

ADAS Subroutine b3leve

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SUBROUTINE B3LEVE( NDLEV , IZDIMD,  
&                IZMAX , Z1A   , IZA   , IZ0A  , IZ1A,  
&                BWNOA , IL    ,  
&                IA    , NA    , WAA    ,  
&                IZS   , IZ0   ,  
&                BWNO  , WAO   )
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C ***** FORTRAN77 SUBROUTINE: B3LEVE *****

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C PURPOSE: TO EVALUATE IONISATION AND LEVEL ENERGIES FOR A SELECTED
C MEMBER OF AN ISOELECTRONIC SEQUENCE FROM THE GENERAL Z DATA

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C CALLING PROGRAM: ADAS203

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C DATA:

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C THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:

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C IONISATION POTENTIAL: WAVE NUMBER (CM-1)

C

C INDEX LEVEL ENERGIES: WAVE NUMBER (CM-1)

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C SUBROUTINE:

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C (I*4) NDSPLN = PARAMETER = MAXIMUM NUMBER OF SPLINE KNOTS

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C INPUT : (I*4) NDLEV = MAXIMUM NUMBER OF LEVELS THAT CAN BE READ

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C INPUT : (I*4) IZDIMD = MAX. NUMBER OF SEQUENCE MEMBERS ALLOWED

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C INPUT : (I*4) IZMAX = NUMBER OF SEQUENCE MEMBERS

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C INPUT : (R*8) Z1A() = SEQUENCE RECOMBINING ION CHARGES READ
C 1ST DIMENSION - SEQUENCE MEMBER INDEX

C

C INPUT : (I*4) IZA() = SEQUENCE RECOMBINED ION CHARGES
C 1ST DIMENSION - SEQUENCE MEMBER INDEX

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C INPUT : (I*4) IZ0A() = SEQUENCE NUCLEAR CHARGES
C 1ST DIMENSION - SEQUENCE MEMBER INDEX

C

C INPUT : (I*4) IZ1A() = SEQUENCE RECOMBINING ION CHARGES READ
C 1ST DIMENSION - SEQUENCE MEMBER INDEX
C (NOTE: IZ1 SHOULD EQUAL IZ+1)

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C INPUT : (R*8) BWNOA() = IONISATION POTENTIALS (CM-1)
C 1ST DIMENSION - SEQUENCE MEMBER INDEX

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

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C INPUT : (I*4) IA() = ENERGY LEVEL INDEX NUMBER

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C INPUT : (I*4) NA() = PRINCIPAL QUANTUM NUMBER OF VALENCE ELECTRON

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C INPUT : (R*8) WAA() = ENERGY RELATIVE TO LEVEL 1 (CM-1) FOR LEVEL
C 'IA()'

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C 1ST DIMENSION - LEVEL INDEX

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C 2ND DIMENSION - SEQUENCE MEMBER INDEX

C INPUT : (I*4) IZS = NUCLEAR CHARGE OF NEUTRAL SEQUENCE MEMBER
 C INPUT : (I*4) IZ0 = NUCLEAR CHARGE OF SELECTED ION
 C
 C OUTPUT: (R*8) BWNO = IONISATION ENERGY OF SELECTED ION (CM-1)
 C OUTPUT: (R*8) WAO() = LEVEL ENERGIES RELATIVE TO LOWEST (CM-1)
 C
 C (I*4) I = GENERAL USE.
 C (I*4) IENDN = SPLINE END CONDITION SWITCH AT LAST POINT
 C (I*4) IEND1 = SPLINE END CONDITION SWITCH AT FIRST POINT
 C (I*4) IFORMS = SPLINE INDEPENDENT VARIABLE FORM SWITCH
 C (I*4) K = GENERAL USE.
 C
 C (R*8) C1(,) = 1ST SPLINE COEFFICIENT MATRIX
 C (R*8) C2(,) = 2ND SPLINE COEFFICIENT MATRIX
 C (R*8) C3(,) = 3RD SPLINE COEFFICIENT MATRIX
 C (R*8) C4(,) = 4TH SPLINE COEFFICIENT MATRIX
 C (R*8) DY = GRADIENT OF SPLINE AT POINT
 C (R*8) ENI = LEVEL PRINCIPAL QUANTUM NUMBER
 C (R*8) EN1 = LOWEST LEVEL PRINCIPAL QUANTUM NUMBER
 C (R*8) E1I = LEVEL ENERGY (RYDBERGS)
 C (R*8) B3FORM = EXTERNAL FUNCTION (SEE SUBROUTINE SECTION)
 C (R*8) REN = GENERAL USE
 C (R*8) XI = GENERAL USE
 C (R*8) XSA() = SPLINE INDEPENDENT VARIABLE AT KNOTS
 C (R*8) Y = SPLINE INTERPOLATED VALUE
 C (R*8) YSA() = SPLINE DEPENDENT VARIABLE AT KNOTS
 C (R*8) Z1 = CURRENT ION CHARGE +1

C ROUTINES:

ROUTINE	SOURCE	BRIEF DESCRIPTION
B2GSPC	ADAS	GENERATES SPLINE COEFFICIENT MATRICES
B2NFAS	ADAS	SETS SPLINE ASYMPTOTIC CONDITIONS
B3FORM	ADAS	INDEPENDENT VARIABLE FUNCTION FOR SPLINE
B2SORT	ADAS	SORTS VECTOR INTO INCREASING ORDER

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 C K1/1/57
 C JET EXT. 4941

C DATE: 08/01/95

C UNIX-IDL PORT:

C VERSION: 1.1

DATE: 20-03-96

C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)

C - PUT UNDER S.C.C.S. CONTROL

C - REPLACED CALLS TO NSORT ROUTINE WITH CALLS TO B2SORT.

C NSORT IS USED TO SORT A REAL ARRAY AND ASSOCIATED

C INTEGER ARRAY WHEREAS WHAT WAS BEING PASSED TO IT WAS

C A REAL ARRAY AND ANOTHER, ASSOCIATED REAL ARRAY. B2SORT

C TAKES 2 REAL ARRAYS AS INPUT AND PERFORMS A BUBBLE SORT

C ON THEM.

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C VERSION: 1.2

DATE: 23-04-07

C MODIFIED: ALLAN WHITEFORD

C - RENAMED FORM SUBROUTINE TO B3FORM.

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INTEGER	IA (NDLEV) ,	IL,	IZ0
INTEGER	IZ0A (IZDIMD) ,		IZ1A (IZDIMD)
INTEGER	IZA (IZDIMD) ,	IZDIMD,	IZMAX, IZS
INTEGER	NA (NDLEV) ,	NDLEV	
REAL*8	BWNO,	BWNOA (IZDIMD)	
REAL*8	WAA (NDLEV, IZDIMD) ,		WAO (NDLEV)
REAL*8	Z1A (IZDIMD)		