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Theoretical lifetimes and Landé g values of Cs II $5p^5\,6p$ levels

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Lifetimes of Cs II $5p^5\,6p$ levels, oscillator strengths to the lower $5p^5\,5d$ and $5p^5\,6s$ levels, Landé g factors and LS compositions of all these levels are presented. Results are in very good agreement with most available experiment. Large correlation effects are associated with those $5p^5\,5d$ and $5p^5\,6s$ states, which strongly interact. [S1050-2947(98)03606-3]

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I. INTRODUCTION

Transition-metal atoms (TM) are technologically important, but difficult to treat accurately, computationally. The difficulty arises for three reasons: (1) correlation effects are difficult to treat due to the presence of open subshell d electrons, (2) the breakdown of LS coupling, and (3) the necessity to include relativistic effects to properly position d^n, $d^{n-1}s$, and $d^{n-2}s^2$ levels relative to each other.

Using a relativistic configuration interaction (RCI) method, we have successfully obtained accurate results for hyperfine structure constants for a series of TM states. The most complicated species studied was Nb II [1] with $n=4$, and the most accurate and recent results are those for La II [2] and Cs II [3]. The relative positioning of the d^{n-1}s states is found to be crucial to accurate determination of some of the hyperfine structure (hfs) constants. In the most recent work [2,3] average errors in energy differences among the above configurations were reduced to $\sim 200\ \mathrm{cm}^{-1}$ (~ 0.025 eV).

We now want to extend our reach to include a perhaps more important property—oscillator strengths. Little *ab initio* theoretical work is available for TM, other than some recent work of ours on Nb II [4], and Luke's work [5,6] on Cr II and V I. Currently, our choice of problem involves three major considerations: (1) whether RCI wave functions are available, so as to reduce computational effort (these may have been previously obtained from hfs studies, for example), (2) availability of at least some experimental results with which to compare (often, such results are in the form of lifetimes, forcing the computationalist to calculate f values for all decay branches), and (3) the technological importance of the species.

Previously, we obtained [4] two lifetimes for Nb II, with the length and velocity results differing by $\sim 10\%$ from the average value, which in turn, differed from experiment by 6% or less. These calculations were quite complicated, and it seemed too much to ask for a much more accurate calculation on such a system, at this time.

We thus looked for a simpler system, subject to the three criteria given above. Cs II appears to be a good case; though it is not normally considered a TM, there is substantial [3] mixing of $5p^5$ 5d and $5p^5$ $6s$ states. Experimentally, lifetime measurements have by made by Alvarez *et al.* [7] and Osherovich and Mikolaich [8]. If we can obtain accurate results for Cs II, it is hoped that detailed analysis can identify the key elements and conclusions, which might be useful for more complicated cases. Such analysis includes trying to answer the following questions: (1) How critical is the relative positioning of states? (2) What are the important configurations, and how useful is the first order theory of oscillator strengths [9] (FOTOS) for *a priori* prediction of configurations? (3) Which gauge is better, length or velocity? A related question is: Does good agreement of the two gauges have any implication regarding the accuracy of the result?

Since our relativistic oscillator strength program [10], RFE, has only been used for Tl II [11] and Nb II [4] f values, we decided to test it more thoroughly, by examing the $2p \rightarrow 3d$ transition in the H atom. This removes any problems treating correlation effects, and maintains the symmetry of the $5p^5\,5d \rightarrow 5p^5\,6p$ transitions, at the one-electron level. Initially, agreement between the two gauges was to 8 digits; theoretically, exact agreement is predicted. Three numerical improvements were introduced, all associated with the radial integral: (1) use a more accurate [12] spherical Bessel function routine, (2) use an improved integration rule, *viz.*, change the two interval Simpson rule, to the 4 interval Bode rule and, (3) double the numerical mesh [13]. Use of all three improved agreement to 10 digits, which we currently consider adequate. Of the three, doubling the mesh is the most important. Comparison with exact results, available [14] only to 4 digits, also indicated no problem.

In this work, we also report Landé g values for all levels (except $J=0$) associated with the transition probabilities. This quantity, which is new to us, can either be computed directly by evaluating [15] $\langle S_z \rangle$, or indirectly [16] once the LS composition of the level is known [17]. For almost all levels, the correlated result differs less than 10% from the Dirac-Fock result, and the correlated values are generally in good agreement with experimental results [18].

In Sec. II, we briefly review the methodology used. In Sec. III we present our Cs II 5p^5 $6p$ lifetime results. We have excluded the $J=0$ states, as they computationally require a modified procedure. Specifically, 2 configuration, $5p^6+5p^5\,6p$, multiconfigurational Dirac-Fock (MCDF) calculations are required; these involve the addition of a kinetic energy term in the inhomogeneous part of the MCDF equations. This is something that the older version of the Desclaux program [13] is not equipped to do. Section III also contains the Landé g value results and the LS percent analysis of the Dirac-Fock functions.

II. METHODOLOGY

We begin by solving the Dirac-Fock (DF) equations, obtained from applying the variational principle to the Dirac-Coulomb Hamiltonian, using a program of Desclaux [13]. In the case of multiple levels (for fixed J), the calculation focuses on one specific level, generally one of the lower ones [3]. Descriptions of the other levels are then corrected during the RCI stage, by the inclusion of symmetry preserving single excitations (''Brillouin'' type).

The form of the correlation portion of the RCI function is created by applying perturbation theory to the DF (MCDF) function. Specifically, single and double excitations are made from each of the outer subshells (generally $5s$, $5p$, $5d$, $6s$, $6p$), except where we have reason to believe that such excitations do not contribute significantly to properties of interest to us—here, hyperfine structure (hfs), energy differences, oscillator strengths and g factors. As Tables II and III of Ref. [3] illustrate, most double excitations from $5p$ subshells are excluded. Selected triples and quadruple excitations are also included. When correlating the $5p^5\,5d/6s/6p$ states, we ''pull them away'' from what used to be energetically nearby Rydberg-like states associated with $5p^5\,nd/ns/np$ configurations. If these play a significant role, as they do for hfs [3], we introduce the equivalent large single and double excitations into these as well. These can be triple excitations with respect to the $5p^5\,5d/6s/6p$ states.

Most excitations are into subshells not present in the DF (MCDF) function. We represent the radial parts of these one-electron functions (called ''virtuals'') with relativistic screened (Z^*) hydrogenic functions, whose effective charge, Z^*, is determined by diagonalizing the energy matrix. Specifically, the lowest energy is sought as a function of Z^*, subject to a ''reasonable'' starting value for Z^*, which we take to mean that the $\langle r \rangle$ of the virtual match the $\langle r \rangle$ of the DF (MCDF) radial it is replacing. Generally, two virtuals of each symmetry type per shell (e.g., excitations from $5s$, $5p$, and $5d$ can share the same set of virtuals) are sufficient to produce about 95% of the possible correlation energy.

The size of the RCI basis set described above may involve from 10^4 to 10^5 functions—too many for our program [19], which is currently limited to 7000 functions. We have introduced [11] and programmed [20] a procedure that minimizes the number of functions, by rotating the original basis, to create the maximum number of functions having a zero interaction with all DF (MCDF) functions, which are then discarded. For complicated states (e.g., d^n or f^n) reductions can be as large as a factor of 100, with little loss (100–200 cm^{-1}) in accuracy.

Once the RCI functions are available, the oscillator strengths can be obtained, following the formalism of Grant [21] as described elsewhere [11]. Results are obtained in both the length and velocity gauges; the results would be identical, if the wave functions were exact. Since the wave functions for each state in the transition are calculated independently, their radial sets are not orthonormal. Thus we have to account for the effects of nonorthonormality (NON). This is done determinant by determinant, following the procedure of King *et al.* [22], specializing it to the electric dipole case, as Westhaus and Sinanoglu [23] first did. This avoids the expensive diagonalization step of the process. Full details may be found elsewhere [11]. An early study [24] of NON for second row (Li-Ne) atoms, suggested that f values may change 20% or so for neutrals, and less for positive ions, when NON is included. In general, such studies are not too meaningful for RCI calculations, as one-electron radial functions for the two transition states are developed completely independently, so it may not be meaningful which would be the ''corresponding'' radial functions between the two sets. If this correspondence could be made, and the size of radial overlap integrals would be the most appropriate means, the program [10] does have the ability to turn NON off.

Computational costs (on a SPARC 10) are up to a few hours for the largest RCI wave functions, and up to 1 h per transition, for the oscillator strength. Ultimately, the latter times will be drastically reduced by processing all transitions associated with a fixed set of J's in one pass.

The expression for the Landé g value may be extracted from Shore and Menzel [15]. It is

$$g-1=(g_S-1)\langle JJ|S_z|JJ\rangle/J. \tag{1}$$

To account for the anomalous magnetic moment of the electron, we take $g_S = 2.002\,319$. The matrix element $\langle S_z\rangle$ may be constructed once the one-electron matrix elements are known. These are

$$\langle n\kappa m|s_z|n'\kappa' m\rangle=\delta_{nn'}\delta_{\ell\ell'} \times\begin{cases}(-1)^{j-\ell-1/2}m/(2\ell+1), & j=j'\\ \sqrt{(2\ell+1)^2-4m^2}/(4\ell+2), & j\neq j'.\end{cases} \tag{2}$$

The g value may also be expressed [16] in terms of pure LS values, as follows:

$$g=\sum_{\gamma SL} g_{SLJ}C^{\gamma}_{SLJ}, \tag{3}$$

where C^{γ}_{SLJ} are the fractional weights of each LS type, and g_{SLJ} is given by

$$g_{SLJ}=1+(g_S-1)\frac{J(J+1)-L(L+1)+S(S+1)}{2J(J+1)}. \tag{4}$$

III. RESULTS AND DISCUSSION

Construction of the wave functions for Cs II $5p^5\,5d/6s$ $J=1,2,3$ states is described by O'Malley and Beck [3]. No correlated results are available for $J=0$ (no hfs) or $J=4$. For Cs II $5p^5\,6p$ levels, correlated results are available [3] for $J=1$ and 2, but not for $J=3$. In this work, we provide the missing correlated functions, but additionally we redid all the $5p^5\,6p$ levels. This was done in an attempt to obtain a smaller (fewer basis functions) wave function that would produce accurate f values. This was successful for the $5p^5\,6p$ levels, but when the same was attempted for the $5p^5\,5d/6s$ $J=1$ levels, f values were not accurate enough. This is attributed to the significant interactions associated with the $5p^5\,5d$ and $5p^5\,6s$ levels.

For the $J=0$ and $J=4$ $5p^5\,5d/6s$ states, the following

TABLE I. RCI f values for Cs II $5p^5\,5d/6s \rightarrow 5p^5\,6p$ transitions. Upper value is velocity, lower value is length result. An * means transition is important for lifetimes. A non-numerical value means the f value is small (see text). The subscript, e.g., 2 in $6p_2$, labels the root number with 1 being lowest. A blank means the f value is zero.

	$6p_1$ $J=1$	$6p_1$ $J=2$	$6p_1$ $J=3$	$6p_2$ $J=1$	$6p_2$ $J=2$	$6p_3$ $J=1$	$6p_4$ $J=1$	$6p_3$ $J=2$
$J=1\ 5d_3$						ΔE	0.0032	0.0037
							0.0060	0.0019
$J=3\ 5d_3$					ΔE			0.1452
								0.1307
$\mathrm{J=2\ 5d_4}$			~ 0	ΔE	ΔE	0.0001	0.1117	0.0116
			~ 0			0.0001	0.1278	0.0111
$J=2\ 5d_3$		ΔE	~ 0	0.0001	0.0001	0.1036	0.0009	.0204
			~ 0	0.0017	~ 0	0.1146	0.0009	0.0202
$J=1\ 5d_2$	0.0015	0.0067		0.0281	0.0009	0.0029	0.0008	0.0945
	0.0005	0.0028		0.0173	~ 0	0.0042	0.0011	0.0806
$J=1\ 6s_2$	0.0008	0.0051		0.0008	~ 0	0.2043	0.1494	0.5297
	~ 0	0.0011		0.0019	0.0010	0.2228	0.1426	0.5567
$J=0\ 6s_1$	0.0026			0.0003		0.3986	0.7483	
	0.0003			0.0001		0.3771	0.7161	
$J=3\ 5d_2$		0.0106	0.0217		0.1206*			~ 0
		0.0084	0.0146		0.0980*			~ 0
$J=2\ 5d_2$	0.0023	0.0414	0.0033	0.0725*	0.0003	0.0075	0.0008	0.0003
	0.0028	0.0363	0.0028	0.0889*	0.0004	0.0058	0.0010	0.0006
$J=3\ 5d_1$		0.0962*	0.0264		0.0018			0.0034
		0.1140*	0.0259		0.0012			0.0036
$J=2\ 5d_1$	0.0008	0.0485	0.0869	0.0248	0.2025*	~ 0	0.0119	0.0042
	0.0003	0.0407	0.0671	0.0257	0.1876*	~ 0	0.0105	0.0063
$J=4\ 5d_1$			0.1475*					
			0.1520*					
$J=1\ 6s_1$	0.0024	0.2338*		0.2923*	0.2601*	0.0054	0.0002	.0003
	0.0023	0.2233*		0.2799*	0.2453*	0.0042	0.0002	.0001
$J=1\ 5d_1$	0.1183*	0.1350*		0.0838*	0.0111	0.0048	0.0006	.0054
	0.1229*	0.1603*		0.0874*	0.0078	0.0091	0.0004	.0097
$J=0\ 5d_1$	0.1465			0.0084		0.0167	0.0078	
	0.1499			0.0102		0.0216	0.0080	
$J=2\ 6s_1$	0.2593*	0.0881*	0.4421*	0.0003	0.1174*	~ 0	~ 0	~ 0
	0.2524*	0.0942*	0.4684*	0.0004	0.1234*	~ 0	~ 0	~ 0

types of correlation were included (all $5p^5\,5d$ and $5p^5\,6s$ levels were used as a reference): (1) Symmetry changing excitations, e.g., $n\ell \rightarrow v(\ell+2)$ where $n\ell = 5s$, $5p$, $5d$, $6s$, (2) pair excitations from $5p$, $5d/6s$ $\rightarrow v\ell v\ell'$ with $\ell \leqslant 4$, (3) the exclusion effects 5s $5d/6s \rightarrow 5p$ $(vp+vf)$ and $5p^2 \rightarrow 5d$ $(vs+vd+5d+vg)$, and (4) the ''Brillouin'' excitations, $n\ell \rightarrow v\ell$ to correct the radial functions ($n\ell = 5s$, $5p$, $5d$, $6s$). Excitations are chosen because they are differentially large; for the most important correlation, two relativistic screened hydrogenic radial functions were used.

For the $5p^5\,6p$ levels, we included the analogous excitations. Additionally, the largest pair excitations from $5s\ 5p$ and $5s\ 6p$ were included. Defining our energy differences relative to the lowest level for the J value of interest, we find an average error of 236 cm^{-1} as compared with experimental values available in Sansonetti and Andrew [25]. This accuracy is comparable to the best achieved so far, e.g., Ref. [3].

The absorption oscillator strengths, f_{ik}, are evaluated with these wave functions, using the experimental [25] energy differences. The correlated results are given in Table I, and the DF results in Table II (All DF results are obtained during the RCI process, so the DF coefficients may vary somewhat from pure [13] DF results.) All possible f values were calculated, except those corresponding to very small (below 0.01 a.u.) energy differences. These are listed in the table as ''ΔE.'' Further, we do not give any result below 0.0001 for the f value—they are just too unreliable; this is indicated as ~ 0. Finally, f values that are exactly zero due to electric dipole selection rules or negative energy differences are left blank.

By examining Tables I and II, one can see that more often than not the velocity result undergoes a larger change than the length result (DF versus correlated result). Also, nonrelativistically speaking, the length result is proportional to the energy difference, and the velocity result inversely proportional to the energy difference. The implication of this is that for the smallest energy differences, the length result is likely to be the more accurate one. From a global perspective, the length result may be the preferred one, but this

TABLE II. Dirac-Fock f values for Cs II $5p^5\ 5d/6s \rightarrow 5p^5\ 6p$ transitions. Upper value is velocity, lower value is length result. A nonnumerical value means the f value is small.

	$6p_1$ $J=1$	$6p_1$ $J=2$	$6p_1$ $J=3$	$6p_2$ $J=1$	$6p_2$ $J=2$	$6p_3$ $J=1$	$6p_4$ $J=1$	$6p_3$ $J=2$
$J=1\ 5d_3$						ΔE	0.0691	0.0100
							0.0045	0.0007
$J=3\ 5d_3$					ΔE			0.2187
								0.1081
$J=2\ 5d_4$			~0	ΔE	ΔE	0.0002	0.1028	0.0104
			~0			0.0002	0.1289	0.0134
$J=2\ 5d_3$		ΔE	0.0003	~0	ΔE	~0	~0	0.0149
			~0	~0		~0	~0	0.0257
$J=1\ 5d_2$	0.0018	0.0145		0.1097	0.0003	0.0079	0.0067	0.0009
	0.0001	0.0015		0.2025	~0	0.0129	0.0104	0.0015
$J=1\ 6s_2$	0.0213	0.0014		0.0005	0.0137	0.2659	0.1571	0.7239
	0.0008	0.0001		~0	0.0020	0.2621	0.1604	0.7406
$J=0\ 6s_1$	0.0744			0.0034		0.0001	1.1400	
	0.0016			0.0003		0.0001	0.6599	
$J=3\ 5d_2$		0.0158	0.0495		0.1956			~0
		0.0078	0.0114		0.0771			~0
$J=2\ 5d_2$	~0	0.0324	0.0023	~0	0.0002	~0	0.0002	0.0002
	~0	0.0450	0.0025	~0	0.0007	~0	0.0009	0.0008
$J=3\ 5d_1$		0.0678	0.0218		0.0027			0.0036
		0.1390	0.0312		0.0010			0.0051
$J=2\ 5d_1$	0.0002	0.0019	0.0052	~0	0.0401	~0	0.0048	0.0012
	0.0002	0.0052	0.0078	~0	0.0792	~0	0.0249	0.0065
$J=4\ 5d_1$			0.1108					
			0.1844					
$J=1\ 6s_1$	0.0301	0.4984		0.4378	0.2785	0.0013	0.0004	~0
	0.0142	0.4024		0.3987	0.2596	0.0029	0.0010	~0
$J=1\ 5d_1$	0.0838	0.0059		~0	0.0156	0.0004	~0	0.0002
	0.1346	0.0131		0.0001	0.0355	0.0024	0.0004	0.0013
$J=0\ 5d_1$	0.1263			0.0039		~0	0.0013	
	0.1712			0.0102		0.0002	0.0061	
$J=2\ 6s_1$	0.2238	0.1250	0.5356	0.0066	0.2282	0.0001	0.0023	.0006
	0.2456	0.1705	0.6866	0.0140	0.3368	0.0002	0.0087	0.0022

observation is not always useful for an individual transition. It should also be noted that these results were obtained from wave functions that contained few excitations from the $n=4$ shell; the specific $n=4$ excitations included have been given in Ref. [3].

In Table I, certain f values have been assigned a ‘‘*.’’ This indicates these transitions are important in determining one or more lifetimes of the 5 energetically lowest $5p^5\ 6p$ levels. The average spread in velocity and length results for these 15 transitions is 5.8%, with the larger ones ($f>0.1$) having a spread around 2%. Although we have made no systematic study of convergence patterns, variations in results for ‘‘near final’’ wave functions seem consistent with these percentages. For these 15 transitions, the largest changes (DF versus correlation) involve the $5d_1$ and $6s_1$ (the subscript labels the root number, with 1 being energetically lowest) wave functions for $J=1,2$, which are just the ones for which the $5d$ and $6s$ interactions are quite large. Specifically, DF weights for these vectors are 0.75 or lower, and they also exhibit big differences in DF and correlation hfs constants [3].

Our oscillator strength program [10] provides all configurational contributions to the transition matrix element. Focusing on the 15 important transitions, it is seen that the greatest correction to the DF value comes from the ‘‘companion’’ configuration in the lower state, e.g., if DF is $5p^5\ 5d$, then $5p^5\ 6s$ is the ‘‘companion.’’ Other important configurations are, for the lower state $5p \rightarrow vp$ from $5p^5\ 5d$, and for the upper state, $5p\ 6p \rightarrow 5d^2 + vs\ vd$. All these configurations are predicted necessary by FOTOS [9], however, in this case, at least, these configurations alone are insufficient. FOTOS-like wave functions were initially constructed during this work, but did not produce satisfactory f values. This may be interpreted to mean that the characteristics of FOTOS configurations are determined in significant part by the presence of non-FOTOS configurations.

Lifetimes can be deduced from our f values using well-known [14,16] formulas; these are displayed in Table III. The agreement between the two gauges is excellent, ranging from 0.5% to 6%. This is actually ‘‘better’’ than that of individual f values, due to the partial cancellation of errors in the f-value sums. The agreement with two of the three

TABLE III. Lifetimes (ns) of Cs II $5p^5$ $6p$ states.

	Theory(RCI)			Experiment	
Level	Velocity	Length	Average [a]	Ref. [7]	Ref. [8]
$6p_1$ $J=1$	6.92	6.99	6.96 ± 0.51%		9.2 ± 0.3
$6p_1$ $J=2$	9.46	8.91	9.19 ± 3.0%		
$6p_1$ $J=3$	6.38	6.57	6.48 ± 1.5%	6.6 ± 0.2	8.9 ± 0.5
$6p_2$ $J=1$	8.04	7.91	7.97 ± 0.84%	7.8 ± 0.2	
$6p_2$ $J=2$	6.78	7.14	6.96 ± 2.6%	9.6 ± 0.3	8.5 ± 0.2
$6p_3$ $J=1$	11.02	9.84	10.43 ± 5.7%		
$6p_4$ $J=1$	5.88	6.02	5.95 ± 1.1%		
$6p_3$ $J=2$	7.20	7.11	7.16 ± 0.70%		

[a] The % gives deviation of length and velocity results from average value.

Alvarez *et al.* [7] values is very good, whereas the three Osherovich and Mikolaich [8] values are considerably larger than our results.

In Table IV, we give our results for Landé g values for all $5p^5$ $5d/6s/6p$ states constructed in this work. Thirteen experimental values [18] are also shown. Only results for $6s_1$, $5d_1$, and $6s_2$ $J=1$ states, which interact strongly, show significant deviation from the experimental values. By ''artificially'' shifting the $5p^5$ $6s$ $J=1$ diagonal matrix elements to bring the RCI $5d_1$-$6s_1$ energy differences into agreement with experiment [25], the g values for the two levels changed 0.015, bringing them closer to the experimental [18] g values. For most levels, DF and correlated values are similar; this makes sense if one realizes that corrections to $\langle S_z \rangle$ occur first in second order, not first order, as indicated by Eq. (2).

Also included in Table IV is the LS composition for the DF solution for each state, calculated using the procedure in Ref. [17]. Specifically, LS eigenstates are constructed by simultaneously diagonalizing the L^2 and S^2 matrices, with the approximations that the radial function's minor component can be neglected, and that the functions are independent of j. For large correlation vectors, construction is inhibited by the need for a large all root diagonalizer. The DF vectors are then decomposed in this basis. The LS eigenstates can be used to predict DF g values [15], which are in good agreement with the directly calculated DF values in Table IV, as they should be. Producing such compositions for the full correlated functions is still a tedious business, but the agreement between the DF and correlated g values, for most states, suggests the LS composition would not change much.

We have also recalculated the $5d_1/6s_1$ $J=1 \rightarrow 6p_{1,2}$ $J=2$ f values with the shifted wave functions. The net effect

TABLE IV. Cs II Landé g values and LS composition.

		g values		
Level	DF	RCI	Expt. [18]	LS % [DF]
$6s_1$ $J=2$	1.501	1.491	1.49 ± 0.03	$^3P(100)$
$5d_1$ $J=1$	1.455	1.416	1.37 ± 0.02	$^1P(0.3)$, $^3P(95.3)$, $^3D(4.3)$
$6s_1$ $J=1$	1.172	1.230	1.29 ± 0.02	$^1P(65.6)$, $^3P(34.4)$
$5d_1$ $J=4$	1.251	1.250		$^3F(100)$
$5d_1$ $J=2$	1.415	1.432		$^3P(78.1)$, $^1D(7.7)$, $^3D(14.2)$
$5d_1$ $J=3$	1.091	1.091		$^3D(8.5)$, $^1F(16.7)$, $^3F(74.7)$
$5d_2$ $J=2$	0.8820	0.8823		$^1D(34.3)$, $^3D(20.2)$, $^3F(45.5)$
$5d_2$ $J=3$	1.203	1.203		$^3D(60.7)$, $^1F(39.2)$, $^3F(0.1)$
$6s_2$ $J=1$	1.293	1.204	1.12 ± 0.02	$^1P(41.4)$, $^3P(58.6)$
$5d_2$ $J=1$	0.6011	0.6851	0.70 ± 0.02	$^1P(10.2)$, $^3P(6.5)$, $^3D(87.3)$
$5d_3$ $J=2$	0.841	0.841		$^3P(0.8)$, $^1D(38.5)$, $^3D(8.0)$, $^3F(52.8)$
$5d_4$ $J=2$	1.188	1.189		$^3P(19.1)$, $^1D(19.9)$, $^3D(59.1)$, $^3F(1.9)$
$5d_3$ $J=3$	1.124	1.124		$^3D(30.7)$, $^1F(44.1)$, $^3F(25.2)$
$5d_3$ $J=1$	0.960	0.965		$^1P(89.1)$, $^3P(1.4)$, $^3D(9.5)$
$6p_1$ $J=1$	1.868	1.867	1.87 ± 0.03	$^3S(76.2)$, $^3P(21.9)$, $^1P(1.0)$, $^3D(0.8)$
$6p_1$ $J=2$	1.125	1.125	1.10 ± 0.02	$^3P(7.4)$, $^1D(39.6)$, $^3D(53.0)$
$6p_1$ $J=3$	1.333	1.333	1.33 ± 0.02	$^3D(1.00)$
$6p_2$ $J=1$	1.024	1.024	1.02 ± 0.02	$^3S(3.6)$, $^3P(18.2)$, $^1P(57.6)$, $^3D(20.6)$
$6p_2$ $J=2$	1.365	1.365	1.34 ± 0.02	$^3P(72.4)$, $^1D(26.1)$, $^3D(1.5)$
$6p_3$ $J=1$	0.6605	0.6609	0.68 ± 0.01	$^3S(1.7)$, $^3P(0.1)$, $^1P(26.8)$, $^3D(71.4)$
$6p_4$ $J=1$	1.448	1.448	1.44 ± 0.02	$^3S(18.5)$, $^3P(59.8)$, $^1P(14.4)$, $^3D(7.3)$
$6p_3$ $J=2$	1.177	1.177	1.12 ± 0.02	$^3P(20.2)$, $^1D(34.3)$, $^3D(45.5)$

is to decrease the average value of the larger $6s_1$ transition by 12% and 3%, respectively. But, the smaller f value gains nearly the same amount, and because the transition energy differences are quite similar, there is little ($<$ 1.8%) change in the lifetimes. This is consistent with the two state approximation (TSA), put forward earlier [26]. TSA says, if two states are nearly degenerate, and fairly isolated from the other RCI basis vectors, and the transition energies are nearly the same, then there is a transfer of oscillator strength from one f value to the other with the sum of the two fixed, as the approximation (e.g., shift versus no shift) is changed. But, this does not work well for these transitions in going from the DF to the RCI results (compare appropriate entries in Tables I and II).

In summary, two of three lifetimes are in good agreement with one experiment [7], whereas the other [8] experimental values are uniformly too high. Most g values are in excellent agreement with experiment [25]. There is some indication that individual f values associated with nearly degenerate states may be uncertain by $\sim$10%, and that this is correlated with the error in splittings of such levels.

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