University of Strathclyde

Atomic Data and Analysis Structure

User manual
Version for UNIX/IDL

H. P. Summers

2nd Edition - Version 2.7

2004

Table of Contents

Introduction

Atomic data entry and verification

Population processing

ADAS215: Specific ion file - temperature regrid

ADAS216: Population and emissivity error analysis

ADAS217: Create hydrogen series limit feature file - **not implemented**

ADAS218: Create helium series limit feature file- **not implemented**

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

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

ADAS315: Comparative display of charge exchange and beam emission coefficients- **not implemented**

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

ADAS417: Apply filter to F_PEC coefficients and F_G(Te,Ne) functions - **not implemented**

General interrogation programs

ADAS501: SXB - graph and fit ionisation per photon coefficients

ADAS502: SZD - graph and fit zero-density ionisation rate coefficients

ADAS503: PEC - graph and fit photon emissivity coefficients

ADAS504: PZD - graph and fit radiated power coefficients

ADAS505: QTX - graph and fit thermal charge exchange coefficients

ADAS506: GFT - graph and fit G(Te) functions

ADAS507: GCF - graph and fit generalised contribution functions

ADAS508: GTN - graph and fit G(Te,Ne) functions

ADAS509: SCX - graph and fit charge exchange cross-sections

ADAS510: F-PEC - graph envelope feature photon emissivity coefficients

ADAS511: F-GTN - graph envelope feature photon emissivity function - **not implemented**

Data analysis and spectral fitting

ADAS601: Differential emission measure analysis

ADAS602: Spectral line profile fitting

ADAS603: Zeeman multiplet line fitting

ADAS604: Dielectronic satellite line profile fitting- **not implemented**

ADAS605: Hydrogen series limit feature fitting- **not implemented**

ADAS606: Helium series limit feature fitting- **not implemented**

ADAS607: Non-Maxwellian electron distribution function fitting- **not implemented**

ADAS608: Molecular band profile fitting- **not implemented**

Creating and using dielectronic data

ADAS701: Autostructure

ADAS702: Postprocessor - Autostructure > adf09 file

ADAS703: Postprocessor - Autostructure > adf04 file

ADAS704: Postprocessor - Autostructure > adf18 file

ADAS705: Merge and bundle partial files > adf04 file- **not implemented**

ADAS706: Calculate doubly excited state populations and satellite line feature file- **not implemented**

ADAS707: Doubly excited populations - process line emissivities- **not implemented**

ADAS708: Calculate l-redistribution for Rydberg DR resonance populations- **not implemented**

Creating and manipulating adf04 files

ADAS801: Calculate Cowan atomic structure

ADAS802: Calculate distorted wave cross-sections

ADAS803: Postprocess distorted wave cross-sections > adf04 file- **not implemented**

ADAS804: Calculate cross-sections and rate coefficients

ADAS805: Calculate radiative Gaunt factors- **not implemented**

ADAS806: Merge, clean and check adf04 files

ADAS807: Prepare cross-referencing files

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

ADAS809: Non-Maxwellian modelling - change adf04 file type

ADAS810: Generate envelope feature photon emissivity coefficient

ADAS811: Compare rate coefficients from adf04 files

Appendix A

ADAS data formats

ADF00: ground configurations and ionisation potentials

ADF01: bundle-n and bundle-nl charge exchange cross-sections

ADF02: ion impact cross-sections with named participant

ADF03: recombination, ionisation and power parameter sets

ADF04: resolved specific ion data collections

ADF05: general z excitation data collections

ADF06: general z recombination/ionisation data collections

ADF07: direct resolved electron impact ionisation data collections

ADF08: direct resolved radiative recombination coefficients

ADF09: direct resolved dielectronic recombination coefficients

ADF10: iso-electronic master files

ADF11: iso-nuclear master files

ADF12: charge exchange effective emission coefficients

ADF13: ionisation per photon coefficients

ADF14: thermal charge exchange coefficients

ADF15: photon emissivity coefficients

ADF16: generalised contribution functions

ADF17: condensed projection matrices

ADF18: cross-referencing data

ADF19: zero density radiative power

ADF20: G(Te) functions

ADF21: effective beam stopping coefficients

ADF22: effective beam emission coefficients

ADF23: state selective electron impact ionisation coefficients

ADF24: state selective charge transfer cross-sections

ADF25: driver data-sets for ADAS204 calculations

ADF26: bundle-n and bundle-nl populations of excited states in beams

ADF27: driver data-sets for ADAS701 calculations

ADF28: driver data-sets for ADAS702 calculations

ADF29: driver data-sets for ADAS707 calculations

ADF30: driver data-sets for ADAS708 postprocessing

ADF31: feature files for satellite line spectral simulation

ADF32: driver data-sets for ADAS802 calculations

ADF33: driver data-sets for ADAS803 postprocessing

ADF34: driver data-sets for ADAS801 calculations

ADF35: spectral filter data

ADF36: feature files for series limit spectral simulation

ADF37: non-Maxwellian distribution function files

ADF38: Seaton - opacity photo-excitation

ADF39: Seaton - opacity - photo-ionisation

ADF40: Envelope feature photon emissivity coefficients

ADF41: driver data-sets for offline ADAS8#1 calculations

ADF42: driver data-sets for ADAS810 calculations

ADF43: GTN photon emissivity functions

ADF44: F_GTN envelope feature emissivity functions

ADF45: feature files for continuum emission

Appendix B

ADAS FORTRAN and IDL subroutine libraries

FORTRAN subroutine and code access from IDL

ADAS offline codes for support calculations

Library index - FORTRAN

Library index - IDL

Appendix C

ADAS-EXCEL spreadsheets