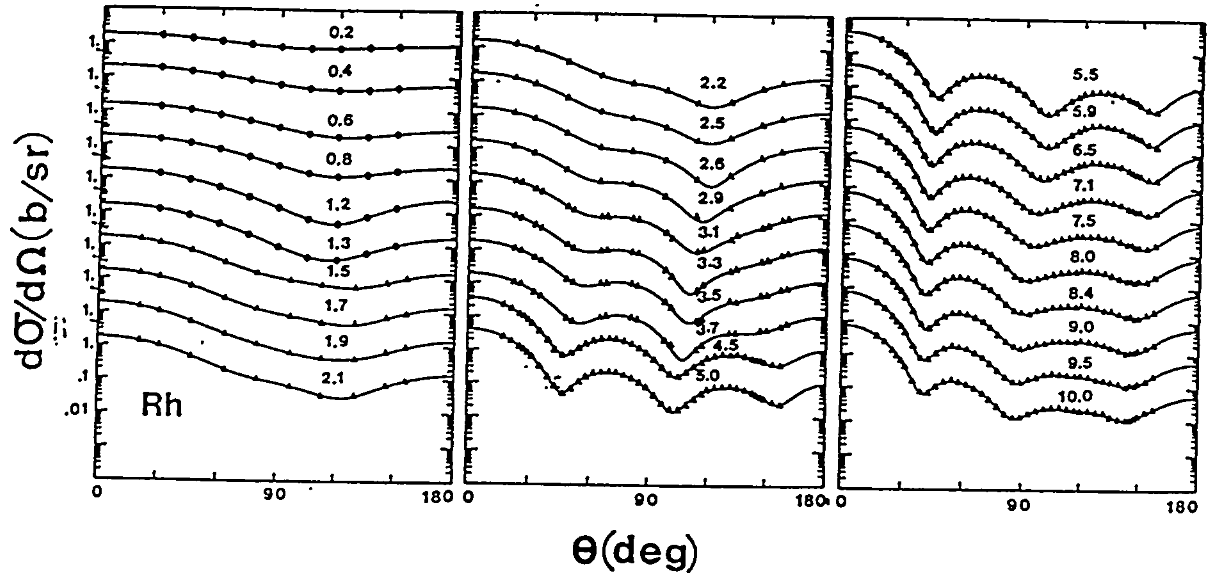
NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-147

ELEMENTAL ABAREX -- A User's Manual

by
A. B. Smith
June 1999



ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

Operated by THE UNIVERSITY OF CHICAGO
for the U. S. DEPARTMENT OF ENERGY
under Contract W-31-109-Eng-38

Argonne National Laboratory

Argonne National Laboratory, with facilities in the states of Illinois and Idaho, is owned by the United States Government, and operated by the University of Chicago under provisions of a contract with the Department of Energy.

Disclaimer

Available to DOE and DOE contractors from the Office
of Scientific and Technical Information, P. O. Box 62,
Oak Ridge, TN 37831; prices available from
(423) 576-8401.

Available to the public from the National Technical
Information Service, U. S. Department of Commerce,
5285 Port Royal Road, Springfield, VA 22161.

PUBLICATIONS IN THE ANL/NDM SERIES

A listing of recent issues in this series is given below. Issues and/or titles prior to ANL/NDM-130 can be obtained from the National Technical Information Service, U. S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161, or by contacting the author of this report at the following address:-

Technology Development Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
USA

A. B. SMITH AND P. T. GUENTHER
Fast-Neutron Interaction with the Fission Product ^{103}Rh
ANL/NDM-130, September 1993

A. B. SMITH AND P. T. GUENTHER
Fast-Neutron Scattering from Vibrational Palladium Nuclei
ANL/NDM-131, October 1993

A. B. SMITH
Neutron Interaction with Doubly-Magic ^{40}Ca
ANL/NDM-132, December 1993

A. B. SMITH
Neutron Scattering at Z = 50:- Tin
ANL/NDM-133, September 1994

A. B. SMITH, S. CHIBA AND J. W. MEADOWS
An Evaluated Neutronic File for Elemental Zirconium
ANL/NDM-134, September 1994

A. B. SMITH
Neutron Scattering from Uranium and Thorium
ANL/NDM-135, February 1995

A. B. SMITH
Neutron Scattering and Models:- Iron
ANL/NDM-136, August 1995

A. B. SMITH
Neutron Scattering and Models:- Silver
ANL/NDM-137, July 1996

A. B. SMITH
Neutron Scattering and Models:- Chromium
ANL/NDM-138, June 1996

W. P. POENITZ AND S. E. AUMEIER
The Simultaneous Evaluation of the Standards and Other Cross Sections of Importance for Technology
ANL/NDM-139, September 1997

J. T.Daly and D. L. Smith
A Compilation of Information on the $^{31}P(p,\gamma)^{32}S$ *Reaction and Properties of Excited Levels in* ^{32}S
ANL/NDM-140, November 1997

A. B. SMITH
Neutron Scattering and Models:- Titanium
ANL/NDM-141, July 1997

A. B. SMITH
Neutron Scattering and Models:- Molybdenum
ANL/NDM-142, July 1999

R. E. MILLER AND D. L. SMITH
A Compilation of Information on the $^{31}P(p,\gamma)^{33}Cl$ *Reaction and Properties of Excited Levels in* ^{33}Cl
ANL/NDM-143, July 1997

R. E. MILLER AND D. L. SMITH
A Compilation of Information on the $^{31}P(p,a)^{28}Si$ *Reaction and Properties of Excited Levels in* ^{28}Si
ANL/NDM-144, November 1977.

R. D. LAWSON AND A. B. SMITH
Abarex-A Neutron Spherical Optical-Statistical Model Code: A User's Manual
ANL/NDM-145, June 1998.

R. T. KLANN AND W. P. POENITZ
Non-destructive Assay of EBR-II Blanket Elements Using Resonance Transmission Analysis
ANL/NDM-146, August 1998.

TABLE OF CONTENTS

ANL/NDM-147

ELEMENTAL ABAREX -- A User's Manual*

by

A. B. Smith

ABSTRACT

ELEMENTAL ABAREX is an extended version of the spherical optical-statistical model code ABAREX, designed for the interpretation of neutron interactions with elemental targets consisting of up to ten isotopes. The contributions from each of the isotopes of the element are explicitly dealt with, and combined for comparison with the elemental observables. Calculations and statistical fitting of experimental data are considered. The code is written in FORTRAN-77 and arranged for use on the IBM-compatible personal computer (PC), but it should operate effectively on a number of other systems, particularly VAX/VMS and IBM work stations. Effort is taken to make the code user friendly. With this document a reasonably skilled individual should become fluent with the use of the code in a brief period of time.

This code and this document have been sent to the NEA Data Bank and the Radiation Safety Information Computational Center (ORNL). Interested users should contact one of these centers. Any suggestions, errors and/or corrections should be communicated to A. B. Smith, Technology Development Division, Bldg. 315, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA.

---

* This work is supported by the United States Department of Energy under contract W-31-109-Eng-38, and by the Nuclear and Energy Engineering Program, College of Engineering and Mines, The University of Arizona.

I. PREFACE

Due to cost and isotope-availability considerations many experimental fast-neutron studies, of necessity, must often employ elemental samples. Thus the resulting measured observables generally refer to an element with varying contributions from a number of isotopes. This situation greatly complicates the experimental interpretation, particularly if one wishes to deduce model parameters by statistical fitting of the data. One such vehicle is the spherical optical-statistical model widely used for the interpretation of fast-neutron total, scattering and reaction cross-section data [FPW54, HF52, Hod63, Hod94, Wol51]. ABAREX is a particularly powerful optical-statistical-model code for interpreting fast-neutron reaction data on an isotopic basis [LS98]. ELEMENTAL ABAREX, described herein, is an extension of ABAREX to elemental interpretations considering up to ten isotopic components. It also will execute nearly all of the calculations of the isotopic ABAREX. ELEMENTAL ABAREX makes possible the interpretation of elemental observables in the context of the spherical optical-statistical model in a manner not here-to-fore easily possible. This document is a user's manual for implementing ELEMENTAL ABAREX. The underlying physical concepts have already been outlined in the report ANL/NDM-145 by R. Lawson and A. Smith [LS98]. The reader is strongly encouraged to become familiar with the latter report as it contains an outline of the physical processes underlying both ABAREX and ELEMENTAL ABAREX, processes which are not defined in any detail in this document. The present report deals only with the implementation of ELEMENTAL ABAREX.

ABAREX, the basis of ELEMENTAL ABAREX, was originally written by P. A. Moldauer using components of the optical-model program ABACUS by E. Auerbach [Aue64]. ABAREX was later extensively modified by R. Lawson and A. Smith, and is defined in ref. [LS98]. ABAREX was first extended to an elemental basis (ELEMENTAL ABAREX) by S. Chiba. The latter elemental version was refined and developed by R. Lawson and A. Smith. Parts of both codes contain non-linear fitting procedures developed by Garbow et al. [Gar68] and Clebsch-Gordon routines originally written by S. Pieper [Pie88]. Like most codes of this type, ELEMENTAL ABAREX is an amalgamation of components from a number of authors.

II. SYSTEM REQUIREMENTS AND EXPERIENCE

ELEMENTAL ABAREX is written in ANSI FORTRAN-77 with several VAX (IBM) extensions. It was developed from ABAREX [LS98] with many common subroutines. The program has been explicitly written for the PC with a 286, 386, 486 or Pentium processor. It will run on a PC with as little as 16 Mb of RAM. Lahey [Lah] and Microsoft [Mic] FORTRAN compilers have been used, and there is every reason to believe that suitable performance can be achieved on VAX [VAX], IBM [IBM] and other work stations. However, there is a VAX-IBM extension in the source Clebsch-Gordon routine. Therefore, the compilation should use the 'VAX option' if available, though it generally will not be necessary. On other facilities some adjustment of constants in the subroutine LMDIF1 may be necessary following the comments given in the source. The little used 'INPUT' option may vary with compilers. What is given here is consistent with VAX/IBM practice. Some systems may require an alternate setup of the I/O files. The user should consult his or her particular system instructions. During the compilation the user may receive a number of "warning" messages. These are generally of two types: i) uninitiated variables, and ii) "common" conflicts. The latter are due to the use of the citation of only the first element of a common variable once it has been fully defined. The former are of no consequence.

The following sections of this report:- i) Define the various input options. Simple outline instructions are also included at the beginning of the FORTRAN source listing. ii) Provide a number of examples illustrating the use of the program. and iii) Give a FORTRAN source listing of the program. The input and output of the examples and the FORTRAN source are on the Diskette of the appendix. Where necessary, some descriptions of the physical basis of the code are given, and these should be augmented by the physical outline of ref. [LS98]. No large code can be guaranteed error free. As illustrated in the examples, a number of internal checks have been made to test for accuracy. In addition parts of the code have been compared with results obtained with the codes SCAT2 [Ber96], JUPITOR [Tam67], ECIS96 [Ray96], PTOLEMY [MP78] and (of course) ABAREX [LS98]. The agreement between the various calculations seems to be acceptable.

ELEMENTAL ABAREX (like ABAREX) is a neutron code. Incident charged-particles can not be treated and the sign of the isospin dependence of the real and imaginary potentials is set to the negative values suitable for neutrons. The code is designed for relatively low energies (e.g. less than 30→50 MeV), and it may give erroneous results at higher energies. The code is not relativistic.

III. CODE OPERATIONS

ELEMENTAL ABAREX input is generally via a set of keyword records consisting of a keyword, an integer and up to seven floating-point numbers. With the exception of the SEARCH image, all keyword records have the Format(A7,I3,7f10.4). Keyword records may be included in any order except for the COMPUTE image. Keyword records not needed for a particular calculation, or erroneous keywords, are ignored. All keywords must be capitalized. The program sorts keywords by using only the first two symbols of the word. Thus 'COMPUTE', 'COMP' or 'CO' are all equivalent, but Compute or compute are not acceptable. The input of every calculation must terminate with a 'COMPUTE' record. That record tells the program to launch the calculation. Any number of problems may be stacked on the input file and they will be processed sequentially. All input is on the input file, not to be confused with keyword 'INPUT', and all problem output is on the file output. In addition, there are two scratch files, templ and temp2. Templ, temp2 and output files should be cleared before attempting to start a problem.

In ELEMENTAL ABAREX all energies are in MeV, all lengths in fermis, all cross sections in the laboratory coordinate system and in barns (b) or barns per steradian (b/sr), and all angles in degrees in the laboratory coordinate system. Generally, ELEMENTAL ABACUS will run the same problems as the parent isotopic ABAREX [LS98] with only several changes to the input. However, there are some limitations as noted below, e.g. ELEMENTAL ABACUS does not do fitting using strength functions as the physical meaning of elemental strength functions is ambiguous, and only elemental average capture and fission cross sections are calculated.

In the following subtopics the various input records are described and their functions outlined. A number of illustrative examples are described, with calculational I/O given in Appendix A and/or on the attached diskette. Each subsection below is introduced with a code line 1234567890123456789012345----- up to 80 columns, followed by the actual input record. The code line is only for identification and not part of the input, as illustrated in the examples. The examples also contain the complete calculational outputs. If the input record requires the full 80 column format it will appear as two lines in the following narrative.

III.1. REAL POTENTIAL

```
1234567890123456789012345678901234567890123456789012345678901234567890...
REAL   KRE   VRE       VRE1      VRE2      R1        A1        VSR
```

The 'REAL' keyword tells the program that the parameters of the real optical potential are to follow. The entry KRE in columns (8-10) indicates the shape of this potential. However, in ELEMENTAL ABAREX (and ABAREX) the potential can have only the Saxon-Woods form [Hod63] given by

$$V_o(r) = -V_o/\{1 + \exp((r-R_v)/a_v)\}, \qquad (1)$$

where a_v is the real-potential diffuseness and R_v its radius. KRE can have any value or be left blank and the default "1" value for the Saxon-Woods form will always be used and printed on the output. <u>It should be clearly understood that ELEMENTAL ABAREX expresses the real (and imaginary) potential in the form</u>

$$V = V_o - V_1 \cdot \eta \qquad (2)$$

$$(\text{and } W = W_o - W_1 \cdot \eta),$$

where V_o is the isoscaler potential, V_1 the isovector potential, and η the nuclear asymmetry equal to (N-Z)/A. The negative sign is for neutrons, as discussed by Lane [Lan62]. <u>This program is only for a neutron interaction. ELEMENTAL ABAREX works with V_o, NOT V</u>, as in ABAREX or as commonly encountered in optical-model calculations. Of course, if the isovector potential is set to zero $V \equiv V_o$. <u>The user must clearly understand the implications of Eq. 2, and its use in the program.</u> VRE of the 'REAL' input is V_o of Eq. 2. Furthermore, V_o can be given up to a quadratic energy dependence of the form

$$V_o = VRE + VRE1 \cdot E + VRE2 \cdot E^2, \qquad (3)$$

where E is the incident neutron energy in the center-of-mass coordinate system. In practice, the E of the laboratory and center-of-mass systems are essentially identical for the considerations of Eq. 3. VRE, VRE1 and VRE2 of the 'REAL' keyword image are given in columns 11→20, 21→30 and 31→40, respectively. VRE1 and VRE2 default values are zero. ELEMENTAL ABAREX expresses the real-potential radius, R, in the reduced form r_o, where

$$R = r_o \cdot A^{1/3}, \qquad (4)$$

and A is the atomic number of the target. On the 'REAL' image $R1 \equiv r_o$ of Eq. 4 appears in columns (41→50). The diffuseness of the Saxon-Woods real potential is A1 of columns (51→60) of the 'REAL' image. If the spin-orbit interaction is real, has the Thomas form, and a geometry identical to that of the real potential, the spin-orbit potential strength can be inserted in columns (61→70) of the 'REAL' image and the 'SO' image, discussed below, omitted. This option will set the isovector potentials to the default values of zero as they are also input from the 'SO' image.

If the 'REAL' image record is omitted, the default values for the spherical optical potential are used. For the real, imaginary and spin-orbit potentials these default values are:

Real potential

$$\begin{aligned} VRE &= V_o = 46.0 \text{ Mev} \\ R1 &= r_v = 1.317 \text{ fm} \\ A1 &= a_v = 0.62 \text{ fm}, \end{aligned}$$

Imaginary potential

$$\begin{aligned} VIM &= W_o = 14.0 \text{ MeV} \\ R2 &= r_w = 1.317 \text{ fm} \\ A2 &= a_w = 0.25 \text{ fm}, \end{aligned}$$

and the Spin-orbit potential

$$\begin{aligned} VSR &= V_{so} = 7.0 \text{ MeV} \\ VSI &= 0 \\ RR1 &= r_{so} = 1.317 \text{ fm} \\ AA1 &= a_{so} = 0.62 \text{ fm}, \end{aligned}$$

where VSI is the imaginary spin-orbit strength and the potential has the Thomas form. The default values of the real and imaginary isovector potentials are identically zero. If any potential is omitted at the input, default values will be used. The 'REAL' image is identical to that of ABAREX except for the distinction between isoscaler and total real potentials.

III.2. IMAGINARY POTENTIAL

```
1234567890123456789012345678901234567890123456789012345678901234567890
IMAG   KIM   VIM       VIM1      VIM2      R2        A2      VIVOL
                                                            1234567890
                                                               VOLRAT
```

The keyword 'IMAG' tells the program that the parameters of the imaginary potential are to follow. The first of these, KIM in columns (8→10), defines the shape of the imaginary potential. When KIM ≡ 1 the imaginary potential is volume absorption with the Saxon-Woods form defined by Eq. 1, above. If KIM ≡ 2 the potential is a surface-peaked gaussian of the form

$$W(r) = -W_o\{\exp((r-R_w)/a_w)^2\}. \qquad (5)$$

When KIM ≡ 4 the potential is a surface-peaked derivative-Saxon-Woods form given by

$$W(r) = -4\cdot W_o\exp((r-R_w)/a_w)/\{1 + \exp((r-R_w)/a_w)\}^2. \qquad (6)$$

The strength of the imaginary potential is given by an expression analogous to that of the real potential given in Eq. 3, where W_o = VIM, W_1 = VIM1, W_2 = VIM2 and E is the center of mass energy of the incident neutron. These three constants are given in columns (11→20), (21→30) and (31→40), respectively. The imaginary potential reduced radius, R2 = r_w, is given in columns (41→50) and the diffuseness A2 = a_w in columns (51→60).

It is possible to have an imaginary potential which is the sum of a surface and a volume part, subject to the restriction that r_w and a_w are the same for the two components. In this case KIM = 3 or 5. There are two ways of communicating the surface and volume strengths to the program. In the first VIM for the surface imaginary component is read in columns (11-20) and the volume strength, VIVOL, is read in columns (61→70). If VIM = 0 the above cited default values will be used. In the second approach the desired surface plus volume strength, VIM + VIVOL, is read in columns (11→20), and the fraction of this total strength that is volume absorption is read in columns (71→80), i.e., VOLRAT = VIVOL/(VIM+VIVOL). In this approach VIVOL in column (61→70) is left blank.

When KIM = 3 the surface absorption has the gaussian form and its strength, together with that of the Saxon-Woods volume absorption is communicated to the calculation using either of the above two methods. The procedure is similar for KIM = 5 except that the surface component has the derivative-Saxon-Woods form. However, if VIVOL is positive and KIM = 4 the same result will be obtained as with KIM = 5, and similarly for KIM = 2 and 3. When r2 and A2 are left blank the program assumes R2 = R1 and A2 = A1, i.e., that $r_w = r_v$ and $a_w = a_v$. If the imaginary record is omitted the default parameters defined above are used. The imaginary image is similar to that of

ABAREX.

III.3. SPIN-ORBIT POTENTIAL

```
1234567890123456789012345678901234567890123456789012345678901234567890...
SO     KSO   VSR       VSI       RR1       AA1       VECR      VECI
```

The keyword 'SO' tells the program that the parameters for the spin-orbit potential and the vector potentials are to follow. KSO, read in columns (8→10), sets the form of the spin-orbit reaction. When KSO = 1 the Thomas form give by

$$V_{so}(r) = (2\underline{L}\cdot\underline{S})V_{so}(2/r)\{d/dr(1/(1+\exp((r-R_{so})/a_{so})))\} \qquad (7)$$

is used, where $\underline{L}$ and $\underline{S}$ are the orbital and spin angular momentum operators, respectively. The spin-orbit potential can take the form V_{so} = VSR +i·VSI where the real (VSR) and imaginary (VSI) strengths are read in columns (11→20) and (21→30), respectively. It has been suggested that the imaginary component of the spin-orbit potential is only a reflection of the neglect of the dispersion effects in most interpretations [Hon+86]. The spin-orbit reduced radius, RR1, and diffuseness, AA1 then follow in columns (31→40) and (41→50). There is no provision for the energy dependence of the spin-orbit potential.

If KSO = 2 the spin-orbit potential takes the Saxon-Woods shape given by

$$V_{so}(r) = -2\underline{L}\cdot\underline{S}(VSR + I\cdot VSI)\{1/[1 + \exp((r-R_{so})/a_{so})]\}, \qquad (8)$$

The parameters are read in the same way as for the KSO = 1 case. This form of the spin-orbit interaction is seldom used.

As discussed above, if the spin-orbit potential is real, $r_{so} = r_v$ (RR1 = R1) and $a_{so} = a_v$ (AA1 = A1), VSR = V_{so} can be entered in columns (61→70) of the REAL image and the 'SO' image omitted. In this case KSO will be equal to 1. If the 'SO' image is omitted and there is no VSO strength on the 'REAL' image the default spin-orbit potential will be used. If the user wishes to make a calculation with zero spin-orbit strength a very small VSR should be used; e.g., $\approx$ 1.0E-6 MeV.

As a convenience, the isovector potentials of Eq. 2 are also read in with the 'SO' keyword. The real vector potential, VECR, is given in columns (51→60) and the imaginary vector potential, VECI, in columns (61→70). The default values for both are zero. There must be a 'SO' input image for non-zero isovector potentials. The 'SO' image is identical to that of ABAREX except for the addition of the real and imaginary isovector terms.

III.4 SURFACE REAL POTENTIAL

```
1234567890123456789012345678901234567890.......
DISP         SURF0     SURF1     SURF2
```

The keyword 'DISP' tells the program that a surface-peaked potential, proportional to the imaginary interaction, is to be added to the real Saxon-Woods potential. The magnitude of this added potential is

$$V_{ADD}(r) = V_{add}\cdot W(r), \tag{9}$$

where W(r) can take either the gaussian or derivative-Saxon-Woods surface form.

$$V_{add} = SURF0 + SURF1\cdot E + SURF2\cdot E^2, \tag{10}$$

where SURF0, SURF1 and SURF2 are from the DISP input image. Again, "E" is the center-of-mass system. The default values of SURF0, SURF1 and SURF2 are all zero. The 'DISP' image is generally used to include the contribution from the dispersion integral as described in ref. [LGS87]. The 'DISP' image is identical to that of ABAREX except that here it deals only with the isoscaler terms in the potential.

III.5. TARGET LEVEL INFORMATION

```
1234567890123456789012345678901234567890123456789012345678901234567890
LEVELS NLE  ZTARGET   ECONT     ESTEP     TAU       EOT       SG
                                                            1234567890
                                                              ABUND
```

The keyword 'LEVELS' indicates that the information on target levels and isotopic abundance is to be provided. NLE in columns (8→10) gives the number of target levels that are to be included in the calculation. In ELEMENTAL ABAREX NLE must be one or larger, to a maximum of 50 levels. ZTARGET (columns (11→20)) is the target charge. If this is omitted (or = 0) no target continuum will be considered. ECONT is the excitation energy at which the target continuum starts. The default value is ECONT = EX(NLE), i.e., the energy of the last discrete level. ECONT should not be less than EX(NLE). When ZTARGET > 0 (i.e., when there is a continuum calculation), width fluctuation considerations will be omitted when the energy of the incident neutron is > ECONT. This is a good approximation as many channels will generally be open. On the other hand, when E ≤ ECONT width fluctuations will be taken into account unless a negative number is read in columns (41→50) of the 'COMPUTE' record, as discussed below. ESTEP (columns (31→40)) is the energy interval for target continuum calculations. Generally, the default value of 0.2 MeV is satisfactory. TAU (columns (41→50)) and EOT (columns (51→60)) are the temperature (TAU = T) and energy-shift parameter (EOT = E_o) of the level density formula

$$\rho(E) = (1/T)\{\exp(E-E_o)/T)\}, \qquad (11)$$

which gives the density of states at relatively low energies [GC65]. SG (columns (61→70)) is the spin cut-off factor [GC65]. All the continuum calculations use optical-model transmission coefficients, the little-used black-nucleus option of ABAREX is not available. The final notation on the LEVELS image is the isotopic abundance, ABUND in columns (71→80), in percentage. It is mandatory. The ABUND of the various isotopes of the input should add up to the elemental 100% or there will be a distortion of the elemental output of the calculation. There is no place for the level-density parameter, α, of the expression [GC65]

$$\rho_2(U) = [\exp(2\sqrt{\alpha U})]/(12\sqrt{2}\cdot\sigma\cdot\alpha^{1/4}U^{5/4}). \qquad (12)$$

If one wishes to specifically define the value of α the 'CAPTURE' image, discussed below, must be included in the input file and the value α = SA is read in columns (61→70) of that image. Otherwise, the default value calculated from [GC65]

$$\alpha = (0.00917\cdot S + 0.142)A, \qquad (13)$$

where S is the shell correction given in Table 3 of Gilbert and Cameron [GC65]. The default values of the spin cut-off parameter, SG = σ, The temperature, TAU = T, and the energy-shift parameter, EOT = E_o, are calculated from

$$\sigma^2 = 0.0888\cdot(\alpha U_x)^{1/2}A^{2/3}, \qquad (14)$$

$$1/T = (\alpha/U_x)^{1/2}-1.5/U_x \qquad (15)$$

and

$$E_o = E_x - T\cdot\ln[T\rho_2(U_x)], \qquad (16)$$

respectively [LS98]. The 'LEVELS' image is the same as for ABAREX, with the addition of the abundance.

The 'LEVELS' image must be followed by NLE records defining the ground state and the excited states, in order of excitation energy. The format of these 'LEVEL' records is (F9.4,F4.1,I2,2I5,3F10.5). The meaning of these various entries is as follows.

EX(I) (columns (1→9)) is the excitation energy of the Ith state in MeV. The excitation energy of the ground state is, of course, zero.

FI(I) (columns (10→13)) is the spin of the Ith target state. The default value is 0.

IPI(I) (columns (14→15)) is the parity, +1 or -1, of the Ith target state. The default value is +1.

KGP(I) (columns (16→20)) is the group number of the I^{th} state. The default value of KGP(I) is I. Cross sections with the same group number are added together and considered as due to single state as far as search and print options are concerned. If KGP(1) is negative only the shape-elastic cross sections are computed and/or fitted. In that case the continuum parameters should be removed from the 'LEVELS' image.

ISORT(I) (columns (21→25)) controls the fitting of inelastically scattered groups. ISORT(I) must be less than or equal to four as only the fitting of a maximum of four inelastically-scattered groups is permitted (in contrast to ABAREX where seven groups are allowed). ISORT(1) ≡ 0, the elastically-scattered neutron group is always fitted. ISORT(I) for I from 2 to NLE may be 0 to 4 depending upon which observed inelastic cross section the the I^{th} excitation of the particular isotope is attributed. ISORT(I) = 0 for I greater than 1 indicates that the I^{th} isotopic excitation is not attributed to any observed inelastically-scattered group. One can combine inelastic excitations so as to attribute more than one level to an observed inelastic group. For example, ISORT(2), ISORT(3) and ISORT(4) = 1 means that inelastic excitations of the first, second and third excited levels of the particular isotope are cumulatively combined to compare with the first observed inelastic group. Such combinations are necessary when dealing with a number of elements and the realities of experimental resolution functions. The use of ISORT will be clarified and illustrated in the examples cited in Section IV, below.

GW(I) (columns 26→35)) is the weight of the I^{th} level in fitting. The default value is unity. In some cases experimental considerations may warrant other than unit weighting to various excitation energies.

ZTT (columns (36→45)), of the ground-state (i.e., I = 1) line only, is the target charge of that particular isotope.

AANO (columns (46→55)), of the ground state (i.e., I = 1) line only, is the target mass in AMU of that particular isotope.

All of the above TARGET LEVEL INFORMATION must be repeated for each of the isotopes of the element under consideration. This total level information can be in several sequential sets or scattered through the input to the problem as long as each 'LEVEL' image is directly followed by the respective NLE level specifications. Examples are given in Section IV illustrating the use of this level information.

III.6. FITTING EXPERIMENTAL DATA

```
123456789012345678901234567890123456789012345678901234567890
SEARCH NOA   E        SGTOT     GWTOT     PRINT     TOL
                                        12345678901234567890
                                        KQ(I).........KQ(20)
```

The keyword 'SEARCH' indicates that optical-model parameters are going to be fitted to experimental data. The Format of this image is (A7,I3,5F10.4,20I1).

The meaning of the entries is as follows:-

NOA is the number of input angles for which differential neutron-scattering data are provided. If NOA = 0 only the total cross section is fitted. The maximum number of NOA depends on the mixture of elastic and inelastic groups, but several hundred is a reasonable working limit, and far larger than the usual experimental data set.

E is the laboratory energy at which the data are given. This energy over-rides the energy given on the 'COMPUTE' image, discussed below.

SGTOT is the experimental total cross section at energy E. When this is blank the total cross section is not fitted.

GWTOT is the weight of the experimental total cross section. The default value is 1.0. That default value weights the total cross section approximately the same as a single differential cross section. Total cross sections are usually far more accurate than differential values and are measured in a quite different manner. Thus, their relative weight in fitting is a matter of judgment. If the total cross section is to have significant impact on the result it must receive a weight considerably larger than unity. The choice of weighting can be a sensitive matter.

PRINT selects what is printed during the fitting. When PRINT = ±1.0 the generated parameters are printed at each step of the search. When PRINT = 0 or is left blank only the final parameter values are printed.

TOL is the relative change in chi-square, defined by

$$\chi^2 = \sum_{i,j} [\{\sigma_{\text{exp}}(i,j) - \sigma_{\text{th}}(i,j)\}/\Delta\sigma(i,j)]^2, \qquad (17)$$

which terminates the search procedures. The default value, TOL = 0.005, is suggested for scattering and total cross-section searches.

KQ(I), for I = 1→16, is either "1" or "0" depending on whether or not the I^{th} optical-model parameter is to be varied. The order of the sixteen parameters that can be varied is VRE, VRE1, VRE2, R1, A1, VIM, VIM1, VIM2, R2, A2, VIVOL, VOLRAT, VSR, VSI, RR1, and AA1. The first 16 KQ values must be either "0" or "1", blanks in the string are <u>not</u> acceptable. The entry in column 80, KQ(20), must be either "0" (or blank) or "5" depending upon whether statistical or experimental errors are to be used in the fitting. In the former case, $\Delta\sigma(i,j)$ is given by

$$\Delta\sigma(i,j) \text{ is proportional to } (\sigma_{\text{exp}}(i,j))^{1/2}, \qquad (18)$$

and in the latter instance by

$$\Delta\sigma(i,j) = \sigma_{\text{exp}}(i,j)\ \text{ERR}(i,j)/100, \qquad (19)$$

where ERR(i,j) is the percentage error in the $(i,j)^{\text{th}}$ differential cross section.

If NOA is not zero, the SEARCH image must be followed by NOA scattering cross sections in the Format (6F10.4).

```
123456789012345678901234567890123456789012345678901234567890
  A(I)    XIN(I,1)  XIN(I,2)  XIN(I,3)  XIN(I,4)  XIN(I,5)
```

where A(I) is the I^{th} laboratory angle in degrees and XIN(I,J) are the differential cross sections for scattering to the J^{th} excited level at the I^{th} angle. The order is elastic-scattering followed by inelastic groups. Only a maximum of four inelastic neutron groups can be fitted and only positive non-zero cross sections are considered. It is recommended that they be presented in order of increasing excitation energy though the order can be changed by the appropriate use of the ISORT index of the 'LEVELS' cards.

If a "5" is inserted in column 80 of the 'SEARCH' image the above NOA angle and cross section records must be followed by the corresponding percentage differential cross-section uncertainties in the format (10X,5F10.4) having the form

```
123456789012345678901234567890123456789012345678901234567890
            ERR(I,1)  ERR(I,2)  ERR(I,3)  ERR(I,4)  ERR(I,5)
```

where ERR(I,J) is the percentage error for scattering to the J^{th} level at the angle A(I).

Data taken at several different neutron energies can be fitted simultaneously, and total- and differential-cross-section values can be intermixed, as illustrated by examples in Section IV. However, if more than one energy is involved and/or 'SEARCH' images with NOA = 0 (i.e., total cross sections only) are present, the final output will not contain the "elemental" cross sections. They can be calculated from the isotopic components which are given on the output but there are ambiguities in the options the user may wish (e.g., are values desired at all SEARCH energies, at those with input differential distributions, etc.). The inclusion of all these possible options can lead to some very extensive outputs and therefore they are not routinely given. A separate 'SEARCH' image and input data set must be provided at each search energy. However, PRINT, TOL and KQ(I) need be specified only once.

ELEMENTAL ABAREX does not offer the option of searching on either the capture cross sections or the strength functions and R^{∞} values (as does ABAREX). Of course, there must be at least as many experimental values in a search mode as parameters to be varied, preferably several times as many. 'SEARCH' and 'SCAN' options can not be used simultaneously.

III.7. CALCULATIONS AT SEVERAL ENERGIES

```
1234567890123456789012345678901234567890123456789012345678901234567890
SCAN        E1        E2        E3        E4        E5        E6
                                                            1234567890
                                                              E7
```

The 'SCAN' image indicates that optical-model calculations are to be carried out at several energies; E1, E2, E3, E4, E5, E6 and E7. A number of SCAN images may be used for a total of 50 or less energies, but 'SCAN' must start each line. The E(I) of the 'SCAN' line overrides the energy given in 'COMPUTE' image discussed below. All energies in the 'SCAN' image must be non-zero until the list is complete. If a "1" is inserted in column 10 of the SCAN image the program interprets E1 as the first energy for which calculations are to be made, E2 = dE as the energy step size, and E3 as the final energy of the sweep. The program then computes the cross sections for energies E1, E1+dE, E1+2dE,.......E1+NdE ≤ E3, with N ≤ (E3-E1)/dE or 50, whichever is smaller.

A 'SCAN' image can lead to a large number of calculations (e.g., the number of isotopes times the number of energies) with correspondingly large elemental cross section outputs. Therefore, elemental cross sections are not calculated when using the 'SCAN' image. They can be derived as desired from the isotopic components which are given.

III.8. RADIATIVE CAPTURE

```
1234567890123456789012345678901234567890123456789012345678901234567890
CAPTURE NZ   TGO       BN        FNUG      EGD       GGD       SA
                                                            1234567890
                                                               SG
```

The 'CAPTURE' image implements the calculation of total gamma-ray production and radiative capture cross sections. The input parameters are as follows:-

NZ is the compound-nucleus charge. If NZ is left blank all further entries on this record are ignored and the gamma-ray transmission coefficients must be read into the program as outlined below.

TGO is the average radiation width-to-spacing ratio for s-wave neutrons near the neutron binding energy. This value should be specific to each isotope but the program uses the approximation of the average elemental value. Values of this quantity can often be constructed from ref. [MDH81]. When TGO is > 0 the transmission coefficients for second-chance neutrons (those emitted after a gamma-decay) are calculated using the Black Nucleus Model, while if TGO < 0 the transmission coefficients are calculated using the optical model. If TGO is left blank the E1 giant dipole gamma-ray strength normalization is computed internally [LS98]. That result should be used with caution.

BN is the neutron binding energy. Values for this quantity can be obtained from ref. [WAH88]. The default value is 8 MeV.

FNUG is the width fluctuation degrees of freedom for the gamma-ray channel.

The default value of 20 is usually used.

EGD is the E1 giant dipole energy. Experimental values of this quantity can often be obtained from ref. [BF75]. When this entry is left blank the EGD is calculated from

$$EGD = \{163\cdot((A + 1 - NZ)NZ)^{1/2}\}/(A + 1)^{4/3}, \qquad (20)$$

where A is the target mass in AMU and NZ the charge.

GGD is the E1 giant dipole width which can often be obtained from ref. [BF75]. The default value is 5 MeV.

SA = α is the level density parameter. Experimental values of this quantity can often be found in Table 4 or 5 of ref. [GC65]. When this entry is left blank SA = α is calculated from

$$\alpha = (0.009175\cdot S + 0.142)A, \qquad (21)$$

where S is the shell correction of Table 3 of ref. [GC65].

SG = σ is the spin cut-off parameter. Experimental values of the quantity sometimes can be found in Table 4 or 5 of ref. [GC65]. When this entry is left blank, SG = σ is calculated using

$$\sigma^2 = 0.0888\ (\alpha U_x)^{1/2}A^{2/3}, \qquad (22)$$

where $U_x = 2.5 + 150/A$.

If the keyword 'CAPTURE' is changed to 'N-GAMMA' only the (n,γ) cross section will be calculated and the capture cross section will be omitted.

When NZ of the 'CAPTURE' (or 'N-GAMMA') image is left blank the record must be followed by an image with the Format(16F5.3),

```
12345678901234567890123456789012345678901234567890.........
TG(1)TG(2)TG(3)...........
```

where TG(K) is the gamma-ray transmission coefficient for the Kth total angular momentum and either parity. Ancillary considerations must be used to provide these coefficients. The user is cautioned that, while the present code treats the TG(I) correctly, the physical results will depend upon how the TG(K) are generated.

Again, the user is cautioned that the 'CAPTURE' and 'N-GAMMA' calculations are based upon average elemental input parameters. The code will calculate the respective capture cross sections for each isotope based upon these average parameters. It will not accept different parameters for different isotopes. In some cases this can lead to significant capture errors, but generally the capture cross sections are small and will have a minor effect on other aspects of the calculations (e.g., on total cross sections). ELEMENTAL ABAREX can be run on a mono-isotopic-element basis. In that mode the particular isotopic capture cross sections can be calculated with the same results as obtained with the isotopic ABAREX.

III.9. PRINTING

```
1234567890123456789012345678 90.........
TRANSM KET
```

The TRANSM image must be included if one wants to print the reflection factors, η_{jl}, the transmission coefficients, $T_{j,l}$, the s- and p-wave strength functions, and/or the potential scattering radius, R′. The KET entry in columns (8→10) tells the program that these quantities are to be printed for the first KET target states. If columns (8→10) are left blank, KET is set equal to NLE, the number of discrete levels in the calculation. The TRANSM printout is inactive when the 'SEARCH' is operational.

III.10. STARTING THE CALCULATION

```
1234567890123456789012345678901234567890123456789012345678901234567890
COMPUTE LM    E      ANO       ANU       FNU       DANG      C1
                                                             1234567890
                                                               PTS
```

The 'COMPUTE' image signals the end of the input data for a given case and starts the calculation for that case. The input quantities are:-

LM specifies the maximum neutron orbital angular momentum. The default value of zero (or a blank) should ordinarily be used, and in this case LM is determined internally for each level with a maximum value of LM = 20. An input LM will be truncated to a maximum of the internally-calculated value.

E is the laboratory energy of the incident neutron in MeV. When using the 'SCAN' or 'SEARCH' options this value is supplanted by that of the 'SCAN' or 'SEARCH' image. The default value is 0.8 MeV.

ANO = A is the mass number of the elemental target. The mass numbers of the various isotopes are given on the respective 'LEVEL' specifications, as cited above. The default value is 55.9349 AMU.

ANU is the projectile mass number. The default value is the neutron mass, 1.008665 AMU. This program does not treat incident charged particles.

FNU is the neutron width fluctuation degrees of freedom. When a zero or blank is used here the program computes FNU internally using the Moldauer formalism [Mol80]. When the incident energy E exceeds that of the start of the continuum (ECONT) no width fluctuation corrections are considered and the Hauser-Feshbach theory is used as many channels are open and the fluctuation corrections are generally not significant. When this entry is negative, the simple Hauser-Feshbach theory is used with no fluctuation corrections. When the entry is positive ν will be calculated using the $F_\nu(x)$ distribution of Eq.

75 of ref. [LS98].

DANG is the angular interval in the printout of the differential cross sections. The default value is 15^{o}. In the 'SEARCH' mode the angles of the experimental data are used.

C1 is the asymptotic matching radius. The default value of 15 fms is generally satisfactory.

PTS is the number of radial integration points. The default value is 301.0. However, if the potential is a rapidly varying function of r a better value is 601.0. PTS should be an odd number.

III.11. CHANGING PARAMETERS

```
123456789012345678901234567890..............
INPUT
```

The 'INPUT' image changes selected input parameters and repeats the calculation. This instruction follows the IBM NAMELIST procedure and may not be available on all Fortran compilers. The quantities that can be changed are:-

NLEVEL, FNU, DANG, LMAX, Z, ANO, EX, FI, IPI, KGP, VRE, VRE1, VRE2, R1, A1, KIM, VIM, VIM1, VIM2, R2, A2, VIVOL, C2, KETA, KSO, VSR, VSI, RR1, AA1, TGO, BN, FNUG, EGD, GGD, SG, NZ, TGG, TFF, FNF, SURFO, SURF1, SURF2, and KSCH,

where C2 = VOLRAT, NLEVEL = NLE, IPI = IP, TGG = TG, KETA = KET and LMAX = LM. The register Z(1) contains the incident neutron energy. KSCH is a keyword set internally by the program, where KSCH = 1 or 0 depending upon whether or not a search is made. The meanings of the other quantities follow from the above discussion. When using the 'INPUT' option the prior input is only modified, thus the input is not repeated in the output listing.

An example of the use of the 'INPUT' option is given in Section IV. The parameters to be changed are followed by ',&END' in VAX/VMS and Lahey Fortran. In Microsoft Fortran this may be replaced by '/'.

III.12. FISSION

```
123456789012345678901234567890.............
FISSION NF
```

The 'FISSION' image calculates the compound-nucleus fission cross section, where NF is the number of total angular momenta in the fission transmission coefficients. This image must be directly followed by lines in the format (16F5.3) as follows:-

```
     5      10      15      20      25      30      35      40...
TF+(1) FN+(1) TF-(1) FN-(1) TF+(2) FN+(2) TF-(2) FN-(2)...
                                                        NF*20
                            TF+(NF) FN+(NF) TF-(NF) FN-(NF),
```

where TF+(I) and TF-(I) are the positive- and negative-parity total fission transmission coefficients of the I^{th} total angular momentum, respectively, and FN+(I) and FN-(I) are the corresponding width-fluctuation degrees of freedom. These fission properties must be obtained from ancillary considerations, and the results will depend on such considerations. Given a reasonable input, the present program yields rational fission cross sections. However, the user is cautioned that the results will be no better than the input parameters. The user is also cautioned that the fission input, like the capture input, is an average elemental input. This a very crude approximation in most cases as the fission process is very isotope dependent and will not be reasonable represented by an elemental average value. For example, in elemental uranium the fission cross sections of ^{235}U and ^{238}U are very different and can not be reasonably represented by a set of elemental average transmission coefficients. The option is retained in ELEMENTAL ABAREX as it is appropriate when dealing with a mono-isotopic element, and it can be used to account for other reaction cross sections in a mono-isotopic context (e.g., charged-particle emission effects).

IV. ILLUSTRATIVE EXAMPLES

ELEMENTAL ABAREX can be used in many ways. This capability makes it a very powerful program but also leads to multitude of input options. Some of these have been outlined in the above remarks and in ref [LS98]. However, the initial user may be somewhat confused. Therefore this document gives a large number of examples illustrating many of the possible options. Further guidance can be obtained from ref. [LS98]. In the following remarks there are a number of narrative discussions of examples, and the input and output of a simpler case is listed in Appendix A. Many of the examples involve extensive output the size of which transcends a reasonable printed report.

Example.1

This is a very simple case calculating the neutron interaction with a mock element consisting of two identical isotopes, each with 50% abundance. The isotopes are actually ^{92}Mo taken from a recent study of the neutron interaction with that isotope [Smi99]. The real potential has the Saxon-Woods shape, the imaginary potential the derivative-Saxon-Woods shape and the spin-orbit potential the Thomas form. There is no imaginary volume potential and the real and imaginary isovector potentials are ≡ zero. Each of the two isotopes has 15 discrete levels and a continuum distribution (in this test case they are identical). This calculation should give the same results as a simple isotopic calculation and therefore is a test of the code. The respective input and output are shown in the listing of Appendix A, and the elemental values agree very well with those obtained with a simple "isotopic" calculation using ABAREX. The last portion of the output listing gives the "elemental" cross sections. This is limited to total, absorption, shape-elastic, total elastic, compound elastic, continuum levels and total compound cross sections. There follow the calculated differential cross sections at 6-deg. angular intervals. These differential values are in the laboratory coordinate system. There is no 'continuum levels' cross section as the energy of the calculation is below the continuum threshold. In this example the differential cross sections are limited to shape-elastic, compound-elastic and total elastic cross sections. The ISORT option was not used in this simple case, but it is illustrated below. The individual inelastic cross sections (angle integrated and differential) are given for each isotope but in this case the input does not define how they are combined in the element so they are ignored in the 'elemental' output.

As this is the first example it is, perhaps, desirable to discuss the details of the output. The output initially reproduces the input parameterization. and then restates the potential parameters. In this particular case there is a real Saxon-woods potential, a derivative-Saxon-Woods imaginary potential. The spin-orbit potential is of the Thomas form. Note that the 'S.O.' line gives the real spin-orbit depth, the imaginary spin-orbit depth (zero), and the spin-orbit radius and diffuseness. The spin-orbit potential does not have an energy dependence. There is no real surface term to the potential ('DISP' = 0) and both real and imaginary vector potentials are zero. The output gives real- and imaginary-potential volume integrals (VOLINT). It should be clearly understood that these integrals refer to the total value of the respective potentials and not V_o or W_o. Furthermore, this initial potential summary of all outputs calculates the volume integrals using the average mass given on the 'COMPUTE' image. Subsequent volume integrals may use isotopic mass values as illustrated below, otherwise it is set to zero. The imaginary volume integral is given only for the derivative-Saxon-Woods form factor. Fluctuation degrees of freedom are computed internally. There follows a calculation for each of the constituent isotopes, in this case with identical results. Three scattering channels are energetically available in each case, leading to the angle-integrated and differential cross sections. The latter consist of shape-elastic, compound elastic, total elastic and two inelastic scattering groups. The calculations involve L-values of ≤ 7 and J-values in the range 0.5→7.5. Finally, the angle-integrated and differential elemental cross section values are presented. The former include total, absorption, shape-elastic, total-elastic, compound-elastic, continuum (in this case zero due the low energies) and the total compound cross sections. In this example, the differential cross sections are the shape-elastic, compound-elastic and total elastic cross sections, in that order.

Example.1A

This calculation is identical to that of Example.1 except that the real and imaginary isovector strengths are set to 24 and 12 MeV, respectively, and these values are clearly noted on the output. They are commonly used values [Hod94]. In evaluating the results one must remember that the potential is given by $V = V_o - V_1 \cdot \eta$ (or $W = W_o - W_1 \cdot \eta$) where η is the nuclear asymmetry, as discussed above, while the volume integrals refer to the full potential V (or W). When this is done the results of Example.1A are in very good agreement with the corresponding simple isotopic calculation.

Example.1B

This calculation is simply Example.1 extended to include the TRANSM printout of ETA, transmission coefficients, Γ^2/D, R^∞, strength functions, and R'. This printout is given for each isotope but not for the elemental results as it is not clear what strength functions of an element mean. In any case, the user can construct the values he or she desires from the isotopic components. The format of the output is essentially self-evident. In addition to the output of Example.1, the format contains a section for each isotope giving ETA and transmission coefficients for all of the L-values and Γ^2/D, R^∞, strength functions and R' for L = 0 and = 1. The P-wave strength function is the sum of the two L = 1 J-components. All the strength functions are referenced to the commonly used 1 eV energy. It is recommended that strength-function calculations be made at low energies; for example at 1 keV as in this example.

Example.1C

This example is, again, Example.1 with the addition of the 'CAPTURE' image. In this case the default capture option was chosen and the capture parameters are calculated internally. As a consequence the EGD value is isotope dependent as give by Eq. 20. The results agree very well with the equivalent simple isotopic calculation. One could use as an alternative the full parameterization of the 'CAPTURE' image. In that case the parameters should be averages of those of the contributing isotopes as there is only one input for all the isotopes. This is an approximation that is generally suitable in most applications since the capture contributions to the reaction are relatively small. However, if the user wishes to deal in detail with the capture process in each isotope, separate isotopic calculations are warranted. The output format is that of Example.1 with the addition of a small section setting forth the parameters of the capture calculation for each isotope and the inclusion of N-GAMMA and RADIATIVE CAPTURE cross sections in the summaries of both isotopic and elemental results.

Example.1D

This example is the same as Example.1B, only with the addition of a 'SCAN' imag consisting of only two energies. The results are identical, with the addition of another energy at 2.3 MeV. This example also illustrates the omission of the final "elemental" tabulation of the output when using either 'SCAN' or 'SEARCH' images (the two can not be used together). This is a matter of expediency as, otherwise, the outputs could become very large. Most 'SCAN' images will include a number of energies, up to a maximum of 50, and for several isotopes.

Example.1E

This example is also an extension of Example.1. ISORT is used to identify the isotopic components contributing to three elemental inelastically-scattered neutron groups consisting of 1.509, 2.283 and 2.520+2.527 MeV isotopic excitations. The results agree very well with those obtained with a simple isotopic calculation using the level structure in an identical manner. In more realistic cases, the elemental inelastic groups can become quite complex, each consisting of a variable assortment of contributions from a number of isotopes.

Example.1F

This example is the same as EXAMPLE.1 except that the energy has been raised to 5 MeV, well above the last discrete excitation energy, thus the continuum excitations are important, amounting to 1.46241 b. In this example the onset of the continuum is the the largest discrete excitation energy (3.621 MeV) and the energy step used in the continuum calculations is 0.2 MeV.

Example.1G

This case is a repeat of Example.1 except that each of the isotopic calculations is confined to shape-elastic processes. When using the shape-elastic input it is suggested that the continuum parameters be removed from the 'LEVELS' image in order to avoid continuum compound-nucleus contributions. Shape-elastic and discrete-level calculations can be intermixed from isotope to isotope in an elemental calculation.

Example.1H

This example is the same as Example.1 with the addition of the 'INPUT' option arranged to repeat the calculation with a change of energy to 5.0 MeV and the real potential to 46.0 MeV. Similar changes can be easily made for any of the variables in the NAMELIST cited above.

Example.2

Example 1 can be easily extended to include the derivation of two parameter values through fitting of total and/or differential scattering cross sections. The case of one elastic distribution, one inelastic distribution (excitation = 1.509 MeV) and a total cross section (with unit weighting) at a single energy for both mock isotopes is given in EXAMPLE.2. Fifteen discrete levels are used for both of two mock isotopes and the isovector potentials are set to zero. The fitting searches, using the normalized least-square methods of Eqs. 17 and 19, for the best values of the real and imaginary potential strengths. With this method, experimental percentage errors are given for all of the experimental quantities being fitted. The convergence criteria is the default value of 0.005. The search converged after 50 calls and the isotopic and elemental cross sections derived. These are essentially identical to the values obtained with a simple isotopic calculation. It should be noted that the output, like those above, initially gives a summary of the input parameters with the associated volume integrals calculated using the mean elemental mass, as above. In addition, after the fitting has finished, a potential summary is given for each of the contributing isotopes. In the latter cases the volume integrals are calculated for the mass of that particular isotope.

Example.2A

This example is a repeat of Example.2 except that the fitting algorithm of Eqs. 17 and 18 is used. This amounts to a different specification of the uncertainties associated with the differential experimental values. The results of this chi-square fitting are significantly different from those given in Example.2. This illustrates the sensitivity of fitting to the uncertainties associated with the experimental data. Unfortunately, experimentalists tend to have widely different concepts of the uncertainties of their experimental results, thus fitting can be as much an "art" as a "science".

Example.3

This example is a real case interpreting elastic scattering from elemental molybdenum at 2.4 MeV [Smi99]. All seven isotopes of the element are considered. There are dispersion effects that result in a surface component of the real potential, and real and imaginary isovector potentials are used. There is one experimental elastic-scattering distribution with experimental errors. The least-square fitting of the elastic distribution involves the adjustment of two parameters, the real and the imaginary isoscaler potentials. After 91 calls there was reasonable convergence to a 'final' parameter set. That potential was then used to calculated the contributions for each of the contributing isotopes which were combined to obtain the final elemental values (remember the interpretation of the volume integrals as cited in Example.2). The internal consistency of the results is very good, and the elemental values are in remarkable agreement with those obtained from a simple calculation using the mean elemental mass of 95.94 AMU and the excited levels of one of prominent even isotopes.

Example.4

This example uses the mock two-isotope element of EXAMPLE.1 and searches ten experimental total cross sections to determine the optimum value of the real and imaginary potentials. Isovector potentials are zero and weighting factors of 3 are used for each total cross section in the least-square fitting. There are no experimental differential distributions in the input. The resulting optical-model parameters are in excellent agreement with those obtained treating only one of the isotopes. The output does not include 'elemental' cross section values. Generally, any time a search extends to more than one energy, 'elemental' values are not given in the output. To do so would lead to very large outputs in most cases. The user can construct 'elemental' values from the isotopic components provided for those energies and/or reactions he or she is interested in.

Example.5

This example is the same as EXAMPLE.4 but with the addition of a pair of differential (elastic and inelastic) distributions and another total cross section at 2.4 MeV. At 2.4 MeV the total cross section weight is only unity. Thus, at this energy, the differential contributions to the fit will be dominant. This example demonstrates the capability to mix total and differential data at a number of energies in experimental fitting. The resulting optical potential is very similar to that obtained fitting on a simple isotopic basis. Again, for conciseness, the 'elemental' output is omitted. The user can obtain it from the isotopic components provided, as desired.

ACKNOWLEDGEMENTS

The author very much acknowledges the work of Dr. S. Chiba. Nearly a decade ago he made the initial extension of ABAREX to what was the basis of the present ELEMENTAL ABAREX. This initial work was invaluable. Drs. R. Lawson and J. Raynal offered a number of corrections and modifications over many years. Finally, the work of P. Moldauer in the formulation of the underlying ABAREX is the essential foundation of the ABAREX code and its derivatives.

REFERENCES

[Aue64] E. Auerbach, Private communication (1964).
[Ber96] J. Bersillon, CEA Report CEA-N-2227 (1981), and revisions from the NEA Data Bank (1996).
[BF75] B. Berman and S. Fultz, Rev. Mod. Phys. 47 713 (1975).
[FPW54] H. Feshbach, C. Porter and V. Wiesskopf, Phys. Rev. 96 448 (1954).
[Gar68] B. Garbow et. al., Argonne National Laboratory Report, ANL-80 (1968).
[GC65] A. Gilbert and A. Cameron, Can. J. Phys. 43 1446 (1965).
[HF52] W. Hauser and H. Feshbach, Phys. Rev. 87 366 (1952).
[Hod63] P. E. Hodgson, The optical model of elastic scattering (Clarendon, Oxford,1963).
[Hod94] P. E. Hodgson, The nucleon optical model (World Sci. Pub., London, 1994).
[Hon+86] G. M. Honore et al., Phys. Rev. C33 1129 (1986).
[IBM] International Business Machines Corp.
[Lah] Lahey Systems Inc., Incline Village, NV.
[Lan62] A. M. Lane, Nucl. Phys. 35 676 (1962).
[LGS87] R. Lawson, P. Guenther and A. Smith, Phys. Rev. C36 1298 (1987).
[LS98] R. Lawson and A. Smith, Argonne National Laboratory Report ANL/NDM-145 (1998).
[Mic] Microsoft Corp., Beaverton, OR.

[Mol80] P. Moldauer, Nucl. Phys. A344 185 (1980).
[MP78] M. MacFarlane and S. Pieper, Argonne National Laboratory Report ANL-76-11 (Rev. 1) (1978).
[MDH81] S. Mughabghab, M. Divadeenam and N. Holden, Neutron cross sections (Academic, New York, 1981)
[Pie88] S. Pieper, private communication (1988).
[Ray96] J.Raynal, CEA Report CEA-N-2772 (1994) and private communications.
[Smi99] A. Smith, The neutron interaction with the isotopes of molybdenum, to be published (1999).
[Tam67] T. Tamura, Oak Ridge National Laboratory Report ORNL-4152 (1967)
[VAX] Digital Equipment Corp., Maynard, MA.
[WAH88] A. Wapstra, G. Audi and R. Hoekstra, At. Data Nucl. Data Tables 39 281 (1988).
[Wol51] L. Wolfenstein, Phys. Rev. 82 690 (1951).

APPENDIX A

An illustrative example is listed in this appendix. The comprehensive set of examples is provided on the attached diskette together with the FORTRAN source. The comprehensive set of examples and the source listing are far too lengthy for listing in printed copies.

EXAMPLE.1

INPUT

```
12345678901234567890123456789012345678901234567890123456789012345678901234567890

################################################################################

LEVELS  15   42.                           0.7250    1.01      3.700       50.0
 .0       0.0+1    1    0             42.     92.
1.509     2.0+1    2
2.283     4.0+1    3
2.520     0.0+1    4
2.527     5.0-1    5
2.612     6.0+1    6
2.761     8.0+1    7
2.850     3.0-1    8
3.007     5.0-1    9
3.064     3.0-1   10
3.091     2.0+1   11
3.369     4.0+1   12
3.542     2.0+1   13
3.580     3.0-1   14
3.621     2.0+1   15
LEVELS  15   42.                           0.7250    1.01      3.700       50.0
 .0       0.0+1    1    0             42.     92.
1.509     2.0+1    2
2.283     4.0+1    3
2.520     0.0+1    4
2.527     5.0-1    5
2.612     6.0+1    6
2.761     8.0+1    7
2.850     3.0-1    8
3.007     5.0-1    9
3.064     3.0-1   10
3.091     2.0+1   11
3.369     4.0+1   12
3.542     2.0+1   13
3.580     3.0-1   14
3.621     2.0+1   15
REAL    1 49.23830    0.00000   0.00000   1.20850   0.6281
IMAG    4  9.36310    0.00000   0.00000   1.25020   0.5025
SO      1  5.94090    0.00000   1.10300   0.5600
COMPUTE 0    2.4000   92.0000                        6.0000              601.0
--------------------------------------------------------------------------------
```

```
OUTPUT

********************************************************************************

                          ELEMENTAL-ABAREX
                          ================

         INPUT DECK :

         LEVELS  15   42.0000    0.0000    0.0000    0.7250    1.0100    3.7000   50.0000
            0.0000 0.0 1    1    0    1.0000   42.0000   92.0000
            1.5090 2.0 1    2    0    1.0000
            2.2830 4.0 1    3    0    1.0000
            2.5200 0.0 1    4    0    1.0000
            2.5270 5.0-1    5    0    1.0000
            2.6120 6.0 1    6    0    1.0000
            2.7610 8.0 1    7    0    1.0000
            2.8500 3.0-1    8    0    1.0000
            3.0070 5.0-1    9    0    1.0000
            3.0640 3.0-1   10    0    1.0000
            3.0910 2.0 1   11    0    1.0000
            3.3690 4.0 1   12    0    1.0000
            3.5420 2.0 1   13    0    1.0000
            3.5800 3.0-1   14    0    1.0000
            3.6210 2.0 1   15    0    1.0000
         LEVELS  15   42.0000    0.0000    0.0000    0.7250    1.0100    3.7000   50.0000
            0.0000 0.0 1    1    0    1.0000   42.0000   92.0000
            1.5090 2.0 1    2    0    1.0000
            2.2830 4.0 1    3    0    1.0000
            2.5200 0.0 1    4    0    1.0000
            2.5270 5.0-1    5    0    1.0000
            2.6120 6.0 1    6    0    1.0000
            2.7610 8.0 1    7    0    1.0000
            2.8500 3.0-1    8    0    1.0000
            3.0070 5.0-1    9    0    1.0000
            3.0640 3.0-1   10    0    1.0000
            3.0910 2.0 1   11    0    1.0000
            3.3690 4.0 1   12    0    1.0000
            3.5420 2.0 1   13    0    1.0000
            3.5800 3.0-1   14    0    1.0000
            3.6210 2.0 1   15    0    1.0000
         REAL     1   49.2383    0.0000    0.0000    1.2085    0.6281    0.0000    0.0000
         IMAG     4    9.3631    0.0000    0.0000    1.2502    0.5025    0.0000    0.0000
         SO       1    5.9409    0.0000    1.1030    0.5600    0.0000    0.0000    0.0000
         COMPUTE  0    2.4000   92.0000    0.0000    0.0000    6.0000    0.0000  601.0000


MASS NUMBERS(MEAN-TARGET/PROJECTILE) = 92.000000/ 1.008665
============
```

```
 OPTICAL MODEL PARAMETERS :          ASYMPTOPIA= 15.0000 FM          601 POINTS
 =======================

  TYPE       DEPTH      (E)       (E*E)      RADIUS     DIFF.   VIVOL      C2    VOLINT

 REAL   1   49.2383   0.0000    0.0000    1.2085    0.6281                     411.6484
 IMAG   4    9.3631   0.0000    0.0000    1.2502    0.5025    0.0000    0.0000   84.0150
 S.O.   1    5.9409   0.0000              1.1030    0.5600
 DISP        0.0000   0.0000    0.0000
 VECR=    0.0000          VECI=    0.0000

 NO. 1 ENERGY(LABORATORY/C.M.)  =  2.400000/ 2.373972 MEV         LAMBDA-BAR =  0.29708 SQRT-BARN
 ============
 NEUTRON CHANNEL WIDTH FLUCTUATION DEGREES OF FREEDOM
 ARE COMPUTED INTERNALLY.

  **** ISOTOPE NUMBER=  1       MASS=     92.00



               TARGET LEVELS
               =============


 LEVEL  GROUP   ENERGY   SPIN   PARITY   WEIGHT

     1     1    0.0000    0.0      1        1.00
     2     2    1.5090    2.0      1        1.00
     3     3    2.2830    4.0      1        1.00

  MAXIMUM NEUTRON L VALUE,(RANGE OF TOTAL J VALUES) =  7, (  0.5,   7.5)

    INTEGRATED CROSS SECTIONS IN BARNS
    ==================================     -

                TOTAL =  4.00124
           ABSORPTION =  2.21846
        SHAPE ELASTIC =  1.78278
        TOTAL ELASTIC =  3.00239
 COMPOUND EXCITATIONS =  1.21961  0.92039  0.07843
       TOTAL COMPOUND =  2.21843

 LABORATORY CROSS SECTION IN BARNS PER STERADIAN
 ===============================================

     ANGLE     S.E.       C.E.   LEVEL GROUP CROSS SECTIONS

     0.00   1.25419   0.23175   1.48594   0.07837   0.00596
```

```
    6.00   1.21951   0.22658   1.44610   0.07837   0.00598
   12.00   1.12075   0.21207   1.33282   0.07837   0.00602
   18.00   0.97254   0.19092   1.16345   0.07833   0.00609
   24.00   0.79565   0.16673   0.96238   0.07819   0.00618
   30.00   0.61268   0.14307   0.75575   0.07791   0.00628
   36.00   0.44371   0.12261   0.56632   0.07746   0.00639
   42.00   0.30307   0.10666   0.40973   0.07684   0.00650
   48.00   0.19787   0.09519   0.29305   0.07607   0.00661
   54.00   0.12819   0.08725   0.21544   0.07520   0.00670
   60.00   0.08879   0.08159   0.17038   0.07428   0.00676
   66.00   0.07149   0.07713   0.14861   0.07339   0.00681
   72.00   0.06746   0.07333   0.14079   0.07258   0.00682
   78.00   0.06906   0.07021   0.13926   0.07191   0.00680
   84.00   0.07077   0.06810   0.13887   0.07140   0.00675
   90.00   0.06946   0.06735   0.13682   0.07106   0.00667
   96.00   0.06402   0.06809   0.13211   0.07092   0.00656
  102.00   0.05477   0.07010   0.12487   0.07095   0.00643
  108.00   0.04295   0.07301   0.11596   0.07114   0.00628
  114.00   0.03020   0.07651   0.10671   0.07144   0.00612
  120.00   0.01835   0.08068   0.09903   0.07182   0.00594
  126.00   0.00912   0.08612   0.09524   0.07223   0.00576
  132.00   0.00403   0.09387   0.09790   0.07261   0.00558
  138.00   0.00407   0.10509   0.10915   0.07291   0.00541
  144.00   0.00955   0.12050   0.13005   0.07311   0.00526
  150.00   0.01987   0.13998   0.15984   0.07319   0.00511
  156.00   0.03350   0.16215   0.19565   0.07317   0.00499
  162.00   0.04817   0.18453   0.23270   0.07309   0.00490
  168.00   0.06124   0.20392   0.26515   0.07299   0.00482
  174.00   0.07025   0.21712   0.28737   0.07291   0.00478
  180.00   0.07347   0.22181   0.29528   0.07288   0.00477

NO. 1 ENERGY(LABORATORY/C.M.)  =  2.400000/ 2.373972 MEV           LAMBDA-BAR =  0.29708 SQRT-BARN
============
NEUTRON CHANNEL WIDTH FLUCTUATION DEGREES OF FREEDOM
ARE COMPUTED INTERNALLY.

 **** ISOTOPE NUMBER=  2       MASS=     92.00



               TARGET LEVELS
               =============


LEVEL  GROUP   ENERGY   SPIN   PARITY   WEIGHT

    1     1    0.0000    0.0      1        1.00
    2     2    1.5090    2.0      1        1.00
    3     3    2.2830    4.0      1        1.00

 MAXIMUM NEUTRON L VALUE,(RANGE OF TOTAL J VALUES) =  7, (  0.5,  7.5)
```

```
   INTEGRATED CROSS SECTIONS IN BARNS
   ==================================

               TOTAL =  4.00124
          ABSORPTION =  2.21846
       SHAPE ELASTIC =  1.78278
       TOTAL ELASTIC =  3.00239
COMPOUND EXCITATIONS =  1.21961  0.92039  0.07843
      TOTAL COMPOUND =  2.21843

LABORATORY CROSS SECTION IN BARNS PER STERADIAN
===============================================

   ANGLE     S.E.       C.E.   LEVEL GROUP CROSS SECTIONS

    0.00   1.25419   0.23175   1.48594   0.07837   0.00596
    6.00   1.21951   0.22658   1.44610   0.07837   0.00598
   12.00   1.12075   0.21207   1.33282   0.07837   0.00602
   18.00   0.97254   0.19092   1.16345   0.07833   0.00609
   24.00   0.79565   0.16673   0.96238   0.07819   0.00618
   30.00   0.61268   0.14307   0.75575   0.07791   0.00628
   36.00   0.44371   0.12261   0.56632   0.07746   0.00639
   42.00   0.30307   0.10666   0.40973   0.07684   0.00650
   48.00   0.19787   0.09519   0.29305   0.07607   0.00661
   54.00   0.12819   0.08725   0.21544   0.07520   0.00670
   60.00   0.08879   0.08159   0.17038   0.07428   0.00676
   66.00   0.07149   0.07713   0.14861   0.07339   0.00681
   72.00   0.06746   0.07333   0.14079   0.07258   0.00682
   78.00   0.06906   0.07021   0.13926   0.07191   0.00680
   84.00   0.07077   0.06810   0.13887   0.07140   0.00675
   90.00   0.06946   0.06735   0.13682   0.07106   0.00667
   96.00   0.06402   0.06809   0.13211   0.07092   0.00656
  102.00   0.05477   0.07010   0.12487   0.07095   0.00643
  108.00   0.04295   0.07301   0.11596   0.07114   0.00628
  114.00   0.03020   0.07651   0.10671   0.07144   0.00612
  120.00   0.01835   0.08068   0.09903   0.07182   0.00594
  126.00   0.00912   0.08612   0.09524   0.07223   0.00576
  132.00   0.00403   0.09387   0.09790   0.07261   0.00558
  138.00   0.00407   0.10509   0.10915   0.07291   0.00541
  144.00   0.00955   0.12050   0.13005   0.07311   0.00526
  150.00   0.01987   0.13998   0.15984   0.07319   0.00511
  156.00   0.03350   0.16215   0.19565   0.07317   0.00499
  162.00   0.04817   0.18453   0.23270   0.07309   0.00490
  168.00   0.06124   0.20392   0.26515   0.07299   0.00482
  174.00   0.07025   0.21712   0.28737   0.07291   0.00478
  180.00   0.07347   0.22181   0.29528   0.07288   0.00477

###################################
##                               ##
##    ELEMENTAL CROSS SECTION    ##
##                               ##
###################################
```

```
    INTEGRATED CROSS SECTIONS IN BARNS
  ==================================

               TOTAL =  4.00124
          ABSORPTION =  2.21846
       SHAPE ELASTIC =  1.78278
       TOTAL ELASTIC =  3.00239
    COMPOUND ELASTIC =  1.21961
    CONTINUUM LEVELS =  0.00000
      TOTAL COMPOUND =  2.21843

LABORATORY CROSS SECTION IN BARNS PER STERADIAN
=============================================

    ANGLE     S.E.       C.E.   LEVEL GROUP CROSS SECTIONS

     0.00   1.25419   0.23175   1.48594
     6.00   1.21951   0.22658   1.44610
    12.00   1.12075   0.21207   1.33282
    18.00   0.97254   0.19092   1.16345
    24.00   0.79565   0.16673   0.96238
    30.00   0.61268   0.14307   0.75575
    36.00   0.44371   0.12261   0.56632
    42.00   0.30307   0.10666   0.40973
    48.00   0.19787   0.09519   0.29305
    54.00   0.12819   0.08725   0.21544
    60.00   0.08879   0.08159   0.17038
    66.00   0.07149   0.07713   0.14861
    72.00   0.06746   0.07333   0.14079
    78.00   0.06906   0.07021   0.13926
    84.00   0.07077   0.06810   0.13887
    90.00   0.06946   0.06735   0.13682
    96.00   0.06402   0.06809   0.13211
   102.00   0.05477   0.07010   0.12487
   108.00   0.04295   0.07301   0.11596
   114.00   0.03020   0.07651   0.10671
   120.00   0.01835   0.08068   0.09903
   126.00   0.00912   0.08612   0.09524
   132.00   0.00403   0.09387   0.09790
   138.00   0.00407   0.10509   0.10915
   144.00   0.00955   0.12050   0.13005
   150.00   0.01987   0.13998   0.15984
   156.00   0.03350   0.16215   0.19565
   162.00   0.04817   0.18453   0.23270
   168.00   0.06124   0.20392   0.26515
   174.00   0.07025   0.21712   0.28737
   180.00   0.07347   0.22181   0.29528
---------------------------------------------------------------------------
```

This is an information copy. As such, it does not include the diskette containing the FORTRAN source and the I/O of the examples as cited in the text. If you wish to use this program the diskette can be obtained from:-

The Radiation Safety Information Computational Center
P. O. Box 2008
Oak Ridge, TN 37831-6362

or by contacting the author at:-

The Technology Development Division, D-315
Argonne National Laboratory
9700 South Cass Ave.
Argonne, IL 60439