

ADAS Subroutine b8scom

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      SUBROUTINE B8SCOM( NDTEM , NDTRN      , NDLEV  , NDMET  ,
&                      IL      , WA      , NPL    , BWNOA  ,
&                      NMET   , IMETR   , NORD   , IORDR  ,
&                      NV     , SCEF    , SCOM   ,
&                      MAXT   , TEA     ,
&                      ICNTS  , ISTRN   , IS1A   , IS2A   ,
&                      LSSETA , SGRDA   , ESGRDA ,
&                      SMETA  , ESMETA  , SORDA  , ESORDA ,
&                      LTRNG
&                      )
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C ***** FORTRAN77 SUBROUTINE: B8SCOM *****

C

C PURPOSE: TO ESTABLISH IONISATION RATE COEFFICIENTS Z --> Z+1 FOR A
C SET OF TEMPERATURES GIVEN BY THE ARRAY 'TEA()' USING CUBIC
C SPLINES ON A SET OF RATE COEFFICIENTS COVERING THE
C TEMPERATURES GIVEN BY THE ARRAY 'SCEF()'.

C

C IONISATION DATA COMES EITHER FROM AN INTERACTIVE SEARCH VIA
C THE ADAS208/ADAS502 ROUTE OR DIRECTLY FROM THE INPUT ADF04
C FILE.

C

C THE OUTPUT IS SEPARATED INTO THE METASTABLE PART (SMETA) AND
C THE ORDINARY LEVEL PART (SORDA) APPROPRIATELY INDEXED.
C EXPONENTIAL FACTORS (ESMETA AND (ESORDA) ARE KEPT SEPARATE
C FROM THE REMAINDER OF THE RATE COEFFICIENTS.

C

C IONISATION TYPE IS SELECTED VIA 'ICNTS' & 'ISTRN'

C

C RATE COEFFICIENTS ARE GIVEN FOR A NUMBER OF IONISING LEVELS
C AND THE ARRAY 'SGRDA(,,)' REPRESENTS COEFFTS. FOR COMB-
C INATIONS OF TEMPERATURE, IONISING LEVEL INDEX AND FINAL
C PARENT INDEX.

C

C SPLINE IS CARRIED OUT USING LOG(RATE COEFFICIENT VALUES)

C

C CALLING PROGRAM: ADAS208

C

C SUBROUTINE:

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C INPUT : (I*4) NDTEM = MAXIMUM NUMBER OF TEMPERATURES ALLOWED
C INPUT : (I*4) NDTRN = MAXIMUM NUMBER OF TRANSITIONS ALLOWED
C INPUT : (I*4) NDLEV = MAXIMUM NUMBER OF ENERGY LEVELS ALLOWED
C INPUT : (I*4) NDMET = MAXIMUM NUMBER OF METASTABLES ALLOWED

C INPUT : (I*4) IL = NUMBER OF ENERGY LEVELS

C INPUT : (R*8) WA() = ENERGY LEVELS RELATIVE TO LOWEST (CM-1)

C INPUT : (I*4) NPL = NUMBER OF PARENTS

C INPUT : (R*8) BWNOA() = PARENT ENERGIES RELATIVE TO RECOMBINED
C ION GROUND LEVEL (CM-1)

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C
C INPUT : (I*4)  NMET      = NUMBER OF RECOMBINED METASTABLES
C INPUT : (I*4)  IMETR() = INDICES OF METASTABLES IN FULL LEVEL LIST
C INPUT : (I*4)  NORD      = NUMBRE OF ORDINARY EXCITED LEVELS
C INPUT : (I*4)  IORDR() = INDICES OF ORDINARY LEVELS IN FULL LEVEL LIST
C
C INPUT : (I*4)  NV        = NUMBER OF TEMPERATURES REPRESENTED IN THE
C                        INPUT DATA SET.
C INPUT : (R*8)  SCEF()   = TEMPERATURES REPRESENTED IN INPUT DATA SET
C INPUT : (R*8)  SCOM(,) = RATE COEFF. REPRESENTED IN INPUT DATA SET
C                        1st DIMENSION: TEMPERATURE INDEX ('SCEF')
C                        2nd DIMENSION: IONISATION INDEX
C                        (SEE: 'ISTRN()')
C
C INPUT : (I*4)  MAXT      = NUMBER OF ISPF SELECTED TEMPERATURES FOR
C                        OUTPUT.
C INPUT : (R*8)  TEA()    = ISPF SELECTED TEMPERATURES FOR OUTPUT.
C
C INPUT : (I*4)  ICNTS    = NUMBER OF SELECTED IONISATIONS
C INPUT : (I*4)  ISTRN() = INDEX VALUES IN MAIN TRANSITION ARRAY WHICH
C                        REPRESENT IONISATIONS OF THE SELECTED
C                        TYPE - USED TO SELECT APPROPRIATE RATE COEFFTS
C                        FOR IONISATION Z --> Z+1 TYPE.
C INPUT : (I*4)  IS1A( ) = PARENT INDEX.
C                        DIMENSION: 'TRANSITION'/IONISATION INDEX
C INPUT : (I*4)  IS2A() = IONISING LEVELS INDICES.
C                        DIMENSION: 'TRANSITION'/IONISATION INDEX
C
C INPUT : (I*4)  LSSETA(,) = .TRUE. => IONISATION DATA FROM ADAS502 ROUTE
C                        .FALSE. => NOT AVAILABLE FROM ADAS502 ROUTE
C                        1ST DIM: METASTABLE INDEX FROM MET. LIST
C                        2ND DIM: PARENT INDEX
C INPUT : (R*8)  SGRDA(,,) = INPUT IONISATION RATE COEFFT. VALUES.
C                        FROM THE ADAS208/ADAS502 LOOP
C                        (EXCLUDING EXPONENTIAL TEMPERATURE FACTOR)
C                        1st DIMENSION: TEMPERATURE INDEX ('TOUT')
C                        2nd DIMENSION: IONISING LEVEL INDEX.
C                        3RD DIMENSION: PARENT INDEX.
C INPUT : (R*8)  ESGRDA(,,) = IONISATION RATE COEFFT. EXPONENTIAL FACTORS
C                        FROM THE ADAS208/ADAS502 LOOP
C                        1st DIMENSION: TEMPERATURE INDEX ('TOUT')
C                        2nd DIMENSION: IONISING LEVEL INDEX.
C                        3RD DIMENSION: PARENT INDEX.
C
C OUTPUT: (R*8)  SMETA(,,) = SPLINED IONISATION RATE COEFFT. VALUES.
C                        FOR THE METASTABLES
C                        (EXCLUDING EXPONENTIAL TEMPERATURE FACTOR)
C                        1st DIMENSION: TEMPERATURE INDEX ('TOUT')
C                        2nd DIMENSION: IONISING METASTABLE INDEX.
C                        3RD DIMENSION: PARENT INDEX.
C OUTPUT: (R*8)  ESMETA(,,) = SPLINED IONISATION RATE COEFFT.
C                        EXPONENTIAL TEMPERATURE FACTORS.
C                        1st DIMENSION: TEMPERATURE INDEX ('TOUT')

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C          2nd DIMENSION: IONISING METASTABLE INDEX.
C          3RD DIMENSION: PARENT INDEX.
C OUTPUT:  (R*8)  SORDA(,,) = SPLINED IONISATION RATE COEFFT. VALUES.
C          FOR THE ORDINARY LEVELS
C          (EXCLUDING EXPONENTIAL TEMPERATURE FACTOR)
C          1st DIMENSION: TEMPERATURE INDEX ('TOUT')
C          2nd DIMENSION: IONISING ORDINARY LEVEL INDEX.
C          3RD DIMENSION: PARENT INDEX.
C OUTPUT:  (R*8)  ESORDA(,,) = SPLINED IONISATION RATE COEFFT.
C          EXPONENTIAL TEMPERATURE FACTORS.
C          1st DIMENSION: TEMPERATURE INDEX ('TOUT')
C          2nd DIMENSION: IONISING ORDINARY LEVEL INDEX.
C          3RD DIMENSION: PARENT INDEX.
C
C OUTPUT:  (L*4)  LTRNG() = .TRUE. => TEMPERATURE VALUES WITHIN RANGE
C          READ FROM INPUT COPASE DATA SET.
C          = .FALSE. => TEMPERATURE VALUE NOT WITHIN RANGE
C          READ FROM INPUT COPASE DATA SET.
C          1st DIMENSION: TEMPERATURE INDEX.
C
C
C          (I*4)  NTDSN   = PARAMETER = MAXIMUM NUMBER OF TEMPERATURES
C                   ALLOWED IN INPUT DATA SET = 14
C          (I*4)  NLTEM   = PARAMETER = MUST BE >= 'NDTEM'
C
C          (I*4)  IOPT    = SPLINE END CONDITIONS/EXTRAPOLATION CONTROL
C                   SWITCH - SEE 'XXSPLE'
C                   I.E. DEFINES THE BOUNDARY DERIVATIVES.
C                   (VALID VALUES = 0, 1, 2, 3, 4)
C          (I*4)  I       = GENERAL INDEX
C          (I*4)  ICAP    = CAPTURING LEVEL INDEX BEING ASSESSED.
C          (I*4)  IC      = RECOMBINATION ARRAY INDEX
C          (I*4)  IP      = PARENT INDEX
C          (I*4)  IT      = TEMPERATURE ARRAY INDEX
C
C          (R*8)  DYIN()  = INTERPOLATED DERIVATIVES
C                   DIMENSION: TEMPERATURE INDEX ('TIN()')
C
C          (L*4)  LSETX   = .TRUE.  => X-AXES ('TIN()' VALUES) NEED TO
C                   SET IN 'XXSPLE'.
C                   .FALSE. => X-AXES ('TIN()' VALUES) HAVE
C                   BEEN SET IN 'XXSPLE'.
C                   (NOTE: 'LSETX' IS RESET BY 'XXSPLE')
C
C          (R*8)  LSCOM() = LOG ( 'SCOM(,)' ) FOR GIVEN IONISING LEVEL
C                   DIMENSION: TEMPERATURE INDEX ('SCEF()')
C          (R*8)  LSGRD() = LOG ( SPLINED IONIS  RATE COEFTS )
C                   DIMENSION: TEMPERATURE INDEX ('TEA()' )
C
C
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C          -----

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C XXSPLE ADAS SPLINE SUBROUTINE (WITH EXTRAP. INFO)

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C AUTHOR: HP SUMMERS, UNIVERSITY OF STRATHCLYDE
C TEL. 0141-548-4196

C

C DATE: 14/09/99

C
C

C VERSION : 1.2

C DATE : 19/12/2000

C MODIFIED : Martin O'Mullane

C - Excluded S values GT 1.0 from the spline fit in order
C to compensate for numerical problems at low temperatures.

C

C VERSION : 1.3

C DATE : 17/02/2006

C MODIFIED : Martin O'Mullane

C - Te values for S-line splining may not be the same
C so set lsetx to TRUE before call to xxspole.

C - Set unused values in redscef and redlscom to 0.0.

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INTEGER	ICNTS,	IL,	IMETR (NDMET)
INTEGER	IORDR (NDLEV) ,		IS1A (NDLEV)
INTEGER	IS2A (NDLEV) ,	ISTRN (NDTRN) ,	MAXT
INTEGER	NDLEV,	NDMET,	NDTEM, NDTRN
INTEGER	NMET,	NORD,	NPL, NV
LOGICAL	LSSETA (NDMET, NDMET) ,		LTRNG (NDTEM)
REAL*8	BWNOA (NDMET)		
REAL*8	ESGRDA (NDTEM, NDMET, NDMET)		
REAL*8	ESMETA (NDTEM, NDMET, NDMET)		
REAL*8	ESORDA (NDTEM, NDLEV, NDMET)		
REAL*8	SCEF (NDTEM) ,	SCOM (NTDSN, NDTRN)	
REAL*8	SGRDA (NDTEM, NDMET, NDMET)		
REAL*8	SMETA (NDTEM, NDMET, NDMET)		
REAL*8	SORDA (NDTEM, NDLEV, NDMET) ,	TEA (NDTEM)	
REAL*8	WA (NDLEV)		