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Multiconfiguration Dirac–Hartree–Fock energy levels and transition probabilities for $3d^5$ in Fe IV

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ABSTRACT

Multiconfiguration Dirac–Hartree–Fock electric quadrupole (E2) and magnetic dipole (M1) transition probabilities are reported for transitions between levels of $3d^5$ in [Fe IV]. The accuracy of the *ab initio* energy levels and the agreement in the length and velocity forms of the line strength for the E2 transitions are used as indicators of accuracy. The present E2 and M1 transition probabilities are compared with earlier Breit–Pauli results and other theories. An extensive set of transition probabilities with indicators of accuracy are reported in Appendices A and B. Recommended values of $A(\mathrm{E2}) + A(\mathrm{M1})$ are listed in Appendix C.

Key words: atomic data – atomic processes.

1 INTRODUCTION

Iron is one of the main contributors to the mass of refractory dust grains (Sofia, Cardelli & Savage 1994). The determination of its gaseous abundance in ionized nebulae of different characteristics can be used to infer the efficiency of dust destruction and formation processes in widely different environments, ranging from H II regions and their associated molecular clouds to planetary nebulae (PNe), the descendants of asymptotic giant branch stars, which are the main source of dust grains in the solar neighbourhood (Whittet 2003).

In these photoionized nebulae, Fe^{3+} is an important ionization state, being the dominant ion in most H II regions and many PNe. Several [Fe IV] lines are expected to appear in the ultraviolet (UV), optical and infrared spectra of these objects but, unfortunately, the more easily accessible optical lines are very weak and difficult to measure. Hence, the first [Fe IV] line observed in an H II region was the UV [Fe IV] 2836.56 Å line, observed by Rubin et al. (1997) in the Orion Nebula with the *Hubble Space Telescope*. Rubin et al. found that the Fe^{3+} abundance implied by this line was much lower than expected. Subsequent observations of this and some weak optical [Fe IV] lines in a handful of H II regions and PNe confirmed the discrepancy (see Rodríguez & Rubin (2005) and references therein). Since the discrepancy translates into a large uncertainty in the iron abundances calculated for most nebulae, it stresses the need for reliable atomic data for the Fe ions, especially the transition probabilities and electron impact excitation collision strengths that are needed to solve the equations of statistical equilibrium for the lower energy levels of these ions (Osterbrock & Ferland 2006).

Because of the rough scaling of the line intensity with the product of the Fe^{3+} density and the electron density, optical [Fe IV] lines are more easily measured in objects with relatively large densities ($N_e \approx 10^6$ cm^{-3}), like some PNe (Rodríguez, Corradi & Mampaso 2001; Zhang & Liu 2002; Zhang et al. 2005). However, these spectra are so cluttered with lines that line identification and deblending can be a problem. This is another instance where reliable atomic data are needed in order to provide good estimates of the relative line intensities.

The first values of radiative transition rates for [Fe IV] were calculated as early as 1958 by Garstang, who used them to confirm the identification by Thackeray (1954) of several [Fe IV] lines in the spectrum of the symbiotic nova RR Telescopii. Forty years later, Froese Fischer & Rubin (1998), motivated by the observation and analysis of [Fe IV] 2836.56 Å in the Orion Nebula by Rubin et al. (1997), provided improved values for the transition probabilities between the 12 lowest levels of Fe^{3+}, the same levels for which effective collision strengths had just become available (Berrington & Pelan 1995, 1996). However, most of the observed [Fe IV] lines arise from higher energy levels, and new calculations that included these levels were not long in coming: collision strengths from Zhang & Pradhan (1997) and transition probabilities from Froese Fischer & Rubin (2004).

The goal of the first Froese Fischer & Rubin (1998) publication was to predict radiative transition probabilities from $3d^5\ {}^4G$, ${}^4P$ and ${}^4D$ levels to the ${}^6S_{5/2}$ ground state. In the process, transition probabilities were also computed for transitions between the levels of the quartet terms. Four theoretical methods were compared and best estimates identified. The multiconfiguration Dirac–Hartree–Fock

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(MCDHF) with the Breit correction was selected in some cases for M1 transitions but there was a strong indication of an error in the code for some E2 transitions. In the second paper (Froese Fischer & Rubin 2004) the multiconfiguration Hartree–Fock (MCHF) work with Breit–Pauli corrections was extended to include all levels of the 3d^5 configuration. In these later calculations, term energy corrections were used to adjust the position of a term to be in close agreement with the values cited in the Atomic Spectra Database (ASD) (ASD 2008), thereby improving the wavefunction LS term composition. Because there are as many as three terms with the same LS value, as for the ^2D (^2_5D, ^2_3D and ^2_1D where the preceding subscript is the seniority), the adjustments were done in groups in order of energy. Thus the final energies are semi-empirical and only the fine structure splitting provides an indication of accuracy. In a more recent paper, Nahar (2006) reported radiative transition rates for a large number of lines that include electric dipole (E1), quadrupole (E2), octupole (E3) and magnetic dipole (M1) transitions in Fe IV. The calculations included only the one-body relativistic corrections of the Breit–Pauli Hamiltonian. Transition calculations were based on the *ab initio* line strength and ASD transition energies.

Assessing the accuracy of theoretical results in the absence of reliable experimental data is as difficult (if not more difficult) than the transition calculations themselves. One way of establishing accuracy is by validating the results through calculations based on different theories. In this paper we report results for fully *ab initio* MCDHF results where relativistic effects are included in the basic theory and not added as a low-order correction as in the Breit–Pauli calculations by Froese Fischer & Rubin (2004) and Nahar (2006). Computed energy levels and their fine structure splitting can be used as an indicator of the accuracy of the wavefunction along with the agreement in the length and velocity forms of the line strength for E2 transitions. All calculations were performed using the most recent revised and corrected parallel GRASP2K code (Jönsson et al. 2007).

2 COMPUTATIONAL PROCEDURE

In the MCDHF approach (Grant 2007) the wavefunction Ψ for a state labelled γJ, where γ represents the configuration and any other quantum numbers required to specify the state, is approximated by an expansion over *jj*-coupled configuration state functions (CSFs)

$$\Psi(\gamma J) = \sum_j c_j \Phi(\gamma_j J). \tag{1}$$

The CSFs $\Phi(\gamma_j J)$ are antisymmetrized linear combinations of products of relativistic orbitals

$$\phi(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\hat{r}) \\ \mathrm{i}Q_{n\kappa}(r)\chi_{-\kappa m}(\hat{r}) \end{pmatrix}. \tag{2}$$

Here κ is the relativistic angular quantum number, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small component radial wavefunctions and $\chi_{\kappa m}(\hat{r})$ is the spinor spherical harmonic in the *lsj* coupling scheme

$$\chi_{\kappa m}(\hat{r}) = \sum_{m_l, m_s} \left\langle l\, \frac{1}{2} m_l m_s \mid jm \right\rangle Y_{lm_l}(\theta, \varphi)\xi_{m_s}(\sigma). \tag{3}$$

The radial functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are numerically represented on a logarithmic grid and are required to be orthonormal within each κ symmetry,

$$\int_0^\infty [P_{n'\kappa}(r)P_{n\kappa}(r) + Q_{n'\kappa}(r)Q_{n\kappa}(r)]\mathrm{d}r = \delta_{n'n}. \tag{4}$$

In the multiconfiguration self-consistent field (MC-SCF) procedure both the radial functions and the expansion coefficients for the CSFs are optimized to self-consistency.

Once a set of radial orbitals has been obtained, relativistic configuration interaction (RCI) calculations can be performed to include the Breit interaction and quantum electrodynamic (QED) effects. At this stage only the expansion coefficients of the CSFs are determined. This is done by diagonalizing the Hamiltonian matrix.

In the RCI calculations the transverse photon interaction

$$\mathcal{H}_{\mathrm{trans}} = -\sum_{i<j}^{N}\left[\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j \cos(\omega_{ij} r_{ij})}{r_{ij}} + (\boldsymbol{\alpha}_i \cdot \nabla_i)(\boldsymbol{\alpha}_j \cdot \nabla_j)\frac{\cos(\omega_{ij} r_{ij}) - 1}{\omega_{ij}^2 r_{ij}}\right] \tag{5}$$

may be included in the Hamiltonian. The photon frequency ω_{ij} used by the RCI program in calculating the matrix elements of the transverse photon interaction is taken to be the difference in the diagonal Lagrange multipliers ϵ_i and ϵ_j associated with the orbitals. In general, diagonal Lagrange multipliers are approximate electron removal energies only when orbitals are spectroscopic and singly occupied. Thus it is not known how well the code can determine the full transverse photon interaction when correlation orbitals are present and orbitals are multiply occupied as in the present case. What can be obtained instead is the low-frequency limit $\omega_{ij} \to 0$ usually referred to as the Breit interaction.

The transition parameters, such as rate and weighted oscillator strength, for a multipole transition of rank K from γJ to $\gamma' J'$ are all related to the reduced transition matrix element

$$\langle \Psi(\gamma J) \| \mathbf{O}^{(K)} \| \Psi(\gamma' J') \rangle, \tag{6}$$

where $\mathbf{O}^{(K)}$ is the relevant transition operator (Grant 1974). In the present study these are the E2 and M1 transitions between levels of 3d^5 but with transitions to the $3d^5\,{}^6S_{5/2}$ ground state being of greatest interest.

3 MCDHF CALCULATION AND RESULTS

A series of calculations were performed that will be identified by the maximum principal quantum number $n = 3, 4, 5, 6$ of orbitals of the wavefunction. In all cases, the $1s^2 2s^2 2p^6$ core was treated as an inactive core. In our first $n = 3$ calculation the wavefunction expansion included all single and double excitations to the 3d subshell or CSFs obtained from $3s \to 3d$ and $3p^2 \to 3d^2$ excitation. All orbitals were varied in an extended optimal level (OL) calculation for all the 37 lowest levels: four for $J = 1/2$, seven for $J = 3/2$, ten for $J = 5/2$, seven for $J = 7/2$, five for $J = 9/2$, three for $J = 11/2$ and one for $J = 13/2$. This calculation accounts for the near degeneracy effects between CSFs in the $n = 3$ shell.

The $n = 4$ calculation included an additional layer of orbitals, namely $\{4s, 4p, 4d, 4f\}$ orbitals with a wavefunction expansion that, in addition to the $n = 3$ CSFs, included single and double (SD) excitations from $3p^6 3d^5$, but with at most one excitation from $3p^6$ as in a core valence calculation, with $3p^6$ being part of the core and $3d^5$ the valence subshell. The latter included 37 486 CSFs. Only the $4l$ orbitals were varied. Since these orbitals are not occupied in the single configuration wavefunction, these orbitals are *virtual* orbitals also referred to as correlation orbitals. The $n = 5$ calculation extended the correlation orbitals to include also $\{5s, 5p, 5d, 5f, 5g\}$ orbitals. The SD excitation process (restricted to at most one excitation from $3p^6$) resulted in a wavefunction expansion of

Table 1. Computed energy levels (in cm^{-1}), splitting (separation between levels of a term), difference from observed (ASD 2008) (computed − observed), and composition of the $3d^5$ levels. The J values within a term that are not in the observed order are preceded by an asterisk.

Level	LS	J	Energy	Splitting	Difference	Composition (per cent)
1	^6S	5/2	0.0	0.0	0.0	97
2	^4G	11/2	33 491.9		1246.4	96
3		9/2	33 538.1	46.2	1245.3	97
4		5/2	33 547.3	9.2	1246.1	97
5		7/2	33 551.6	4.3	1245.9	97
6	^4P	5/2	35 721.3		467.5	$93 + 3\,^4D$
7		3/2	35 791.4	70.2	458.1	$94 + 2\,^4D$
8		1/2	35 850.1	58.7	443.5	96
9	^4D	7/2	39 837.1		1057.7	96
10		1/2	39 945.5	108.4	1048.8	96
11		5/2	39 963.9	18.4	1028.8	$94 + 3\,^4P$
12		3/2	39 973.2	9.2	1035.0	$94 + 2\,^4P$
13	^2I	11/2	49 190.0		2099.5	96
14		13/2	49 202.9	12.8	2112.4	96
15	^2_5D	5/2	50 558.7		1017.2	$55 + 22\,^2_3F + 18\,^2_1D$
16		3/2	51 043.7	484.9	992.3	$70 + 23\,^2_1D + 3\,^4F$
17	^2_3F	7/2	52 442.9		1049.7	$94 + 1\,^4F + 1\,^2_5F$
18		5/2	53 192.8	749.9	1026.1	$70 + 7\,^4F + 14\,^2_5D + 4\,^2_1D$
19	^4F	9/2	53 833.1		1212.4	$95 + 1\,^2G$
20		7/2	53 896.4	63.3	1201.0	$95 + 1\,^2_3F$
21		*3/2	54 022.3	125.9	1185.2	$93 + 3\,^2_5D + 1\,^2_1D$
22		*5/2	54 007.1	-15.2	1169.1	$88 + 4\,^2_3F + 3\,^2_5D$
23	^2H	9/2	57 734.1		1675.8	$84 + 12\,^2G$
24		11/2	58 007.6	273.5	1638.8	96
25	$^2_5$G	7/2	59 234.6		1826.6	96
26		9/2	59 504.8	270.3	1783.6	$83 + 12\,^2_3H + 1\,^4F$
27	^2_5F	5/2	62 901.4		1744.8	95
28		7/2	62 999.2	97.8	1744.8	$96 + 1\,^2_3F$
29	^2S	1/2	68 332.5		1612.3	96
30	^2_3D	3/2	75 648.8		1552.2	96
31		5/2	75 686.5	37.7	1573.4	96
32	^2_3G	9/2	85 049.1		2154.3	96
33		7/2	85 050.3	1.1	2153.0	96
34	^2P	3/2	102 444.0		2326.0	96
35		1/2	102 447.9	3.9	2321.9	96
36	^2_1D	5/2	110 374.1		2122.0	$72 + 23\,^2_5D$
37		3/2	110 392.0	17.9	2133.7	$72 + 23\,^2_5D$

213 037 CSFs for our range of J. The final $n = 6$ calculation introduced $\{6s, 6p, 6d, 6f, 6g\}$ orbitals but the only CSFs added to the expansion were those from SD excitations from $3d^5$. Because of the importance of the $J = 5/2$ levels in this work, this last set of orbitals was optimized for the ten $J = 5/2$ levels. Once optimized radial functions were determined, RCI calculations were performed to include the Breit correction. The sizes of the matrices were 18 350, 33 356, 42 642, 45 325, 42 221, 35 117 and 26 359, respectively, for $J = 1/2$ to 13/2.

In this description, we have used a non-relativistic terminology, but the JJGEN program (Sturreson, Jönsson & Froese Fischer 2007) used to generate the CSFs translates the terminology to the relativistic framework where a $4p$ orbital, for example, is either a $4p_{1/2}$ or $4p_{3/2}$ orbital and the coupling of each CSF is described in terms of jj coupling.

Since the present calculations are entirely *ab initio*, our measure of accuracy will be the energy level structure of terms and their fine structure. The $3d^5\,^6S$ ground state, where all spin quantum numbers are the same, has some correlation in the motion of the electrons included already at the single-configuration DHF level through the antisymmetry requirement of the CSF. In fact the correlation correction to the total energy for the ^6S term is much smaller than for other terms. Thus we cannot expect the higher energy levels relative to ^6S to be in good agreement with observed levels (ASD 2008), but they should be in better relative agreement with each other. In particular the difference between the computed and observed level structure should be essentially constant within a term.

The final ($n = 6$) energy levels relative to the ground state for these calculations are reported in Table 1. The energy levels of the lowest term (^4G) differ from observed by 3.7 per cent but those of the highest term (^2_1D) are accurate to 2.0 per cent and compare favourably with errors of more than 10 per cent for lower and 5 per cent for the higher levels reported by Nahar (2006). The MCDHF energies include the Breit correction which is important in changing the order of the levels for the ^4G term from [5/2, 7/2, 9/2, 11/2] to the observed order of [11/2, 9/2, 5/2, 7/2]. In addition the energies relative to the lowest ($^4G_{11/2}$) of [46.2, 56.0, 60.0] cm^{-1} are in excellent agreement with observed values of [47.3, 55.7, 60.2] (ASD 2008), respectively. The only fine-structure levels not in their observed order are the $J = 5/2$, 3/2 levels of ^4F: our calculated values are separated by 15.2 cm^{-1} whereas the observed $J = 3/2$ should be lower than $J = 5/2$ by 0.9 cm^{-1}. However, this does

Table 2. Comparison of $J = 5/2$ energy level separation (in cm^{-1}) with observed.

Term	Level (Obs)	Separation Obs	Separation Calc	Ratio (Calc/obs)
^6S	0			
^4G	32 301	32 301	33 547	1.04
^4P	35 254	2953	2174	0.74
^4D	38 935	3681	4243	1.15
^2_5D	49 542	10 606	10 595	1.00
^2_3F	52 167	2625	2634	1.00
^4F	52 838	671	814	1.21
^2_5F	61 157	8319	8894	1.07
^2_3D	74 133	12 977	12 785	0.99
^2_1D	108 242	34 109	34 687	1.02

not directly contribute to the error in the wavefunction since only CSFs of the same parity and J have non-zero interaction matrix elements. Comparing the wavefunction composition to the earlier MCHF Breit–Pauli term composition, there is a general reduction in the admixture of different LS terms. For example, whereas the present $^2_3F_{5/2}$ has a dominant contribution of 70 per cent it was only 60 per cent in the earlier work.

What may be important for the accuracy of the wavefunction is the separation of levels of the same J and parity. Table 2 shows the ten lowest observed $J = 5/2$ levels and, for each level except the lowest, the difference in energy of the level from the one immediately preceding it in the table. This difference represents the separation between levels of the same J. Also reported is the ratio of the present and observed separation. The greatest deviation from unity (with a ratio of 0.74) is for the separation between the $^4G_{5/2}$ and the $^4P_{5/2}$ levels: the calculated separation of 2174 cm^{-1} is too small compared with the observed separation of 2953 cm^{-1}. The second largest deviation from unity (with a ratio of 1.21) is for the separation of the ^2_3F and ^4F $J = 5/2$ levels. The important separations are those where configuration mixing occurs. A more detailed analysis of the wavefunction composition of the ground state shows that the largest admixture is $^4P_{5/2}$, and that the $^6S_{5/2}$ –$^4P_{5/2}$ energy separation is accurate to 1.3 per cent; the largest admixture to $^4G_{5/2}$ is from ^{2,4} $F_{5/2}$ and the energy separation of the latter two with respect to $^4G_{5/2}$ has similar accuracy. This suggests that the compositions of the $^6S_{5/2}$ and $^4G_{5/2}$ wavefunctions are reliable. Table 1 shows the larger admixture of $^4D_{5/2}$ in the $^4P_{5/2}$ wavefunction and vice versa. The separation of these energy levels is in error by 15 per cent. It is reasonable to assume that the energy adjusted results from the MCHF calculation yield the more accurate transition probability when this mixing is important.

Table 3 reports transition probability data for E2 and M1 transitions to the ground state for all levels considered in this paper except for a few weak lines from $J = 1/2$ levels. Included in this table is the observed wavelength (in vacuum) and the computed line strength S, the weighted oscillator strength gf, the transition rate A_{ki}(N) normalized to the observed wavelength and the *ab initio* unnormalized A_{ki}(U) value, both in s^{-1}. Thus the normalized value is obtained from the computed line strength and the observed wavelength. All these values are computed in the length form. Also included are 'indicators of accuracy' (Froese Fischer 2008). The factor $\delta E = \Delta E(\text{calc})/\Delta E(\text{obs}) - 1$ is a measure of the accuracy of the transition energy and is always positive for the transitions considered in this table. Consequently, normalization reduces all these transition rates. The factor

$$\delta T = |S(\text{length}) - S(\text{velocity})|/\max(S(\text{length}), S(\text{velocity}))$$

is a measure of the agreement in length and velocity values of the line strength S for E2 transitions. Because all of the transitions in this table are LS forbidden with contributions arising from small components of the wavefunction, some δT factors are relatively large. Generally the length form of the line strength is the more stable value as more correlation is included in the calculation.

A complete list of similar data for all multiplets between different LS terms of $3d^5$ is provided in Table A1 (for E2) and Table A2 (for M1) transitions of the Appendix. Not included are transitions between levels within an LS term for which the transition energy is less than 100 cm^{-1}.

4 COMPARISON OF TRANSITION PROBABILITIES

In order to further assess the accuracy of these results, we compare in Table 4 the present transition probabilities between ^6S and the ^4G,^4P, and ^4D terms with previously published values. Included are Garstang's early calculations, results from the semi-empirical orthogonal operator method (Raassen & Uylings private communication), the one-body Breit–Pauli results reported by (Nahar 2006), the two-body MCHF (Froese Fischer & Rubin 2004) Breit–Pauli values, as well as the present normalized (N) and unnormalized (U) values. With only one exception, namely the transition from $^4G_{9/2}$, the process of normalizing to the observed wavelength has reduced the transition rate to values below those reported for MCHF previously. Since the separation of ^4P and ^4D is too large (see Table 2) the mixing of these terms is less than in MCHF. The latter calculation used the LS term energy corrections to improve the wavefunction composition, a correction we were not able to perform in this paper. For transitions from ^4G levels, the Nahar (2006) values are considerably smaller, possibly because of the restricted Breit–Pauli operators that were included. As mentioned earlier, for these levels the Breit correction was needed to produce levels in the observed order. The low-order version of this correction consists of the two-body Breit–Pauli operators that were omitted in Nahar's calculations. What is striking is that, when there is excellent agreement among the last three columns (and possibly others), there is also agreement within 10 per cent with Garstang's 1958 result. Examples are some of the transitions from ^4P. Exceptions tend to be the very small values for which the transition rate is $<10^{-9}$ s^{-1}.

Table 5 compares LS allowed values for E2 and M1 transitions. All results are now the normalized values. In the majority of the cases there is agreement to within 3 per cent between the two theories over a wide range of transition rates.

Both the Breit–Pauli MCHF method with term energy corrections and the present fully relativistic MCDHF method have points in their favour. In order to establish a set of 'best' values, the two sets were merged and agreement in length and velocity used to select between them. Exceptions are the 1/2–1/2 transitions for which E2 transitions are not allowed. In this case the value selected was from the same calculation as for a 3/2–1/2 transition of the same multiplet. These values are reported in Table A3 of the Appendix. Transitions are identified by the index of the lower and upper level (as given in Table 1) and the data include the wavelength (in vacuum), A_{ki}(E2),

Table 3. Observed vacuum wavelength λ (Å) and calculated line strength S, weighted absorption oscillator strength gf and radiative transition rate A_{ki} (s^{-1}) for E2 and M1 transitions to the ground state. Transition rates normalized to observed wavelengths [A_{ki}(N)] and unnormalized *ab initio* values [A_{ki}(U)] are reported. Also included are the accuracy indicators: $\delta E = \Delta E(\text{calc})/\Delta E(\text{obs}) - 1$ and $\delta T = S(\text{length}) - S(\text{velocity})/\max(S(\text{length}), S(\text{velocity}))$.

Term	J	λ(vac)		S	gf	A_{ki}(N)	A_{ki}(U)	δE	δT
^4G	9/2	3096.67	E2	2.361(−08)	1.335(−16)	9.285(−09)	1.122(−08)	0.037	0.038
	5/2	3095.86	E2	2.033(−08)	1.150(−16)	1.334(−08)	1.612(−08)	0.037	0.066
			M1	1.400(−07)	1.828(−13)	2.120(−05)	2.375(−05)		
	7/2	3095.43	E2	2.417(−08)	1.368(−16)	1.190(−08)	1.438(−08)	0.037	0.109
			M1	1.883(−10)	2.460(−16)	2.141(−08)	2.398(−08)		
^4P	5/2	2836.57	E2	3.862(−05)	2.841(−13)	3.925(−05)	4.192(−05)	0.013	0.016
			M1	6.642(−03)	9.468(−09)	1.308	1.361		
	3/2	2830.19	E2	1.484(−05)	1.099(−13)	2.288(−05)	2.441(−05)	0.013	0.031
			M1	2.855(−03)	4.080(−09)	8.494(−01)	8.829(−01)		
^4D	7/2	2578.69	E2	8.962(−04)	8.776(−12)	1.100(−03)	1.259(−03)	0.027	0.077
			M1	1.565(−06)	2.455(−12)	3.078(−04)	3.337(−04)		
	1/2	2570.91	E2	3.499(−05)	3.458(−13)	1.828(−04)	2.088(−04)	0.018	0.033
	5/2	2568.38	E2	6.436(−04)	6.378(−12)	1.075(−03)	1.225(−03)	0.026	0.090
			M1	1.240(−04)	1.953(−10)	3.291(−02)	3.559(−02)		
	3/2	2568.17	E2	2.518(−04)	2.496(−12)	6.312(−04)	7.196(−04)	0.026	0.089
			M1	3.969(−05)	6.250(−11)	1.580(−02)	1.710(−02)		
^2_5D	5/2	2018.51	E2	1.979(−08)	4.040(−16)	1.102(−07)	1.220(−07)	0.020	0.175
			M1	1.699(−06)	3.404(−12)	9.287(−04)	9.871(−04)		
	3/2	1997.95	E2	9.416(−10)	1.982(−17)	8.281(−09)	9.135(−09)	0.019	0.402
			M1	1.278(−07)	2.587(−13)	1.081(−04)	1.146(−04)		
^2_3F	7/2	1945.74	E2	2.233(−07)	5.090(−15)	1.121(−06)	1.240(−06)	0.020	0.080
			M1	5.087(−11)	1.057(−16)	2.328(−08)	2.474(−08)		
^4F	9/2	1900.39	E2	5.032(−06)	1.231(−13)	2.274(−05)	2.548(−05)	0.023	0.025
	7/2	1897.70	E2	2.295(−06)	5.639(−14)	1.305(−05)	1.461(−05)	0.022	0.016
			M1	7.864(−11)	1.676(−16)	3.880(−08)	4.151(−08)		
	5/2	1892.58	E2	6.260(−07)	1.550(−14)	4.812(−06)	5.369(−06)	0.022	0.002
			M1	4.785(−08)	1.022(−13)	3.173(−05)	3.388(−05)		
	3/2	1892.61	E2	7.415(−08)	1.836(−15)	8.550(−07)	9.553(−07)	0.022	0.003
			M1	3.149(−09)	6.728(−15)	3.132(−06)	3.348(−06)		
^2H	9/2	1783.86	E2	9.799(−09)	2.898(−16)	6.075(−08)	7.040(−08)	0.029	0.113
^2_5G	7/2	1741.92	E2	6.819(−10)	2.166(−17)	5.953(−09)	6.962(−09)	0.031	0.303
			M1	1.319(−14)	3.062(−20)	8.413(−12)	9.242(−12)		
	9/2	1732.47	E2	3.157(−08)	1.019(−15)	2.265(−07)	2.637(−07)	0.030	0.136
^2_5F	5/2	1635.15	E2	2.997(−10)	1.151(−17)	4.786(−09)	5.508(−09)	0.028	0.127
			M1	1.421(−12)	3.514(−18)	1.461(−09)	1.590(−09)		
	7/2	1632.54	E2	6.856(−09)	2.646(−16)	8.277(−08)	9.525(−08)	0.028	0.285
			M1	5.094(−12)	1.262(−17)	3.947(−09)	4.294(−09)		
^2_3D	3/2	1349.59	E2	1.282(−08)	8.756(−16)	8.017(−07)	8.892(−07)	0.021	0.381
			M1	4.080(−12)	1.222(−17)	1.119(−08)	1.191(−08)		
	5/2	1349.29	E2	4.692(−08)	3.207(−15)	1.958(−06)	2.175(−06)	0.021	0.379
			M1	7.206(−11)	2.160(−16)	1.319(−07)	1.405(−07)		
^2_3G	9/2	1206.35	E2	2.668(−07)	2.552(−14)	1.170(−05)	1.330(−05)	0.025	0.111
	7/2	1026.31	E2	2.147(−08)	2.054(−15)	1.177(−06)	1.338(−06)	0.025	0.108
		1206.35	M1	9.927(−16)	3.328(−21)	1.907(−12)	2.059(−12)		
^2P	3/2	998.82	E2	3.434(−07)	5.786(−14)	9.672(−05)	1.085(−04)	0.023	0.149
			M1	1.911(−10)	7.738(−16)	1.293(−06)	1.386(−06)		
	1/2	998.74	E2	9.615(−08)	1.621(−14)	5.537(−05)	6.209(−05)	0.023	0.149

A_{ki}(M1), A_{ki}(Total) and a symbol for the source: B for the earlier Breit–Pauli MCHF data and G for the present results obtained using the GRASP program. A total of 315 G transitions were selected and 150 B transitions. It should be noted that the agreement in the length and velocity values is not a definitive indicator of accuracy, but is a reasonable one. All the present normalized values of Table 4 were selected as the 'best' by this process.

The publications over the last decade reporting transition data for transitions between levels of $3d^5$ in [Fe IV] illustrate the difficulty of establishing the accuracy of transition rates in complex cases. Garstang computed many values fifty years ago. Progress has been made but agreement between the MCHF Breit–Pauli and MCDHF values for more transitions would be desirable.

In Table A3 we have listed our recommended transition rates for both E2 and M1 transitions as well as their sum for the convenience of the community.

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Table 4 Comparison of E2 and M1 transition rates $A_{J'J}$ (in s^{-1}) for transitions to the ground state for different theories: (1) from Garstang (1958), (2) from Raassen & Uylings (1997, private communication) (3) from Nahar (2006), Froese Fischer & Rubin (2004) and present normalized (N) and unnormalized (U) MCDHF values.

LS	J	Obs ΔE	Semi-empirical			MCHF	Present calculation	
			(1)	(2)	(3)		(N)	(U)
E2 transitions								
^4G	9/2	32 292.8	<1.0(−09)	6.92(−12)	3.06(−10)	1.85(−09)	9.29(−09)	1.12(−08)
	5/2	32 301.2	<1.0(−09)	1.95(−08)	7.64(−09)	2.30(−08)	1.33(−08)	1.61(−08)
	7/2	32 305.7	<1.0(−09)	3.18(−08)	1.19(−08)	3.32(−08)	1.19(−08)	1.44(−08)
^4P	5/2	35 253.8	3.9(−05)	4.26(−05)	6.28(−05)	4.02(−05)	3.93(−05)	4.19(−05)
	3/2	35 333.0	1.5(−05)	1.99(−05)	3.52(−05)	1.21(−05)	2.29(−05)	2.44(−05)
	1/2	35 406.6	very small	1.67(−06)	7.11(−06)	1.47(−05)	5.52(−06)	5.87(−06)
^4D	7/2	38 779.4	1.1(−03)	1.13(−03)	1.22(−03)	1.27(−03)	1.10(−03)	1.26(−03)
	1/2	38 897.7	1.8(−04)	1.97(−04)	2.00(−04)	2.17(−04)	1.83(−04)	2.08(−04)
	5/2	38 935.1	1.0(−03)	1.09(−03)	1.15(−03)	1.23(−03)	1.08(−03)	1.22(−03)
	3/2	38 938.2	6.2(−04)	6.72(−04)	6.80(−04)	7.33(−04)	6.31(−04)	7.12(−04)
M1 transitions								
^4G	5/2	32 301.2	1.0(−05)	1.53(−05)	2.16(−06)	2.16(−05)	2.12(−05)	2.38(−05)
	7/2	32 305.7	<1.0(−07)	3.78(−08)	8.29(−09)	5.72(−08)	2.14(−08)	2.40(−08)
^4P	5/2	35 253.8	1.4	1.42	1.21	1.56	1.31	1.36
	3/2	35 333.3	8.8(−01)	9.23(−01)	7.92(−01)	1.02	8.49(−01)	8.83(−01)
^4D	7/2	38 779.4	2.0(−04)	5.90(−04)	3.33(−04)	7.67(−04)	3.08(−04)	3.34(−04)
	5/2	38 935.1	5.1(−02)	5.69(−02)	1.11(−02)	6.64(−02)	3.29(−02)	3.56(−02)
	3/2	38 938.2	3.8(−02)	2.75(−02)	3.56(−02)	3.33(−02)	1.58(−02)	1.71(−02)

Table 5. Comparison of MCHF Breit–Pauli and present normalized transition rates $A_{J'J}$ (in s^{-1}) for LS allowed E2 and M1 transitions between excited states.

Transition				E2 transition		M1 transition	
LS	L′S′	J	J'	MCHF	Present	MCHF	Present
^2I	^2_3G	11/2	7/2	5.00	4.92		
			9/2	1.50(−01)	1.47(−01)	2.24(−05)	2.28(−05)
		13/2	9/2	4.82	4.78		
	^2H	11/2	9/2	5.77(−04)	5.67(−04)	8.27(−02)	8.24(−02)
			11/2	2.58(−05)	2.43(−05)	2.05(−01)	1.92(−01)
		13/2	9/2	1.52(−05)	1.71(−05)		
			11/2	6.60(−04)	6.54(−04)	1.07(−01)	1.03(−01)
^2F	^2P	7/2	3/2	7.33	7.14		
		5/2	1/2	8.86	8.63		
			3/2	1.22	1.18	9.04(−05)	1.10(−04)
^4G	^4F	5/2	3/2	2.00(−01)	1.93(−01)	1.59(−01)	1.38(−01)
			5/2	6.36(−02)	6.39(−02)	2.91(−01)	2.05(−01)
			7/2	6.69(−03)	6.52(−03)	1.58(−02)	1.27(−02)
			9/2	8.95(−05)	8.96(−05)		
		7/2	3/2	8.00(−02)	7.85(−02)		
			5/2	1.10(−01)	1.21(−01)	2.11(−02)	2.67(−03)
			7/2	7.17(−02)	7.03(−02)	1.56(−01)	1.29(−01)
			9/2	3.91(−03)	3.89(−03)	1.25(−02)	9.85(−03)
		9/2	5/2	6.00(−02)	6.57(−02)		
			7/2	1.55(−01)	1.53(−01)	5.12(−02)	3.75(−02)
			9/2	4.71(−02)	4.66(−02)	7.31(−02)	6.40(−02)
		11/2	7/2	4.33(−02)	4.26(−02)		
			9/2	2.23(−01)	2.20(−01)	1.60(−01)	1.36(−01)

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SUPPORTING INFORMATION

The following supporting information is available for this article.

Table A1. E2 transition data and accuracy.
Table A2. M1 transition data and accuracy.
Table A3. Recommended values from MCDHF (G) and MCHF (B).

Supporting Information may be found in the online version of this article:

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APPENDIX

Table A1. E2 transition data and accuracy (see the online version for the complete Table).

L	U	L(vac)	S	gf	A_{ki}(N)	A_{ki}(U)	δE	δT
1	3	3096.67	2.361e−08	1.335e−16	9.285e−09	1.122e−08	0.04	0.04
1	4	3095.86	2.033e−08	1.150e−16	1.334e−08	1.612e−08	0.04	0.07
1	5	3095.43	2.417e−08	1.368e−16	1.190e−08	1.438e−08	0.04	0.11
1	6	2836.57	3.862e−05	2.841e−13	3.925e−05	4.192e−05	0.01	0.02
1	7	2830.19	1.484e−05	1.099e−13	2.288e−05	2.441e−05	0.01	0.03
1	8	2824.33	1.770e−06	1.319e−14	5.515e−06	5.869e−06	0.01	0.16
1	9	2578.69	8.963e−04	8.776e−12	1.100e−03	1.259e−03	0.03	0.08
1	10	2570.91	3.667e−05	3.623e−13	1.828e−04	2.088e−04	0.03	0.09
1	11	2568.38	6.436e−04	6.378e−12	1.075e−03	1.225e−03	0.03	0.09
1	12	2568.17	2.518e−04	2.496e−12	6.312e−04	7.196e−04	0.03	0.09
1	15	2018.51	1.979e−08	4.040e−16	1.102e−07	1.220e−07	0.02	0.17
1	16	1997.95	9.416e−10	1.982e−17	8.281e−09	9.135e−09	0.02	0.40
1	17	1945.74	2.233e−07	5.090e−15	1.121e−06	1.240e−06	0.02	0.08
1	18	1916.93	8.228e−14	1.961e−21	5.933e−13	6.540e−13	0.02	1.00
1	19	1900.39	5.032e−06	1.231e−13	2.274e−05	2.548e−05	0.02	0.03
1	20	1897.70	2.295e−06	5.639e−14	1.305e−05	1.461e−05	0.02	0.02
1	21	1892.58	6.260e−07	1.550e−14	4.812e−06	5.369e−06	0.02	0.00
1	22	1892.61	7.415e−08	1.837e−15	8.550e−07	9.553e−07	0.02	0.00
1	23	1783.86	9.799e−09	2.898e−16	6.076e−08	7.040e−08	0.03	0.11
1	25	1741.92	6.819e−10	2.166e−17	5.953e−09	6.962e−09	0.03	0.30
1	26	1732.47	3.157e−08	1.019e−15	2.265e−07	2.638e−07	0.03	0.14
1	27	1635.15	2.997e−10	1.151e−17	4.786e−09	5.508e−09	0.03	0.13
1	28	1632.54	6.856e−09	2.646e−16	8.277e−08	9.525e−08	0.03	0.28
1	29	1498.80	2.266e−09	1.130e−16	1.678e−07	1.890e−07	0.02	0.48
1	30	1349.59	1.282e−08	8.756e−16	8.017e−07	8.892e−07	0.02	0.38
1	31	1349.29	4.692e−08	3.207e−15	1.958e−06	2.175e−06	0.02	0.38
1	32	1206.35	2.668e−07	2.552e−14	1.170e−05	1.330e−05	0.03	0.11
1	33	1206.31	2.147e−08	2.054e−15	1.177e−06	1.338e−06	0.03	0.11
1	34	998.82	3.434e−07	5.786e−14	9.672e−05	1.085e−04	0.02	0.15
1	35	998.74	9.826e−08	1.656e−14	5.537e−05	6.209e−05	0.02	0.15
1	36	923.77	7.402e−10	1.577e−16	2.054e−07	2.263e−07	0.02	0.55
1	37	923.72	2.841e−11	6.053e−18	1.183e−08	1.304e−08	0.02	0.61
2	9	15 304.79	6.930e−02	3.246e−12	1.155e−05	9.979e−06	−0.03	0.99
2	13	6736.27	4.331e−05	2.379e−14	2.914e−07	3.853e−07	0.05	0.02
2	14	6736.27	1.139e−03	6.254e−13	6.567e−06	8.719e−06	0.06	0.00
2	17	5222.29	1.705e−04	2.010e−13	6.145e−06	5.834e−06	−0.01	1.00
2	19	4907.93	5.591e+00	7.941e−09	2.199e−01	2.181e−01	−0.00	0.16
2	20	4890.00	7.959e−02	1.143e−10	3.985e−03	3.941e−03	−0.00	0.58
2	23	4199.42	1.055e−02	2.391e−11	9.044e−04	9.889e−04	0.02	0.11
2	24	4145.37	5.317e−06	1.253e−14	4.054e−07	4.394e−07	0.02	0.18

Table A2. M1 transition data and an indicator of accuracy (see online version for the complete Table).

L	*U*	*L*(vac)	*S*	*gf*	A_{ki}(N)	A_{ki}(U)	δE
1	4	3095.86	1.400E−07	1.828E−13	2.121E−05	2.375E−05	0.04
1	5	3095.43	1.883E−10	2.460E−16	2.141E−08	2.398E−08	0.04
1	6	2836.57	6.642E−03	9.468E−09	1.308E+00	1.361E+00	0.01
1	7	2830.19	2.855E−03	4.080E−09	8.494E−01	8.829E−01	0.01
1	9	2578.69	1.565E−06	2.455E−12	3.078E−04	3.337E−04	0.03
1	11	2568.38	1.240E−04	1.953E−10	3.291E−02	3.559E−02	0.03
1	12	2568.17	3.969E−05	6.250E−11	1.580E−02	1.710E−02	0.03
1	15	2018.51	1.699E−06	3.404E−12	9.287E−04	9.871E−04	0.02
1	16	1997.95	1.278E−07	2.587E−13	1.081E−04	1.146E−04	0.02
1	17	1945.74	5.087E−11	1.057E−16	2.328E−08	2.474E−08	0.02
1	18	1916.93	1.614E−07	3.406E−13	1.030E−04	1.092E−04	0.02
1	20	1897.70	7.864E−11	1.676E−16	3.880E−08	4.151E−08	0.02
1	21	1892.58	4.785E−08	1.022E−13	3.173E−05	3.388E−05	0.02
1	22	1892.61	3.149E−09	6.728E−15	3.132E−06	3.348E−06	0.02
1	25	1741.92	1.319E−14	3.062E−20	8.413E−12	9.242E−12	0.03
1	27	1635.15	1.421E−12	3.514E−18	1.461E−09	1.590E−09	0.03
1	28	1632.54	5.094E−12	1.262E−17	3.947E−09	4.294E−09	0.03
1	30	1349.59	4.080E−12	1.222E−17	1.119E−08	1.191E−08	0.02
1	31	1349.29	7.206E−11	2.160E−16	1.319E−07	1.405E−07	0.02
1	33	1206.31	9.927E−16	3.328E−21	1.907E−12	2.059E−12	0.03
1	34	998.82	1.911E−10	7.738E−16	1.293E−06	1.386E−06	0.02
1	36	923.77	1.655E−08	7.243E−14	9.436E−05	1.000E−04	0.02
1	37	923.72	1.137E−09	4.979E−15	9.731E−06	1.032E−05	0.02
2	13	6736.27	7.257E−04	4.356E−10	5.337E−03	6.311E−03	0.05
2	14	6736.27	2.613E−05	1.568E−11	1.647E−04	1.952E−04	0.06
2	19	4907.93	5.968E−03	4.918E−09	1.362E−01	1.355E−01	−0.00
2	23	4199.42	3.010E−04	2.898E−10	1.096E−02	1.157E−02	0.02
2	24	4145.37	1.449E−02	1.413E−08	4.571E−01	4.798E−01	0.02
2	26	3925.31	1.029E−07	1.060E−13	4.590E−06	4.886E−06	0.02
2	32	1974.36	3.760E−04	7.701E−10	1.318E−01	1.390E−01	0.02
3	9	15 416.40	9.453E−04	2.480E−10	8.699E−04	7.966E−04	−0.03
3	13	6757.81	2.316E−04	1.386E−10	1.687E−03	1.996E−03	0.06
3	17	5235.22	2.126E−02	1.642E−08	4.997E−01	4.844E−01	−0.01
3	19	4919.35	2.825E−03	2.322E−09	6.401E−02	6.370E−02	−0.00
3	20	4901.34	1.311E−03	1.081E−09	3.753E−02	3.729E−02	−0.00
3	23	4207.78	4.653E−03	4.471E−09	1.685E−01	1.778E−01	0.02
3	24	4153.51	5.982E−03	5.824E−09	1.877E−01	1.970E−01	0.02
3	25	3981.65	1.437E−06	1.459E−12	7.674E−05	8.219E−05	0.02
3	26	3932.61	3.101E−04	3.188E−10	1.375E−02	1.464E−02	0.02
3	28	3452.85	5.929E−05	6.944E−11	4.856E−03	5.112E−03	0.02
3	32	1976.20	2.793E−05	5.716E−11	9.762E−03	1.030E−02	0.02

Table A2 – *continued.*

L	*U*	*L*(vac)	*S*	*gf*	A_{ki}(N)	A_{ki}(U)	δE
3	33	1976.11	7.253E−05	1.484E−10	3.169E−02	3.343E−02	0.02
4	6	33 868.45	1.249E−03	1.491E−10	1.445E−04	5.768E−05	−0.36
4	7	32 980.44	9.245E−05	1.134E−11	1.738E−05	7.046E−06	−0.35
4	9	15 436.39	1.065E−04	2.791E−11	9.766E−05	8.938E−05	−0.03
4	11	15 074.09	6.507E−04	1.746E−10	8.540E−04	7.728E−04	−0.03
4	12	15 067.05	1.855E−04	4.979E−11	3.657E−04	3.319E−04	−0.03
4	15	5800.36	5.904E−03	4.116E−09	1.360E−01	1.307E−01	−0.01
4	16	5633.74	2.730E−04	1.960E−10	1.030E−02	9.862E−03	−0.01
4	17	5237.52	5.864E−04	4.527E−10	1.376E−02	1.334E−02	−0.01
4	18	5033.85	5.289E−03	4.249E−09	1.864E−01	1.803E−01	−0.01
4	20	4903.35	4.438E−04	3.660E−10	1.269E−02	1.261E−02	−0.00
4	21	4869.31	5.263E−03	4.371E−09	2.049E−01	2.026E−01	−0.00
4	22	4869.52	2.364E−03	1.964E−09	1.381E−01	1.369E−01	−0.00
4	25	3982.98	9.461E−06	9.606E−12	5.049E−04	5.407E−04	0.02
4	27	3465.57	1.134E−09	1.324E−15	1.225E−07	1.290E−07	0.02
4	28	3453.85	3.544E−06	4.150E−12	2.900E−04	3.053E−04	0.02
4	30	2392.61	2.419E−08	4.088E−14	1.191E−05	1.217E−05	0.01
4	31	2391.66	4.852E−08	8.204E−14	1.594E−05	1.632E−05	0.01
4	33	1976.44	2.945E−04	6.025E−10	1.286E−01	1.356E−01	0.02
4	34	1474.56	4.830E−10	1.324E−15	1.016E−06	1.065E−06	0.02
4	36	1316.64	1.026E−09	3.152E−15	2.021E−06	2.092E−06	0.01
4	37	1316.53	5.360E−09	1.646E−14	1.584E−05	1.640E−05	0.01
5	6	33 920.15	2.500E−04	2.980E−11	2.880E−05	1.148E−05	−0.36
5	9	15 447.12	1.147E−03	3.002E−10	1.049E−03	9.601E−04	−0.03
5	11	15 084.32	2.438E−07	6.535E−14	3.193E−07	2.890E−07	−0.03
5	15	5801.88	5.814E−03	4.052E−09	1.338E−01	1.286E−01	−0.01
5	17	5238.76	3.235E−03	2.497E−09	7.587E−02	7.354E−02	−0.01

Table A3. Recommended values from MCDHF (G) and MCDHF (B) (see online version for the complete Table).

L	U	λ(vac)	A_{ki}(E2)	A_{ki}(M1)	A_{ki}(Total)	
1	3	3096.67	9.285e−09	–	9.285e−09	G
1	4	3095.86	1.334e−08	2.121e−05	2.122e−05	G
1	5	3095.43	1.190e−08	2.141e−08	3.331e−08	G
1	6	2836.57	3.925e−05	1.308e+00	1.308e+00	G
1	7	2830.19	2.288e−05	8.494e−01	8.494e−01	G
1	8	2824.33	5.515e−06	–	5.515e−06	G
1	9	2578.69	1.100e−03	3.078e−04	1.408e−03	G
1	10	2570.91	1.828e−04	–	1.828e−04	G
1	11	2568.38	1.075e−03	3.291e−02	3.399e−02	G
1	12	2568.17	6.312e−04	1.580e−02	1.643e−02	G
1	15	2018.51	1.102e−07	9.287e−04	9.288e−04	G
1	16	1997.95	8.281e−09	1.081e−04	1.081e−04	G
1	17	1945.74	1.121e−06	2.328e−08	1.144e−06	G
1	19	1900.39	2.274e−05	–	2.274e−05	G
1	20	1897.70	1.305e−05	3.880e−08	1.309e−05	G
1	21	1892.58	4.812e−06	3.173e−05	3.654e−05	G
1	22	1892.61	8.550e−07	3.132e−06	3.987e−06	G
1	23	1783.86	6.076e−08	–	6.076e−08	G
1	25	1741.92	5.953e−09	8.413e−12	5.961e−09	G
1	26	1732.47	2.265e−07	–	2.265e−07	G
1	27	1635.15	4.786e−09	1.461e−09	6.247e−09	G
1	28	1632.54	8.277e−08	3.947e−09	8.672e−08	G
1	29	1498.80	1.678e−07	–	1.678e−07	G
1	30	1349.59	9.912e−07	2.533e−08	1.016e−06	B
1	31	1349.29	1.958e−06	1.319e−07	2.090e−06	G
1	32	1206.35	1.170e−05	–	1.170e−05	G
1	33	1206.31	1.177e−06	1.907e−12	1.177e−06	G
1	34	998.82	9.672e−05	1.293e−06	9.801e−05	G
1	35	998.74	5.537e−05	–	5.537e−05	G
1	36	923.77	2.054e−07	9.436e−05	9.457e−05	G
1	37	923.72	1.183e−08	9.731e−06	9.743e−06	G
2	9	15 304.79	2.591e−07	–	2.591e−07	B
2	13	6736.27	2.914e−07	5.337e−03	5.337e−03	G
2	14	6736.27	6.567e−06	1.647e−04	1.712e−04	G
2	17	5222.29	3.562e−04	–	3.562e−04	G
2	19	4907.93	2.199e−01	1.362e−01	3.561e−01	G
2	20	4890.00	4.305e−02	–	4.305e−02	G
2	23	4199.42	9.044e−04	1.096e−02	1.187e−02	G
2	24	4145.37	4.054e−07	4.571e−01	4.571e−01	G
2	25	3974.17	2.216e−04	–	2.216e−04	G
2	26	3925.31	4.151e−03	4.590e−06	4.156e−03	G
2	28	3447.22	1.686e−05	–	1.686e−05	G
2	32	1974.36	1.474e−06	1.318e−01	1.318e−01	G
2	33	1974.26	8.495e−05	–	8.495e−05	G
3	6	33 772.37	7.025e−10	–	7.025e−10	B
3	9	15 416.40	2.743e−06	1.088e−03	1.091e−03	B
3	11	15 055.03	9.560e−07	–	9.560e−07	G
3	13	6757.81	2.270e−06	1.687e−03	1.689e−03	G
3	14	6757.81	8.992e−07	–	8.992e−07	B
3	15	5797.54	2.672e−04	–	2.672e−04	B
3	17	5235.22	1.030e−03	4.997e−01	5.007e−01	G
3	18	5031.73	5.715e−03	–	5.715e−03	G
3	19	4919.35	4.669e−02	6.401e−02	1.107e−01	G
3	20	4901.34	1.528e−01	3.753e−02	1.903e−01	G
3	21	4867.32	6.565e−02	–	6.565e−02	G
3	23	4207.78	2.439e−04	1.685e−01	1.687e−01	G
3	24	4153.51	1.077e−07	2.288e−01	2.288e−01	B
3	25	3981.65	6.697e−04	7.674e−05	7.464e−04	G
3	26	3932.61	1.107e−03	1.375e−02	1.486e−02	G
3	27	3464.56	4.393e−04	–	4.393e−04	G
3	28	3452.85	4.275e−03	4.856e−03	9.131e−03	G
3	31	2391.18	7.762e−07	–	7.762e−07	G
3	32	1976.20	1.588e−05	9.762e−03	9.778e−03	G
3	33	1976.11	2.378e−05	3.962e−02	3.964e−02	B

Table A3 – *continued.*

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