Modelling spectral emission from fusion plasmas

H. P. Summers, N. R. Badnell, A. R. Foster, A. Giunta, F. Guzmán et al.

Citation: AIP Conf. Proc. **1438**, 181 (2012); doi: 10.1063/1.4707875
View online: http://dx.doi.org/10.1063/1.4707875
View Table of Contents: http://proceedings.aip.org/dbt/dbt.jsp?KEY=APCPCS&Volume=1438&Issue=1
Published by the American Institute of Physics.

Modelling spectral emission from fusion plasmas

H. P. Summers[a], N. R. Badnell[a], A. R. Foster[b], A. Giunta[a], F. Guzmán[a], L. Menchero[a], C. H. Nicholas[a], M. G. O'Mullane[a], A. D. Whiteford[a], A. Meigs[c], and JET-EFDA Contributors[d]

[a]*Department of Physics, University of Strathclyde, Glasgow G4 0NG, UK*
[b]*Smithsonian Astrophysical Observatory, Cambridge, MA 02138, USA*
[c]*Association EURATOM-CCFE Culham Science Centre, Abingdon, OX14 3DB, UK*
[d]*JET-EFDA, Culham Science Centre, Abingdon, OX14 3DB, UK*[1]

Abstract. The paper is a tribute to Nicol Peacock and has a focus on interests and developments at Culham Laboratory from $\sim$ 1970 when Nicol led the UKAEA spectroscopy team. The paper charts a little of the evolution of these models and their data through the seventies and eighties on into this century at Culham. The paper concludes with the state of efforts to enable easy, universal access to spectral analysis across the scope of Culham activity, of which it is hoped Nicol would approve.

Keywords: Atomic physics, spectroscopy, plasmas, fusion
PACS: 39.30,52.55,52.25, 96.60

INTRODUCTION

It is interesting to look back to the very early days of fusion in the UK from an atomic modelling perspective. Work notes of Thonemann[2], an originator of the toroidal confinement approach, include quite detailed considerations of impurity ions in magnetically confined plasmas, such as relaxation of metastable states - which will be returned to later. First efforts to predict electron temperatures in ZETA from line ratios were however misleading because of errors in assumed cross-sections. Pioneering work by Bates, Kingston and McWhirter [1] on collisional-radiative theory in the early sixties and first R-matrix calculations of cross-sections by Burke had not changed the view of senior management at UKAEA Culham Laboratory in the early seventies that atomic physics and diagnostic spectroscopy was not to be trusted. In any case spectroscopists and atomic physicists at Culham Laboratory were mostly more interested in VUV and soft X-ray observations of the sun's upper atmosphere from space. Nonetheless Culham had a new divertor tokamak experiment (DITE) coming on-stream which incidentally had molybdenum limiters. So radiant losses from impurity species, including heavy species, mattered and predictive modelling from atomic physics was required and tolerated. It was then, in the early seventies, that one of us (Summers) first became involved in magnetic confinement fusion at Culham. In fact this was with Nicol Peacock, who had kept faith with atomic modelling for plasmas and wished for some calculations on ionisation state

[1] See the Appendix of F. Romanelli et al., Proceeedings of the 23rd IAEA Fusion Energy Conference 2010, Daejeon, Korea

[2] Private communication and notebook archives from R. W. P. McWhirter

The 17th International Conference on Atomic Processes in Plasmas (ICAPiP)
AIP Conf. Proc. 1438, 181-188 (2012); doi: 10.1063/1.4707875

and radiated power of species in DITE. So, from that point in time, a connection was established with Nicol which has continued on through the eighties into this century with the JET Joint Undertaking. It was of course clear that lack of accurate knowledge of electron-ion reaction rates limited our work and fortunately, in the late eighties, another of us (Badnell) started a crucial, long-term focus on precision cross-sections which continues to this day. To complete the story, another of us (O'Mullane) a research student with Nicol Peacock in the nineties continues our efforts into ITER and the future and in fact wrote Nicol's last paper with him [2]. It must be said that Nicol did not stand still, but was always enthused by the latest ideas. So the rest of this paper is not a historical work, but rather a tribute, showing where the engagement with Nicol has led us to now.

POPULATION STRUCTURE AND IONISATION STATE

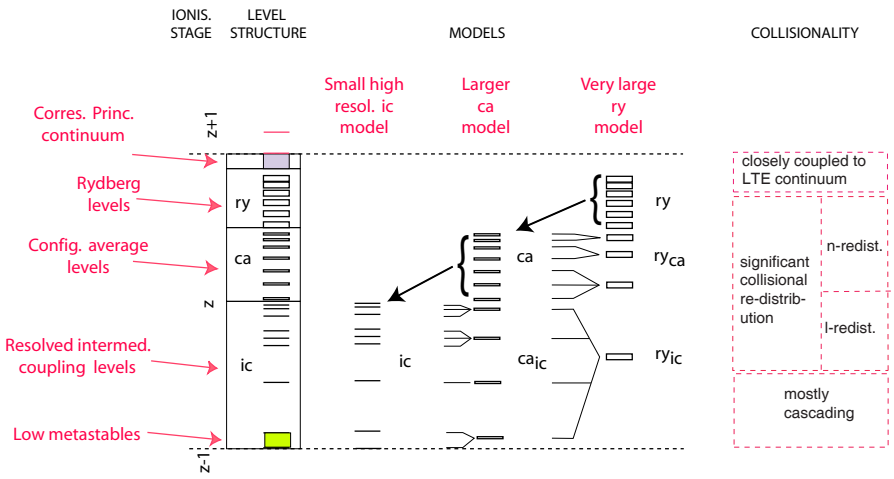

FIGURE 1. Population modelling zones and organisation of collisional-radiative calculations. *ic*, *ls*, *ca* and *ry* denote intermediate coupling level, term, configuration-average valence orbital and valence n-shell population grouping. Diagonal arrows indicate projection of the indicated partition of the source population model and expansion onto the target population model. The procedure terminates at the lowest lying metastables of the system. It yields effective coefficients coupling metastables of the $z-1$, z and $z+1$ ionisation stages and matching emissivity coefficients driven by each metastable.

In our Cambridge ivory tower in the early seventies, Nicol appeared one day excited about titanium ions and wanting to model the low level population structure so that he could predict the emissivities of the associated VUV lines. This was an interesting departure, since at that time our main concern was dielectronic recombination and its sensitivity to finite plasma density - a very highly excited Rydberg level problem. Also, Nicol was concerned about the emission of O VII lines in the recombining environment of the peripheral DITE plasma which seemed to reveal differential behaviour of ground and metastables in radial transport. Again this was intriguing, since early errors were made in effective dielectronic recombination from neglect of abundant metastable recombining target ions. Later, at the JET Joint Undertaking in the middle eighties, related questions, associated with impurity influx from localised surfaces contacted by the

plasma, arose. Spectral observations of such inflowing ions are conveniently performed in the visible and so arise from excited levels in higher n-shells for light element ions. A typical transition is O II ($2s^2 2p^2 3p\ ^4P - 2s^2 2p^2 3s\ ^4S$) whose emissivity is driven from the $2s^2 2p^3\ ^4S$ ground primarily. But the $2s^2 2p^2 3p\ ^4P$ level is relatively long-lived, since it cannot decay to the ground. It is therefore susceptible to collisional re-distribution at tokamak densities and also to augmentation by cascade from higher n-shells. Although JET was a machine following a light element first wall strategy (beryllium and carbon), influx of more complex heavier elements such as Cr (JET antennae screens) and Mo (DITE and ALCATOR) were of interest. These motivations set in train the pattern of excited population and ionisation state modelling which, in a more refined form, we use and continue to develop today. This can be summarised as trying to address the whole excited population structure of an ion, ground to continuum, recognizing metastability, including all relevant collisional processes, adopting collisional-radiative principles on timescale ranking to obtain 'effective coefficients', using varying resolutions (in a shell, term or level sense) and population grouping to make the problem computationally manageable (see figure 1). The realisation of these principles in codes, together with all the data, fundamental and derived, necessary to make it practical and relevant became ADAS, the Atomic Data and Analysis Structure[3]. The ADAS Project is grateful to Nicol for his encouragement in this area over many years.

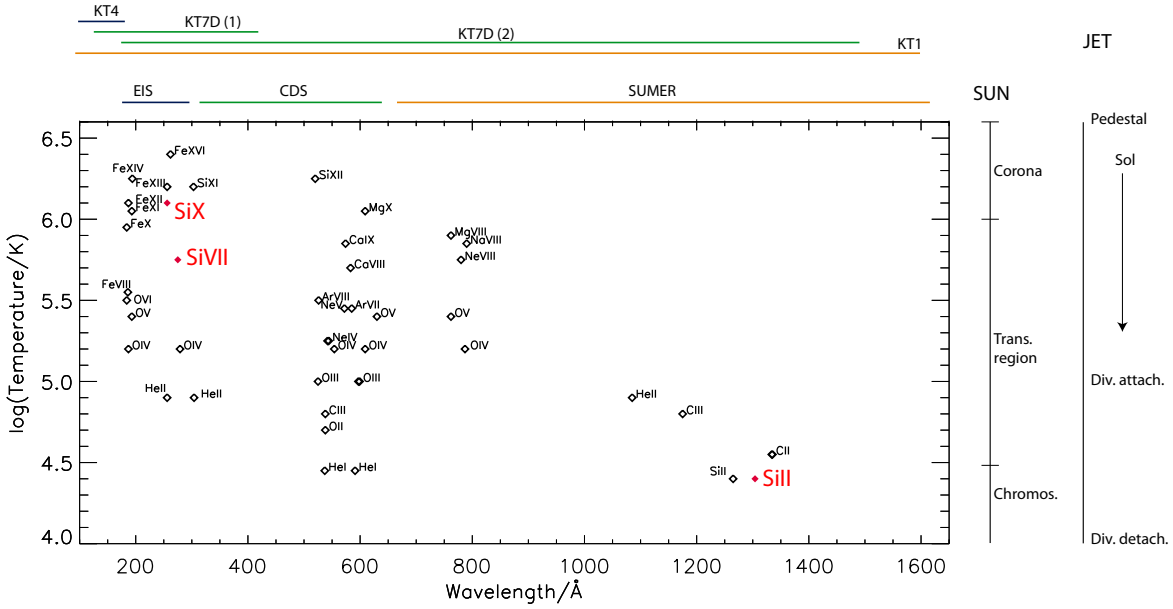

FIGURE 2. Emission lines observed by SUMER, CDS and EIS in the joint solar observations JOP220/HOP109 on 17^{th} April 2009 [5] together with the instrument wavelength coverages. The temperatures of line formation have been shown, in order to indicate the solar atmosphere layer from which the indicated lines arise. The spectral ranges of JET spectrometers becoming operational in the EP2 extended performance upgrade and relevant divertor zones are also indicated for comparison.

[3] URL: http://www.adas.ac.uk

To elaborate a little on the present state of affairs, ADAS population modelling, at its highest precision, has been targetted at the ions of the elements hydrogen to neon. The details of the methods are described in Summers *et al.*[3], which develops the simplified schematic shown in figure 1 (see also [4]). Comprehensive derived effective coefficient data are available to support modelling of the separate dominant metastables of light elements in plasma transport equations and prediction of associated spectral emission. Periodic updates of the data occur in response to improved calculations of electron-impact cross-sections between low levels (see figure 1). However, new differential emission measure (DEM) analyses in the lower temperature solar chromosphere/transition region (Giunta [5]), and of course preparations for ITER in fusion, have compounded pressure to extend the range of species to argon and possibly iron. This is further justified by new state-resolved dielectronic recombination, ionisation cross-section and R-matrix excitation cross-section calculations which provide underpinning fundamental data. Silicon is now complete and magnesium will soon follow. Recent analyses using these new data do indicate that all of the ingredients summarised in the previous paragraph matter. The studies confirm that truncation of the population structure at a set of low levels and failure to include the finite-density suppression of dielectronic recombination, even with good low-level fundamental data, does lead to mis-interpretation [5]. In such development, fusion and astrophysics can be mutually supportive. Figure 2 shows our current focus of interest in solar observations and the relationship to divertor spectrometry and species at Culham laboratory (JET and MAST). Attention is drawn to the spectrum lines Si II(1309.3Å), Si VII(275.7Å) and Si X(256.4Å) in figure 2 which influence chromosphere DEM. The derived atomic data required for DEM analysis are contribution functions (theoretical combinations of emissivities and ionisation fractional abundances), but their ingredients (effective emissivity, ionisation and recombination coefficients) allow equivalent prediction in non-stationary transport regimes and transients of both the solar atmosphere and tokamak divertors (except that the tokamak evolution is about one thousand times faster).

It is though the change of emphasis in population and emissivity modelling from light to heavy elements which has been the main pre-occupation. The methods being used for heavy element ions were outlined in Summers *et al.*[6] and in O'Mullane *et al.*[7] and since then they have become more refined, systematised and tested. Superstaging has now been carried into 2-D transport modelling enabling studies of tungsten (Strachan *et al.*[8]). This has encouraged efforts to improve the baseline approximations used in ADAS and to target selected ions at the highest precision. Figure 3 shows a partition which isolates the ions W^{+20} and W^{+44} from the grosser superstages. Within the JET scope of core electron temperature, W^{+44} stands out as a somewhat simpler system (JET baseline modelling includes $\sim 2 \times 10^4$ lines) with predicted spectral emission in the range of the KX1 soft X-ray spectrometer. First relativistic, R-Matrix, radiation damped cross-section calculations have been carried out by Ballance and Griffin [9], but omit the observable lines which are $3d - 4f$ core excited. Further very large calculations are in preparation to explore this. The W^{+20} ion with a partially filled f-shell is a formidable system (JET baseline modelling includes $\sim 2 \times 10^5$ lines) with a quasi-continuum of emission, yet marks (to lower ionisation stages) the divertor relevant stages. In ionisation, the CADW approximation of Loch *et al.* [10] (see also Loch *et al.* [11]) raises our baseline, but measurements by Borovik *et al.*[12] still indicate discrepancies

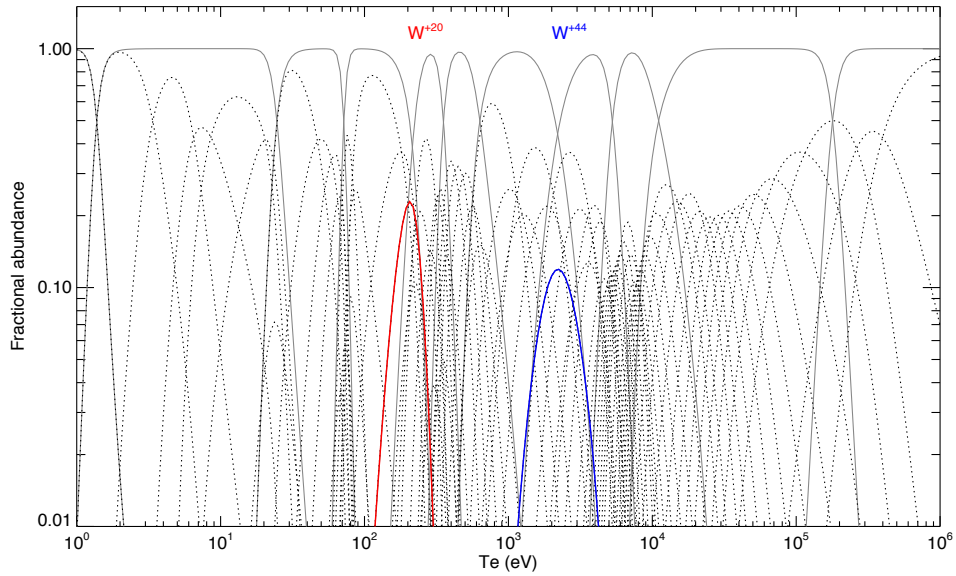

FIGURE 3. Tungsten ionisation balance in superstage partitioning with separate W^{+20} and W^{+44} stages. Superstages in solid lines, normal stages in dotted lines.

even at quite high charge states from REDA-like structures. AUTOSTRUCTURE raises our baseline for dielectronic recombination (see Badnell *et al.*[13]), and is being pushed towards more complex systems (Badnell *et al.*[14]). These comparative calculations suggest a varying bundling and resolution approach, along with approximations such as BBGP [13], is the way forward. Such an approach can probably make manageable both the low temperature and high temperature needs. Again the measurements (Schippers *et al.*[15]) show that very large low energy resonances can influence the high temperature dielectronic rates. Our current work moves forward in all these aspects, but in a strongly targetted manner driven by observability as indicated above.

NEUTRAL BEAMS AND CHARGE EXCHANGE SPECTROSCOPY

Nicol was not too enthused by charge exchange spectroscopy (CXS) or at least by that conducted at visible wavelengths and directed at inferring concentrations. Partly this reflected his VUV and shorter wavelength preference, but also because the observations are of emission from sub-dominant levels of the receiver with rather a long trail of atomic modelling involving, sometimes, poorly known cross-sections. He would therefore be shocked by figure 4, an estimate designed to examine how much tungsten active signals could affect fast helium concentration deduction from charge exchange spectroscopy.
However CXS certainly was and remains a subject of interest and much discussion. State selective charge exchange data from neutral hydrogen ground state and excited donors to fully stripped light impurity nuclei as receivers has improved. Recent studies consolidate and extend the coverage with precision methods such as CCMO for B^{+5}

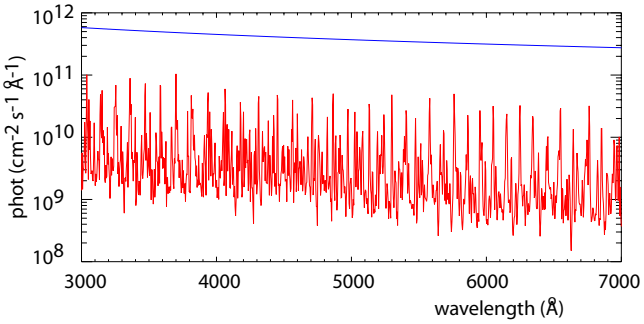

FIGURE 4. Predicted tungsten CXS emission for ITER, in red, contrasted with Bremsstrahlung, in blue: 50keV/amu D beam, JNBI=300Am^{-2}, INBI=60A; ITER scneario 2 (Te=20keV core, Ne=1.0^{14} cm^{-3}; no transport, vertical view, no beam attenutation, W conc = 10^{-6} of N_H.

(Guzman *et al.*[16]) and CCAO for Be^{+4} (Igenbergs *et al.*[17]) and N^{+7} (Igenbergs - private communication). Extension to argon is the prize because of ITER relevance and also because it allows (by simultaneous observation of Ar^{+15}, Ar^{+16} and Ar^{+17} CXS emission in the visible) a direct connection with impurity transport. Differences and discontinuities between methods (CTMC, modified CTMC and CCMO) in the key $\sim$ 50keV/amu region are an anxiety. Calculations by Igenbergs (private communication) in CCAO approximation will hopefully clarify the situation. Meanwhile, the existing database does allow the preparation of universal semi-empirical z-scaled parametric forms for the state selective data (Foster [18]) which have been included in ADAS and used for extrapolation to high Z (see figure 4). Further studies on CXS of a Kr^{+36} receiver in the modified CTMC approach (Illescas - private communication) and the Ar^{+18} revision will strengthen the universal parametric form. The conversion of such data to emissivities uses the similar models as discussed in figure 1.

SPECIAL FEATURES AND SPECTRAL ANALYSIS

The now extensive population and ionisation state models of ADAS, which span most fusion plasma environments and species to some measure, combined with their delivery of derived coefficients in precisely defined data formats, provide a basis for spectral diagnostics. Helium-/lithium-like satellite lines, Balmer decrements, Zeeman pattern lines and so on are just groupings of related lines exploited as special features because of their special sensitivity. Ad hoc models and codes abound to expedite such exploitation. The comprehensive character of ADAS has encouraged us to explore and expand the atomic physics link so that the special features may be realised as a universal mathematical/computational construct for use in spectral modelling and fitting. In close association with ADAS, one of us (Nicholas) [19] has sought to empower special feature analysis by implementing such generalised computational structures — AFG (ADAS Feature Generator) and FFS (Framework for Feature Synthesis). These allow both a pedagogical insight into the capabilities of each special feature as well as practical execution of optimised spectral fitting and plasma parameter extraction. The methods, based

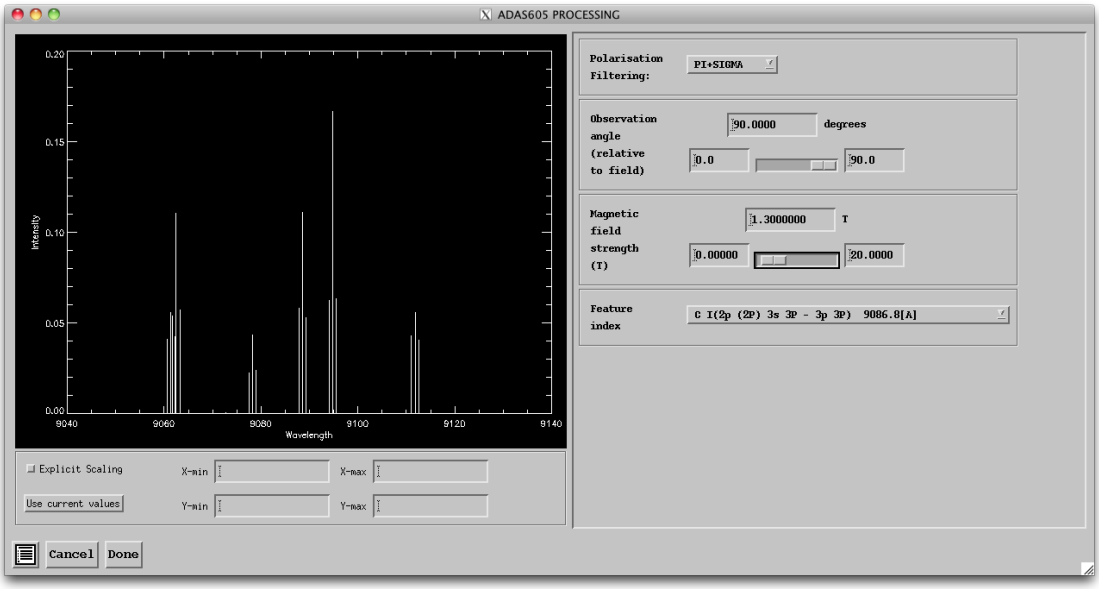

FIGURE 5. ADAS605 processing screen: allows interactive manipulation of the chosen feature via custom control widgets in the right hand panel, with graphical output in the left panel.

on object-oriented programming, are universal including aspects such as self-generating graphical user interfaces and an algebra of parametric feature creation. An illustration from JET is shown in figure 5. In order to specify the construct for an arbitrarily complex model spectra, a LISP-like model definition language (MDL) has been set up. Details of initial user model optimising, allowing substitution of analytic derivatives and hence very substantial fitting speed-up are beyond this short paper (see Nicholas [19]). Special features were close to Nicol's heart and so this paper concludes with figure 6, an illustration of our latest methods on selected JET spectra.

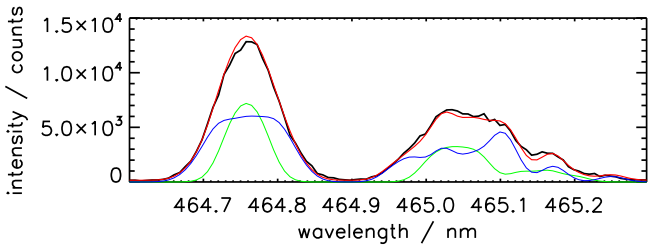

FIGURE 6. C III ($1s^2 2s3s\,^3S$ – $1s^2 2s3p\,^3P$) multiplet at $\sim$ 465 nm as recorded by KS8 at JET, pulse #75898. The in-board and out-board emission, differentially perturbed by the magnetic field and flow, along a mid-plane, horizonal line-of-sight, form the observational feature. The fitted FFS model is shown in red, with the low-field and high-field side Zeeman components indicated in green and blue, respectively.

CONCLUSIONS AND ACKNOWLEDGMENTS

Nicol was a fusion and spectroscopy enthusiast who freely shared information, ideas and results. He facilitated engagement between experimental spectroscopists, theoretical atomic physicists and plasma physicists. Also, he had an outward looking perspective from Culham Laboratory which allowed external university scientists to become fully engaged. We believe this was very fruitful as indicated by this brief survey of what was started and where it has got to now. His legacy at Culham is evident. ITER is our next target in which Nicol would surely have concurred.

This work was supported by EURATOM and carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission. Two of us (Foster, Nicholas) acknowledge EPSRC CASE studentships with CCFE Culham Laboratory. One of us (Giunta) acknowledges a Faculty scholarship from the University of Strathclyde.

REFERENCES

1. D. R. Bates, A. E. Kingston and R. W. P. McWhirter *Proc. Roy. Soc. A*, **267**, 297 (1962).
2. N. J. Peacock, M. G. O'Mullane, R. Barnsley and M. Tarbutt *Can. J. Phys.* **86**, 277–284 (2008).
3. H. P. Summers, W. J. Dickson, M. G. O'Mullane, N. R. Badnell, A. D. Whiteford, D. H. Brooks, J. Lang, S. D. Loch and D. C. Griffin, *Plasma Phys. Control. Fusion*, **48**, 263–293 (2006).
4. H. P. Summers and M. G. O'Mullane, *Amer. Inst. Phys. Conf. Series* **1344**, 179–187 (2011).
5. A. Giunta, *Spectral analysis of the solar atmosphere at the chromosphere-corona boundary*, Ph. D. Thesis, University of Strathclyde (2011). `http://www.adas.ac.uk/theses/giunta_thesis.pdf`.
6. H. P. Summers, M. G. O'Mullane, A. D. Whiteford, N. R. Badnell and S. D. Loch, *Amer. Inst. Phys. Conf. Series* **901**, 239–248 (2007).
7. M. G. O'Mullane,A. R. Foster, A. D. Whiteford, H. P. Summers, S. D. Loch and L. Lauro-Taroni *Amer. Inst. Phys. Conf. Series* **1161**, 43–50 (2009).
8. J. D. Strachan, G. Corrigan, D. Harting *et al.*, *J. Nucl. Mater.* **doi:** 10.1016 (2010).
9. C. P. Ballance and D. C. Griffin *J. Phys. B: At. Mol. Phys.Proc.* **40**, 247 (2007).
10. S. D. Loch, J. Ludlow, M. S. Pindzola, A. D. Whiteford and D. C. Griffin, *Phys. Rev. A*, **72**, 052716 (2005).
11. S. D. Loch, M. S. Pindzola and D. C. Griffin, *Int. J. Mass Spectrom.* **271**, 58 (2008).
12. A. Borovik, S. Schippers and A. Müller, *Atom. and Plasma-Mater. Inter. Data for Fusion* - in preparation (2011).
13. N. R. Badnell, M. G. O'Mullane, H. P. Summers, Z. Altun, M. A. Bautista, J. Colgan, T. W. Gorczyca, D. M. Mitnik, M. S. Pindzola and O. Zatsarinny, *Astron. and Astrophys.*, **406**, 1151–1165 (2003).
14. N. R. Badnell, A. Foster, D. C. Griffin, D. Kilbane, M. G. O'Mullane, H. P. Summers, *J. Phys. B: At. Mol. Phys.Proc.* **44**, 135201 (2011).
15. S. Schippers, D. Bernhardt, A. Müller, C. Krantz, M. Grieser, R. Repnow, A. Wolf, M. Lestinsky, M. Hahn, O. Novotný and D. W. Savin *Phys. Rev. A* **83**, 012711 (2011).
16. F. Guzmán, L. F. Errea, C. Illescas, L. Méndez and B. Pons, *J. Phys. B: At. Mol. Phys.Proc.* **43**, 144007 (2010).
17. K. Igenbergs, J. Schweinzer and F. Aumayr, *J. Phys. B: At. Mol. Phys.Proc.* **42**, 235206 (2009).
18. A. R. Foster, *On the Behaviour and Radiating Properties of Heavy Elements in Fusion Plasmas*, Ph. D. Thesis, University of Strathclyde (2008). `http://www.adas.ac.uk/theses/foster_thesis.pdf`.
19. C. H. Nicholas, *Special features and spectral analysis for fusion plasmas*, Ph. D. Thesis, University of Strathclyde (2011). `http://www.adas.ac.uk/theses/nicholas_thesis.pdf`.