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SUBC2: Sub-contract specifications, deliverables, integration and analysis

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Abstract: *The second set of ADAS-EU sub-contracts, issued in 2012, comprised four work packages. One of these was authorised under Amendment no. 1 to the ADAS-EU agreement. Three packages were issued to university groups in Europe and targetted critical specialised data in which these groups have unique capability - especially difficult areas in heavy element structure and electron impact excitation. These activities successfully addressed the developing needs for fusion in Europe and ITER. The fourth sub-contract was placed with a computer software company in Glasgow, Scotland for an update of the OPEN-ADAS world-wide-web dissemination site whereby free access is provided to key ADAS data and resulting data from ADAS-EU. This report is a comprehensive document bringing together the objectives of the sub-contracts, the datasets and machinery resulting from them, the analysis, placing and integration of these items into ADAS modelling*

Contents

Chapter 1

Introduction

As reported in report SUBC1, sub-contract 6, the last of the primary set of sub-contracts was with Professor Hoekstra, KVI, Universoity of Groningen. Changes in direction at KVI meant that it was not possible to complete the work according to the original contract. The contract was terminated with approximately 1/4 completed.

The evolving fusion needs during the first years of ADAS-EU, clearly identified the atomic physics modelling of tungsten ions in the fusion plasma as critical. The first wave of ADAS-EU sub-contracts, in particular S2 with the University of Mons-Hainaut, S4 with Justus-Liebig University and S3 with the University of Vilnius, were therefore very well targetted. The new methodologies enabled with these first contracts, were in consequence in place and essential for further progress. In the meantime, the planned sub-contract S7 for line broadening development had become secondary to other methods. It was therefore decided to use available funds for S1, S6 residue and S7 for three further sub-contracts pursuing a set of tungsten issues. S1, as originally planned, was placed with Queen's University Belfast for studies enabling R-matrix cross-sections for tungsten ions around W^{+44}, a test semi-relativistic case of considerable complexity potentially observable in the soft X-ray spectrometry at EFDA-JET. The replacement sub-contract S6 was placed with the University of Mons-Hainaut for further optimised near neutral system structure for coupling to ADAS modelling and structure codes. Sub-contract S7 was moved to a second tranche of quasi-relativistic treatments of low ionisation stages of tungsten in the Jucys methodology, again linked to ADAS codes and moving the Vilnius structure work into the collisional domain. These three sub-contracts completed successively and are described in the following chapters.

Amendment No. 1 to the ADAS-EU contract was agreed. Its purpose was to use some residual monies of ADAS-EU to place a sub-contract for the updating of the OPEN-ADAS website provision. This upgrade was an orginal part of the ADAS-EU plan, but was not possible with the loss of Dr. Allan Whiteford from the ADAS-EU core team. Dr. Whiteford, now manages a small computer software company in Glasgow. It was decided to place sub-contract S9 for ther OPEN-ADAS upgrade with this company, being the only possible route for upgrading within the ADAS-EU time-frame. This sub-contract has also completed with an outstanding delivery.

In summary, ADAS-EU has completed all nine (eight + one) contracts successfully. The alterations to two of the sub-contracts in fact enhanced the achievements of ADAS-EU in-so-far as they were able to respond to changes in need. The delivery from this last phase of sub-contracts are of particular benefit to ITER and to the extended experimental programme at EFDA-JET with the ITER-like wall.

Chapter 2

Atomic structure and electron data for heavy element ions - S6 (modification)

(1) THE IONS W+3 TO W+5 AND ADJACENT ELEMENT NEUTRAL/NEAR-NEUTRAL IONS
(2) ATOMIC STRUCTURE MAPPING BETWEEN CODES

The authors of this chapter are Partick Palmeri, Pascal Quinet, Emile Biemont, Nigel Badnell, Martin O'Mullane and Hugh Summers. It incorporates the report on ADAS-EU sub-contract S2 prepared by the Astrophysics and Spectroscopy group, University of Mons, Belgium dated 3 February 2013. See also appendix A.

2.1 Introduction

One of the main goals of the Atomic Data and Analysis Structure (ADAS) Project is to provide, with an appropriate accuracy, all the atomic data required for global modelling and quantitative spectroscopic diagnosis and analysis of fusion plasmas. The system is based on the initial preparation of collections of fundamental atomic transition probability and excitation rate data for selected ions called specific ion files. Several ADAS computer codes then prepare all the derived data (such as net power loss coefficients, spectral line contribution functions, ...) in a form directly usable in experimental analysis and in plasma models. The effectiveness and precision in the applications depends of course on the availability and quality of fundamental data. In that context a specific need is enhanced provision for low ionisation stages of heavy elements up to and including tungsten, this latter element playing a very important role since it will be used in divertor tiles of the ITER tokamak. One of the main sources of spectroscopic properties of such heavy atoms and ions is the Astrophysics and Spectroscopy (ASPECT) group of Mons University (Belgium). This group has developed and systematised methods of atomic structure calculations essentially based on the relativistic Hartree-Fock (HFR) approach of Cowan [1] in which core-polarization has been included [2] giving rise to the so-called HFR+CPOL method. This theoretical approach, combined with a semi-empirical adjustment of the radial parameters in order to minimize the discrepancies between calculated and available experimental energy levels, has been proven to provide reliable transition probabilities in many complex systems such as neutral and lowly ionized atoms belonging to the fifth, the sixth and the lanthanide groups of the periodic table. In a large number of cases, the accuracy of the calculations has been assessed through comparisons with experimental measurements of radiative lifetimes using laser-induced fluorescence (LIF) spectroscopy.

2.2 Atomic structure calculations in W^{3-5+} ions

During the past year, the ASPECT group of Mons University has carried out atomic structure calculations in W IV-VI. To do so, the semi-empirical HFR+CPOL method mentioned above has been used with the physical models reported in Table 1. As no measurements of radiative lifetimes are available for these three ions, the accuracy of the transition probabilities has been assessed through comparisons with independent theoretical models (MCDF, FAC, RMBPT, RCI). The final sets of transition probabilities were published in several papers [3-5] and in the DESIRE atomic database [6].

Table 1. Electronic configurations and core-polarization parameters used in atomic structure calculations of W IV, W V and W VI.

W IV		WV		W VI	
Even parity	Odd parity	Even parity	Odd parity	Even parity	Odd parity
$5d^3$	$5d^26p$	$5d^2$	5d6p	6s	6p
$5d^26s$	$5d^25f$	5d6s	5d7p	7s	7p
$5d6s^2$	$5d^26f$	5d7s	5d5f	5d	5f
$5d^26d$	5d6s6p	5d6d	5d6f	6d	6f
$5d6p^2$	5d6s5f	5d7d	5d7f	5g	7f
$5d^6d^2$	5d6s6f	$6s^2$	6s6p	6g	
$5d5f^2$	5d6p6d	6s6d	6s7p	7g	
$5d6f^2$	5d6d5f	6s7d	6s5f		
5d6s6d	5d6d6f	6s7s	6s6f		
5d6p5f	$6s^26p$	$6p^2$	6s7f		
5d6p6f	$6s^25f$	6p7p	6p6d		
$6s^26d$	$6s^26f$	6p5f	6p7d		
$6s6p^2$	$6p^25f$	6p6f	6p7s		
$6s6d^2$	$6p^26f$	6p7f	6d7p		
$6d^3$	$6p^3$	$6d^2$	6d5f		
$6s5f^2$	$6p6d^2$	6d7s	6d6f		
$6d5f^2$	$6d^25f$	6d7d	6d7f		
$6s6f^2$	$6d^26f$	$7s^2$	7s5f		
$6d6f^2$	$6p5f^2$	7p2	7s6f		
	$6p6f^2$	7s7d	7s7f		
	$5f^26f$	7p5f	7s7p		
	$5f6f^2$	7p6f	7p7d		
		7p7f			
W VII ionic core:		W VII ionic core:		W VII ionic core:	
α_d = 2.5 a_0^3		vα_d = 2.5 a_0^3		α_d = 2.5 a_0^3	
r_c = 1.2 a_0		r_c = 1.2 a_0		r_c = 1.2 a_0	

2.3 Integration of the lowly-ionized heavy ion data into ADAS

Two input files of the Cowan code (ing11 files) per ion, one for the radiative data and a second one for the collision data, containing the optimized radial parameters (Slater, spin- orbit, radiative transition, and Bessel radial integrals) have been transferred to generate higher quality plane-wave Born (PWB) collision strengths and transition probabilities on the basis of accurate atomic structures. The concerned ions were the following: Mo II [7], Hf III [8], W IV [3], W V [4], W VI [5], Re I [9], Re II [10], Au I [11], Au II [11,12], Au III [13]. This part of the work has been performed in collaboration with ADAS-EU staff during a one- week stay (9-15 December 2012) of one of us (P. Palmeri) at the JET facility. The ADAS staff will then produce the data (such as photon emissivity coefficients, ...) for transitions of interest for fusion influx spectroscopy.

2.4 Upgrading collision strengths to distorted-wave quality

During the one-week visit of P. Palmeri at JET, he and N.R. Badnell investigated the possibility of upgrading the HFR+CPOL collision strengths to distorted-wave quality by considering an interface between HFR [1] and AUTOSTRUCTURE [14]. They found that this interface needs a long term effort essentially because the construction of the Hamiltonian matrix elements is very different in these two programs, i.e. HFR builds its Hamiltonian with respect to configuration average energies, while this is not the case with AUTOSTRUCTURE which considers all the core-orbital Slater integrals. Another idea was explored consisting in building AUTOSTRUCTURE models in order to reproduce the high-energy limits of the HFR+CPOL PWB collision strengths. Tests were carried out in W V and agreements between both sets of high-energy limits reached about 20% validating this idea.

2.5 Perspectives and recommendations

In view of the success of atomic data transfer between the Mons group and the ADAS team, this work should continue for other elements of interest for fusion. Among these elements, let us mention Ta I, Ta II, Ta III for which atomic structure calculations have already been published [15-17]. Concerning the upgrading of HFR+CPOL PWB collision strengths, AUTOSTRUCTURE calculations should be carried out in collaboration with N.R. Badnell beginning in first priority with the tungsten ions. In a longer term effort, this collaboration should set up an efficient interface between HFR and AUTOSTRUCTURE.

2.6 References

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Chapter 3

Atomic structure and electron data for heavy element ions, part 2 - S7 (replacement)

(1) PRODUCTION OF CONFIGURATION INTERACTION, QUASI-RELATIVISTIC ATOMIC STRUCTURE AND CROSS-SECTIONS FOR THE ADAS DATABASE.
(2) ATOMIC STRUCTURE INTERCHANGE.

The authors of this chapter are Alicija Kupliauskiene, Pavel Bogdanovich, Olga Rancova, Valdez Jonauskas, Romas Kiselius, Nigel Badnell and Hugh Summers. It incorporates the brief report on ADAS-EU sub-contract S4 prepared by the Institute of Theoretical Physics and Astronomy, University of Vilnius, Lithuania (P. Bogdanovitch) dated 5 February 2013. See also appendix B.

3.1 Introduction

The work consisted of three parts:

1. Evaluation of atomic structure, Born collision cross-sections and generation of ADAS *adf04 type 1* and *3* datasets for W^{+2}–W^{+5} (with open $5d$ shell) and related iso-electronic sequence members of chemical elements hafnium, tantalum and rhenium.
2. Inclusion of the $5d - 5f$ transitions in the Bogdanovich quasi-relativistic (TRO) approach. The configuration interaction will be restricted initially to at most one or two f-electrons promotions from closed shells. The $5d - 5f$ transition array contribution to total radiated line power will be assessed for W^{+2}. The possibilities for extending the numbers of equivalent f-shell electron capability will be explored with Prof. G. Gaigalas.
3. Investigation of the transfer of an orthogonal basis of radial wave functions from the Bogdanovich multi-configurational with virtual excitations and TRO codes as inputs for the AUTOSTRUCTURE.

3.2 Approach used

The software exploited is created for *ab initio* calculations of spectra of atoms and ions within the quasirelativistic approach. This approach significantly differs from the widely known program based on methods described in the monograph by R.D. Cowan [1]. The quasirelativistic equations used to obtain the radial orbitals (RO) are of the following form:

$$\left\{\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(nl|r) - \varepsilon_{nl}\right\} P(nl|r) - X(nl|r) + \frac{\alpha^2}{4}\left(\varepsilon_{nl} + V(nl|r)\right)^2 P(nl|r) + \frac{\alpha^2}{4}\left(\varepsilon_{nl} + V(nl|r)\right) X(nl|r) + \frac{\alpha^2}{4}\left(1 - \frac{\alpha^2}{4}\left(\varepsilon_{nl} + V(nl|r)\right)\right)^{-1} D(nl|r)P(nl|r) = 0. \quad (3.1)$$

The first part of the equation coincides with the usual Hartree-Fock equations, where $X(nl|r)$ denotes the exchange part of the potential, and $V(nl|r)$ denotes the direct part of it including an interaction of an electron with a nucleus $U(r)$ and with other electrons. The finite size of a nucleus is taken into account within the interaction with a nucleus potential $U(r)$ [2] thus enabling us to derive a simple expansion of RO in powers of the radial variable in the nucleus region. Two terms containing the multiplier $(\varepsilon + V(nl|r))$ squared and that in the first order describe the relativistic correction of the mass dependence on the velocity. The last term on the left side of the equation (1) describes the potential of the contact interaction of the electrons with the nucleus. Here the contact interaction with the nucleus is taken into account not only for s-electrons, but also for some part of p-electrons:

$$D(nl|r) = \left(\delta(l,0) + \frac{1}{3}\delta(l,1)\right)\frac{dU(r)}{dr}\left(\frac{d}{dr} - \frac{1}{r}\left(\alpha^2 Z^2 \delta(l,1)\left(-\frac{37}{30} - \frac{5}{9n} + \frac{2}{3n^2}\right) + 1\right)\right). \quad (3.2)$$

Special features of the equation (1) are described in details in [3], [4], and their solution technique can be found in [5], [6].

Energy spectra are calculated within Breit-Pauli approach adjusted for the application of the quasirelativistic radial orbitals (RO). A single joint integral [7] is used to describe the one-electron interactions, both the non-relativistic and the relativistic ones, independent of the total angular momentum J:

$$L_{\mathrm{QR}}(n'l, nl) = -\int_0^\infty P(n'l|r)U(r)P(nl|r) + \int_0^\infty \left(1 - \frac{\alpha^2}{4}\left(\varepsilon_{nl} + V(nl|r)\right)\right)^{-1} P(n'l|r)\left\{\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right\} P(nl|r)dr + \frac{\alpha^2}{4}\int_0^\infty \left(1 - \frac{\alpha^2}{4}\left(\varepsilon_{nl} + V(nl|r)\right)\right)^{-2} P(n'l|r)D(nl|r)P(nl|r)dr. \quad (3.3)$$

Here one must apply the symmetrization procedure for the integrals within the inter-configuration matrix elements because of their non-symmetric form:

$$L_{\mathrm{S}}(n'l, nl) = \frac{1}{2}\left(L_{\mathrm{QR}}(nl, n'l) + L_{\mathrm{QR}}(n'l, nl)\right). \quad (3.4)$$

Special features of the quasirelativistic RO and the finite size of the atomic nucleus are taken into account while evaluating the spin-orbit interaction. This results in the spin-orbit interaction parameter acquiring the following form [4]:

$$\eta_{\rm QR}(nl) = \frac{\alpha^2}{8}\int_0^\infty \frac{P(nl|r)\frac{1}{r}\frac{dU(r)}{dr}P(nl|r)}{1-\frac{\alpha^2}{4}\left(\varepsilon_{nlj}+V(r)\right)}dr. \tag{3.5}$$

All two-electron interactions are taken into account in the same way as it is usually done within the Breit-Pauli approach. This similarity with the conventional approach enabled us to use the program [8] for calculation of the angular integrals of the energy operator matrix elements, and the program [9] for calculations of the electron transition characteristics along with the program [10] upgraded for the use of the quasirelativistic RO. Our own original codes are used in the remaining calculations.

To take into account the correlation effects, the transformed radial orbitals (TRO) are used to describe the virtually excited electrons. The TRO were initially introduced for non-relativistic calculations [11] and their advantages are confirmed by numerous non-relativistic researches (see for example [12],[13],[14],[15] and references therein). The TRO with two free parameters k and B are utilized within the present calculations:

$$\begin{aligned} P_{\rm TRO}(nl|r) = N\Big(r^{l_0-l+k}\exp(-Br)P(n_0l_0|r) \\ -\textstyle\sum_{n'<n}P(n'l|r)\int_0^\infty P(n'l|r)r^{l-l_0+k}\exp(-Br)P_{\rm QR}(n_0l_0|r)dr\Big). \end{aligned} \tag{3.6}$$

These parameters are varied in order to ensure the maximum of the averaged energy correction to the energy of the configuration under research expressed in the second order of the perturbation theory. The same set of RO is used to describe both even and odd configurations thus avoiding any problems caused by the non-orthogonality of RO while calculating the transition characteristics.

Employing the TRO one can generate a very large basis of radial orbitals. Consequently, the number of possible admixed configurations increases rapidly. Therefore it becomes necessary to select the admixed configurations that have the largest influence on the configuration being adjusted. The mean weight of the admixed configuration within the wave function of the adjusted configuration expressed in the second order of perturbation theory is used as a selection criterion

$$W_{\rm PT}(K_0,K') = \frac{\sum_{TLST'}(2L+1)(2S+1)\langle K_0TLS||H||K'T'LS\rangle^2}{g(K_0)\left(\bar{E}(K')-\bar{E}(K_0)\right)^2}. \tag{3.7}$$

Only the configurations having $W_{PT}(K_0,K')$ larger than a specified small parameter S are used in the calculations. This method coincides completely with the one exploited in the non-relativistic calculations [12], [16], [17]. The configuration state functions of the selected configurations were utilized to form the energy operator matrices. The approach employed is more thoroughly described in [7] and references therein. The examples of applications of the approach are available in [18], [19].

Electron-impact excitation of atoms is computed in the Born approximation [20]. The calculation consists of two parts. First of all, we determine the angular integrals for all required matrix elements. For this purpose we adopt the computer code [9] which determines angular integrals for the matrix elements of radiative transitions. Secondly, the special code to calculate the parameters for the electron-impact excitation in Born approximation was created. This program utilizes the eigenvalues and eigenvectors obtained from the Hamiltonian matrix in quasirelativistic approach to compute the excitation cross-sections and collision strengths in multiconfiguration approximation. The main task of this code is to determine the radial integrals containing the spherical Bessel functions. In our code these integrals are calculated for each electron energy in order to avoid possible computational errors. We apply a logarithmic step for the numerical integration of radial integral over the wave-vector facilitating the reduction of computing time. The analysis of computed integral values have demonstrated that it is enough to use only 25 integration points.

Obtained data for energy level spectra and collision strengths were transferred to the ADAS *adf04 type 1* files. Because of the requirement to present the ionization energy in this file, a special subroutine to derive and to include necessary information retrieved from to the NIST database [21]. After that *adf04 type 2* files were generated using code "adf04.om2ups.f".

3.3 Calculation results

3.3.1 Investigation of $5d - 6p$ excitation

According to the first task of Sub-Contract, the energy level spectra and Born collision cross sections were investigated for the hafnium, tantalum, tungsten and rhenium ions with open $5d^N, N = 1, 2, 3, 4$ shell. It is well known that the electrons from $5d$ shell have energies very close to $6s$ shell electron energies in a case of low-ionized atoms. Therefore the ion energy eventually is not affected by the $5d - 6s$ excitation, the spectral lines are greatly mixed and configurations interact strongly. Therefore, instead of investigating one ground configuration, one must consider configuration complex $5d^N + 5d^{N-1}6s + 5d^{N-2}6s^2$. After the excitation of $5d$ electron to the $6p$ shell, another complex of strongly interacting configurations $5d^{N-1}6p + 5d^{N-2}6s6p + 5d^{N-3}6s^26p$ arises. Therefore, one must consider three even-parity configurations and three odd-parity configurations at once.

All radial orbitals for the above configuration complexes were determined in quasirelativistic approximation. In a following step, the radial orbital basis was complemented by TRO having the principal quantum number n from 7 to 9 and all allowed values of the orbital quantum number l. One- and two-electron excitations from $5p$, $5d$, $6s$ and $6p$ shells of everyone configuration under investigation (adjusted configuration) to all possible states of our defined basis were considered while constructing the basis of admixed configurations. The excitation of $5s$ electrons did not make a significant influence, therefore it was not included in further calculations. When the number of electrons in $5d$ shell was small ($N = 1$ or 2), the value of configuration selection parameter from Eq. 3.7 adapted was small ($W = 10^{-7}$). From the experience of previous calculations we can definitely state that this value is small enough.

When the number of electrons in investigated configurations increases, the number of LS-terms increases significantly. The number of these terms in admixed configurations increases even faster. In order to run the job on our computer clusters, we had to increase the value of selection parameter W. In the case of lutetium isoelectronic sequence ($N = 3$), we have chosen $W = 10^{-6}$, in the case of hafnium isoelectronic sequence ($N = 4$), $W = 10^{-5}$. Even if these selection parameter values are significantly larger than those for configurations with small number of d electrons, the selected admixed configurations have enabled us to include most important correlation effects.

Some parameters of our applied CI expansion are given in Table 1. The first column (Ion) gives the ion description and the number of electrons (N) in open shells. The second column (P) gives parity of the investigated configurations. A row with the symbol "e" describes properties of the $5d^N + 5d^{N-1}6s + 5d^{N-2}6s^2$ shells, and a row with the symbol "o" describes properties of the shells $5d^{N-1}6p + 5d^{N-2}6s6p + 5d^{N-3}6s^26p$. Column $N_{\rm lev}$ gives the number of investigated levels in these shells. Column $N_{\rm conf}$ describes the number of selected configurations in CI wavefunction expansion. Parameter $N_{\rm conf}$ tends to decrease along isoelectronic sequence when the ionization degree increases. This is caused by decreasing influence of correlation effects. On the other hand, the number of admixed configurations (we investigate one odd-parity configuration for the hafnium isoelectronic sequence) rises and the number of available virtual excitation channels increases, when the number of electrons N increases. The correlation effects become stronger for bigger N numbers. Consequently, the number of selected admixed configurations for the hafnium isoelectronic sequence is significantly larger comparing to the case of Tm-like ions even if the selection parameter differs by two orders of magnitude.

The column T_0 gives the total number of configuration state functions (CSF) in full CI wavefunction expansion. Applying our methods to reduce the number of CSF in CI wavefunction expansion [17],[22], the initial number T_0 was reduced to the number $T_{\rm R}$, which was specifically used in our calculations. It is well established that such a reduction of the number of CSF does not decrease the accuracy of determined results. As one can see from Table 1, the reduction of CSF numbers have decreased the number of necessary CSF by up to one hundred times. As a consequence, the size of Hamiltonian matrix and the size of the determined eigenfunction expansion has decreased by the same factor. Without that reduction we could not perform CI calculations with such numbers $N_{\rm conf}$ on our computer clusters or these calculations would take substantially more time than the whole current project duration. Although the reduction significantly decreases the number of included CSF, the number $T_{\rm R}$ increases fast with the increase of N. In real calculations, the computational times of all physical parameters, such as eigenvalues and eigenfunctions, radiative transition data, collision strengths, increase as a square function of the size of adopted CSF basis in wavefunction expansion.

The number of investigated energy levels $N_{\rm lev}$ increases rapidly with increase of the number of electrons in open shells. This causes fast increase of the number of possible electron-impact excitation channels $N_{\rm cs}$. The row "e" gives

Table 3.1: Parameters of adopted CI wavefunction expansion

Ion	P	N_{lev}	N_{conf}	T_0	T_R	N_{cs}
Hf IV, $N = 1$	e	3	353	121,320	1,692	3
	o	2	216	64,617	578	6
Ta V, $N = 1$	e	3	345	119,878	1,630	3
	o	2	210	64,016	546	6
W VI, $N = 1$	e	3	340	119,760	1,728	3
	o	2	213	63,893	517	6
Re VII, $N = 1$	e	3	278	103,011	1,511	3
	o	2	196	58,596	550	6
Hf III, $N = 2$	e	14	706	679,333	17,850	79
	o	16	604	738,718	16,469	186
Ta IV, $N = 2$	e	14	703	671,254	17,780	79
	o	16	607	732,100	16,643	186
W V, $N = 2$	e	14	700	677,081	16,974	79
	o	16	618	743,042	16,161	182
Re VI, $N = 2$	e	14	633	623,011	17,080	79
	o	16	544	675,614	15,533	180
Hf II, $N = 3$	e	37	696	1,712,870	74,580	661
	o	70	742	2,898,127	89,874	2,182
Ta III, $N = 3$	e	37	738	1,778,745	79,562	661
	o	70	785	3,008,006	95,404	2,439
W IV, $N = 3$	e	37	700	1,739,538	74,840	661
	o	70	750	2,945,969	89,155	2,438
Re V, $N = 3$	e	37	643	1,590,725	72,307	661
	o	70	689	2,699,768	87,267	2,399
Hf I, $N = 4$	e	81	495	2,481,662	155,336	2,880
	o	212	501	5,873,610	273,076	8,772
Ta II, $N = 4$	e	81	441	2,346,219	149,158	2,880
	o	212	461	5,590,700	251,392	13,630
W III, $N = 4$	e	81	443	2,172,778	152,473	2,880
	o	212	458	5,114,420	246,644	14,309
Re IV, $N = 4$	e	81	373	1,755,935	134,624	2,880
	o	212	391	4,138,893	235,030	14,233

N_{cs} for the excitations between the levels of even-parity configurations (even excitations), and the row "o" gives the number of electron-impact excitations from the even-parity configurations to those of odd parity (odd excitations). The numbers of even excitations are constant for all ions of the same isoelectronic sequence. They increase rapidly with increase of N. The numbers of odd excitations increase even faster with increase of N. Their values can change for the different ions in the same isoelectronic sequence.

This can be explained very easily. When the number of electrons in open shells N increases, the number of energy levels increases also. The energy levels of different parities begin to overlap. That will decrease the number of computed electron-impact excitation channels because our codes do not calculate the excitation when the final levels is lower than the initial one. Since the positions of energy levels are specific for each ion, the N_{cs} values differ slightly.

A large number of possible excitation channels had caused a situation that the most of computational time resources

was devoted to calculate parameters of electron-impact excitation, after all angular integrals for transition matrix elements were determined already. The calculation of a single excitation for all necessary electron energies in the case of Tm-like ions required only 0.2 second of CPU time. For the ions of hafnium isoelectronic sequence, that kind of calculation required 100 − 110 seconds. As a result, the calculation of just odd excitation cross-sections took around 3 weeks of CPU time. Even if all calculations were distributed between several CPUs (up to 8 CPUs simultaneously), it took approximately one month time for each ion to determine collision data in the case of hafnium isoelectronic sequence.

Our calculation results were transformed into *adf04 type 1* and *type 3* files and submitted to contractor.

3.3.2 Calculation of $5d - 5f$ excitation in W^{+2} ion

According to the second task of the current Sub-Contract, we have investigated electron-impact excitation of $5d$ electrons to the $5f$ shell in doubly-ionized tungsten. In this case three initial even-parity configurations remain the same $5d^4 + 5d^3 6s + 5d^2 6s^2$ as in previously discussed excitation to the $6p$ shell. We need to include three strongly interacting configurations with $5f$ electron: $5d^3 5f + 5d^2 5f 6s + 5d5f6s^2$. Since the energies of these configurations are higher than those of the configurations with $6p$ electrons $5d^3 6p + 5d^2 6s6p + 5d6s^2 6p$, the latest complex of configurations must be included into the list of adjusted configurations and the admixed configurations have to be selected for it.

While performing calculations of W^{+2}, the quasirelativistic function basis, comparing to that described in Sect. 3.1, was complemented with RO for $5f$ electron. Afterwards, the radial orbital basis was supplemented with transformed RO, having the main quantum number $7 \leq n \leq 9$ and all allowed values of the orbital quantum number l. This procedure was the same as in earlier case.

Further calculations were performed by utilizing virtual electron excitations from the $5p$, $5d$, $6s$ and $6p$ shells of every adjusted configuration into all allowed states. For the even-parity configurations, the selection parameter was set to $W = 10^{-5}$, the same value as in the previous calculations. This did not cause any problems. The complex of three odd-parity configurations with $5f$ electrons can generate a big number of LS-terms. The number of fine-structure levels arising from them $N_{\rm lev} = 388$ was almost two times larger comparing to configurations with $6p$ electrons. After applying selection parameter values $W = 10^{-5}$ for configuration with $5f$ electron and $W = 10^{-3}$ for the configurations with $6p$ electron, we have acquired these parameters for the CI wavefunction expansion: $N_{\rm conf} = 443$, $T_0 = 9,714,778$, $T_{\rm R} = 758,212$.

Although the number of selected configurations was not large, the number of their LS-terms was significantly to large for use in our computing facilities. Therefore the selection parameter for the configurations with $5f$ electron was increased to $W = 10^{-4}$ and for the configurations with $6p$ electron it was increased to $W = 5 \times 10^{-2}$. Using these selection parameters, we have acquired $N_{\rm conf} = 150$, $T_0 = 2,514,778$, $T_{\rm R} = 298,843$ for the wavefunction extension parameters. The total number of excitation channels between even-parity and odd-parity configurations was 28392. The computational time for one excitation channel and all electron energies was approximately 53 seconds. The total computational time to determine data in employed approximation took over 18 days.

Determined data results were submitted to contractor in the *adf04 type 1* and *type 3* files.

One part of Task 2 in current Sub-Contract Agreement was planned for the calculations with electrons virtually excited from the $4f$ shell. Unfortunately, we have encountered significant technical problems when trying to perform such calculations. When the selection parameter $W = 10^{-4}$ and the virtual excitation from the $4f$ shell is included, the CI parameters are $N_{\rm conf} = 356$, $T_0 = 41,704,388$, $T_{\rm R} = 3,541,293$. After increasing the selection parameter value to $W = 10^{-3}$, the CI parameters decrease to $N_{\rm conf} = 88$, $T_0 = 9,388,040$, $T_{\rm R} = 623,301$. Even at that small number of interacting configurations, the acquired number of LS-terms does not allow to perform calculations on our computer clusters. A further increase of selection parameter W restricts the number of admixed configurations even more significantly. Therefore even the data from the energy level calculation become unstable because for a part of the levels correlation corrections become large while for another part of the levels they are too small. Such a situation significantly distorts determined eigenvalues and eigenfunctions. Consequently, calculation results are unreliable.

There is one more issue in performing electron-impact excitation calculations with inclusion of virtual excitations from the $4f$ shell. Prof. G. Gaigalas, on top of his task to include f electrons into transition operator angular integrals

calculation code, was planning to remake it substantially and to improve it in order to achieve a higher reliability and computing speed. This work is rather complicated. It had required more time and effort than it was planned initially. Therefore Prof. G. Gaigalas did not succeed in time to extend his code which determines transition operator matrix element angular integrals for f electrons.

On the other hand, our experience in such calculations point out to a conclusion that the inclusion of polarization does not lead to any significant changes when investigating transition parameters. Therefore it is reasonable to expect that determined collision strengths both for the transitions inside the even-configurations and for the transitions from the $5d$ shell to the $6p$ and $5f$ shells are reliable enough.

3.3.3 Investigation of the applicability of the quasirelativistic radial orbitals as inputs for the AUTOSTRUCTURE

We have determined quasirelativistic radial orbitals under request of contractor. The RO basis was to include required transformed radial orbitals. The file with these data was submitted to contractor.

Each RO present in that file is described by following information.

Record 1.
FORMAT(A2,2X,A8,F6.2,F10.5,F6.2,1X,A3,2I3,I5,F20.12,2L3,2X,A1):
Atomic symbol, name of atom, nuclear charge, nuclear mass, ionization degree (spectroscopic notation), nl, n value, l value, number of points N in RO, one-electron energy (in a.u.), two logical variables and parameter used in solving equations.

Record 2.
FORMAT(4(1PD20.13)/):
Value of the first point r_1 of RO, the nuclear radius, two parameters describing the way to include spin-orbit interaction in solving equations.

Records 3 - 8.
FORMAT(6(5(1PD20.13)/)):
Coefficients describing expression of RO by powers of radial variable for 6 points inside nuclear charge.

Records with RO.
FORMAT(5(1PD20.14)):
The values of radial orbital N points $\bar{P}(nl|r)$ at logarithmic step.

$$\bar{P}(nl|r) = r^{1/2}R(nl|r) = r^{-1/2}P(nl|r).$$

The logarithmic step was defined according the relation $r_{i+1} = r_i \exp(0.01)$.

Records after text the record with text "TOLIAU VARDIKLIS".
FORMAT(5(1PD20.13)):
Values of the N logarithmic-step points of the denominator used to solve the quasirelativistic equations (3.1) and to determine quasirelativistic energy corrections (3.3),(3.5).

The routine to read RO from the described file into computer memory and the routines to calculate the average integrals of radial variable and all radial integrals of energy operator can be submitted to contractor at his request.

3.4 Conclusion

We may conclude, that all tasks included in the Sub-Contract Agreement between University of Strathclyde and Institute of Theoretical Physics and Astronomy (ITPA) of Vilnius University have been achieved. Larger calculations can be performed on computer clusters with bigger numbers of CPU available and bigger amount of RAM and higher CPU clock rate.

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Chapter 4

Electron collision cross-sections for heavy element ions - S1

(1) PILOT R-MATRIX CALCULATIONS FOR TUNGSTEN
(2) W XLV: ATOMIC DATA FOR ITER DIAGNOSTICS

The authors of this chapter are Cathy Ramsbottom, Alan Hibbert, Penny Scott, L. Spencer, Nigel Badnell and Hugh Summers. It incorporates the brief report on ADAS-EU sub-contract 1 prepared by the Centre for Theoretical Atomic, Molecular and Optical Physics School of Mathematics and Physics, Queen's University Belfast (QUB), Northern Ireland, De (C. Ramsbottom) dated 15 February 2013. See also appendix C.

4.1 Introduction

The role of tungsten as a suitable thermally resistant plasma facing wall component for the divertors of fusion machines has stimulated fresh studies of the atomic physics of tungsten. This is so that its impact on radiated power can be assessed and so that key quantities such as tungsten influx from surfaces may be measured for current machines such as AUG, JET EP2 and predicted for future machines - especially ITER. Tungsten will be present in the neutral form inflowing from plasma contacted surfaces, in low stages of ionisation up to W^{+20} in the divertor, and in ionisation stages up to W^{+60} at the highest temperatures of the central confined plasma of ITER.

This work focuses on W^{+44} , W XLV, a spectrum line emitter in the EFDA-JET experiment soft x-ray regime and a reference species for complex semi-relativistic or relativistic electron impact cross-sections calculations. A 311-state structure description is required for accurate representation of the primary observable transitions. For high precision reference studies of electron impact cross sections, an associated R-matrix calculation, towards the limit of current capability, is required. Our goal is to undertake this calculation, using CIV3 [1] for the atomic structure calculations and the R-matrix package for the collsional work. The first half of this report focuses on atomic structure aspects of the problem and the second half concentrates on the collision calculation. For such a heavy ion, we would expect a fully relativistic calculation to be more accurate than a Breit-Pauli calculation. However, it is interesting to see how well a Breit-Pauli approach can model the atomic structure.

4.2 Atomic Structure Calculations

4.2.1 LS calculations

First, to assess the extent to which we have included electron correlation, we consider a non-relativistic calculation. We customarily begin with Hartree-Fock (HF) orbitals for (typically) the ground state. However, we had access to no HF for the $4s^2\ ^1S$ state, so we determined our orbitals sequentially as follows:

Orbitals	Method of determination
1s,2s,2p	HF orbitals of W II (see [2])
3s,3p,3d	Optimised on $3s^2\ 3p^6\ 3d^{10}\ ^1S$ of W XLVII
4s	Optimised on $4s^2\ ^1S$ of W XLV
4p	Optimised on $4s4p\ ^1P^o$ of W XLV
4d	Optimised on $4s4d\ ^1D$ of W XLV
4f	Optimised on $4s4p\ ^1F^o$ of W XLV

We calculated ^1S - $^1P^o$ LS oscillator strengths using the following configurations:

Even parity
$3d^{10}4s^2$, $3d^{10}4p^2$, $3d^{10}4d^2$, $3d^{10}4f^2$, $3d^9 4s4d4f$
Odd parity
$3d^{10}4s4p$, $3d^{10}4p4d$, $3d^{10}4d4f$, $3d^9 4s^2\ 4p$, $3d^9 4p^3$, $3d^9 4s^2\ 4f$, $3d^9 4p^2 4f$,
$3d^9 4s4p4d$, $3d^9 4p4d^2$, $3d^9 4d^2 4f$, $3d^9 4s4p4f$

The oscillator strengths, in length and velocity form are

Transition		Length	Velocity	ΔE
$3d^{10}\ 4s^2\ 1\ S$	- $3d^{10}\ 4s4p\ ^1P^o$	0.703	0.722	3.59697
	- $3d^9\ 4s^2\ 4p\ ^1P^o$	0.299	0.305	65.48634
	- $3d^9\ 4s^2\ 4f\ ^1P^o$	7.472	6.892	78.80619

The good agreement between length and velocity forms demonstrates that there is sufficient correlation included in the calculation.

4.2.2 LSJ calculations

For heavier ions, relativistic effects contribute not only to the energies, but also to the radial distribution of the orbitals. Within the Breit-Pauli (BP) approximation, Cowan and Griffin [3] pointed out that the relativistic adjustment of the orbitals is achieved by including the mass-correction and Darwin BP terms in the optimisation process. The problem is that the Darwin term contains a Dirac delta function, and so for s-electrons the Hamiltonian is not bounded. Cowan and Griffin

replaced the normal expressions of these operators by

$$\begin{aligned} \text{mass correction :} \quad & - \quad \frac{1}{2}\alpha^2 \left[\epsilon_i - V(r)\right]^2 \\ \text{Darwin :} \quad & - \quad \delta_{l0}\frac{1}{4}\frac{dV}{dr}\left(\frac{d}{dr} - \frac{1}{r}\right) \end{aligned} \tag{4.1}$$

for the potential $V(r)$ describing the W XLVII core. Mohan and Hibbert [4], in work on Hg I, expressed $V(r)$ as a sum $V_D(r) + V_E(r)$ of direct and exchange potentials, and used simple local expressions for these operators. We followed a similar pattern for W XLV, writing

$$\begin{aligned} V_D(r) &= -\frac{Z - N_c}{r} - \frac{N_c}{r}\exp(-\alpha r) \\ V_E(r) &= C\exp(-\beta r) + Dr\exp(-\gamma r) \end{aligned} \tag{4.2}$$

where Z=74 and N_c =28, the number of core electrons. The parameters were determined by fitting the matrix elements of these operators to those of the all-electron values: α =13.64(s), 13.56(p), 13.36(d or f); β = 7.236; γ = 6.541; C = -13.5; D = -0.11. However, when we used these operators to model the BP operators in the optimisation of the orbitals, we found the fine structure separations were substantally overestimated. So instead, we took the non-relativistic orbitals (expressed in terms of Slater-type orbitals (STOs)) and varied the exponent of the outermost STO so that the energy separations between certain pure (ie no significant CI mixing) levels were given to reasonable accuracy in a single configuration approximation:

4f : optimised using the BP operators, 4s4f $^3F^o$
4d : to fit the separation between 4s4d $^3D_1$ and $^3D_3$
4p : to fit the separation between 4s4p $^3P^o_0$ and $^3P^o_2$
4s : to fit the separation between $4s^2$ $^1S_0$ and $4p^2$ $^3P_1$

What is remarkable is that the fine structure splittings of the $4p^2$ levels is also given well by these orbitals, while the 4s4d levels, although higher than experimental levels [5] are fairly consistent among themselves.the energies (in atomic units) are shown below.

Level		Expt [5]	This work
$4s^2$	$^1S_0$	0.000	0.000
4s4p	$^3P^o_0$	3.165	3.165
	$^3P^o_1$	3.429	3.423
	$^3P^o_2$	6.809	6.833
	$^1P^o_1$	7.478	7.486
$4p^2$	$^3P_0$	7.235	7.245
	$^3P_1$	10.688	10.687
	$^1D_2$	10.766	10.752
	$^3P_2$	14.630	14.690
	$^1S_0$	14.805	14.812
4s4d	$^3D_1$	12.679	12.976
	$^3D_2$	12.801	13.085
	$^3D_3$	13.413	13.709
	$^1D_2$	13.617	13.839

4.2.3 Inner-shell excitations

The LS calculations show that the strongest resonance lines involve transitions from the 3d sub-shell, particularly to 4f. We included all configurations of the form $3d^{10}\ 4l^2$ and $3d^9\ 4l4l'\ 4l''$, for ^{1}S and ^{3}P J=0 even parity, and 1 Po , 3 Po and 3 Do J=1 odd parity. We did however omit $3d^94s^24d$, since it corresponds to a configuration correcting the 3d orbital, and this is not matched by a corresponding CSF in the $3d^9$ configurations. This gives us 99 even parity and 259 odd parity CSFs.

The upper levels are more properly expressed in terms of j-j rather than LSJ coupling, although there is a recoupling transformation matrix between the two representations. If we consider the 3d9 4s2 4p states and write the possible couplings as

LSJ - Φ_i: $^1P^o_1$, $^3P^o_1$, $^3D^o_1$;
j-j - Ψ_j: $(\frac{5}{2},\frac{3}{2})_1$, $(\frac{3}{2},\frac{3}{2})_1$, $(\frac{3}{2},\frac{1}{2})_1$;

the transformation between them is $\Phi = U\Psi$ where

$$U = \begin{pmatrix} \sqrt{\frac{3}{5}} & -\sqrt{\frac{1}{15}} & \sqrt{\frac{1}{3}} \\ \sqrt{\frac{3}{10}} & \sqrt{\frac{8}{15}} & -\sqrt{\frac{1}{6}} \\ -\sqrt{\frac{1}{10}} & \sqrt{\frac{2}{5}} & \sqrt{\frac{1}{2}} \end{pmatrix}$$

and we find that, following this transformation of our results, the three J=1 levels are at least 99% pure when labelled (from lowest to highest in energy) as $(\frac{3}{2},\frac{1}{2})_1$, $(\frac{5}{2},\frac{3}{2})_1$, $(\frac{3}{2},\frac{3}{2})_1$, in agreement with [5].

The oscillator strengths for the three transitions from the ground state are

Upper level	fl	fv	Ref [6]
$(\frac{3}{2},\frac{1}{2})_1$	0.080	0.094	0.122
$(\frac{5}{2},\frac{3}{2})_1$	0.197	0.220	0.188
$(\frac{3}{2},\frac{3}{2})_1$	0.027	0.029	0.019

where we also compare with the Relativistic Parametric Potential calculations of [6]. Both sets of calculations are *ab initio*.

By contrast, the $3d^9\ 4s^2$ 4f levels are heavily mixed with $3d^9$ 4s4p4d, and the large ^1S - ^1P_o oscillator strength is somewhat dispersed across several transitions. There are 36 couplings of the angular momenta, and only four of these are given in the NIST tables, all showing strong mixing. In fact $3d^9\ 4s^2$ 4f is distributed across all 36, but with varying strengths. In particular, we concur with the mixings given by NIST for the level at 17 337 000 cm^{-1} and at 17 399 900 cm^{-1}, though our *ab initio* calculations did not clearly identify the labelling for the other two lines in [5]. For the former two lines, the oscillator strengths are (f_l ,f_v) = (2.212,2.039) and (1.343, 1.203), with several other lines having f-values in the range 0.5-0.9.

4.3 The Collision Calculations

The orbital parameters defined above for the structure calculations will now be utilized in the electron-impact excitation evaluations for W XLV to derive the collision strengths and effective collision strengths for forbidden and allowed lines. These collision calculations will include for the first time atomic data for the main predicted radiative loss transition, $3d^{10}$ $4s^2$ - $3d^9$ $4s^2$ 4f, representing an opening of the 3d shell. To compute the collision cross sections we aim to use two sets of parallel R-matrix codes. Initially the LS orbital parameters defined above will be included in PRMAT [7] and FINE95 [8], the RMATRXII suite of codes which adopts the LS coupling scheme in the internal region evaluations followed by a unitary transformation from LSπ to Jπ coupling on the boundary. At the present time we are midway through the internal region computations for this initial calculation. As already stated for heavy ions, such as W XLV, relativistic effects should contribute. In order to test and corroborate these initial evaluations we aim to perform a second collision calculation adopting the LSJ orbital parameters defined above in the Breit-Pauli suite of computer codes. If we find that the collision cross sections agree for both evaluations and that either a semi-relativistic BP or non-relativistic PRMAT R-matrix approach may be adopted in the collision calculations, then for the first time we may be in a position to tackle these complicated heavy systems. We will thus be able to include in the model a number of high-lying important levels that have never been investigated before. The subsequent benefit to the plasma physics community as well as other theoreticians would be great. The model developed to represent the W XLV target in both collision calculations consists of 141 LS target states which arise from the $3d^{10}4s^2$, $3d^{10}4p^2$, $3d^{10}4d^2$, $3d^{10}$ 4s4p, $3d^{10}$ 4s4d, $3d^{10}$ 4s4f, $3d^{10}$ 4p4d, $3d^{10}$ 4p4f, $3d^{10}$ 4d4f, $3d^9 4s^2 4p$, $3d^9 4s^2 4d$, $3d^9 4s^2 4f$, $3d^9 4s 4p^2$ and $3d^9 4s 4d^2$ configurations. This represents a formidable 311 fine- structure levels, 1905 coupled channels and a total of 48,205 individual forbidden and allowed lines. The only other theoretical work to compare with this is the collision evaluation of Ballance and Griffin [8] who performed a 168-level parallel Dirac R-matrix calculation. We note that this work did not include the $3d^9 4s^2 4f$ levels important in the present work. Comparisons between all three sets of atomic data for a selection of transitions will allow us to systematically investigate the inclusion of relativistic effects for these heavy species.

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Chapter 5

OPEN-ADAS upgrade - S9

The authors of this chapter are Allan Whiteford, Andy Armstrong, Martin O'Mullane and Hugh Summers. It incorporates the report on ADAS-EU sub-contract 9 prepared by A. Whiteford dated 21 February 2013. See also appendix D. The present document details changes made to the OPEN-ADAS system as part of a sub-contract awarded to 256 Kelvin Limited from the ADAS-EU project. The primary purpose of the sub-contract was to enhance and reinforce the online distribution mechanism for OPEN-ADAS. A significant security review was performed and the re-write of front-end infrastructure gave opportunity to also address some of the visual aspects of the site.

5.1 Background

OPEN-ADAS is the name of the path for release of ADAS data and support software into the public domain. It is an agreed and shared project between ADAS and the International Atomic Energy Agency, Atomic and Molecular Data Unit, Nuclear Data Section (IAEA) in Vienna. As agreed in the ADAS-EU proposal, OPEN-ADAS is used for public domain release of fundamental and derived atomic data which enters the ADAS databases from ADAS-EU activities. The web server is located at the Physics Department, University of Strathclyde and is linked via the IAEA web pages. The development of OPEN-ADAS was substantively finished early in the ADAS-EU project with the addition of free-form search capability. During the first 18 month reporting period the number of users increased steadily each month and came from very many countries. The principal aims of the project had been realized and it had settled down to high-availability but low-maintenance web service.

In June 2010 email attacks began. The webserver logs showed a few SQL injection attacks every few weeks which is not unexpected on the public internet. However around the end of May 2011 the volume rose sharply. The reasons are unclear but news of a successful exploit probably circulates quickly in the anarchistic world of web breaking. Ameliorating steps were taken. The usual way of ameliorating such an attack is via a captcha. Before implementing such a system a simpler text challenge field was tried: requesting the correspondent to type 'not spam' into the appropriate box. This proved to be successful initially so the more invasive captcha system was not deployed. The OPEN-ADAS web site required a simple sign-up resulting in an account with a password. The name and email address were not verified before creating the account so a degree on anonymity was possible. This enabled us to produce accurate usage statistics since the number of hits is a very poor metric. Reports that a list of the OPEN-ADAS user names and passwords

were available on the 'pastebin' web site came to us in the first week of June 2011. A serious security breach had occurred.

It should be noted that the actual attack vector was suspected to be another site hosted on the same server but that it is still deemed necessary at this point to do a thorough security audit of OPEN-ADAS.

It was decided that the most effective way to prevent a further occurrence was to remove the registration requirement. All data from OPEN-ADAS can now be downloaded anonymously. The removal of the code for registration, sanitizing the MySQL queries and trapping all input resulted in the OPEN-ADAS website being unavailable until 4 September 2011 — a two month interruption which also displaced other activities. The disadvantages in not knowing the OPEN-ADAS users are the loss of statistics and the ability to inform people who downloaded data of any subsequent improvements. Given the time pressures on the staff, this was an acceptable compromise.

5.2 Site security and Infrastructure

The public-facing website was given a thorough overhaul as a primary objective of this work. The underlying logic on searching for data has remained largely unaltered. Although it should be noted that there is a significant change in display (see section 5.3.1) and navigation (see section 5.3.2) along with enhanced data coverage (see section 5.4).

5.2.1 SQL Injection Attacks

A complete re-write of the way in which input data is processed was undertaken. This primarily involved rationalisation of data into distinct classes with well defined input and output characteristics. Whereas before each data class had it's own custom code, each class now has a file associated with it which transfers information about search parameters etc. to a more generalised searching mechanism.

This allows much less repetition of code and, critically for the security of the site, means that there orders of magnitude less places for security vulnerabilities to occur. Previously a file such as `adf15.php` had code like:

```
@$element   = $_GET['element'];
@$charge    = $_GET['charge'];
@$wave_min  = $_GET['wave_min'];
@$wave_max  = $_GET['wave_max'];
@$resolveby = $_GET['resolveby'];
```

it would have been necessary to modify **each** line to contain a call to `mysql_real_escape_string` and then repeat this exercise for **every** data class.

There is now a single place of code where search parameters come in which looks like:

```
$searchparams=$adf->searchparams();
foreach(array_keys($searchparams) as $p)
```

```
{
        if (isset($_REQUEST[$p]))
            $searchparams[$p]=mysql_real_escape_string($_REQUEST[$p]);
}
```

Such an approach makes it much less likely for an unescaped string to be able to be passed into SQL and also has the advantage of meaning there is less code so that future maintenance of the system will be much more straightforward.

5.2.2 Removal of user database

The original OPEN-ADAS system consisted of two MySQL databases:

- A read only database containing metadata about each file
- A read-write database containing user information

The need for login and capture of user information was removed some time ago but part of this upgrade fully cleansed any reliance on the user database existing at all.

5.2.3 URL Structure

The URL structure of the site was changed significantly, urls such as:

- `http://open.adas.ac.uk/adf08.php`
- `http://open.adas.ac.uk/filedetail.php?id=16300`
- `http://open.adas.ac.uk/aboutoa.php`

were changed to:

- `http://open.adas.ac.uk/adf08`
- `http://open.adas.ac.uk/detail/adf08/radrec/lilike/lilike_c3ls.dat`
- `http://open.adas.ac.uk/about-open-adas`

There is no inherent security advantage in this approach but it does obscure somewhat the technology being used and the fact there is a database with ‘id’s etc.

The two main advantages are that it is much better suited for search engine optimisation and also that links to files are persistent. Previously the file with an id of ‘16300’ would change between versions of the ADAS database. By mapping the URL to a pathname similar to that of the underlying database URLs can be shared and stored which are more predictable. Note that because the character ‘#’ has a special meaning in a URL it cannot be used in file URLs. Unfortunately, ADAS makes extensive use of the ‘#’ character so in URLs we replace this with the string ‘][’.

5.3 Visual design and user experience

The overall user experience of the OPEN-ADAS site was upgraded significantly. Emphasis and attention was given to user flow both for the non-expert and expert user.

5.3.1 Design aesthetics

The design aesthetics of the site were completely redone. Figure 5.1 shows a screenshot from the new site. There are a number of specific issues to note versus the old design which are drawn attention to here.

Colour has been used with blue representing the site generally along with headings etc. Orange has been used for derived data and purple for fundamental data. Blue was chosen as the base colour to match current ADAS branding but the shade of blue was changed very slightly to be less imposing on the screen and easier on the eyes. Orange is then a natural companion to blue. There was an attempt made to make the purple shade match H_α emission but this was, unfortunately, not aesthetically appropriate.

It should also be noted that orange has been used for general searching (top right) even though these searches (with the exception of wavelength) search both fundamental and derived data. This is to subtly shift the emphasis of the site to derived data.

Note also the line at the top of the screen stretching from the blue logo to the orange buttons. The 'spectrum' band between the two colours corresponds to an inverse linear dispersion of 3.2 Å / px converted to an RGB representation using Bruton's algorithm with a gamma value of 0.8. The orange and blue used in the design do not correspond exactly to a spectral colour (pure spectral colours do not work well in web design as they tend to be too bright and reduce contrast when against a white background). To deal with this problem and to prevent a sharp jump in colour there are ten pixels used at the short wavelength and five at the long wavelength to blend to the design colours .

As the mouse is moved by the user, a spectrum line moves along the top of the screen corresponding to a line at the wavelength of that pixel position. The movement is reasonably gentle and doesn't cause much distraction but the implication is that horizontal spectroscopy is so trivial that it's been relegated to a neat graphical effect so that the serious business of vertical spectroscopy can be done.

5.3.2 Navigation scheme

The navigation scheme was also re-done completely. In particular there are now three parts to the navigation:

1. General search boxes at the top right in a toolbox style arrangement.
2. All of the data classes are present down the left hand side of the screen.
3. Ancillary links have been moved to the footer.

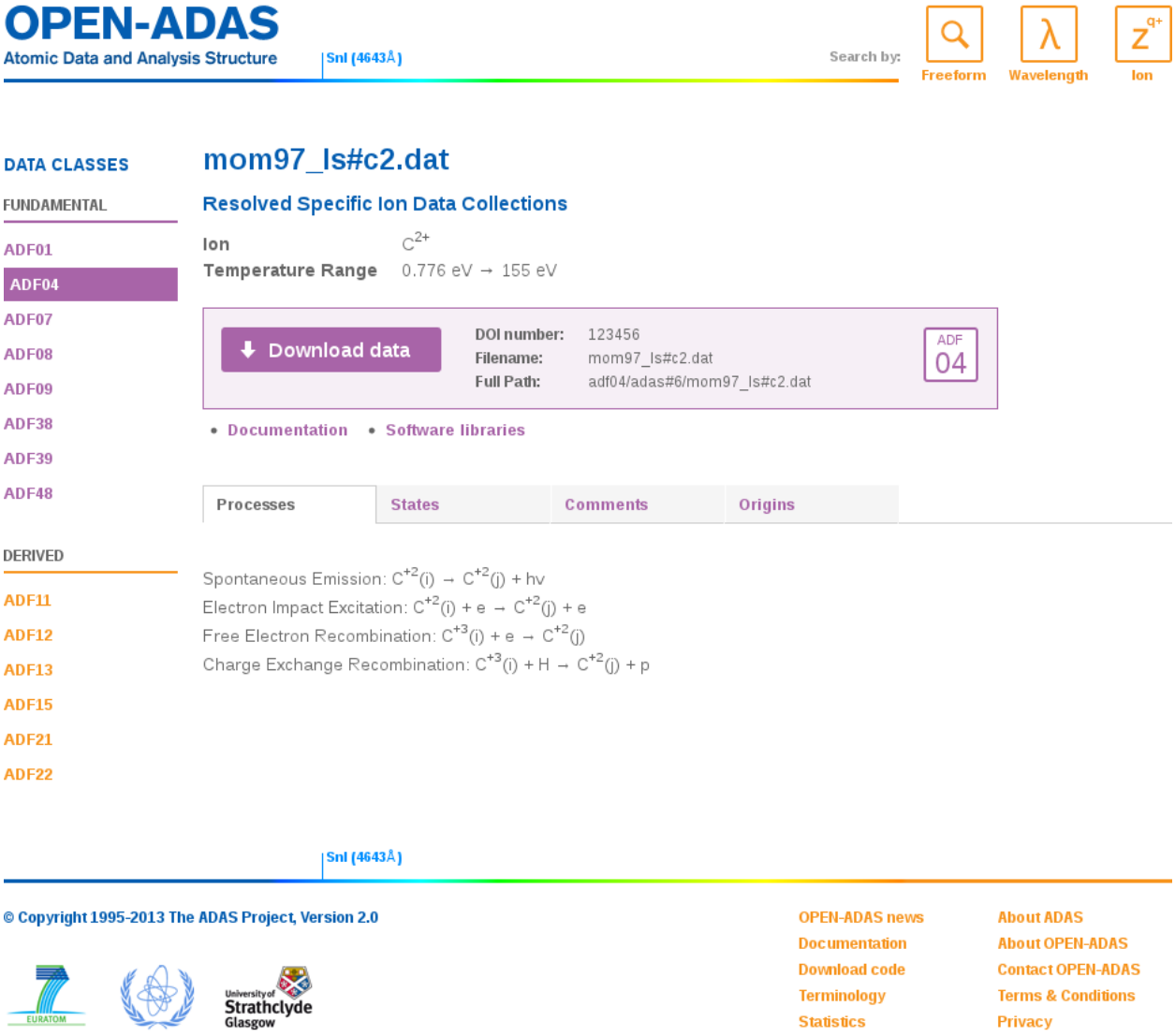

Figure 5.1: New design of OPEN-ADAS site

A number of things have been achieved by these changes. Specifically the ADAS data classes now play a more front and centre role to the navigation, previously they were hidden behind a 'search by dataclass' link. The links themself have also become (intentionally) ambiguous. Rather than saying explicitly that they are for searching, the contents behind the link now gives some information about the data class and additionally allows one to search.

The fact the link is now simply the data class name allows unambiguous highlighting of it after a user navigates to it irrespective of the route they chose to get there. The previous version of OPEN-ADAS suffered in that if a user navigated to a file using freeform search then they would end up in a state where 'search by dataclass' was highlighted and the dataclass appearing on the tabbed navigation even though they had never explicitly chosen this route or option. The new navigation scheme, by design, eliminates these problems entirely.

The links at the left serve to remind the non-expert user about the extent and organisation of OPEN-ADAS and they also allow the expert user to quickly search for a specific data class.

5.3.3 Home page

The home page of the OPEN-ADAS system was given particular attention so that the non-expert user can quickly understand what the system is for, The previous home page was simply a freeform search box and some navigation. The new homepage is shown in figure 5.2.

This new home page frames the idea of OPEN-ADAS and has some positioning paragraphs for the new user. It also puts front and centre the three different ways of cross-class searching (freeform, wavelength, ion).

Finally, it explains each data class and what they are, encouraging the user to click on a data class of interest — this gives a new user an immediate overview of the coverage of OPEN-ADAS in terms of types of data.

5.4 Expansion of data coverage

As part of this project, a number of new data classes were added to OPEN-ADAS, these are detailed below. Most of these files are quite similar in structure (from the point of view of parsing the data) and searching parameters (from the point of view of the user searching for data) to ADF09 files.

5.4.1 ADF38

The basic process is

$$1s^2 nl + \gamma \rightarrow 1snln'l' \rightarrow 1sn''l'' + e \tag{5.1}$$

A separate file is provided for each n , which contains data for all n'¿ n . Note however that

$$1snln'l' \leftrightarrow 1s2n'l' + \gamma \tag{5.2}$$

has to be considered consistently at the same time to avoid multiple counting. Separate files are given for term (LS) coupling and intermediate (IC) coupling.

About OPEN-ADAS

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS).

ADAS is a computer program managed by the University of Strathclyde and made up of a consortium of over twenty members.

The OPEN-ADAS system enables non-members, with an interest in fusion and astrophysics, to download and use ADAS data.

More about OPEN-ADAS

01 Feb 2013 – Major update to the website

The OPEN-ADAS website has been updated with a new visual interface and the addition of three new data classes... Read more

Freeform search

Search

Freeform search examples
Carbon
C
C+3
C+3 3000-4000A
C+3 3000-4000A ADF13

Freeform search | Search by wavelength | Search by ion

The OPEN-ADAS data classes

The data contained within ADAS is strictly organised and precisely formatted. There are over fifty distinct types of data file. The scope of OPEN-ADAS is targetted on and limited to the release and organisation of general user relevant data from the ADAS databases and the provision of code, subroutines and procedures to enable such users of OPEN-ADAS to read the released data. These data classes are given below.

FUNDAMENTAL CLASSES

ADF 01 – Charge exchange cross sections
nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

ADF 04 – Resolved specific ion data collections
Coefficient data for a given ion which includes spontaneous emission coefficients and electron impact collisional rates and other optional processes.

ADF 07 – Electron impact ionisation coefficients
Collections of Maxwell averaged electron impact ionisation rate coefficients for both direct ionisation and excitation/autoionisation.

ADF 08 – Radiative recombination coefficients
Maxwell-averaged radiative recombination coefficients i.e. spontaneous free-bound transitions of Maxwellian electrons excluding dielectronic recombination.

ADF 09 – Resolved dielectronic recombination coefficients
Collections of state-selective dielectronic recombination coefficients of Maxwellian free electrons resolved by initial and final metastable and captured n-shell.

ADF 38 – Photoexcitation-autoionisation rate coefficients
Fundamental data for inner shell excitation followed by autoionisation

ADF 39 – Photoionisation cross-sections
Fundamental data for direct (including and especially inner shell) photoionisation.

ADF 48 – Radiative recombination rate coefficients
Partial final-state resolved radiative recombination rate coefficients from both ground and metastable levels.

DERIVED CLASSES

ADF 11 – Iso-nuclear master files
Effective (collisional–radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

ADF 12 – Charge exchange effective emission coefficients
Collections of effective emission coefficients for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms.

ADF 13 – Ionisation per photon coefficients
Data collections useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface.

ADF 15 – Photon emissivity coefficients
Fully density dependent and metstable resolveed effective emissitivy coeffeicients from a collisional–radiative model.

ADF 21 – Effective beam stopping/excitation coefficients
They are effective ionisation coefficients, including charge transfer losses, which leave the beam atoms ionised.

ADF 22 – Effective beam emission/population coefficients
Coefficients for the emission from a beam when it enters an ionised plasma including impurities. Results are fully density dependent output from a collisional–radiative model.

Figure 5.2: Home page of OPEN-ADAS site

5.4.2 ADF39

The basic process is inner shell photo-ionisation:

$$(n_c l_c)^q \, nl + \gamma \rightarrow (n_c l_c)^{q-1} \, nl + \mathrm{e} \tag{5.3}$$

A separate file is provided for each n shell. Separate files are given for term (LS) coupling and intermediate (IC) coupling. Outer shell photo-ionisation is included for completeness. Where inner shell photo-ionisation is present, the atomic structure is optimised for the inner-shell processes.

5.4.3 ADF48

ADF48 files contain partial final-state resolved radiative recombination rate coefficients from both ground and metastable levels.

5.4.4 DOI

DOI numbers are issued by a number of different registries, the two which are most relevant for OPEN-ADAS are (descriptions taken from official DOI website):

- **CrossRef**
  - Scholarly and professional research content.
  - Journal articles, books, conference proceedings, etc.
  - Reference linking and searchable metadata database.
- **DataCite**
  - DataCite is focused on improving the scholarly infrastructure around datasets. There will be a set of activities around establishing and sharing best-practices, identifying and solving some of the unique issues that arise with datasets.
  - DataCite is focused on working with data centres and organisations that hold data. The details of their business models, workflows, and other requirements do not appear to be identical to those of publishers producing traditional journals.
  - DataCite has a business model that meets the needs of non-commercial and sometimes smaller organisations; larger national-scale organisations (e.g., TIB, BL) carry the basic infrastructure costs and will reclaim where appropriate within their domain.

It was decided, on balance, to firstly pursue the DateCite registry. An initial approach was made to the British library who are the UK body responsible for administering DateCite (typically participants do not approach DOI or even DateCite directly). Initial discussions were positive that DateCite via the British Library was an appropriate route to go down. These discussions are ongoing with the British Library.

5.5 Back end data processing and organisation

5.5.1 File tagging

A system was added whereby files could be excluded from OPEN-ADAS. This has initially been used to exclude older ADF38 and ADF39 files where levels and rates were split across separate files.

5.5.2 SQL population

The process of taking tag files and moving them into the relational (i.e. MySQL) database was increased by several orders of magnitude as part of this work. This was not a objective of the work but proved worthwhile to do in order to speed up testing of processing new files.

5.5.3 Code organisation

The code was reorganised and moved into a subversion repository. A detailed set of instructions for installing and updating OPEN-ADAS was also produced.

Most of the code reorganisation was done to the PHP front-end of OPEN-ADAS as necessitated to make it easier to add future data classes and also to deal with security concerns (see section 5.2 for more details).

5.6 Other considerations

5.6.1 News

Infrastructure for a news item was added to the site, this is an optional panel on the home page in addition to a link in the footer to see previous news items.

5.6.2 Privacy policy

A privacy policy page was added to the site, the specifics of this page are not finalised at the time of writing.

Appendix A

ADAS-EU: Sub-contract S6

ADAS-EU CONTRACT

ATOMIC STRUCTURE AND ELECTRON DATA FOR HEAVY ELEMENT IONS

THE IONS W^{+3} TO W^{+5}AND ADJACENT ELEMENT NEUTRAL/NEAR-NEUTRAL IONS

ATOMIC STRUCTURE MAPPING BETWEEN CODES

H. P. Summers

25 May 2012

1. Summary

It is proposed to place an ADAS-EU [1] follow-up contract with Prof. Emile Biémont, Department of Physics, University of Mons-UMONS, Belgium, to provide further compilations of atomic energy levels and transition probabilities and associated optimized parameter sets for atomic structure calculations linked to ADAS. In the initiating sub-contract (see ADAS-EU report SUBC1 [2]), a pathway was successfully created for the Mons assessments of atomic energy levels and transition probabilities for the ions W^{+0}, W^{+1} and W^{+2} to be carried into the ADAS database [3], extended into the Born collisional regime and assembled as data format adf04. This is enabled by the Mons group optimising fitting parameters for Cowan atomic structure calculations to laser induced fluorescence observational data. Parameter datasets are then transferred to ADAS for completion processing. These reference studies provided, inter alia, data for W^{0} and have allowed production of the first comprehensive set of derived photon efficiencies for W^{0} - a priority need for fusion (see ADAS-EU report SUBC1 [2]) .

Two consolidating and exploiting further actions are proposed for part 2 and will be led by Drs. Quinet and Palmeri and co-workers at UMONS and overseen by Dr. O'Mullane and Prof. Badnell for ADAS-EU. The first is organisation and transfer of a priority list of further parameter sets for ions including W^{+3} - W^{+5}, Mo^{+1}, Re^{0} - Re^{+1}, Hf^{0}, Hf^{+2}, Au^{0} - Au^{+2}, Sn^{0} and Sn^{+2}. The second action will be an investigation of how to implement University of Strathclyde AUTOSTRUCTURE calculations which are matched to the optimised Cowan structure calculations of UMONS as above. In the latter, two steps will be examined, firstly a mechanism for transfer of the radial wavefunctions will be put in place on a minimal calculation. The second step will be the inclusion of the scaling, polarization, α, β, γ and T optimizing parameters within the AUTOSTRUCTURE framework. Mo^{0} will be used as a test species for the interchange format. This important step, can extend the UMONS species optimizations further into the collisional domain, by enabling distorted wave cross-section production through AUTOSTRUCTURE. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [4].

The duration of the project will be six months (1 Jul. 2012 - 31 Dec. 2012) at a fixed price of [redacted]

2. Background

The background and broad strategy were described in the initiating sub-contract proposal. The appropriateness of this strategy and the effective implementation has been demonstrated over the last three years. The primary ADAS capability for handling heavy species has been developed and now provides the baseline of atomic modelling support for nearly all fusion plasma models. Also, the selective targetting of difficult systems for special studies, reinforced by ADAS-EU sub-contracts has worked. In line with the interests of ITER, EFDA-JET EP2 and the international fusion community, special attention has been given to tungsten ions enabling spectroscopic diagnostic analysis, such as for tungsten influx, to proceed and allowing accurate input to forward planning of the future ITER diagnostics (see ADAS-EU report ITER1 [5]).

As described in the initiating sub-contract proposal, the Astrophysics and Spectroscopy Group, University of Mons, has a long history of research on the energy levels and transition probabilities of complex neutral and near-neutral atoms. They are pre-eminent in the world on lanthanides and maintain the DREAM and DESIRE databases [6]. With the initiating sub-contract, a link was successfully set up between UMONS and ADAS enabling utilisation of these studies for the ADAS database and the preparation of relevant derived data for application by ADAS codes. UMONS is therefore uniquely able to extend the benefit to the ADAS-EU Project by further exploitation of the link, in accordance with the planning decisions of the ADAS-EU Electron Collision Working Party.

The Electron Collision Working Party (ECWP) of the ADAS-EU project is the vehicle for coordinating and planning action on the fundamental atomic structure and collision data for ADAS (see ADAS-EU report ECWP1 [7]). It ensures the movement of data and methods into the codes suites used by ADAS. Prof. Badnell, who leads the Atomic Molecular and Diagnostic Processes in Plasmas group of the Department of Physics at the University of Strathclyde also directs the ECWP on behalf of ADAS-EU.

3. The proposed work

The work falls into two parts.

(1) Exploitation of the transfer path established in the initiating sub-contract for optimised parameter transfer to the ADAS implementations of Cowan atomic structure calculations. This allows generation of the key ADAS datasets in adf04 format with Born collisional rate coefficients and then production of necessary derived data, especially photon efficiencies of format adf13. Information to be organised and transferred will include data sets of in36, ing11.omega and ing11.e1m1 types for the ions W^{+3} - W^{+5}, Mo^{+1}, Re^{0} - Re^{+1}, Hf^{0}, Hf^{+2}, Au^{0} - Au^{+2}, Sn^{0} and Sn^{+2}. Dr. O'Mullane will oversee these transfers and consequential calaculations for ADAS-EU.

(2) The more fundamental transfer of radial wavefunction and optimized parameters to the Strathclyde AUTOSTRUCTURE code of Prof. Badnell will be investigated. With AUTOSTRUCTURE structure calculations then exactly matched to Cowan calculations, the power of AUTOSTRUCTURE would be available for cross-section calculations in the distorted wave approximation. Such higher quality data, including spin changing rates will replace the simpler Born variant. This study and implementation will be carried out in two steps with Mo^{0} as the test species.

(a) An additional optional output will be made from the Mons-Hainaut rationalised Cowan structure code (ADAS8#1) to provide the RCN orbital information for input to the AUTOSTRUCTURE radwin.for subroutine, with restructuring of radwin.for as necessary.

(b) Additions to AUTOSTRUCTURE will be made to allow utilisation of the scaling, polarization, α, β, γ and T optimizing parameters in radial functions and integrals to match the Cowan code. This will be implemented in a collaboration between Dr. Palmeri and Prof. Badnell. Prof. Badnell will oversee the development for ADAS-EU.

Integration of data into ADAS will be executed by staff of ADAS-EU, including the conversion to the key derived data format adf04. ADAS-EU staff will pay working visits to Mons-Hainaut to assist with execution of the above tasks as appropriate.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (1 Jul. 2012 - 31 Dec. 2012). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators Dr. Palmeri, Dr. Quinet) and their research staff. No travel funds or computation costs are sought.

Item	€
Univ. Mons (fixed price)	[redacted]
total	[redacted]

References

[1] http://www.adas-fusion.eu
[2] "SUBC1: Sub-contract specifications, deliverables, integration and analysis" (2012), ADAS-EU R(12)SU01
[3] http://www.adas.ac.uk
[4] http://www.open.adas.ac.uk
[5] "ITER1: ITER visits and support activities Report 1" (2012), ADAS-EU R(12)SU03
[6] "ECWP1: Electron Collision Working Party Report 1" (2012), ADAS-EU R(12)SU02
[7] http://w3.umh.ac.be/astro/desire.shtml

Appendix B

ADAS-EU: Sub-contract S7

ADAS-EU CONTRACT

ATOMIC STRUCTURE AND ELECTRON DATA FOR HEAVY ELEMENT IONS - PART 2.

(1) PRODUCTION OF CONFIGURATION INTERACTION, QUASI-RELATIVISTIC ATOMIC STRUCTURE AND CROSS-SECTIONS FOR THE ADAS DATABASE.

(2) ATOMIC STRUCTURE INTERCHANGE.

H. P. Summers

28 May 2012

1. Summary

It is proposed to place an ADAS-EU [1] follow-up contract with Prof Alicija Kupliauskiene, acting for the Department of Theory of Atom, Institute of Theoretical Physics and Astrophysics, Vilnius University, Vilnius, Lithuania, to provide further calculations of atomic structure and linked atomic cross-section calculations. Inter alia, in the initiating sub-contract (see ADAS-EU report SUBC1 [2]), a pathway was successfully created for the Bogdanovich *ab initio* large scale configuration interaction, quasi-relativistic and relativistic atomic structure calculations into the Born collisional regime and ADAS [3] datasets. These reference theoretical studies provided a key cross-validation for W^{+2} of the large scale parametrically adjusted methods, based on LIF measurements carried out by the University of Mons group for ADAS-EU (see ADAS-EU report SUBC1 [2]) .

Three consolidating and exploiting further steps are proposed for part 2 and will be led by Prof. Bogdanovich, Prof. Gaigalas and co-workers at Vilnius and overseen by Prof. Badnell for ADAS-EU. These include evaluation of further tungsten ions, extension of the Bogdanovich method to handle limited f-shell promotions and associated configuration interaction, and development of a transfer method for radial wave function for input to Strathclyde AUTOSTRUCTURE and R-matrix codes . The calculations will be performed at the Institute for Theoretical Physics and Astrophysics, University of Vilnius, Vilnius. The data will be organised and relayed from Vilnius to ADAS in established specific ion data formats with the assistance of ADAS-EU staff. Conversion to spectrum line photon efficiencies and similar derived data will take place at the EFDA-JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [4].

The duration of the project will be six months (1 Jul. 2012 – 31 Dec. 2012) at a fixed price of [redacted]

2. Background

The background and broad strategy were described in the initiating sub-contract proposal. The appropriateness of this strategy and the effective implementation has been demonstrated over the last three years. The primary ADAS capability for handling heavy species has been developed and now provides the baseline of atomic modelling support for nearly all fusion plasma models. Also, the selective targetting of difficult systems for special studies, reinforced by ADAS-EU sub-contracts has worked. In line with the interests of ITER, EFDA-JET EP2 and the international fusion community, special attention has been given to tungsten ions enabling spectroscopic diagnostic analysis, such as for tungsten influx, to proceed and allowing accurate input to forward planning of the future ITER diagnostics (see ADAS-EU report ITER1 [5]).

As described in the initiating sub-contract proposal , the Department of the Theory of the Atom at the Institute for Theoretical Physics and Astrophysics, has a long history of research in complex atomic structure and unique capabilities in very large multi-configuration approaches and efficient algebraic methods, stemming from the original work of Prof. Yutsis (Jucys) on through the work of Prof. Rudzikas through to the present day and the work of Profs. Bogdanovich and Gaigalas. For the present proposal, it is the modified radial orbital (RO) approach combined with the very large multi-configuration approach with ‘virtual excitations’ of Prof. Bogdanovich and Dr Rancova, extended to quasi-relativistic transformed radial orbitals (TROs) which is to be exploited further. Also, the group of Prof. Gaigalas's special interests in efficient coding of spin algebra for Dirac-Fock codes and the correct handling of f-states will be of benefit.

The Electron Collision Working Party (ECWP) of the ADAS-EU project is the vehicle for coordinating and planning action on the fundamental atomic structure and collision data f or ADAS (see ADAS-EU report ECWP1 [6]). It ensures the movement of data and methods into the codes suites used by ADAS. Prof. Badnell, who leads the University of Strathclyde's atomic collisions group, also directs the ECWP on behalf of ADAS-EU.

3. The proposed work

The work falls into three parts exploiting *ab initio* structure and transition probability calculations in the large scale multi-configurational approach with virtual excitations and TROs for low and medium charge states of very heavy systems.

(1) Evaluation of atomic structure, Born collision cross-sections and generation of ADAS adf04 type 1 and 3 datasets for W^{+2} - W^{+5} (with open 5d shell) and related iso-electronic sequence members of elements hafnium, tantalum and rhenium .

(2) Inclusion of the 5d-5f transitions in the Bogdanovich quasi-relativisitic (TRO) approach. The configuration interaction will be restricted initially to at most one or two f-electrons promotions from closed shells. The 5d-5f transition array contribution to total radiated line power will be assessed for W^{+2}. The possibilities for extending the numbers of equivalent f-shell electron capability will be explored with Prof. Gaigalas.

(3) Investigation of the transfer of an orthogonal basis of radial wave functions. from the Bogdanovich multi-configurational with virtual excitations and TRO codes as inputs for the AUTOSTRUCTURE.

Integration of data into the ADAS system will be executed by staff of ADAS-EU. ADAS-EU staff will engage closely with ITPA in the study. ADAS-EU staff will pay working visits to University of Vilnius to assist with execution of the above tasks as appropriate.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of six months (Jul. 2012 - Dec. 2012). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators (Prof. Bogdanovich, Prof. Gaigalas) and their research staff. No travel funds or computation costs are sought.

~~Item~~	€
University of Vilnius (fixed price)	[redacted]
total	[redacted]

References

[1] http://www.adas-fusion.eu

[2] "SUBC1: Sub-contract specifications, deliverables, integration and analysis" (2012), ADAS-EU R(12)SU01

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

[4] http://www.open.adas.ac.uk

[5] "ITER1: ITER visits and support activities Report 1" (2012), ADAS-EU R(12)SU03

[6] "ECWP1: Electron Collision Working Party Report 1" (2012), ADAS-EU R(12)SU02

Appendix C

ADAS-EU: Sub-contract S1

ADAS-EU CONTRACT

ELECTRON COLLISION CROSS-SECTIONS FOR HEAVY ELEMENT IONS

(1) PILOT R-MATRIX CALCULATIONS FOR TUNGSTEN

H. P. Summers

5 July 2012

1. Summary

It is proposed to contract with Dr Penny Scott, Centre for Theoretical Atomic, Molecular and Optical Physics School of Mathematics and Physics, Queen's University Belfast (QUB), Northern Ireland, UK, to provide a CIV3, RMATRX-II, PFARM study of electron impact cross-sections for the ion W^{+44}. It will be a preliminary set-up study as a step towards substantive calculations on complex tungsten ions on supercomputers for fusion.

W^{+44} is a spectrum line emitter in the EFDA-JET experiment soft x-ray regime and a reference species for complex semi-relativistic/relativistic electron impact cross-sections calculations. A three hundred and twenty-six state structure description is required for accurate representation of the primary observable transitions. Thus W^{+44} is a suitable ion for initial high precision reference studies of electron impact cross-sections, in R-matrix calculation, in the advance towards tungsten ions at the limit of current capability on supercomputers. Two parallelized atomic structure/collision calculation approaches are relevant, namely the CIV3, RMATRX-II, PFARM approach of QUB and the AUTOSTRUCTURE, parallel Breit-Pauli RMATRX-I and PSTGF approach of Auburn University and University of Strathclyde. The former will be used by QUB for W^{+44} for this contract and contrasted with the latter, carried out by the ADAS Project. QUB computations will be executed on local UK computer systems and the ADAS calculations on the HPC-FF machine at the Juelich Supercomputer Centre, Forschungzentrum Juelich, Germany. The comparison of results and methodologies will guide future structure and R-matrix cross-section calculations for other ions of tungsten and similar heavy species for fusion.

The specific data for W^{+44} will be organised and relayed from Queen's University of Belfast to ADAS in established specific ion data formats with the assistance of ADAS-EU staff. The fundamental and derived data in appropriate ADAS[1] data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [2].

The duration of the project will six months (1 Jul. 2012 – 31 Dec. 2012) at a fixed price of [redacted]

2. Background

The role of tungsten as a suitable thermally resistant plasma facing wall component for the divertors of fusion machines has stimulated fresh studies of the atomic physics of tungsten. This is so that its impact on radiated power can be assessed and so that key quantities such as tungsten influx from surfaces may be measured for current machines such as AUG, JET EP2 and predicted for future machines - especially ITER. Tungsten will be present in the neutral form W^{+0} inflowing from plasma contacted surfaces, in low stages of ionisation up to ~W^{+20} in the divertor, and in ionisation stages up to ~W^{+60} at the highest temperatures of the central confined plasma of ITER. Most of these ions, with many bound electrons, have atomic structure of such complexity that atomic cross-section calculations, of the type necessary for population modelling and spectral emissivity predictions, can only be done in a simplified form. The ADAS-EU Project has developed and utilised approximations such as configuration average structure, Born approximation cross-sections and superstage compression to enable plasma model predictions for ITER. This is called baseline ADAS atomic modelling for tungsten and other heavy elements. With new spectroscopic measurements from the ITER-like wall of the extended performance upgrade (EP2) of the EFDA-JET facility, as well as on-going measurements at AUG, progress is required in finer precision atomic modelling for selected ions. In the ADAS-EU Project, this is called 'lifting the baseline' and is part of the heavy element theme of the Project. To this end, ADAS-EU has set-up the Electron Collision Working Party (ECWP) led by Prof. Nigel Badnell, to chart the important and feasible steps which can be made and to maintain connection and coordinate action with university research groups which can assist. In the field of the calculation of electron impact cross-sections of complex ions, the R-matrix method alone is capable of delivering cross-sections of the highest precision. The primary development of this method for electron collisions took place at QUB, led by Prof. Philip Burke (see Burke (2011) for a detailed

description of the current state of R-matrix calculations for atoms and ions) and QUB remains a pre-eminent exponent of the method, along with Strathclyde University, in Europe and groups associated with them in other parts of the world - especially in the USA. Current supercomputer power is such that most of the lower ionisation stages of tungsten remain outside the scope of R-matrix calculation at this time. A relatively simple ion (W^{+44}) has been identified as a test-case which is relevant to JET core diagnostics. Its emission is expected in the wavelength range of the revamped KX1 X-ray spectrometer at the JET Facility. It has some R-matrix calculations (Ballance and Griffin, 2007) but which do not open the 3d shell to which the main predicted radiative loss transition occurs.

The relevant computer codes break down into two groups – those based on fully relativistic Dirac wavefunctions and the Breit-Pauli (BP) ones, which currently use non-relativistic or kappa averaged wavefunctions. The former include the structure code GRASP and the R-matrix code DARC while the latter cover the codes CIV3 and AUTOSTRUCTURE on the structure side and FINE/RMATRX-II and ICFT/BP/RMATRX-I on the collisional side. Complex, multi-state R-matrix calculations require the power of parallelized versions of these codes optimised for scaling on supercomputers. Of the BP variants, two parallelized atomic collision calculation packages are relevant for this proposal, namely the RMATRX-II, PFINE and PFARM approach of QUB, called PRMAT (see for example Cassidy et al., 2010) and the parallel Breit-Pauli RMATRX-I, ICFT and PSTGF approach of Auburn University and University of Strathclyde (see for example Ludlow et al., 2011). It is likely that all will use the same outer region PSTGF suite, which simplifies deliverables to the ADAS Project data classes (via the post-processing code ADASEXJ).

A key issue and prelude to an R-matrix calculation, is establishment of a satisfactory target ion structure. A preliminary study by the Electron Collision Working Party study on whether the 'BP' models can be used for W^{+44} (and/or similar residual charge states) indicated that, provided appropriate configuration interaction (especially the $3d^{9}4s4p4d$ configuration) was included, a semi-relativistic description of the structure is sufficient (Badnell - private communication) for the observable spectral emission of W^{+44}. Badnell, using AUTOSTRUCTURE, found particularly that the kappa-averaged orbital solution gave very good agreement with the fully relativistic GRASP code for the most important levels. Further attention needs to given however to comparison with CIV3. It is noted that CIV3 does not use kappa-averaged orbitals, but the expectation is that the CIV3 structure will be satisfactory (due its large number of adjustable parameters which can be utilized to mimic such relativistic effects) and be able to provide the necessary inputs to the QUB R-matrix calculations of W^{+44}. This will also enable the special expertise of Allan Hibbert (see for example [6]) in structure calculations for complex systems with CIV3 to be brought to bear. Within the BP suites it seems unlikely that a full BP calculation is necessary (re-coupling before H(N+1) diagonalization) and that "FINE" (recoupling the R-matrix, before outer-region solution) and/or ICFT (recoupling the K-matrix) should suffice and is highly beneficial since diagonalization is an N^{3} process. It is likely that AUTOSTRUCTURE and CIV3 are interchangeable between the "BP" collision codes. AUTOSTRUCTURE is of special use for its ability to generate comparative plane-wave Born (PWB) and distorted wave (DW) collision strengths and the infinite energy Born limit points. Also relevant is the AUTOSTRUCTURE Auger rate capability. It is noted that radiation damping was found to be important [a] on effective collision strengths for certain transitions below T=1000eV in W^{+44} in the study by Ballance & Griffin (2007).

3. The proposed work

A set-up study of atomic structure and electron impact cross-sections of W^{+44} will be carried out to include up to three hundred and twenty-six states and the spectroscopic configurations $3d^{10}4l4l'$ (l,l'=0-3) , $3d^{9}4s^{2}4l$ (l=0-3), $3d^{9}4s4p4d$. There are three steps: (1) a Breit-Pauli examination of the above W^{+44} structure using CIV3. Outcomes will be orbital parameters for R-matrix calculation and alignment of CIV3 structure with the results of AUTOSTRUCTURE. The latter will be assisted by ADAS-EU staff; (2) Set-up R-matrix calculations of electron impact cross-sections using the PRMAT package for the above optimised atomic structure of W^{+44}. The expected outcomes, in the available time, will be the collisional model preparation infrastructure and R-matrix runs of a set of low partial wave cross-sections using local UK computers; (3) Comparison of the above results with similar results using the parallel BP/ICFT RMATRX-I, and PSTGF approach calculated by the ADAS Project at Strathclyde University. ADAS-EU staff will work with QUB in the preparation of ADAS datasets [8], especially of format adf04 type 1 and type 3 for W^{+44} from the results of the above studies.

ADAS-EU staff will use the set-up studies and associated guidance from QUB and Strathclyde University to build pilot, massively parallel, R-matrix calculations for tungsten ions on the Juelich HPC-FF supercomputer for fusion in Europe.

ADAS-EU staff will pay working visits to QUB to assist with execution of the above tasks as appropriate.

4. The Financial Provision

The operations and calculations outlined in the previous section will be carried out over a period of six months (1 Jul. 2012 - 31 Dec. 2012). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigator and her research staff. No travel funds or computation costs are sought.

Item	€
Queen's University of Belfast (fixed price)	[redacted]
total	[redacted]

References

[1] http://www.adas.ac.uk
[2] http://www.open.adas.ac.uk
[3] P. G. Burke (2011) 'R-Matrix Theory of Atomic Collisions: Application to Atomic, Molecular and Optical Processes' (Springer).
[4] C. M. Cassidy, C. A. Ramsbottom, M. P. Scott and P. G. Burke (2010) A&A **513**, A55.
[5] J. A. Ludlow, T. G. Lee, C. P. Ballance, S. D. Loch, and M. S. Pindzola (2011) Phys. Rev. A **8**4, 022701.
[6] P. Oliver and A. Hibbert (2010) J. Phys. B: At. Mol. Opt. Phys. **43**, 074013.
[7] C P Ballance and D C Griffin (2007) J. Phys. B: At. Mol. Opt. Phys. **40** 247.
[8] H. P. Summers (2010) The ADAS-Manual (http://www.adas.ac.uk/manual.php).

Appendix D

ADAS-EU: Sub-contract S9

ADAS-EU CONTRACT

OPEN-ADAS UPDATE

H. P. Summers

7 Nov. 2012

1. Summary

It is proposed to commission an update to the OPEN-ADAS computer software. OPEN-ADAS is the mechanism for free release of ADAS [1] fundamental and derived atomic data and associated user access software to the public domain.

OPEN-ADAS[2], as an open web site, is subject to mischievous attack. An increase in the security of OPEN-ADAS, in line with current best practice, will be carried out. Enhancement to the user interface will be made to improve the user experience. New ADAS data classes will be added to those currently available through OPEN-ADAS in line with the very substantial extension in the ADAS database during the ADAS-EU Project.

The duration of the project will be three months (Oct. 2012 - Dec. 2012) at a fixed price of [redacted]

2. Background

OPEN-ADAS is the name of the path for release of ADAS data and support software into the public domain. It is an agreed and shared project between ADAS and the International Atomic Energy Agency, Atomic and Molecular Data Unit, Nuclear Data Section (IAEA) in Vienna. As agreed in the ADAS-EU proposal, OPEN-ADAS is used for public domain release of fundamental and derived atomic data which enters the ADAS databases from ADAS-EU activities. The web server is located at the Physics Department, University of Strathclyde and is linked via the IAEA web pages. The development of OPEN-ADAS was substantively finished early in the ADAS-EU project with the addition of free-form search capability. During the first 18 month reporting period the number of users increased steadily each month and came from very many countries. The principal aims of the project had been realized and it had settled down to high-availability but low-maintenance web service.

In June 2010 email attacks began. The webserver logs showed a few SQL injection attacks every few weeks which is not unexpected on the public internet. However around the end of May 2011 the volume rose sharply. The reasons are unclear but news of a successful exploit probably circulates quickly in the anarchistic world of web breaking. Ameliorating steps were taken. The usual way of ameliorating such an attack is via a captcha. Before implementing such a system a simpler text challenge field was tried: requesting the correspondent to type 'not spam' into the appropriate box. This proved to be successful initially so the more invasive captcha system was not deployed. The OPEN-ADAS web site required a simple sign-up resulting in an account with a password. The name and email address were not verified before creating the account so a degree on anonymity was possible. This enabled us to produce accurate usage statistics since the number of hits is a very poor metric. Reports that a list of the OPEN ADAS user names and passwords were available on the 'pastebin' web site came to us in the first week of June 2011. A serious security breach had occurred.

It was decided that the most effective way to prevent a further occurrence was to remove the registration requirement. All data from OPEN-ADAS can now be downloaded anonymously. The removal of the code for registration, sanitizing the MySQL queries and trapping all input resulted in the OPEN-ADAS website being unavailable until 4 September 2011— a two month interruption which also displaced other activities. The disadvantages in not knowing the OPEN-ADAS users are the loss of statistics and the ability to inform people who downloaded data of any subsequent improvements. Given the time pressures on the staff, this was an acceptable compromise.

The opportunity is now taken to improve OPEN-ADAS security, restore its statistics logging and at the same time to enhance its facilities for the user.

3. The proposed work

1. Make the OPEN-ADAS site as secure as possible in line with current best practice. Review the *mysql* and *php* settings and eliminate the errors that are seen in the logs, even if they are only warnings due to deprecated features. In particular make sure that the *mysql* settings are secure with separate processes for different aspects. Also isolate the web servers into containers if deemed necessary.

2. Review the functional flow of website - at an early stage of the contract establish the look of the site in line with current expectations. The basic functionality is to remain, ie full datasets are returned and a lightweight, mostly pure HTML web page delivery is retained but enhanced CSS styles could be used to improve the user experience. The addition of new *adf* data classes may necessitate a more hierarchical webpage structure.

3. Document and streamline the back-end database generation. The current system is a series of *perl* scripts from which the metadata for the *mysql* is derived.

4. Add new ADAS data classes - *adf00, adf38, adf39, adf48.*

5. Add a news and privacy section and ensure the site's use of cookies is compatible with current legislation.

6. Make funding contributors, particularly FP7 and IAEA more prominent.

7. Attribution of effort in increasingly important if OPEN-ADAS is to be positioned as a primary publication vehicle. Improve the back-end extraction of this data and make recommendations for changes to the ADAS workflow and comment inclusion.

8. References such as 'data from ADAS', or the slightly better 'data downloaded from OPEN-ADAS July 2012' show that it is not sufficiently fine grained. The document object identifier system (*doi*) is a way to make a permanent link to an object, in this case an ADAS dataset. The *doi* system is not confined to academic publishing, although is has established an authoritative position there. Explore the cost, both initial and ongoing, for tagging each ADAS file with a *doi*. This will make referencing simple and acceptable to the journals. If this proves affordable add a *doi* resolver box to OPEN-ADAS. If the cost is prohibitive, on an ongoing basis, develop our own unique url identifier scheme.

9. Reinstate the statistics which was removed after the hacking incident. Anonymous provision of data removes effort in maintaining the system but the valuable knowledge of where the data was used was lost. Add a system to parse the access logs for unique access and reference to geo-location.

10. Oversight of the contract will be by phone and video conference but two formal meeting, one early on to approve the design aspects and a wrap-up meeting are planned.

11. Contract supervision and completion approval by Dr. Martin O'Mullane for ADAS-EU.

12. Duration 3 months - 1 Oct. 2012 to 31 Dec. 2012.

13 Deliverables are (a) Working OPEN-ADAS with updated code (b) Summary report on update and guide for users.

4. The Financial Provision

The computational developments outlined in the previous section will be carried out over a period of three months (1 Oct. 2012 - 31 Dec. 2012). Funds are provided for staff time on the OPEN-ADAS computer software development. No travel funds are sought.

Item	£
256 Kelvin Limited (fixed price)	[redacted]
total	[redacted]

References

[1] http://www.adas.ac.uk

[2] http://open.adas.ac.uk