

Appendix B

ADAS FORTRAN and IDL subroutine libraries

For subroutine naming, codes series 1-7 are labelled alphabetically a-g. A subroutine associated with series 1 begins with the letter 'a', a subroutine associated with series 2 begins with letter 'b' and so on. A subroutine associated with a particular member of a code series has the code number as the second character of the subroutine name. Thus the name of a subroutine associated with the code ADAS403 begins with the letters 'd3' (e.g. 'd3spf0'). The name of a general subroutine from a code series but not restricted to a specific code has 'x' as the second character of its name (e.g. 'bxdata'). A general subroutine, not restricted to a single code series begins with the letters 'xx' (e.g. 'xxuid'). General functions are preceded by 'I4', 'R8', 'C' depending on the type of function value returned.

FORTRAN subroutine names have the terminator '.for', IDL subroutines have the terminator '.pro'. FORTRAN subroutine source code is not accessible, but the headers, including call parameters, description of the routine and all variables and declaration statements are available in the separate document 'Usernotes'. IDL code is accessible. It is to be noted that IDL procedures are often grouped to provide complete self-managing widgets.

The FORTRAN scannable libraries are located as follow:

../adas/idl_adas/fortran/libadaslib.a	'XX','I4', 'R8' and 'C' general fortran subroutines and functions
../adas/idl_adas/fortran/libadas1xx.a	'AX', 'A1', 'A2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas2xx.a	'BX', 'B1', 'B2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas3xx.a	'CX', 'C1', 'C2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas4xx.a	'DX', 'D1', 'D2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas5xx.a	'EX', 'E1', 'E2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas6xx.a	'FX', 'F1', 'F2', ... fortran subroutines and functions
../adas/idl_adas/fortran/libadas7xx.a	'GX', 'G1', 'G2', ... fortran subroutines and functions

The IDL scannable libraries are located as follow:

../adas/idl_adas/idl/adaslib.a	'xx', 'i4', 'r8' and 'c' general idl procedures
../adas/idl_adas/idl/adas1xx.a	'ax', 'a1', 'a2', ... idl procedures
../adas/idl_adas/idl/adas2xx.a	'bx', 'b1', 'b2', ... idl procedures
../adas/idl_adas/idl/adas3xx.a	'cx', 'c1', 'c2', ... idl procedures
../adas/idl_adas/idl/adas4xx.a	'dx', 'd1', 'd2', ... idl procedures
../adas/idl_adas/idl/adas5xx.a	'ex', 'e1', 'e2', ... idl procedures
../adas/idl_adas/idl/adas6xx.a	'fx', 'f1', 'f2', ... idl procedures
../adas/idl_adas/idl/adas7xx.a	'gx', 'g1', 'g2', ... idl procedures

Library index - FORTRAN

The available subroutines are summarised below. Page references are to the ADAS Usernotes manual.

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D6MPOP	calculation of metastable resolved ionisation stage populations of a particular element for a given temperature and density.	753
D6OTG1	passes graphics data to idl. provides graph of metastable fractional abundances. a single graph will contain up to seven metastables. (if more than seven metastables are present extra graphs will be output as required).	756
D6OTG2	passes graph data to idl. provides graph of metastable fractional line energy functions. a single graph will contain up to seven metastables. (if more than seven metastables are present extra graphs will be output as required).	759
D6OTG3	communicates graph data to idl provides graph of selected gcf function and its components.....	763
D6OTG4	communicates graph data to idl provides graph of erb, erc, elt and total energy excess/deficit functions.	767
D6OUT0	to print primary output from transient ionisation program adas406.	771
D6SCRIP	to read script file and access emissivity data on spectral lines requested for further processing in equilibrium ionisation codes.	775
D6SGCF	to assemble gcf functions and their components using fractional metastable abundances.....	777
D6SPEC	to calculate photon emissivity coefficients for spectral lines identified in script file.....	780
D6SPOW	to assemble radiated energy excess functions using fractional metastable abundances integral excesses.	783
D6WR11	to output data to gcf passing file.....	787
DIEL	purpose unknown.....	627
DIELCL	to generate dielectronic recombination data.	330
DPMPAR	This function provides double precision machine parameters when the appropriate set of data statements is activated (by removing the c from column 1) and all other data statements are rendered inactive. Most of the parameter values were obtained from the corresponding Bell Laboratories Port Library function.	789
EIQIP	purpose unknown.....	627
FIND	find values from line and store only not repeated values.	627
FINTB	define interpolation independent variable.....	331
FINTER	purpose unknown.....	628
FITSP	purpose unknown.....	628
GBB	purpose unknown.....	629
GBF	purpose unknown.....	629
GENTAB	send data to stream '10' for subsequent table production.	629
GSPC	purpose unknown.....	630
I4EIZ0	to return the nuclear charge for the element symbol esym (integer*4 function version of 'xxeiz0').....	5
I4FCTN	convert an integer number stored in the string 'str' into a integer*4 variable.	6
I4IDFL	returns a unique index number based on the value of the n and l quantum numbers passed to it.....	8
I4IDFM	returns a unique index number based on the value of the n, l and m quantum numbers passed to it.....	8
I4IDLI	returns a unique index number based on the value of the n, l and m quantum numbers passed to it.....	9
I4IDLI	returns the index number of the predicted spectrum line tables given the orbital quantum number of the initial state and the principal and orbital quantum numbers of the final state.	9
I4JGAM	uses index to reference 'jgam' table generated by subroutine 'xxgama'.	10
I4JGRP		

returns decimal form of eissner single hex character orbital.....	11	access specific higher quality data for h population structure calculation in the bundle-n approximation.	633
I4LGRP		PHOTOLT	
returns angular momentum quantum number of orbital given in the eissner single hexadecimal character form.....	11	variant of photo	
returns angular momentum quantum number of orbital given in the eissner single hexadecimal character	12	multiplies prec by exp(xnt) if n<ncut.	332
I4NGRP		PYPR	
returns n quantum number given in the eissner single hexadecimal character form	12	calculates py factor (cf. van regemorter,1962) using percival,richard and coworker cross-sections.	636
I4PGRP		PYVR	
returns parity of orbital given the eissner single hexadecimal character form	13	calculates van regemorter's p factor for electron collisions with atoms and ions.....	637
I4SCHR		QH	
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I4UNIT		QLPR	
to reset or return a stored integer*4 value greater than or equal to zero. This is used within adas to store the stream/unit number for the output of error messages (to the screen).....	14	calculates lodge-percival-richards ion impact excitation cross-sections in original form.....	640
INITPOS		QPR78	
purpose unknown.	630	calculates electron collision cross-sections for transitions between principal quantum shells in hydrogen and hydrogenic ions.	641
LENSTR		QVAIN	
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LH404RR		R2PHOTO	
to fetch data from master condensed parent/metastable resolved collisional dielectronic files and prepare resolved isonuclear (adf11) master files.....	792	updated version of rphoto to allow return of energy averaged electron cooling coefficient.	332
LH404RU		R8AH	
to fetch data from master condensed parent/metastable resolved collisional dielectronic files, bundle them, and prepare unresolved isonuclear (adf11) master files. also check for an equivalently named adf15 files and bundle resolved data blocks into unresolved ones.....	796	calculates a-values for hydrogen.	17
LINFIT		R8ATAB	
subroutine to perform linear interpolation.....	15	calculates hydrogenic l resolved A-values.	18
LOWPOP		R8BCON	
calculate populations of low excited populations of ions.....	631	to convert a beam energy into specified units (double precision function version of 'xxbcon').....	19
MATINV		R8DCON	
matrix inversion with accompanying solution of linear equations	16	to convert a density into specified units (double precision function version of 'xxdcon').....	20
METRD		R8ECIP	
to fetch data from <i>adf10</i> 'met' files and spline onto the requested temperature/density grid.	800	calculates the shell contribution to the ionisation rate coefficient in the ecip approximation of Burgess. 21	
NGFFMH		R8ECON	
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NSORT		R8FBCH	
subroutine to sort an array so that it is increasing order	16	evaluates a shell contribution to the ionisation rate coefficient in the burgess-chidichimo approximation.	23
NSUPH1		R8FCTN	
		to convert a floating point number stored in the string 'str' into a real*8 variable.....	25
		R8FEEI	
		evaluates the exponential integral exp(x)E1(x).....	26
		R8FORM	

calculates charge exchange l-resolved cross-section as a fraction of the corresponding n-resolved cross-section.	28		
R8FUN1			
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R8FUN2			
r8fun2 = 1 / (z + 1)	30		
R8GAM			
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R8GBF			
calculates hydrogenic n-shell bound-free gaunt factor gii	32		
R8GIIH			
calculates bound-free g-factors for angularly resolved levels uses hydrogenic matrix elements.	33		
R8OVLP			
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R8RD2B			
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R8RD2F			
calculates hydrogenic bound-free radial integrals using recurrence relations.	39		
R8SCON			
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R8TCON			
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R8WIG6			
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evaluates ion impact rate coefficients of vainshtein et al.	643		
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		V2BNMOD	
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		XX0000	
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		XXADAS	
		gets an 80 byte character string header containing the adas release & version, the executing program name & version, and the current date & time from idl via the pipe.	48
		XXBCON	
		to convert an array of beam energies into specified units.....	48
		XXCEIA	
		converts ionisation potentials from wave numbers to rydbergs and fills in any missing values up to an ion charge of 50. (if 'eia()' is all zero - return).....	49
		XXCFTR	
		converts a configuration character string, such as occurs in a specific ion file level list, between eissner and standard forms	51
		XXCHEB	
		carry out chebyshev polynomial fit algorithm (direct replacement for nag minimax polynimial coef. routine e02acf - has same argument list).	52
		XXDATE	
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		to convert an array of densities into specified units..	54
		XXDELT	
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XXEIGN		XXLIM4	
finds the eigenvalues and eigenvectors of a general real matrix. replaces nag routine f02agf although there are several differences	63	finds maxima and minima of a list of x values and returns the scale range for plotting on a log to the base 10 grid.	87
XXEIZ0		XXLIM8	
to return the nuclear charge iz0 for the element symbol esym.....	64	finds maxima and minima of a list of x values and returns the scale range for plotting on a log to the base 10 grid.	88
XXELEM		XXLM28	
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XXERYD		XXMADD	
to calculate the energy levels in rydbergs (from wave num- bers) relative to level 1, and the energies (also in ryd.) relative to the ionisation potential.	66	adds two matrices with multiplier for each.	90
XXFCHR		XXMCPY	
to identify the first and last occurrence of sstrng in cstrng, the values of which are ifirst , ilast.	66	copies one matrix to another.	91
XXFLNM		XXMINO	
to prepare a unix dataset name from a string which may include an adas environment leader and comments.	67	inverts a matrix.	92
XXFLSH		XXMINV	
routine for setting call to "flush" command depending on operating system specifics.....	68	matrix inversion with accompanying solution of linear equations if requested.....	93
XXGAMA		XXMMUL	
set up gamma function tables for integer arguments.	69	multiplies two matrices.	95
XXGTSL		XXMNMX	
given a general tridiagonal matrix and a right hand side will find the solution of the associated system of linear equations.....	70	to evaluate the taylor coefficients of the minimax polynomial using a call to a nag library routine. ..	96
XXGUID		XXOPEN	
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XXHKEY		XXRATE	
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XXIDTL		XXREIA	
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XXIDTM		XXSIM	
inverse of function i4idfm. returns the unique n, l and m quantum numbers which generate the given index when passed to i4idfm.	74	solves the system of simultaneous equations ax=b using the netlib linalg routine lsqr. this routine replaces nag library routine f04atf.	104
XXIN17		XXSLEN	
to open and acquire data from the following master condensed collisional-dielectronic files	75	to identify the first and last non-blank character in a string. (if input string is blank ifirst=ilast=0.....	106
XXIN80		XXSPLE	
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XXSTNP	
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XXSTUC	
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XXTCON	
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XXTERM	
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XXUID	
adas routine - sets up the default userid which stores the data to be read using standard adas data reading routines.	123
XXWORD	
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