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Review of Current Light Species Electron-impact Excitation Data in the CFADC Database

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ABSTRACT: An update is given on the recommended electron-impact excitation data currently available for light species (H through to Ne) in the Controlled Fusion Atomic Data Center (CFADC) database. This data is unlikely to undergo significant revision for most of the ion stages in this range. The ion stages that require further study are indicated.

1. INTRODUCTION

Electron-impact excitation is the dominant means of populating excited states of atoms in a wide range of laboratory and astrophysical plasmas. Emission from excited levels that are populated via electron-impact excitation thus provide diagnostic information on a wide range of astrophysical objects, including H II regions [1], planetary nebulae [2], supernova remnant plasmas [3], and stellar coronae [4]. Similar diagnostics exist in laboratory plasmas such as fusion tokamaks [5], helicon plasmas [6], and light sources [7].

The quality of any spectral diagnostic based on emission from such plasmas thus depends critically on the quality of the electron-impact excitation data that the collisional-radiative modeling is based upon. For example, the need for accurate temperature diagnostics of planetary nebulae was the driving force behind the application of close coupling methods, such as the *R*-matrix approach, to atomic systems. A range of methods can be used to calculate electron-impact excitation data, including plane-wave Born methods [8], distorted-wave methods [9], and non-perturbative methods such as the *R*-matrix methods [10].

For light species, particularly for their lower charge states, it has been demonstrated that close-coupling methods are needed to account for the effects of correlation on the collision processes [11-13]. More recently, it was shown that for *R*-matrix calculations, continuum coupling effects must be included in the near neutral ion stages via the use of the *R*-matrix with pseudostates (RMPS) method [14-16].

In this paper we present a brief summary of the data that forms the currently recommended data for light species (H through to Ne) in the CFADC [17] database. Significant effort has been put into calculating accurate atomic data for such light species, so the currently recommended data is unlikely to undergo significant changes. The excitation data within the CFADC database has been generated largely from the groups at Strathclyde University in the UK, Rollins College in Florida and Auburn University in Alabama. So while other datasets exist for these ions, produced by other groups, we present a summary of just the data files that were made for the CFADC database. All of the files are in standard ADAS adf04 file format [18]. Fortran subroutines for reading the adf04 files are available from the OPEN-ADAS web page [19].

2. THEORY

Electron-impact excitation of atomic systems can proceed via direct excitation, or resonant excitation (resonant capture followed by autoionization to an excited state). For light species, due to the relatively small effect of the

spin-orbit interaction, it is usually sufficient to generate the atomic data in LS coupling, and to assume that any J-resolved spectral lines have upper levels within an LS term that are statistically populated.

All of the recommended atomic data for H through to Ne in the CFADC database was generated using the *R*-matrix approach. *R*-matrix theory accounts for interaction between the direct and indirect excitation processes.

As mentioned above, the RMPS method [14, 15] is required for near neutral systems, to account for continuum coupling effects [16]. Our codes are based upon signficantly modified versions of the serial RMATRIX I programs [10]. The basis used to represent the (N + 1)-electron continuum is made orthogonal to the pseudo orbitals using a method developed by Gorczyca and Badnell [15]. In recent years, the codes have undergone significant parallelization to optimize their use on supercomputers [20, 21].

R-matrix theory dictates that the configuration space describing the scattering processes is split into two regions. In the inner region, which encompasses the N-electron target, the total wavefunction for a given LS symmetry is expanded in basis states given by:

$$\Psi_k^{N+1} = A\sum_{i,j} a_{ijk}\psi_i^{N+1}\frac{u_{ij}\left(r_{N+1}\right)}{r_{N+1}} + \sum_i b_{ik}\chi_i^{N+1} \tag{1}$$

where A is an antisymmetrization operator, ψ_i^{N+1} are channel functions obtained by coupling N-electron target states with the angular and spin functions of the scattered electron, u_{ij} are radial continuum basis functions, and χ_i^{N+1} are bound functions which ensure completeness of the total wavefunction. The coefficients a_{ijk} and b_{ik} are determined by diagonalization of the total (N + 1)-electron Hamiltonian. The availability of massively parallel computers permits the concurrent parallel diagonalisation of every Hamiltonian utilizing ScaLapack libraries [22], from which the resulting eigenvalues and eigenvectors are subsequently used in the formation of the *R*-matrix.

In the outer region, the total wavefunction for a given $LS\Pi$ symmetry is expanded in basis states given by:

$$\Psi_k^{N+1} = \sum_{i,j}\psi_i^{N+1}\frac{v_{ij}\left(r_{N+1}\right)}{r_{N+1}} \tag{2}$$

There are a range of implementations of the *R*-matrix approach, including semi-relativistic approaches such as the Breit-Pauli *R*-matrix (BPRM) method and the intermediate coupling frame transformation (ICFT) *R*-matrix method. Fully relativistic effects are included in the Dirac *R*-matrix approach (DRM). Pseudostates can also be used to include the effects of coupling to the target continuum, and is often referred to as the *R*-matrix with pseudostates (RMPS) method.

The *R*-matrix calculations return all of the excitation cross sections between levels of the target system. We note that the focus of these calculations is on achieving high quality collision data, and as such they are usually based upon restricted structure calculations. To achieve spectroscopically accurate wavelength positions that can be compared with observation, the data user should use the wavelength data such as that in the NIST database [23].

3. SUMMARY OF RECOMMENDED DATA

3.1. Hydrogen

The data for neutral hydrogen is based upon the *R*-matrix calculation of Anderson *et al.* [24,25]. The data consists of excitation between all terms of the first 5 n-shells.

3.2. Helium

The data currently available for neutral helium is from the *R*-matrix with pseudostates calculation of Ballance *et al.* [6], and consists of all excitations between the 1s nl configurations, with $1s \le nl \le 4f$. The data for He^+ comes from

the RMPS calculation of Ballance *et al.* [26] and contains all transitions within the 15 terms of the first 5 n-shells, excluding transitions between degenerate terms. All of the H-like data in the CFADC database excludes transitions between such degenerate terms or levels. We note that the excitation data for H, He and He^+ have been combined with ionization and recombination rate coefficients, and processed into generalized collisional-radiative coefficients commonly used in plasma transport codes [27].

3.3. Lithium

The data for Li consists of the RMPS calculation of Griffin *et al.* [28] and includes all excitations within the 9 terms of the 1s *nl* configurations ($2s \le nl \le 4f$). The data for Li^+ originates from the RMPS calculation of Ballance *et al.* [16] and includes excitation between the 19 LS terms of the 1s and 1s *nl* ($2s \le nl \le 4f$) configurations. The data for Li^{2+} consists of RMPS data from Ballance *et al.* [26] and includes excitation between the 15 LS terms of the first 5 n-shells of the ion. We note that GCR data for Li has also been generated and is reported in Loch *et al.* [29].

3.4. Beryllium

The data for all of the ion stages of Be consists of RMPS calculations and were reported by Ballance *et al.* [30]. For neutral Be, the data includes transitions within the 19 terms of the $1s^22s^2$, $1s^22s2p$, $1s^22p^2$, and the $1s^22s$ *nl* configurations ($3s \le nl \le 4f$). The data for Be^+ includes all transitions within the 9 terms of the $1s^2nl$ ($2s \le nl \le 4f$) configurations. The data for Be^{2+} includes all transitions within the $1s^2$ and 1s*nl* ($2s \le nl \le 4f$) configurations. The data for Be^{3+} includes transitions between the 10 LS terms of the first 4 *n*-shells of this hydrogenic system. The data for Be has been processed into GCR coefficients [31].

3.5. Boron

The data for the B iso-nuclear sequence were reported in Ballance *et al.* [32] for neutral B, in Badnell *et al.* [33] for B^+, in and Griffin *et al.* [34] for B^{2+}. The unpublished calculations for B^{3+} by Ballance were performed to complete the data required for the B iso-nuclear sequence. The data for B^{4+} was taken from Ballance *et al.* [26]. All of these were RMPS calculations. The data for neutral B includes all transitions within the $2s^2$ 2p, 2s $2p^2$, and $2s^2$ *nl* ($3s \le nl \le 4f$) configurations. The data for B^+ includes transitions amongst the $2s^2$, $2p^2$, and 2s *nl* ($2p \le nl \le 4f$) configurations. The data for B^{2+} includes all transitions between the $1s^2$ *nl* ($2s \le nl \le 4f$) configurations. For B^{3+} all transitions within the $1s^2$, 1s*nl* ($2s \le nl \le 4f$) are included. The data for B^{4+} includes all transitions within the first 5 *n*-shells.

3.6. Carbon

For the carbon isonuclear sequence, data exists for C^{3+} [34] and C^{2+} [35]. The data for C^{4+} are unpublished calculations of Ballance, and were calculated to complete higher members of the C iso-nuclear sequence. The calculations for C^{5+} are reported in [26]. Calculations for neutral C and C^+ are underway. The data for C^{2+} includes transitions between the 24 terms of the $2s^2$, 2s2p, $2p^2$, and the 2s*nl* ($3s \le nl \le 4f$) configurations. The data for C^{3+} includes transitions between the 9 terms of the 1s *nl* ($2s \le nl \le 4f$) configurations. For C^{4+} all transitions within the 1s, 1s*nl* ($2s \le nl \le 4f$) are included. The data for C^{5+} includes all the transitions between the 15 terms of the first 5 *n*-shells.

3.7. Oxygen

The data currently available on the CFADC web page for O consists of O^{5+} [34] and O^{7+}, with the H-like data coming from Ballance *et al.* [26]. For O^{5+}, all transitions within the $1s^2$ *nl* ($2s \le nl \le 4f$) configurations are included, and for O^{7+}, all transitions within the first 5 *n*-shells are included.

3.8. Neon

The data available for neutral Ne are term-resolved, while the data for the ions are level-resolved. The data of Ballance and Griffin [36] is used for neutral Ne, the data of Griffin *et al.* [37] for Ne^+, the data of McLaughlin *et al.*

[38] for Ne^{2+}, the data of Ludlow *et al.* [39] for Ne^{3+} and Ne^{6+}, the data of Griffin *et al.* [40] for Ne^{4+}, the data of Mitnik *et al.* [41] for Ne^{5+}. The data for the charge states greater than Ne^{6+} have been evaluated by other groups [42-44], but no data has been uploaded to the CFADC web page yet.

For neutral Ne, all transitions within the 61 terms of the $2p^6$, and $2p^5nl$ ($3s \le nl \le 5g$) configurations are included. For Ne^+, all transitions within the 138 levels of the $2s^22p^5$, $2s2p^6$, and $2s^22p^4nl$ ($3s \le nl \le 4f$) are included. For Ne^{2+}, all transitions within the 554 levels of the $2s^22p^4$, $2s^22p^3nl$ ($3s \le nl \le 4f$), $2s\ 2p^4nl$ ($3s \le nl \le 4f$), $2p^5\ nl$ ($3s \le nl \le 4f$), and the $2p^6$ configurations are included. For Ne^{3+}, all transitions within the 581 levels of the $2s^2\ 2p^3$, $2s\ 2p^4$, $2p^5$, $2s\ 2p^3nl$ ($3s \le nl \le 4f$), $2p^4nl$ ($3s \le nl \le 3d$), and $2s^22p^2\ nl$ ($3s \le nl \le 4f$) configurations are included. For Ne^{4+}, all transitions within the 49 levels of the $2s^22p^2$, $2p^4$, $2s2p^3$, $2s^22p\ nl$ ($3s \le nl \le 3d$), and $2s\ 2p^2\ nl$ ($3s \le nl \le 3d$) configurations are included. For Ne^{5+}, all transitions within the 180 levels of the $2s^22p$, $2s2p^2$, $2p^3$, $2s^2nl$ ($3s \le nl \le 4f$), $2s2pnl$ ($3s \le nl \le 4d$), and $2p^2nl$ ($3s \le nl \le 3d$) configurations are included. For Ne^{6+}, all transitions within the 171 levels of the $2s^2$, $2s2p$, $3s^2$, $2p^2$, $2s\ nl$ ($3s \le nl \le 5g$), and $2p\ nl$ ($3s \le nl \le 5g$) configurations are included.

All of the above data is summarized in tables 1 and 2.

Table 1
Summary of Electron-impact Excitation Data Files Available for H-O

Atomic system	*Reference*	*Configurations*	*Number of LS terms*
H	Anderson *et al.* [24,25]	1s - 5g	15
He	Ballance *et al.* [6]	$1s^2$, 1s *nl* ($2s \le nl \le 4f$)	19
He^+	Ballance *et al.* [26]	1s - 5g	15
Li	Griffin *et al.* [28]	$1s^2$ *nl* ($2s \le nl \le 4f$)	9
Li^+	Ballance *et al.* [16]	$1s^2$, 1s *nl* ($2s \le nl \le 4f$)	19
Li^{2+}	Ballance *et al.* [26]	1s - 5g	15
Be	Ballance *et al.* [30]	$2s^2$, 2s 2p, $2p^2$, 2s *nl* ($3s \le nl \le 4f$)	19
Be^+	Ballance *et al.* [30]	$1s^2$ *nl* ($2s \le nl \le 4f$)	9
Be^{2+}	Ballance *et al.* [30]	$1s^2$, 1s nl ($2s \le nl \le 4f$)	19
Be^{3+}	Ballance *et al.* [26]	1s-4f	10
B	Ballance *et al.* [32]	$2s^2$ 2p – 2s $2p^2$, $2s^2$ *nl (3s ≤ nl ≤ 4f)*	11
B^+	Badnell *et al.* [33]	$2s^2$, 2s 2p, $2p^2$, 2s *nl* ($3s \le nl \le 5s$)	19
B^{2+}	Griffin *et al.* [34]	1s2 *nl* ($2s \le nl \le 4f$)	9
B^{3+}	Ballance (unpublished)	$1s^2$, 1s *nl* ($2s \le nl \le 4f$)	19
B^{4+}	Ballance *et al.* [26]	1s-5g	15
C^{2+}	Mitnik *et al.* [35]	$2s^2$, 2s 2p, $2p^2$, 2s *nl* ($3s \le nl \le 4f$)	19
C^{3+}	Griffin *et al.* [34]	$1s^2$ *nl* ($2s \le nl \le 4f$)	9
C^{4+}	Ballance	$1s^2$, 1s*nl* ($2s \le nl \le 4f$)	19
C^{5+}	Ballance *et al.* [26]	1s-5g	15
O^{5+}	Griffin *et al.* [34]	$1s^2$ *nl* ($2s \le nl \le 4f$)	19
O^{7+}	Ballance *et al.* [26]	1s-5g	15

Table 2
Summary of electron-impact excitation data files available for Ne

System	*Reference*	*Configurations*	*Number of LSJ levels or LS terms*
Ne	Ballance and Griffin *et al.* [36]	$2p^6$ and $2p^5nl$ ($3s \le nl \le 5g$)	61 terms
Ne^+	Griffin *et al.* [37]	$2s^2\,2p^5$, $2s\,2p^6$, and $2s^22p^4nl$ ($3s \le nl \le 4f$)	138 levels
Ne^{2+}	McLaughlin *et al.* [38]	$2s^22p^4$, $2s^22p^3nl$ ($3s \le nl \le 4f$), $2s2p^4nl$ ($3s \le nl \le 4f$), $2p^5nl$ ($3s \le nl \le 4f$), and $2p^6$	554
Ne^{3+}	Ludlow *et al.* [39]	$2s^22p^3$, $2s\,2p^4$, $2p^5$, $2s\,2p^3nl$ ($3s \le nl \le 4f$), $2p^4nl$ ($3s \le nl \le 3d$), and $2s^22p^2\,nl$ ($3s \le nl \le 4f$)	581
Ne^{4+}	Griffin *et al.* [40]	$2s^22p^2$, $2p^4$, $2s2p^3$, $2s^22p\,nl$ ($3s \le nl \le 3d$), and $2s2p^2nl$ ($3s \le nl \le 3d$)	49
Ne^{5+}	Mitnik *et al.* [41]	$2s^22p$, $2s2p^2$, $2p^3$, $2s^2\,nl$ ($3s \le nl \le 4f$), $2s2pnl$ ($3s \le nl \le 4d$), and $2p^2nl$ ($3s \le nl \le 3d$)	180
Ne^{6+}	Ludlow *et al.* [39]	$2s^2$, $2s2p$, $3s^2$, $2p^2$, $2s\,nl$ ($3s \le nl \le 5g$), and $2p\,nl$ ($3s \le nl \le 5g$)	171

4. CONCLUSIONS

A brief report has been presented on the data currently available for light species in the CFADC database. In all cases, the data was generated using the *R*-matrix method. All of the data is available for download at the CFADC web page. While most of the fusion-relevant species are reasonable complete, a few ion stages remain to be added to the database.

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