Atomic data from the Iron Project. LXIV. Radiative transition rates and collision strengths for Ca II *

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ABSTRACT

Aims. This work reports radiative transition rates and electron impact excitation rate coefficients for levels of the n= 3, 4, 5, 6, 7, 8 configurations of Ca II.

Methods. The radiative data were computed using the Thomas-Fermi-Dirac central potential method in the frozen core approximation and includes the polarization interaction between the valence electron and the core using a model potential. This method allows for configuration interactions (CI) and relativistic effects in the Breit-Pauli formalism. Collision strengths in LS-coupling were calculated in the close coupling approximation with the R-matrix method. Then, fine structure collision strengths were obtained by means of the intermediate-coupling frame transformation (ICFT) method which accounts for spin-orbit coupling effects.

Results. We present extensive comparisons with the most recent calculations and measurements for Ca II as well as a comparison between the core polarization results and the “unpolarized” values. We find that core polarization affects the computed lifetimes by up to 20%. Our results are in very close agreement with recent measurements for the lifetimes of metastable levels. The present collision strengths were integrated over a Maxwellian distribution of electron energies and the resulting effective collision strengths are given for a wide range of temperatures. Our effective collision strengths for the resonance transitions are within ~11% from previous values derived from experimental measurements, but disagree with latter computations using the distorted wave approximation.

Key words. atomic data - atomic processes - line: formation - stars: Eta Carinae - Active Galactic Nuclei

1. Introduction

Ca II plays an prominent role in astrophysics. The so-called H and K lines of this ion are important probes of solar and stellar chromospheres (Rauscher & Marcy 2000). In the red spectra of Active Galactic Nuclei (AGN) the infrared triplet of Ca II in emission has been used to investigate the correlations with optical Fe II (Joly 1989) and their implications on the physical conditions of the emitting gas (Ferland & Persson 1989). [Ca II] optical emission lines together with the infrared [Fe II] are often used as probe of dust content of AGNs (Shields et al. 1999).

Ca II has been addressed by numerous theoretical and experimental groups. The lifetimes τ for the 4p 2P0 and 3d 2D levels have been measured with high precision (Jin & Church 1993; Kreuter et al. 2005). Various theoretical methods have been used in trying to match these experimental values. The most recent calculations of Liaw (1995) using the Brueckner approximation with third-order correction agree within ~1% with the experimental lifetime for the 4p 2P0 levels but are ~11% too small for the 3d 2D metastable levels. The calculations of Kreuter et al. (2005), using a relativistic all-order method which sums infinite sets of many-body perturbation theory terms, agree within ~0.3% with the experimental lifetimes of the 3d 2D metastable levels of Ca II, but offer no data for other levels. Guet & Johnson (1991) computed lifetimes using relativistic many-body perturbation theory that agree within ~2% with experimental values for the 4p 2P0 levels and within ~6% for the metastable states. In the present work we use the Thomas-Fermi-Dirac central potential with core polarization interaction to provide a complete set of accurate A-values for allowed and forbidden transitions to be used in modeling Ca II spectra.

Various calculations of collision strengths have been performed for the resonance transitions in Ca II (see Zatsarinny et al. 1991; Chidichimo 1983; Kennedy et al. 1978; Saraph 1974). Osterbrock & Wallace (1977) derived effective collision strengths from experimental cross sections of the resonance K and H lines of Ca II at 3934 and 3968 Å by Taylor & Dunn (1973). Later, Zapesochnyi et al. (1975) published cross sections for exciting 5s and 4d levels from the ground state, which are important to estimate the contribution to the 4p level by cascade. Mitroy et al. (1988) presented a detailed study of...
the electron-impact excitation of the (4s-4p) transitions using the close-coupling approximation including a polarization potential. More recently [Burgess et al. (1995)] used a non-exchange distorted wave approximation including the lowest 7 Ca II terms.

The IRON Project is an international enterprise devoted to the computation of accurate atomic data for the iron group elements [Ulmer et al. (1993)]. A complete list of publications from this project can be found at http://www.iron-project.de. Within this project we have been systematically working on the data for the low ionization stages of iron peak elements, e.g. radiative and collisional rates for Fe I–IV (Bautista & Pradhan 1998), Ni II (Bautista 2001), Ni III (Bautista 2004), Ni IV (Eissner et al. 1974), but incorporates various improvements and new capabilities like two-body non-fine-structure operators of the Breit-Pauli Hamiltonian and polarization terms.

The objective of the present work is to provide accurate and complete atomic data for a detailed spectral modeling of Ca II. Such a model should be large enough to account for various processes such as collisional excitation including cascades from high levels, fluorescence by line and continuum radiation, and line optical depth effects.

2. Atomic data

2.1. Atomic structure calculations

We use the atomic structure code AUTOSTRUCTURE (Badnell 1984, 1997) to reproduce the structure of the Ca II ion. This code is based on the program SUPERSTRUCTURE originally developed by Eissner et al. (1974), but incorporates various improvements and new capabilities like two-body non-fine-structure operators of the Breit-Pauli Hamiltonian and polarization models. In this approach, the wave functions are written as configuration interaction expansions of the type:

\[ \psi_i = \sum_j \phi_j c_{ji}, \]

where the coefficients \( c_{ji} \) are determined by diagonalization of \( \langle \psi_i | H | \psi_i \rangle \). Here \( H \) is the Hamiltonian and the basic functions \( \phi_j \) are constructed from one-electron orbitals generated using the Thomas-Fermi-Dirac model potential (Eissner & Nussbaumer 1969), including \( \lambda_{nl} \) scaling parameters which are optimized by minimizing a weighted sum of energies. The basic list of configurations and scaling parameters used in this work are listed in Table 1.

Relativistic effects are included in the calculation by means of the Breit-Pauli operators in the form:

\[ H = H_{\text{nr}} + H_{\text{bp}}, \]

where \( H_{\text{nr}} \) is the usual non-relativistic Hamiltonian and \( H_{\text{bp}} \) is the Breit-Pauli perturbation, which includes one- and two-body operators (Jones 1970, 1971; Eissner et al. 1974).

2.2. Model potential

In order to obtain accurate orbitals in our multiconfiguration frozen-core approximation we include the polarization interaction between the valence electron and the core in a model potential. We used a model potential \( V_{\text{pol}} \) of the form described by Norcross & Seaton (1976):

\[ V_{\text{pol}}(r, \rho) = -\alpha_d \left[ 1 - \exp(-\rho/r)^6 \right], \]

where \( \alpha_d \) is the static dipole core polarizability of the ion Ca III and \( \rho \) is adjusted empirically to yield good agreement with experimental energies. Valley (1926) using the “non-penetrating” orbitals theory obtained \( \alpha_d = 3.31 \) for the d, f and g states. We adopt \( \rho = 2.25 \) the cut-off parameter. This yields accurate binding energies for the \( n=3,4,5,6,7 \) and 8 configurations of Ca II.

The expansion considered here for the Ca II system includes 23 LS terms. Table 2 presents the complete list of states included as well as a comparison between the calculated and observed target term energies, averaged over fine structure. Here, we show the energies without polarization interaction (w/o PI) and those with polarization interaction.

Table 1. Configuration expansion for Ca II, and scaling parameters \( \lambda_{nl} \) for each orbital of the configurations \( 1s^22s^22p^63s^23p^6nl \) in the Thomas-Fermi-Dirac potential

<table>
<thead>
<tr>
<th>( nl ) Configurations</th>
<th>( \lambda_{nl} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3d, 4s, 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 6f, 6g, 7s, 7d, 7f, 7g, 8s, 8d, 8f, 8g</td>
<td>1.438820, 2s: 1.11310, 2p: 1.05670, 3s: 1.10580, 3p: 1.09850, 3d: 1.07950, 4s: 1.08770, 4p: 1.07730, 4d: 1.07690, 4f: 1.05000, 5s: 1.08510, 5p: 1.07690, 5d: 1.07660, 5f: 1.04950, 5g: 1.01940, 6s: 1.08480, 6p: 1.07820, 6d: 1.07690, 6f: 1.04960, 6g: 1.01920, 7s: 1.08510, 7d: 1.07760, 7f: 1.05010, 7g: 1.01930, 8s: 1.08590, 8d: 1.07860, 8f: 1.05120, 8g: 1.01950</td>
</tr>
</tbody>
</table>

Table 2. Term energies for Ca II (in Ryd). The table shows results computed without PI (w/o PI), with PI and experimental energies from NIST V.3.1.0

<table>
<thead>
<tr>
<th>TERM</th>
<th>w/o PI</th>
<th>PI</th>
<th>NIST</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 4s 2S</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>2 3d 2D</td>
<td>0.147449</td>
<td>0.124596</td>
<td>0.124721</td>
</tr>
<tr>
<td>3 4p 2P</td>
<td>0.219659</td>
<td>0.232855</td>
<td>0.230916</td>
</tr>
<tr>
<td>4 5s 2S</td>
<td>0.454729</td>
<td>0.478864</td>
<td>0.475380</td>
</tr>
<tr>
<td>5 4d 2D</td>
<td>0.500830</td>
<td>0.524648</td>
<td>0.518602</td>
</tr>
<tr>
<td>6 5p 2P</td>
<td>0.529136</td>
<td>0.555242</td>
<td>0.552092</td>
</tr>
<tr>
<td>7 4f 2F</td>
<td>0.593486</td>
<td>0.623006</td>
<td>0.620180</td>
</tr>
<tr>
<td>8 6s 2S</td>
<td>0.618814</td>
<td>0.647386</td>
<td>0.644061</td>
</tr>
<tr>
<td>9 5d 2D</td>
<td>0.639097</td>
<td>0.667632</td>
<td>0.662741</td>
</tr>
<tr>
<td>10 6p 2P</td>
<td>0.652978</td>
<td>0.682121</td>
<td>0.678980</td>
</tr>
<tr>
<td>11 5f 2F</td>
<td>0.683576</td>
<td>0.713962</td>
<td>0.711101</td>
</tr>
<tr>
<td>12 5g 2G</td>
<td>0.683935</td>
<td>0.715180</td>
<td>0.712289</td>
</tr>
<tr>
<td>13 7s 2S</td>
<td>0.697115</td>
<td>0.727147</td>
<td>0.723986</td>
</tr>
<tr>
<td>14 6d 2D</td>
<td>0.707827</td>
<td>0.737833</td>
<td>0.733791</td>
</tr>
<tr>
<td>15 6f 2F</td>
<td>0.732574</td>
<td>0.763404</td>
<td>0.760526</td>
</tr>
<tr>
<td>16 6g 2G</td>
<td>0.732824</td>
<td>0.764166</td>
<td>0.761272</td>
</tr>
<tr>
<td>17 8s 2S</td>
<td>0.740613</td>
<td>0.771273</td>
<td>0.768206</td>
</tr>
<tr>
<td>18 7d 2D</td>
<td>0.749577</td>
<td>0.777594</td>
<td>0.779387</td>
</tr>
<tr>
<td>19 7f 2F</td>
<td>0.762129</td>
<td>0.793202</td>
<td>0.790315</td>
</tr>
<tr>
<td>20 7g 2G</td>
<td>0.762303</td>
<td>0.793703</td>
<td>0.790807</td>
</tr>
<tr>
<td>21 8d 2D</td>
<td>0.771345</td>
<td>0.802302</td>
<td>0.789935</td>
</tr>
<tr>
<td>22 8f 2F</td>
<td>0.781312</td>
<td>0.812527</td>
<td>0.809636</td>
</tr>
<tr>
<td>23 8g 2G</td>
<td>0.781436</td>
<td>0.812872</td>
<td>0.809975</td>
</tr>
</tbody>
</table>
tion (PI). It can be seen that the contribution of PI can reach up to 15%, especially for the lower energy terms.

In the calculation of radiative rates, fine-tuning of eigenstates is performed with term energy corrections (TEC), where the improved relativistic wave function, \(\psi_i^{\text{R}}\), is obtained in terms of the non-relativistic functions

\[
\psi_i^{\text{R}} = \psi_i^{\text{LS}} + \sum_{j \neq i} \psi_j^{\text{LS}} \times \frac{\langle \psi_j^{\text{LS}} | H_{\text{lp}} | \psi_i^{\text{LS}} \rangle}{E_i^{\text{LS}} - E_j^{\text{LS}}},
\]

with the LS energy differences \(E_i^{\text{LS}} - E_j^{\text{LS}}\) adjusted to fit weighted averaged energies of the experimental multiplets (Zeippen et al. 1977).

In our best target representation, which accounts for the interaction between the valence electron and the core, the theoretical energies for all 23 terms are typically within 2% of the experimental values before any further empirical correction. After TEC, the agreement with experimental energies is better than 1%.

For dipole-allowed transitions, spontaneous decay rates are given by

\[
A_{ij}^{E1} = 2.6774 \times 10^9 (E_i - E_j)^{3/2} \frac{1}{g_i} S_{ij}^{E1} \quad (s^{-1}),
\]

while for forbidden transitions we consider electric quadrupole (E2) and magnetic dipole (M1) transition rates given by

\[
A_{ij}^{E2} = 2.6733 \times 10^9 (E_i - E_j)^{3/2} \frac{1}{g_i} S_{ij}^{E2} \quad (s^{-1})
\]

and

\[
A_{ij}^{M1} = 3.5644 \times 10^4 (E_i - E_j)^{3/2} \frac{1}{g_i} S_{ij}^{M1} \quad (s^{-1}).
\]

Here, \(g_i\) is the statistical weight of the upper initial level \(i\), \(S_{ij}\) is the line strength and \(E\) is the energy in Rydbergs.

Eqs. (5,6 and 7) show that the transition rates are sensitive to the accuracy of the energy levels, particularly for forbidden transitions among nearby levels. Thus, we perform further adjustments to the transition rates by correcting our best calculated energies to experimental values.

In Fig. 1 we plot the \(gf\)-values for dipole allowed transitions among fine structure levels computed in the length gauge vs. those in the velocity gauge. We present the \(gf\)-values without PI (a) and with PI (b). The overall agreement between the two gauges is around 5% for \(\log\langle gf\rangle\)-values greater than -3 when accounting for PI and greater than 15% without PI. This is a good indicator of the quality of the dipole allowed radiative data.

In Table 3 we present an extensive comparison between the present results and previous lifetimes for the metastable levels 3d \(^2D_{3/2}\) and 3d \(^2D_{5/2}\). These levels are of particular astrophysical interest because they yield the prominent spectral lines \(\lambda\lambda\ 7293, 7326\ \text{Å}\). Our results including PI and TEC are in excellent agreement with experimental values, while the results that neglect PI are \(\sim 10\%\) too low.

### Table 3. Lifetimes of the metastable 3d \(^2D\) levels of Ca II

<table>
<thead>
<tr>
<th>Level</th>
<th>Present (w/o) PI</th>
<th>PI</th>
<th>Other</th>
<th>(\text{Experiment}(\tau(s)))</th>
</tr>
</thead>
<tbody>
<tr>
<td>3d (^2D_{3/2})</td>
<td>0.926</td>
<td>1.107</td>
<td>1.081 (1.176\pm0.011)^5</td>
<td>1.16^2</td>
</tr>
<tr>
<td>3d (^2D_{5/2})</td>
<td>0.901</td>
<td>1.08</td>
<td>1.058</td>
<td>1.168\pm0.009^5</td>
</tr>
</tbody>
</table>


In Table 3 we compare the calculated lifetimes for short-lived levels of Ca II from the present calculations with other theoretical and experimental values. For the lower levels \(4p\ \text{or}^2P_{1/2}\) and \(4p\ ^2P_{3/2}\) the effect of polarization interaction is \(\sim 20\%\). Overall, the differences between the results of our best model and experimental values are less than 5%, except for the level 5d \(^2D_{5/2}\). For this level, our result agrees with previous independent calculations but is about 40% below the experimental values of Andersen et al. (1970). A new measurement of this lifetime would be very important.

In Table 4 we present a comparison between calculated and experimental oscillator strengths in absorption. For the calculated oscillator strengths we choose the most complete and representative set of values as well as the most cited. We compare with previous calculations by Vaeck et al. (1992) where they use a multiconfiguration Hartree-Fock method with core polarization included variationally (SECP) using a model potential of the form de-
Table 4. Ca II lifetimes (in ns). The second column gives the results with neither PI (w/o PI) nor TECs (w/o TECs), the third column gives the results without PI (w/o PI) but with TEC, the fourth columns gives results with PI but no TEC, and the fifth column shows the results with both PI and TEC. Theoretical (Other) and experimental (Experiment) values from other authors are given in the sixth and seventh columns, respectively.

<table>
<thead>
<tr>
<th>Level</th>
<th>Present</th>
<th>Other</th>
<th>Experiment</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>w/o PI</td>
<td>TEC</td>
<td>w/o PI</td>
</tr>
<tr>
<td>4p 2P^0_{1/2}</td>
<td>6.978</td>
<td>5.734</td>
<td>6.697</td>
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<td></td>
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<tr>
<td>4p 2P^0_{3/2}</td>
<td>6.797</td>
<td>5.577</td>
<td>6.508</td>
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<td></td>
</tr>
<tr>
<td>4d 2D^2_{3/2}</td>
<td>2.963</td>
<td>2.779</td>
<td>2.781</td>
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<tr>
<td>4d 2D^2_{5/2}</td>
<td>2.981</td>
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<tr>
<td>4f 2F^5_{5/2}</td>
<td>3.625</td>
<td>2.656</td>
<td>3.487</td>
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<tr>
<td>4f 2F^7_{3/2}</td>
<td>3.625</td>
<td>2.654</td>
<td>3.486</td>
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<tr>
<td>5s 2S^1_{1/2}</td>
<td>4.310</td>
<td>3.833</td>
<td>3.886</td>
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<tr>
<td>5p 2P^0_{1/2}</td>
<td>40.195</td>
<td>34.903</td>
<td>36.541</td>
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<tr>
<td>5p 2P^0_{3/2}</td>
<td>38.987</td>
<td>33.755</td>
<td>35.783</td>
</tr>
<tr>
<td>5d 2D^2_{3/2}</td>
<td>5.960</td>
<td>5.625</td>
<td>5.895</td>
</tr>
<tr>
<td>5d 2D^2_{5/2}</td>
<td>6.002</td>
<td>5.669</td>
<td>5.944</td>
</tr>
<tr>
<td>6s 2S^1_{1/2}</td>
<td>7.007</td>
<td>6.390</td>
<td>6.391</td>
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<td>6p 2P^0_{1/2}</td>
<td>114.06</td>
<td>98.569</td>
<td>93.141</td>
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<tr>
<td>6p 2P^0_{3/2}</td>
<td>111.23</td>
<td>95.788</td>
<td>92.262</td>
</tr>
</tbody>
</table>


The inclusion of PI can affect the oscillator strengths by up to 12%. One finds very good agreement between the present calculation, previous calculations and experimental values.
In the close coupling (CC) approximation the total wave
function of the electron-ion system is represented as
\[ \psi(E; LS\pi) = A \sum_i \chi_i \theta_i + \sum_j c_j \Phi_j \] (8)
where \( \chi_i \) is the target ion wave function in a specific state
\( LS_i \), \( \theta_i \) is the wave function of the free electron, \( \Phi_j \) are short range correlation functions for the bound (\( e^+ \)ion) system, and \( A \) is the antisymmetrization operator.

The variational procedure gives rise to a set of coupled integro-differential equations that are solved with the R-matrix technique (Burke et al. 1971; Berrington et al. 1978, 1993). We use the LS-coupling R-matrix method that includes mass-velocity and Darwin operators and the polarization model potential. Note that the scattering calculations include one-body relativistic operators while the atomic structure calculations using AUTOSTRUCTURE include two-body operators of the Breit-Pauli Hamiltonian namely (two-body) fine-structure operators and (two-body) non-fine-structure operators.

The S-matrix elements determine the collision strength for a transition from an initial target state \( i \) to a final target state \( f \),
\[ \Omega_{if} = \frac{1}{2} \sum w |S_{if} - \delta_{if}|, \] (9)
where \( w = (2L+1)(2S+1) \) or \( (2J+1) \) depending on the coupling scheme, and the summation runs over the partial waves and channels coupling the initial and final states of interest.

In order to derive fine-structure results out of the LS-coupling calculation we employ the intermediate-coupling frame transformation (ICFT) method of Griffin et al. (1998). The ICFT method uses the multi-channel quantum defect theory (MQDT) to generate the LS-coupled unphysical \( K \)-matrices. In this approach one treats all scattering channels as open and calculates the term-coupling coefficients (TCCs) to transform the unphysical \( K \)-matrices to full intermediate coupling. Finally, we can generate the physical \( K \)-matrices on a fine energy mesh. Because all channels are treated as open this method eliminates the problems associated with the transformation of the physical \( S \)-matrices with closed channels and consequently yields accurate results for both background and resonances of the collision strengths at all energies.

The computations were carried out with the RMATRIX package of codes (Berrington et al. 1993) and also include the dipole polarization potential for the interaction of the valence electron and the core. The set of \((N+1)\)-electron wave functions to the right of the CC expansion in Eq. (8) includes all the configurations that result from adding an additional electron to the target configurations.

In Fig. 2 we compare the collision strengths for different target expansions. For the various close-coupling expansions we include all the terms that arise from the \( n=3, 4, 5, 6, 7 \) and 8 configurations. It is interesting to note that by increasing the number of terms in the close-coupling expansion the resonances tend to become better organized and blended, leading to regular broad series of structures. This is because of the increasing number of channels for decay of autoionizing levels. We adopt the expansion up to \( n=8 \) for all further calculations.

Partial wave contributions to the summation in Eqn. 3 were included from 162 \( SL\pi \) total symmetries with angular momentum \( L = 0 \rightarrow 40 \), total multiplicities \( (2S+1) = 1 \) and 3, and parities even and odd. As for the number of background waves, we consider all \( S \) states and \( J \) states up to \( J = 8 \). The various close-coupling expansions include all terms that arise from the \( n=3, 4, 5, 6, 7 \) and 8 configurations. It is interesting to note that by increasing the number of terms in the close-coupling expansion the resonances tend to become better organized and blended, leading to regular broad series of structures. This is because of the increasing number of channels for decay of autoionizing levels. We adopt the expansion up to \( n=8 \) for all further calculations.

### Table 5. Oscillator strengths for Ca II. The oscillator strengths from previous calculations of Vaeck et al. (1992), Theodosiou (1989), Guet & Johnson (1991) and Brage et al. (1993), and experimental data from Gallagher (1967) are also given.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Present</th>
<th>Vaek</th>
<th>Theodosiou</th>
<th>Guet</th>
<th>Brage</th>
<th>Experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td>4s S1/2 - 4p P1/2</td>
<td>0.364</td>
<td>0.323</td>
<td>0.318</td>
<td>0.316</td>
<td>0.320</td>
<td>0.321</td>
</tr>
<tr>
<td>4s 2S1/2 - 4p 2P3/2</td>
<td>0.734</td>
<td>0.652</td>
<td>0.641</td>
<td>0.637</td>
<td>0.645</td>
<td>0.649</td>
</tr>
<tr>
<td>3d 2D3/2 - 4p 2P1/2</td>
<td>0.0478</td>
<td>0.0537</td>
<td>0.0547</td>
<td>0.0473</td>
<td>0.0494</td>
<td>0.0524</td>
</tr>
<tr>
<td>3d 2P3/2 - 4p 2P1/2</td>
<td>0.0098</td>
<td>0.0110</td>
<td>0.0112</td>
<td>0.0096</td>
<td>0.0101</td>
<td>0.0107</td>
</tr>
<tr>
<td>3d 2D5/2 - 4p 2P3/2</td>
<td>0.0584</td>
<td>0.0656</td>
<td>0.0666</td>
<td>0.0574</td>
<td>0.0601</td>
<td>0.0637</td>
</tr>
</tbody>
</table>

### Table 6. Electric quadrupole (E2) and magnetic dipole (M1) transitions probabilities of [Ca II]. We compare our results with previous calculated values of Zeippen (1990), Ali & Kim (1988) and Vaeck et al. (1992).

<table>
<thead>
<tr>
<th>A(( s^{-1} ))</th>
<th>Type</th>
<th>Present</th>
<th>Zeippen</th>
<th>Ali and Kim</th>
<th>Vaeck</th>
</tr>
</thead>
<tbody>
<tr>
<td>3d 2D5/2 - 4s 2S1/2</td>
<td>E2</td>
<td>0.905</td>
<td>0.925</td>
<td>1.02</td>
<td>0.84</td>
</tr>
<tr>
<td>3d 2D5/2 - 4s 2S1/2</td>
<td>E2</td>
<td>0.928</td>
<td>0.945</td>
<td>1.05</td>
<td>0.86</td>
</tr>
<tr>
<td>3d 2D5/2 - 3d 2D3/2</td>
<td>M1</td>
<td>2.41×10^{-6}</td>
<td>2.45×10^{-6}</td>
<td>2.45×10^{-6}</td>
<td>2.45×10^{-6}</td>
</tr>
</tbody>
</table>
graphs represents the infinite energy limit of the collision
energies mapped onto the interval \([0,1]\). The last point in these
approach allows us to visualize the complete range of ener-
gies. We compare them with our present calculation
Ref. [Burgess & Tully (1992)]. This approach allows us to visualize the complete range of ener-
gies mapped onto the interval \([0,1]\). The last point in these
graphs represents the infinite energy limit of the collision
strengths \((\Omega)\). In Fig. 3 we plot reduced collision
strengths \((\Omega_r)\) as function of reduced energy \((E_r)\) follow-
ing the procedure describe by Ref. [Burgess & Tully (1992)].
This approach allows us to visualize the complete range of ener-
gies mapped onto the interval \([0,1]\). The last point in these
graphs shows good progression of the resonance structures for accurate calculations of effective
collision strengths for temperatures above \(\sim 5000\, \text{K}\).

A dimensionless thermally-averaged effective collision strength results from integrating the collision strength over
a Maxwellian distribution of electron velocities

\[
\Upsilon_{if} = \int_0^\infty \Omega_{if} \exp \left(\frac{-\epsilon_f}{kT}\right) d(\epsilon_f/kT),
\]

where \(\epsilon_f\) is the kinetic energy of the outgoing electron, \(T\)
the electron temperature in Kelvin and \(k = 6.339 \times 10^{-6}\,
\text{Ry/K}\) is the Boltzmann constant.

In Table 7 we compare the present effective collision strengths for the \(4s\rightarrow 4p\) transition of \(\text{CaII}\). We show
the values obtained by Ref. [Osterbrock & Wallace (1977)]
where they used experimental results of Ref. [Taylor & Dunn (1973)],
as reduced to collision strengths by Ref. [Seaton (1975)]. We also
present the values from Ref. [Burgess et al. (1995)] as we use their five point cubic spline fitting parameters to tabulate
the \(\Upsilon(T)\) using the procedure described in Ref. [Burgess & Tully (1992)]. We compare them with our present calculation
without PI in the target representation and in the scattering calculations \((\text{w/o PI})\); without PI in the R-matrix calculations
only \((\text{PI-S})\) and with PI. Our best results agree
within 11% of Ref. [Osterbrock & Wallace (1977)] values. On the other hand, the results of Ref. [Burgess et al. (1995)]
obtained with the non-exchange distorted wave approximation appear
overestimated by \(\sim 50\%\). In this calculation, the \(\text{CaII}\) target is represented in the frozen core approximation
neglecting polarization. As we pointed out before the main contribution of the dipole polarization potential is in the
representation of the target ion. Further, our effective collision
strengths when neglecting polarization are overestimated by 30% in closer agreement with Ref. [Burgess et al. (1995)].

3. Conclusions
We have computed radiative data, collision strengths and effective collision strengths for transitions among 41 levels
from the \(n=3, 4, 5, 6, 7\) and 8 configurations of \(\text{CaII}\). The
...
Fig. 4. Comparison between collision strengths for the Ca\textsuperscript{II} ion. The solid and dashed lines depict the results with and without model potential interaction respectively. The transitions are: (a) \(^3\text{D}_3/2 - 4\text{s}\(^2\text{S}_1/2\); (b) \(^3\text{D}_5/2 - 4\text{s}\(^2\text{S}_1/2\); (c) \(^2\text{P}^0_1/2 - 4\text{s}\(^2\text{S}_1/2\); (d) \(^2\text{P}^0_3/2 - 4\text{s}\(^2\text{S}_1/2\); (e) \(^3\text{D}_3/2 - 4\text{p}\(^2\text{P}^0_3/2\) and (f) \(^3\text{D}_5/2 - 4\text{p}\(^2\text{P}^0_3/2\).

Table 7. Effective collision strengths for the \(^4\text{s}\text{S} - 4\text{p}\text{P}^0\) transition Ca\textsuperscript{II}. The first three lines correspond to results of the present calculations for the cases of no PI in either the target orbitals of scattering calculation (w/o PI), PI in the scattering calculation only (PI-S), and PI in the target and scattering calculations (PI). These results are compared with values deduced from experimental cross sections (Osterbrock & Wallace 1977) (OW) and the most recent theoretical calculations (Burgess et al. 1995) (BCT).

<table>
<thead>
<tr>
<th>(T (k))</th>
<th>5000</th>
<th>10000</th>
<th>15000</th>
<th>20000</th>
</tr>
</thead>
<tbody>
<tr>
<td>w/o PI</td>
<td>19.03</td>
<td>20.82</td>
<td>22.45</td>
<td>24.03</td>
</tr>
<tr>
<td>PI-S</td>
<td>16.96</td>
<td>19.34</td>
<td>21.35</td>
<td>23.13</td>
</tr>
<tr>
<td>PI</td>
<td>17.07</td>
<td>19.44</td>
<td>21.45</td>
<td>23.23</td>
</tr>
<tr>
<td>OW</td>
<td>15.6</td>
<td>17.5</td>
<td>19.2</td>
<td>20.8</td>
</tr>
<tr>
<td>BCT</td>
<td>24.87</td>
<td>27.50</td>
<td>29.88</td>
<td>32.04</td>
</tr>
</tbody>
</table>

Radiative data were calculated using the Thomas-Fermi-Dirac central potential with a model core potential that account for dipole polarization interaction of the valence electron with the core. We also present an extensive comparison between our results and the most recent experiments and calculations for the lifetimes of Ca\textsuperscript{II}.

Effective collision strengths are available for various temperatures that expand from 3000 K to 38000 K. The whole set of data reported here including energy levels, infinite energy limit Born collision strengths, transition probabilities and effective collision strengths can be obtained in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5), via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/ or by request to the authors.

References
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