

# Spectral properties of In II from MCDHF calculations

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Received 19 April 2007, in final form 10 May 2007

Published 5 June 2007

Online at [stacks.iop.org/JPhysB/40/2417](http://stacks.iop.org/JPhysB/40/2417)

## Abstract

We report extensive relativistic multiconfiguration Dirac–Hartree–Fock calculations of oscillator strengths and hyperfine structures for a large number of electric dipole transitions in In II. Results for the  $5s^2\ ^1S_0$ – $5s5p\ ^3P_0^o$  hyperfine induced transition are also presented. Core polarization is accounted for by means of explicit CI. To describe spin–polarization effects configuration state functions obtained by single excitations from all core-shells are included in the expansions. The computed oscillator strength for the  $5s^2\ ^1S_0$ – $5s5p\ ^3P_1^o$  intercombination transition is in good agreement with laser spectroscopy measurements of  $\text{In}^+$  ions in a radio-frequency trap. The calculated magnetic dipole hyperfine interaction constants agree very well with experimental constants derived from Fourier transform spectra. The problem with off-diagonal interactions affecting the hyperfine structures in closely spaced fine-structure levels is discussed.

## 1. Introduction

There are a number of highly accurate measurements of various spectral properties in In II. New wavelengths, energy levels and hyperfine structure constants for a large number of states have been derived from Fourier transform spectra [1]. The isotope structure of the  $5s^2\ ^1S_0$ – $5s5p\ ^3P_1^o$  line has been studied by means of laser spectroscopy of ions in a radio-frequency trap [2]. In the same experiment the lifetimes of the  $^3P_1^o$  and  $^3P_0^o$  states were determined using intensity-modulated laser excitation. The decay of the  $^3P_0^o$  state is strictly forbidden. However, for atoms with nuclear spin the hyperfine interaction opens decay channels through the admixture of  $^1P_1^o$  and  $^3P_1^o$ . This effect has been theoretically studied in a number of cases e.g. [3–5], but there are only a few experimental values to compare with. The hyperfine structures of levels in the  $5s^2\ ^1S_0$ – $5s5p\ ^3P_1^o$  and  $5s5p\ ^3P_{1,2}^o$ – $5s6s\ ^3S_1$  transitions were accurately determined by Larkins and Hannaford [6] using a high-resolution scanning echelle monochromator. In addition to these measurements, there are also beam–foil measurements corrected by the arbitrarily normalized decay curve (ANDC) technique of lifetimes for 12 states [7].

During the years there have been several calculations of transition probabilities using different methods. Among the more recent efforts we mention the work by Hibbert [8],

Migdalek and Baylis [9], Migdalek and Bojara [10], Das and Idrees [11], Chou and Huang [12], Chou *et al* [13], Lavin and Martin [14], Biémont and Zeippen [15] and Biémont *et al* [16]. To the knowledge of the authors hyperfine structures and isotope shifts have so far not been theoretically investigated.

Indium is also of astrophysical interest. Indium shows the largest discrepancy between the photospheric and meteoritic values of abundance among all elements with  $Z > 3$  [17]. The photospheric value is determined from a single In I line at 451.1 nm in the solar spectrum and one may suspect that unidentified blends cause the discrepancy. No In II lines have been identified in the solar spectrum even though such lines could be expected due to the low ionization energy of In I.

The purpose of the present work is to improve and complement the dataset for In II and to explore the capacity of the grasp2K multiconfiguration Dirac–Hartree–Fock package [18] to predict oscillator strengths and hyperfine structures in ‘spectrum calculations’ including states high up in the Rydberg series.

## 2. Theory

### 2.1. MCDHF

The multiconfiguration Dirac–Hartree–Fock (MCDHF) method [19], as implemented in the grasp2K program package [18], was used in the present work. Starting from the Dirac–Coulomb Hamiltonian

$$H_{\text{DC}} = \sum_i (c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_i^N) + \sum_{i>j} 1/r_{ij}, \quad (1)$$

where  $V^N$  is the monopole part of the electron–nucleus Coulomb interaction, the atomic state functions were obtained as linear combinations of symmetry adapted configuration state functions (CSFs)

$$|\Gamma P J M_J\rangle = \sum_{j=1}^N c_j |\gamma_j P J M_J\rangle. \quad (2)$$

Here  $J$  and  $M_J$  are the angular quantum numbers and  $P$  is the parity.  $\gamma$  denotes other appropriate labelling of the configuration state function, for example orbital occupancy and coupling scheme. Normally the label  $\Gamma$  of the atomic state function is the same as the label of the dominating CSF. The configuration state functions were built from products of one-electron Dirac orbitals. In the relativistic self-consistent field procedure both the radial parts of the Dirac orbitals and the expansion coefficients were optimized to self-consistency. The Breit interaction

$$B_{ij} = -\frac{1}{2r_{ij}} \left[ \alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot \mathbf{r}_{ij})(\alpha_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right] \quad (3)$$

was included in subsequent configuration interaction (CI) calculations [20].

### 2.2. Isotope shift

Corrections to the calculated energy structure due to isotope-dependent recoil motion of the nucleus and finite nuclear volume effects were included in first-order perturbation theory with the atomic state functions as zero-order functions. The corrections can be written as

$$E_M = (S_{\text{nms}} + S_{\text{sms}}) \frac{1}{M} + \frac{2}{3} \pi Z \rho(0) \langle r_M^2 \rangle \quad (4)$$

where

$$S_{\text{nms}} = \langle \Gamma P J M_J | \sum_i (c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2) | \Gamma P J M_J \rangle \quad (5)$$

and

$$S_{\text{sms}} = \langle \Gamma P J M_J | \sum_{i < j} \mathbf{p}_i \cdot \mathbf{p}_j | \Gamma P J M_J \rangle \quad (6)$$

are, respectively, the normal and specific mass shift parameters and

$$\rho(0) = \langle \Gamma P J M_J | \sum_i \delta(\mathbf{r}_i) | \Gamma P J M_J \rangle \quad (7)$$

the electron density at the site of the nucleus [21].  $M$  is the mass of the nucleus and  $\langle r_M^2 \rangle$  is the root-mean-square radius, both in atomic units. From these quantities, the transition isotope shift  $\Delta E_{M',M}$  between two isotopes  $M'$  and  $M$  was obtained as

$$\Delta E_{M',M} = (\Delta S_{\text{nms}} + \Delta S_{\text{sms}}) \left( \frac{1}{M'} - \frac{1}{M} \right) + \frac{2\pi}{3} Z \Delta \rho(0) (\langle r_{M'}^2 \rangle - \langle r_M^2 \rangle), \quad (8)$$

where the differences in the electronic quantities are between the values of upper and lower levels in the transition.

### 2.3. Hyperfine structure and Landé factors

The two stable isotopes of indium,  $^{115}\text{In}$  (95.7 %) and  $^{113}\text{In}$  (4.3 %), both have nuclear spin  $I = 9/2$  and the fine-structure levels are split into closely spaced hyperfine levels. The splittings of the fine-structure levels are to first order given by the magnetic dipole  $A_J$  and electric quadrupole  $B_J$  hyperfine interaction constants:

$$A_J = \frac{\mu_I}{I} \frac{1}{\sqrt{J(J+1)(2J+1)}} \langle \Gamma P J \| \sum_j -i\sqrt{2}\alpha r_j^{-2} (\alpha_j \mathbf{C}^{(1)}(j))^{(1)} \| \Gamma P J \rangle, \quad (9)$$

$$B_J = 2Q \sqrt{\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)}} \langle \Gamma P J \| \sum_j -r_j^{-3} \mathbf{C}^{(2)}(j) \| \Gamma P J \rangle. \quad (10)$$

The hyperfine levels of closely spaced fine-structure levels are also affected by the off-diagonal hyperfine interaction [22]. The hyperfine interaction constants as well as the Landé  $g_J$ -factors

$$g_J = \frac{2}{\sqrt{J(J+1)(2J+1)}} \langle \Gamma P J \| \sum_j -i \frac{\sqrt{2}}{2\alpha^2} r_j (\alpha_j \mathbf{C}^{(1)}(j))^{(1)} + \frac{g_s - 2}{2} \beta_j \Sigma_j \| \Gamma P J \rangle \quad (11)$$

were calculated using the HFSZEEMAN program [23, 24]. The nuclear magnetic dipole moment  $\mu_I$  and the nuclear quadrupole moment  $Q$  were taken from a recent compilation by Stone [25] and we use the values  $\mu_I = 5.5408\mu_N$  and  $Q = 0.81(5)$  barns for  $^{115}\text{In}$ .

### 2.4. Transition parameters

The transition parameters, such as weighted oscillator strengths, for multipole transitions between two atomic states  $\Gamma P J M_J$  and  $\Gamma' P' J' M'_J$  can be expressed in terms of the reduced transition matrix element

$$\langle \Gamma P J \| \mathbf{Q}_k^{(\lambda)} \| \Gamma' P' J' \rangle, \quad (12)$$

where  $Q_{kq}^{(\lambda)}$  is the electromagnetic multipole operator of order  $k$  in Coulomb or Babushkin gauge [26]. The superscript designates the type of multipole:  $\lambda = 1$  for electric multipoles and  $\lambda = 0$  for magnetic multipoles. To compute the transition matrix element between two atomic state functions described by independently optimized orbital sets, biorthogonal transformations of the atomic state functions were performed [27]. In the new representation, the evaluation of the matrix element was done using standard Racah-algebra techniques.

### 3. Calculations

#### 3.1. Spectrum

It is, from some perspectives, desirable to perform separate calculations for each of the studied atomic states. This approach, however, is impractical and time consuming when considering large portions of a spectrum. In this work, the atomic state functions were instead determined simultaneously in extended optimal level (EOL) calculations on the weighted energy average of the states [28]. As a starting point two MCDHF calculations were performed in the EOL scheme: one calculation with 24 CSFs describing each of the even parity states up to  $5s7d\ ^1D_2$ , and one calculation with 20 CSFs describing each of the odd parity states up to  $5s5f\ ^1F_3^o$ . These calculation were followed by calculations with expansions including CSFs obtained by single(S) and double(D) excitations from, respectively, the studied even and odd state reference configurations to active sets of orbitals. Of the excitations from the even and odd state reference configurations at most one was allowed from the outer 4d core-shell. The active sets for the even and odd parity states consisting of spectroscopic orbitals from the initial MCDHF calculations were consecutively enlarged by adding three layers of correlation orbitals. Each layer contained orbitals with s, p-, p, d-, d, f-, f symmetries. For the even states one layer also included orbitals with g-, g symmetries. For the odd states two layers included orbitals with g-, g symmetries and one layer contained orbitals with h-, h symmetries. Due to stability problems in the relativistic self-consistent field procedure only the outermost layers of orbitals could be optimized each time. The largest calculation for the even parity states included 49 relativistic orbitals and around 157 000 CSFs. The largest calculation for the odd parity states was based on 52 relativistic orbitals and more than 235 000 CSFs. All calculations were done on an ordinary PC under Linux.

The MCDHF calculations were followed by relativistic CI calculations including Breit and some QED effects. To account for spin-polarization which is important for the hyperfine interaction constants [29], additional CI calculations were performed. The expansions for these CI calculations were obtained by augmenting the largest expansion from the previous CI calculations with CSFs generated by allowing single excitations from all shells of the initial reference configurations to the active set of orbitals.

#### 3.2. Ground and first excited states

In EOL calculations, the included correlation orbitals correct a number of states at the same time. Obviously this will give less accurate results compared to the case where the correlation orbitals are obtained in separate calculations for each of the states. To check the accuracy of the spectrum calculations described above, separate calculations were performed for the  $5s^2\ ^1S_0$  ground state and the excited  $5s5p\ ^3P_{0,1,2}^o, ^1P_1^o$  states. The expansions for the ground state were obtained by allowing SD-excitations from the  $5s^2, 5p^2$  and  $5d^2$  complex to an active set. As before at most one excitation was allowed from the outer 4d core-shell. The  $5s5p\ ^3P_{0,1,2}^o, ^1P_1^o$  states were treated together in an EOL scheme. The expansions for these states were obtained

by allowing SD-excitations from the  $5s5p$  and  $5p5d$  complex to an active set. The active sets were increased by adding five layers of correlation orbitals. All calculations were followed by relativistic CI calculations including Breit and some QED effects. To account for spin-polarization additional CI calculations were again performed with the expansions from the previous CI calculations augmented by CSFs generated by allowing single excitations from all shells of the initial reference configurations to the active set of orbitals.

## 4. Results and discussion

### 4.1. Spectrum properties

The energy values from the different spectrum calculations are displayed in table 1. The inclusion of the three layers of correlation orbitals improves the initial energies dramatically. Although the Breit and QED effects in the CI calculations slightly act in the wrong direction, the final energies are in very good agreement with experiment. All levels except  $5p^2\ ^1S_0$  are a few hundred  $\text{cm}^{-1}$  too high relative to the ground level indicating that less correlation has been captured for the latter. In table 2 calculated hyperfine structure constants from the CI wavefunctions including spin-polarization are compared with experimental values of Karlsson and Litzén derived from Fourier transform spectra [1]. The calculated and experimentally determined  $A$  factors are in very good agreement. For the  $B$  factors the situation is different and in many cases there are substantial differences between theory and experiment. In the paper by Karlsson and Litzén it is, however, pointed out that for some levels different transitions did not give quite consistent results for the  $B$  factors and the given values, except for the lowest configurations, should therefore mainly be considered as parameters useful together with the  $A$  values for describing the observed structure in a model accounting only for diagonal hyperfine interaction. Details of the fitting procedures can be found in the thesis by Karlsson [30]. The large differences between the calculated and experimentally determined  $B$  factors indicate that the neglected off-diagonal hyperfine interactions are indeed important for some of the levels. The off-diagonal interaction shifts the positions of the hyperfine levels and, more important, leads to a redistribution of the oscillator strength that modifies the line profiles. The effect of the off-diagonal interaction has been investigated for the  $4s4d\ ^3D-4s4f\ ^3F^o$  transition in the homologous Ga II [22] and a similar study of the unanalysed lines of the  $5s5d\ ^3D-5s4f\ ^3F^o$  transition in In II is in progress [31]. In the last two columns of table 2 the calculated Landé  $g_J$  values are compared with values assuming pure  $LS$  coupling. There is a close agreement between the two sets of  $g_J$  values although one sees that term mixing in  $5snp\ ^1,3P_1$  becomes more important higher up in the Rydberg series, gradually changing the  $g_J$  values away from the  $LS$  limit.

Calculated oscillator strengths in the Coulomb or Babushkin gauges from the CI wavefunctions are presented in table 3. To save space only transitions with  $gf > 10^{-3}$  are included. The agreement between the two gauges is very good. All values are completely *ab initio* and for some transitions with small transition energies the calculated values may be improved by scaling the  $gf$  values with the experimental transition energies. In table 4 the present values are compared with experiment and selected values from the semi-empirical HFR calculations by Biémont and Zeippen [15]. The values from the two calculations are in good agreement, the value for the weak  $5s^2\ ^1S_0-5s6p\ ^1P_1^o$  transition being an exception. For this transition the difference between the two gauges is also large, indicating difficulties of some sort. A survey of previous calculations can be found in table 5 of [15].

**Table 1.** Calculated and experimental energy levels in  $\text{cm}^{-1}$ . Column 1 displays energies from calculations where the configuration expansion were generated by excitations to the initial spectroscopic orbitals. Columns 2–4 show energies from calculations where the active set consisting of the spectroscopic orbitals were enlarged by, respectively, one, two and three layers of correlation orbitals. Column 5 shows the final energy values from the CI calculations including Breit and leading QED effects.

Level	Spectroscopic orbitals	Corr. 1	Corr. 2	Corr. 3	CI	Experimental
$5s^2\ ^1S_0$	0.000	0.000	0.000	0.000	0.000	0.000
$5s5p\ ^3P_0^o$	36 519.60	41 292.83	42 195.51	42 164.18	42 084.92	42 275.997
$5s5p\ ^3P_1^o$	37 588.00	42 371.49	43 262.85	43 232.97	43 141.86	43 350.583
$5s5p\ ^3P_2^o$	39 867.69	44 823.79	45 715.42	45 696.12	45 575.11	45 829.257
$5s5p\ ^1P_1^o$	65 526.23	63 612.94	63 044.28	62 907.36	62 779.58	63 038.534
$5s6s\ ^3S_1$	85 766.18	92 854.78	93 930.45	93 791.42	93 651.19	93 923.883
$5s6s\ ^1S_0$	90 391.54	96 055.62	97 071.36	96 981.07	96 841.35	97 030.201
$5s5d\ ^1D_2$	87 470.27	97 393.20	97 879.05	97 717.15	97 527.55	97 628.421
$5p^2\ ^3P_0$	94 994.22	100 684.72	101 392.41	101 386.10	101 181.84	101 607.7
$5s5d\ ^3D_1$	93 870.75	101 754.01	102 377.13	101 956.81	101 791.86	102 088.975
$5s5d\ ^3D_2$	93 942.86	101 839.70	102 464.33	102 044.53	101 877.06	102 174.924
$5s5d\ ^3D_3$	94 056.44	101 964.08	102 595.13	102 179.22	102 007.98	102 308.387
$5p^2\ ^3P_1$	96 220.86	102 225.83	103 013.72	103 005.72	102 777.42	103 248.84
$5p^2\ ^3P_2$	98 310.97	104 543.41	105 358.30	105 331.00	105 078.02	105 565.275
$5s6p\ ^3P_0^o$	98 570.47	106 042.40	107 620.57	107 357.57	107 215.95	107 662.708
$5s6p\ ^3P_1^o$	98 775.17	106 225.84	107 809.24	107 538.71	107 395.76	107 841.992
$5s6p\ ^3P_2^o$	99 266.96	106 761.15	108 398.07	108 124.32	107 973.87	108 430.336
$5s6p\ ^1P_1^o$	103 101.40	108 552.52	109 975.04	109 546.86	109 401.41	109 780.223
$5p^2\ ^1D_2$	108 433.85	114 632.02	114 706.85	114 003.51	113 791.25	113 884.903
$5p^2\ ^1S_0$	122 885.97	120 500.03	121 550.50	121 555.39	121 364.45	121 289.09
$5s7s\ ^3S_1$	111 677.79	119 811.43	121 305.91	121 362.58	121 206.33	121 442.542
$5s7s\ ^1S_0$	113 397.06	124 453.17	123 770.64	123 589.69	123 208.79	123 372.851
$5s4f\ ^3F_2^o$	113 858.17	121 913.41	123 378.67	123 372.00	123 211.89	123 643.132
$5s4f\ ^3F_3^o$	113 856.93	121 911.23	123 378.67	123 375.18	123 220.92	123 648.050
$5s4f\ ^3F_4^o$	113 855.29	121 908.54	123 389.00	123 384.36	123 263.56	123 664.787
$5s4f\ ^1F_3^o$	114 110.21	122 119.00	123 405.15	123 426.91	123 376.22	123 699.154
$5s6d\ ^3D_1$	114 915.61	123 310.86	124 629.89	124 661.88	124 496.62	124 742.729
$5s6d\ ^3D_2$	114 947.35	123 344.87	124 664.17	124 694.04	124 527.77	124 776.712
$5s6d\ ^3D_3$	114 995.25	123 396.95	124 717.44	124 744.44	124 576.64	124 830.174
$5s6d\ ^1D_2$	119 780.17	126 202.87	126 899.47	126 651.38	126 476.24	126 670.945
$5s7p\ ^3P_0^o$	116 946.39	124 809.95	126 608.99	126 664.90	126 512.01	
$5s7p\ ^3P_1^o$	117 033.36	124 882.62	126 677.44	126 728.39	126 575.30	126 994.866
$5s7p\ ^3P_2^o$	117 247.29	125 117.43	126 934.55	126 983.02	126 826.69	127 254.061
$5s7p\ ^1P_1^o$	118 790.12	125 689.56	127 366.69	127 333.16	127 180.18	127 573.302
$5s8s\ ^3S_1$	128 719.49	131 265.27	132 847.63	132 935.20	132 776.25	133 072.509
$5s8s\ ^1S_0$	129 180.40	131 767.57	133 305.51	133 405.01	133 245.69	133 554.383
$5s5f\ ^3F_2^o$	123 796.71	131 866.77	133 576.51	133 662.06	133 499.86	133 940.984
$5s5f\ ^3F_3^o$	123 795.69	131 864.93	133 581.39	133 664.78	133 502.54	133 944.832
$5s5f\ ^3F_4^o$	123 794.34	131 862.75	133 586.65	133 672.12	133 509.81	133 960.864
$5s5f\ ^1F_3^o$	123 982.67	132 012.81	133 598.24	133 697.86	133 535.58	
$5s7d\ ^3D_1$	124 477.90	133 007.73	134 509.34	134 590.81	134 424.80	134 726.488
$5s7d\ ^3D_2$	124 494.43	133 025.14	134 526.52	134 607.42	134 440.93	134 744.017
$5s7d\ ^3D_3$	124 519.45	133 052.05	134 553.72	134 633.93	134 466.68	134 771.894
$5s7d\ ^1D_2$	127 336.35	134 218.44	135 333.37	135 290.22	135 120.94	135 400.325

**Table 2.** Calculated hyperfine interaction constants for  $^{115}\text{In}$  (in MHz) compared with experimental values derived from Fourier transform spectra [1]. In the two last two columns the calculated Landé  $g_J$  factors are compared with values  $g_{LSJ}$  derived in pure  $LS$  coupling.

Level	$A$	$B$	$A_{\text{exp}}$	$B_{\text{exp}}$	$g_J$	$g_{LSJ}$
$5s5p\ ^3P_1^o$	6832	-407	$6949 \pm 24$	-420	1.4982	1.5011
$5s5p\ ^3P_2^o$	5014	737	$5088 \pm 27$	629	1.5011	1.5011
$5s5p\ ^1P_1^o$	-229	546			1.0028	1.0000
$5s6s\ ^3S_1$	11 758	0.2	$12049 \pm 12$	0	2.0021	2.0023
$5s5d\ ^1D_2$	521	611	$549 \pm 21$	570	1.0090	1.0000
$5s5d\ ^3D_1$	-4845	23.2			0.5042	0.4988
$5s5d\ ^3D_2$	1778	339	$1865 \pm 30$	-600	1.1673	1.1670
$5s5d\ ^3D_3$	3340	94.9	$3388 \pm 60$	-60	1.3341	1.3341
$5p^2\ ^3P_1$	-123	360			1.4959	1.5011
$5p^2\ ^3P_2$	648	-776	$666 \pm 45$	-629	1.4821	1.5011
$5s6p\ ^3P_1^o$	7841	-74.7	$8148 \pm 15$	-480	1.4828	1.5011
$5s6p\ ^3P_2^o$	5156	155	$5297 \pm 18$	210	1.5011	1.5011
$5s6p\ ^1P_1^o$	-2245	176	$-2278 \pm 24$	149	1.0183	1.0000
$5p^2\ ^1D_2$	455	753	$480 \pm 60$	659	1.0094	1.0000
$5s7s\ ^3S_1$	10 927	-0.006	$11167 \pm 36$	-180	2.0023	2.0023
$5s4f\ ^3F_2^o$	-3381	11.0			0.6659	0.6659
$5s4f\ ^3F_3^o$	-285	12.1			1.0804	1.0835
$5s4f\ ^3F_4^o$	2543	15.5			1.2506	1.2506
$5s4f\ ^1F_3^o$	1141	17.2	$1736 \pm 21$	-690	1.0031	1.0000
$5s6d\ ^3D_1$	-5094	9.4	$-5228 \pm 24$	360	0.4988	0.4988
$5s6d\ ^3D_2$	1902	13.4	$1931 \pm 24$	-2008	1.1670	1.1670
$5s6d\ ^3D_3$	3431	25.8	$3477 \pm 30$	-1678	1.3341	1.3341
$5s6d\ ^1D_2$	-97.3	112			1.0003	1.0000
$5s7p\ ^3P_1^o$	8550	-24.9	$9000 \pm 45$	-1319	1.4664	1.5011
$5s7p\ ^3P_2^o$	5156	60.0	$5297 \pm 30$	300	1.5011	1.5011
$5s7p\ ^1P_1^o$	-3209	69.2	$-3424 \pm 27$	-29	1.0348	1.0000
$5s8s\ ^3S_1$	10 631	-0.004	$10 894 \pm 30$	209	2.0023	2.0023
$5s5f\ ^3F_2^o$	-3401	6.1			0.6659	0.6659
$5s5f\ ^3F_3^o$	-399	6.5			1.0798	1.0835
$5s5f\ ^3F_4^o$	2557	8.1			1.2506	1.2506
$5s5f\ ^1F_3^o$	1257	9.6			1.0037	1.0000
$5s7d\ ^3D_1$	-5147	4.3	$-5312 \pm 36$	869	0.4988	0.4988
$5s7d\ ^3D_2$	1979	6.2	$1970 \pm 36$	-3837	1.1669	1.1670
$5s7d\ ^3D_3$	3448	11.8	$3508 \pm 45$	-2128	1.3341	1.3341
$5s7d\ ^1D_2$	-227	31.1			1.0002	1.0000

#### 4.2. The resonance transition

In table 5 transition energies and weighted oscillator strengths in Coulomb and Babushkin gauges for the  $5s^2\ ^1S_0-5s5p\ ^3P_1^o$  and  $5s^2\ ^1S_0-5s5p\ ^1P_1^o$  transitions are shown. The values were obtained from increasingly large CI calculations including the Breit interaction and leading QED effects. The oscillator strengths converge rapidly with the active sets and basically only two levels of correlation orbitals are needed. Comparing the weighted oscillator strengths with those from the spectrum calculation we see that there is a fairly good consistency. For  $5s^2\ ^1S_0-5s5p\ ^3P_1^o$  there is no difference at all, but for the intercombination transition  $5s^2\ ^1S_0-5s5p\ ^1P_1^o$  the more extensive calculations with correlation orbitals targeted only for the states in the transition, and not for the whole spectrum, give somewhat larger values in better agreement

**Table 3.** Calculated weighted oscillator strengths in Coulomb and Babushkin gauges for E1 transitions in In II. The oscillator strengths have been obtained with the theoretical energy differences.

Transition	$\Delta E_{\text{exp}}$	$\Delta E$	$gf_B$	$gf_C$
5s6d $^1D_2$ -5s7p $^3P_1^o$	324	99	4.23 [-3]	1.10 [-1]
5s5f $^1F_3^o$ -5s7d $^3D_2$	757	905	9.35 [-2]	5.28 [-2]
5s5f $^1F_3^o$ -5s7d $^3D_3$	785	931	9.29 [-3]	5.35 [-3]
5s5f $^3F_2^o$ -5s7d $^3D_1$	786	924	1.01 [+0]	5.52 [-1]
5s5f $^3F_3^o$ -5s7d $^3D_2$	799	938	1.42 [+0]	7.85 [-1]
5s5f $^3F_2^o$ -5s7d $^3D_2$	803	941	1.89 [-1]	1.05 [-1]
5s5f $^3F_4^o$ -5s7d $^3D_3$	811	956	2.23 [+0]	1.26 [+0]
5s5f $^3F_3^o$ -5s7d $^3D_3$	827	964	1.84 [-1]	1.04 [-1]
5s5f $^3F_2^o$ -5s7d $^3D_3$	831	966	5.55 [-3]	3.15 [-3]
5s6d $^1D_2$ -5s7p $^1P_1^o$	902	703	4.58 [-1]	1.19 [+0]
5s4f $^1F_3^o$ -5s6d $^3D_2$	1078	1264	2.70 [-2]	4.08 [-2]
5s4f $^3F_2^o$ -5s6d $^3D_1$	1100	1287	3.73 [-1]	5.63 [-1]
5s4f $^3F_3^o$ -5s6d $^3D_2$	1129	1315	5.36 [-1]	8.06 [-1]
5s4f $^1F_3^o$ -5s6d $^3D_3$	1131	1313	2.86 [-3]	4.46 [-3]
5s4f $^3F_2^o$ -5s6d $^3D_2$	1134	1318	7.05 [-2]	1.06 [-1]
5s4f $^3F_4^o$ -5s6d $^3D_3$	1165	1355	8.38 [-1]	1.25 [+0]
5s4f $^3F_3^o$ -5s6d $^3D_3$	1182	1364	6.98 [-2]	1.04 [-1]
5s4f $^3F_2^o$ -5s6d $^3D_3$	1187	1367	2.08 [-3]	3.11 [-3]
5s5f $^1F_3^o$ -5s7d $^1D_2$	1413	1585	2.34 [+0]	1.72 [+0]
5s5f $^3F_3^o$ -5s7d $^1D_2$	1455	1618	1.57 [-1]	1.15 [-1]
5s6d $^3D_1$ -5s7p $^3P_0^o$	2189	2015	4.12 [-1]	5.02 [-1]
5s6d $^3D_2$ -5s7p $^3P_1^o$	2218	2047	8.87 [-1]	1.08 [+0]
5s6d $^3D_1$ -5s7p $^3P_1^o$	2252	2078	2.95 [-1]	3.58 [-1]
5s6d $^3D_3$ -5s7p $^3P_2^o$	2424	2250	1.90 [+0]	2.31 [+0]
5s6d $^3D_2$ -5s7p $^3P_2^o$	2477	2298	3.43 [-1]	4.16 [-1]
5s6d $^3D_1$ -5s7p $^3P_2^o$	2511	2330	2.30 [-2]	2.78 [-2]
5s6d $^3D_2$ -5s7p $^1P_1^o$	2797	2652	6.63 [-2]	7.94 [-2]
5s6d $^3D_1$ -5s7p $^1P_1^o$	2831	2683	2.64 [-2]	3.17 [-2]
5s4f $^1F_3^o$ -5s6d $^1D_2$	2972	3212	1.10 [+0]	1.36 [+0]
5s4f $^3F_3^o$ -5s6d $^1D_2$	3023	3264	5.69 [-2]	7.12 [-2]
5s7s $^1S_0$ -5s7p $^3P_1^o$	3622	3199	3.71 [-2]	4.56 [-2]
5s6p $^1P_1^o$ -5p $^2$ $^1D_2$	4105	4389	5.18 [-1]	3.40 [-1]
5s7s $^1S_0$ -5s7p $^1P_1^o$	4200	3803	5.79 [-1]	6.81 [-1]
5p $^2$ $^3P_2$ -5s6p $^1P_1^o$	4215	4323	2.40 [-2]	2.81 [-2]
5p $^2$ $^3P_1$ -5s6p $^3P_0^o$	4414	4438	1.62 [-3]	2.05 [-3]
5s7s $^3S_1$ -5s7p $^3P_0^o$	5489	5305	5.99 [-1]	6.24 [-1]
5s7p $^1P_1^o$ -5s8s $^3S_1$	5499	5596	1.07 [-1]	8.07 [-2]
5s7s $^3S_1$ -5s7p $^3P_1^o$	5552	5368	1.68 [+0]	1.75 [+0]
5s5d $^3D_1$ -5s6p $^3P_0^o$	5574	5424	2.33 [-1]	2.50 [-1]
5s5d $^3D_2$ -5s6p $^3P_1^o$	5667	5518	5.20 [-1]	5.60 [-1]
5p $^2$ $^1S_0$ -5s7p $^3P_1^o$	5706	5210	7.33 [-2]	7.79 [-2]
5s5d $^3D_1$ -5s6p $^3P_1^o$	5753	5603	1.74 [-1]	1.87 [-1]
5s7s $^3S_1$ -5s7p $^3P_2^o$	5812	5620	3.08 [+0]	3.21 [+0]
5s7p $^3P_2^o$ -5s8s $^3S_1$	5818	5949	2.45 [+0]	1.82 [+0]
5s7p $^1P_1^o$ -5s8s $^1S_0$	5981	6065	1.21 [+0]	1.08 [+0]
5s6p $^3P_1^o$ -5p $^2$ $^1D_2$	6043	6395	2.48 [-2]	1.88 [-2]
5s7p $^3P_1^o$ -5s8s $^3S_1$	6078	6200	1.30 [+0]	9.73 [-1]
5s5d $^3D_3$ -5s6p $^3P_2^o$	6122	5965	1.07 [+0]	1.15 [+0]
5s7s $^3S_1$ -5s7p $^1P_1^o$	6131	5973	1.31 [-1]	1.36 [-1]



**Table 3.** (Continued.)

Transition	$\Delta E_{\text{exp}}$	$\Delta E$	$gf_B$	$gf_C$
5s7p $^3P_0^o$ -5s8s $^3S_1$	6141	6264	4.62 [-1]	3.44 [-1]
5s5d $^3D_2$ -5s6p $^3P_2^o$	6255	6096	1.93 [-1]	2.07 [-1]
5p $^2$ $^1S_0$ -5s7p $^1P_1^o$	6284	5815	1.03 [+0]	1.10 [+0]
5s5d $^3D_1$ -5s6p $^3P_2^o$	6341	6182	1.26 [-2]	1.34 [-2]
5s7p $^3P_1^o$ -5s8s $^1S_0$	6560	6670	7.93 [-2]	7.00 [-2]
5s7p $^1P_1^o$ -5s7d $^3D_1$	7153	7244	7.39 [-2]	6.10 [-2]
5s7p $^1P_1^o$ -5s7d $^3D_2$	7171	7260	1.70 [-1]	1.38 [-1]
5s6d $^1D_2$ -5s5f $^3F_3^o$	7274	7026	3.47 [-1]	3.84 [-1]
5s6d $^1D_2$ -5s5f $^1F_3^o$	7316	7059	5.59 [+0]	6.15 [+0]
5s7p $^3P_2^o$ -5s7d $^3D_1$	7472	7598	6.66 [-2]	5.46 [-2]
5s7p $^3P_2^o$ -5s7d $^3D_2$	7490	7614	9.93 [-1]	8.14 [-1]
5s7p $^3P_2^o$ -5s7d $^3D_3$	7518	7639	5.52 [+0]	4.53 [+0]
5s5d $^3D_2$ -5s6p $^1P_1^o$	7605	7524	2.24 [-2]	2.34 [-2]
5s5d $^3D_1$ -5s6p $^1P_1^o$	7691	7609	8.19 [-3]	8.76 [-3]
5s7p $^3P_1^o$ -5s7d $^3D_1$	7732	7849	8.82 [-1]	7.21 [-1]
5s7p $^3P_1^o$ -5s7d $^3D_2$	7749	7865	2.67 [+0]	2.19 [+0]
5s7p $^3P_0^o$ -5s7d $^3D_1$	7795	7912	1.24 [+0]	1.01 [+0]
5s7p $^1P_1^o$ -5s7d $^1D_2$	7827	7940	2.96 [+0]	2.79 [+0]
5s7p $^3P_1^o$ -5s7d $^1D_2$	8405	8545	1.50 [-1]	1.42 [-1]
5s6d $^3D_3$ -5s5f $^3F_2^o$	9111	8923	1.70 [-2]	1.82 [-2]
5s6d $^3D_3$ -5s5f $^3F_3^o$	9115	8925	5.65 [-1]	6.06 [-1]
5s6d $^3D_3$ -5s5f $^3F_4^o$	9131	8933	6.87 [+0]	7.38 [+0]
5s6d $^3D_3$ -5s5f $^1F_3^o$	9157	8958	2.91 [-2]	3.14 [-2]
5s6d $^3D_2$ -5s5f $^3F_2^o$	9164	8972	5.90 [-1]	6.32 [-1]
5s6d $^3D_2$ -5s5f $^3F_3^o$	9168	8974	4.44 [+0]	4.76 [+0]
5s6d $^3D_1$ -5s5f $^3F_2^o$	9198	9003	3.17 [+0]	3.39 [+0]
5s6d $^3D_2$ -5s5f $^1F_3^o$	9210	9007	2.75 [-1]	2.95 [-1]
5p $^2$ $^1D_2$ -5s4f $^3F_3^o$	9763	9420	9.14 [-2]	9.36 [-2]
5p $^2$ $^1D_2$ -5s4f $^1F_3^o$	9814	9472	2.02 [+0]	2.04 [+0]
5s5d $^1D_2$ -5s6p $^3P_1^o$	10 214	9868	2.62 [-2]	2.46 [-2]
5s6s $^1S_0$ -5s6p $^3P_1^o$	10 812	10 554	3.92 [-2]	4.28 [-2]
5s6p $^1P_1^o$ -5p $^2$ $^1S_0$	11 509	11 963	5.14 [-1]	4.88 [-1]
5s6p $^1P_1^o$ -5s7s $^3S_1$	11 662	11 804	3.68 [-2]	3.20 [-2]
5s4f $^1F_3^o$ -5s7d $^1D_2$	11 701	11 857	9.00 [-3]	2.58 [-2]
5s5d $^1D_2$ -5s6p $^1P_1^o$	12 152	11 873	7.29 [-1]	6.85 [-1]
5s6s $^1S_0$ -5s6p $^1P_1^o$	12 750	12 560	1.19 [+0]	1.28 [+0]
5s6p $^3P_2^o$ -5s7s $^3S_1$	13 012	13 232	1.51 [+0]	1.36 [+0]
5p $^2$ $^1D_2$ -5s7p $^3P_1^o$	13 110	12 784	2.25 [-2]	1.88 [-2]
5s6p $^3P_1^o$ -5p $^2$ $^1S_0$	13 447	13 968	1.64 [-2]	1.63 [-2]
5s6p $^1P_1^o$ -5s7s $^1S_0$	13 593	13 974	3.35 [-1]	3.17 [-1]
5s6p $^3P_1^o$ -5s7s $^3S_1$	13 601	13 810	8.29 [-1]	7.62 [-1]
5p $^2$ $^1D_2$ -5s7p $^1P_1^o$	13 688	13 388	2.56 [-1]	2.22 [-1]
5s6s $^3S_1$ -5s6p $^3P_0^o$	13 739	13 564	4.41 [-1]	4.61 [-1]
5s6p $^3P_0^o$ -5s7s $^3S_1$	13 780	13 990	2.81 [-1]	2.60 [-1]
5s6s $^3S_1$ -5s6p $^3P_1^o$	13 918	13 744	1.29 [+0]	1.34 [+0]
5s6s $^3S_1$ -5s6p $^3P_2^o$	14 506	14 322	2.29 [+0]	2.39 [+0]
5s6p $^1P_1^o$ -5s6d $^3D_1$	14 963	15 095	3.09 [-2]	2.92 [-2]
5s6p $^1P_1^o$ -5s6d $^3D_2$	14 996	15 126	7.18 [-2]	6.76 [-2]
5s6p $^3P_1^o$ -5s7s $^1S_0$	15 531	15 980	9.99 [-3]	1.03 [-2]
5s6s $^3S_1$ -5s6p $^1P_1^o$	15 856	15 750	5.24 [-2]	5.48 [-2]
5s6p $^3P_2^o$ -5s6d $^3D_1$	16 312	16 522	5.16 [-2]	4.98 [-2]

**Table 3.** (Continued.)

Transition	$\Delta E_{\text{exp}}$	$\Delta E$	$gf_B$	$gf_C$
5s6p $^3P_2^0$ -5s6d $^3D_2$	16 346	16 553	7.71 [-1]	7.44 [-1]
5s6p $^3P_2^0$ -5s6d $^3D_3$	16 400	16 602	4.29 [+0]	4.14 [+0]
5s6p $^1P_1^0$ -5s6d $^1D_2$	16 891	17 074	2.22 [+0]	2.23 [+0]
5s6p $^3P_1^0$ -5s6d $^3D_1$	16 901	17 100	7.15 [-1]	6.96 [-1]
5s6p $^3P_1^0$ -5s6d $^3D_2$	16 935	17 132	2.15 [+0]	2.09 [+0]
5s6p $^3P_0^0$ -5s6d $^3D_1$	17 080	17 280	9.76 [-1]	9.53 [-1]
5p $^2$ $^3P_2$ -5s4f $^3F_3^0$	18 083	18 133	2.12 [-2]	2.16 [-2]
5p $^2$ $^3P_2$ -5s4f $^1F_3^0$	18 134	18 185	1.58 [-1]	1.59 [-1]
5s6p $^3P_1^0$ -5s6d $^1D_2$	18 829	19 080	5.53 [-2]	5.76 [-2]
5p $^2$ $^1D_2$ -5s5f $^3F_3^0$	20 060	19 711	4.80 [-3]	3.89 [-3]
5p $^2$ $^1D_2$ -5s5f $^1F_3^0$	20 102	19 744	7.06 [-2]	5.91 [-2]
5p $^2$ $^3P_1$ -5s4f $^3F_2^0$	20 394	20 431	1.16 [-2]	1.17 [-2]
5s5d $^3D_3$ -5s4f $^3F_2^0$	21 335	21 200	1.51 [-2]	1.49 [-2]
5s5d $^3D_3$ -5s4f $^3F_3^0$	21 340	21 203	5.08 [-1]	5.04 [-1]
5s5d $^3D_3$ -5s4f $^3F_4^0$	21 356	21 212	6.17 [+0]	6.11 [+0]
5s5d $^3D_3$ -5s4f $^1F_3^0$	21 391	21 255	2.20 [-2]	2.17 [-2]
5s5d $^3D_2$ -5s4f $^3F_2^0$	21 468	21 331	5.28 [-1]	5.23 [-1]
5s5d $^3D_2$ -5s4f $^3F_3^0$	21 473	21 334	4.05 [+0]	4.01 [+0]
5s5d $^3D_2$ -5s4f $^1F_3^0$	21 524	21 386	1.85 [-1]	1.84 [-1]
5s5d $^3D_1$ -5s4f $^3F_2^0$	21 554	21 416	2.84 [+0]	2.81 [+0]
5s6p $^1P_1^0$ -5s8s $^3S_1$	23 292	23 374	4.00 [-3]	2.69 [-3]
5s6p $^1P_1^0$ -5s8s $^1S_0$	23 774	23 844	1.05 [-1]	1.02 [-1]
5s6p $^3P_2^0$ -5s8s $^3S_1$	24 642	24 802	1.97 [-1]	1.40 [-1]
5s5d $^3D_3$ -5s7p $^3P_2^0$	24 946	24 818	2.92 [-3]	1.02 [-3]
5s6p $^1P_1^0$ -5s7d $^3D_1$	24 946	25 023	3.75 [-3]	2.97 [-3]
5s6p $^1P_1^0$ -5s7d $^3D_2$	24 964	25 039	7.82 [-3]	5.96 [-3]
5s6p $^3P_1^0$ -5s8s $^3S_1$	25 231	25 380	1.14 [-1]	8.41 [-2]
5s6p $^3P_0^0$ -5s8s $^3S_1$	25 410	25 560	3.95 [-2]	2.93 [-2]
5s6p $^1P_1^0$ -5s7d $^1D_2$	25 620	25 719	4.59 [-1]	4.55 [-1]
5s6p $^3P_1^0$ -5s8s $^1S_0$	25 712	25 849	4.09 [-3]	4.24 [-3]
5s5d $^1D_2$ -5s4f $^3F_3^0$	26 020	25 684	1.20 [-1]	1.17 [-1]
5s5d $^1D_2$ -5s4f $^1F_3^0$	26 071	25 736	2.87 [+0]	2.81 [+0]
5s6p $^3P_2^0$ -5s7d $^3D_1$	26 296	26 450	7.55 [-3]	6.20 [-3]
5s6p $^3P_2^0$ -5s7d $^3D_2$	26 314	26 467	1.13 [-1]	9.34 [-2]
5s6p $^3P_2^0$ -5s7d $^3D_3$	26 342	26 492	6.42 [-1]	5.28 [-1]
5s6p $^3P_1^0$ -5s7d $^3D_1$	26 884	27 029	1.11 [-1]	9.31 [-2]
5s6p $^3P_1^0$ -5s7d $^3D_2$	26 902	27 045	3.39 [-1]	2.84 [-1]
5s6p $^3P_0^0$ -5s7d $^3D_1$	27 064	27 208	1.54 [-1]	1.30 [-1]
5s6p $^3P_1^0$ -5s7d $^1D_2$	27 558	27 725	1.33 [-2]	1.40 [-2]
5p $^2$ $^3P_2$ -5s5f $^3F_3^0$	28 422	28 457	7.45 [-3]	8.17 [-3]
5s5d $^1D_2$ -5s7p $^3P_1^0$	29 366	29 047	3.06 [-3]	2.36 [-3]
5s5d $^1D_2$ -5s7p $^1P_1^0$	29 945	29 652	5.80 [-2]	4.67 [-2]
5s5p $^1P_1^0$ -5s6s $^3S_1$	30 885	30 871	4.08 [-3]	4.04 [-3]
5s5d $^3D_3$ -5s5f $^3F_2^0$	31 633	31 491	1.29 [-3]	1.35 [-3]
5s5d $^3D_3$ -5s5f $^3F_3^0$	31 636	31 494	4.38 [-2]	4.57 [-2]
5s5d $^3D_3$ -5s5f $^3F_4^0$	31 652	31 501	5.57 [-1]	5.79 [-1]
5s5d $^3D_3$ -5s5f $^1F_3^0$	31 678	31 527	2.66 [-3]	2.73 [-3]
5s5d $^3D_2$ -5s5f $^3F_2^0$	31 766	31 622	4.68 [-2]	4.87 [-2]
5s5d $^3D_2$ -5s5f $^3F_3^0$	31 770	31 625	3.63 [-1]	3.78 [-1]
5s5d $^3D_2$ -5s5f $^1F_3^0$	31 812	31 658	2.11 [-2]	2.20 [-2]
5s5d $^3D_1$ -5s5f $^3F_2^0$	31 852	31 708	2.57 [-1]	2.68 [-1]

**Table 3.** (Continued.)

Transition	$\Delta E_{\text{exp}}$	$\Delta E$	$gf_B$	$gf_C$
5s6s $^3S_1$ -5s7p $^3P_1^0$	33 071	32 924	3.23 [-3]	2.05 [-3]
5s6s $^3S_1$ -5s7p $^3P_2^0$	33 330	33 175	1.39 [-2]	1.01 [-2]
5s6s $^3S_1$ -5s7p $^1P_1^0$	33 649	33 528	1.07 [-3]	8.56 [-4]
5s5p $^1P_1^0$ -5s6s $^1S_0$	33 992	34 061	4.59 [-1]	4.50 [-1]
5s5p $^1P_1^0$ -5s5d $^1D_2$	34 590	34 747	1.14 [-1]	8.69 [-2]
5s5d $^1D_2$ -5s5f $^3F_3^0$	36 316	35 975	2.42 [-2]	2.37 [-2]
5s5d $^1D_2$ -5s5f $^1F_3^0$	36 358	36 008	4.67 [-1]	4.65 [-1]
5s5p $^1P_1^0$ -5p $^2$ $^3P_0$	38 569	38 402	1.42 [-3]	1.05 [-3]
5s5p $^1P_1^0$ -5s5d $^3D_1$	39 050	39 012	3.56 [-3]	3.61 [-3]
5s5p $^1P_1^0$ -5s5d $^3D_2$	39 136	39 097	7.56 [-3]	7.40 [-3]
5s5p $^1P_1^0$ -5p $^2$ $^3P_1$	40 210	39 997	1.37 [-3]	1.47 [-3]
5s5p $^1P_1^0$ -5p $^2$ $^3P_2$	42 527	42 298	6.98 [-2]	6.97 [-2]
5s $^2$ $^1S_0$ -5s5p $^3P_1^0$	43 351	43 141	4.91 [-3]	5.86 [-3]
5s5p $^3P_2^0$ -5s6s $^3S_1$	48 095	48 076	8.08 [-1]	7.76 [-1]
5s5p $^3P_1^0$ -5s6s $^3S_1$	50 573	50 509	4.80 [-1]	4.62 [-1]
5s5p $^1P_1^0$ -5p $^2$ $^1D_2$	50 846	51 011	3.68 [+0]	3.87 [+0]
5s5p $^3P_0^0$ -5s6s $^3S_1$	51 648	51 566	1.61 [-1]	1.56 [-1]
5s5p $^3P_2^0$ -5s5d $^1D_2$	51 799	51 952	3.00 [-2]	3.25 [-2]
5s5p $^3P_1^0$ -5s6s $^1S_0$	53 680	53 699	2.45 [-3]	2.55 [-3]
5s5p $^3P_1^0$ -5s5d $^1D_2$	54 278	54 385	9.31 [-3]	1.07 [-2]
5s5p $^3P_2^0$ -5s5d $^3D_1$	56 260	56 216	2.26 [-2]	2.23 [-2]
5s5p $^3P_2^0$ -5s5d $^3D_2$	56 346	56 301	5.51 [-1]	5.54 [-1]
5s5p $^3P_2^0$ -5s5d $^3D_3$	56 479	56 432	3.43 [+0]	3.47 [+0]
5s5p $^3P_2^0$ -5p $^2$ $^3P_1$	57 420	57 202	6.60 [-1]	7.09 [-1]
5s5p $^1P_1^0$ -5p $^2$ $^1S_0$	58 251	58 584	9.98 [-2]	9.66 [-2]
5s5p $^3P_0^0$ -5p $^2$ $^3P_0$	58 257	58 039	5.04 [-1]	5.41 [-1]
5s5p $^3P_1^0$ -5s5d $^3D_1$	58 738	58 650	5.37 [-1]	5.40 [-1]
5s5p $^3P_1^0$ -5s5d $^3D_2$	58 824	58 735	1.86 [+0]	1.88 [+0]
5s5p $^3P_2^0$ -5p $^2$ $^3P_2$	59 736	59 502	1.94 [+0]	2.08 [+0]
5s5p $^3P_0^0$ -5s5d $^3D_1$	59 813	59 706	8.77 [-1]	8.89 [-1]
5s5p $^3P_1^0$ -5p $^2$ $^3P_1$	59 898	59 635	4.39 [-1]	4.71 [-1]
5s5p $^1P_1^0$ -5s7s $^1S_0$	60 334	60 596	5.62 [-1]	5.49 [-1]
5s5p $^3P_0^0$ -5p $^2$ $^3P_1$	60 973	60 692	4.40 [-1]	4.77 [-1]
5s5p $^3P_1^0$ -5p $^2$ $^3P_2$	62 215	61 936	6.15 [-1]	6.63 [-1]
5s $^2$ $^1S_0$ -5s5p $^1P_1^0$	63 039	62 779	1.56 [+0]	1.70 [+0]
5s5p $^1P_1^0$ -5s6d $^1D_2$	63 632	63 696	9.62 [-1]	1.00 [+0]
5s5p $^3P_2^0$ -5p $^2$ $^1D_2$	68 056	68 216	4.05 [-2]	4.34 [-2]
5s5p $^1P_1^0$ -5s8s $^1S_0$	70 516	70 466	3.57 [-2]	3.77 [-2]
5s5p $^1P_1^0$ -5s7d $^1D_2$	72 362	72 341	2.59 [-1]	2.76 [-1]
5s5p $^3P_2^0$ -5s7s $^3S_1$	75 613	75 631	1.17 [-1]	1.05 [-1]
5s5p $^3P_1^0$ -5p $^2$ $^1S_0$	77 939	78 222	1.98 [-3]	2.28 [-3]
5s5p $^3P_1^0$ -5s7s $^3S_1$	78 092	78 064	6.57 [-2]	5.86 [-2]
5s5p $^3P_2^0$ -5s6d $^3D_1$	78 913	78 921	4.17 [-3]	4.37 [-3]
5s5p $^3P_2^0$ -5s6d $^3D_2$	78 947	78 952	6.29 [-2]	6.57 [-2]
5s5p $^3P_2^0$ -5s6d $^3D_3$	79 001	79 001	3.49 [-1]	3.63 [-1]
5s5p $^3P_0^0$ -5s7s $^3S_1$	79 167	79 121	2.12 [-2]	1.89 [-2]
5s5p $^3P_1^0$ -5s6d $^3D_1$	81 392	81 354	6.37 [-2]	6.65 [-2]
5s5p $^3P_1^0$ -5s6d $^3D_2$	81 426	81 385	1.91 [-1]	1.99 [-1]
5s5p $^3P_0^0$ -5s6d $^3D_1$	82 467	82 411	8.60 [-2]	8.96 [-2]
5s5p $^3P_1^0$ -5s6d $^1D_2$	83 320	83 334	2.46 [-3]	2.61 [-3]
5s5p $^3P_2^0$ -5s8s $^3S_1$	87 243	87 201	3.79 [-2]	3.47 [-2]

**Table 3.** (Continued.)

Transition	$\Delta E_{\text{exp}}$	$\Delta E$	$gf_B$	$gf_C$
5s5p $^3P_2^0$ -5s7d $^3D_1$	88 897	88 849	1.13 [-3]	1.22 [-3]
5s5p $^3P_2^0$ -5s7d $^3D_2$	88 915	88 865	1.72 [-2]	1.85 [-2]
5s5p $^3P_2^0$ -5s7d $^3D_3$	88 943	88 891	9.69 [-2]	1.04 [-1]
5s5p $^3P_1^0$ -5s8s $^3S_1$	89 722	89 634	2.14 [-2]	1.98 [-2]
5s5p $^3P_0^0$ -5s8s $^3S_1$	90 797	90 691	6.98 [-3]	6.47 [-3]
5s5p $^3P_1^0$ -5s7d $^3D_1$	91 376	91 282	1.78 [-2]	1.93 [-2]
5s5p $^3P_1^0$ -5s7d $^3D_2$	91 393	91 299	5.41 [-2]	5.86 [-2]
5s5p $^3P_0^0$ -5s7d $^3D_1$	92 450	92 339	2.43 [-2]	2.64 [-2]

with experiment. The good overall agreement, however, strengthens our confidence in the spectrum calculations, indicating that these include the same correlation effects as do the calculations targeted for the individual states. In table 5 values from the HFR calculations of Biémont and Zeippen [15] and the HFR and MCDHF calculations of Biémont *et al* [16] are also presented. The MCDHF calculations include the same correlation effects as the present calculations but the  $^1P_1^0$  state is separately optimized in one calculation and the three  $^3P^0$  states in another. One notes the large effect of the optimization scheme on the oscillator strength of the allowed transition in Coulomb gauge. The updated HFR calculation for the intercombination transition is in very good agreement with the present value from the CI calculation.

Hyperfine structure constants obtained from the CI wavefunctions including spin-polarization are displayed in table 6. Both diagonal and off-diagonal parameters are shown. The diagonal and off-diagonal constants show a similar convergence pattern and are fairly stable after three layers of correlation orbitals. The hyperfine constants from the more extensive calculations with correlation orbitals targeted for the particular state seem to be somewhat more accurate than the constants from the spectrum calculation. The differences between the two sets of calculations are however small.

In table 7 the differences  $\Delta S_{\text{nms}}$ ,  $\Delta S_{\text{sms}}$  and  $\Delta \rho(0)$  between the upper and lower state isotope shift parameters in the  $5s^2\ ^1S_0$ - $5s5p\ ^3P_1^0$  transition are shown as functions of the increasing active set of orbitals. The computed quantities converge after three layers of correlation orbitals. Combining the computed differences in electronic quantities with differences in nuclear quantities according to equation (9) we obtain the isotope shift  $\Delta \nu = \nu_{115} - \nu_{113}$ . The difference in the root-mean-square radius between  $^{115}\text{In}$  and  $^{113}\text{In}$  is  $-0.128(8)\text{ fm}^2$  and was taken from Eberz *et al* [32]. The calculated isotope shift is compared with the experimental shift in table 8. As suggested by Peik *et al*, the shift is dominated by the volume effect. Accounting for the uncertainties in the difference in the root-mean-square radius the calculated total shift  $-0.515\text{ GHz}$  is within the error bars of the experiment. The main uncertainty in the calculation comes from  $\Delta S_{\text{sms}}$ . This quantity is sensitive to correlation effects in the core and is known to be extremely difficult to compute accurately.

#### 4.3. The $5s^2\ ^1S_0$ - $5s5p\ ^3P_0^0$ hyperfine induced transition

The hyperfine interaction, although weak, not only shifts and splits individual  $J$  levels, but also mixes wavefunctions with different  $J$  quantum numbers. The wavefunction for the  $5s5p\ ^3P_0^0$  state can, when the hyperfine interaction is included, be written as

$$|5s5p\ ^3P_0^0 I F'\rangle = c_0 |5s5p\ ^3P_0^0 I F\rangle + \sum_i c_i |\gamma_i J_i I F\rangle, \quad (13)$$

**Table 4.** Comparison of the present calculated weighted oscillator strengths in Coulomb and Babushkin gauges with previous theoretical and experimental results.

Transition	$\Delta E_{\text{exp}}$	$gf_B$	$gf_C$	$gf^a$	
$5s^2\ ^1S_0-5s5p\ ^3P_0^o$	43 351	4.91 [-3]	5.86 [-3]	7.3 [-3]	5.44(45) [-3] <sup>b</sup>
$5s^2\ ^1S_0-5s5p\ ^1P_1^o$	63 039	1.56 [+0]	1.70 [+0]	1.64 [+0]	1.43(9) [+0] <sup>c</sup>
$5s^2\ ^1S_0-5s6p\ ^1P_1^o$	109 780	7.80 [-4]	3.79 [-3]	2.7 [-3]	
$5s5p\ ^1P_1^o-5s6s\ ^1S_0$	33 992	4.59 [-1]	4.50 [-1]	6.81 [-1]	
$5s6s\ ^1S_0-5s6p\ ^1P_1^o$	12 750	1.19 [+0]	1.28 [+0]	1.32 [+0]	
$5s5p\ ^3P_2^o-5s6s\ ^3S_1$	48 095	8.08 [-1]	7.76 [-1]	8.15 [-1]	
$5s5p\ ^3P_1^o-5s6s\ ^3S_1$	50 573	4.80 [-1]	4.62 [-1]	5.13 [-1]	
$5s5p\ ^3P_0^o-5s6s\ ^3S_1$	51 648	1.61 [-1]	1.56 [-1]	1.76 [-1]	
$5s5p\ ^3P_2^o-5s7s\ ^3S_1$	75 613	1.17 [-1]	1.05 [-1]	1.2 [-1]	
$5s5p\ ^3P_1^o-5s7s\ ^3S_1$	78 092	6.57 [-2]	5.86 [-2]	7.5 [-2]	
$5s5p\ ^3P_0^o-5s7s\ ^3S_1$	79 167	2.12 [-2]	1.89 [-2]	2.5 [-2]	
$5s5p\ ^3P_2^o-5s8s\ ^3S_1$	87 243	3.79 [-2]	3.47 [-2]	4.5 [-2]	
$5s5p\ ^3P_1^o-5s8s\ ^3S_1$	89 722	2.14 [-2]	1.98 [-2]	2.8 [-2]	
$5s5p\ ^3P_0^o-5s8s\ ^3S_1$	90 797	6.98 [-3]	6.47 [-3]	9.5 [-3]	
$5s6s\ ^3S_1-5s6p\ ^3P_2^o$	14 506	2.29 [+0]	2.39 [+0]	2.46 [+0]	
$5s6s\ ^3S_1-5s6p\ ^3P_1^o$	13 918	1.29 [+0]	1.34 [+0]	1.37 [+0]	
$5s6s\ ^3S_1-5s6p\ ^3P_0^o$	13 739	4.41 [-1]	4.61 [-1]	4.65 [-1]	
$5s5p\ ^3P_2^o-5s5d\ ^3D_3$	56 479	3.43 [+0]	3.47 [+0]	3.36 [+0]	
$5s5p\ ^3P_2^o-5s5d\ ^3D_2$	56 346	5.51 [-1]	5.54 [-1]	5.90 [-1]	
$5s5p\ ^3P_2^o-5s5d\ ^3D_1$	56 260	2.26 [-2]	2.23 [-2]	4.0 [-2]	
$5s5p\ ^3P_1^o-5s5d\ ^3D_2$	58 824	1.86 [+0]	1.88 [+0]	1.89 [+0]	
$5s5p\ ^3P_1^o-5s5d\ ^3D_1$	58 738	5.37 [-1]	5.40 [-1]	6.24 [-1]	
$5s5p\ ^3P_0^o-5s5d\ ^3D_1$	59 813	8.77 [-1]	8.89 [-1]	8.55 [-1]	
$5s5p\ ^3P_2^o-5s6d\ ^3D_3$	79 001	3.49 [-1]	3.63 [-1]	3.9 [-1]	
$5s5p\ ^3P_2^o-5s6d\ ^3D_2$	78 947	6.29 [-2]	6.57 [-2]	7.10 [-2]	
$5s5p\ ^3P_2^o-5s6d\ ^3D_1$	78 913	4.17 [-3]	4.37 [-3]	4.7 [-3]	
$5s5p\ ^3P_1^o-5s6d\ ^3D_2$	81 426	1.91 [-1]	1.99 [-1]	2.17 [-1]	
$5s5p\ ^3P_1^o-5s6d\ ^3D_1$	81 392	6.37 [-2]	6.65 [-2]	7.20 [-2]	
$5s5p\ ^3P_0^o-5s6d\ ^3D_1$	82 467	8.60 [-2]	8.96 [-2]	9.8 [-2]	
$5s5p\ ^3P_2^o-5s7d\ ^3D_3$	88 943	9.69 [-2]	1.04 [-1]	1.2 [-1]	
$5s5p\ ^3P_2^o-5s7d\ ^3D_2$	88 915	1.72 [-2]	1.85 [-2]	2.2 [-2]	
$5s5p\ ^3P_2^o-5s7d\ ^3D_1$	88 897	1.13 [-3]	1.22 [-3]	1.5 [-3]	
$5s5p\ ^3P_1^o-5s7d\ ^3D_2$	91 393	5.41 [-2]	5.86 [-2]	6.93 [-2]	
$5s5p\ ^3P_1^o-5s7d\ ^3D_1$	91 376	1.78 [-2]	1.93 [-2]	2.3 [-2]	
$5s5p\ ^3P_0^o-5s7d\ ^3D_1$	92 450	2.43 [-2]	2.64 [-2]	3.10 [-2]	

<sup>a</sup> HFR calculations. Biémont and Zeippen [15].<sup>b</sup> Intensity modulated laser excitation. Peik *et al* [2].<sup>c</sup> Beam-foil (ANDC). Ansbacher *et al* [7].

where  $I$  is the nuclear spin and  $F(=I)$  is the total angular momentum quantum number. The use of quotation marks in the left-hand wavefunction emphasizes the fact that the notation is just a label indicating the dominant character of the eigenvector. Clearly, the one-photon  $5s5p\ ^3P_0^o \rightarrow 5s^2\ ^1S_0$  transition now becomes allowed via the mixing of functions with  $J$  different from zero.  $|5s5p\ ^3P_0^o IF\rangle$  and  $|5s5p\ ^1P_1^o IF\rangle$  are the only important contributors to wavefunction expansion and in this work we model the  $5s5p\ ^3P_0^o$  state as

$$|5s5p\ ^3P_0^o IF\rangle = c_0|5s5p\ ^3P_0^o IF\rangle + c_1|5s5p\ ^3P_1^o IF\rangle + c_2|5s5p\ ^1P_1^o IF\rangle. \quad (14)$$

The mixing coefficients are obtained by constructing and diagonalizing the Hamiltonian matrix in the presence of the hyperfine interaction. Once the mixing coefficients have been determined

**Table 5.** Energies (in  $\text{cm}^{-1}$ ) and weighted oscillator strengths in Coulomb and Babushkin gauges for the  $5s^2\ ^1S_0\text{-}5s5p\ ^3P_1^o$  and  $5s^2\ ^1S_0\text{-}5s5p\ ^1P_1^o$  transitions from CI calculations with increasingly large configuration expansions. The first active set consists of the 5s, 5p-, 5p-, 5d-, 5d orbitals in the complex. The active set is enlarged by up to five layers of correlation orbitals.

Active set	$5s^2\ ^1S_0\text{-}5s5p\ ^1P_1^o$			$5s^2\ ^1S_0\text{-}5s5p\ ^3P_1^o$		
	$\Delta E$	$gf_B$	$gfc$	$\Delta E$	$gf_B$	$gfc$
Complex	64 726	2.12	1.87	39 753	2.12 [-3]	2.99 [-3]
Corr. 1	62 953	1.65	1.65	43 293	4.90 [-3]	5.37 [-3]
Corr. 2	62 939	1.59	1.69	43 427	5.16 [-3]	5.96 [-3]
Corr. 3	62 806	1.58	1.71	43 401	5.16 [-3]	5.99 [-3]
Corr. 4	62 785	1.57	1.71	43 387	5.14 [-3]	5.99 [-3]
Corr. 5	62 773	1.57	1.71	43 382	5.13 [-3]	5.99 [-3]
Spectrum	62 779	1.56	1.70	43 141	4.91 [-3]	5.86 [-3]
HFR <sup>a</sup>		1.64			7.3 [-3]	
HFR <sup>b</sup>		1.522			5.19 [-3]	
MCDHF <sup>b</sup>	62 714	1.562	1.538	43 655	4.71 [-3]	5.07 [-3]
Experiment	63 039	1.43(9) <sup>c</sup>		43 351	5.44(45) [-3] <sup>d</sup>	

<sup>a</sup> Biéumont and Zeippen [15].

<sup>b</sup> Biéumont *et al* [16].

<sup>c</sup> Beam-foil (ANDC) (Ansbacher *et al* [7]).

<sup>d</sup> Intensity modulated laser excitation (Peik *et al* [2]).

**Table 6.** Magnetic dipole,  $A$ , and electric quadrupole,  $B$ , hyperfine interaction constants (in Mhz) for  $5s5p\ ^3P_0$  in  $^{115}\text{In}$  from calculations with increasingly large configuration expansions including single excitations from all core shells. The first active set consists of the 5s, 5p-, 5p-, 5d-, 5d orbitals in the complex. The active set is then enlarged by up to five layers of correlation orbitals.

Active set	$A(^3P_1^o)$	$B(^3P_1^o)$	$A(^3P_2^o)$	$B(^3P_2^o)$	$A(^3P_1^o, ^3P_0^o)$	$A(^1P_1^o, ^3P_0^o)$
Complex	5644	-305	4362	540	5633	3733
Corr. 1	6519	-381	4814	688	6148	4152
Corr. 2	6700	-394	4916	715	6296	4141
Corr. 3	6907	-413	5056	750	6433	4258
Corr. 4	6898	-416	5046	753	6417	4237
Corr. 5	6948	-422	5082	765	6452	4270
Spectrum	6832	-407	5014	737		
Experiment <sup>a</sup>	$6961 \pm 6$	$-477 \pm 27$	$5093 \pm 12$	$629 \pm 180$		
Experiment <sup>b</sup>	$6949 \pm 24$	-420	$5088 \pm 27$	629		

<sup>a</sup> High-resolution scanning echelle monochromator (Larkins and Hannaford [6]).

<sup>b</sup> Fourier transform spectra (Karlsson and Litzén [1]).

the transition rate can be computed as

$$A(5s5p\ ^3P_0^o \rightarrow 5s^2\ ^1S_0) = \frac{2.026\ 13 \times 10^{18}}{3\lambda^3} |c_1 \langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^3P_1^o \rangle + c_2 \langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^1P_1^o \rangle|^2 \quad (15)$$

where the decay rate is in  $\text{s}^{-1}$  and  $\lambda$  is the wavelength in  $\text{\AA}$  for the transition.  $\langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^3P_1^o \rangle$  and  $\langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^1P_1^o \rangle$  are reduced matrix elements for the electric dipole operator [5]. The reduced transition matrix elements can be obtained as square roots of the corresponding line strengths. The phase is such that we have constructive

**Table 7.** Differences  $\Delta S_{\text{nms}}$ ,  $\Delta S_{\text{sms}}$  and  $\Delta\rho(0)$  between the upper and lower state isotope shift parameters in the  $5s^2\ ^1S_0$ – $5s5p\ ^3P_1^o$  transition from CI calculations with increasingly large configuration expansions. The first active set consists of the 5s, 5p-, 5p-, 5d-, 5d orbitals in the complex. The active set is enlarged by up to five layers of correlation orbitals.

Active set	$\Delta S_{\text{sms}}$	$\Delta\rho(0)$	$\Delta S_{\text{nms}}$
Complex	–0.401 31	–26.170	–0.104 88
Corr. 1	–0.587 62	–30.032	–0.165 04
Corr. 2	–0.595 22	–29.951	–0.141 31
Corr. 3	–0.566 57	–30.378	–0.189 93
Corr. 4	–0.561 83	–30.213	–0.191 24
Corr. 5	–0.561 25	–30.279	–0.192 19

**Table 8.** Computed and experimental transition isotope shift  $\Delta\nu = \nu_{115} - \nu_{113}$  (in GHz) for  $5s^2\ ^1S_0$ – $5s5p\ ^3P_1^o$ .

$\Delta\nu_{\text{nms}}$	$\Delta\nu_{\text{sms}}$	$\Delta\nu_{\text{vol}}$	$\Delta\nu_{\text{tot}}$
0.107	0.312	–0.935	–0.515
			–0.64(7) <sup>a</sup>

<sup>a</sup> Peik *et al* [2].

interference. To obtain a good value for the rate, both the hyperfine interaction and the transition matrix elements must be calculated with high accuracy. The off-diagonal magnetic hyperfine interaction constants needed to construct the Hamiltonian matrix elements are  $A(^3P_1^o, ^3P_0^o) = 3928$  MHz and  $A(^1P_1^o, ^3P_0^o) = 2916$  MHz. The reader may consult [29] for explicit formulae relating the interaction constants and the matrix elements. The off-diagonal magnetic hyperfine interaction constants give mixing coefficients  $c_1 = 1.02 \times 10^{-3}$  and  $c_2 = 3.47 \times 10^{-5}$  in good agreement with the values  $c_1 = 1.1 \times 10^{-3}$  and  $c_2 = 3.5 \times 10^{-5}$  derived by Peik *et al* from the Breit–Wills theory for a hyperfine structure in intermediate coupling. Using the transition matrix elements  $\langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^3P_1^o \rangle = 3.89 \times 10^{-2}$  and  $\langle 5s^2\ ^1S_0 \| \mathbf{Q}_1^{(1)} \| 5s5p\ ^1P_1^o \rangle = 8.21$  from the calculations reported in table 5 we obtain a transition rate  $A = 4.61\ \text{s}^{-1}$  corresponding to a lifetime  $\tau = 0.217\ \text{s}$  of the  $^3P_0^o$  state. This value should be compared with the experimental value  $\tau = 0.14(2)\ \text{s}$  determined by Peik *et al* [2]. One explanation for the difference between theory and experiment may be that the current calculation underestimates the transition matrix element for the intercombination transition. Another explanation could be that the neglected two-photon decay channel may be important. More work, both theoretical and experimental, is needed to clarify the situation.

## 5. Summary and conclusions

We report on relativistic multiconfiguration Dirac–Hartree–Fock calculations of oscillator strengths for electric dipole transitions in In II. In addition hyperfine structure constants and Landé  $g_J$ -factors are given. On the whole the calculations, that account for core polarization by means of explicit CI, give a good description of the energy structure. The calculated hyperfine magnetic dipole interaction constants are in excellent agreement with constants derived from Fourier transform spectra. For the electric quadrupole interaction constants the situation is different. Here there are substantial differences especially for the  $5snd\ ^3D$  states. These differences indicate that parameterizations using only diagonal interaction constants are

inadequate and that accurate descriptions of the experimental, partly resolved, line profiles must include also off-diagonal contributions [22].

Looking at the oscillator strengths there is good agreement between the results in the Coulomb and Babushkin gauges. The oscillator strengths from the spectrum calculations were compared with more accurate calculations for the  $5s^2\ ^1S_0-5s5p\ ^3P_1^o$  and  $5s^2\ ^1S_0-5s5p\ ^1P_1^o$  transitions where the correlation orbitals were targeted only on the states in the transition. The agreement between the two different sets of calculations is good, showing that the major correlation effects are captured in the spectrum calculations.

The calculated  $^{115-113}\text{In}$  isotope shift for the  $5s^2\ ^1S_0-5s5p\ ^3P_1^o$  transition is within the experimental error bars. The major uncertainty is the specific mass shift contribution which is very difficult to obtain accurately. Using calculated off-diagonal hyperfine interaction constants and electric dipole transition matrix elements the lifetime for the  $5s5p\ ^3P_0^o$  state was determined to 0.217 s. The computed lifetime is considerably longer than the experimental lifetime of 0.14(2) s, and the difference may be due to underestimated transition matrix elements.

## Acknowledgment

Financial support by the Swedish Research Council is gratefully acknowledged.

## References

- [1] Karlsson H and Litzén U 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 4475
- [2] Peik E, Hollemann G and Walther H 1994 *Phys. Rev. A* **49** 402
- [3] Indelicato P, Parente F and Marrus R 1989 *Phys. Rev. A* **40** 3505
- [4] Aboussaïd A, Godefroid M R, Jönsson P and Froese Fischer C 1995 *Phys. Rev. A* **51** 2031
- [5] Johnson W R, Cheng K T and Plante D R 1997 *Phys. Rev. A* **55** 2728
- [6] Larkins P L and Hannaford P 1993 *Z. Phys. D* **27** 313
- [7] Ansbacher W, Pinnington E H, Kernahan J A and Gosselin R N 1986 *Can. J. Phys.* **64** 1365
- [8] Hibbert A 1982 *Nucl. Instrum. Methods* **202** 323
- [9] Migdalek J and Baylis W E 1986 *J. Phys. B: At. Mol. Phys.* **19** 1
- [10] Migdalek J and Bojara A 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2221
- [11] Das B P and Idrees M 1990 *Phys. Rev. A* **42** 6900
- [12] Chou H-S and Huang K-N 1992 *Phys. Rev. A* **46** 3725
- [13] Chou H-S, Chi H-C and Huang K-N 1993 *Phys. Rev. A* **48** 2453
- [14] Lavin C and Martin I 1994 *J. Quant. Spectrosc. Radiat. Transfer* **52** 21
- [15] Biémont E and Zeippen C J 1999 *At. Data Nucl. Data Tables* **72** 101
- [16] Biémont E, Froese Fischer C, Godefroid M R, Palmeri P and Quinet P 2000 *Phys. Rev. A* **62** 032512
- [17] Asplund M, Grevesse N and Sauval A J 2005 *Cosmic Abundances as Records of Stellar Evolution and Nucleosynthesis in Honor of David L Lambert (ASP Conference Series vol 336)* ed T G Barnes III and F N Bash p 25
- [18] Jönsson P, He X, Froese Fischer C and Grant I P 2007 *Comput. Phys. Commun.* submitted
- [19] Grant I P 2007 *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation (Springer Series on Atomic, Optical, and Plasma Physics)* (Berlin: Springer)
- [20] McKenzie B J, Grant I P and Norrington P H 1980 *Comput. Phys. Commun.* **21** 233
- [21] Jönsson P and Froese Fischer C 1997 *Comput. Phys. Commun.* **100** 81
- [22] Andersson M, Jönsson P and Sabel H 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 4239
- [23] Jönsson P, Parpia F A and Froese Fischer C 1996 *Comput. Phys. Commun.* **96** 301
- [24] Andersson M and Jönsson P 2007 *Comput. Phys. Commun.* at press
- [25] Stone N J 2005 *At. Data Nucl. Data Tables* **90** 75
- [26] Grant I P 1974 *J. Phys. B: At. Mol. Opt. Phys.* **7** 1458
- [27] Olsen J, Godefroid M, Jönsson P, Malmqvist P Å and Froese Fischer C 1995 *Phys. Rev. E* **52** 4499
- [28] Dyall K G, Grant I P, Johnson C T, Parpia F A and Plummer E-P 1989 *Comput. Phys. Commun.* **55** 425



- 
- [29] Froese Fischer C, Brage T and Jönsson P 1997 *Computational Atomic Structure—An MCHF Approach* (Bristol: Institute of Physics Publishing)
- [30] Karlsson H 2002 *Spectroscopic Studies of the Elements Ba, Fe, Ga, In and Ru* (Lund University, Sweden: Atomic Astrophysics Lund Observatory)
- [31] Andersson M, Bieroń J and Jönsson P 2007 in preparation
- [32] Eberz J *et al* 1987 *Nucl. Phys. A* **464** 9