

Ab initio lifetimes, Landé g-values and hyperfine structure for Ta II states

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Abstract. *Ab initio* Dirac-Coulomb (Breit) configuration-interaction calculations have been done for the lowest 4 (8, 12) $J = 0$ ($J = 1, 2$) $(5d+6s)^4$ states and the lowest 12 $(5d+6s)^36p$ $J = 1$ states of Ta II. Nearly 20 000 basis functions were used for each state. Energy differences, magnetic dipole hyperfine constants and Landé g-values were calculated, and are in good agreement with available experiment. Lifetimes and branching ratios were calculated for the odd parity levels, and agree well with experiment, except in one case.

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1. Introduction

Lifetimes and hyperfine structure of Ta II levels are of interest to the astrophysical community [1, 2] for abundance determination and spectrum synthesis. The spectrum of this system is a complex one [3, 4, 5], as it involves interpenetration of $(5d+6s)^4$ [$(5d+6s)^3 6p$] levels, and experimental corrections to the energy levels have been made as late as 1990 [5]. Henderson *et al* in their 1999 work [2] recognized that “an elaborate calculation would be required to determine quantitatively the [odd parity] wavefunctions”, and instead restricted their studies to qualitative estimates of branching ratios, using semi-empirical methods. Our work provides the elaborate quantitative calculations needed.

The work reported here involves the 12 lowest odd parity $J = 1$ states (33 706 to 49 887 cm^{-1}), and, because of electric dipole (E1) selection rules, all $J = 0, 1, 2$ even parity $(5d+6s)^4$ states constituting significant decay branches for these $(5d+6s)^3 6p$ levels. We report oscillator strengths for each of the significant branches. Because of the high Z ($Z = 73$), relativistic effects must be included from the beginning. Additionally, correlation plays a crucial role, especially due to the interpenetration within $(5d+6s)^4$ [$(5d+6s)^3 6p$] states, and it is difficult to treat, because of the number of open d-shell electrons.

The approach used here is that of relativistic configuration interaction (RCI). We begin by using a Dirac-Coulomb (or Dirac-Breit) Hamiltonian, and solve multiconfigurational Dirac-Fock (MCDF) equations, using the algorithm of Desclaux [6] for the $(5d+6s)^4$ and $(5d+6s)^3 6p$ configurations, to provide reference wavefunctions. Correlation is then included by creating new configurations through, mainly, single and double subshell excitations from the valence and shallow core reference subshells. Correlation coefficients and correlation radial functions are then determined by employing the energy variational principle.

Very recently [7], we increased the RCI matrix limit from 7000 to 20 000 vectors. Without this increase, the calculations on Ta II would not have been possible. The limit is imposed by our current desire to have all non-zero matrix elements reside in memory. For this work, we have also dramatically (by a factor of ~ 300) speeded up calculation times for the f-values, by taking advantage of the long wavelength characteristic of the transitions of interest. In this regime, the length (velocity) f-value scales as the energy difference (inverse of energy difference), and all transitions for a fixed J , parity pair may be done at once. Calculation time is then reduced to about 30 minutes on a 500 MHz Alpha workstation, including full treatment of non-orthonormality effects, based [8] on the work of King *et al* [9].

Earlier, we reported work on $(d+s)^4 \rightarrow (d+s)^3 p$ transitions in Nb II [10] and Fe V [7]. The 1995 work [10] was much less (at least a factor of 2) accurate and extensive,

while the more recent Fe V calculations were simpler because the ionicity produced a good separation of d^4 , d^3s and d^2s^2 [d^3p , d^2sp and ds^2p] states, so that it was not necessary to treat all three configurations on an equal footing, as is needed for Ta II.

In Fe V [7] and here, we find that it is very important that energy differences between adjacent nearly degenerate states (same J , parity) are accurately determined. It would be preferable to have these be in error less than $\sim 10\%$ or 200 cm^{-1} , whichever is smaller. For some of the higher odd parity levels of Ta II, we have not been able to accomplish this, and possibly as a consequence, of the five measured lifetimes [2, 11, 12, 13], our *ab initio* RCI results are only in very good to good agreement with four of them. The difficulty may arise because our correlation tends to emphasize the lower (odd parity) states, artificially pulling the twelve states away from $(5d+6s)^3(5p+4f)$ states, which need to be more carefully correlated. Due to the size of the matrix, it is not now possible to do this in an *ab initio* manner. Instead, we artificially shift the diagonal matrix elements of the $(5d+6s)^3(5p+4f)$ basis members, which decreases the energy separation errors, but with little effect on the lifetimes of Ta II. Thus, the reason for the experimental-theoretical discrepancy of the seventh odd parity level, at $44\,206 \text{ cm}^{-1}$, is not understood.

2. Methodology

The relativistic configuration interaction (RCI) methodology employed is based on a Dirac-Coulomb or Dirac-Breit Hamiltonian. The bound state wavefunction is represented by a linear combination of basis functions, each of which is an eigenstate of the J^2 , J_z and relativistic parity operators, and has a unique relativistic configuration. The basis functions are linear combinations of Slater determinants, whose elements are four-component spinors, constructed from major and minor radial and angular factors. The angular factors are of the hydrogen type, and the radial functions are to be determined.

It is desirable to have an economical, general and well-converged expansion of the wavefunction. To accomplish this, we divide the wavefunction configurations into two classes—those few providing $\sim 90\%$ of the wavefunction, by weight, which typically appear as spectroscopic labels [3] of the levels of interest, and the remainder. For the former, the energy variational principle is applied to determine both the spinor radial functions and the coefficients of the N-electron basis functions. This requires solving a coupled set of first-order inhomogeneous integro-differential equations, known as the Dirac-Fock equations. This is done using a modified version [14] of Desclaux’s algorithm [6].

Since the spinor’s angular functions are known, the angular integrations can be done, and the energy functional reduced to a linear combination of one- and two-particle radial integrals. This reduction is greatly aided by the fact that the N-electron basis functions

are fully orthonormal; the necessary angular algebra has been provided by Grant [15]. Further details of the wavefunction methodology may be found in Ref. [16].

Because the remainder of the wavefunction, i.e., the correlation part, is mainly determined by the Coulomb operator, as well as for reasons of bookkeeping, it is useful to refer to all relativistic configurations reducing to a common non-relativistic configuration, as $c \rightarrow \infty$, as a manifold. The MCDF or reference function then consists of three manifolds $(5d+6s)^4 [(5d+6s)^3 6p]$, depending on how the three electrons are distributed between the 5d and 6s subshells. The principal manifolds to be included in the correlation function, χ , are determined by appealing to first-order perturbation theory, which leads us to include single and double excitations from the MCDF manifolds.

As part of the specification of the correlation function, new radial functions are needed, which are called virtuals. As has been known from the 1960's [17], such functions must represent the localized portion of the Rydberg and continuum series of the same symmetry (e.g., $v f_{5/2}$ represents $4f_{5/2}, 5f_{5/2}, \dots, \epsilon f_{5/2}, \dots$). Simultaneously, in the relativistic case, we must avoid variational collapse into the positron sea [18]. We find that representing virtuals with relativistic screened (Z^*) hydrogenic functions, RSHF, produces up to 90% of the correlation energy achievable, with much slower convergence as more virtuals are added, as is typical of single particle expansions. Usually, from two to three virtuals produce an adequately converged result. The single parameter, Z^* , is estimated by matching the $\langle r \rangle$ between the MCDF radial being replaced and the virtual. Final adjustment is made at the RCI diagonalization stage.

Because Z^* tends to maximize the overlap of the MCDF and virtual radial charge densities, different MCDF shells require different sets of virtuals. Calculation begins with the outermost shell(s) (5d, 6s and 6p here), where most of the physics is, and where there is more near degeneracy between the correlation and MCDF manifolds. As part of the determination of this valence correlation, selected triple and quadruple excitations, characteristic of a second-order wavefunction, are explored. The largest of these should be formed by products of the largest single-pair and pair-pair excitations [19].

One then excites from the shallow core, bearing in mind that this can considerably increase the size of the calculation. Not only can core (core-valence) manifolds involve lots of complicated basis functions (large number of determinants), and new virtuals, but they may require that second-order effects be added to the valence correlation. This can arise because the MCDF manifolds are being preferentially correlated [20], as compared to nearly degenerate valence correlation manifolds. As an illustration, if the excitation $5p^2 \rightarrow 5d^2$ were made for the MCDF manifold $5p^6 5d^2 6s^2$, then it probably should be made for the $5p^6 5d^2 v p^2$ valence correlation manifold. For Ta II, we have chosen the shallow core to be the 5s and 5p subshells.

To diagonalize the RCI matrix, we use a modified [21, 22] form of Weber's [23] diagonalizer, which is based on the algorithm of Davidson [24]. This is a multi-root large-scale diagonalizer, with the attractive attribute that it needs only the non-zero matrix elements, one row at a time. Our current preference, for reasons of efficiency, is to have the non-zero portion of the matrix (typically $\sim 70\%$ sparse) reside in memory. Formerly, this meant restricting matrix sizes to 7000 or less, but with the acquisition of additional memory, this has just been increased to 20 000, which makes the treatment of Ta II much more convenient. In the past, we have only been interested in the lowest roots, but for the Ta II odd parity levels, we looked at the lowest 25, which include all the levels measured by Kiess [4], accepted by Wyart and Blaise [5]. To make sure the top roots were being determined accurately enough, the two tolerance parameters of the diagonalizer were slightly adjusted, until errors fell below 1 cm^{-1} .

Inclusion of the Breit operator in the RCI matrix increases computation times approximately fourfold, so we do it originally with just the MCDF manifolds. If energy differences are changed by less than 200 cm^{-1} (our current average error goal), then the Breit operator is not included in the RCI matrix, which is the case for the Ta II levels (the average Breit contribution to odd parity energy differences is 60 cm^{-1}).

Once the odd and even parity wavefunctions are obtained, the oscillator strengths (f-values) are computed using the formalism of Grant [25], as discussed in Ref. [26]. Since we have obtained the odd and even parity wavefunctions from different basis sets, non-orthonormality effects must be included in this evaluation. This is done by using a modified version [10, 26] of the method of King *et al* [9], which for parity-changing transitions (e.g., $E1$) eliminates the need for performing the expensive diagonalization step for each pair of determinants, and minimizes the number of determinantal matrix elements that need to be evaluated, by using symmetry to *a priori* remove the maximum number of zero interactions. A further efficiency gain is made by recognizing that many core radial functions are nearly identical for both states.

Despite these efficiencies, due to the large size of the basis set ($\sim 16\ 000$ – $18\ 000$ members), a single f-value calculation takes nearly 30 minutes on a 500 MHz Alpha workstation. But, from the formalism [25], we can establish that for long wavelength (small energy difference, dE) transitions, such as we have here, the length (Babuskin) gauge result is proportional to dE , and the velocity (Coulomb) gauge result is proportional to $1/dE$, as is true non-relativistically. We have used this property to do all f-values at once, for a fixed (J, J') . The efficiency occurs because each surviving pair of determinantal matrix elements is evaluated once only (and not for each pair of transitions) and then distributed over all transition pairs. A typical energy difference is chosen (necessary for the spherical Bessel function argument), and the f-values rescaled to the correct energy differences, at the end. Several transitions were computed exactly, and then with this method, with no discernible change. We use the experimental energy

difference for the transitions, as these are known, whereas the wavefunctions (and hence, transition matrix elements) are not.

3. Results

3.1. *Odd parity wavefunctions*

Relative energies, Landé g -values, and magnetic dipole hyperfine structure constants are shown for the lowest 12 odd parity $J = 1$ Ta II levels in Table 1. Our results are consistent with Wyart and Blaise’s [5] rejection of the Kiess [4] levels at 31 212 and 47 620 cm^{-1} . Though we calculated all 25 remaining odd parity $J = 1$ levels reported by Kiess [4], we are only including the bottom 12, as the upper 13 are not accurately enough determined to warrant inclusion in this work. This inaccuracy stems from three sources, we believe; the first is the worsening ability of the MCDF radials determined for the lowest odd parity $J = 1$ level to represent higher levels. For example, MCDF calculations produce a splitting between the ground and third excited state odd parity levels 591 cm^{-1} lower than an RCI calculation for the same manifolds. This is solely due to the difference in radial functions. RCI uses a single set, obtained for the ground level. This deficiency chiefly occurs for the valence radials, and is substantially corrected for within RCI, by including $6p \rightarrow vp$ and $5d \rightarrow vd$ excitations. For the full RCI calculation, second-order effects and/or shifts may be necessary.

The second source is the growing importance of $(5d+6s)^37p$ and $4f$ manifolds with increasing energy, because of near degeneracy effects and the greater need to adequately correlate them (second-order effects). Finally, the third source is our exclusion of certain first-order excitations based on the bottom 7 roots (our original focus), which may be of greater importance for the higher energies. In principle, all these problems can be removed, but at the cost of a much larger calculation than the ones reported here. However, the five measured lifetimes are for levels 2, 3, 7, 10 and 12 (the lowest odd parity $J = 1$ level is numbered 1), and we have values for all of these, in addition to seven other unmeasured levels.

Relative to the $J = 1$ odd parity lowest state, our average energy difference is in error by 262 cm^{-1} , and the average absolute energy difference between adjacent levels is in error by 157 cm^{-1} (14.4%) for all 12 levels; for the bottom 7 levels the error is considerably less. This second quantity (157 cm^{-1}) we believe is a better figure of merit, because it more correctly represents how well nearly degenerate basis functions are “mixed” into the states. The worst adjacent separations are for levels 7 and 8, and levels 11 and 12.

The composition of the odd parity levels is complex, and only a crude account has been given in Table 1 [“Label”]. In Table 2, all contributions to the MCDF manifolds greater than 1% after integer truncation are given. These are determined from the final

RCI wavefunction, by decomposing the jjJ MCDF basis functions into an approximate (but complete, within the manifolds) LSJ set, obtained by diagonalization of L^2 and S^2 matrices, with the conditions that the minor radial component is ignored, and the major radial component is assumed independent of j (e.g., so $5d_{3/2}$ and $5d_{5/2}$ are assumed to have the same radial function). Most of the levels have $5d^26s6p$ character, but levels 2, 7, 8 and 10 are $5d^36p$; this changing character with level means that there is less cancellation of differential correlation effects.

The Landé g -values are computed from the full RCI wavefunction, which has 16 160 basis functions built from 211 000 determinants, and ~ 5 million coefficients. The relativistic operator of Armstrong [27] is used; this does not include the anomalous g -value, but our errors due to missing correlation effects are at least 10 times larger. Specifically, the average absolute g -value error is 0.036, which is to be contrasted with the MCDF error of 0.565, as computed from a common set of radial functions, with no correlation configurations present. From Table 1, one may observe that a good portion of this error occurs because some levels are flipped, at the MCDF level. We also note that the ‘‘MCDF’’ values extracted from the full RCI run are consistently close to the full RCI values. We take this as a reflection of the fact that corrections to $\langle S_z \rangle$ and $\langle L_z \rangle$, the non-relativistic Landé g -value operators, must be of second order.

Table 1 also contains results for the magnetic dipole hyperfine structure constants, for $\mu = 2.3$ and $I = 3/2$. These values, especially the smaller ones, are not too well determined (perhaps to ~ 100 MHz), for two reasons: (1) the smaller ones are quite sensitive to remaining errors in the positioning of energy levels, as we discuss below, and (2) more excitations from core subshells, e.g., $4s \rightarrow s$, need to be included, based on past experience.

In Table 3, we present the contributions of the significant (10 meV or higher) ‘‘first order’’ manifolds to the correlation energy. For reasons of brevity, all contributions are given relative to the lowest odd parity $J = 1$ state, and all contributions involving the same symmetry (e.g., $6p \rightarrow vp+vp'+\dots$) are collected into a single entry ($6p \rightarrow vp$). In intermediate normalization, the RCI wavefunction, ψ , may be written

$$\psi = \phi + \sum_i [c(i)/c(\phi)] * \chi(i) \quad (1)$$

where ϕ represents the normalized MCDF manifolds portion of the wavefunction, $\chi(i)$ the i th correlation function, with $\langle \phi | \chi(i) \rangle = 0$. If the coefficient of ϕ in the normalized (original) ψ is $c(\phi)$ and that of $\chi(i)$ is $c(i)$, then the i th correlation function contributes $[c(i)/c(\phi)] * \langle \phi | H | \chi(i) \rangle$ to the correlation energy. Within this first-order ‘‘concept’’, all higher-order effects, whether due to explicit triple or quadruple excitations, or to pair-pair interactions implicitly present in the RCI matrix, enter only through the value of $c(i)$.

For space reasons, correlation manifolds in Table 3 are indicated as single or double

excitations from a specified (by n = number of d electrons) MCDF manifold. Many configurations can arise from more than one MCDF manifold; we have chosen the one with highest n arbitrarily.

Single excitations of the type $nl \rightarrow n(l+2)$ or $v(l+2)$ are known [28] to be large both totally and differentially, the latter because they depend on the interactions with open subshell electrons, which vary from state to state. In the present instance, $5p$ ($6p$) $\rightarrow vf$ falls into this category. The pair excitation $(nl)^2 \rightarrow [v(l+1)]^2$ is also large [28, 29], totally and differentially. The latter effect arises from both the different coupling of the $(nl)^2$ electrons, and the total number of nl electrons in the states. From Table 3, we see that $5d^2 \rightarrow vf^2+vd^2$ are both important. Exclusion effects described by $nl \rightarrow n'l'$ and $nl n'l' \rightarrow n''l'' x$, where $x = n'''l'''$ or vl , can also be important; if $x = nl'''$ and $n' = n'' = n$, these excitations are also complex-preserving. From Table 3, we find that $5p^2 \rightarrow 5d^2$, $5p6p \rightarrow 5d^2$ and $5p \rightarrow 6p$ are important contributors in this category. We also find $6p$ ($5p$) $\rightarrow vp$ to be an important contributor, likely because the MCDF radials are best suited to the bottom roots, not the upper ones. Finally, $5p5d \rightarrow vdvf$ is important because of the varying occupancies of the $5d$ electrons in the states. It can be shown [28, 30] that for any pair excitation involving at least one closed-core subshell, the correlation energy associated with that excitation is proportional to the occupancy of the other shell, assuming no variation in the radial functions with state. Additionally, past experience, e.g., [29], has demonstrated that the $vdvf$ combination along with vfv and $vpvd$, are the largest ones.

Many manifolds included in the final RCI odd parity wavefunctions were too small (relative contributions below 10 meV) to be included in Table 3. As a general rule, there are three correlation configurations for each excitation type, if allowed in first order. For example, $5d^2 \rightarrow vf^2$, $5d6s \rightarrow vf^2$ and $6s^2 \rightarrow vf^2$ are all present. Additionally, there are excitation types which were included, but do not appear in Table 3. These are the following: $5d6s \rightarrow vpvf$; $5d^2 \rightarrow vsvd+vp^2+vs^2+6pvp$; $5d6p \rightarrow vpvf+vsvp+vsvf+vfv$; $5p6p \rightarrow 5dvs+vpvf$; $5s \rightarrow vd$; $5s^2 \rightarrow 5d^2$ and $5d^3 \rightarrow vdvf^2+6pvdvf$.

Additionally, other configurations were investigated, found to be small, and deleted from the final wavefunction. These included the exclusion excitations: $(5s^2+5s5d+5p^2) \rightarrow 6p^2$; $5p^4 \rightarrow 5d^4$; $5p^3 \rightarrow 5d^2vf$; $5p5d \rightarrow 6p(vs+vd)$; $5s5p \rightarrow (5d+6s)6p$; $5s5d \rightarrow 6pvd$. Also, to examine the completeness of the angular pair excitations, we included: $5d^2 \rightarrow vdv$; $5p6p \rightarrow vf^2+vpv$; $5p(5d+6s) \rightarrow vpvf+vsvf$; and $5s5d \rightarrow vsvf$. Finally, single excitations $6p \rightarrow vh$ and $5d \rightarrow vi$ and the triple excitation $5p5d^2 \rightarrow vf^3$ were tried.

In addition to the basis set deficiencies noted earlier for the higher states, we have not included the excitation $5p^2 \rightarrow 5dvd$. While this is significant on its own, it increases the basis size substantially, and should be partially compensated by a larger virtual basis set for $5p5d$ pair excitations. The fact that these two tend to cancel can be understood by realizing that the first (second) is larger when fewer (more) $5d$ electrons are present.

The effect of improving the energy level positions has been explored semi-empirically by shifting RCI diagonal matrix elements associated with $(5d+6s)^3(vp+vp'+vf+vf')$ manifolds, and re-diagonalizing the RCI matrix. The shift is adjusted from its initial estimate until the best match to the experimental energy spectrum is achieved. The motivation behind this choice is that these manifolds represent nearly degenerate manifolds, compared to $(5d+6s)^36p$, which tends to lose this property as the MCDF manifolds are correlated (e.g., there is no $5p^2 \rightarrow 5d^2$ for $(5d+6s)^3vp$). A shift is estimated by using a value nearly equal to the total correlation energy of the MCDF reference, viz. -0.090 a.u. The consequence is that the average error in the spacings between adjacent levels has been reduced to 109 cm^{-1} (9.3%), and the average Landé g-value error reduced to 0.029. In order of increasing energy, the shifted values for A (in MHz) are: -1876, 1767, -1334, 541, 3168, 2136, 644, 1135, 1367, 11, 46, 1920. This corresponds to an average change in the magnitude of A of 48 MHz. The effect on the lifetimes is marginal, as is noted below in Section 3.3.

3.2. Even parity wavefunctions

Energy differences (separately zeroed for each J), Landé g-values and magnetic dipole hyperfine constants are given in Table 4 for the RCI wavefunctions, and compared with experiment. The average separation error for all three J 's is 398 cm^{-1} , about 2.5 times larger than for the odd parity levels. Despite the larger errors, there does not seem to be a substantial impact on the lifetimes due to the relatively poorer positioning of the levels, as the shift studies reported below and in Section 3.3 indicate. Furthermore, the Landé g-values agree well with experiment.

The even parity states are labelled following Moore [3], but this does not adequately characterize the levels, so we have given the LS percentages, for the MCDF manifolds, in Table 5. These are normalized to 100%, but the totals are somewhat less than that, as we present only contributions of 1% or higher, and truncate. As the MCDF manifolds constitute at least 92.7%, by weight, of each wavefunction, these results should characterize the entire wavefunction rather well.

For the even parity states, all three configurations $(5d+6s)^4$ play an important role ($5d6s^26p$ plays a subdued role for odd parity $J = 1$), complicating the treatment of correlation. This is undoubtedly one of the causes of the larger errors, which are most likely associated with the changing occupation of 5d electrons. Differential correlation contributions exceeding 10 meV are given in Tables 6, 7 and 8. The largest contributors are: $5d^2 \rightarrow vp^2+vd^2+vf^2+vpvf$; $5p \rightarrow vp+vf$; $5p^2 \rightarrow 5d^2+5dvd+vd^2$ and $5p5d \rightarrow vpvd+vdvf$.

The sizes of the RCI matrices were 9245, 17 617 and 18 208 for $J = 0, 1, 2$ respectively. CPU times on a 500 MHz Alpha workstation were about 2.0 hours for

each final matrix, of which, characteristically, assembly of the energy matrix element structure (i.e., determination of the coefficients of the radial integrals, for each matrix element) was about 75% of CPU time. Excitations included in the final matrix, but not shown in Tables 6, 7 or 8 are, for $J = 0$: $5d^2 \rightarrow vs^2$, $5s5d \rightarrow vp^2 + vpvf$; $5p5d^2 \rightarrow vd^2vf + vf^3$; $5d^3 \rightarrow vd^3 + vdv^2 + vdvf^2 + vdvvpv$ and $5d^4 \rightarrow vd^4 + vd^2vf^2 + vf^4$. Present for $J = 1$ is: $5d^2 \rightarrow vs^2 + vh^2$; $5d^3 \rightarrow vd^3 + vdv^2 + vdvf^2 + vdvvpv$ and $5s5d \rightarrow vp^2$. Finally, for $J = 2$, we also included: $5d^3 \rightarrow vd^3$ and $5s5d \rightarrow vp^2 + vpvf$.

Among the lower levels, which are the most important for lifetimes, the $5d^4$ levels are furthest out of place (see Table 4). We correct the positions of these levels by shifting the diagonal matrix elements of the $5d^4$ basis members by an amount which gives the best match to experiment, for that level, after diagonalization of the shifted RCI matrix. We shifted $J = 0, 1, 2$ by -0.0175 , -0.0067 and -0.006 a.u., respectively. For $J = 0$, we also shifted $5d^36s$ diagonal elements by -0.0175 a.u.

While these shifts had little effect on the uppermost levels, they reduced the average absolute error for the lower 2 (6, 7) levels for $J = 0$ (1, 2) to 147 cm^{-1} (525 cm^{-1} , 189 cm^{-1}) from their unshifted values of 819 cm^{-1} (884 cm^{-1} , 406 cm^{-1}), respectively. For $J = 1$, the small average Landé g-value error of 0.017 increased to 0.036, and for $J = 2$ it decreased from 0.049 to 0.029 for all 12 levels.

As we have come to expect, the effect of shifting on magnetic dipole hyperfine structure constants can be substantial, when relative level positions are changing significantly, or when the constants are small. For shifted $J = 1$, in order of increasing energy, A (MHz) = $-5013, 2017, 10\ 527, -973, -3778, -4828, 8913$ and -3712 . For shifted $J = 2$, we have A (MHz) = $1888, 1047, 3027, 2534, 4723, 1396, -333, 2974, -2470, -1708, 991$ and 4442 . Generally, the effect of shifting is least for the lowest level, larger for the levels being shifted, and largest for the levels with the smallest A 's (sign reversal is possible), as well as the highest levels. These differences are likely not completely adequate to establish errors for the A 's, as excitations like $4s \rightarrow s$ are needed. We also note that throughout this paper the shifted results are only presented in the text, and not in the tables.

3.3. Lifetimes

In Table 9, we present the lifetimes for the 12 lowest $J = 1$ odd parity levels. Decays to all $J = 0, 1, 2$ even parity levels at or below $28\ 044 \text{ cm}^{-1}$ [3, 4] were calculated, and those branches contributing $>1\%$ of the total spontaneous emission probability, A_{ki} (s^{-1}), are shown. Experimental energy differences [3, 4] were used. Smaller values of A_{ki} are more uncertain, contribute little to the lifetime, and waste space, so they have not been given. Since the lowest odd parity level is at $33\ 706 \text{ cm}^{-1}$, with the highest treated here at $49\ 887 \text{ cm}^{-1}$, a cutoff of the even parity levels at $28\ 044 \text{ cm}^{-1}$ seems reasonable. This is

also consistent with the observation that the highest significant level (5% of the total) is at 23 295 cm⁻¹ for odd parity level 12.

Both length (Babuskin) and velocity (Coulomb) gauge results are given for A_{ki} . For the total A_{ki} , the average gauge spread for all 12 odd parity levels is only 3.4%. This small value is due in part to the fortuitous cancellation of A_{ki} sums for (J, J') pairs [$J = 1; J' = 0, 1, 2$]. For other levels, such as 7, 9 and 10, there is no such cancellation, and the gauge spread reaches 8.1%. No significant cancellation of spreads occurs within (J, J') pairs.

Lifetimes for 5 of the levels have been measured, and we are in excellent agreement (within a few percent) for levels 2 [11] and 3 [11, 12, 13]. For levels 10 and 12, our results are in good agreement [2, 13] (20-30%), but for level 7, our results are 2.4 times smaller than the experimental value [13]. For level 10, experimental branching ratios obtained from Corliss and Bozman [31] have been given [2] for three branches at 12 601, 5658 and 1031 cm⁻¹, in order of decreasing importance. Our results, given in Table 9, bear little resemblance to these; the major branches are to 1031, 0 and 5658 cm⁻¹, in order of decreasing importance.

We would like to determine the size and source of the remaining errors in the calculated lifetimes. One measure of the quality of our wavefunctions should be how well they account for measured adjacent energy differences, dE, and Landé g-values. The lifetimes which have the largest experimental-theoretical discrepancy are levels 7 and 10. Table 1 indicates that these levels also exhibit relatively large differences for dE and g. From Table 9, the most important (>30%) even parity contributors to the lifetimes are: levels 1, 2 for $J = 1$; levels 1, 2, 3, 4 and 7 for $J = 2$; and level 1 for $J = 0$. Table 4 indicates that any $J = 2$ level 3 or above, and $J = 0$ level 1 might be improved.

In past work on f-values, hyperfine structure and electron affinities, e.g., [7, 20], it was found necessary to correlate nearly degenerate manifolds in the same way as the MCDF manifolds. In some of these cases, it was possible to include at least a portion of these second-order effects directly in the RCI matrix, while the remainder were approximated by shifting the appropriate diagonal matrix elements. Due to the large size of the Ta II wavefunctions, only shifting is a viable option here. As explained in Section 3.1, for the odd parity levels, we have shifted the $(5d+6s)^3(vp+vp'+vf+vf')$ diagonal matrix elements for the odd parity basis by -0.090 a.u., which significantly improved dE and g. We have also shifted the even parity wavefunctions, as explained in Section 3.2. The effect on the lifetimes (and gauge spreads) of the lifetimes of levels 7 and 10, however, is quite minimal (a few percent) for all shifts.

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Table 1. Ta II (5d+6s)³6p $J = 1$ properties

Label	dE (cm ⁻¹)			Landé g-value			A (MHz)
	Expt [3,4]	DF	RCI	Expt [3,4]	DF	RCI	RCI
d ² sp [⁵ F+ ³ D]	0	0	0	0.285	0.147	0.228	-1888
d ³ p [³ D]	3283	4693	3286	0.685	0.706	0.669	1747
d ² sp [³ D+ ⁵ F]	4829	6401	4950	0.472	0.905	0.495	-1266
d ² sp [⁵ D]	6599	7651	6574	1.225	0.823	1.230	513
d ² sp [³ S]	7649	8870	7612	1.885	2.026	1.917	3168
d ² sp [⁵ D]	9849	11010	9993	?	1.454	1.449	2158
d ³ p [⁵ F]	10500	13072	10997	0.242	1.476	0.274	734
d ³ p+d ² sp [⁵ D+ ³ P]	11527	15013	11862	1.458	0.336	1.448	1099
d ² sp+d ³ p [⁵ D+ ³ P]	12468	16275	12773	1.367	1.564	1.361	1212
d ³ p+d ² sp [⁵ D]	13890	17315	14474	1.520	1.926	1.564	5
d ² sp+d ³ p+ds ² p [³ D]	15070	19489	15690	0.746	1.488	0.850	128
d ² sp+d ³ p [⁵ P]	16181	20230	16393	2.006	0.627	1.936	1972
avg. absolute error		2561	262		0.565	0.036	
avg. absolute separation error			157 (14.4%)				

Table 2. Percent LS composition of Ta II $J = 1$ levels

Level	d ³ p							d ² sp							ds ² p	
	⁵ F	⁵ D	⁵ P	³ D	³ P	³ S	¹ P	⁵ F	⁵ D	⁵ P	³ D	³ P	³ S	¹ P	³ D	³ P
1	12			10				49	2		19				4	
2	6	5		47	2				9		22	2				
3		2		17	3		1	34	3		26	2			6	
4		7		14	3	2		8	45		3	9	5			
5		2	5		4	17			11	13		1	41			
6		15			4				49			14			2	7
7	67			6	4			3	4		7	1			3	
8		16			13		2		22	6	5	16	2		2	8
9	6	13		3	27				31			12	2			
10		48	2			12			8	12	2	7				
11		8	4	24		4			2	1	26	4	2	16		1
12		8	16	3	4	5		2	35			12	1	2		

Table 3. Ta II $(5d+6s)^36p$ $J = 1$ correlation energy (in meV) relative to lowest root. A positive difference means the separation is increased by this contribution. Excitations with no contribution >10 meV have been omitted.

Config.	d^n	Root Number										
		12	11	10	9	8	7	6	5	4	3	2
6p \rightarrow vp	3	-65	-78	-146	-63	-51	-131	-9	-12	-19	-20	-18
6p \rightarrow vp	2	-10	-16	-13	-12	-21	-14	-9	-9	-19	-9	-5
6p \rightarrow vf	3	-19	-19	-45	-18	-27	-6	-7	3	4	-8	-1
6p \rightarrow vf	2	-24	-75	-23	-20	-16	-49	-11	-7	-21	-14	-8
5d \rightarrow vs	2	-1	-12	4	2	-27	2	-15	6	-3	-8	4
5d \rightarrow vd	3	3	-29	43	16	12	18	16	-28	9	-1	-34
5d \rightarrow vd	2	11	-20	19	16	0	18	11	15	-4	1	13
5d \rightarrow vd	1	4	-28	8	8	-4	1	-4	7	7	-4	6
5d \rightarrow vg	2	8	-3	9	2	1	7	-1	11	3	2	10
5d6p \rightarrow vdvf	3	-15	-16	-44	-21	-10	-48	0	-4	-5	-4	-28
5d6p \rightarrow vdvf	2	4	22	18	6	0	27	2	5	-2	3	21
5d ² \rightarrow 6p ²	3	4	-23	1	-1	-8	1	-20	6	7	5	-10
5d ² \rightarrow 6pvf	3	12	5	5	22	19	32	7	5	18	-4	35
5d ² \rightarrow 6pvf	2	0	-19	2	1	-4	0	-2	1	-1	0	1
5d ² \rightarrow vd ²	3	-21	-24	-41	-30	-11	-55	0	-10	-4	-2	-43
5d ² \rightarrow vd ²	2	-6	2	5	-2	0	14	-11	-11	-5	-2	7
5d ² \rightarrow vf ²	3	-49	-62	-84	-71	-33	-103	-8	-22	-6	-6	-88
5d ² \rightarrow vf ²	2	-45	-20	-10	-24	-9	20	-47	-57	-27	-10	-1
5d ² \rightarrow vg ²	3	-8	-11	-13	-12	-6	-16	-1	-4	-1	-1	-14
5d ² \rightarrow vg ²	2	-9	-5	-3	-6	-2	2	-9	-12	-6	-2	-1
5p \rightarrow 6p	3	-15	-2	-40	-33	-38	-22	-1	-4	-10	-33	36
5p \rightarrow 6p	2	7	-31	18	21	-26	18	-6	10	-10	-13	24
5p \rightarrow vp	3	-3	16	-9	-9	3	-5	9	-7	-6	-1	-6
5p \rightarrow vp	2	15	-21	33	26	-12	33	-11	12	7	-8	30
5p \rightarrow vf	3	-145	-168	-410	-237	-65	-568	11	-38	-27	5	-401
5p \rightarrow vf	2	139	281	313	183	136	431	62	48	22	47	297
5p \rightarrow vf	1	11	-55	21	19	-25	7	-25	18	14	-14	17
5p \rightarrow vh	3	-6	-7	-21	-10	-2	-29	1	0	-1	1	-18
5p \rightarrow vh	2	12	17	18	13	9	22	8	7	3	4	17
5p6p \rightarrow 5d ²	2	-16	-25	-67	-39	-30	-56	2	-2	-11	-18	-28
5p6p \rightarrow 5d ²	1	12	11	6	10	4	8	16	-4	11	4	12
5p6p \rightarrow 5dvd	3	-14	-17	-30	-22	-11	-43	-2	-5	-3	0	-30
5p6p \rightarrow 5dvd	2	5	17	15	6	8	28	1	-2	-8	-8	22

$5p5d \rightarrow vdvf$	3	-60	-71	-146	-94	-35	-194	1	-21	-11	-6	-146
$5p5d \rightarrow vdvf$	2	38	84	98	58	38	140	11	6	0	11	97
$5p5d \rightarrow vdvf$	1	3	-18	6	5	-7	1	-7	5	5	-4	5
$5p5d \rightarrow vfvf$	3	-30	-35	-73	-46	-18	-95	0	-11	-6	-3	-71
$5p5d \rightarrow vfvf$	2	17	37	44	27	16	64	5	2	0	5	44
$5p^2 \rightarrow 5d^2$	3	-107	-140	-239	-170	-77	-315	-2	-50	-18	-23	-253
$5p^2 \rightarrow 5d^2$	2	94	254	280	162	116	424	8	-7	-18	28	282
$5p^2 \rightarrow 5d^2$	1	20	-130	39	38	-47	5	-45	37	34	-23	32
$5s \rightarrow vs$	3	-2	-3	-8	-4	-1	-11	0	0	0	0	-8
$5s \rightarrow 5d$	3	-11	-11	-9	-12	-4	-12	-2	-12	-3	-2	-16
$5s \rightarrow 5d$	2	-22	-7	-9	-11	0	1	-24	-18	-6	-1	-3

Table 4. Ta II (5d+6s)⁴ $J = 0, 1, 2$ properties

Label	dE (cm ⁻¹)			Landé g-value			A (MHz)
	Expt [3]	DF	RCI	Expt [3]	DF	RCI	RCI
d ² s ² [³ P ₀]	0	0	0				
d ⁴ [⁵ D ₀]	8476	-9800	9393				
d ³ s [³ P ₀]	12163 ^a	6320	13058				
d ³ s [³ P ₀]	19256	3485	20709				
avg. absolute error		13297	1088				
avg. absolute separation error			499				
d ³ s [⁵ F ₁]	0	0	0	0.000	0.016	0.028	-5013
d ² s ² [³ P ₁]	5331	26342	5416	1.555	1.600	1.554	2141
d ³ s [⁵ P ₁]	10713	12690	10884	2.374	2.367	2.399	10483
d ⁴ [⁵ D ₁]	13475	16570	14759	1.510	1.490	1.499	-1156
d ³ s [³ D ₁]	14628	21839	16189	0.850	0.685	0.859	-3922
d ³ s [³ P ₁]	17375	26298	18716	1.171	1.335	1.157	-4690
d ³ s [¹ P ₁]	23406	28202	25786	1.15	1.039	1.185	9276
d ³ s [³ P ₁]	26235 ^a	27391	28640	1.332 ^a	1.462	1.317	-4318
avg. absolute error		6881	1318		0.079	0.017	
avg. absolute separation error			406				
d ³ s [⁵ F ₂]	0	0	0	1.008	1.003	1.007	1880
d ² s ² [³ F ₂]	2149	12253	2069	0.750	1.329	0.740	1043
d ² s ² [³ P ₂]	4627	23159	4722	1.340	0.864	1.369	3092
d ³ s [³ F ₂]	8659	16935	9200	1.063	1.389	1.134	2643
d ³ s [⁵ P ₂]	10844	14739	11136	1.48	1.211	1.480	4627
d ² s ² [¹ D ₂]	12529	26463	12956	1.111	1.464	0.958	1577
d ⁴ [⁵ D ₂]	13464	16485	14548	1.472	0.917	1.474	-446
d ³ s [³ D ₂]	16137	22516	17010	1.211	1.165	1.210	3148
d ³ s [³ P ₂]	17469	28480	18460	1.462	1.486	1.454	-2744
d ³ s [³ F ₂]	21897	28299	23571	0.700	0.694	0.909	-993
d ³ s [¹ D ₂]	22263	33448	23758	1.120	1.096	1.017	-321
d ³ s [³ P ₂]	27013	25810	28271	1.358 ^a	1.373	1.358	4402
avg. absolute error		8539	800		0.223	0.049	
avg. absolute separation error			288				

^aExperimental value from [4]

Table 5. Percent LS composition of even parity Ta II $J = 0, 1, 2$ levels

Level	d^3s							d^2s^2				d^4					
	5F	5P	3F	3D	3P	1D	1P	3F	1D	3P	1S	5D	3F	3D	3P	1D	1S
$J = 0$																	
1					43					33		2			19		
2					6					7		77			7		
3					45					12		17			23		
4					52					25	8				5		7
$J = 1$																	
1	95			4													
2	1	7		1	44					32		1			13		
3		90			2					4		1			2		
4					4					3		85			4		
5	2			49	17		12			6		1		4	5		
6	1			31	37					1		9		1	17		
7				1	12		57			22				1	3		
8				3	40		24			22				3	4		
$J = 2$																	
1	94			3													
2			4		1	2		75	9	1		3					
3	1	10	2	2	33	5		7	4	23		1			5	1	
4		24	23		4	16		1	19			2	1				4
5		54	20		4					12		1			3		
6		6	37	3	4	6		4	25	1		1	1		1	3	
7				4	1							89		1	1		
8	1		4	63	7	1				7		3		6	3		
9				9	56	1						4			25		
10			31	1	5	19		2	11	6		11	2				5
11		2	12	6	4	10		1	1	3		25		5	26		
12		1	1	3	34	5				9	33				1	9	

Table 6. Ta II $(5d+6s)^4 J = 0$ correlation energy in meV, relative to lowest root, $5d^26s^2$. A positive difference means the separation is increased by this contribution. Excitations with no contribution >10 meV have been omitted.

Config.	d^n	Root			Config.	d^n	Root		
		4	3	2			4	3	2
6s \rightarrow 5d	3	816	-574	582	5p $^2\rightarrow$ 5dvg	2	40	40	40
5d \rightarrow 6s	3	942	-14	47	5p $^2\rightarrow$ 5dvg	3	-34	-36	0
5d \rightarrow 6s	4	1445	1445	1490	5p $^2\rightarrow$ 5dvg	4	0	0	-31
5d \rightarrow vs	3	-108	-24	-25	5p $^2\rightarrow$ vp 2	2	51	51	51
5d \rightarrow vs	4	-47	-74	-2	5p $^2\rightarrow$ vp 2	3	-52	-55	0
5d \rightarrow vd	2	142	153	152	5p $^2\rightarrow$ vp 2	4	0	0	-57
5d \rightarrow vd	3	-23	-46	30	5p $^2\rightarrow$ vd 2	2	301	301	301
5d \rightarrow vd	4	39	-16	0	5p $^2\rightarrow$ vd 2	3	-303	-303	0
5d \rightarrow vg	3	-146	-50	-16	5p $^2\rightarrow$ vd 2	4	0	0	-317
5d \rightarrow vg	4	-26	-36	-25	5p5d \rightarrow vsvp	3	66	68	80
5d $^2\rightarrow$ vp 2	2	42	42	42	5p5d \rightarrow vsvp	4	-39	-39	-18
5d $^2\rightarrow$ vp 2	3	-112	-7	35	5p5d \rightarrow vpvd	2	119	119	119
5d $^2\rightarrow$ vp 2	4	167	53	167	5p5d \rightarrow vpvd	3	-72	-68	119
5d $^2\rightarrow$ vd 2	2	46	46	46	5p5d \rightarrow vpvd	4	-60	-57	-261
5d $^2\rightarrow$ vd 2	3	-143	-125	-7	5p5d \rightarrow vdvf	2	170	170	170
5d $^2\rightarrow$ vd 2	4	-11	-4	-232	5p5d \rightarrow vdvf	3	-231	-233	20
5d $^2\rightarrow$ vf 2	2	138	138	138	5p5d \rightarrow vdvf	4	-60	-57	-261
5d $^2\rightarrow$ vf 2	3	-339	-295	-26	5p5d \rightarrow vfv	2	64	64	64
5d $^2\rightarrow$ vf 2	4	-23	-3	-451	5p5d \rightarrow vfv	3	-103	-101	0
5d $^2\rightarrow$ vg 2	2	22	22	22	5p5d \rightarrow vfv	4	20	10	-120
5d $^2\rightarrow$ vg 2	3	-54	-48	-7	5p5d \rightarrow vsvf	2	20	20	20
5d $^2\rightarrow$ vg 2	4	-8	-3	-66	5p5d \rightarrow vsvf	3	-34	-32	0
5d $^2\rightarrow$ vh 2	3	-14	-12	-2	5p5d \rightarrow vsvf	4	0	0	-45
5d $^2\rightarrow$ vh 2	4	-3	-6	-16	5s \rightarrow 5d	2	-15	-33	20
5d $^2\rightarrow$ vsvd	3	71	76	76	5s \rightarrow 5d	3	-34	-17	-98
5d $^2\rightarrow$ vsvd	4	-61	-55	0	5s \rightarrow 5d	4	-4	-8	-16
5d $^2\rightarrow$ vpvf	3	210	296	313	5s \rightarrow vs	2	13	13	13
5d $^2\rightarrow$ vpvf	4	-297	-349	-72	5s \rightarrow vs	3	-2	-15	0
5d $^2\rightarrow$ vdvg	3	18	18	19	5s \rightarrow vs	4	0	0	-26
5d $^2\rightarrow$ vdvg	4	-10	-16	-1	5s \rightarrow vd	2	-9	-1	19
5p \rightarrow vp	2	133	129	137	5s \rightarrow vd	3	-22	-8	-21
5p \rightarrow vp	3	523	503	591	5s \rightarrow vd	4	-11	-6	-21
5p \rightarrow vp	4	-230	-235	-258	5s5d \rightarrow vsvd	2	19	19	19
5p \rightarrow vf	2	665	655	672	5s5d \rightarrow vsvd	3	-28	-30	0
5p \rightarrow vf	3	-745	-818	14	5s5d \rightarrow vsvd	4	0	0	-38
5p \rightarrow vf	4	-28	-37	-1036	5s5d \rightarrow 5dvp	2	30	30	39

$5p \rightarrow vh$	2	25	25	25	$5s5p \rightarrow 5dvp$	3	-34	-35	-18
$5p \rightarrow vh$	3	-32	-38	0	$5s5p \rightarrow 5dvp$	4	0	0	-33
$5p \rightarrow vh$	4	0	0	-49	$5s5p \rightarrow 5dvf$	2	57	57	57
$5p^2 \rightarrow 5d^2$	2	640	648	649	$5s5p \rightarrow 5dvf$	3	-51	-50	0
$5p^2 \rightarrow 5d^2$	3	-551	-501	-4	$5s5p \rightarrow 5dvf$	4	0	0	-43
$5p^2 \rightarrow 5d^2$	4	0	0	-337	$5s^2 \rightarrow vd^2$	2	14	14	14
$5p^2 \rightarrow 5dvd$	2	859	859	862	$5s^2 \rightarrow vd^2$	3	-14	-14	0
$5p^2 \rightarrow 5dvd$	3	-760	-756	-6	$5s^2 \rightarrow vd^2$	4	0	0	-15
$5p^2 \rightarrow 5dvd$	4	0	0	-663					

Table 7. Ta II $(5d+6s)^4$ $J = 1$ correlation energy in meV, relative to the lowest root. A positive difference means the separation is increased by this contribution. Excitations with no contribution >10 meV have been omitted.

Config.	d^n	Root						
		8	7	6	5	4	3	2
6s \rightarrow 5d	3	69	-59	-573	-289	5	-28	-460
5d \rightarrow 6s	3	562	303	-14	-27	19	-28	1
5d \rightarrow 6s	4	0	0	0	0	-27	0	-1484
5d \rightarrow vs	3	-62	-68	-8	-21	2	0	-54
5d \rightarrow vs	4	-8	-19	-3	-7	-1	-1	0
5d \rightarrow vd	2	-8	-5	-1	-1	0	0	-67
5d \rightarrow vd	3	-23	-24	-16	-13	2	-4	-50
5d \rightarrow vd	4	-14	-23	-45	-27	-155	-11	-61
5d \rightarrow vg	3	-79	-73	-17	-27	13	-16	19
5d \rightarrow vg	4	-23	-35	-15	-11	-7	8	29
5d $^2\rightarrow$ vp 2	2	0	0	0	0	0	0	-17
5d $^2\rightarrow$ vp 2	3	-63	-53	-25	-38	17	-16	-6
5d $^2\rightarrow$ vp 2	4	-106	-147	-114	-94	-49	1	-252
5d $^2\rightarrow$ vd 2	2	0	0	0	0	0	0	-45
5d $^2\rightarrow$ vd 2	3	-38	-32	-26	-36	100	-13	92
5d $^2\rightarrow$ vd 2	4	0	-1	2	1	-192	0	4
5d $^2\rightarrow$ vf 2	2	0	0	0	0	0	0	-123
5d $^2\rightarrow$ vf 2	3	-107	-101	-88	-98	172	-75	197
5d $^2\rightarrow$ vf 2	4	-6	-6	4	0	-384	1	12
5d $^2\rightarrow$ vg 2	2	0	0	0	0	0	0	-11
5d $^2\rightarrow$ vg 2	3	-13	-11	-11	-11	14	-9	19
5d $^2\rightarrow$ vg 2	4	-4	-4	-1	-2	-36	0	0
5d $^2\rightarrow$ vsvd	3	-1	0	0	0	0	0	-63
5d $^2\rightarrow$ vsvd	4	-11	-14	-11	-9	-55	1	56
5d $^2\rightarrow$ vpvf	3	-15	-7	2	-2	18	9	-173
5d $^2\rightarrow$ vpvf	4	-36	-48	-34	-29	120	-2	151
5d $^2\rightarrow$ vdvg	4	-5	-8	-8	-6	12	-1	-11
5p \rightarrow vp	2	6	6	3	3	12	0	-172
5p \rightarrow vp	3	68	66	44	43	133	-3	-456
5p \rightarrow vp	4	41	47	26	24	22	8	267
5p \rightarrow vf	2	-22	6	3	2	17	-9	-674
5p \rightarrow vf	3	93	108	80	101	898	51	880
5p \rightarrow vf	4	-4	-5	-6	-4	-1043	1	22
5p $^2\rightarrow$ 5d 2	2	-6	-4	-2	-1	-1	0	-690
5p $^2\rightarrow$ 5d 2	3	-83	-85	-61	-90	502	-43	506
5p $^2\rightarrow$ 5d 2	4	0	0	0	0	-349	0	0

$5p^2 \rightarrow 5dvd$	2	0	0	0	0	4	0	-850
$5p^2 \rightarrow 5dvd$	3	3	2	1	-1	743	-1	751
$5p^2 \rightarrow 5dvd$	4	0	0	0	0	-654	0	0
$5p^2 \rightarrow 5dvg$	2	0	0	0	0	0	0	-16
$5p^2 \rightarrow 5dvg$	3	1	0	0	0	14	-1	14
$5p^2 \rightarrow 5dvg$	4	0	0	0	0	-13	0	0
$5p^2 \rightarrow vp^2$	2	0	0	0	0	0	0	-23
$5p^2 \rightarrow vp^2$	3	2	2	1	2	26	0	3
$5p^2 \rightarrow vp^2$	4	0	0	0	0	-27	0	0
$5p^2 \rightarrow vd^2$	2	0	0	0	0	0	0	-411
$5p^2 \rightarrow vd^2$	3	4	5	3	3	412	0	412
$5p^2 \rightarrow vd^2$	4	0	0	0	0	-418	0	0
$5p5d \rightarrow vsvp$	3	0	0	0	0	0	0	-44
$5p5d \rightarrow vsvp$	4	1	2	1	1	17	0	31
$5p5d \rightarrow vpv d$	2	0	0	0	0	0	0	-92
$5p5d \rightarrow vpv d$	3	4	2	3	0	152	3	83
$5p5d \rightarrow vpv d$	4	1	1	1	1	-167	-1	34
$5p5d \rightarrow vdvf$	2	0	0	0	0	0	0	-259
$5p5d \rightarrow vdvf$	3	6	5	3	2	380	1	345
$5p5d \rightarrow vdvf$	4	0	1	1	1	-476	1	19
$5p5d \rightarrow vfv g$	2	0	0	0	0	0	0	-51
$5p5d \rightarrow vfv g$	3	-3	-2	-2	-2	79	-1	71
$5p5d \rightarrow vfv g$	4	0	0	0	0	-107	1	5
$5p5d \rightarrow vsvf$	2	0	0	0	0	0	0	-18
$5p5d \rightarrow vsvf$	3	2	0	2	0	32	3	32
$5p5d \rightarrow vsvf$	4	0	0	0	0	-42	0	0
$5s \rightarrow 5d$	2	-6	-8	-8	-5	0	0	-45
$5s \rightarrow 5d$	3	-18	-14	-30	-27	-22	-34	5
$5s \rightarrow 5d$	4	-1	0	-4	-3	-15	0	2
$5s \rightarrow vs$	2	0	0	0	0	0	0	-18
$5s \rightarrow vs$	4	0	0	0	0	-26	-2	0
$5s \rightarrow vd$	2	-10	-7	-2	-1	13	0	-5
$5s \rightarrow vd$	3	-19	-16	-8	-8	-18	-18	2
$5s \rightarrow vd$	4	-2	-1	9	1	-13	0	9
$5s5d \rightarrow vsvd$	2	0	0	0	0	0	0	-22
$5s5d \rightarrow vsvd$	3	2	2	1	1	37	1	37
$5s5d \rightarrow vsvd$	4	0	0	0	0	-46	0	0
$5s5d \rightarrow vpvf$	4	0	0	0	0	-14	0	0

$5s5p \rightarrow 5dvp$	2	-1	-1	-1	0	5	0	-21
$5s5p \rightarrow 5dvp$	3	3	3	2	1	16	1	27
$5s5p \rightarrow 5dvp$	4	0	0	0	0	-27	0	0
$5s5p \rightarrow 5dvp$	2	0	0	0	0	0	0	-119
$5s5p \rightarrow 5dvp$	3	-3	-2	-2	-3	103	-1	103
$5s5p \rightarrow 5dvp$	4	0	0	0	0	-88	0	0
$5s^2 \rightarrow 5d^2$	2	0	0	0	0	-1	0	-12
$5s^2 \rightarrow 5d^2$	3	-1	0	-2	-3	9	-1	9

Table 8. Ta II $(5d+6s)^4 J = 2$ correlation energy in meV, relative to lowest root, $5d^36s$. A positive difference means the separation is increased by this contribution. Excitations with no contribution >10 meV have been omitted.

Config.	d^n	Root										
		12	11	10	9	8	7	6	5	4	3	2
6s→5d	3	-243	-249	-539	-793	-293	6	-209	14	15	16	17
5d→6s	3	1133	-43	529	6	-31	11	7	-117	-322	-341	-187
5d→6s	4	0	0	0	0	0	-27	-576	0	0	-1208	-224
5d→vs	2	-1	-3	1	0	-2	0	-28	0	-3	-5	-4
5d→vs	3	-51	44	-22	-2	-17	1	-57	-4	-18	-57	-5
5d→vs	4	5	-54	3	0	2	0	1	-8	-8	1	1
5d→vd	2	-8	4	-4	0	0	0	-85	1	2	-74	-107
5d→vd	3	-23	43	-26	-13	-11	4	-15	-6	-8	-39	-11
5d→vd	4	-25	-29	-39	-64	-23	-207	-46	-14	-23	-55	-46
5d→vg	2	2	31	-7	-1	-1	0	-44	0	-3	-10	-16
5d→vg	3	-122	49	-94	-16	-29	16	-6	-12	-5	22	-28
5d→vg	4	4	-26	5	-16	1	-10	14	-7	-17	14	14
5d ² →vs ²	4	0	0	0	0	0	0	-12	0	0	-10	-13
5d ² →vp ²	2	0	0	0	0	0	0	-32	0	0	-24	-4
5d ² →vp ²	3	-123	-123	-84	-27	-64	25	-69	-14	-2	-25	-103
5d ² →vp ²	4	-49	-203	-59	-158	-67	-52	-338	-61	-112	-303	-347
5d ² →vd ²	2	0	0	0	0	0	0	-40	0	0	-38	-26
5d ² →vd ²	3	-34	-14	-42	-19	-31	96	99	-12	-15	104	97
5d ² →vd ²	4	1	7	3	4	1	-189	-5	0	1	0	-7
5d ² →vf ²	2	0	0	0	0	0	0	-83	0	0	-91	-40
5d ² →vf ²	3	-128	-142	-96	-76	-89	161	166	-54	-40	185	156
5d ² →vf ²	4	0	2	6	4	0	-384	-5	-3	-2	5	-6
5d ² →vg ²	2	0	0	0	0	0	0	-15	0	0	-17	-6
5d ² →vg ²	3	-26	-6	-21	-17	-21	25	26	-11	-9	31	23
5d ² →vg ²	4	0	-4	1	0	0	-61	-2	-1	-1	1	-2
5d ² →vsvd	3	-5	0	-2	0	-1	0	-73	0	1	-72	-73
5d ² →vsvd	4	7	50	6	12	5	64	64	4	7	64	64
5d ² →vpvf	2	0	0	0	0	0	0	-22	0	0	-5	-15
5d ² →vpvf	3	-88	-67	-89	9	-20	38	-311	19	20	-267	-314
5d ² →vpvf	4	-40	-409	-41	-106	-52	162	233	-45	-77	233	233
5d ² →vdvg	3	1	1	0	0	0	1	-18	0	0	-20	-17
5d ² →vdvg	4	-1	-12	-2	-5	-2	11	12	-1	-3	12	12
5p→vp	2	9	19	7	5	0	12	-139	1	1	-147	-126
5p→vp	3	79	12	71	48	45	128	-389	14	22	-436	-387
5p→vp	4	14	-107	7	26	16	21	257	15	23	257	257

5p→vf	2	15	5	8	1	1	17	-638	0	-3	-677	-700
5p→vf	3	118	-543	44	43	115	904	889	43	40	-888	-888
5p→vf	4	-3	15	-4	-8	-3	-1056	21	-3	-6	21	21
5p ² →5d ²	2	-10	2	-6	-2	0	-1	-691	1	1	-680	-670
5p ² →5d ²	3	-86	-32	-64	-43	-83	490	493	-34	-42	493	493
5p ² →5d ²	4	0	0	0	0	0	-339	0	0	0	0	0
5p ² →5dvd	2	0	0	0	0	0	0	-755	0	0	-756	-757
5p ² →5dvd	3	6	355	1	4	2	678	679	3	0	679	679
5p ² →5dvd	4	0	0	0	0	0	-604	0	0	0	0	0
5p ² →5dvg	2	0	0	0	0	0	0	-38	0	0	-39	-39
5p ² →5dvg	4	0	0	0	0	0	-32	0	0	0	0	0
5p ² →vp ²	2	0	0	0	0	0	0	-49	0	0	-50	-50
5p ² →vp ²	3	5	40	4	2	3	57	57	1	1	57	57
5p ² →vp ²	4	0	0	0	0	0	-59	0	0	0	0	0
5p ² →vd ²	2	0	0	0	0	0	0	-277	0	0	-278	-276
5p ² →vd ²	3	4	240	1	3	1	285	285	1	1	285	285
5p ² →vd ²	4	0	0	0	0	0	-296	0	0	0	0	0
5p5d→vsvp	3	0	14	1	1	0	15	-59	1	0	-60	-60
5p5d→vsvp	4	1	28	1	3	1	22	42	1	2	42	42
5p5d→vpvd	2	0	0	0	0	0	0	-111	0	0	-115	-116
5p5d→vpvd	3	4	45	2	5	4	191	90	4	2	88	92
5p5d→vpvd	4	1	-35	1	3	1	-197	54	1	2	54	54
5p5d→vdvf	2	0	0	0	0	0	0	-157	0	0	-157	-158
5p5d→vdvf	3	6	-42	3	3	1	239	217	0	0	218	217
5p5d→vdvf	4	0	-3	1	1	0	-313	12	0	0	12	12
5p5d→svsf	2	0	0	0	0	0	0	-20	0	0	-20	-23
5p5d→svsf	3	2	22	1	2	1	35	35	2	0	35	35
5p5d→svsf	4	0	0	0	0	0	-48	0	0	0	0	0
5s→5d	2	-8	-22	-10	-13	-3	0	-32	-4	-2	-36	-16
5s→5d	3	-13	2	-23	-29	-30	-19	8	-23	-20	5	9
5s→5d	4	-2	4	-2	-5	-3	-15	2	-1	-1	2	2
5s→vs	2	0	0	0	0	0	0	-15	0	0	-18	-16
5s→vs	4	0	0	0	0	0	-26	0	0	0	0	0
5s→vd	2	-18	7	-10	-4	-2	11	-5	-1	1	-2	-3
5s→vd	3	-19	23	-17	-9	-5	-16	-2	-11	-5	2	-3

$5s5d \rightarrow vsvd$	2	0	0	0	0	0	0	-18	0	0	-18	-19
$5s5d \rightarrow vsvd$	3	3	10	2	1	1	32	32	1	1	32	32
$5s5d \rightarrow vsvd$	4	0	0	0	0	0	-39	0	0	0	0	0
$5s5p \rightarrow 5dvp$	2	-1	7	-1	-1	0	8	-27	0	0	-28	-30
$5s5p \rightarrow 5dvp$	3	6	17	4	4	3	21	38	2	1	38	38
$5s^2 \rightarrow 5d^2$	2	0	0	0	0	0	-1	-12	0	0	-11	-11

Table 9. Branching contributions of Ta II $J = 1$ lifetimes. Only branches $>1\%$ of the total are shown. Sums and lifetimes include branches not shown.

Label	LS	J	E_i (cm^{-1})	State A		State B	
				A_{ki} (s^{-1})		A_{ki} (s^{-1})	
				Vel	Len	Vel	Len
				State 1		State 2	
5d ³ 6s	⁵ F	1	0	0.937+7	0.859+7	0.955+7	0.123+8
5d ³ 6s	⁵ F	2	1031			0.406+7	0.493+7
5d ² 6s ²	³ F	2	3180	0.869+7	0.110+8		
5d ² 6s ²	³ P	0	4125	0.747+7	0.842+7	0.386+8	0.379+8
5d ² 6s ²	³ P	1	5331	0.274+7	0.229+7	0.737+7	0.109+8
5d ² 6s ²	³ P	2	5658	0.114+7	0.130+7		
5d ³ 6s	³ F	2	9691	0.245+7	0.210+7	0.386+7	0.326+7
5d ³ 6s	⁵ P	1	10713			0.100+7	0.554+6
5d ³ 6s	⁵ P	2	11875	0.119+7	0.761+6	0.446+7	0.373+6
5d ⁴	⁵ D	0	12601	0.133+7	0.998+6	0.294+7	0.241+7
5d ⁴	⁵ D	1	13475	0.110+7	0.571+6		
5d ² 6s ²	¹ D	2	13560	0.954+6	0.481+6	0.381+7	0.318+7
5d ³ 6s	³ P	0	16288			0.122+7	0.676+6
			Sum	0.372+8	0.369+8	0.789+8	0.809+8
			RCI τ (ns)	26.86	27.06	12.68	12.35
			Avg. (% spread)	26.98	(0.4%)	12.52	(1.3%)
			Expt. [11]			12.2(8)	
			E_k (cm^{-1})	33706.47		36987.71	

			State 3		State 4		
5d ³ 6s	⁵ F	1	0	0.422+8	0.483+8		
5d ³ 6s	⁵ F	2	1031	0.342+8	0.365+8	0.442+8	0.485+8
5d ² 6s ²	³ F	2	3180	0.141+8	0.134+8	0.555+7	0.628+7
5d ² 6s ²	³ P	0	4125	0.329+8	0.364+8		
5d ² 6s ²	³ P	1	5331			0.485+8	0.517+8
5d ² 6s ²	³ P	2	5658	0.905+7	0.995+7	0.812+7	0.909+7
5d ³ 6s	³ F	2	9691	0.243+7	0.225+7	0.705+7	0.600+7
5d ³ 6s	⁵ P	2	11875	0.283+7	0.222+7		
5d ⁴	⁵ D	0	12601			0.263+7	0.180+7
5d ⁴	⁵ D	1	13475			0.247+7	0.140+7
5d ² 6s ²	¹ D	2	13560	0.166+7	0.948+6	0.201+7	0.169+7
5d ⁴	⁵ D	2	14495			0.362+7	0.229+7
5d ³ 6s	¹ D	2	23295	0.500+7	0.520+5		
			Sum	0.148+9	0.153+9	0.130+9	0.133+9
			RCI τ (ns)	6.74	6.54	7.71	7.54
			Avg. (% spread)	6.64	(1.5%)	7.63	(1.0%)
			Expt.	7.1(3) [11]			
				6.6(6) [13]			
				6.9(4) [12]			
			E_k (cm ⁻¹)	38535.21		40304.79	

			State 5		State 6		
5d ³ 6s	⁵ F	1	0	0.605+7	0.708+7	0.191+7	0.151+7
5d ³ 6s	⁵ F	2	1031	0.227+7	0.241+7	0.969+6	0.486+6
5d ² 6s ²	³ P	0	4125	0.172+8	0.196+8		
5d ² 6s ²	³ P	1	5331	0.264+8	0.322+8	0.634+6	0.396+6
5d ² 6s ²	³ P	2	5658	0.239+7	0.302+7		
5d ³ 6s	³ F	2	9691	0.170+7	0.206+7		
5d ³ 6s	⁵ P	1	10713	0.606+7	0.526+7	0.423+6	0.120+7
5d ³ 6s	⁵ P	2	11875	0.100+7	0.969+6		
5d ⁴	⁵ D	0	12601			0.292+7	0.270+7
5d ⁴	⁵ D	1	13475	0.243+7	0.186+7	0.160+7	0.125+7
5d ² 6s ²	¹ D	2	13560			0.592+6	0.551+6
5d ⁴	⁵ D	2	14495	0.595+7	0.438+7	0.122+8	0.103+8
5d ³ 6s	³ D	1	14628			0.297+6	0.360+6
5d ³ 6s	³ P	0	16288			0.485+7	0.434+7
5d ³ 6s	³ D	2	17168			0.407+6	0.677+6
5d ³ 6s	³ P	1	17375	0.126+7	0.958+6	0.550+6	0.459+6
5d ³ 6s	³ P	2	18501	0.719+7	0.482+7	0.680+6	0.496+6
5d ³ 6s	¹ D	2	23295			0.128+6	0.639+6
Sum				0.832+8	0.874+8	0.296+8	0.272+8
RCI τ (ns)				12.03	11.45	33.82	36.71
Avg. (% spread)				11.74	(2.5%)	35.27	(4.1%)
E _k (cm ⁻¹)				41355.11		43553.67	

			State 7		State 8		
5d ³ 6s	⁵ F	1	0	0.293+9	0.366+9	0.362+8	0.418+8
5d ³ 6s	⁵ F	2	1031	0.833+8	0.950+8	0.155+9	0.173+9
5d ² 6s ²	³ F	2	3180			0.126+8	0.161+8
5d ² 6s ²	³ P	0	4125	0.986+7	0.109+8	0.891+7	0.873+7
5d ² 6s ²	³ P	1	5331	0.699+7	0.944+7	0.289+8	0.310+8
5d ² 6s ²	³ P	2	5658			0.537+8	0.625+8
5d ³ 6s	³ F	2	9691	0.548+7	0.472+7		
5d ³ 6s	⁵ P	2	11875			0.350+7	0.341+7
5d ⁴	⁵ D	0	12601	0.970+7	0.105+8	0.526+7	0.592+7
5d ⁴	⁵ D	1	13475	0.182+8	0.137+8		
5d ⁴	⁵ D	2	14495			0.898+7	0.769+7
5d ³ 6s	¹ D	2	23295			0.444+7	0.624+6
Sum				0.443+9	0.522+9	0.325+9	0.356+9
RCI τ (ns)				2.26	1.92	3.07	2.81
Avg. (% spread)				2.09	(8.1%)	2.94	(4.4%)
Expt. [13]				5.0(5)			
E _k (cm ⁻¹)				44206.24		45233.91	

			State 9		State 10		
5d ³ 6s	⁵ F	1	0	0.691+8	0.871+8	0.976+8	0.123+9
5d ³ 6s	⁵ F	2	1031	0.442+7	0.593+7	0.286+9	0.328+9
5d ² 6s ²	³ F	2	3180			0.831+7	0.938+7
5d ² 6s ²	³ P	0	4125	0.153+8	0.147+8	0.243+8	0.269+8
5d ² 6s ²	³ P	1	5331	0.211+8	0.273+8		
5d ² 6s ²	³ P	2	5658	0.814+8	0.887+8	0.514+8	0.622+8
5d ³ 6s	⁵ P	1	10713	0.376+8	0.392+8		
5d ³ 6s	⁵ P	2	11875	0.510+7	0.439+7		
5d ⁴	⁵ D	0	12601			0.381+8	0.375+8
5d ⁴	⁵ D	1	13475	0.412+7	0.287+7	0.152+8	0.128+8
5d ⁴	⁵ D	2	14495	0.777+7	0.684+7	0.331+8	0.298+8
5d ³ 6s	³ D	1	14628	0.425+7	0.356+7		
Sum				0.259+9	0.290+9	0.567+9	0.644+9
RCI τ (ns)				3.86	3.45	1.76	1.55
Avg. (% spread)				3.66	(5.5%)	1.66	(6.0%)
Expt. [2]						2.5(6)	
E _k (cm ⁻¹)				46174.60		47595.98	

			State 11		State 12		
5d ³ 6s	⁵ F	1	0	0.186+8	0.225+8	0.119+8	0.158+8
5d ³ 6s	⁵ F	2	1031			0.412+8	0.482+8
5d ² 6s ²	³ F	2	3180	0.192+8	0.249+8	0.302+7	0.361+7
5d ² 6s ²	³ P	0	4125			0.224+7	0.239+7
5d ² 6s ²	³ P	1	5331	0.351+7	0.348+7	0.907+6	0.211+7
5d ² 6s ²	³ P	2	5658			0.559+8	0.667+8
5d ³ 6s	³ F	2	9691	0.147+9	0.154+9	0.247+8	0.278+8
5d ³ 6s	⁵ P	1	10713	0.405+7	0.552+7		
5d ³ 6s	⁵ P	2	11875	0.643+7	0.476+7	0.778+7	0.824+7
5d ⁴	⁵ D	1	13475	0.298+7	0.381+7	0.257+7	0.263+7
5d ² 6s ²	¹ D	2	13560	0.131+8	0.111+8		
5d ³ 6s	³ D	1	14628	0.289+7	0.307+7	0.106+8	0.117+8
5d ³ 6s	³ P	0	16288	0.310+7	0.345+7		
5d ³ 6s	³ D	2	17168	0.947+7	0.831+7		
5d ³ 6s	³ P	1	17375			0.612+7	0.605+7
5d ³ 6s	³ P	2	18501			0.143+8	0.134+8
5d ³ 6s	³ F	2	22929	0.384+7	0.274+7		
5d ³ 6s	¹ D	2	23295	0.214+8	0.802+6	0.124+8	0.164+7
5d ³ 6s	³ P	0	23381	0.565+7	0.329+7		
5d ³ 6s	¹ P	1	23406	0.277+7	0.244+7	0.353+7	0.359+7
Sum				0.272+9	0.262+9	0.205+9	0.218+9
RCI τ (ns)				3.68	3.82	4.89	4.60
Avg. (% spread)				3.75	(1.9%)	4.75	(2.9%)
Expt. [13]						6.2(6)	
E _k (cm ⁻¹)				48776.29		49886.97	