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Letter to the Editor

The collision strength of the [Ne V] infrared fine-structure lines*

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Abstract. The calculation of accurate collision strengths for atomic transitions has been a long standing problem in quantitative spectroscopy. Most modern calculations are based on the R-matrix method and problems pertaining to the use of this method have led to a discussion of the accuracy of these results. More in particular, based on an analysis of the spectra of NGC 3918 and NGC 6302, Clegg et al. (1987) and Oliva et al. (1996) have questioned R-matrix calculations for the infrared [Ne V] fine-structure transitions. Using improved flux measurements for the [Ne V] lines, we show that the conclusion that these collision strengths would be too high, is not correct. The discrepancies found by Clegg et al. (1987) can be explained by the inaccuracy of the [Ne V] 342.6 nm flux they adopted. The discrepancies found by Oliva et al. (1996) can be explained by the inaccuracy of the *LRS* flux for the [Ne V] 14.32 μm line. Based on the data presented in this paper there is *no reason* to assume that there are any problems with the R-matrix calculations for Ne^{4+} of Lennon & Burke (1994). We show that the data are accurate at the 30 % level or better. This confirms the validity of the close coupling method.

Key words: atomic data – plasmas – ISM: planetary nebulae: individual: NGC 3918 – ISM: planetary nebulae: individual: NGC 6302 – ISM: planetary nebulae: individual: NGC 7027 – infrared: ISM: lines and bands

1. Introduction

The calculation of accurate collision strengths for atomic transitions has been a long standing problem in the field of quantitative spectroscopy. Any calculation involving atoms in non-LTE conditions requires the knowledge of vast numbers of collision strengths in order to make these calculations realistic and accurate. Until recently the computing power was simply not available to calculate collision strengths in a systematic way. One either had to resort to simpler and more approximate methods or one had to limit the calculations to only the most important transitions. This situation has now changed with the start of the Iron Project (Hummer et al. 1993), which aims to produce a large database of accurately calculated collision strengths.

The collision strength for an atomic transition depends strongly on the energy of the colliding electron and shows many resonances (e.g., Aggarwal 1984). Such resonances occur when the total energy of the target ion and the colliding electron correspond to an auto-ionizing state. In order to calculate these resonances accurately, a fine grid of energy points is necessary. This is a type of problem for which R-matrix methods are very well suited. However, a source of uncertainty in these calculations is that the energies of most auto-ionizing states have not been measured in the laboratory and therefore need to be derived from calculations. It is a well known fact that the resulting energies are not very accurate and hence the positions of the resonances are also uncertain. Since the collision strengths are usually folded with a Maxwellian energy distribution, this is not a major problem for high temperature (i.e., X-ray) plasmas where the distribution is much broader than the uncertainty in the position of the resonances. However, for low temperature (e.g., photo-ionized) plasmas this can lead to problems if a resonance is present near the threshold energy for the transition. If only the high-energy tail of the Maxwellian distribution is capable of inducing a collisional transition, then a small shift in the position of a near-threshold resonance can have a severe impact on the effective collision strength. This effect would be even more pronounced if the resonance shifts below the transition threshold and disappears completely.

The inclusion of resonances in the calculation of collision strengths can lead to much higher values than were previously published (see Table 2 in Oliva et al. 1996). This is also illustrated in Table 1 where we show various calculations of the effective collision strength of transitions within the ground term of Ne^{4+}. One can see that the R-matrix calculations of Aggarwal (1983) and Lennon & Burke (1991, 1994) yield substantially larger results than the previous calculations. This is caused by the presence of a large complex of strong resonances at low

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Table 1. Comparison of various determinations of the effective collision strengths for transitions within the ground term of Ne^{4+}. The values are for T_e = 10 000 K.

ref.	$^3P_0 - ^3P_1$	$^3P_0 - ^3P_2$	$^3P_1 - ^3P_2$
Blaha (1969)	0.251	0.132	0.611
Osterbrock (1974)	0.23	0.11	0.53
Aggarwal (1983)	1.463	1.810	5.901
Lennon & Burke (1991)	1.401	1.766	5.725
Lennon & Burke (1994)	1.408	1.810	5.832

Table 2. Log of the *SWS* observations. The AOT's are described in de Graauw et al. (1996), SWS01–4 stands for SWS01 speed 4.

Source	Date	Rev.	AOT	$F(14.32)$	$F(24.32)$
				10^{-14} W m^{-2}	
NGC 7027	11 Dec 1995	24	SWS01–4	160.	47.0
NGC 7027	19 Dec 1995	32	SWS02	136.	40.9
NGC 7027	6 Nov 1996	356	SWS02	141.	47.1
NGC 6302	19 Feb 1996	94	SWS01–4	65.2	29.7
NGC 6302	20 Feb 1997	462	SWS06	63.4	30.8

energies (see Fig. 5 in Aggarwal 1984). This large difference has led to a discussion of the validity the R-matrix calculations (Clegg et al. 1987, C87; Oliva et al. 1996, O96). Both authors tested the calculations by comparing predicted flux ratios with observations and both concluded that the R-matrix calculations yielded results that are too high. Nebulae offer powerful tests of atomic physics, and have revealed incomplete treatment in the past (Péquignot et al. 1978, Harrington et al. 1980). However, both C87 and O96 base their conclusions on only one nebula and both include *LRS* data in their analysis. Since the accuracy of *LRS* data is limited to approximately 30 % (Pottasch et al. 1986), a re-analysis based on more accurate *SWS* data is warranted. In this paper we will present a test of the R-matrix calculations for Ne^{4+} by applying them to observational data of NGC 3918, NGC 6302 (the nebulae studied by C87 and O96, respectively) and NGC 7027. This will yield a larger and more accurate sample for the discussion.

2. The observational data and analysis

Several *SWS* observations were obtained for the objects studied in this paper. A log of the observations is shown in Table 2. The instrument is described in de Graauw et al. (1996). The observations used three different templates: SWS01 – a spectral scan from 2.4 μm to 45 μm, SWS02 – a set of grating scans of individual lines, and SWS06 – a high resolution grating scan. All *SWS* spectra of NGC 7027 were obtained during calibration time. The complete SWS06 spectrum of NGC 6302 is published in Beintema & Pottasch (1999). An *SWS* spectrum of NGC 3918 was also obtained, but not used. Due to inaccurate pointing the source was partially outside the aperture.

The line fluxes were measured in spectra reduced with the *SWS* interactive-analysis software. The line fluxes were virtually identical to those derived from the standard *ISO* auto-analysis products. The various *SWS* measurements were subsequently averaged. Table 3 shows the dereddened line fluxes we have adopted for our study. The values adopted by C87 and O96 are also shown for comparison. The extinction corrected [Ne V] 342.6 nm fluxes were taken from the original publications. Both for NGC 7027 and NGC 6302 the dereddening is complicated by the fact that the extinction varies over the nebula. The correction for the blend in NGC 3918 is discussed below. The infrared line fluxes were dereddened using the law from Mathis (1990).

Table 3. The values for the line fluxes (corrected for reddening) and the extinction adopted in this work. Entries in italics are assumed. The rows labeled O96 and C87 give the values adopted by Oliva et al. (1996) and Clegg et al. (1987).

source	$F(342.6)$	$F(14.32)$	$F(24.32)$	$c(\mathrm{H}\beta)$
		10^{-14} W m^{-2}		dex
NGC 7027	204.[a]	153.	46.9	1.37±0.05[a]
NGC 6302	70.[b]	67.2	31.4	1.23±0.10[c]
O96	86.[c]	45.7[d]	32.3[d]	1.23±0.10[c]
NGC 3918	7.4[e]:	12.[f]	*8.1*	0.43±0.05[g]
C87	20.[g]	12.[f]	—	0.43±0.05[g]

[a] Middlemass (1990) [b] Beintema & Pottasch (1999) [c] Oliva et al. (1996) [d] Rowlands et al. (1994) [e] Aller & Faulkner (1964), corrected for blend [f] Pottasch et al. (1986) [g] Clegg et al. (1987)

Table 4. This table first shows the observed line flux ratios, R_1 and R_2. Next it shows the derived values for the electron temperature and density and finally the expected values for these quantities. Entries in italics are assumed.

	NGC 3918	NGC 6302	NGC 7027
R_1	1.65±0.74	0.96±0.42	0.75±0.17
R_2	*1.50*	2.14±0.29	3.26±0.29
T_e/K	18 000±2400	20 800±3000	20 400±1700
n_e/cm^{-3}	*4 900*	12 300±3300	26 900±4100
T_e/K (exp.)	13 900	19 000	18 000
n_e/cm^{-3} (exp.)	4 900	15 000	37 100

To calculate the diagnostic diagrams we used the effective collision strengths given in Lennon & Burke (1994) and adopted the transition probabilities from Baluja (1985). We used a 5-level atom to calculate the relative level populations. The results of our analysis are shown in Table 4 and Fig. 1. The line flux ratios are defined as: $R_1 = I(14.32)/I(342.6)$ and $R_2 = I(14.32)/I(24.32)$. To determine the uncertainties in the line ratios we included contributions from the absolute calibration accuracy of the UV and IR data, the internal calibration accuracy of the SWS data and the uncertainty in the extinction correction. We will now discuss the results for each nebula separately.

2.1. NGC 7027

We have included this nebula in our sample because it is bright and well studied. This assures that accurate values for the

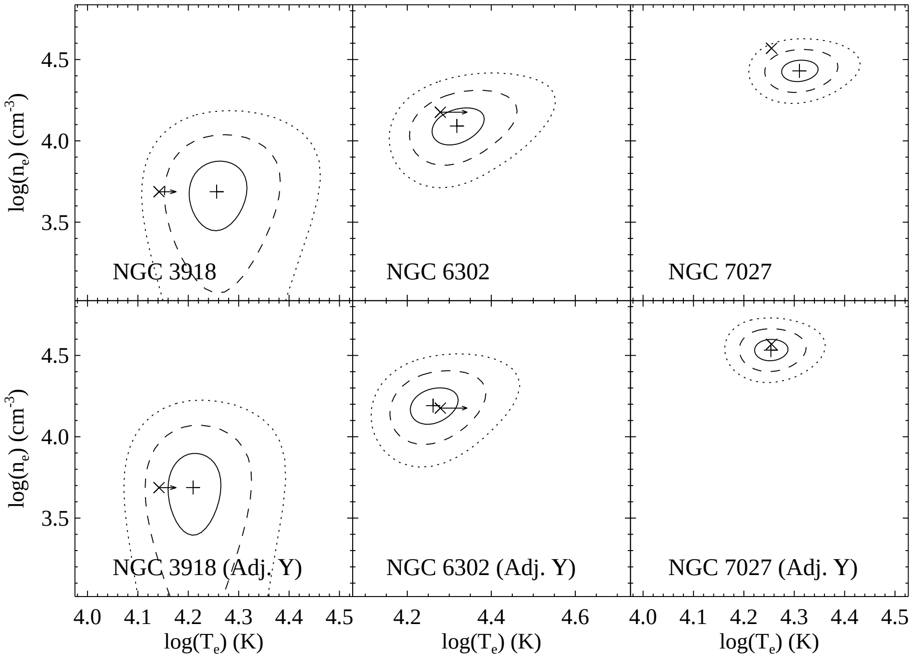

Fig. 1. In these graphs the electron temperature and density derived from the [Ne V] lines is marked with a $+$. The solid, dashed and dotted lines are the 1 σ, 2 σ and 3 σ contours respectively. The expected value of the electron temperature and density, based on either photo-ionization modeling or other line-ratio diagnostics, is indicated with an $\times$. An arrow indicates the estimated increase of the electron temperature if temperature stratification is taken into account. The top row was obtained using the effective collision strengths Υ given by Lennon & Burke (1994), the bottom row was obtained by lowering the Υ's for transitions within the ground term by 30 %.

Table 5. The temperature stratification in NGC 7027, derived from our photo-ionization model (Beintema et al. 1996). The temperature is defined as $\int n_{\rm e} n_{\rm ion} T_{\rm e} {\rm d}V / \int n_{\rm e} n_{\rm ion} {\rm d}V$.

ion	$\chi_{\rm ion}$/eV	$T_{\rm e}$/K	ion	$\chi_{\rm ion}$/eV	$T_{\rm e}$/K
O^0	13.62	10 450	O^{2+}	54.94	13 520
N^+	29.60	12 140	Ar^{3+}	59.81	14 670
Ar^{2+}	40.74	12 990	Ar^{4+}	75.02	16 180
S^{2+}	34.83	13 100	Ne^{3+}	97.12	16 350
C^{2+}	47.89	13 440	Ne^{4+}	126.2	17 990

fluxes needed in our analysis are available. Additionally, we have a detailed photo-ionization model (Beintema et al. 1996) which allows us to derive good estimates for the expected electron temperature and density. For a high excitation nebula like NGC 7027, significant temperature stratification of the plasma can be expected. We have illustrated this effect in Table 5 where we show the average electron temperature in various line forming regions. One can see that the electron temperature rises almost monotonically with the ionization potential $\chi_{\rm ion}$. It is important to note that the temperature in the Ne^{4+} region is substantially higher than the temperature in any other line forming region observed in the spectrum. The expected values for the electron temperature and density are based on our photo-ionization model. The analysis of the [Ne V] lines gives a result which deviates less than 3 σ from these values.

2.2. NGC 6302

This is the nebula studied by O96. The [Ne V] temperature and density for this nebula were already derived from the SWS06 spectrum by Pottasch & Beintema (1999). In our analysis we will include the SWS01–4 spectrum as well. The expected values for the electron temperature and density are those of O96. Our analysis gives a result which deviates slightly more than 1 σ from these values. The preferred temperature of O96 is based on various determinations using ions with lower ionization potentials than Ne^{4+}. In view of the discussion in the previous section concerning temperature stratification, this estimate is probably too low. Especially in view of the temperatures derived by O96 from rather low excitation line ratios like [S III], [Ar III] and [O III] which range between 18 100 K and 19 400 K, the [Ne V] temperature may be expected to be considerably higher than 19 000 K. A temperature of 22 000 K is more realistic (see the discussion in Pottasch & Beintema 1999). This value for the temperature is indicated by an arrow in Fig. 1. After this correction the discrepancy is slightly less than 1 σ.

2.3. NGC 3918

This is the nebula studied by C87. The intensity for the [Ne V] 342.6 nm line is in doubt. C87 quote $I(342.6) = 80$, but it is not clear how this value was obtained. We decided to use the value quoted in Aller & Faulkner (1964) instead. From the discussion in that article it is not clear whether the data were corrected for interstellar extinction. The intensities they quote for other strong blue emission lines compare well with the dereddened intensities given by C87 and we therefore assume that the Aller & Faulkner (1964) data are corrected for interstellar extinction. They give $I(342.6{+}342.9{+}344.4) = 60$. The correction for the blend with the O III 342.9 nm and 344.4 nm Bowen resonance-fluorescence lines is easy, since the O III 313.3 nm line has been measured by C87. The O III 313.3 nm, 342.9 nm and 344.4 nm lines all originate from the same upper level ($2s^2\,2p\,3d\,^3P^\circ_2$) and the intensity ratio of the lines is simply given by the ratio of the transition probabilities times the photon energy. Using Opacity Project data (Luo et al. 1989) one finds $I(313.3) : I(342.9) :$

$I(344.4)$ = 10.94 : 1.00 : 2.94. C87 gives $I(313.3) = 85$. Hence $I(342.9 + 344.4) = 30.6$ and $I(342.6) = 29.4$. This result is substantially lower than the value used by C87. We were not able to correct the *SWS* spectrum accurately for aperture effects and therefore preferred to use the *LRS* flux for the [Ne V] 14.32 μm line. To complete the data set, we assumed a value for the 24.32 μm flux such that the resulting density agreed with the expected value. None of the flux values we adopted for this nebula can be considered accurate and re-measurement is warranted. The expected values for the electron temperature and density were determined by averaging the data in Table 12 of C87. For the temperature we only used the values derived from the [Ar V], [Ne IV] and [Ne V] line ratios, for the density we used all values except those derived from [Mg I], [N IV] and [O IV] lines. One can see that there is a slightly more than 2 σ discrepancy for the electron temperature. Again the expected value for the electron temperature may be underestimated due to temperature stratification. We think 15 000 K is in all probability a more realistic, though still conservative, estimate. This value for the temperature is indicated by an arrow in Fig. 1. After this correction there is a 1.5 σ discrepancy.

3. Discussion

A major advance in atomic theory in the past decade has been close coupling calculations that include resonances. These new calculations (carried out with an R-matrix code) can raise the collision strength by an order of magnitude or more compared to older calculations. These large differences have led to a discussion of the validity of these calculations. Nebulae offer powerful laboratories for verifying atomic processes, and two studies (C87 and O96) used this approach to test the R-matrix calculations for Ne^{4+}. They found that spectra of planetary nebulae did not agree with the R-matrix results. This casted doubt on the validity of the close coupling calculations.

In this paper we have redone the analysis carried out by C87 and O96 using newer, more accurate data. We also included the well studied nebula NGC 7027 in the analysis to obtain a larger sample. We found that the expected values of the electron temperature and density all were within 3 σ of our results. Hence there is no proof for significant problems with the R-matrix calculations. On closer inspection one sees that the largest discrepancy is for NGC 7027, the best studied nebula. Also the electron temperature derived from our analysis is systematically higher than the expectation value for all nebulae. This could point to inaccuracies in the collision strengths. To check this point further, we have re-analyzed our sample using effective collision strengths which were lowered by 30 % for transitions within the ^3P ground term. The results are shown in the bottom row of Fig. 1. They are in good agreement with the expected values. Hence the R-matrix calculations for Ne^{4+} could be off by 30 %, but certainly not more. We point out that this is significantly less than the factor ~2.7 suggested by O96. An alternative explanation could be that the [Ne V] 342.6 nm fluxes are systematically overestimated due to a problem with the extinction curve, or a combination of the two effects.

We reach the following main conclusions:

1. The discrepancies found by C87 can be explained by the inaccuracy of the [Ne V] 342.6 nm flux they adopted. The discrepancies found by O96 mainly stem from the inaccuracy of the *LRS* measurement of the [Ne V] 14.32 μm line.
2. Based on the data presented in this paper there is *no reason* to assume that there are any problems with the collision strengths for Ne^{4+} calculated by Lennon & Burke (1994). Our analysis has shown that the data are accurate at the 30 % level or better. This confirms the validity of close coupling calculations.

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