

ADAS Subroutine e5spln

```
SUBROUTINE E5SPLN( NTRDIM , NTDDIM ,  
&                 ITRA   , ITDA   , ITVAL  ,  
&                 AMSRA  , AMSDA  , RMASS  , DMASS  ,  
&                 TFRA   , TFDA   , TREVA  , TDEVA  ,  
&                 QFTCXA ,          QTCXA  ,  
&                 LTRRNG , LTDRNG  
&                 )
```

```
C-----  
C  
C ***** FORTRAN77 SUBROUTINE: E5SPLN *****  
C  
C PURPOSE:  
C     PERFORMS CUBIC SPLINE ON LOG(TEMP.) VERSUS LOG(RATE-COEFT)  
C     INPUT DATA FOR A GIVEN DONOR/RECEIVER DATA-BLOCK.  
C  
C     USING TWO-WAY SPLINES IT CALCULATES THE RATE-COEFFICIENTS  
C     FOR 'ITVAL' PAIRS OF RECEIVER/DONOR TEMPERATURES FROM THE  
C     TWO-DIMENSIONAL TABLE OF RECEIVER/DONOR TEMPERATURES READ  
C     IN FROM THE INPUT FILE. IF A VALUE CANNOT BE INTERPOLATED  
C     USING SPLINES IT IS EXPLICITLY EXTRAPOLATED.  
C  
C CALLING PROGRAM: ADAS505/SQTCX  
C  
C  
C SUBROUTINE:  
C  
C INPUT : (I*4)  NTRDIM  = MAX NUMBER OF RECEIVER TEMPERATURES ALLOWED  
C INPUT : (I*4)  NTDDIM  = MAX NUMBER OF DONOR      TEMPERATURES ALLOWED  
C  
C INPUT : (I*4)  ITRA    = INPUT DATA FILE: NUMBER OF RECEIVER TEMPERA-  
C                       TURES READ FOR THE DATA-BLOCK BEING ASSESSED  
C INPUT : (I*4)  ITDA    = INPUT DATA FILE: NUMBER OF DONOR      TEMPERA-  
C                       TURES READ FOR THE DATA-BLOCK BEING ASSESSED  
C INPUT : (I*4)  ITVAL   = NUMBER OF ISPF ENTERED RECEIVER/DONOR TEMP-  
C                       ERATURE PAIRS FOR WHICH RATE-COEFFICIENTS  
C                       ARE REQUIRED FOR TABULAR/GRAPHICAL OUTPUT.  
C  
C INPUT : (R*8)  AMSRA   = INPUT DATA FILE: RECEIVER ATOMIC MASS FOR  
C                       THE DATA-BLOCK BEING ASSESSED.  
C INPUT : (R*8)  AMSDA   = INPUT DATA FILE: DONOR      ATOMIC MASS FOR  
C                       THE DATA-BLOCK BEING ASSESSED.  
C INPUT : (R*8)  RMASS   = USER ENTERED: RECEIVER ISOTOPIC ATOMIC MASS  
C INPUT : (R*8)  DMASS   = USER ENTERED: DONOR      ISOTOPIC ATOMIC MASS  
C  
C INPUT : (R*8)  TFRA()  = INPUT DATA FILE: RECEIVER TEMPERATURES (EV)  
C                       FOR THE DATA-BLOCK BEING ASSESSED.  
C                       DIMENSION: RECEIVER TEMPERATURE INDEX  
C INPUT : (R*8)  TFDA()  = INPUT DATA FILE: DONOR      TEMPERATURES (EV)  
C                       FOR THE DATA-BLOCK BEING ASSESSED.  
C                       DIMENSION: DONOR      TEMPERATURE INDEX  
C INPUT : (R*8)  TREVA() = USER ENTERED: RECEIVER TEMPERATURES (EV)  
C                       DIMENSION: RECEIVER/DONOR TEMP. PAIR INDEX
```

```

C INPUT : (R*8) TDEVA() = USER ENTERED: DONOR TEMPERATURES (EV)
C DIMENSION: RECEIVER/DONOR TEMP. PAIR INDEX
C
C
C INPUT : (R*8) QFTCXA(,) = INPUT DATA FILE: FULL SET OF RATE-COEFFTS.
C (UNITS: CM**3/SEC) FOR THE DATA-BLOCK BEING
C ANALYSED.
C 1ST DIMENSION: DONOR TEMPERATURE INDEX
C 2ND DIMENSION: RECEIVER TEMPERATURE INDEX
C OUTPUT: (R*8) QTCXA() = SPLINE INTERPOLATED OR EXTRAPOLATED RATE-
C COEFFICIENTS FOR THE USER ENTERED RECEIVER/
C DONOR TEMPERATURE PAIRS (UNITS: CM**3/SEC)
C DIMENSION: RECEIVER/DONOR TEMP. PAIR INDEX
C
C OUTPUT: (L*4) LTRRNG() = .TRUE. => OUTPUT 'QTCXA()' VALUE WAS INTER-
C POLATED FOR THE USER ENTERED
C RECEIVER TEMPERATURE 'TREVA()'.
C .FALSE. => OUTPUT 'QTCXA()' VALUE WAS EXTRA-
C POLATED FOR THE USER ENTERED
C RECEIVER TEMPERATURE 'TREVA()'.
C DIMENSION: RECEIVER/DONOR TEMP. PAIR INDEX
C
C OUTPUT: (L*4) LTDRNG() = .TRUE. => OUTPUT 'QTCXA()' VALUE WAS INTER-
C POLATED FOR THE USER ENTERED
C DONOR TEMPERATURE 'TDEVA()'.
C .FALSE. => OUTPUT 'QTCXA()' VALUE WAS EXTRA-
C POLATED FOR THE USER ENTERED
C DONOR TEMPERATURE 'TDEVA()'.
C
C (I*4) NIN = PARAMETER = MAX. NO. OF INPUT TEMPERATURE
C VALUES. MUST BE >= 'ITRA' & 'ITDA'
C (I*4) NOUT = PARAMETER = MAX. NO. OF OUTPUT TEMPERATURE
C PAIRS. MUST BE >= 'ITVAL'
C (I*4) L1 = PARAMETER = 1
C
C (I*4) ITD = ARRAY SUBSCRIPT USED INPUT FILE DONOR
C TEMPERATURES.
C (I*4) ITR = ARRAY SUBSCRIPT USED INPUT FILE RECEIVER
C TEMPERATURES.
C (I*4) IT = ARRAY SUBSCRIPT USED FOR USER ENTERED
C TEMPERATURE PAIRS .
C (I*4) IOPT = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C SPLINE ROUTINE 'XXSPLE', SEE 'XXSPLE'.
C (VALID VALUES = <0, 0, 1, 2, 3, 4)
C
C (L*4) LSETX = .TRUE. => SET UP SPLINE PARAMETERS RELATING
C TO 'XIN' AXIS.
C .FALSE. => DO NOT SET UP SPLINE PARAMETERS
C RELATING TO 'XIN' AXIS.
C (I.E. THEY WERE SET IN A PREVIOUS
C CALL )
C (VALUE SET TO .FALSE. BY 'XXSPLE')
C

```

```

C      (R*8)  R8FUN1  = FUNCTION - (SEE ROUTINES SECTION BELOW)
C      (R*8)  LOGSFR  = LOG( SCALING FACTOR FOR DATA FILE RECEIVER
C                    TEMPERATURES )
C      (R*8)  LOGSFD  = LOG( SCALING FACTOR FOR DATA FILE DONOR
C                    TEMPERATURES )
C      (R*8)  RMR     = RECIPROCAL OF 'RMASS' - USED IN EXTRAPOLATN.
C      (R*8)  DMD     = RECIPROCAL OF 'DMASS' - USED IN EXTRAPOLATN.
C      (R*8)  AMR     = RECIPROCAL OF 'AMSRA' - USED IN EXTRAPOLATN.
C      (R*8)  AMD     = RECIPROCAL OF 'AMSDA' - USED IN EXTRAPOLATN.
C      (R*8)  RDMIN   = FACTOR USED IN EXTRAPOLATION OF DONOR
C                    TEMPERATURES BELOW THE MINIMUM DATA VALUE.
C      (R*8)  RDMAX   = FACTOR USED IN EXTRAPOLATION OF DONOR
C                    TEMPERATURES ABOVE THE MAXIMUM DATA VALUE.
C      (R*8)  RRMIN   = FACTOR USED IN EXTRAPOLATION OF RECEIVER
C                    TEMPERATURES BELOW THE MINIMUM DATA VALUE.
C      (R*8)  RRMAX   = FACTOR USED IN EXTRAPOLATION OF RECEIVER
C                    TEMPERATURES ABOVE THE MAXIMUM DATA VALUE.
C      (R*8)  VAL1    = VALUE USED IN EXTRAPOLATION.
C      (R*8)  VAL2    = VALUE USED IN EXTRAPOLATION.
C      (R*8)  COEF1   = COEFFICIENT USED TO CALC. EXTRAPOLTED VALUE
C      (R*8)  COEF2   = COEFFICIENT USED TO CALC. EXTRAPOLTED VALUE
C
C      (R*8)  XIN( )  = 1) LOG( DATA FILE DONOR   TEMPERATURES )
C                    2) LOG( DATA FILE RECEIVER TEMPERATURES )
C      (R*8)  YIN( )  = LOG( DATA FILE RATE-COEFFICIENTS )
C      (R*8)  XOUT( ) = 1) LOG( SCALED USER ENTERED DONOR   TEMPS.)
C                    2) LOG( SCALED USER ENTERED RECEIVER TEMPS.)
C      (R*8)  YOUT( ) = LOG( OUTPUT GENERATED RATE COEFFICIENTS )
C      (R*8)  YPASS( , ) = LOG( RATE COEFFICIENTS ) INTERMEDIATE ARRAY
C                    WHICH STORES INTERPOLATED/EXTRAPOLATED RATE
C                    COEFFICIENT VALUES BEWTEEN THE TWO SPLINE
C                    SECTIONS.
C      (R*8)  DF( )   = SPLINE INTERPOLATED DERIVATIVES

```

C NOTE:

C ROUTINES:

ROUTINE	SOURCE	BRIEF DESCRIPTION
XXSPLE	ADAS	SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
R8FUN1	ADAS	REAL*8 FUNCTION: (X -> X)

C AUTHOR: PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 4569

C DATE: 21/02/91

C UNIX-IDL PORT:

C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)

C DATE: 22TH MARCH 1996
 C
 C VERSION: 1.1 DATE: 22-03-96
 C MODIFIED: WILLIAM OSBORN
 C - FIRST VERSION
 C
 C VERSION: 1.2 DATE: 02-03-96
 C MODIFIED: WILLIAM OSBORN
 C PROPER HEADER INFORMATION ADDED
 C
 C VERSION: 1.3 DATE: 7-11-97
 C MODIFIED: Martin O'Mullane
 C increased NOUT to 24
 C

C-----
 C
 C-----

INTEGER	ITDA,	ITRA,	ITVAL,	NTDDIM
INTEGER	NTRDIM			
LOGICAL	LTDRNG (ITVAL) ,		LTRRNG (ITVAL)	
REAL*8	AMSDA,	AMSRA,	DMASS	
REAL*8	QFTCXA (NTDDIM, NTRDIM) ,		QTCXA (ITVAL)	
REAL*8	RMASS,	TDEVA (ITVAL)		
REAL*8	TFDA (ITDA) ,	TFRA (ITRA) ,	TREVA (ITVAL)	