

Effective collision strengths^{*} for fine-structure transitions for the electron impact excitation of N II

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Abstract. We present effective collision strengths for the electron impact excitation of singly ionized nitrogen which have been calculated using the *R*-matrix method. The 23 lowest *LS* states are included in the expansion of the total wavefunction. These target states arise from the $2s^22p^2$, $2s2p^3$ and $2s^22p3l$ ($l = s, p, d$) configurations, leading to 41 fine structure levels and 820 possible transitions. The fine-structure collision strengths were obtained by transforming to a *jj*-coupling scheme using the JAJOM program of Saraph and have been determined at a sufficiently fine energy mesh to delineate properly the resonance structure. The effective collision strengths were calculated by averaging the electron collision strengths over a Maxwellian distribution of velocities. Tabulations of the non-zero effective collision strengths are given for electron temperatures (T_e) in the range $\log_{10} T_e(\text{K}) = 2.0\text{--}5.5$.

Key words. atomic processes – line: formation – methods: analytical

1. Introduction

The elements of carbon and nitrogen are amongst the most chemically abundant, and are of obvious importance to life on Earth. As such there has been much investigation into the role these elements and their ions play in terrestrial and extra-terrestrial processes. The data from astrophysical observations can be analysed and used to form plasma diagnostics for electron temperature and density.

For example, in the Orion Nebulae, Rubin et al. (2003) estimate electron temperature (T_e) and the fractional mean-square T_e variations (t_A^2) in the N^+ region of the nebula using emission lines at optical wavelengths of 5756 and 6585 Å. These lines arise from the $2s^22p^2\ ^1D_2^e\text{--}2s^22p^2\ ^1S_0^e$ and the $2s^22p^2\ ^3P_2^e\text{--}2s^22p^2\ ^1D_2^e$ transitions in N II. Observations from the ultraviolet spectrum are also used to form diagnostics – Czyzak et al. (1986) form electron and temperature diagnostics using the $2s^22p^2\ ^3P_1^e\text{--}2s2p^3\ ^5S_2^o$ and $2s^22p^2\ ^3P_2^e\text{--}2s2p^3\ ^5S_2^o$ transitions observed at 2139.7 and 2143.5 Å, in conjunction with optical lines at 6549.9 and 6585.2 Å. Infra-red emission lines have also been used – Keenan et al. (2001) base an electron density diagnostic on the 122 and 205 μm lines arising from the ($J = 1\text{--}2$) and ($J = 0\text{--}1$) transitions in the ground state 3P term of N II.

Two previous *R*-matrix calculations exist and provide effective collision strengths which are used to establish line

ratios, and from these electron temperature and density can be determined. The calculation of Lennon & Burke (1994) uses 12 *LS* target states whilst the calculation of Stafford et al. (1994) uses 13 *LS* target states. However, we note that the effective collision strengths from these two calculations are not in agreement. These discrepancies have been observed by Keenan et al. (2001), Rubin et al. (2003) and by Rodríguez (1999), who also uses the intensity ratio $I(\lambda 6548 + \lambda 6583)/I(\lambda 5754)$ to calculate the electron temperature in Galactic H II regions. Rodríguez (1999) notes that some of the abundance ratios derived are very sensitive to temperature, and the discrepancies between the two previous *R*-matrix calculations lead to differing estimates for the electron temperature $T_e[\text{N II}]$ – the results of Lennon & Burke (1994) imply temperatures ~ 200 K higher than those from Stafford et al. (1994).

The aim of the current work was initially to resolve the differences between the two previous *R*-matrix calculations and so produce a set of effective collision strengths that could be used with confidence. Thirteen of the transitions (those between the first 6 fine structure levels) have been examined in detail by the current authors (see Hudson & Bell 2004a) and we note that these effective collision strengths are in much better agreement with the calculation of Lennon & Burke (1994) than with the Stafford et al. (1994) data. We find that the agreement with Lennon & Burke (1994) is typically to within a few percent, and at worst no more than 10% at some high/low temperature extremities.

We can therefore have confidence that the work of Hudson & Bell (2004a) provided accurate effective collision strengths

* Table 2 is only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via <http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/430/725>

and that the approach can be extended to provide effective collision strengths for other transitions. Apart from data for individual transitions, there is a requirement for bulk data. Both neutral and singly-ionized nitrogen are known to be affected by non-LTE effects (Dufton & Hibbert 1981), and model atom for non-LTE line formation calculations require such bulk data.

The Hudson & Bell (2004a) work has therefore been extended and we here present effective collision strength data for all the transitions between the 41 fine structure levels included, with the temperature range of our data being extended to include temperatures down to 100 K so that we here give data in the electron temperature range of $\log_{10} T_e(\text{K}) = 2.0\text{--}5.5$.

2. Calculation details

The multi-channel R -matrix method as described by Berrington et al. (1987) is used to calculate the collision strengths for electron impact excitation of N II. The effective collision strength Ω_{if} can be expressed in terms of the cross section σ_{if} between an initial state i and a final state f as

$$\sigma_{if} = \Omega_{if} \frac{\pi a_0^2}{\omega_i k_i^2} \quad (1)$$

in which a_0 is the Bohr radius, ω_i is the statistical weight of the initial target level and k_i^2 is the incident kinetic energy in rydbergs. In this calculation, configuration-interaction (CI) wavefunctions were constructed for the 23 lowest N II states, namely $2s^2 2p^2 \ ^3P, \ ^1D, \ ^1S; 2s^2 2p^3 \ ^5S^o, \ ^3D^o, \ ^3P^o, \ ^1D^o, \ ^3S^o, \ ^1P^o; 2s^2 2p 3s \ ^3P^o, \ ^1P^o; 2s^2 2p 3p \ ^3P, \ ^3D, \ ^3S, \ ^3P, \ ^1D, \ ^1S; 2s^2 2p 3d \ ^3F^o, \ ^1D^o, \ ^3D^o, \ ^3P^o, \ ^1F^o, \ ^1P^o$. Each target state is represented by a configuration-interaction wavefunction expansion, constructed from the following set of orthogonal one-electron basis functions: $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f$. The radial part of each orbital is expressed as

$$P_{nl}(r) = \sum_{jnl} c_{jnl} r^{l_{jnl}} \exp(-\zeta_{jnl} r). \quad (2)$$

The orbital parameters c_{jnl} , l_{jnl} and ζ_{jnl} were optimised using the CIV3 program of Hibbert (1975). These optimisations and the orbital parameters obtained are given in Hudson & Bell (2004a) and will not be reproduced here. With the orbitals obtained, wavefunctions for the 23 N II target states are constructed using configurations generated by a two-electron replacement on the $2s^2 2p^2$ basis distribution, with the $1s$ shell being kept closed.

In Table 1, we compare the calculated LS target state energies (in rydbergs) for N II relative to the $2s^2 2p^2 \ ^3P$ ground state with experimental values from the NIST database available at <http://www.physics.nist.gov>. Such a comparison provides a useful test of the wavefunctions employed. From the ‘‘difference’’ column in Table 1 where we consider how close to experiment the calculated energies lie, we see that the agreement between the present theory and observed values is excellent. Thus we conclude that the wavefunctions employed are of sufficient accuracy for the R -matrix collision strength calculation. In Table 1 we also display the J -values available to each LS state and assign a J -level index to each of the 41 J -resolved levels.

Using these target state wavefunctions, the $(N + 1)$ ‘‘ion-plus-electron’’ system is described using the R -matrix method outlined by Burke & Robb (1975). Configurations describing the $(N + 1)$ -electron symmetries were generated through the addition of one electron from the orbital set to those configurations generated above by a two-electron replacement on the basis configuration. The R -matrix radius was calculated to be 18.0 atomic units and for each orbital angular momentum, 30 Schmidt-orthogonalized continuum orbitals were included, ensuring that a converged collision strength was obtained up to an incident electron energy of 14 Rydbergs ($1 \text{ Ryd} = 2.17987 \times 10^{-18} \text{ J}$). The correct positioning of resonances relative to the target states included in the calculation was ensured by adjusting our theoretical energies to the NIST values, prior to diagonalization of the Hamiltonian matrix. We note that for the close-lying thirteenth and fourteenth LS target states – $2s^2 2p^3 \ ^1P^o$ and $2s^2 2p 3p \ ^3S$ – the calculated energy levels differ in order from those in the NIST database. For these two levels, the calculated energies were adjusted to the arithmetic mean of the NIST values, i.e. 1.5294 Ryd.

In forming the $(N + 1)$ symmetries, we include all total angular momenta $0 \leq L \leq 12$ for both even and odd parities and doublet, quartet and sextet multiplicities. For dipole-allowed transitions, however, it was necessary to consider the effect of higher partial waves with $L > 12$ because they have a significant effect upon the collision strengths. The contributions from these higher partial waves is approximated by assuming the partial collision strengths form a geometric series expansion, with a geometric scaling factor given by the ratio of two adjacent terms. This ‘‘topping-up’’ procedure has been used successfully in similar calculations by Bell & Ramsbottom (2000), and Ramsbottom et al. (2001).

For small energy intervals between fine-structure levels, it is possible to recouple the matrices obtained from non-relativistic calculations in LS coupling to obtain the electron collision strengths between these levels. Above all the thresholds the effects of intermediate coupling in the target can be included by using this method. In the current work, the program of Saraph (1978) is used to carry out this recoupling procedure. Further details of the coupling scheme are given by Bell & Ramsbottom (2000).

Effective collision strengths Υ_{if} for a particular electron temperature T_e (in Kelvin) were obtained by averaging the electron collision strengths Ω_{if} over a Maxwellian distribution of velocities, so that

$$\Upsilon_{if}(T_e) = \int_0^\infty \Omega_{if}(E_f) \exp(-E_f/kT_e) d(E_f/kT_e) \quad (3)$$

where E_f is the final free electron energy after excitation and k is Boltzmann’s constant.

3. Results and discussion

The collision strengths presented in this work have been evaluated for a fine mesh of incident impact energies, at energy intervals typically in the region of 0.0001 Rydbergs across the energy range considered (0 to 14 Ryd). This ensured that the

Table 1. Energy levels in Rydbergs for the 23 LS target states included in the calculation, relative to the $2s^22p^2\ ^3P^e$ ground state. Also shown are the experimental values of NIST and the difference between the calculated and observed energies. The J -values arising from each LS state are also noted along with the J level index assigned to each of the fine structure levels.

LS state	Current LS	Observed LS	Difference	J -value	J -index
	Energy (Ryd)	Energy (Ryd)			
$2s^22p^2\ ^3P^e$	0.0000	0.0000	0.0000	0	1
				1	2
				2	3
$2s^22p^2\ ^1D^e$	0.1485	0.1396	0.0089	2	4
$2s^22p^2\ ^1S^e$	0.3155	0.2979	0.0176	0	5
$2s2p^3\ ^5S^o$	0.4114	0.4263	0.0149	2	6
$2s2p^3\ ^3D^o$	0.8454	0.8406	0.0048	1	7
				2	8
				3	9
$2s2p^3\ ^3P^o$	1.0108	0.9953	0.0155	0	10
				1	11
				2	12
$2s2p^3\ ^1D^o$	1.3350	1.3139	0.0211	3	13
$2s^22p3s\ ^3P^o$	1.3560	1.3579	0.0019	0	14
				1	15
				2	16
$2s^22p3s\ ^1P^o$	1.3615	1.3595	0.0020	1	17
$2s2p^3\ ^3S^o$	1.4389	1.4136	0.0253	1	18
$2s^22p3p\ ^1P^e$	1.5240	1.5000	0.0240	1	19
$2s^22p3p\ ^3D^e$	1.5413	1.5183	0.0230	1	20
				2	21
				3	22
$2s2p^3\ ^1P^o$	1.5605	1.5197	0.0408	1	23
$2s^22p3p\ ^3S^e$	1.5587	1.5391	0.0196	1	24
$2s^22p3p\ ^3P^e$	1.5690	1.5550	0.0140	0	25
				1	26
				2	27
$2s^22p3p\ ^1D^e$	1.5987	1.5875	0.0112	2	28
$2s^22p3p\ ^1S^e$	1.6315	1.6245	0.0070	0	29
$2s^22p3d\ ^3F^o$	1.7006	1.7003	0.0003	2	30
				3	31
				4	32
				2	33
$2s^22p3d\ ^1D^o$	1.7056	1.7049	0.0007	2	33
$2s^22p3d\ ^3D^o$	1.7085	1.7084	0.0001	1	34
				2	35
				3	36
$2s^22p3d\ ^3P^o$	1.7218	1.7212	0.0006	0	37
				1	38
				2	39
$2s^22p3d\ ^1F^o$	1.7279	1.7253	0.0026	3	40
$2s^22p3d\ ^1P^o$	1.7366	1.7325	0.0041	1	41

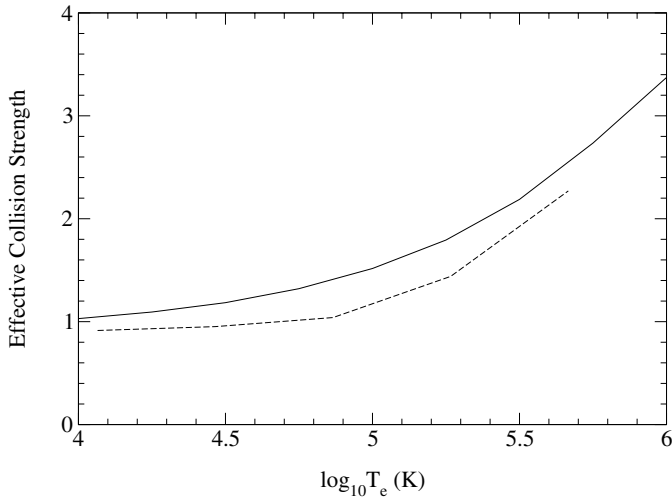


Fig. 1. Effective collision strengths for the $2p^2 \ ^1D-3s \ ^1P^o$ allowed transition in N II as a function of the electron temperature (in K): — present, - - - Frost et al.

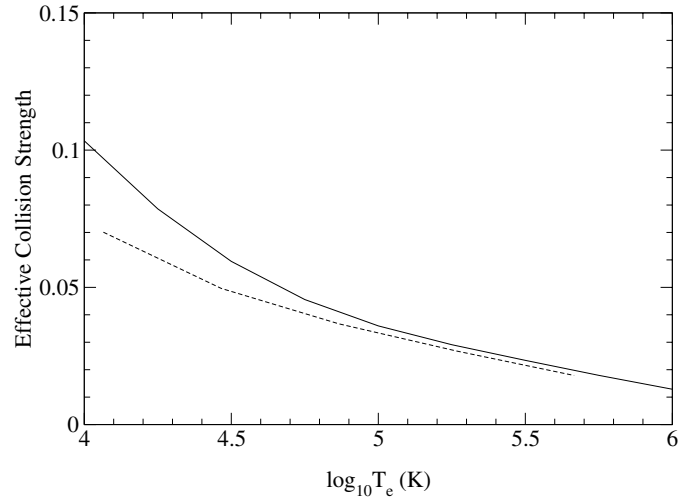


Fig. 2. Effective collision strengths for the $2p^2 \ ^1S-3p \ ^1P$ forbidden transition in N II as a function of the electron temperature (in K): — present, - - - Frost et al.

autoionizing resonances which converge to the target state thresholds were fully delineated.

Those resonances located at energies lower than the highest target threshold considered in this work ($2s^2 2p 3d \ ^1P^o$) are physically meaningful; however at higher energies (i.e. above 1.7325 Ryd) pseudo-resonances appear. These arise from the inclusion of pseudo-orbitals in the wavefunction expansion (Burke et al. 1981). At higher temperatures the high-impact energy region is much more important and so it is necessary to properly average over the pseudo-resonances to prevent distortion of the correct results in the calculation of the effective collision strengths.

We note that a slightly finer mesh was used here than for the 13 transitions given in Hudson & Bell (2004a). However, we find that this has very little impact on the effective collision strengths – at most a difference of about 1% is observed at the high temperature extremity for these transitions. For the majority of the transitions the difference is negligible, but we highlight this difference here to account for minor discrepancies between the data presented in this paper and those given by Table 3 in Hudson & Bell (2004a). The values which have been affected are for the temperature $\log_{10} T_e(\text{K}) = 5.0$ and for the transitions labelled 1–2, 1–3, 2–3 and 4–5.

The inclusion of the 23 *LS* target states leads to 41 *J* levels and a total of 820 transitions. In Table 2 available at the CDS we present the 805 non-zero effective collision strengths for a range of electron temperatures [$\log_{10} T_e(\text{K}) = 2.0-5.5$] suitable for application in plasma and astronomical diagnostics. Table 2 contains the following information: Col. 1 lists the transitions between fine-structure states indicated as initial–final according to the *J*-index assigned to each fine-structure level in Table 1. For example, 1–14 denotes the transition $2s^2 2p^6 \ ^3P_0-2s^2 2p 3s^3 P_0^o$. The remaining 12 columns list the effective collision strengths for each transition at the following logarithmic electron temperatures $\log_{10} T_e(\text{K}) = 2.00, 2.25, 2.50, 2.75, 3.00, 3.25, 3.50, 3.75, 4.00, 4.50, 5.00, 5.50$.

As noted above, comparisons of some of the low-lying transitions with the work of Lennon & Burke (1994) and Stafford et al. (1994) were performed by the current authors in Hudson & Bell (2004a). For these low-lying transitions, we found better agreement with Lennon & Burke (1994) than with Stafford et al. (1994). The present calculation contains additional target states than were used in the work of Stafford et al. (1994) and so achieves a better representation. The current work also ensured that the resonance structure was properly defined, particularly above threshold.

We have also (see Hudson & Bell 2004b) performed comparisons with experimental data – measured rate coefficients for six transitions – obtained by Frost et al. (1998). The Frost et al. paper also gives effective collision strengths obtained from a 23-state *R*-matrix calculation, and as reported in Hudson & Bell (2004b), for the six experimental transitions discussed, we find good agreement with the Frost et al. (1998) calculated values.

The six transitions discussed are excitations from the ground state $2s^2 2p^2 \ ^3P$ level, and we here present effective collision strengths for two transitions involving excitations from the second and third lowest lying *LS* states – $2s^2 2p^2 \ ^1D$ and $2s^2 2p^2 \ ^1S$. The calculation of Frost et al. (1998) was performed in *LS* coupling, thus only giving effective collision strengths for transitions between *LS* levels, and without the use of pseudo-orbitals. Figure 1 displays the effective collision strengths from the current work along with the Frost et al. data for the excitation from the $2p^2 \ ^1D$ level to the $3s \ ^1P^o$ level. We have displayed the data over the range of electron temperatures given in Frost et al. In Fig. 2 we show the $2p^2 \ ^1S-3p \ ^1P$ forbidden transition.

For both the transitions in Figs. 1 and 2, we find that the current work gives an effective collision strength which is slightly higher than that of Frost et al. (1998). For the allowed transition in Fig. 1, the current calculation gives an effective collision strength which is about 14% higher than Frost et al. (1998) at

the low temperature end of the graph. This rises to a difference of about 35% around $\log_{10} T_e(\text{K}) = 5.0$ before the two sets of data begin to converge again at higher temperatures. For the forbidden transition shown in Fig. 2, the differences exhibited are about 40% in the initial region, falling to 10% at the high temperature extremity.

These two transitions are indicative of the accuracy of the present calculation which we believe to be more sophisticated than any previous calculation. Thus at the higher temperatures an accuracy of better than 10% may be expected for transitions from lower levels of N II. For transitions from higher levels and for lower temperatures the accuracy may not be as good.

4. Conclusions

In this paper we extend a previous calculation of effective collision strengths for electron impact excitation of the N II ion. These astrophysically important atomic data are evaluated for a large range of electron temperatures, ($\log_{10} T_e(\text{K}) = 2.0\text{--}5.5$) and for all transitions among the lowest 23 *LS* states of N II, corresponding to 41 fine-structure levels and 820 individual transitions. From earlier comparisons carried out by the present authors (Hudson & Bell 2004a,b) we believe that the present results are the most accurate currently available.

All the effective collision strength data for the transitions noted in Table 2 over the temperature range $\log_{10} T_e(\text{K}) = 2.0\text{--}5.5$ (in steps of 0.1 dex) are available, along with the electron collision strengths, by contacting the authors.

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