



Weaknesses in ADAS models and how to put them right

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- Comments on selected ADAS series codes and plans for them
- Some additional notes on superstage datasets
- Mass production of baseline data for heavy elements.
- Configuration average adf04 and adf11/plt production
- Outstanding issues

ADAS series 3

Charge exchange processing

ADAS301: State selective charge exchange data - graph and fit cross-section

ADAS302: Ion/atom data - graph and fit cross-section

ADAS303: Effective charge exchange spectroscopy emission data - graph and fit coefficient

ADAS304: Effective beam emission spectroscopy stopping data - graph and fit coefficient

ADAS305: Generate hydrogen beam Stark features and emissivities

ADAS306: Charge exchange spectroscopy - process effective coefficients: j-resolved

ADAS307: Charge exchange spectroscopy - process effective coefficients: j-resolved/scan

ADAS308: Charge exchange spectroscopy - process effective coefficients: l-resolved

ADAS309: Charge exchange spectroscopy - process effective coefficients: l-resolved/scan

ADAS310: Beam emission spectroscopy - process beam stopping and emission : H-beam

ADAS311: Beam emission spectroscopy - process beam stopping and emission : He-beam

ADAS312: Post-process population data for hydrogen beam stopping and emission

ADAS313: Post-process population data for helium beam stopping and emission

ADAS314: Convert QCX to effective cross-sections

ADAS317: Prepare high n-shell level assignments and bundles for heavy element ions

ADAS319: Generate baseline adf01 files for heavy element ions

ADAS series 4

Recombination and ionisation processing

ADAS401: Isoelectronic sequence data - graph and fit coefficient

ADAS402: Isonuclear sequence data - graph and fit coefficient

ADAS403: Merge iso-electronic master files

ADAS404: Isonuclear master data - extract from isoelectronic master data

ADAS405: Equilibrium ionisation - process metastable populations and emission functions

ADAS406: Transient ionisation - process metastable populations and emission functions

ADAS407: Iso-nuclear parameter sets - prepare optimised power parameters

ADAS408: Iso-nuclear master data - prepare from iso-nuclear parameter sets

ADAS409: Equilibrium ionisation – prepare G(Te,Ne) function tables

ADAS410: Dielectronic recombination – graph and fit data

ADAS411: Radiative recombination – graph and fit data

ADAS412: Equilibrium ionisation - prepare G(Te) function tables

ADAS413: Collisional ionisation – graph and fit data

ADAS414: Prepare soft X-ray filter file

ADAS415: Display spectral filter file

ADAS416: Create child partition – prepare GCR, PEC, F-PEC,GTN,F-GTN data

adf11 tungsten acd

an unresolved - #01 partition level

```
74      8      24      1      6      /TUNGSTEN      /ACD /GCR PROJECT
-----
//#02/p00/ 00 01/
  p01/ 02 03 04 05/
  p02/ 06 07 08 09 10 11 12/
  p03/ 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27/
  p04/ 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45/
  p05/ 46 47 48 49 50 51 52 53 54 55/
  p06/ 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74/
//#01/p00/ 00/p01/ 01/p02/ 02/p03/ 03/p04/ 04/p05/ 05/p06/ 06/p07/ 07/
  p08/ 08/p09/ 09/p10/ 10/p11/ 11/p12/ 12/p13/ 13/p14/ 14/p15/ 15/
  p16/ 16/p17/ 17/p18/ 18/p19/ 19/p20/ 20/p21/ 21/p22/ 22/p23/ 23/
  p24/ 24/p25/ 25/p26/ 26/p27/ 27/p28/ 28/p29/ 29/p30/ 30/p31/ 31/
  p32/ 32/p33/ 33/p34/ 34/p35/ 35/p36/ 36/p37/ 37/p38/ 38/p39/ 39/
  p40/ 40/p41/ 41/p42/ 42/p43/ 43/p44/ 44/p45/ 45/p46/ 46/p47/ 47/
  p48/ 48/p49/ 49/p50/ 50/p51/ 51/p52/ 52/p53/ 53/p54/ 54/p55/ 55/
  p56/ 56/p57/ 57/p58/ 58/p59/ 59/p60/ 60/p61/ 61/p62/ 62/p63/ 63/
  p64/ 64/p65/ 65/p66/ 66/p67/ 67/p68/ 68/p69/ 69/p70/ 70/p71/ 71/
  p72/ 72/p73/ 73/p74/ 74/
-----
10.00000 10.67128 11.34256 12.01384 12.68513 13.35641 14.02769 14.69897
-0.30103 -0.13086 0.03930 0.20947 0.37963 0.54980 0.71996 0.89013
 1.06030  1.23046  1.40063  1.57079  1.74096  1.91113  2.08129  2.25146
 2.42162  2.59179  2.76195  2.93212  3.10229  3.27245  3.44262  3.61278
-----/ ISPP= 1 / ISPB= 1 /-----/ S1= 1 / DATE= 12:09:05
-11.64510 -11.66588 -11.69610 -11.71692 -11.74369 -11.74369 -12.74277 -12.74277
```

partition
specification



unresolved child
partition level
#02

adf11 format class extensions

<u>class index</u>		<u>type</u>	<u>content</u>
1	acd		effective recombination coefficients
2	scd		effective ionisation coefficients
3	ccd		CX recombination coeffts
4	prb		recomb/brems power coeffts
5	prc		CX power coeffts
6*	qcd		base meta. coupl. coeffts
7*	xcd		parent metastable coupling coeffts
8	plt		low level line power coeffts
9	pls		representative line power coefficient
10	zcd		effective charge
11	ycd		effective squared charge
12	ecd		effective ionisation potential

* Only present with metastable resolved cases (1996 data)

ADAS series 8

Creating and manipulating adf04 files

ADAS801: Calculate Cowan atomic structure

ADAS804: Calculate cross-sections and rate coefficients

ADAS806: Merge, clean and check adf04 files

ADAS807: Prepare cross-referencing files

ADAS808: Create composite iso-nuclear adf34, adf40 and adf41 driver files

→

`run _adas808`

ADAS809: Non-Maxwellian modelling - change adf04 file type

ADAS810: Generate envelope feature photon emissivity coefficient

ADAS811: Compare rate coefficients from adf04 files

Baseline mass data production for heavy species

run_adas808

- set up the default promotion rules
- generate the configurations for each ion in turn.
- prepare the output adf34 and adf42 driver and data file names
- create the configuration average adf04 data files
- create the ls and ic adf04 data files
- prepare adf15, adf40 and adf11 data file names of ls, ic and ca type
- create the ls, ic and ca adf15, adf40 and adf11 data files

run archive_scripts

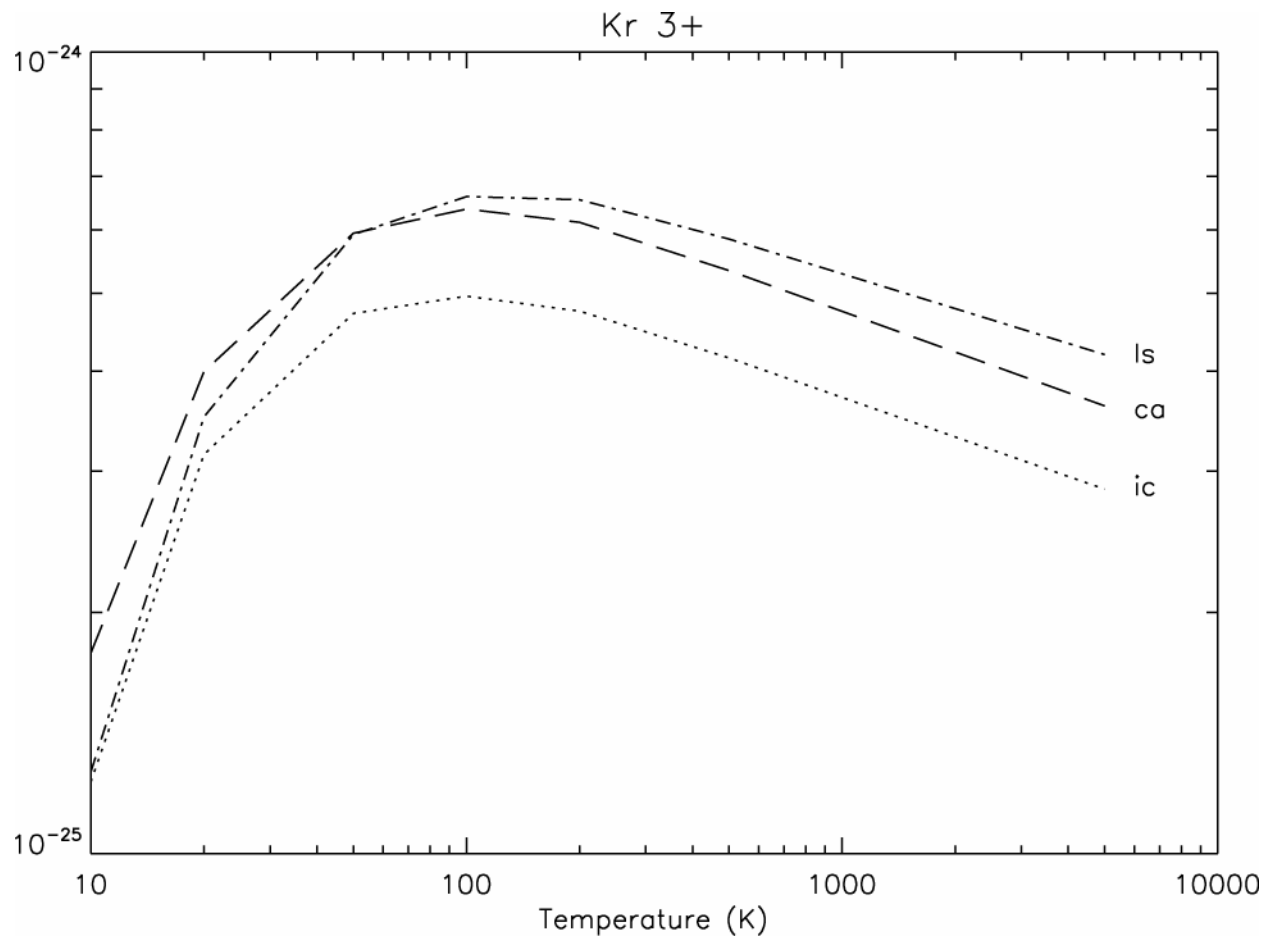
Configuration generation based on all possible ground configurations

n=4 l=f

config_ref,

```
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f8',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p6',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f7',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p5',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f6',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p4',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f5',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p3',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f4',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p2',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f3',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2 5p1',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f2',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s2',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f1',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d9 4f0 5s2',  
'1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p6 4d10 4f0 5s1'
```


adf11/plt generated by run_adas808



Offline-ADAS

ADAS3#1: Calculate high n-shell precision energy levels for heavy element ions

ADAS8#1: Calculate Cowan atomic structure

ADAS8#2: Calculate configuration average ionisation cross-sections

ADAS8#3: Automated R-matrix calculations

Outstanding issues for heavy species

- Difficult ions which are computing power/space limited
- Raising the baseline for ionisation (cf. adf23 – config. average)
- Raising the baseline for recombination (cf. DR – BBGP)
- Completing the baseline for all heavy species
- Valid operational scenarios for superstaging
- CXS emissivity predictive code update for heavy elements
- (Jp)nljJ based generalised-collisional radiative-code for targetted heavy element ions