

# *Ab Initio* Electric Dipole $f$ Values for Fe II (3d+4s)<sup>7</sup> $J=9/2 \rightarrow (3d+4s)^6 4p J=11/2$ Transitions

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**Abstract.** Relativistic Configuration Interaction  $f$  values have been obtained for all transitions between the energetically lowest 17  $J=9/2$  and the lowest 27  $J=11/2$  (odd) levels. Thirty-five of these  $f$  values exceed .01 and are published here. The  $3d^5(^4G)4s4p z ^6G$  ( $z ^6H$ ) levels have been located for the first time. Many of the odd levels are so nearly degenerate that the introduction of small semiempirical corrections are necessary. Landé  $g$ -values are calculated for all levels and a systematic way of estimating radial convergence is introduced.

## 1. Introduction

Fe II is one of the most astrophysically important of the transition metal ions, yet is so complex that few *ab initio* calculations have been done for it, and only a few experimental  $f$  values, determined from lifetime combined with branching ratios are available. Recent reviews involving Fe II include that of Johansson *et al* [1], that of Hibbert and Correge [2] and NIST's critical compilation co-authored by Fuhr and Wiese which is now in press [3]. An up-to-date listing Fe II energy levels as well as references to existing work can be found in the NIST data base [4].

In this work, we apply the relativistic configuration interaction (RCI) methodology to the low lying  $9/2 \rightarrow 11/2$  (odd) transitions in Fe II. Since this work is an extension of our recent work [5] on the  $9/2 \rightarrow 9/2$  (odd) transitions, we will only provide here details essential for the understanding for the results reported here. The treatment of any of the transition metal ions requires the simultaneous inclusion of both relativistic and correlation effects. Simply stated, relativistic effects for 3d and 4s electrons differ by  $\sim 0.1$  eV [6], and this amount of energy is of at least moderate size as compared to the near degeneracies observed in these species. Secondly, for these complicated open d-subshell ions, *ab initio* treatments of electron correlation optimistically can probably do no better than  $\sim 200$  cm<sup>-1</sup> for energy differences, thus requiring some sort of "extra" correction for very closely spaced levels. Failure to accurately account for energy differences between closely spaced levels can mean that basis functions are not properly mixed into computed wavefunctions, which can lead to erroneous predictions for other properties such as  $f$  values. This accuracy limit will be decreased in the

future, of course, as it has been in the recent past. We believe that most improvement in the near future will come through systematically improving radial convergence, and computational efficiencies, which would allow larger basis sets to be used.

The  $J=9/2$  (even) wavefunction is nearly the same as what was previously [5] used. The main change is to generate 6 more levels, associated with the  $3d^5 4s^2$ ,  $3d^6 5s$  and  $3d^6 4d$  manifolds, and make modest improvements in the radial set (e.g. a  $5s$  from  $3d^6 5s$  was added to improve the  $f$  values). Consequently, we will limit most of our remarks to generation of the  $J=11/2$  (odd) wavefunctions.

For  $J=11/2$  (odd) we began by calculating numerical radial functions for the lowest ( $z^6F$ )  $3d^6 4p$  root. This procedure does not produce a “reasonable”  $4p_{1/2}$  radial because for the  $z^6F$  state, the  $3d^6$  electrons are almost 100% coupled to a  $^5D$ . This requires a  $4p_{3/2}$  function to “reach” the requested  $J=11/2$ . Numerically, we observed that all  $3d^6 4p_{1/2}$  basis functions have small coefficients which lead to an “unreasonable”  $4p_{1/2}$  (both the  $\langle r \rangle$  and the one electron energy eigenvalue differs considerably from those of  $4p_{3/2}$ ). A solution is to generate the  $4p_{1/2}$  from a higher  $3d^6 4p$  root. A numerical  $4s$  was generated from the energetically lowest root of  $3d^5 4s 4p$  ( $z^6F$ ). Radial variations among the levels are accounted for at the RCI stage, which also generates  $f$  radials needed to represent the two  $3d^6 4f$  levels included.

## 2. Methodology

The Hamiltonian used to generate the radial functions is the Dirac-Coulomb one with a uniform charge distribution nuclear model. Magnetic Breit effects are inserted in the later stages of the RCI calculations.

In RCI, the wavefunctions are eigenstates of  $J^2$ ,  $J_z$ , and parity, and are separated into reference and correlation parts. Usually, the reference part consists of the single non-relativistic manifold that dominates the levels of interest. A manifold consists of all relativistic configuration reducing to the same non-relativistic configuration in the  $c \rightarrow \infty$  limit. The first important decision to be made is how many energy levels are desired for each  $J$ , parity as this determines the reference space. All reference basis functions are determined numerically by solving the Dirac-Fock-Coulomb equations using Desclaux’s algorithm [7]. The  $jj$  eigenstates are then transformed into eigenstates of  $L^2$  and  $S^2$  [5] to facilitate analysis and to allow us to shift the diagonal matrix elements only (“fine tuning” of energy differences). Each reference function is “equivalently” correlated, i.e. has the same single and pair excitations (e.g.  $3d^2 \rightarrow vf^2$ ) generated from it.

To introduce correlation, we apply perturbation theory to suggest what additional manifolds are needed in the wavefunction. We find that single and double excitations from the outer subshells ( $3s$ ,  $3p$ ,  $3d$ ,  $4s$ ,  $4p$ ) suffice [5]. The additional radial functions needed, called virtuals ( $vl$ ), are represented by relativistic screened hydrogenic (RSH) functions, with a single parameter,  $Z^*$ , the effective charge. These virtuals represent the compact portion of an entire Rydberg and continuum series, and  $\sim 2$  per symmetry ( $\kappa$ ) are sufficient to capture  $\sim 90\%$  of the correlation energy. A method of estimating

the degree of radial convergence is discussed below.

Estimates for each  $Z^*$ , which are fine tuned during the RCI diagonalization, are made by matching the RSH  $\langle r \rangle$  to that of the numerical radial it is replacing. Virtual orbital symmetries higher than  $l=5$  contribute  $< 100\text{cm}^{-1}$  to energy differences and are not included [5].

Radial convergence can be determined by the use of a very large number of radial functions with a numerical solution of the Dirac-Fock equations [8], but this can be very time consuming, especially for the complicated open d-subshell species, where tens of thousands of N-electron basis functions may be needed. An alternative we have used in the past is to split the calculation into a series of smaller ones involving the reference space and one correlation manifold (e.g.  $3d^2 \rightarrow vf^2$ ) to develop the radial sets [9]. But the question of radial convergence exists for each of these smaller calculations too.

Past non-relativistic work on light atoms has shown [10] that the total “dynamical” (i.e. having 2 virtuals) pair correlation energy can be expressed as a sum of products of group theoretical factors ( $\beta$ s) and radial pair energies ( $\epsilon$ s). For low  $Z$  atoms, it was found that the radial pair energies were fairly invariant to  $Z$  and ionization stages [10]. An explicit formula has been given [11] for the  $\beta$ s and a computer program to evaluate them was written some time ago [12].

Assuming radial transferability, its value lies in the possibility of doing the calculation on a simpler (but nearby) species, such as one possessing just (or nearly so) closed subshells for which reaching satisfactory radial convergence may be much easier. These radial pair energies ( $\epsilon$ s) are then used with the angular factors ( $\beta$ s) of the original species to provide estimates of convergence limits for the RCI basis sets being developed.

This has proven effective both for transition metals and lanthanides, even though these species involve significant relativistic effects. It should be noted that the method permits the angular coupling to change due to the presence of relativistic effects. The key assumption is that the radial basis convergence properties are little affected by relativity.

In our previous work [5], for the Fe III  $J=4$  levels, the average energy error between adjacent energy levels was  $452\text{ cm}^{-1}$  (or 12.2%). By using the Jankowski *et al* [13] results for Zn III (closed subshells), we were able to extract partial wave contributions to the  $3d^2$  radial pair energies ( $\epsilon$ s). These were then combined with the proper angular factors for Fe III to produce estimated limits which we compared with our RCI results [5]. Removal of deficiencies in  $3d^2 \rightarrow vpvf+vdvg+vgvi$  correlation were the most important improvements made. The net result was to reduce the average adjacent error in the Fe III  $J=4$  levels to  $159\text{ cm}^{-1}$  (9.4%).

Sometimes it is not possible to include enough correlation to adequately position the levels, and the prediction of properties is insufficiently accurate. A crude, by reasonably effective way to improve the situation is to shift the energy of a few of the basis functions, i.e. the diagonal matrix element is shifted by a bit more than the desired change. For  $J=11/2$  the  $3d^5 4s 4p$ ,  $3d^6 (5p+4f)$  basis functions are insufficiently correlated relative

to  $3d^6 4p$  so they have been shifted (each) as a unit so their lowest term agrees well with the observed levels [4]. The missing correlation is mainly associated with absent core-valence correlation effects. Here, the shift could have been determined computationally, i.e. in the absence of observed spectra, by doing separate RCI calculations with, for example, just  $3d^5 4s 4p$  as a reference. The remaining shifts of  $\sim 200-300 \text{ cm}^{-1}$  are within  $3d^6 4p$  to adjust positions of nearby degenerate levels arising from  $3d^6$  ( $^3F$ ,  $^1G$  and  $^1I$ ). The commonality of the  $3d^6$  coupling suggests possible radial incompleteness for  $3d^2$  pairs for  $^3F$ ,  $^1G$  and  $^1I$  couplings.

Two efficiency improvements have been made: (1) the REDUCE procedure by which the number of basis functions is dramatically lowered [5] has been speeded up by about 3x by using bit-packed determinants (this allows speedier comparisons of determinants), (2) 2 AMD 2.4GHz PCs have replaced our 500 MHz Alpha workstation, for an improvement of 6x.

### 3. Results

#### 3.1. Fe II $J=11/2$ (odd) Energy Levels

The results for energy differences and Landé  $g$  values for the lowest 27  $J=11/2$  Fe II levels are given in Table 1. The average error between the adjacent energy levels is  $100 \text{ cm}^{-1}$  (14%). This could have been reduced by narrowing the  $5p z ^6F$  and  $3d^6(^3F)4p ^4G$  energy difference, thus changing the mixing of the basis functions of the same “name”, but there are no  $f$  values  $> .01$  involving either level, so this was not done.

Two new levels  $3d^5(^4G) 4s 4p z ^6G$  and  $z ^6H$  are predicted to lie at 85271 and 86874  $\text{cm}^{-1}$  respectively (all levels in the table are relative to  $3d^6 4p z ^6F$  at 41968  $\text{cm}^{-1}$ ). As explained in the Table, the predictions are made by subtracting the error for the  $y ^6F$  from the RCI  $z ^6G$  and  $z ^6H$  values.

The labelling of the levels is the author’s. It is based on two “non-traditional” aspects: (1) The LS percentage is determined from the re-normalized reference portion of the wavefunction. This avoids the potentially messy computation of producing LS eigenstates for the correlation basis functions. This will tend to increase my basis function weights over more conventional ones, (2) no “fractional parentage” is used, because the author feels use of such does not lead to a “purer” basis. So, weights for basis functions with the same LS designations are simply summed together. If published [4] weights don’t include all basis functions with the same LS, then my weights will tend to also be the larger ones. Finally, it may be observed weights of specific manifolds are not good quantum numbers, and may vary from one work to the next depending on how the calculations are done [completeness, (non-)inclusion of magnetic Breit effects, etc].

All this said, the labels of Table 1 are in good agreement with published [4] results for the  $3d^6 4p$  levels, with the exception of the state at 73604  $\text{cm}^{-1}$  which is nearly an equal mixture of  $3d^6(^1G)$  and  $3d^6(^1I)$ . Although the ( $^1I$ ) percentage is slightly smaller, we have chosen to label this level with that, to distinguish it from the level at 72262

cm<sup>-1</sup>. Our choice agrees with the published label [4], which however is missing one of the two <sup>1</sup>G's, so we can't be sure just how large that percentage is. We also provide labels for the lowest lying 3d<sup>5</sup> 4s 4p and 3d<sup>6</sup> 4f levels which are not included in the published table [4].

For the weight values, there is less agreement, particularly for the levels at 60888, 61587, 65364, and 65580 cm<sup>-1</sup> in addition to the two levels above. There is an apparent difference for the 63876 level, although there is not certain, as the weight of one of the two (<sup>3</sup>F)<sup>4</sup>G is missing [4]. All these levels exhibit substantial basis function mixing which may have an impact on their  $f$  values (discussed below). Finally, we provide Landé  $g$ -values for the 27 levels. Agreement with the few available experimental values [4] is good.

### 3.2. $f$ values

Our  $f$  values are computed in the length and velocity gauges, and include the effects of non-orthogonality between the wavefunctions [5]. Frequently a few manifolds need to be added to the basis sets before computation. These are predicted by applying the First Order Theory of Oscillator Strengths (FOTOS [14]) and mainly serve to improve the velocity gauge result. In FOTOS, one formally applies the dipole operator (e.g.  $\vec{r}$ ) to the main configurations in one of the two wavefunctions to predict what should appear in the other. In the current instance "exciting" a 3p electron to a 3d electron by means of the dipole operator should appear. Thus, from the 3p<sup>6</sup> 3d<sup>6</sup> 4s manifold we would produce 3p<sup>5</sup> 3d<sup>7</sup> 4s in the other state. These effects are not always initially included in the RCI wavefunction because their relative energy contribution may be limited.

In order to improve the predictability of what FOTOS manifolds may be important for  $f$  values, a standalone algorithm which evaluates the radial dipole length integral has been written for this work. Evaluation of the integrals  $\langle ns|\vec{r}|mp\rangle$  and  $\langle np|\vec{r}|md\rangle$  shows that in addition to the important  $n = m$  case (above), only the  $\langle 5s|\vec{r}|4p\rangle$  integral is relatively important (as compared to  $\langle 4s|\vec{r}|4p\rangle$ ) and that is why 3d<sup>6</sup> 5s is added [5] to the  $J=9/2$  basis set. The impact of 3d<sup>6</sup> 5s is also dependent on its coefficient in the RCI wavefunction. For the a <sup>6</sup>D<sub>9/2</sub>  $\rightarrow$  z <sup>6</sup>F<sup>o</sup><sub>11/2</sub> transition, it changed both the velocity and length gauge result by .01, improving their agreement.

Our  $f$  value results are given in Table 2, along with the semiempirical values of Kurucz [15] and Raassen [16] as well as a few experimental results [17-20] which are quoted in the new NIST compilation [3]. All 35  $f$  values  $> 0.01$ , out of the 459 computed ones, are displayed in the table. The average gauge spread is 3.6% and all  $f$  values are computed using the observed energies [4]. Overall, the RCI results are in best agreement with the Raassen [16] values, although for a few individual  $f$  values they may be closer to Kurucz [15] or experiment [3]. It is perhaps interesting to note that the theoretical  $f$  values for the resonance transition a <sup>6</sup>D<sub>9/2</sub>  $\rightarrow$  z <sup>6</sup>F<sup>o</sup><sub>11/2</sub> exceed the composite experimental  $f$  value [3].

Frequently, the sum of  $f$  values from one level to a group of closely spaced levels may

be nearly conserved for similar calculations, as been shown formally [21]. A corollary is that if a basis function that makes a significant contribution to the sum is missing, the sum will be too small. This assumes the missing function does not make a significant contribution to an  $f$  value not included in the sum.

Here, this near conservation of the sum is exhibited for three groups of transitions:  $c\ ^2G \rightarrow x\ ^2H + w\ ^2H$ ,  $a\ ^4H \rightarrow z\ ^4H + z\ ^4I$  and  $a\ ^4G \rightarrow z\ ^4H + z\ ^4I$ . There is enough LS percentage detail available (Table 1 and [3]) to see what is happening for the  $z\ ^4H$  and  $z\ ^4I$  levels – the distribution of the  $(^3H)^4H$  and  $(^3H)^4I$  basis functions over the two levels differs, but their sum is nearly constant.

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*Ab Initio Electric Dipole f Values for Fe II (3d+4s)<sup>7</sup> J=9/2→(3d+4s)<sup>6</sup> 4p J=11/2 Transitions*

**Table 1.** Fe II (3d+4s)<sup>6</sup> 4p J=11/2 Energy levels (in cm<sup>-1</sup>) referenced to z <sup>6</sup>F (at 41968 cm<sup>-1</sup>)

Label	Energy(cm <sup>-1</sup> )		Adj. dE <sup>a</sup>		Landé g		Add. Label <sup>c</sup>
	Expt <sup>b</sup>	RCI	Expt	RCI	RCI	Expt	
3d <sup>6</sup> ( <sup>5</sup> D)4p z <sup>6</sup> F	0	0			1.453		100%
3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> G	18657	19668			1.269	1.24	70%; 25% ( <sup>3</sup> F) <sup>4</sup> G
3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> H	18920	20007	263	332	1.088		62%; 27% ( <sup>3</sup> H) <sup>4</sup> I; 8% ( <sup>3</sup> G) <sup>4</sup> H
3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> I	19619	20731	699	724	1.012		69%; 26% ( <sup>3</sup> H) <sup>4</sup> H
3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> I	20694	21868	1075	1137	.930	.910	93%
3d <sup>6</sup> ( <sup>3</sup> F)4p y <sup>4</sup> G	21908	22904	1214	1036	1.266	1.24	70%; 26% ( <sup>3</sup> H) <sup>4</sup> G
3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> H	23396	24425	1488	1521	1.120	1.07	55%; 20% ( <sup>3</sup> G) <sup>4</sup> G; 15% ( <sup>3</sup> G) <sup>2</sup> H
3d <sup>6</sup> ( <sup>3</sup> G)4p x <sup>4</sup> G	23612	24617	216	192	1.225		71%; 12% ( <sup>3</sup> G) <sup>2</sup> H; 8% ( <sup>3</sup> H) <sup>2</sup> H
3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>4</sup> H	24496	25576	884	959	1.131	1.13	79%; 7% ( <sup>3</sup> H) <sup>2</sup> H; 6%( <sup>3</sup> H) <sup>4</sup> H
3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>2</sup> H	25548	26595	1052	1019	1.097	1.07	59%; 25% ( <sup>3</sup> H) <sup>2</sup> H; 10% ( <sup>3</sup> G) <sup>4</sup> H
3d <sup>6</sup> ( <sup>1</sup> G)4p x <sup>2</sup> H	30293	31392	4745	4787	1.090	1.08	51%; 41% ( <sup>1</sup> I) <sup>2</sup> H; 5% ( <sup>3</sup> G) <sup>2</sup> H
3d <sup>6</sup> ( <sup>1</sup> I)4p w <sup>2</sup> H	31636	32718	1343	1336	1.082		41%; 47% ( <sup>1</sup> G) <sup>2</sup> H; 5% ( <sup>1</sup> I) <sup>2</sup> I
3d <sup>6</sup> ( <sup>1</sup> I)4p y <sup>2</sup> I	32001	33131	365	413	0.933		94%; 5% ( <sup>1</sup> I) <sup>2</sup> H
3d <sup>5</sup> ( <sup>4</sup> G)4s4p z <sup>6</sup> G	43333	44378	d		1.338		94%
3d <sup>5</sup> ( <sup>4</sup> G)4s4p z <sup>6</sup> H	44906	45951	d		1.209		96%
3d <sup>5</sup> ( <sup>4</sup> G)4s4p y <sup>6</sup> F	45372	46417			1.452		92%
3d <sup>6</sup> ( <sup>5</sup> D)5p x <sup>6</sup> F	47956	49401	2584	2984	1.454		89%
3d <sup>6</sup> ( <sup>3</sup> F)4p <sup>4</sup> G	48247	49966	291	565	1.272		99%
3d <sup>5</sup> ( <sup>4</sup> G)4s4p x <sup>4</sup> H	50199	51923	1957	1951	1.137		96%
3d <sup>5</sup> ( <sup>4</sup> D)4s4p <sup>6</sup> F	50464	52235	265	312	1.451		92%; 5% ( <sup>4</sup> G) <sup>6</sup> F
3d <sup>5</sup> ( <sup>4</sup> G)4s4p w <sup>4</sup> G	52222	53782	1758	1547	1.270		97%
3d <sup>5</sup> ( <sup>4</sup> G)4s4p v <sup>2</sup> H	54094	55969	1812	2187	1.092		98%
3d <sup>6</sup> ( <sup>1</sup> G)4p <sup>2</sup> H	56311	58389	2217	2420	1.091		99%
3d <sup>5</sup> ( <sup>2</sup> I)4s4p <sup>4</sup> K	60372	62436	4061	4047	0.826		71%; 27% ( <sup>2</sup> I) <sup>4</sup> I
3d <sup>6</sup> ( <sup>5</sup> D) 4f <sup>6</sup> G	60863	62882	491	446	1.380		53%; 39% ( <sup>5</sup> D) <sup>6</sup> F
3d <sup>6</sup> ( <sup>5</sup> D) 4f <sup>4</sup> G	60925	62947	62	65	1.262		75%; 13% ( <sup>5</sup> D) <sup>4</sup> H
3d <sup>5</sup> ( <sup>2</sup> I)4s4p <sup>4</sup> I	61012	63007	87	60	0.913		68%; 28% ( <sup>2</sup> I) <sup>4</sup> K

<sup>a</sup> E<sub>n</sub>−E<sub>n−1</sub> for nth level

<sup>b</sup> From [4]

<sup>c</sup> the 1st number gives the percent weight of the lead term; the 2nd (3rd) gives the percent weight and label

<sup>d</sup> the “experimental” value is computed by subtracting 1045 (determined from RCI−Expt for 4s4p y <sup>6</sup>F) from the RCI value

**Table 2.** Fe II  $(3d+4s)^7 J=9/2 \rightarrow (3d+4s)^6 4p J=11/2$  RCI  $f$ -values (using experimental [4] dE; only values greater than 0.01 shown). The “spread” is defined by  $|f_l - f_v|/f_{avg} \times 50$ .

Transition	RCI			Kurucz <sup>a</sup>	Raassen <sup>b</sup>	Expt
	Vel	Len	Spread			
3d <sup>6</sup> 4s a <sup>6</sup> D $\rightarrow$ 3d <sup>6</sup> ( <sup>5</sup> D)4p z <sup>6</sup> F	.327	.352	3.6%	.359	.344	.320 <sup>c,d</sup>
$\rightarrow$ 3d <sup>5</sup> ( <sup>4</sup> G)4s4p z <sup>6</sup> F	.105	.091	7.1%	.148	.109	.083 <sup>e</sup>
$\rightarrow$ 3d <sup>5</sup> ( <sup>4</sup> D)4s4p <sup>6</sup> F	.011	.010	5.1%	.022	.013	
3d <sup>7</sup> a <sup>4</sup> F $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> G	.055	.054	1.2%	.089	.053	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> F)4p y <sup>4</sup> G	.027	.026	1.6%	.048	.031	
$\rightarrow$ 3d <sup>6</sup> ( <sup>5</sup> D)4f <sup>4</sup> H	.021	.025	8.8%		.017	
3d <sup>7</sup> a <sup>2</sup> G $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> H	.021	.020	3.4%	.026	.019	
$\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> G)4p x <sup>2</sup> H	.036	.036	1.1%	.061	.037	
3d <sup>7</sup> a <sup>2</sup> H $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> I	.023	.023	0.5%	.031	.017	.021 <sup>f</sup>
$\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> I)4p y <sup>2</sup> I	.033	.032	1.8%	.052	.029	
3d <sup>6</sup> 4s a <sup>4</sup> H $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> H	.038	.040	2.4%	.049	.078	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> I	.272	.289	3.1%	.233	.239	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> I	.013	.013	2.2%	.013	.015	.014 <sup>f</sup>
$\rightarrow$ 3d <sup>5</sup> ( <sup>2</sup> I)4s4p <sup>4</sup> I	.034	.029	7.9%		.037	
3d <sup>6</sup> 4s b <sup>4</sup> F $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> G	.080	.082	1.6%		.082	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> F)4p y <sup>4</sup> G	.226	.244	4.0%	.236	.233	
$\rightarrow$ 3d <sup>5</sup> ( <sup>4</sup> G)4s4p w <sup>4</sup> G	.021	.017	9.3%	.025	.019	
3d <sup>6</sup> 4s a <sup>4</sup> G $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> H	.010	.010	0.6%	.0085	.0068	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>4</sup> I	.011	.011	1.5%	.021	.018	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> I	.014	.014	1.3%	.016	.018	.017 <sup>f</sup>
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> H	.011	.011	0.3%	.015	.010	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>4</sup> H	.248	.267	3.7%	.261	.251	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>2</sup> H	.022	.024	4.1%	.020	.022	
3d <sup>6</sup> 4s b <sup>2</sup> H $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> I	.275	.282	1.3%	.284	.265	.258 <sup>f</sup>
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>4</sup> H	.019	.021	3.5%	.023	.026	
3d <sup>6</sup> 4s b <sup>2</sup> G $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> H)4p z <sup>2</sup> H	.049	.051	1.6%	.044	.071	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> G)4p x <sup>4</sup> G	.038	.039	2.0%	.051	.022	
$\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> G)4p y <sup>2</sup> H	.189	.197	2.1%	.203	.183	
$\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> G)4p x <sup>2</sup> H	.019	.021	3.6%	.020	.018	
$\rightarrow$ 3d <sup>5</sup> ( <sup>4</sup> G)4s4p v <sup>2</sup> H	.017	.014	9.2%	.018	.013	
3d <sup>6</sup> 4s c <sup>2</sup> G $\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> G)4p x <sup>2</sup> H	.166	.173	2.3%	.181	.158	
$\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> I)4p w <sup>2</sup> H	.149	.160	3.5%	.154	.161	
3d <sup>6</sup> 4s c <sup>4</sup> F $\rightarrow$ 3d <sup>6</sup> ( <sup>3</sup> F)4p <sup>4</sup> G	.296	.321	4.1%	.314	.301	
$\rightarrow$ 3d <sup>5</sup> ( <sup>4</sup> G)4s4p w <sup>4</sup> G	.018	.014	12.0%	.021	.022	
3d <sup>6</sup> 4s d <sup>2</sup> G $\rightarrow$ 3d <sup>6</sup> ( <sup>1</sup> G)4p <sup>2</sup> H	.296	.321	4.0%	.316	.305	

<sup>a</sup> From [15]   <sup>b</sup> From [16]   <sup>c</sup> From [17]   <sup>d</sup> From [20]   <sup>e</sup> From [18]   <sup>f</sup> From [19]