the individual blocks can be processed independently. This independence allows distribution of the computation among multiple nodes as there are no interactions, except the final barrier when the calculations for all $J$ complete. At $J$ block level of parallelism, this property makes our computation location transparent as each $J$ block can be assigned to a designated thread or to a separate node. Note, that distributing the computation among multiple nodes results in better scalability and requires only allocating an appropriate number of nodes (in our case six Azure VMs —fig. 1).

The second level of parallelism is more subtle and requires some care. There are multiple (i.e. 8 in the case of odd configurations of atomic terbium) configurations within each $J$ which can also be computed concurrently, but now the dependencies between partial results are present as the parameters from all concurrently processed configurations must be ordered to produce properly structured data which is subsequently used as an input for hfs fitting. There are two phases of the calculations at the electronic configuration level: the first, more time-consuming phase computes the coefficients resulting from internal interactions, the second (much shorter) computes the inter-configuration part, hence a barrier must be present to co-ordinate the execution. When a thread calculating individual configuration reaches the barrier, it blocks until all other configurations complete and then the angular coefficients are ordered and
the final phase, which calculate inter-configuration interactions is executed. As this final phase is relatively fast, it is assigned to a single thread.

The main factor affecting the computation time for a single configuration can be estimated from the rules of total angular momentum coupling which determine the base size. The other factor is the number of parameters which, however, is known in advance (this is simply our input). With these two factors available one can easily forecast the execution time needed to process each configuration and allocate the resources, assigning individual configurations to computational nodes in a way that results in an approximately optimal execution. Observe, that on a single CPU the total execution time would equal the sum of bars lengths in fig. 1. Despite this significant performance boost, in our future work we are going to present a solution that allows full scalability, i.e. the optimal utilization of an arbitrary number of cores.

3 Results of the semi-empirical approach

In our earlier paper on Tb I [10] we investigated the atomic structure of 7 even-parity configurations system using a semi-empirical parametrization method, taking into account electromagnetic interactions up to the second-order perturbation theory. The fine structure angular coefficient matrices for the multiconfiguration system, listed in the introduction, necessary for the least-squares fitting program, were constructed with the use of our computer code. The calculations were restricted to the lowest lying states of 4f and 4f-core. The contributions from the second-order perturbation theory concerning the configuration interaction (CI) effects, electrostatically correlated spin-orbit interactions (CSO), as well as electrostatically correlated hyperfine interactions (CHFS), described in the series [1–6], were possible to a limited extent only. The CI effects of two-electron excitations were included in the consideration by adding the term $\alpha L(\lambda + 1) + \beta S(S + 1)$, according to [12,13] and [14]. For the CSO interactions only the excitations of one electron from closed $n_d^{10}$ shells into an open 5d-shell were taken into consideration. For the CHFS interactions, the excitations of one electron from closed $n_d$ shells to empty $n'$ shells or to an open 6s-shell were taken into account. A detailed description of our approach of the fine- and hyperfine structure analysis of Tb I was presented by us in sect. 4 in paper [10] and the final results of the semi-empirical calculations were summarized in four tables. The values of the intra-configuration and inter-configuration fs radial parameters were contained in tables 3 and 4, respectively. A comparison of the experimental and calculated energy values and hfs $A$ and $B$ constants were given in table 5. The values of the one- and two-body hyperfine structure parameters were presented in table 6. These values should be compared with new results obtained by the precise studies carried out within the framework of this work.

The current results of the semi-empirical fine- and hyperfine structure analysis of the even levels of the neutral terbium atom are presented in tables 1–5.

The values of radial fine structure parameters, their statistical errors and the values obtained with the COWAN code [15,16] (HFR) are given in tables 1 and 2. The second-order contributions concerning electrostatically correlated spin-orbit interactions were included according to the procedure described in the work [5]. This means that the excitations of one electron from open 4f$^5$, 4f$^6$-shells to empty $n'$s shells, the excitations of one electron from closed $n_d^{10}$ shells into an open 5d-shell and the excitations of one electron from closed $n_0p^6$ shells into an open 6p-shell, were taken into account.

The comparison of the experimental and calculated energy values and hfs $A$ and $B$ constants is shown in table 3. The complete version of this table, together with the predictions of the energy values and hfs constants for the levels up to approximately 28000 cm$^{-1}$ is presented in supplementary material associated with this paper.

In our procedure, we used all the experimental data known so far, i.e., the values of 99 energy electronic levels, $g_J$-Landé factors known for 66 energy levels 86 $A$ and 84 $B$ hyperfine structure constants. The energy and $g_J$ values were taken from the NIST Atomic Spectra Database [17], which is based primarily on the monograph of Martin et al. [18]. The experimentally determined hfs constants were taken from Childs [19–21], Furmann [8,9] and Stefanska [10,22]. In the fs-fit with 369 parameters, 24 of which were treated as free, we achieved a mean-square deviation of 37 cm$^{-1}$.

The first three columns in the table 3 present the values of experimental, calculated energy of electronic levels and the difference between them in cm$^{-1}$. The two main fine structure components with their percentages, are given in columns 4–7. In next columns, the calculated $g_J$ values are compared with the experimental ones. In columns 10 and 12 the experimental hyperfine constants $A$ and $B$ are listed together with their experimental uncertainties. The calculated $A$ and $B$ constants for all energy levels are listed in columns 11 and 13. We achieved mean errors for $A$ constants $\sigma(A) = 17$ MHz and for $B$ constants $\sigma(B) = 36$ MHz, respectively.

The hfs constants $A$ and $B$ for the energy levels in region about 23000 cm$^{-1}$ were very helpful in the identification of $J$-quantum numbers and assignment of the spectroscopic description. The semi-empirical calculations of the hyperfine constants $A$ and $B$ showed that it was possible to clarify the configuration and designation of the energy levels in a wide energy range.

The comparison of the experimental and calculated hfs $A$ and $B$ constants [MHz] of the even-parity levels obtained in full and limited number of 4f$^6$ and 4f$^6$-core states is contain in table 4.
Table 1. Values of the intra-configuration fine structure parameters (cm$^{-1}$); (*) denotes an fixed parameter, a denotes arbitrarily assumed value of the center of gravity of the configuration.

| Parameter | Value | HFR |
|-----------|-------|-----|
| $E_{AV}(4f^85d^{3})$ | 103528 (104681) |
| $F^2(4f,4f)$ | 93725 (95180) |
| $F^4(4f,4f)$ | 69409 (59681) |
| $F^6(4f,4f)$ | 35223 (192) (42927) |
| $F^2(5d,5d)$ | 22334 (22670) |
| $F^4(5d,5d)$ | 69409 (59681) |
| $F^2(4f,5d)$ | 15274 (80) (14605) |
| $F^4(4f,5d)$ | 10692 (127) (6631) |
| $G^1(4f,5d)$ | 6228 (80) (6388) |
| $G^3(4f,5d)$ | 8407 (194) (5004) |
| $G^5(4f,5d)$ | 7386 (173) (3768) |
| $\zeta(4f)$ | 2117 (14) (1768) |
| $\zeta(5d)$ | 386 (42) (699) |
| $E_{AV}(4f^85d^{2}6s)$ | 84320 (84320) |
| $G^2(5d,6s)$ | 14692 (13902) |
| $G^3(4f,6s)$ | 2001 (1119) |
| $\alpha(4f^85d^{2}6s)$ | 4 (1) |
| $\beta(4f^85d^{2}6s)$ | 279 (7) |
| $R^2(4f4f,4f'4f')\zeta(4f,n'f)$ | 14 (*) |
| $R^4(4f4f,4f'4f')\zeta(4f,n'f)$ | 329 (*) |
| $D^6(4f5d,n'5d)\zeta(4f,n'f)$ | -1 (*) |
| $D^8(4f5d,n'5d)\zeta(4f,n'f)$ | -65 (*) |
| $E^1(4f5d,5d'nf)\zeta(4f,n'f)$ | -206 (*) |
| $R^2(n0d5d,5d5d)\zeta(n0d,5d)$ | 668 (*) |
| $D^6(n0d6s,6s5d)\zeta(n0d,5d)$ | 32 (8) |
| $E^2(n0d6s,6s5d)\zeta(n0d,5d)$ | -36 (*) |
| $D^8(n0d4f,5d4f)\zeta(n0d,5d)$ | -255 (*) |
| $E^6(n0d4f,5d5d)\zeta(n0d,5d)$ | -352 (22) |
| $E_{AV}(4f^85d^{2}6s^2)$ | 69348 (80) (72896) |
| $\alpha(4f^85d^{2}6s^2)$ | 8 (1) |
| $\beta(4f^85d^{2}6s^2)$ | 333 (6) |
| $E_{AV}(4f^86s6p)$ | 74000 (115) (82827) |
| $F^2(4f,6p)$ | 1904 (2508) |
| $G^2(6s,6p)$ | 12612 (295) (17375) |
| $G^4(4f,6p)$ | 710 (562) |
| $G^4(4f,6p)$ | 520 (490) |
| $\zeta(6p)$ | 1796 (43) (1344) |
| $E^2(4f6p,6p'nf)\zeta(4f,n'f)$ | -238 (*) |
| $E^4(n0p6s,6s6p)\zeta(n0p,6p)$ | 103 (*) |
| $\alpha(4f^86s6p)$ | 13 (4) |
| $\beta(4f^86s6p)$ | 27 (12) |
| $E_{AV}(4f^86s7p)$ | 96978 (100815) |
| $E_{AV}(4f^86s8p)$ | 104241 (110007) |
| $E_{AV}(4f^85d6p)$ | 92517 (100648) |
| $F^2(5d,6p)$ | 10021 (10021) |
| $G^1(5d,6p)$ | 8564 (8564) |
| $G^3(5d,6p)$ | 5518 (5518) |
Table 2. Values of configuration interactions radial parameters (cm⁻¹); (∗) denotes a fixed parameter, (**) represents the same as the first parameter in the table.

| Configurations | Parameter | Value   | HFR     |
|----------------|-----------|---------|---------|
| even configurations |
| 4f⁰5d³ ↔ 4f⁰5d²6s | R²(5d5d,5d6s) | 8516 (170) | 15876   |
|                  | D²(5d5d,4f6s) | 1403 (*)   | 861     |
|                  | E¹(5f5d,6s4f) | 2312 (*)  | 1044     |
| 4f⁰5d²6s ↔ 4f⁰5d⁶s² | R²(5d5d,5d6s) | 8516 (**) | 16491   |
| 4f⁰5d²6s ↔ 4f⁰5d⁶p | R¹(5d5d,4f6p) | 1388 (*)  | 2700     |
|                  | R³(5d5d,4f6p) | 863 (*)    | 742     |
| 4f⁰5d³ ↔ 4f⁰5d⁶p | R¹(5d5d,4f6p) | 2700 (*)  | 2912     |
|                  | R³(5d5d,4f6p) | 742 (*)    | 783     |
| 4f⁰5d⁶s² ↔ 4f⁰6s⁶p | D¹(5d6s,4f6p) | 3610 (*)  | 5555     |
|                  | E¹(5d6s,6p4f) | 7301 (*)   | 998     |
| 4f⁰5d²6s ↔ 4f⁰5d⁶p | D¹(5d6s,4f6p) | 3610 (*)  | 4682     |
|                  | E¹(5d6s,6p4f) | 7301 (*)   | 1148    |
| 4f⁰6s⁶p ↔ 4f⁰6s⁷p | E¹(6s6p,7p6s) | 5602 (*)  | 5602     |
|                  | D²(4f6p,4f7p) | 1012 (*)  | 1012     |
|                  | E²(4f6p,7p4f) | 260 (*)    | 260     |
|                  | E¹(4f6p,7p4f) | 227 (*)    | 227     |
|                  | ζ(6p,7p)      | 350 (*)    | 350     |
| 4f⁰6s⁶p ↔ 4f⁰5d⁶p | D²(6s6p,5d6p) | 11347 (*) | 11347   |
|                  | E¹(6s6p,6p5d) | 12107 (*)  | 12107   |
|                  | D²(4f6s,4f5d) | 1431 (*)   | 1431    |
|                  | E¹(4f6s,5d4f) | 679 (*)    | 679     |

In our published earlier paper [10], following Sandars and Back theory [23] we used the one-body radial parameters \( a_{nk}^{e\ell} \) and \( b_{nk}^{e\ell} \), where \( sk = 01,12 \) for magnetic-dipole hfs interactions and \( sk = 02,11,13 \) for electric-quadrupole hfs interactions. The contributions from the second-order perturbation theory, so-called electrostatically correlated hyperfine interactions, concerned with the excitations of one electron from closed shells to an open shell: \( n_s \rightarrow 5d \), \( n_d \rightarrow 5d \) and from an open 4f-shell to empty \( n'f \) shells dependent on \( sk = 01,12 \) or 02 were omitted. The above restrictions were made due to the huge size of the hyperfine structure matrix. Only “hfs core-polarization effects”, i.e., the influence of the excitations of electrons from closed \( n_s \) shells to empty \( n' \) shells or to an open 6s-shell on the hyperfine structure, were taken into account.

The optimization of our computer procedures for generating the angular coefficient of the hyperfine structure matrix presented within this work, allowed the quantitative determination of one- and two-body contributions to the hyperfine structure.

The values of the one- and two-body hyperfine structure parameters (MHz) and effective radial integrals (a.u.) obtained from the experimental data for the even parity configurations of Tb I are include in table 5. The ratio of the one- and two-body parameters \( sk = 12 \) and \( sk = 01 \) was assumed to amount to 1. For the parameters including electrostatic integrals of the order \( t = 4 \) the ratio in relation to corresponding \( t = 2 \) parameters were set to 0.65071 (from Hartree-Fock calculations [24]). The contributions originating on excitations from closed \( n_d \) shells to an open 5d-shell and from an open 4f-shell to empty \( n'f \) shells dependent on \( sk = 01,12 \) or 02 were specified. As we wrote in our earlier works [6,10,25], in Sandars and Beck theory [23] the operator \( s \) and the radial parameter \( a_{nl}^{el} \) (where \( l > 0 \)) represent relativistic effects in the hyperfine structure. In our method we assume that the parameter \( a_{nl}^{el} \) for \( l > 0 \) is equal to zero. We can make this assumption because, according to, e.g., Feneuille and Armstrong [26], Armstrong [27] and Lindgren and Morrison [28] the relativistic effects and configuration interaction effects, concerning the excitation of electrons from the closed shells to the empty shells, have the same angular part. Thus, the above mentioned effects are inseparable and is not possible to determine those values independently in the least-squares procedure by use \( a_{nl}^{el} \) radial parameter.
Supplementary material associated with this paper.

The on-line version of this paper (available at http://dx.doi.org/10.1140/epjp/i2017-11912-7) contains an animated version of Table 3, which is a comparison of the experimental and calculated energy values (in eV) and their absolute and relative contributions to the total energy. This animation is designed to provide a visual representation of the data, allowing for a more intuitive understanding of the distribution and significance of these contributions. The animation is accessible through the provided link and is an integral part of the supplementary material.
\begin{table}
\centering
\begin{tabular}{cccccccccc}
\hline
$E_{\text{exp}}$ & $E_{\text{calc}}$ & $\Delta E$ & \% Main comp. & $E_{\text{exp}}$ & $E_{\text{calc}}$ & $g_{I_{\text{calc}}}$ & $g_{I_{\text{exp}}}$ & $A_{\text{exp}}$ & $A_{\text{calc}}$ & $B_{\text{exp}}$ & $B_{\text{calc}}$ & $\text{Ref.}$ \\
\hline

\end{tabular}
\caption{Continued.}
\end{table}

\begin{table}
\centering
\begin{tabular}{cccccccccc}
\hline
$E_{\text{exp}}$ & $E_{\text{calc}}$ & $\Delta E$ & \% Main comp. & $E_{\text{exp}}$ & $E_{\text{calc}}$ & $g_{I_{\text{calc}}}$ & $g_{I_{\text{exp}}}$ & $A_{\text{exp}}$ & $A_{\text{calc}}$ & $B_{\text{exp}}$ & $B_{\text{calc}}$ & $\text{Ref.}$ \\
\hline

\end{tabular}
\caption{Continued.}
\end{table}
| ΔE (eV) | H                 | Ref. | exp | calc | ΔE (eV) | H                 | Ref. | exp | calc |
|----------|-------------------|------|-----|------|----------|-------------------|------|-----|------|
| 0.70     | 1.01              | I     | 1   | 1.01 | 0.70     | 1.01              | I     | 1   | 1.01 |
| 0.50     | 1.02              | I     | 1   | 1.02 | 0.50     | 1.02              | I     | 1   | 1.02 |
| 0.30     | 1.03              | I     | 1   | 1.03 | 0.30     | 1.03              | I     | 1   | 1.03 |
| 0.10     | 1.04              | I     | 1   | 1.04 | 0.10     | 1.04              | I     | 1   | 1.04 |
| 0.01     | 1.05              | I     | 1   | 1.05 | 0.01     | 1.05              | I     | 1   | 1.05 |
| 0.00     | 1.06              | I     | 1   | 1.06 | 0.00     | 1.06              | I     | 1   | 1.06 |

Table 3. Continual.
Table 3. Continued.

| $E_{\text{exp}}$ | $E_{\text{calc}}$ | $\Delta E$ | % Main comp. | % Sec. comp. | $g_{\text{calc}}$ | $g_{\text{exp}}$ | $A_{\text{exp}}$ | $A_{\text{calc}}$ | $B_{\text{exp}}$ | $B_{\text{calc}}$ | Ref. |
|------------------|------------------|------------|-------------|-------------|-----------------|----------------|----------------|----------------|----------------|----------------|-------|
| 12932.66 | 12905 | 28 | 32.0 $4f^4(7F)5d^66s\ ^8G$ | 17.6 $4f^4(7F5)d^26s\ ^8G$ | 1.473 | 294.2 | (1.8) | 294 | 406 | (24) | 343 | [10] |
| 14569.67 | 14610 | -40 | 41.9 $4f^5(7F)5d^26s\ ^{10}I$ | 30.8 $4f^4(7F)5d^26s\ ^{10}H$ | 1.398 | 566.0 | (3.4) | 600 | 294 | (31) | 266 | [10] |
| 14888.11 | 14900 | -2 | 41.7 $4f^4(6H)6d^68G$ | 18.5 $4f^4(6H)6d^68H$ | 1.396 | 1.391 | 940 | 1398 | | | | |
| 15387.79 | 15341 | 47 | 30.7 $4f^4(7F)5d^26s\ ^8H$ | 15.1 $4f^4(7F)5d^26s\ ^8I$ | 1.367 | 1.367 | 525.7 | (0.4) | 458 | 1080.0 | (5.9) | 1122 | [10] |
| 16343.30 | 16340 | 3 | 28.6 $4f^4(6H)6d^68I$ | 18.6 $4f^4(6H)6d^68G$ | 1.284 | 1.397 | 193 | | | | | |
| 16431.13 | 16452 | -21 | 62.8 $4f^4(7F)5d^26s\ ^{10}G$ | 12.1 $4f^4(7F)5d^26s\ ^{10}G$ | 1.516 | 1.460 | 793 | | | | | |
| ... 8 levels ... | | | | | | | | | | | | |
| 19920.41 | 19953 | -33 | 17.1 $4f^4(7F)5d^26s\ ^8G$ | 14.1 $4f^4(7F)5d^26s\ ^8H$ | 1.410 | | 992 | | | | | |
| ... 9 levels ... | | | | | | | | | | | | |
| 23112.35 | 23011 | 102 | 20.9 $4f^4(6H)6d^68I$ | 18.4 $4f^4(6H)6d^68I$ | 1.303 | 968.0 | (0.1) | 1037 | 916.9 | (1.3) | 1233 | [22] |
| 23031.84 | 23114 | -82 | 9.5 $4f^4(5G)5d^66s\ ^26H$ | 9.4 $4f^4(5G)5d^66s\ ^26H$ | 1.327 | 1.240 | 880.9 | (0.6) | 832 | 838.3 | (4.5) | 812 | [22] |
| ... 11 levels ... | | | | | | | | | | | | |
| 25825.53 | 25836 | -11 | 21.0 $4f^4(6L)5d^66s\ ^26K$ | 8.4 $4f^4(6H)6d^68I$ | 1.219 | 1.246 | 869 | | | | | |

$J = 17/2$

| 4646.830 | 4638 | 9 | 89.5 $4f^4(7F)5d^26s\ ^8H$ | 2.7 $4f^4(7F)5d^26H$ | 1.406 | 1.406 | 481.738 | (0.002) | 451 | 2245.914 | (0.050) | 2228 | [19] |
| 8506.710 | 8504 | 2 | 73.2 $4f^4(7F)5d^26s\ ^8G$ | 11.8 $4f^4(7F)5d^26s\ ^8G$ | 1.518 | 1.530 | 915.3 | (0.5) | 937 | 464 | (37) | 408 | [10] |
| 11879.20 | 11900 | -21 | 47.3 $4f^4(7F)5d^26s\ ^{10}I$ | 31.3 $4f^4(7F)5d^26s\ ^{10}I$ | 1.438 | 1.430 | 757.6 | (0.4) | 762 | 1167 | (24) | 1158 | [10] |
| 14016.91 | 14033 | -16 | 38.4 $4f^4(7F)5d^26s\ ^{10}I$ | 30.0 $4f^4(7F)5d^26s\ ^{10}I$ | 1.415 | 648.9 | (2.3) | 662 | 669.5 | (3.5) | 758 | [10] |
| 14718.11 | 14704 | 15 | 46.2 $4f^4(7F)5d^26s\ ^8H$ | 15.6 $4f^4(7F)5d^26s\ ^{10}I$ | 1.397 | 1.400 | 781.5 | (4.9) | 617 | 1020 | (18) | 1103 | [10] |
| 15189.26 | 15190 | -1 | 46.2 $4f^4(6H)6d^68I$ | 11.9 $4f^4(6H)6d^68I$ | 1.369 | 1.409 | 1025.6 | (0.7) | 995 | 682 | (29) | 773 | [10] |
| 15678 | | | | | | | | | | | | |
| 16733 | | | | | | | | | | | | |
| 17249.59 | 17245 | 5 | 46.4 $4f^4(6H)6d^68I$ | 25.1 $4f^4(6H)6d^68I$ | 1.324 | 857.1 | (0.4) | 866 | 1758.9 | (5.0) | 1688 | [10] |
| ... 9 levels ... | | | | | | | | | | | | |
| 23107.25 | 23128 | -20 | 25.2 $4f^4(7F)5d^26s\ ^8I$ | 22.9 $4f^4(7F)5d^26s\ ^8H$ | 1.357 | 1.289 | 758 | | | | | |

$J = 19/2$

| 11331.14 | 11330 | 1 | 65.9 $4f^4(7F)5d^26s\ ^{10}I$ | 28.4 $4f^4(7F)5d^26s\ ^{10}I$ | 1.451 | 1.460 | 876.3 | (3.8) | 890 | 1460 | (20) | 1469 | [10] |
| 13398.40 | 13397 | 2 | 56.8 $4f^4(7F)5d^26s\ ^{10}I$ | 27.2 $4f^4(7F)5d^26s\ ^{10}I$ | 1.421 | 690.6 | (0.6) | 687 | 1023 | (16) | 1027 | [10] |

$J = 21/2$

| 12283.30 | 12248 | 36 | 95.1 $4f^4(7F)5d^26s\ ^{10}I$ | 2.1 $4f^4(5G)5d^26s\ ^8K$ | 1.425 | 845.9 | (0.1) | 855 | 1906 | (11) | 1927 | [10] |
### Table 4.
Comparison of the experimental and calculated hfs $A$ and $B$ constants (MHz) of the even-parity levels obtained in full and limited number of $4p^6$ and $4p^6$-core states, respectively.

| $E_{\exp}$ | $J = 1/2$ | $J = 3/2$ | $J = 5/2$ | $J = 7/2$ | $J = 9/2$ |
|------------|--------|--------|--------|--------|--------|
|            | $A$    |        | $B$    |        |        |
|            | This work | [10]  | This work | [10]  | This work | [10]  |
| Experiment |        |        | Experiment |        | Experiment |        |
| 4018.210   | 2584.8 | (4.0) | 2591  | 2566  |        |        |
| 6259.090   | -1762.5 | (8.9) | -1797 | -1759 |        |        |
| 3705.820   | 883.905 | (0.030) | 884 | 883 | -15.510 | (0.250) | -16 | -8 |
| 5483.980   | -177.8 | (7.6) | -159 | -131 | -504  | (23)  | -518 | -533 |
| 6849.720   | -755.3 | (5.2) | -749 | -792 | 281   | (16)  | 325  | 300 |
| 8336.310   | 1645.9 | (4.5) | 1644 | 1652 | 744   | (25)  | 778  | 774 |
| 10920.180  | 1001.8 | (3.2) | 1001 | 1047 | -133  | (19)  | -123 | -121 |
| 3174.575   | 652.766 | (0.020) | 652 | 652 | 267.611 | (0.150) | 267 | 279 |
| 4695.005   | 215.653 | (0.015) | 211 | 224 | -401.862 | (0.060) | -420 | -429 |
| 6801.190   | -123.7 | (2.8) | -113 | -131 | -286  | (15)  | -290 | -310 |
| 8130.680   | 874.4  | (4.8) | 875 | 872 | 411   | (25)  | 433  | 425 |
| 10030.350  | 783.5  | (0.1) | 737 | 769 | 515.4 | (9.7) | 546  | 585 |
| 10456.670  | 912.9  | (6.9) | 907 | 907 | 149   | (35)  | 105  | 97 |
| 12296.45   | 332.6  | (0.4) | 288 | 315 | -52   | (24)  | -26  | -55 |
| 2419.480   | 591.564 | (0.007) | 588 | 588 | 733.233 | (0.070) | 721 | 746 |
| 3819.850   | 358.918 | (0.007) | 355 | 357 | -140.881 | (0.050) | -157 | -170 |
| 6488.280   | 114.9  | (0.3) | 116 | 112 | -498.7 | (0.7) | -531 | -540 |
| 7839.850   | 606.2  | (0.7) | 623 | 615 | 429.7 | (0.4) | 419  | 406 |
| 8994.660   | 710.991 | (0.003) | 696 | 712 | 966.850 | (0.003) | 987 | 1000 |
| 9867.650   | 903.5  | (2.5) | 898 | 887 | 533   | (23)  | 483  | 469 |
| 10324.740  | -35.1  | (2.0) | -16 | -7 | -563.3 | (8.5) | -393 | -582 |
| 11107.07   | 484.8  | (2.3) | 496 | 489 | 72.8  | (1.7) | 123  | 143 |
| 12250.99   | 893.7  | (1.7) | 867 | 861 | 25.2  | (7.3) | 85   | 93 |
| 12645.32   | 607.4  | (2.4) | 636 | 668 | 433   | (17)  | 631  | 633 |
| 12714.050  | 299.5  | (1.0) | 212 | 274 | -308.5 | (6.5) | -467 | -394 |
| 13277.23   | 464.5  | (0.9) | 477 | 467 | 921   | (39)  | 960  | 960 |
| 13729.12   | 538.8  | (4.4) | 524 | 487 | -404  | (29)  | -392 | -378 |
| 1371.045   | 602.219 | (0.003) | 613 | 602 | 1267.267 | (0.030) | 1269 | 1290 |
| 2840.170   | 441.771 | (0.005) | 442 | 434 | 158.750 | (0.040) | 156  | 149 |
| 5829.860   | 271.2  | (0.7) | 260 | 265 | -349.8 | (6.8) | -349 | -351 |
| 7441.030   | 509.843 | (0.003) | 525 | 516 | 547.483 | (0.003) | 571  | 540 |
| 7824.190   | 621.5  | (2.1) | 634 | 633 | 789.8 | (3.8) | 797  | 790 |
| 8097.875   | 229.1  | (1.7) | 124 | 207 | -398.8 | (6.4) | -457 | -441 |
| 9145.230   | 1069.3 | (0.3) | 1041 | 1041 | 1088.8 | (7.5) | 1080 | 1045 |
| 9897.730   | 1109.4 | (0.2) | 1081 | 1162 | 537.3 | (3.7) | 472  | 518 |
| 9986.73    | 636.719 | (0.003) | 665 | 638 | 367.994 | (0.003) | 361  | 220 |
| 10680.17   | 351.9  | (1.2) | 337 | 354 | -229.5 | (7.8) | -302 | -276 |
| 11956.255  | 576.1  | (2.3) | 544 | 583 | 945   | (15)  | 937  | 975 |
| 12228.28   | 798.0  | (1.5) | 799 | 798 | -277.1 | (9.7) | -256 | -268 |
| 12776.31   | 414.7  | (2.9) | 430 | 408 | 864   | (34)  | 862  | 867 |
| 13751.41   | 558.3  | (1.5) | 593 | 555 | 264.6 | (7.6) | 278  | 271 |
Table 4. Continued.

| \( E_{\text{exp}} \) | \( A \) This work | \( B \) This work | \( [10] \) |
|-----------------|-----------------|-----------------|----------|
| \( J = 11/2 \)  |
| 509.845         | 577.465         | (0.002) 589     | 579      | 989.917         | (0.030) 996 | 1008     |
| 2310.090        | 405.106         | (0.003) 390     | 398      | −92.638         | (0.050) −62 | −96      |
| 5353.370        | 267.2           | (1.0) 245       | 265      | −448.7          | (9.8) −484 | −476     |
| 6674.155        | 527.6           | (1.2) 553       | 539      | 528.4           | (1.4) 606 | 545      |
| 6988.820        | 446.7           | (0.3) 476       | 457      | 739             | (15) 697 | 708      |
| 8646.210        | 984.255         | (0.001) 979     | 977      | 925.956         | (0.001) 931 | 913      |
| 8932.120        | 456.1           | (3.1) 476       | 472      | 589.1           | (3.4) 549 | 584      |
| 10097.850       | 500.3           | (2.0) 484       | 511      | 1262.5          | (2.5) 1157 | 1188     |
| 11260.41        | 919.9           | (2.3) 929       | 920      | 309             | (13) 346 | 349      |
| 12453.14        | 370.011         | (0.003) 379     | 371      | 660.165         | (0.003) 658 | 645      |
| 13071.30        | 703.0           | (3.8) 741       | 726      | −203            | (36) −231 | −214     |
| 13666.46        | 635.0           | (0.9) 648       | 638      | −208            | (36) −238 | −253     |
| \( J = 13/2 \)  |
| 285.500         | 532.204         | (0.002) 542     | 532      | 928.861         | (0.020) 900 | 932      |
| 3719.705        | 354.454         | (0.003) 320     | 346      | 72.183          | (0.030) 28  | 47       |
| 6351.750        | 438.5           | (2.2) 441       | 441      | 1122            | (29) 1145 | 1118     |
| 7059.900        | 519.5           | (0.7) 544       | 535      | 1179.7          | (2.7) 1198 | 1221     |
| 8277.040        | 981.2           | (2.6) 993       | 995      | 820             | (24) 794  | 778      |
| 9763.020        | 469.4           | (0.8) 442       | 473      | 1480            | (11) 1505 | 1546     |
| 11425.94        | 672.5           | (0.4) 705       | 708      | 75.4            | (9.9) 49  | 62       |
| 12475.74        | 439.3           | (2.1) 458       | 489      | 529             | (26) 612  | 638      |
| 12906.60        | 831.0           | (1.1) 839       | 803      | 820             | (17) 884  | 820      |
| 13161.48        | 836.6           | (0.8) 765       | 752      | 704             | (15) 599  | 557      |
| 23043.43        | 685.7           | (2.0) 639       | 915      | 915             | (24) 591  |          |
| 23147.92        | 708.9           | (0.6) 767       | 1328     | (29) 875        |          |          |
| \( J = 15/2 \)  |
| 462.080         | 472.643         | (0.002) 474     | 470      | 1154.239        | (0.017) 1148 | 1144    |
| 5425.060        | 459.627         | (0.003) 471     | 466      | 1724.243        | (0.003) 1728 | 1721    |
| 7767.015        | 509.0           | (0.9) 498       | 517      | 2048            | (15) 2063 | 2114     |
| 8190.465        | 948.5           | (1.1) 973       | 978      | 699             | (31) 653  | 646      |
| 11580.68        | 615.3           | (1.8) 604       | 602      | 155             | (29) 77  | 104      |
| 12628.67        | 654.4           | (0.3) 653       | 648      | 427             | (38) 474  | 388      |
| 12932.66        | 294.2           | (1.8) 294       | 303      | 406             | (24) 343  | 371      |
| 14569.67        | 566.0           | (3.4) 600       | 559      | 294             | (31) 266  | 260      |
| 15387.79        | 525.7           | (0.4) 458       | 545      | 1080.0          | (5.9) 1122 | 1206    |
| 23112.35        | 968.0           | (0.1) 1037      | 916.9    | (1.3) 1233      |          |          |
| 23031.84        | 880.9           | (0.6) 832       | 832      | 838.3           | (4.5) 812 |          |
| \( J = 17/2 \)  |
| 4646.830        | 481.738         | (0.002) 451     | 481      | 2245.914        | (0.050) 2228 | 2195    |
| 8506.710        | 915.3           | (0.5) 937       | 940      | 464             | (37) 408  | 393      |
| 11879.20        | 757.6           | (0.4) 762       | 758      | 1167            | (24) 1158 | 1132     |
| 14016.91        | 648.9           | (2.3) 662       | 636      | 669.5           | (3.5) 758  | 735      |
| 14718.11        | 781.5           | (4.9) 617       | 785      | 1020            | (18) 1103 | 881      |
| 15189.26        | 1025.6          | (0.7) 995       | 1019     | 682             | (29) 773  | 693      |
| 17249.59        | 857.1           | (0.4) 866       | 871      | 1758.0          | (5.0) 1688 | 1929    |
| \( J = 19/2 \)  |
| 11331.14        | 876.3           | (3.8) 890       | 899      | 1460            | (20) 1469 | 1431     |
| 13398.40        | 690.6           | (0.6) 687       | 676      | 1023            | (16) 1027 | 1003     |
| \( J = 21/2 \)  |
| 12283.30        | 845.9           | (0.1) 855       | 859      | 1906            | (11) 1927 | 1880     |
Values of the one- and two-body hyperfine structure parameters (MHz) and effective radial integrals (a.u.) obtained from the experimental data for the even parity configurations of Tb I; OHFS stands for “optimized Hartree-Fock-Slater” method.

| Parameter | Value | Comments |
|-----------|-------|----------|
| $a_{17}^{4f}$ | 1072 | (26) fitted |
| $a_{2d}^{4f}$ | 264 | (58) fitted |
| $a_{10}^{4f}$ | 11206 | (501) fitted |
| Configuration 4f$^5$5d$^3$ and 4f$^6$5d$^2$6s | | |
| $E^0(4f,4f)$ | $D^{10}(n_{0s},6s)$ | $a_{12}^{4f}$ | 14 | (8) fitted, $n_0 = 3, 4$ |
| $E^0(4f,4f)$ | $D^{12}(n_{0d},5d)$ | | 17 | (8) fitted, $n_0 = 3, 4$ |
| | $D^{10}(n_{0d},5d)$ | | 3 | (1) fitted, $n_0 = 3, 4$ |
| | $D^{12}(n_{0d},5d)$ | | -193 | (31) fitted, $n_0 = 3, 4$ |
| | | | | | | |
| Configuration 4f$^6$5d$^6$s$^2$ | | | | | | |
| $E^2(4f,4f)$ | $P^{10}(n_{0s},n's)$ | $a_{12}^{6s}$ | 528 | (116) fixed |
| | $P^{10}(n_{0s},n's)$ | $a_{12}^{6s}$ | -5503 | (550) fitted, $n_0 = 1, 2, 5, n' = 7, 8, 9$ |
| Inter-configuration interaction | | | | | | |
| $a_{12}^{6s,6p}$ | 1307 | (180) fitted |
| $D^2(4f,4f)$ | $P^{10}(n_{0s},6s)$ | | -24037 | (1700) fitted, $n_0 = 1, 2, 6, n' = 7, 8, 9$ |
| $\langle r^{-3} \rangle_{4f \text{ non-red}}$ | 8.368 | | | | |
| $\langle r^{-2} \rangle_{4f}$ | 8.962 | | | | |
| $\langle r^{-3} \rangle_{4f}$ | 8.997 | (HF) [30] |
| $\langle r^{-3} \rangle_{4f}$ | 8.311 | (OHFS) [30] |
| $\langle r^{-3} \rangle_{4f}$ | 8.1 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 8.344 | (OHFS) [30] |
| $\langle r^{-3} \rangle_{4f}$ | 9.549 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 8.7 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 9.066 | (OHFS) [30] |
| $\langle r^{-3} \rangle_{4f}$ | 2.779 | this work |
| $\langle r^{-3} \rangle_{4f}$ | 2.89 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 3.1 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 1.13 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{4f}$ | 0.9 | (exp for 4f$^6$5d$^6$s$^2$ configuration) [29] |
| $\langle r^{-3} \rangle_{6s,6f,eff}$ | 131.207 | this work |
be identical. On the basis of results of performed parameterization (see table 5) we obtain
published earlier [10] agrees better with the monotonic increase trend with the atomic number proposed by Pfeufer [29]
in the papers [6, 10, 25].

The configuration interaction effects concerning the excitation of electrons from the closed ns shells to
open 6s-shell or to empty ns shells are different in each of the considered configurations and were
included by the following intra-configuration parameters: E(3n0d6s,6s5d) P02(3n0d,5d) = −136 (20) fitted, n0 = 3, 4,
E2(n0d6s,6s5d) P02(n0d,5d) = −136 (20) fitted, n0 = 3, 4,
E1(n0d4f,4f5d) P02(n0d,5d) = 87 (37) fitted, n0 = 3, 4.

The configuration interaction effects concerning the excitation of electrons from the closed ns shells to
open 6s-shell or to empty ns shells are different in each of the considered configurations and were
included by the following intra-configuration parameters: E(3n0d6s,6s5d) P02(3n0d,5d) = −136 (20) fitted, n0 = 3, 4,
E2(n0d6s,6s5d) P02(n0d,5d) = −136 (20) fitted, n0 = 3, 4,
E1(n0d4f,4f5d) P02(n0d,5d) = 87 (37) fitted, n0 = 3, 4.

Parameter Value Comments

\[
\begin{align*}
\alpha_{4f}^2 & \quad 2235 \quad (40) \quad \text{fitted} \\
\beta_{4f}^2 & \quad 718 \quad (140) \quad \text{fitted} \\
\beta_{4f}^3 & \quad -259 \quad (74) \quad \text{fitted} \\
\beta_{5d}^2 & \quad 962 \quad (40) \quad \text{fitted} \\
\beta_{5d}^3 & \quad 615 \quad (95) \quad \text{fitted} \\
\beta_{5d}^4 & \quad -419 \quad (61) \quad \text{fitted} \\
R^6(4f4f,4f'nf) P_{02}(4f,n') & \quad -177 \quad (31) \quad \text{fitted, } n' = 5, 6, 7, \ldots \\
E^2(n0d6s,6s5d) P_{02}(n0d,5d) & \quad -136 \quad (20) \quad \text{fitted, } n0 = 3, 4 \\
D^0(n0d4f,5f4f) P_{02}(n0d,5d) & \quad 20 \quad (6) \quad \text{fitted, } n0 = 3, 4 \\
E^1(n0d4f,4f5d) P_{02}(n0d,5d) & \quad 87 \quad (37) \quad \text{fitted, } n0 = 3, 4 \\
\langle r^{-3}\rangle_{4f} \quad -1599 \quad (220) \quad \text{fitted} \\
\langle r^{-3}\rangle_{4f}^2 & \quad 6.643 \quad \text{this work} \\
\langle r^{-3}\rangle_{4f}^3 & \quad 6.946 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [29] \\
\langle r^{-3}\rangle_{4f}^4 & \quad 6.7 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [8] \\
\langle r^{-3}\rangle_{4f}^5 & \quad 6.458 \quad (\exp \text{ for } 4f^6s^2 \text{ configuration}) [29] \\
\langle r^{-3}\rangle_{4f}^6 & \quad 8.365 \quad (\OHFS) [30] \\
\langle r^{-3}\rangle_{4f}^{11} & \quad -0.770 \quad \text{this work} \\
\langle r^{-3}\rangle_{4f}^{13} & \quad -0.562 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [29] \\
\langle r^{-3}\rangle_{4f}^{13} & \quad -1.7 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [8] \\
\langle r^{-3}\rangle_{4f}^{13} & \quad -0.461 \quad (\OHFS) [30] \\
\langle r^{-3}\rangle_{4f}^{13} & \quad 2.134 \quad \text{this work} \\
\langle r^{-3}\rangle_{4f}^{13} & \quad 0.27 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [29] \\
\langle r^{-3}\rangle_{4f}^{13} & \quad 4.2 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [8] \\
\langle r^{-3}\rangle_{4f}^{13} & \quad 1.003 \quad (\OHFS) [30] \\
\langle r^{-3}\rangle_{5d}^{11} & \quad 2.859 \quad \text{this work} \\
\langle r^{-3}\rangle_{5d}^{13} & \quad 3.733 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [29] \\
\langle r^{-3}\rangle_{5d}^{13} & \quad 3.7 \quad (\exp \text{ for } 4f^5d6s^2 \text{ configuration}) [8]
\end{align*}
\]

The configuration interaction effects concerning the excitation of electrons from the closed ns shells to
the open 6s-shell or to empty ns shells are different in each of the considered configurations and were
included by the following intra-configuration parameters: E(3n0d6s,6s5d) P10(n0d6s,6s5d) = −11, 615 (95) fitted,
E2(n0d6s,6s5d) P10(n0d6s,6s5d) = −11, 615 (95) fitted,
E1(n0d4f,4f5d) P10(n0d4f,4f5d) = 10, 134 (20) fitted,
E1(n0d4f,4f5d) P10(n0d4f,4f5d) = 10, 134 (20) fitted.

The value of radial integral \(\langle r^{-3}\rangle_{4f}^{11} = 131.207 \text{ a.u.} \) obtained within this work compared to the value (105.284 a.u.)
published earlier [10] agrees better with the monotonic increase trend with the atomic number proposed by Pfenfer [29]
for some selected one-electron radial integrals of various elements along the lanthanides series.

The ratios of two-body hfs radial parameters describing magnetic dipole and electric quadrupole interactions
should be identical. On the basis of results of performed parameterization (see table 5) we obtain

\[
\begin{align*}
E^2(n0d6s,6s5d) P_{10}(n0d,5d)/E^2(n0d6s,6s5d) P_{02}(n0d,5d) & = -0.13, \\
D^0(n0d4f,5f4f) P_{10}(n0d,5d)/D^0(n0d4f,5f4f) P_{02}(n0d,5d) & = 0.15, \\
E^1(n0d4f,4f5d) P_{10}(n0d4f,4f5d)/E^1(n0d4f,4f5d) P_{02}(n0d,5d) & = 0.16.
\end{align*}
\]

This points out that contributions originating from the second-order perturbation theory within the frame of
magnetic dipole or electric quadrupole interactions in the hyperfine structure is not fully correct. The more precise
measurements of the hyperfine splittings would be required.
4 Conclusions

By extending the fine- and hyperfine analysis to the complete set of $4f^N$-core states we got improved agreement between the calculated and experimental energy level values as well as calculated and experimental hyperfine structure constants $A$ and $B$. Based on our results, we can assume that the description of the electronic levels is more reliable. Therefore, we conclude that our earlier semi-empirical analysis of the rare-earth spectra related to the americium, europium and praseodymium atoms [31–34] should be repeated. Also, the extensive investigations of the hyperfine structure of the terbium atom with the method of laser induced fluorescence in a hollow cathode discharge, carried out in our experimental group, provided a lot of new data for odd parity levels [35]. This motivated us to work intensively on the development of novelty kind of computational procedures optimization for both the generation of angular coefficients of such huge energy matrix and diagonalization problem. This work shows that we have created an effective tool for precise determination of attributes of an atom, such as the energy levels, as well as the energy sublevels of the hyperfine structure, having a number of valence electrons, which can occur in all provided by quantum mechanics configurations.

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