

Mo V $J = 0, 1$ Energy Levels, Oscillator Strengths, and Landé g -values

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Abstract

Relativistic Configuration Interaction results are obtained for the lowest 9 $J = 0$ even parity and the lowest 30 $J = 1$ odd parity levels of Mo V. Some of the levels (e.g. $4p^5 4d^3$) are new to this work, and several of the others (e.g. $5s^2$, $5p^2$, $4d6d$ and $5s5p \ ^1P_1$) are repositioned. Average errors for the remaining energy differences are 229 cm^{-1} ($J = 0$) and 368 cm^{-1} ($J = 1$). All 360 electric dipole f -values connecting these levels have been obtained, and average gauge agreement for the 88 transitions with $f > .01$ is 3.1%.

I. Introduction

In this work we continue our study of the Sr I isoelectronic sequence with Mo V. Like the Zr III and Nb IV members we previously studied [1], there are examples of nearly degenerate $J = 1$ states in Mo V which require careful treatment. For Mo V there are no published f -values, and two experimental studies [2, 3] of energy levels, from the mid 1980's which are not always in good agreement for $J = 0$. For these reasons, we undertook an *ab initio* study with simultaneous treatment of relativity and correlation, using a Relativistic Configuration Interaction (RCI) methodology.

The frequent near degeneracy of nd and $(n + 1)s$ electrons and the differing relativistic effects for them (> 0.1 eV [4]) mean that relativistic effects must be included from the first, and that a multi-reference $(d+s)^2 J = 0$ [($d+s$) p for $J = 1$] zeroth order wavefunction must be used. Relativity is incorporated using a Dirac+Breit Hamiltonian, and approximate wavefunctions are built from linear combinations of Slater determinants whose elements are spinors composed of products of to-be-determined radial parts (major and minor) and spin-angular functions, as in the relativistic treatment of the hydrogen atom. The linear combinations are chosen, to the extent possible, by making the approximate functions eigenstates of J^2 and J_z , which remain good quantum numbers. In zeroth order, we determine the radial functions by solving the Dirac-Fock equations numerically, using the computer program of Desclaux [5].

Ten $J = 0$ and fourteen $J = 1$ levels have been experimentally identified. Roughly in order of increasing energy, these are associated with the $4d^2$, $5s^2$, $4d5d$, $5p^2$, $4d6d$ and $5s6s$ configurations for $J = 0$, and with the $4d5p$, $5s5p$, $4d4f$, $4d6p$, $4d5f$ and $5s6p$ configurations for $J = 1$ [2, 3]. To form our reference list of configurations, we have modified this list to add $4d7d$ ($J = 0$), and for $J = 1$ deleted $5s6p$ and $4d5f$ (high energy) but added the previously unknown $4p^5 4d^3$ configuration, whose lowest levels lie between the highest $4d6p$ $J = 1$ level and the lowest $4d5f$ $J = 1$ level. In this work, we provide results for the 9 lowest $J = 0$ levels, and the 30 lowest $J = 1$ levels. Electric dipole oscillator strengths are calculated for all 360 possible transitions.

Once the reference space is selected, construction of the correlation function begins by making single and double excitations from each reference configuration. Radial functions of unoccupied subshells (virtuals) are represented by relativistic screened hydrogenic (RSH) functions whose effective charge (Z^*) is determined as part of the energy variational process. This form of virtual helps prevent variational collapse into the "positron sea". For the accuracies desired: ~ 200 cm^{-1} in energy level differences, and 5% spreads in the f -value length and velocity gauges, limiting azimuthal symmetries to $l < 5$ appears adequate [1]. Good convergence of the virtual radial space is achieved with a principle quantum number $n = l + 1$, except for s-radials, where $n = 2$ is found most effective. Generally 2 virtuals/ l originating shell are adequate.

Because of the near degeneracy of some levels (within 1-2000 cm^{-1}) and the large size of some correlation effects (up to ~ 2.0 eV as in $4p^2 \rightarrow 4d^2$), it is necessary that each and every reference configuration be equivalently correlated. Furthermore, differentially large first order correlation effects such as $5pvd$ for the $5s5p$ 1P level must also be so correlated (e.g. $4p \rightarrow f$ must appear for all of them). To make sure all such excitations are present,

a small analysis computer program was used, which was introduced in the earlier work [1]. With a smaller reference space, as we had traditionally used, some of these correlation effects would be classified as second order in nature. A more detailed description of the methodology may be found in reference [1], and references therein.

The principle results of this work are as follows:

(1) We are in better agreement with the newer measurements [3] for $J = 0$. The $4d^2 \ ^1S$ and the two $4d5d$ levels are on average 229 cm^{-1} lower relative to $4d^2 \ ^3P_0$ with RCI than experiment [3]. RCI has the $5s^2$ level 4559 cm^{-1} higher, the $4d6d \ ^3P_0$ level 210 cm^{-1} lower, the $4d6d \ ^1S$ level 3493 cm^{-1} lower, and the two $5p^2$ levels $\sim 22\text{-}23 \ 000 \text{ cm}^{-1}$ higher than the older measurement [2]. The largest difference between the two measurements is 1236 cm^{-1} for the $4d5d \ ^1S$ level.

(2) For the lowest ten measured $J = 1$ energy differences, our average error [3] is 368 cm^{-1} . Of these the position of $5s5p \ ^1P$ is most in error, by $\sim 1600 \text{ cm}^{-1}$. Difficulty with this level was also apparent in Zr III and Nb IV. All other errors were below 500 cm^{-1} . We have located the lowest 16 out of 19 $4p^5 \ 4d^3 \ J = 1$ levels. Due to our current 30 level limit [9] the 3 uppermost levels remain unknown.

(3) We have calculated f -values for the 360 electric dipole transitions, and find an average gauge spread of 3.1% for all f -values $> .01$.

II. $J = 0$ Wavefunctions and Energy Levels

The numerical radial functions for $1s \cdots 4d$, $5s$ and $5p$ were generated as in ref [1] from Desclaux's code [5]. Generation of the $5d$, $6d$ and $7d$ radials required a different approach due to the indeterminacy associated with use of orthogonal radials (which we require) for $(nlj)^q (n'lj)^q \ J$ levels for which the $(nlj)^{2q} \ J$ level exists. [6]. One often first encounters this problem in dealing with the He I $1s \ 2s \ J = 0$ state. A straightforward solution to this problem [6] is to do a 2-configuration calculation ($(nlj)^{2q} + (nlj)^q (n'lj)^q$) for this J . This however introduces the one particle kinetic energy operator into the inhomogeneous part of the Dirac-Fock equations, which can not be handled with the version of the algorithm we are using [5]. Other approaches also exist [7, 8]. We instead worked our way around this difficulty by calculating the $5d_{3/2}$ radial for the $4d_{3/2} \ 5d_{3/2} \ J = 3$ level and the $5d_{5/2}$ from the $4d_{5/2} \ 5d_{5/2} \ J = 5$ level. There is neither a $(4d_{3/2})^2 \ J = 3$ nor a $(4d_{5/2})^2 \ J = 5$ level, so the problem no longer exists. A similar approach [6] has been taken for non-relativistic calculations. These $5d$ radials (and those for $6d$ and $7d$) are then used in the $J = 0$ calculation. Any differences from the correct Dirac-Fock radials for $J = 0$ will then be corrected at the correlation stage.

In constructing the correlated $J = 0$ wavefunction, the $1s \cdots 3d$ subshells were kept closed, as for Zr III and Nb IV [1]. For Mo V $J = 0$, a smaller separate calculation with $3d$ open showed that the $4d^2 \ ^3P_0\text{-}5s^2$ energy difference to be increased by 172 cm^{-1} , which we consider negligible. The valence excitations (from $4d$, $5s$, $5p$, $5d$, $6d$, $7d$) satisfactorily converged with a single RSH function, except for f and g symmetries which required two RSHs. In opening the $4s$ and $4p$ subshells, a new set of virtuals was added, as the $\langle r \rangle$ for these subshells differs significantly from that of the valence space. Finally, a fourth set of virtuals was added to assure adequate radial convergence.

Due to the larger number of $J = 0$ levels considered, and the more thorough calculation,

the energy matrix size increased from [1] 3557 to 18 141. The current limit on our RCI matrix size is 20 000 [9]. Calculation times, with the Breit operator turned on, were ~ 2 days on a Blade 2000 (with no Breit, calculation is $4\times$ faster). The largest effect of the Breit operator on energy differences is to raise the $5s^2$ level 520 cm^{-1} relative to the $4d^2\ ^3P_0$ level. The average effect is a raise of 177 cm^{-1} .

The differentially most important correlation effects for energy differences are associated with the excitations: $4p^2 \rightarrow 4d^2+4d5d+4dvd$; $4p \rightarrow 5p+vp+vf$; $4p\text{ valence} \rightarrow vfv$; $4p\text{ valence} \rightarrow (5s+4d)5p+(5s+4d)vp$; $4s \rightarrow 4d+5s$; $4p5p \rightarrow 4d5d+4d5s+4dvd$ and $4s4p \rightarrow 4dvd$.

Our results for the Mo V $J = 0$ energy levels are in Table 1. Comparing to the 3 energy differences available from Cabeza *et al* [3] for the $4d^2$ and $4d5d$ levels, we have an average error of 229 cm^{-1} , quite good. On the other hand, we are in substantial disagreement with Tauheed *et al* [2] for the remaining levels, except for $4d6d\ ^3P$, where we are within 210 cm^{-1} . For $5s^2$ we are 4559 cm^{-1} higher, and for the $5p^2$ levels $22\text{-}23\ 000\text{ cm}^{-1}$ higher relative to $4d^2\ ^3P$ than Tauheed *et al* [2]. It is not clear how reliable these values are, however. Both experimenters give the position of $4d5d\ ^1S$, but they differ by 1236 cm^{-1} . Clearly, MoV $J = 0$ states deserve further experimental attention.

III. $J = 1$ Wavefunctions and Energy Levels

Initially our reference space contained the $4d5p$, $5s5p$, $4d4f$ and $4d6p$ configurations, as only these had been observed [2, 3], for a total of 11 levels. Numerical radial functions were obtained [5] for the $1s \dots 4d$ subshells from the $4d5p\ ^3D_1$ level, and for $5s$ and $5p$ from the $5s5p\ ^3P_1$ level, as we did in Zr III and Nb IV. Experimentally, positioning the $5s5p\ ^1P$ and $5s^2\ ^1S$ levels is not easy [10] because neither level is involved in a very strong transition, except with its companion. Consequently, we made some extra effort to correctly position the $5s5p\ ^1P$ level.

The splitting of the $5s5p\ ^3P$ and $5s5p\ ^1P$ levels is large, because of the large exchange integral. In Mo V, at the Dirac-Fock level, it is $34\ 874\text{ cm}^{-1}$ whereas the experimental value is $26\ 399\text{ cm}^{-1}$ and the RCI value is $28\ 422\text{ cm}^{-1}$. Clearly correlation effects are very large in Mo V, as they are for Zr III and Nb IV [1] (we discuss the RCI experimental discrepancy later). But we need also to be concerned about how well the $5s5p\ ^3P$ radials do in representing the $5s5p\ ^1P$ radials. Calculation shows a loss of 1040 cm^{-1} in the 1P energy, using these radials. Of this amount, all but 336 cm^{-1} can be recovered through symmetry preserving Brillouin excitations from the $5p$, $5s$ and $4p$ subshells. Such excitations are included as part of the correlation function.

A first order (in form) wavefunction was created from these reference configurations, first by exciting from the valence ($4d$, $5s$, $5p$, $6p$, $4f$) subshells. Virtual symmetries up to $l = 4$ were used, and generally $1\text{ RSH}/l$ was adequate. Next, single and double excitations from the $4p$ subshell were introduced, with a second set of virtual RSH functions used, because of the substantial change in $\langle r \rangle$ from the valence space. In order to keep the size of the total wavefunction below 20 000 basis functions, the REDUCE procedure [11] was used. Very briefly, this rotates the complete set of basis functions for a given correlation configuration so as to maximize the number of rotated basis functions having zero interactions with the reference space [1]. Rotated basis functions producing all zero interactions are then discarded.

In relatively “simple” cases like Mo V, size reductions of 10-100 times can be routine.

With 4p open, the diagonalizer was asked to generate 30 roots, the current limit [9]. Levels from the previously unknown [2, 3] $4p^5 4d^3$ configuration appeared, along with 3 $4d7p$ levels and, initially, 1 $4d5f$ level. We then enlarged our reference space to include these configurations, and added new virtuals to both represent the “Dirac-Fock” radials and correlation effects. Excitations from the 4s subshell were also permitted.

Properly correlating the $4p^5 4d^3$ wavefunctions relative to the $4p^6 nl n'l'$ wavefunctions requires some care because the number of electrons in the core and valence space are changing. Crudely [12] one may estimate that the $4p^2$ pair energy in $4p^5$ is 2/3 of that in $4p^6$, and that $(1s \cdots 4s)4p$ pairs in $4p^5$ have 5/6 of the pair energy present in $4p^6$. A separate calculation on $1s^2 \cdots 4p^6$ Mo VII $J = 0$, chosen for its closed shell simplicity, suggests the net differential effect for $4p^2$ to be 1.47 eV and for $4s4p$ pairs (presumably the largest) to be 0.19 eV. However, the $4p^2 \rightarrow 4d^2+4dvd$ excitations are already included in the RCI function, as they are important differential contributors within the $4p^6 nl n'l'$ levels [1]. This reduces the 1.47 eV above by 0.99 eV. Other correlation effects, not included, tend to preferentially lower the $4p^5 4d^3$ levels. These include single symmetry changing (e.g. $4s \rightarrow vd$) and exclusion effects (e.g. $4s^2 \rightarrow 4pvp$) out of the core, and additional valence correlation from $4d^3$, as there are now 3 not 2 valence electrons. While it is difficult to quantitatively estimate the net effect of all this, we would not be surprised if the accurate positions of the $4p^5 4d^3$ levels were a few thousand cm^{-1} away from our current predictions, and more likely to be above where we have them. This assessment is based on our observation of how these levels changed positions as we added correlation effects.

The $J = 1$ results for energy levels and Landé g values are shown in Table II. Magnetic Breit effects are included; relative to $4d5p^3D$, they raise or lower levels a few hundred cm^{-1} at most, with the effects larger for the $4p^5 4d^3$ levels. The effect of retardation on the $5s5p^1P$, 3P splitting was calculated [9], but found to be negligible ($\sim 0.3 \text{ cm}^{-1}$). Our Landé g values do not account for the anomalous g -factor. Correlation errors probably considerably exceed this correction. We found many of the $4p^5 4d^3$ levels to be so LS impure that we didn’t label them in Table 2. Instead we give an LS breakdown for each of these levels in Table 3, along with g values for pure LS states.

The final RCI wavefunction contains 16 943 basis functions. Because of the large reference space, there are few important second order effects. An exception are the $4p^4 \rightarrow 4d^4$ excitations which differentially can contribute as much as 400 cm^{-1} . Each reference function is automatically checked [1] to make sure it has the same (or equivalent) excitations in it as the $4d5p^3D_1$ state. Differentially, the largest contributions to the $5s5p^1P$, 3P splitting are $5pvd$ and $4p^5 4d (5s^2+5p^2)$. A more detailed analysis has been given for Zr III $J = 1$ in ref. [1]. Care has been taken to make sure correlation effects are included which properly correlate these basis functions as well (second order effects). In the past, we have sometimes tried to estimate the importance of missing second order effects by shifting nearly degenerate diagonal matrix elements. However, in moderately to highly ionized species like Mo V, energy denominators appearing in second order perturbation theory can be quite large, so any reasonable choice for the shift has little impact. Correlation errors in these cases may be more associated with numerator problems (off diagonal matrix elements).

IV. Mo V Electric Dipole f -values

In Table IV we give the velocity (Coulomb) and length (Babuskin) gauges for the 88 largest electric dipole f -values. F -values smaller than .01 are not displayed, as they are not likely to be reliable. The two gauges agree on average to 3.1%, which is good for RCI. Where the gauges differ significantly, some preference may be given to the length form, as the outer regions of the atomic wavefunctions are probably better correlated than the mid regions. This is even more true for the smaller energy differences (e.g. $< 10\,000\text{ cm}^{-1}$), as significant cancellation may be required for the velocity radial integral to achieve satisfactory accuracy. About 20 transitions with f -values $> .01$ were not included due to large gauge discrepancies. These either involved small energies, or double (triple) electron “jumps”; in the latter case $4p^5\ 4d^3$ levels were always involved.

Our calculations include full treatment of non-orthonormality [13, 14], (NON), the magnetic Breit operator, with $1s \cdots 3d$ subshells closed. It may be noted that several of the tabulated transitions involve “double jumps”, which means the f -value would vanish at the Dirac-Fock level, assuming complete orthonormality. All 360 transitions were obtained with our “one-pass” algorithm [15] which computes all transitions simultaneously for a fixed energy difference, and then scales appropriately the individual f -values with the experimental energy difference [3] when available. This approach is restricted to “optical” transitions, where the small r expansion of the spherical Bessel function is valid. Calculation time on a Blade 2000 was 2.2 hours. If all 360 transitions had been done one at a time, the estimated calculation time would have been 1 month!

Except for the $5s^2 \rightarrow 5s5p\ ^1P, ^3P_1$ transitions, the RCI f -values presented here are the only available ones. Migdalek and Stanek [16] have presented multi-configurational Dirac-Fock f -values for these two transitions. Including effects of core polarizations and using the length gauge and theoretical energy differences their results are .00352 (3P) and 1.99 (1P). RCI values are .010 and 1.07 respectively (see Table IV). For the allowed transition, the variation in their f -value as the approximations are improved (from 3.02 to 1.99) and their use of a theoretical energy difference of uncertain accuracy (a 14% error in Y II) [16], seemingly does not challenge the RCI result.

V. Discussion

If the Cabeza *et al* [3] position for $5s5p\ ^1P$ is correct, and Tauheed *et al* [2] have correctly assigned the observed wavelength to the $5s^2\text{--}5s5p\ ^1P_1$ transition, then their [2] position for $5s^2$ should be lowered 3274 cm^{-1} in Table I. This increases the discrepancy with the RCI result.

As a precaution, we undertook to evaluate the contribution of radiative effects at the screened hydrogenic level, using the Welton picture. This is built into the second version of Desclaux’s code [19]. Relative to $4d^2\ ^3P$, we find that $5s^2$ is raised $+274\text{ cm}^{-1}$ (this includes a moderate retardation correction of -25 cm^{-1}). In Zr III and Nb IV, these effects are $+136\text{ cm}^{-1}$ and $+198\text{ cm}^{-1}$ respectively. No radiative corrections are included in any of the tables. For the odd parity $J = 1$ states, $5s5p$ is raised $+151\text{ cm}^{-1}$ and $4p^5\ 4d^3$ lowered -42 cm^{-1} in Mo V relative to $4d5p\ ^3D_1$. While these effects are of some importance (e.g. by reducing

the $5s5p\ ^3P$ discrepancy in Mo V), they do not improve the agreement for $5s5p\ ^1P$ with the newer experiment [3].

A possible source of the discrepancy in the position of $5s5p\ ^1P_1$ may be due to the following: Reader and Acquista, in their work on Zr III [10], have noted the difficulty in locating the $5s^2\ ^1S$ level as it has only one strong combination, that to $5s5p\ ^1P$. They postponed trying to locate $5s^2\ ^1S$ until nearly all the strong lines in the region of the predicted wavelength for $5s^2\ ^1S_0 \rightarrow 5s5p\ ^1P_1$ were accounted for. The remaining strong line in this region was then assigned to this transition. In earlier work [17] it had been assigned to a completely different transition $5s4f\ ^1F_3 \rightarrow 5s5g\ ^1G_4$. Both the $5s^2\ ^1S$ and $5s5p\ ^1P_1$ levels in Zr III [10] and the $5s^2\ ^1S$ level in Nb IV [18] had their positions significantly changed. Because of these circumstances, we looked over our RCI results to see if there were any other strong transitions ($f > 0.4$) with an similar energy difference ($74\ 882\ \text{cm}^{-1}$, using the RCI $5s^2$ result and an experimental position for $5s5p\ ^1P_1$ [3]). Two other transitions were found: each involves a transition from $4d5d$ to $4p^5\ 4d^3$ at $75\ 264$ and $75\ 303\ \text{cm}^{-1}$ with $f = .431$ and $.758$ respectively.

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Table I. *Mo V J = 0 Energy Levels(in cm⁻¹)*

Label	RCI	Expt ^a		
4d ² ³ P	0	0	0	
4d ² ¹ S	26202	26577	26782	T
5s ² ¹ S	185556		180997	
4d5d ³ P	230900	231001	230999	
4d5d ¹ S	239669	239932	241168	
5p ² ³ P	301282		279503	
4d6d ³ P	307622		307832	
4d6d ¹ S	309864		313357	
5p ² ¹ S	330445		307246	

^a The first number, when present, is from ref. [3]. The second number is from ref. [2], unless marked with a T. In that case, it is from M. W. Trawick, Phys. Rev. A **48**, 223 (1935)

Table II. *Mo V J = 1 Energy Levels and Landé g-values*

Label	RCI	Expt		Landé <i>g</i>
		(b)	(c)	
4d5p ³ D	0	0	0	.536
4d5p ³ P	7646	7668	7667	1.415
4d5p ¹ P	13457	13308	13308	1.048
5s5p ³ P	97499	97851	95787	1.421
4d4f ³ D	99380	98984	97851	.603
4d4f ³ P	103810	103700	99796	1.475
4d4f ¹ P	107311	106992	108663	.999
5s5p ¹ P	125921	124250	127524	.971
4d6p ³ D	128164	128240	125735	.549
4d6p ³ P	131538	131557	130866	1.460
4d6p ¹ P	137065	136670	136676	1.022
4p ⁵ 4d ³ R1	133101			1.342
4p ⁵ 4d ³ R2	140721			.230
4p ⁵ 4d ³ R3	153004			1.113
4p ⁵ 4d ³ R4	157353			.862
4p ⁵ 4d ³ R5	164756			1.547
4p ⁵ 4d ³ R6	165760			.703
4p ⁵ 4d ³ R7	171411			1.682
4p ⁵ 4d ³ R8	173066			1.413
4p ⁵ 4d ³ R9	175230			.793
4p ⁵ 4d ³ R10	178401			1.370
4p ⁵ 4d ³ R11	180042			1.496
4p ⁵ 4d ³ R12	182582			1.594
4p ⁵ 4d ³ R13	186962			1.020
4p ⁵ 4d ³ R14	187753			.821
4p ⁵ 4d ³ R15	191796			1.452
4d7p ¹ P+ ³ P	193189			.555
4d7p ³ D+ ³ P	194760			1.386
4d7p ¹ P+ ³ P	198100			1.084
4p ⁵ 4d ³ R16	222261			.551

^a This work. Includes the magnetic part of the Breit operator.

^b Ref. [3]

^c Ref. [2]

Table III. *Mo V J = 1 4p⁵ 4d³ LS Composition*

Root #	¹ P	³ S	³ P	³ D	⁵ P	⁵ D	⁵ F
1	0.000	0.000	0.005	0.005	0.001	0.886	0.102
2	0.003	0.000	0.004	0.148	0.000	0.097	0.748
3	0.001	0.039	0.616	0.279	0.000	0.000	0.065
4	0.081	0.021	0.333	0.475	0.000	0.015	0.075
5	0.011	0.059	0.606	0.049	0.120	0.150	0.004
6	0.058	0.027	0.021	0.713	0.030	0.148	0.004
7	0.044	0.138	0.139	0.040	0.406	0.230	0.003
8	0.137	0.237	0.010	0.169	0.116	0.328	0.004
9	0.260	0.036	0.065	0.606	0.006	0.008	0.018
10	0.064	0.039	0.206	0.255	0.331	0.104	0.000
11	0.035	0.161	0.300	0.159	0.207	0.138	0.000
12	0.016	0.230	0.266	0.145	0.169	0.174	0.000
13	0.451	0.026	0.234	0.250	0.000	0.037	0.002
14	0.018	0.000	0.337	0.632	0.009	0.003	0.000
15	0.141	0.217	0.490	0.091	0.056	0.006	0.000
16	0.020	0.001	0.034	0.944	0.001	0.000	0.000
Pure <i>g</i>	1.000	2.000	1.500	0.500	2.500	1.500	0.000

Table IV. $Mo V 4d^2 + 5s^2 + 4d(5d + 6d) + 5p^2 J = 0 \rightarrow 4d(5p + 6p + 4f) + 5s5p + 4p^54d^3$
 $J = 1 f$ -values^a

Transition	Vel	Len	Avg	Spread
$4d^2 \ ^3P \rightarrow 4d5p \ ^3D$.094	.093	.093	0.5%
$4d^2 \ ^3P \rightarrow 4d5p \ ^3P$.163	.161	.162	0.4%
$4d^2 \ ^3P \rightarrow 4d5p \ ^1P$.024	.023	.023	0.5%
$4d^2 \ ^3P \rightarrow 5s5p \ ^3P$.117	.123	.120	2.7%
$4d^2 \ ^3P \rightarrow 4d4f \ ^3D$.564	.590	.577	2.3%
$4d^2 \ ^3P \rightarrow 4d4f \ ^3P$.107	.111	.109	1.7%
$4d^2 \ ^3P \rightarrow 4d6p \ ^3D$.010	.010	.010	2.5%
$4d^2 \ ^3P \rightarrow 4d6p \ ^3P$.022	.023	.022	1.9%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R3$.050	.051	.051	0.7%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R9$.045	.049	.047	4.1%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R10$.083	.089	.086	3.6%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R11$.020	.020	.020	0.6%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R12$.019	.021	.020	5.2%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R13$.114	.119	.117	2.1%
$4d^2 \ ^3P \rightarrow 4p^54d^3 \ R16$.184	.199	.191	4.1%
$4d^2 \ ^1S \rightarrow 4d5p \ ^3P$.013	.013	.013	1.9%
$4d^2 \ ^1S \rightarrow 4d5p \ ^1P$.218	.211	.214	1.7%
$4d^2 \ ^1S \rightarrow 4d4f \ ^1P$.812	.843	.827	1.9%
$4d^2 \ ^1S \rightarrow 5s5p \ ^1P$.032	.034	.033	1.6%
$4d^2 \ ^1S \rightarrow 4d6p \ ^1P$.098	.102	.100	1.6%
$4d^2 \ ^1S \rightarrow 4p^54d^3 \ R8$.070	.074	.072	2.9%
$4d^2 \ ^1S \rightarrow 4p^54d^3 \ R14$.066	.071	.068	3.8%
$4d^2 \ ^1S \rightarrow 4d7p \ ^3P$.025	.026	.025	3.3%
$4d^2 \ ^1S \rightarrow 4d7p \ ^1P$.023	.027	.025	9.3%
$4d^2 \ ^1S \rightarrow 4p^54d^3 \ R16$.045	.050	.048	4.6%
$5s^2 \ ^1S \rightarrow 4d5p \ ^1P$	-.022	-.022	-.022	1.0%
$5s^2 \ ^1S \rightarrow 5s5p \ ^3P$.010	.010	.010	2.9%
$5s^2 \ ^1S \rightarrow 4d4f \ ^1P$.294	.294	.294	0.0%
$5s^2 \ ^1S \rightarrow 5s5p \ ^1P$	1.06	1.08	1.07	0.6%
$5s^2 \ ^1S \rightarrow 4d6p \ ^3D$.112	.118	.115	2.4%
$5s^2 \ ^1S \rightarrow 4d6p \ ^3P$.070	.073	.071	2.0%
$5s^2 \ ^1S \rightarrow 4d6p \ ^1P$.314	.322	.318	1.4%
$5s^2 \ ^1S \rightarrow 4p^54d^3 \ R8$.028	.031	.030	4.6%
$4d5d \ ^3P \rightarrow 4d5p \ ^3D$	-.207	-.209	-.208	0.5%
$4d5d \ ^3P \rightarrow 4d5p \ ^3P$	-.368	-.372	-.370	0.5%

Table IV. *Continued*

Transition	Vel	Len	Avg	Spread
4d5d ³ P → 4d5p ¹ P	-.026	-.027	-.027	1.6%
4d5d ³ P → 4d4f ³ P	.026	.019	.022	15.%
4d5d ³ P → 5s5p ¹ P	.037	.033	.035	5.7%
4d5d ³ P → 4d6p ³ D	.051	.049	.050	2.0%
4d5d ³ P → 4d6p ³ P	.202	.198	.200	0.9%
4d5d ³ P → 4d6p ¹ P	.010	.011	.010	2.5%
4d5d ³ P → 4p ⁵ 4d ³ R3	.159	.173	.166	4.4%
4d5d ³ P → 4p ⁵ 4d ³ R4	.093	.095	.094	1.2%
4d5d ³ P → 4p ⁵ 4d ³ R5	.392	.421	.406	3.6%
4d5d ³ P → 4p ⁵ 4d ³ R7	.038	.038	.038	0.3%
4d5d ³ P → 4p ⁵ 4d ³ R9	.030	.030	.030	0.7%
4d5d ³ P → 4p ⁵ 4d ³ R10	.080	.080	.080	0.0%
4d5d ³ P → 4p ⁵ 4d ³ R11	.012	.011	.012	2.8%
4d5d ³ P → 4p ⁵ 4d ³ R13	.023	.022	.022	3.7%
4d5d ¹ S → 4d5p ³ P	-.013	-.013	-.013	1.2%
4d5d ¹ S → 4d5p ¹ P	-.512	-.509	-.510	0.4%
4d5d ¹ S → 5s5p ¹ P	.202	.180	.191	5.7%
4d5d ¹ S → 4d6p ³ D	.013	.014	.014	3.7%
4d5d ¹ S → 4d6p ¹ P	.108	.086	.097	11.%
4d5d ¹ S → 4p ⁵ 4d ³ R6	.014	.015	.014	2.5%
4d5d ¹ S → 4p ⁵ 4d ³ R8	.731	.758	.744	1.8%
4d5d ¹ S → 4p ⁵ 4d ³ R9	.015	.016	.015	1.6%
4d5d ¹ S → 4p ⁵ 4d ³ R10	.045	.046	.045	1.6%
4d5d ¹ S → 4p ⁵ 4d ³ R11	.012	.013	.013	1.3%
4d5d ¹ S → 4p ⁵ 4d ³ R14	.024	.024	.024	0.1%
4d5d ¹ S → 4d7p ¹ P	.026	.028	.027	5.3%
5p ² ³ P → 4d5p ³ D	-.313	-.337	-.325	3.6%
5p ² ³ P → 4d5p ³ P	-.034	-.040	-.037	8.5%
5p ² ³ P → 5s5p ³ P	-.346	-.354	-.350	1.1%
5p ² ³ P → 4d4f ³ D	-.065	-.059	-.062	5.0%
5p ² ³ P → 4d4f ³ P	-.117	-.110	-.114	3.0%
5p ² ³ P → 5s5p ¹ P	-.050	-.061	-.055	10.%
5p ² ³ P → 4d6p ³ D	-.018	-.021	-.019	7.8%
5p ² ³ P → 4d6p ³ P	-.080	-.095	-.087	8.9%
4d6d ³ P → 4d5p ³ D	-.164	-.162	-.163	0.7%
4d6d ³ P → 4d5p ³ P	-.044	-.041	-.042	3.4%

Table IV. *Continued*

Transition	Vel	Len	Avg	Spread
4d6d ³ P → 4d5p ¹ P	-.009	-.010	-.009	7.3%
4d6d ³ P → 5s5p ³ P	-.146	-.134	-.140	4.2%
4d6d ³ P → 5s5p ¹ P	-.102	-.115	-.108	6.0%
4d6d ³ P → 4d6p ³ D	-.124	-.129	-.127	1.9%
4d6d ³ P → 4d6p ³ P	-.453	-.445	-.449	0.9%
4d6d ³ P → 4p ⁵ 4d ³ R3	-.044	-.045	-.044	0.5%
4d6d ¹ S → 5s5p ¹ P	-.329	-.374	-.352	6.4%
4d6d ¹ S → 4d6p ³ D	-.051	-.054	-.053	3.1%
4d6d ¹ S → 4d6p ³ P	-.036	-.038	-.037	3.5%
4d6d ¹ S → 4d6p ¹ P	-.368	-.358	-.363	1.4%
5p ² ¹ S → 4d5p ³ P	-.032	-.031	-.032	1.2%
5p ² ¹ S → 4d5p ¹ P	-.443	-.447	-.445	0.4%
5p ² ¹ S → 4d4f ¹ P	-.127	-.143	-.135	6.1%
5p ² ¹ S → 5s5p ¹ P	-.241	-.268	-.254	5.2%
5p ² ¹ S → 4d6p ³ D	-.032	-.032	-.032	0.8%
5p ² ¹ S → 4d6p ³ P	-.027	-.025	-.026	4.1%
5p ² ¹ S → 4d6p ¹ P	-.287	-.240	-.263	9.0%

^a Only f -values $> .01$ are listed. Experimental Energies are used when available, otherwise we use RCI energies. The length value is preferred. A negative sign means the $J = 0$ state(i) is higher in energy than the $J = 1$ state(k). To convert the emission f -value to its absorption form, use

$$f_{k,i} = -\frac{1}{3}f_{i,k}$$

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