

ADAS Subroutine effz3

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      subroutine effz3( jealfa , n      , l      , e      , qd      ,  
&                    jsn      , z0      , nshell , nc      , numel ,  
&                    alfa     , jalfl1 , jalfl2 ,  
&                    x0      , x1      , x2      , d      , m0  
&                    )
```

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C  
C ***** fortran77 program: effz3.for *****
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C Purpose: Searches for the effective potential for a single electron  
C          distorted wave function for a specified screening or a  
C          specified energy.  
C          (original by A. Burgess, DAMTP, University of Cambridge)
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C Subroutine:
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C input : (i*4) jealfa = <0 => search for energy e  
C          = >0 => search for screening parameter alfa  
C input : (i*4) n      = principal quantum number  
C input : (i*4) l      = orbital quantum number  
C i/o   : (i*4) e      = energy (Ryd) for electron.  
C          (NB -ve for a bound state)  
C input : (i*4) qd     = quantum defect for valence electron  
C input : (i*4) jsn    = -1 => Jucys potential form adopted  
C          = 0  => Slater potential form adopted  
C input : (i*4) z0     = nuclear charge  
C input : (i*4) nshell = number of screening shells  
C input : (i*4) nc()   = principal quantum number of screening shell  
C          1st dim: index of screening shells  
C input : (i*4) numel() = number of electrons in screening shell  
C i/o   : (r*8) alfa() = screening parameters  
C          1st dim: initial (1) and final (2) states  
C          2nd dim: screening shell index.  
C input : (i*4) jalfl1 = first screening shell for optimising  
C input : (i*4) jalfl2 = last screening shell for optimising  
C output: (i*4) x0     = inner turning point  
C output: (i*4) x1     = outer turning point  
C output: (i*4) x2     = range for active electron wave function  
C input : (i*4) d      = search accuracy setting  
C output: (i*4) m0     = number of nodes in wave function
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C Routines:
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C      routine      source      brief description  
C-----  
C      zeff         adas  
C      zser         adas  
C      fcf6         adas  
C      i4unit       adas      fetch unit number for output of messages
```

C
C Author: H. P. Summers, University of Strathclyde
C ja7.08
C tel. 0141-548-4196
C
C Date: 24/02/03
C
C Update: HP Summers 24/05/04 restructure and added standard warning
C
C-----

INTEGER	JALF1,	JALF2,	JEALFA,	JSN
INTEGER	L,	M0,	N,	NC(10)
INTEGER	NSHELL,	NUMEL(10)		
REAL*8	ALFA(10),	D,	E,	QD
REAL*8	X0,	X1,	X2,	Z0