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STATEFIT: A COMPUTER PROGRAM TO FACILITATE THE INTERPRETATION OF SPECTROSCOPIC DATA

by

S. B. Burson, G. T. Wood, and C. H. Batson

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STATEFIT: A COMPUTER PROGRAM TO FACILITATE THE
INTERPRETATION OF SPECTROSCOPIC DATA

S. B. BURSON,* G. T. WOOD,** and C. H. BATSON

Argonne National Laboratory, Argonne, Illinois 60439

The authors have a limited number
of copies for general distribution.
Anyone who desires a copy should
contact them directly.

*Present address: Office of Research, United States Nuclear Regulatory
Commission, Washington, D. C., 20555

**Present address: Cleveland State University, Cleveland, Ohio

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STATEFIT: A COMPUTER PROGRAM TO FACILITATE THE INTERPRETATION OF SPECTROSCOPIC DATA

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Abstract

STATEFIT is a program written in Fortran IV for the IBM 370/195 computer to facilitate the interpretation of spectroscopic data. A list containing all the experimentally determined γ -ray energies, their relative intensities, the uncertainties in each, and when known, the total internal conversion coefficients is supplied as input. A preliminary partial decay scheme is assumed to already exist, and a second list specifying those γ rays representing transitions between members of this group of energy levels is also provided as input data. Before execution is allowed to proceed, the two lists are subjected to ten different tests to locate possible user errors and if any are found, they are noted. Identification of a fatal error such as the inadvertent assignment of two different gamma rays between one pair of states, causes termination. The energies of the presumed states are not estimated, but are treated as variable parameters. For purposes of the calculation, each state is identified by an arbitrary index number. The best energy values of the states are determined by making a least-squares fit of the level energies to the network of assigned gamma rays. Transition intensities $R_T = R_r (1 + \alpha)$ are calculated, and for radioactive samples the fractional beta feeding to each state is computed. A table of all possible transitions between the calculated states is then computed and listed in

monotonically increasing order. The complete list of experimentally observed gamma rays is then searched for additional acceptable assignments. The acceptance criterion for selection of such possible additional assignments is externally adjustable. Space required for 20 excited states, 50 assigned gamma rays and 100 observed gamma rays is $15C60_{16}(89,184_{10})$ bytes. Space required for 120 excited states, 500 assigned gamma rays and 1200 observed gamma rays is $61A58_{16}(399,960_{10})$ bytes.

1. Introduction

Advances in electronic technology and the widespread application of solid-state radiation detectors with high sensitivity and resolution have stimulated the development of more sophisticated methods of processing and interpreting spectroscopic data. It has become relatively commonplace for experimenters to identify literally hundreds of transitions within a few hundred kilovolts of energy in the gamma-ray spectrum of a single nuclide. The processing and interpretation of such data demands the use of contemporary computer facilities and sound statistical methods.

The development of a consistent nuclear level system from raw spectroscopic data has never been a simple matter; and, although the vastly improved experimental apparatus holds great promise of significant breakthroughs in nuclear theory, the problem of data analysis has been correspondingly augmented.

The construction of a decay scheme is usually approached by first considering those transitions with the greatest intensity and highest energy precision to establish a skeletal system of levels upon which less reliable extensions may be built. The natural disposition to employ this procedure is quite apparent when one contemplates a table containing a hundred or more gamma transitions together with their relative intensities. As the level scheme becomes more and more complex, the necessity of maximizing the reliability of each preceding step becomes more stringent and

the probability for human error increases. Merely keeping track of which transitions have been placed in the system becomes a serious clerical problem.

The computer program described does not purport to interpret data, or to create developmental steps in the course of such interpretation. It does provide a convenient tool to assist the experimenter in the sometimes overwhelming task of handling in a systematic way the large number of tables and lists of numbers which may be generated in the process of developing the decay scheme. The most significant function of the program is to determine, by a conventional least-squares procedure, the best values for a set of tentative energy levels between which a number of gamma rays have already been assigned.

An example is to be found in the report¹⁾ on the study of the levels in $^{182}_{75}\text{Re}$, where STATEFIT was applied to determine the "best" energies of 14 excited states; in this case, 41 out of 57 experimentally observed γ rays were assigned between the levels. Concurrent with the preparation of this report, the program is being used to analyze data on the reaction $^{159}\text{Tb}(n,\gamma)^{160}\text{Tb}$. Over 400 low-energy gamma rays (23-1300 keV) and over 125 high-energy (5460-6380 keV) have been included on the input list of data. The least-squares portion of the program has been expanded to accommodate up to 120 levels.

The input data for the program comprises two lists. The first list contains all of the experimentally determined γ -ray energies and relative intensities, together with their associated uncertainties. In addition, for each γ ray, the total internal-conversion coefficient (if known) is supplied along with a confidence rating that reflects in a qualitative way the experimenter's subjective judgment as to the merit of the data. This confidence 'rank' is not used in the calculations. The second list is a subset of the first list and specifies those transitions which are assigned among the excited states. Each of the entries in the second list contains only the γ -ray energy and two additional numbers—these are integer tags, or "names" which identify the initial and final levels connected by the transition.

Since the function being fitted is linear, no input estimates are necessary and the "best" energy values of the presumed states are derived from a single matrix inversion. By the customary method of error propagation, the statistical uncertainties of the level energies are calculated.

After the "best" energy values of the excited states have been determined, a complete list of all possible transitions between these levels is computed and put into monotonically increasing order of energy. The list of observed gamma rays is then searched to ascertain if there are any others which might be acceptable for assignment. To perform this search, a "window" is established by the user as a criterion for acceptance. When a member of the list is found to fall within these limits, the instance is noted on the output so that subsequent decisions can be made.

2. Program STATEFIT—Mathematical Structure

Program STATEFIT was written in Fortran IV, but since other languages are preferred by various people, the mathematical structure is presented in considerable detail so that the functional aspects of the program will not be language oriented. Table 1 defines the experimentally determined quantities that are introduced as input data. Table 2 has been prepared to demonstrate how the entire body of experimental data can be kept intact while those gamma rays that are to be used in the calculation are contained in a separate list. It is the numerical identity of the energy value that specifies to the computer where to draw the auxiliary information about each assigned gamma ray.

2.1 INPUT DATA—PROGRAM SECTION 1

GIVEN:

A set of experimentally measured gamma-ray energy values:

$$G_1, G_2, \dots, G_j, \dots, G_J \quad (2.1.1)$$

together with their experimental uncertainties

TABLE 1
Input data - definitions

Complete list of J experimentally determined gamma rays

- G_j - gamma-ray energy
 ΔG_j - uncertainty in energy of gamma ray
 R_j - relative intensity of the gamma ray
 ΔR_j - uncertainty in relative intensity
 C_j - comment (any user determined values and/or letters)
 a_j - total internal-conversion coefficient

List of K assigned gamma rays

- G_k - assigned gamma-ray energy (each G_k must be identical to a single value from the complete list, i. e., for some j, $G_k \equiv G_j$)
 JU_k - initial level index (L_m)
 JL_k - final level index ($L_{m'}$)

TABLE 2-A
OBSERVED GAMMA RAYS

CARD NO. j	ENERGY G_j	ERROR ΔG_j	INTENSITY R_j	ΔR_j	RANK C_j	ALPHA a_j
1	23.000	0.300	122	91	B	0.0
2	33.020	0.150	334	27	C	0.0
3	39.100	0.800	365	212	D	0.0
4	41.890	0.075	834	83	E	4.40
5	51.219	0.090	1169	35	D	4.00
6	63.580	0.120	833	8	A	13.50
7	68.402	0.105	28	2	C	0.0
8	74.620	0.085	1049	157	D	0.68
9	75.610	0.090	50	13	D	8.20
10	83.894	0.078	41	9	C	0.0
11	93.010	0.095	106	2	C	0.0
12	101.066	0.076	13	1	C	0.0
13	117.956	0.095	14	1	A	0.0
14	129.120	0.180	5	1		0.0
15	6152.120	0.420	1	~0	D	0.0
16	6173.650	0.230	2	~0	B	0.0
17	6217.400	0.220	84	2	A	0.0
18	6218.250	0.210	30	3	C	0.0
19	6235.030	0.250	15	1	B	0.0
20	6241.370	0.260	22	1	B	0.0
21	6269.190	0.280	21	1	A	0.0
22	6311.140	0.260	20	~0	A	0.0
23	6374.940	0.350	2	~0	C	0.0

TABLE 2-B
ASSIGNED GAMMA RAYS

CARD NO. k	ENERGY G_k	INITIAL LEVEL, JU_k	FINAL LEVEL, JL_k
1	23.000	156	133
2	33.020	138	105
3	63.580	63	0
4	74.620	138	63
5	75.610	139	63
6	93.010	156	63
7	6218.250	1	156
8	6235.030	1	139
9	6241.370	1	133
10	6269.190	1	105
11	6374.940	1	0

$$\Delta G_1, \Delta G_2, \dots, \Delta G_j, \dots, \Delta G_J \quad (2.1.2)$$

the corresponding relative intensity values

$$R_1, R_2, \dots, R_j, \dots, R_J \quad (2.1.3)$$

and their uncertainties

$$\Delta R_1, \Delta R_2, \dots, \Delta R_j, \dots, \Delta R_J \quad (2.1.4)$$

Experimenters' comments

$$C_1, C_2, \dots, C_j, \dots, C_J \quad (2.1.5)$$

and the total internal-conversion coefficient

$$a_1, a_2, \dots, a_j, \dots, a_J \quad (2.1.6)$$

Table 2-A is representative of such a list of gamma rays. The entries in the table were selected from data obtained in experiments done using the reaction $^{159}\text{Tb}(n,\gamma)^{160}\text{Tb}$. The experimental data contains over 125 high-energy γ rays in the primary spectrum and approximately 400 between 23 and 1300 keV. Since the sample used to illustrate the operation of the computer program is necessarily very small, the measured values were modified slightly in order to simulate the statistical distribution normally observed when a larger body of data is being processed. For this reason, the reader should not expect the energies and errors of the γ rays listed to agree with values published in the literature on ^{160}Tb .

The gamma rays G_j represent transitions between various pairs of excited states in the same nucleus. Failure to supply intensities and/or their errors R_j and ΔR_j will not interfere with the least-squares part of the program but will, of course, prohibit the calculation of the intensity balance. The same holds true for the values of the total internal-conversion coefficients a_j . When the conversion coefficients are supplied, the intensity values R_j are corrected for internal conversion before the intensity balance or beta-feeding calculation is begun, i.e.,

$$R_j \rightarrow (1 + a_j) R_j \quad (2.1.7)$$

The column headed "RANK" contains a subjective evaluation of the experimenter's confidence in each transition. These entries are qualitative and are not involved in the calculation. The program will run satisfactorily if nothing more than the gamma-ray energies G_j and their errors ΔG_j are entered on the input cards.

From any given body of experimental data such as that represented in Table 2-A, we wish to develop a nuclear decay scheme. For purposes of this discussion, we assume that the data have been purged of any spurious entries that may have been caused by impurities so that all entries do represent transitions between various pairs of excited states in the same nucleus.

Before the calculation is made, we assume that the approximate location of some of the excited states has been determined and that a number of the observed gamma rays (Table 2-B) contained in the total list (Table 2-A) have been assigned between various pairs of these levels. For purposes of the calculation the energies of the states are designated by the variables ϵ_m , i. e.,

$$\epsilon_0 \equiv 0, \epsilon_1, \epsilon_2, \dots, \epsilon_m, \dots, \epsilon_M. \quad (2.1.8)$$

The principal purpose of the program is to determine the "best" values of the energies of these M states by making a least-squares fit of the ϵ_m 's to the assigned gamma rays. The solution of the problem is represented by the "best" energy values e_m , i. e.,

$$e_0 \equiv 0, e_1, e_2, \dots, e_m, \dots, e_M. \quad (2.1.9)$$

To state that a γ ray is assigned between two levels m and m' , expresses the relationship

$$\tau_k = \epsilon_m - \epsilon_{m'} = G_k \pm \Delta G_k, \quad (2.1.10)$$

where G_k is any one of the assigned γ rays (see Table 1). Each assigned γ ray is thus a measurement of the difference in energy τ_k between two of the excited states. In the example (Table 2-B), it can be seen that the

assigned gamma rays

$$G_1, G_2, \dots, G_k, \dots, G_K \quad (2.1.11)$$

form a subset of the total list of observed energy values G_j (2.1.1). The errors in the energies ΔG_k , the relative intensities R_k and their errors ΔR_k along with the values of a_k that are associated with these assigned gamma rays are not entered in Table 2-B, but are obtained by the computer from the total list in Table 2-A.

The indices j and k serve merely to identify members in the two lists, respectively. For every value G_k in the assigned list, there must exist an identical entry G_j in the complete list such that

$$G_k \equiv G_j. \quad (2.1.12)$$

Since the indices are not in one-to-one correspondence, we can write

$$G_k = G_{j(k)}. \quad (2.1.13)$$

To make the least-squares fit of the energy variables ϵ_m to the data, we must specify the pair of states m_k and m'_k , connected by each γ ray G_k .

Each state must be identified in some manner in advance so that its memory location can be specified and so that the user can stipulate the two levels between which each of the γ rays G_j is to be assigned. The state subscripts m are used for this purpose internally in the program. However, since these numbers have no significance in themselves, it is more convenient to provide a set of level index numbers that carry some mnemonic value. For this purpose, each state is assigned an arbitrary integer name, or tag, L_m , referred to as the LEVEL INDEX.

The LEVEL INDEX tags are in one-to-one correspondence with the sequential integer subscript numbers m in the list of M excited states. The values of L_m are completely arbitrary, but it is usually convenient to choose integers close to the energy where the computed value is expected to be found, e.g., in the preliminary decay scheme presented in Fig. 1, there is a gamma ray of 63.58 keV depopulating

the first excited state to the ground state, and so the integer index "63" was chosen as the "name" of that state. By contrast, and to further demonstrate the flexibility of the numbering system, the level-index tag "1" was chosen to identify the capture state whose energy is, in fact, approximately 6375 keV.

Fig. 1. Preliminary partial decay scheme for ^{160}Tb . The level index tags, L_m , are completely arbitrary and are used to identify the excited states whose energies are to be determined by making a least-squares fit to the gamma rays (solid lines) that have been assigned between the levels. The column on the right shows the results of an actual fit. The gamma rays in dotted lines were then selected by the computer from the total list of observed data as being eligible for subsequent assignment. (Neg. No. 209-4380R1; Phg 12585)

In similar fashion, the variables JU_k and JL_k associated with the assigned gamma rays G_k take on values of L_m , i.e.,

$$JU_k = L_m \text{ and } JL_k = L_{m'}, \quad (2.1.14)$$

representing the states connected by the assigned γ ray G_k .

Figure 1 represents a preliminary decay scheme containing 7 excited states whose "best" energy values are to be determined by STATEFIT. The LEVEL-INDEX numbers in the left-hand column are the integer identifiers L_m that have been assigned to each state. The second column represents the set of level energies ϵ_m to be determined by the least-squares calculation. For convenience, the computed "best" values e_m (the results of an actual fit) are entered in the right-hand column of the figure. The gamma-ray transitions drawn in solid lines are those shown in Table 2-B and are the ones used in the calculation yielding the energies on the right. The transitions drawn in with dotted lines represent other gamma rays that were picked out in the search portion of the program (see 3.4 and 3.5) and may be assigned in the next calculation.

2.2 TESTS MADE ON INPUT DATA

When the amount of data being processed becomes large, and the complexity of the decay scheme grows, the probability of human error correspondingly increases. When there are several hundreds of cards in the deck and the execution of the program is terminated by the machine because of an error in the input data, it is frequently difficult to locate where the error was made. For this reason, a variety of tests are performed on the two lists of γ rays immediately after they have been read in and before execution of the program is attempted. For fatal mistakes, the error is noted, and execution is automatically terminated. For mistakes that are not fatal, an error message is written at the end of Sec. 1 but execution is allowed to proceed. The testing routine is always carried to completion even though one of the earlier tests may have indicated

termination. There are ten such tests, as follows:

2.2.1. TEST 1. Each assigned γ ray G_k must connect two different excited states. Thus if the same LEVEL INDEX has been entered for both initial and final levels, the mistake is fatal, i. e., if for any k , $JU_k = JL_k$. Execution is terminated.

2.2.2. TEST 2. For each card in the list of assigned γ rays, there must be one, and only one, card in the list of observed γ rays bearing the identical energy value. This mistake can be made in either of two ways: an erroneous value may have been punched on the assignment card, or, for some reason, the observed γ -ray card may be missing from the deck. Failure to fulfill this requirement is fatal, since all of the additional information about each assigned γ ray is derived from the entry in the complete list. Thus, for every G_k in the list of assigned γ rays, there must exist a G_j in the complete list such that $G_j \equiv G_k$. If this condition is not satisfied, the error is noted and execution is terminated.

2.2.3. TEST 3. Values of the experimental uncertainties in the energies of the assigned γ rays are indispensable to performance of the least-squares calculation. The list of observed γ rays is searched to ascertain if any of the energy errors ΔG_j is zero. If any such error is found, the consequence depends upon whether the mistake relates to an assigned or to an as yet unassigned γ ray, i. e., (a) if $\Delta G_j = 0$ and the γ ray is not found in the list of assigned γ rays, the error is not fatal but is noted. (b) If the uncertainty in energy, ΔG_k , equals zero for any of the assigned γ rays, the error is noted and execution is terminated.

2.2.4. TEST 4. No more than one γ ray may be assigned between the same two excited states. To do so, of course, contradicts the physics involved. However, there is real danger of such an error being made, since, in the search portion of the program, a very close-lying transition may be picked out as falling within the test criterion and the assignment be made without noting the previous one that had been made. The mistake is fatal. The list of assigned γ -ray cards is searched to ensure that no

two pairs of initial and final level indices are alike. I.e., if for any two assigned γ rays G_k and $G_{k'}$, $JU_k = JU_{k'}$ and $JL_k = JL_{k'}$, the mistake is noted and execution is terminated.

2.2.5. TEST 5. No two entries in the list of observed γ rays may have the same energy value. Thus, if $G_j = G_{j'}$ for any two observed γ rays j and j' , the error is noted and execution is terminated. Note: This test is not applied to the list of assigned γ rays since, if at a specific energy one might believe there to be an unresolved doublet comprising two different γ rays with the identical energy, the user may elect to temporarily assign this transition to two different places in the decay scheme. Such "double assignments" are not considered to be errors, but since keeping track of them may sometimes be difficult, such double assignments are noted in Secs. 3, 4, and 5 of the output.

2.2.6. TEST 6. The number "0" must never be used for the LEVEL INDEX number of any excited state. Use of the LEVEL INDEX number zero is exclusively reserved for the ground state. The set of values JU_k on the list of assigned γ rays is searched to see if any zero value appears. Thus, if for any k , $JU_k = 0$, the error is noted and execution is terminated.

2.2.7. TEST 7. The zero reference for the energies of the excited states is the ground state; there must be at least one of the assigned γ rays that depopulates to the ground state. The list of assigned γ rays is searched to ensure that the value 0 appears at least once in the list of JL . I.e., $JL_k = 0$. If not, the error is noted and the execution is terminated.

2.2.8. TEST 8. The core demand of the program is determined by values assigned to 5-dimension parameters. The program constants NDIMA, NDIMB, and NDIMC determine the maximum allowable number of assigned γ rays, observed γ rays, and excited states, respectively. The constants NDIMAF and NDIMCF are the maximum dimensions of the observation matrix F used in the least-squares calculation and indicate the assigned gamma-ray axis and excited-state axis, respectively.

The actual number of observed and assigned γ rays and the total number of excited states in any particular fit, LISTG, NGAM, and NLEV are checked against the program dimensions to ensure that the capacity of the program has not been exceeded. In addition, the size of the matrix used in the least-squares calculation which is independently specified is also tested. I. e., if

$$\text{NGAM} > \text{NDIMA} \quad (\# \text{ of assigned gammas})$$

or

$$\text{LISTG} > \text{NDIMB} \quad (\# \text{ of observed gammas})$$

or

$$\text{NLEV} > \text{NDIMC} \quad (\# \text{ of excited states})$$

or, for the matrix dimensions, if

$$\text{NGAM} > \text{NDIMAF}$$

or

$$\text{NLEV} > \text{NDIMCF},$$

the error(s) is (are) noted and execution is terminated.

2.2.9. TEST 9. Ordering of the data deck. Handling of the list of observed γ rays is facilitated by maintaining the list in monotonically increasing order of γ -ray energy. However, there may be times when the user will find it desirable to arrange the deck differently. Failure to have the data ordered is not fatal and is merely noted. I. e., if for any j , $G_j > G_{j+1}$, the discrepancy is noted.

2.2.10. TEST 10. A blank card should be placed between the deck of observed γ rays and the deck of assigned γ rays as a separator. Failure to include this card is not fatal, but the error is noted.

2.3 LEAST-SQUARES CALCULATION OF THE "BEST" ENERGY VALUES OF THE EXCITED STATES (PROGRAM SEC. 2)

We assume that the existence of a number M of excited nuclear states has already been established. These levels have energies

$$\epsilon_0 \equiv 0, \epsilon_1, \dots, \epsilon_m, \dots, \epsilon_M \quad (2.1.8)$$

but, at the outset, we do not know the precise values of these energies. We also have a set of K experimentally measured γ rays

$$G_1, \dots, G_k, \dots, G_K \quad (2.1.11)$$

that have been assigned with some confidence as representing nuclear transitions between various pairs of the levels. An example of such a system is represented in Fig. 1.

We wish to determine the "best" energy values,

$$e_1, \dots, e_m, \dots, e_M \quad (2.1.9)$$

of the set of M unknown energies, e_m , (2.1.8) by making a least-squares fit of the latter to the set of K assigned γ rays. There must, of course, be more assigned γ rays than there are levels, i.e., $K > M$, and at least one of them must depopulate to the ground state in order to provide an energy reference for the system. In addition to the measured energy of each gamma ray, G_k , the available experimental data usually include the relative intensity, R_k , together with the experimental uncertainties ΔG_k and ΔR_k , and may include an associated internal-conversion coefficient α_k . The total body of data available for use in the calculation is thus represented symbolically in Table 3. The quantities R_k , ΔR_k , and α_k , when available, are used to compute the intensity balance of the system of excited states.

The only information needed to make the least-squares calculation is the energy of each assigned γ ray G_k , its associated error ΔG_k , and the identification of the two levels connected by the γ ray (Table 3). The quantities JU_k and JL_k are used in the input data to specify the upper and lower levels, respectively, and are expressed in terms of the set of integer names L_m that have arbitrarily been given to the levels. Thus for every γ ray, $G_k(JU, JL)$, assigned between the levels m and m' ,

$$JU_k = L_m \text{ and } JL_k = L_{m'}. \quad (2.3.1)$$

TABLE 3

Data used to make least-squares calculation of the "best" energy values and to compute the intensity balance for M excited states.

Gamma No.	Energy	Error	Intensity		Alpha	Initial Level ^a	Final Level ^a	Initial ^b Level	Final ^b Level
k	G _k	ΔG _k	R _k	ΔR _k	α _k	JU _k (L _m)	JL _k (L _{m'})	μ _k (m)	λ _k (m')
1	G ₁	ΔG ₁	R ₁	ΔR ₁	α ₁	JU ₁	JL ₁	μ ₁	λ ₁
2	G ₂	ΔG ₂	R ₂	ΔR ₂	α ₂	JU ₂	JL ₂	μ ₂	λ ₂
...	...	...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...	...	...
...	...	...	...	...	...	...	...	...	...
K	G _K	ΔG _K	R _K	ΔR _K	α _K	JU _K	JL _K	μ _K	λ _K

^a Each of the M excited states is assigned an arbitrary integer "name" L_m by the user; assignment of each γ ray is specified by giving the initial and final level numbers JU_k and JL_k in terms of these arbitrary tags.

^b The quantities μ_k and λ_k (to the right of the double line) are the initial and final level numbers in terms of the sequential integers m; the correspondence between the user assigned "names" L_m and the internal sequence number m is established automatically by the computer.

However, the computer must carry out the calculation in terms of memory locations m , where the M values of the calculated state energies are to be stored. For purposes of the calculation, then, instead of using the variables JU_k and JL_k which are in terms of the set of identifiers L , the quantities μ_k and λ_k are used; these literally take on the values m and m' from the set of M sequential indices representing the states. Each gamma ray may thus be alternatively written $G_k(\mu, \lambda)$ where μ is the state index number (m) of the level being depopulated and λ the index number (m') of the populated state. Thus, in Table 3, the entries in the columns JU_k and JL_k are the identifying tags selected by the user, and the columns to the right of the double line μ_k and λ_k are the corresponding values used internally. After the data are read into the computer, this correspondence is established automatically in a table of L vs m , i.e.,

$$\begin{aligned}
 L_m &\rightarrow m \\
 JU_k &\rightarrow \mu_k \\
 JL_k &\rightarrow \lambda_k \\
 (JU_k = L_m) &\rightarrow (\mu_k = m) \\
 (JL_k = L_{m'}) &\rightarrow (\lambda_k = m')
 \end{aligned} \tag{2.3.2}$$

thus $G_k(JU, JL) \rightarrow G_k(\mu, \lambda)$.

At the end of the calculations, the levels are again identified in terms of L_m and the indices m used internally are never printed.

We seek to find the "best" energy values e_m of the M excited states. The information about how the K gamma rays are assigned among the M excited states is formalized in an observation matrix F (Table 4). The matrix has dimensions K by M , where each column corresponds to one of the excited states ϵ_m and each row corresponds to one of the assigned gamma rays G_k . No column exists for the ground state ϵ_0 , since it is the zero reference of energy and is not a variable, i.e.,

$$e_0 \equiv \epsilon_0 \equiv 0. \tag{2.3.3}$$

TABLE 4

Observation Matrix $\underline{F}$ used in least-squares calculation.

G_k	k	L_m	= 156 133 138 105 63 1 139						
		m	= 1 2 3 4 5 6 7						
6241.37	1		0	-1	0	0	0	+1	0
6235.03	2		0	0	0	0	0	+1	-1
6374.94	3		0	0	0	0	0	+1	0
6269.19	4		0	0	0	-1	0	+1	0
6218.25	5		-1	0	0	0	0	+1	0
23.00	6		+1	-1	0	0	0	0	0
63.58	7		0	0	0	0	+1	0	0
93.01	8		+1	0	0	0	-1	0	0
33.02	9		0	0	+1	-1	0	0	0
74.62	10		0	0	+1	0	-1	0	0
75.61	11		0	0	0	0	-1	0	+1

If the k^{th} γ ray depopulates level L_m , $F_{km} = +1$.

If the k^{th} γ ray populates level $L_{m'}$, $F_{km'} = -1$.

All other elements of row $k = 0$.

The observation matrix $\underline{F}$ is constructed by entering +1 for the element $f_{k\mu}$ if the k^{th} gamma ray depopulates the μ^{th} level ϵ_μ , while the element $f_{k\lambda}$ is entered as -1 if the k^{th} gamma ray populates the λ^{th} state ϵ_λ . All other elements in this row (f_{km}) are given the value zero. Each row of the matrix $\underline{F}$ thus contains two entries, +1 and -1, in the columns corresponding to the energy levels ϵ_μ and ϵ_λ connected by the gamma ray represented by that particular row.

Exception: The row will contain only one nonzero element, +1, if the transition terminates on the ground state ϵ_0 .

Table 4 is the observation matrix representing the ^{160}Tb data listed in Table 2-B and depicted in Fig. 1 (solid lines).

The unknown "best" energy values for the M excited states are represented by the column vector $\underline{\epsilon}$; the calculated "best" energy values are represented by the corresponding solution vector $\underline{e}$. When the ground state is taken together with any set of M excited states, then $M(M+1)/2$ possible transitions may occur. We thus define the complete list T_n of "best" possible transition energies

$$T_1, T_2, \dots, T_n, \dots, T_N \quad (2.3.4)$$

where $N = M(M+1)/2$. There exists a subset T_k of the complete list T_n , i.e.,

$$T_1, T_2, \dots, T_k, \dots, T_K. \quad (2.3.5)$$

There is a one-to-one correspondence between the entries in the list T_k and the list G_k (2.1.11), i.e., any value T_k is the "best" energy difference between the two states connected by the assigned gamma ray G_k . Since the set of "best" transition energies T_k is not known until the calculation has been made, we identify the corresponding set of variable parameters τ_k , i.e.,

$$\tau_k(\mu, \lambda) = \epsilon_\mu - \epsilon_\lambda = \sum_{m=1}^{m=M} f_{km} \epsilon_m. \quad (2.3.6)$$

The deviation x_k between the energy difference $\tau_k(\mu, \lambda)$ and the assigned gamma ray $G_k(\mu, \lambda)$ is

$$x_k = G_k(\mu, \lambda) - \tau_k(\mu, \lambda). \quad (2.3.7)$$

To determine the "best" energy values for the excited states (contained in the list of ϵ_m 's) (2.1.8) by the method of least-squares, we form the function

$$\theta(\epsilon_1, \dots, \epsilon_m, \dots, \epsilon_M) = \sum_{k=1}^{k=K} w_k x_k^2. \quad (2.3.8)$$

The weights w_k are obtained from the experimental uncertainties in the gamma-ray energy values, i.e.,

$$w_k = \frac{1}{(\Delta G_k)^2}. \quad (2.3.9)$$

Thus the function becomes

$$\theta(\epsilon_1, \dots, \epsilon_m, \dots, \epsilon_M) = \sum_{k=1}^{K} \frac{(G_k - \sum_{m=1}^M f_{km} \epsilon_m)^2}{(\Delta G_k)^2}. \quad (2.3.10)$$

The "best" values of the variable parameters ϵ_m are designated e_m and are found by determining the minimum value of θ

$$\chi^2 = \theta_{\min}. \quad (2.3.11)$$

This is done by solving the set of equations

$$\frac{\partial \theta}{\partial \epsilon_1} = 0, \quad \frac{\partial \theta}{\partial \epsilon_2} = 0, \quad \dots, \quad \frac{\partial \theta}{\partial \epsilon_M} = 0 \quad (2.3.12)$$

for all of the M parameters ϵ_m

$$\frac{\partial \theta}{\partial \epsilon_m} = -2 \sum_{k=1}^K \frac{f_{km}}{\Delta G_k} (G_k - \sum_{i=1}^M f_{ki} \epsilon_i) \quad (2.3.13)$$

Since $\partial \theta / \partial \epsilon_m = 0$, it follows

$$\sum_{k=1}^K \sum_{i=1}^M \frac{f_{km} f_{ki} \epsilon_i}{\Delta G_k} = \sum_{k=1}^K \frac{f_{km} G_k}{\Delta G_k}. \quad (2.3.14)$$

The M equations may be represented in matrix form

$$\underline{A} \underline{\epsilon} = \underline{b} \quad (2.3.15)$$

where $\underline{A}$ contains M rows and M columns. The general matrix element is written

$$a_{mi} = \sum_{k=1}^{k=K} \frac{f_{km} f_{ki}}{\Delta G_k^2} . \quad (2.3.16)$$

The general element of the constant vector $\underline{b}$ is

$$b_m = \sum_{k=1}^{k=K} \frac{f_{km} G_k}{\Delta G_k^2} . \quad (2.3.17)$$

Thus to obtain the solution vector $\underline{e}$ representing the "best" energy values for the excited states, we must calculate the inverse matrix $\underline{A}^{-1}$ and solve the equation

$$\underline{e} = \underline{A}^{-1} \underline{b} . \quad (2.3.18)$$

Thus the "best" energy values for each of the M excited states is given by

$$e_m = \sum_{i=1}^{i=M} a_{mi}^{-1} b_i . \quad (2.3.19)$$

Also, from the solution vector $\underline{e}$, the list of "best" energy differences between any two states is given by

$$T_k = e_\mu - e_\lambda . \quad (2.3.20)$$

The goodness of fit χ^2 is determined by evaluating the function (2.3.10), that is,

$$\chi^2 = \sum_{k=1}^{k=K} \frac{(G_k - \sum_{m=1}^{m=M} f_{km} e_m)^2}{\Delta G_k^2} . \quad (2.3.21)$$

The normalized function chi-squared per degree of freedom is given by

$$\chi_n^2 = \frac{\chi^2}{K - M} . \quad (2.3.22)$$

2.4 CALCULATION OF ERRORS

The statistical uncertainty Δe_m in any state e_m is given by

$$(\Delta e_m)^2 = \sum_{k=1}^{k=K} \left(\frac{\partial e_m}{\partial G_k} \Delta G_k \right)^2, \quad (2.4.1)$$

thus substituting for e_m with (2.3.19) and using the relationships shown in (2.3.17) we have

$$(\Delta e_m)^2 = \sum_{k=1}^{k=K} \left[\frac{\partial}{\partial G_k} \left(\sum_{i=1}^{i=M} a_{mi}^{-1} \times \sum_{k'=1}^{k'=K} \frac{f_{k'i} G_{k'}}{\Delta G_{k'}^2} \right) \Delta G_k \right]^2. \quad (2.4.2)$$

Then

$$(\Delta e_m)^2 = \sum_{k=1}^{k=K} \left(\sum_{i=1}^{i=M} a_{mi}^{-1} \times \frac{f_{ki}}{\Delta G_k^2} \times \Delta G_k \right)^2 \quad (2.4.3)$$

or

$$(\Delta e_m)^2 = \sum_{k=1}^{k=K} \left(\sum_{i=1}^{i=M} \frac{a_{mi}^{-1} f_{ki}}{\Delta G_k} \right)^2. \quad (2.4.4)$$

So

$$(\Delta e_m)^2 = \sum_{i=1}^{i=M} a_{mi}^{-1} \sum_{\rho=1}^{\rho=M} a_{m\rho}^{-1} \times \sum_{k=1}^{k=K} \frac{f_{ki} f_{k\rho}}{\Delta G_k^2} \quad (2.4.5)$$

and using (2.3.16) we can say

$$(\Delta e_m)^2 = \sum_{i=1}^{i=M} a_{mi}^{-1} \sum_{\rho=1}^{\rho=M} a_{m\rho}^{-1} a_{i\rho}. \quad (2.4.6)$$

So

$$(\Delta e_m)^2 = \sum_{i=1}^{i=M} a_{mi}^{-1} \delta_{mi} = a_{mm}^{-1}. \quad (2.4.7)$$

That is, the error Δe_m in each of the excited states e_m is

$$\Delta e_m = \sqrt{a_{mm}^{-1}}. \quad (2.4.8)$$

The error in the "best" transition energy is given by combining in quadrature the statistical uncertainties of the two states involved, i.e., for $T_n = e_\mu - e_\lambda$

$$\Delta T_n = \sqrt{\Delta e_\mu^2 + \Delta e_\lambda^2}. \quad (2.4.9)$$

2.5. CALCULATION OF INTENSITY BALANCE (IBETA=0)/ FRACTIONAL BETA FEEDING (IBETA=1)

2.5.1 Intensity balance. The intensity balance (in γ -ray intensity units) of any excited state is given by the difference between the total intensity of the depopulating γ rays and the total intensity of the transitions populating the state. Thus the intensity balance of any level may be represented by

$$\rho_m = \sum_{k=1}^{k=K} f_{km} R_k, \quad (2.5.1.1)$$

where f_{km} is an element of the observation matrix $\underline{F}$ (Table 4). The quantity ρ_m is always computed for each state; if it has a positive value, there is an excess of depopulations over populations. This means that there may be one or more populating transitions missing in the decay scheme, and in addition, in the case of a radioactive sample, there is probably beta feeding into the state. In either case, if the data have not been corrected for internal conversion the values of ρ_m are unreliable and should not be used literally. If the γ -ray intensity values R_k have been corrected for internal conversion, $R_k \rightarrow R_k(1 + \alpha_k)$, (2.1.7) where α_k is the total internal-conversion coefficient, then the values of the intensity balance ρ_m of the states are useful in the interpretation.

2.5.2 Fractional beta feeding. If the data under analysis relate to a radioactive sample, where it is expected that beta feeding occurs to one or more of the levels, the user may elect to print the intensity balance of each state as a fraction of the total excess feeding into all of the levels rather than in terms of γ -ray intensity units. The total excess feeding into all of the excited states is

$$B = \sum_{m=1}^{m=M} \rho_m. \quad (2.5.2.1)$$

The fractional beta feeding, i. e., the total strength of the components feeding the m 'th state (beta feeding plus possible unassigned populating gamma rays) is thus given by

$$\beta_m = \frac{\rho_m}{B}. \quad (2.5.2.2)$$

3. Operation of the Program

Operation of the program and the functions that are performed are described in terms of the printed output sections that are produced.

3.1. OPERATING INSTRUCTIONS AND INPUT DATA

3.1.1 Operating instructions. The first printed output (Table 5) is a set of OPERATING INSTRUCTIONS. These instructions are written into the program and are always reproduced as a convenience for the user.

The input data deck comprises a title card, a control card and two lists of experimental data. The first card is a label, or TITLE containing the run identification information.

The second card contains two control constants. The first of these is a real number WIDE, this number establishes the criterion used in Secs. 4 and 5 where the search for acceptable as-yet-unassigned γ rays is made. The value of WIDE is usually of the order of unity since for that value, gamma rays lying within one standard deviation of the combined errors of the transition and the experimental uncertainty of the

TABLE 5

PROGRAM STATEFIT

WRITTEN BY
S. B. BURSON
G. T. WOOD, AND
C. H. BATSON

PHYSICS DIVISION
ARGONNE NATIONAL LABORATORY
ARGONNE, ILLINOIS

JOB TITLE: STATEFIT RUN FOR DISPLAY IN REPORT

OPERATING INSTRUCTIONS

DATA DECK ORGANIZATION

FIRST CARD: TITLE CARD, (ANY 80 CHARACTERS.)
FORMAT(10A8)

SECOND CARD: WIDE, IBETA
FORMAT(F6.0,I6)

WIDE DETERMINES WIDTH OF WINDOW USED TO SEARCH COMPLETE LIST OF OBSERVED GAMMA RAYS (SECTION 1-A) FOR POSSIBLE ASSIGNMENTS.

$E(T) = \text{CALCULATED TRANSITION ENERGY} = E(JU) - E(JL)$

$\Delta = \text{ABS}(E(T) - E(\text{GAMMA}))$

$\text{ERR}(\Delta) = \text{COMPUTED STATISTICAL ERROR IN } \Delta$

A GAMMA RAY IS SELECTED FROM THE COMPLETE LIST

(SECTION 1-A) IF: $\Delta < \text{WIDE} * \text{ERR}(\Delta)$.

WIDE IS NORMALLY SET EQUAL TO 1 OR APPROXIMATELY SO

IBETA MAY EQUAL ONE OR ZERO. IF IBETA=0, THE INTENSITY BALANCE(OF EACH STATE) IS:

$\text{XTFEED} = \text{TOTAL DEPOPULATING INTENSITY} - \text{TOTAL POPULATING INTENSITY}$.

IF IBETA=1 (FOR RADIOACTIVE SAMPLES), XTFEED

FOR EACH STATE IS DIVIDED BY THE TOTAL BETA

FEEDING TO ALL EXCITED STATES.

NEXT LISTG CARDS: CEN, DELCEN, RINT, DINT, CONF, COM, ALPHA

FORMAT (4F12.0,A4,A8,E12.0)

(THESE LISTG CARDS ARE THE EXPERIMENTALLY OBSERVED GAMMA RAYS (SECTION 1-A), 1 GAMMA RAY PER CARD. LISTG IS NOT TO EXCEED THE PROGRAM CONSTANT "NDIMB", 5000 SERIES LINE NUMBERS)

(CEN = EXPERIMENTALLY OBSERVED GAMMA RAY ENERGY IN KEV.)

WARNING! THE ENERGY VALUE EG OF ANY ASSIGNED GAMMA RAY MUST BE IDENTICALLY EQUAL TO THE CORRESPONDING ENERGY VALUE CEN IN THIS LIST OF OBSERVED GAMMA RAYS OR EXECUTION WILL TERMINATE.

(DELCEN = EXPERIMENTAL ERROR IN CEN.)

(RINT = RELATIVE INTENSITY OF THE GAMMA RAY IN ARBITRARY UNITS.)

(DINT = EXPERIMENTAL ERROR IN RINT.)

(CONF+COM=CONFIDENCE RATING OF OBSERVED GAMMA RAY (OR COMMENT) ARBITRARILY ASSIGNED BY EXPERIMENTER.)

(ALPHA = THE TOTAL INTERNAL CONVERSION COEFFICIENT.)

TABLE 5 (contd.)

(OPERATING INSTRUCTIONS CONTINUED)

NEXT CARD: BLANK CARD; THIS CARD IS OPTIONAL AND IS USED
TO SEPERATE THE DATA DECKS. OMISSION
WILL NOT CAUSE PROGRAM TO TERMINATE.

NEXT NGAM CARDS: EG, JU, JL

FORMAT(1F12.0,2I6)

(THESE NGAM CARDS ARE ASSIGNED GAMMA RAYS (SECTION 1-B),
1 GAMMA RAY PER CARD. NGAM IS NOT TO EXCEED THE PROGRAM
CONSTANT "NDIMA" IN THE 5000 SERIES LINE NUMBERS)
(EG IS GAMMA RAY ENERGY IN KEV. WARNING! EG MUST BE
IDENTICALLY EQUAL TO CORRESPONDING ENERGY VALUE CEN
IN COMPLETE LIST OF OBSERVED GAMMA RAYS.)
(JU AND JL ARE THE INTEGER INDEX NUMBERS OF THE
UPPER AND LOWER EXCITED STATES, WHICH NEED NOT BE CONSECUTIVE
INTEGERS AND NEED NOT BE ASSIGNED IN ASCENDING ENERGY ORDER)
(RESTRICTIONS: FOR THE GROUND STATE,
JL=0; ALL JU VALUES MUST BE NON ZERO)

LAST CARD: BLANK CARD; THIS CARD SIGNALS END OF DATADECK,
OMISSION WILL CAUSE ABNORMAL TERMINATION.

PROGRAM ALTERATIONS

SET NDIMA(LINE 5100)=MAXIMUM NGAM EXPECTED.
SET NDIMB(LINE 5200)=MAXIMUM LISTG EXPECTED.
SET NDIMC(LINE 5300)=MAXIMUM NLEV EXPECTED(NO.LEVELS TO BE FITTED).
SET MATRIX GAMMA AXIS NDIMAF(LINE 5500) EQ/LT NDIMA
SET MATRIX EXCITED-STATE AXIS NDIMCF(LINE 5510) EQ/LT NDIMC
SET NDIMD(LINE 5400)=NDIMCF*(NDIMCF+1)/2
NDIMD=TOTAL TRANSITIONS BETWEEN NDIMCF EXCITED STATES
(INCLUDING GROUND STATE)
REDIMENSIONING ARRAYS - REFER TO 5000 SERIES LINE NUMBERS
SET DIMENSIONS IN LINES 5101-5104 TO NDIMA
SET DIMENSIONS IN LINES 5201&5202 TO NDIMB
SET DIMENSIONS IN LINES 5301-5303 TO NDIMC
SET DIMENSIONS IN LINE 5401 TO NDIMD
SET DIMENSIONS IN LINE 5501 TO NDIMCF BY NDIMAF
SET DIMENSIONS IN LINES 5516&5517 TO NDIMCF BY NDIMCF
THESE LINES ARE IN SUBROUTINE LEASQE

(END OF OPERATING INSTRUCTIONS)

γ ray are selected (see Sec. 3.4.1). In the early stages of development of the decay scheme, the experimenter will make assignments with a high degree of caution and so will limit the acceptance window rather severely. When the final decay scheme has been determined, the window can be broadened so that the search procedure will be more "liberal" in picking out additional candidates for assignment. One would expect the final analysis to reflect a normal distribution of the individual CHI values [see Eq. (3.3.2)].

The second constant IBETA is set equal to 1 or left blank on the card. If the constant is omitted from the card (IBETA=0), the "Intensity Balance" to each state is computed in terms of γ -ray intensity units and is the difference between the total depopulations and populations to each state (see Secs. 2.5 and 3.2.3). Also, the intensities R_j are corrected for internal conversion and are referred to as "TRANSITION INTENSITY" in output sections 3 and 7.

If the data relates to radioactive samples, the constant "IBETA" is set equal to 1. The beta feeding to each state is then computed in terms of its fraction of the total excess feeding to all the excited states. The intensities of the assigned γ rays R_k , after being corrected for internal conversion, are divided by the total feeding and referred to as "NORMALIZED INTENSITY" in output section 3.

The TITLE card and control card are followed by the cards containing the complete list of experimentally observed γ rays (see Sec. 2.1), usually in order of ascending energy. This set of cards is terminated by a blank card which serves as a separator and also to signal the computer that the first list is complete.

Finally, the set of cards containing the list of assigned gamma rays is entered. These cards are usually grouped in terms of depopulations from each state, with the states arranged in order of increasing energy. If one wishes to add a new state, the depopulations are inserted into the deck as a package and the feedings are entered into the clusters of high lying levels at the appropriate points. It should be emphasized that the

ordering of either list is totally optional with the user and the above recommendations are based entirely on the experience of the authors.

3.1.2 Modification of program dimensions (output section 0). The space required by the program should be adjusted to accommodate the amount of data to be processed and may, of course, be limited by the capacity of the computer. Both running costs and turn-around time increase rapidly with the space required and so the dimensions should be revised from time to time.

Modification of the space requirements is considered at two levels. The size of the input list of observed γ rays is determined by the experiments while the number of assignments and the number of excited states to be fitted depends upon the degree to which the development of the decay scheme has advanced. At the outset, there may be need to store a list of several hundred observed γ rays while only ten or fifteen states are to be fitted. The size of the arrays required for the observation matrix F and the energy matrices used in the least-squares calculation increase rapidly with the number of states and so it is advantageous to monitor the size of these areas.

The constant NDIMB is used throughout the program as the terminal index of all the lists containing information about the observed gamma rays. It need only be as large as the maximum number of data cards to be entered. The lists containing this information are accordingly dimensioned to the size NDIMB. The constant NDIMA bears the corresponding relationship to the assigned gamma rays and the lists accommodating them are dimensioned to that value. NDIMA need never exceed NDIMB, and can usually be set somewhat smaller since it is seldom possible to develop a decay scheme that will accommodate all of the observed data.

The constant NDIMC specifies the maximum number of excited states that can be processed by the program and may be specified according to the degree of advancement of the analysis.

The constants NDIMAF and NDIMCF are the maximum dimensions of the observation matrix F used in the least-squares calculation and

indicate the assigned gamma-ray axis and excited-state axis, respectively. The space needed increases as the product of the two axes; it is advisable to specify these dimensions independently from time to time, depending upon the immediate demand for the space. The OPERATING INSTRUCTIONS include detailed information for making these changes.

The constant NDIMD is used as the terminal index for the complete list of possible transitions and must always be modified whenever NDIMC, the maximum number of excited states, is changed. The formula for this adjustment is described in the instructions.

3.1.3 Output section 1, reproduction of input information. The options expressed on the control card for the particular run are reprinted (Table 6). The space capacity of the program is then printed, i. e., the size of the arrays available for the two lists of data and the number of

TABLE 6

PROGRAM STATEFIT
INPUT INFORMATION

JOB TITLE: STATEFIT RUN FOR DISPLAY IN REPORT

NOTE! IF EXECUTION TERMINATES AT THIS POINT, CHECK FOR ERRORS
IN DATA DECK. BLANK CARD OR EOF CARD MAY BE MISSING
AT END OF DATA.

CONTROL CARD: WIDE = 1. IBETA = 0

PROGRAM DIMENSIONS

ASSIGNED GAMMA RAYS (NDIMA) = 50
OBSERVED GAMMA RAYS (NDIMB) = 100
NO. OF EXCITED STATES (NDIMC) = 20

F MATRIX (NDIMCF BY NDIMAF)
EXCITED STATE AXIS: (NDIMCF) = 20
ASSIGNED GAMMA AXIS: (NDIMAF) = 50
NO. POSSIBLE TRANSITIONS: (NDIMD) = 210

PROGRAM UTILIZATION

	ASSIGNED GAMMA RAYS	OBSERVED GAMMA RAYS	EXCITED STATES
STORAGE CAPACITY	50	100	20
STORAGE NEEDED	11	23	7

excited states that can be accommodated. As the data are read in, the demand for space is determined and under the title PROGRAM UTILIZATION, these quantities are listed. If any of the dimensions are inadvertently exceeded, this error is noted and execution is terminated.

After the above preliminary information is printed, the major output is begun; it is presented in 7 sections.

The complete list of experimentally observed γ rays (Sec. 2.1) is printed as it appears in the data deck. This is followed by the list of assigned γ rays. Table 7 is a representative sample of this section of the output; it contains the data used in the fit shown in the decay scheme (Fig. 1).

TABLE 7
Input data used for the decay scheme shown in fig. 1.

SECTION 1-A		COMPLETE INPUT LIST OF OBSERVED GAMMA RAY ENERGIES				
CARD NUMBER	GAMMA RAY ENERGY	GAMMA RAY ERROR	RELATIVE INTENSITY	INTENSITY ERROR	CONFIDENCE LEVEL&I.D.	CONVERSION COEFFICIENT
1	23.000	0.300	12.170	9.130	B	0.0
2	33.020	0.150	33.450	2.680	C	0.0
3	39.100	0.800	36.500	21.170	D	0.0
4	41.890	0.075	83.440	8.340	E	4.40D 00
5	51.219	0.090	116.880	3.510	D	4.00D 00
6	63.580	0.120	83.250	0.830	A	1.35D 01
7	68.402	0.105	2.810	0.170	C	0.0
8	74.620	0.085	104.900	15.740	D	6.80D-01
9	75.610	0.090	5.000	1.250	D	8.20D 00
10	83.894	0.078	4.060	0.890	C	0.0
11	93.010	0.095	10.570	0.210	C	0.0
12	101.066	0.076	1.330	0.050	C	0.0
13	117.956	0.095	1.430	0.090	A	0.0
14	129.120	0.180	0.520	0.050		0.0
15	6152.120	0.420	0.050	0.010	D	0.0
16	6173.650	0.230	0.200	0.020	B	0.0
17	6217.400	0.220	8.410	0.170	A	0.0
18	6218.250	0.210	3.000	0.300	C	0.0
19	6235.030	0.250	1.490	0.050	B	0.0
20	6241.370	0.260	2.180	0.060	B	0.0
21	6269.190	0.280	2.050	0.050	A	0.0
22	6311.140	0.260	2.010	0.030	A	0.0
23	6374.940	0.350	0.220	0.040	C	0.0

SECTION 1-B: LIST OF ASSIGNED GAMMA RAYS

CARD NUMBER	GAMMA RAY ENERGY	INITIAL LEVEL	FINAL LEVEL
1	6241.370	1	133
2	6235.030	1	139
3	6374.940	1	0
4	6269.190	1	105
5	6218.250	1	156
6	23.000	156	133
7	63.580	63	0
8	93.010	156	63
9	33.020	138	105
10	74.620	138	63
11	75.610	139	63

3.1.4 Tests made on the input data. After the input data are read into the computer, the ten tests described in detail in Sec. 2.2 are then carried out. Table 8 shows a set of input data, where an example of each kind of mistake has been deliberately made; Table 9 is the computer output resulting from these tests. The paragraph titled TESTS MADE IN SECTION 1 is always printed along with the subsequent heading, ERRORS FOUND. If there are no errors, the output proceeds immediately to the next section.

TABLE 8

Input data containing typical user mistakes to demonstrate operation of the error-search procedure.

SECTION 1-A		COMPLETE INPUT LIST OF OBSERVED GAMMA RAY ENERGIES				
CARD NUMBER	GAMMA RAY ENERGY	GAMMA RAY ERROR	RELATIVE INTENSITY	INTENSITY ERROR	CONFIDENCE LEVEL&I.D.	CONVERSION COEFFICIENT
1	23.000	0.300	791.000	593.000	D	0.0
2	39.100	0.0	2372.000	1383.000	D	0.0
3	41.890	0.0	1404.000	280.000	E	0.0
4	50.869	0.002	1452.000	300.000	D	4.00D 00
5	63.686	0.003	4596.000	250.000	A	1.10D 01
6	64.110	0.003	3717.000	250.000	D	0.0
7	68.402	0.013	316.000	20.000	C	0.0
8	68.402	0.013	316.000	20.000	C	0.0
9	75.790	0.003	302.000	80.000	D	8.20D 00
10	75.050	0.003	6215.000	1000.000	D	6.80D-01
11	83.894	0.007	362.000	81.000	C	0.0
12	92.765	0.011	106.000	30.000	C	0.0
13	101.066	0.004	95.000	4.000	C	0.0
14	117.956	0.006	99.000	6.000	A	0.0
15	129.120	0.180	34.000	4.000	.	0.0
16	6152.120	0.670	0.050	0.010	D	0.0
17	6173.650	0.370	0.200	0.020	B	0.0
18	6217.400	0.360	8.410	0.170	A	0.0
19	6218.250	0.300	3.000	0.300	C	0.0
20	6235.130	0.370	1.490	0.050	B	0.0
21	6241.370	0.370	2.180	0.060	B	0.0
22	6269.190	0.380	2.050	0.050	A	0.0
23	6311.140	0.400	2.010	0.030	A	0.0
24	6374.940	0.480	0.220	0.040	C	0.0
25	6464.590	0.480	0.350	0.030	C	0.0

SECTION 1-B:

LIST OF ASSIGNED GAMMA RAYS

CARD NUMBER	GAMMA RAY ENERGY	INITIAL LEVEL	FINAL LEVEL
1	23.000	133	133
2	33.159	138	105
3	41.890	105	63
4	63.686	63	2
5	64.110	63	2
6	75.050	138	63
7	75.790	0	63
8	75.790	139	63
9	92.765	156	63
10	50.869	156	105
11	6218.250	1	156
12	6235.130	1	139
13	6241.370	1	133
14	6269.190	1	105
15	6311.140	1	63
16	6374.940	1	2

TABLE 9
Demonstration - results of the error search made on the synthesized data shown in Table 8.

TESTS MADE IN SECTION 1

ERROR NO.1: THE SAME INDEX NUMBER MUST NOT BE USED TO IDENTIFY BOTH UPPER AND LOWER LEVELS ON AN ASSIGNED GAMMA RAY CARD.
 ERROR NO.2: FOR EVERY ASSIGNED GAMMA RAY, THERE MUST BE A CORRESPONDING CARD IN THE COMPLETE LIST OF OBSERVED GAMMA RAYS (SECTION 1-A). THE TWO ENERGY VALUES MUST BE IDENTICALLY EQUAL.
 ERROR NO.3: TOTAL LIST OF OBSERVED GAMMA RAYS IS CHECKED TO SEE IF ERRORS HAVE BEEN ASSIGNED TO ALL ENERGY VALUES. (DOES NOT CAUSE TERMINATION UNLESS GAMMA RAY IS ASSIGNED.)
 ERROR NO.4: TWO DIFFERENT GAMMA RAYS CANNOT BE ASSIGNED TO THE SAME TRANSITION, NOR CAN A SINGLE GAMMA RAY ASSIGNED TO ONE TRANSITION BE LISTED TWICE.
 ERROR NO.5: TWO OBSERVED GAMMA RAYS SHOULD NOT HAVE THE SAME ENERGY
 ERROR NO.6: AN ASSIGNED GAMMA RAY HAS BEEN GIVEN AN UPPER LEVEL OF ZERO.
 ERROR NO.7: AT LEAST ONE TRANSITION MUST POPULATE THE GROUND STATE
 ERROR NO.8: THE ARRAY SPACE PROVIDED HAS BEEN EXCEEDED BY THE INPUT EXCESS IS IGNORED AND EXECUTION TERMINATED
 ERROR NO.9: THE LIST OF OBSERVED GAMMA RAYS SHOULD BE ORDERED BY INCREASING ENERGY; IF NOT, AN ERROR MESSAGE WILL BE PRINTED, BUT EXECUTION WILL CONTINUE.
 ERROR NO.10: A BLANK CARD BETWEEN THE DATA DECKS IS MISSING.

OCCURRENCE OF ANY ERROR EXCEPT 9 AND 10 TERMINATES EXECUTION OF PROGRAM

ERRORS FOUND

ERROR NO.1: ASSIGNED GAMMA RAY HAS THE SAME UPPER AND LOWER LEVEL NUMBER.
 ASSIGNMENT CARD 1: 23.000 133 133

ERROR NO.2: ASSIGNED GAMMA RAY NOT FOUND IN LIST OF OBSERVED GAMMA RAYS.
 ASSIGNMENT CARD 2: 33.159 138 105

ERROR NO.3: A MEMBER OF THE LIST OF OBSERVED GAMMA RAYS DOES NOT HAVE AN ERROR ASSIGNED TO THE ENERGY.
 OBSERVED CARD 2: 39.100 0.0 2372.000 1383.000 D 0.0

ERROR NO.3: ASSIGNED GAMMA RAY DOES NOT HAVE AN ENERGY ERROR
 OBSERVED CARD 3: 41.890 0.0 1404.000 280.000 E 0.0
 ASSIGNMENT CARD 3: 41.890 105 63 63

ERROR NO. 4: TWO ASSIGNED GAMMA RAYS HAVE THE SAME INITIAL AND FINAL LEVEL NUMBERS.
 ASSIGNMENT CARD 4: 63.686 63 2
 ASSIGNMENT CARD 5: 64.110 63 2

ERROR NO.5: TWO OBSERVED GAMMA RAYS HAVE THE SAME ENERGY.
 OBSERVED CARD 7: 68.402
 OBSERVED CARD 8: 68.402

ERROR NO.6: A GAMMA RAY HAS BEEN ASSIGNED WITH AN UPPER LEVEL OF ZERO
 ASSIGNMENT CARD 7: 75.790 0 63

ERROR NO.7: NO GAMMA RAYS POPULATE THE GROUND STATE

ERROR NO.8: THE DIMENSION OF AT LEAST ONE ARRAY HAS BEEN EXCEEDED BY AN EXCESSIVE AMOUNT OF INPUT DATA
 ARRAY DIMENSIONS ALLOW NO MORE THAN 5 EXCITED STATES, BUT THE INPUT DATA REQUIRE SPACE FOR AT LEAST 18
 THE OBSERVATION MATRIX "P" HAS MAXIMUM DIMENSIONS OF 20 BY 6
 BUT THE INPUT DATA REQUIRE AT LEAST 18 BY 16

ERROR NO.9: THE INPUT DECK OF OBSERVED GAMMA RAYS IS NOT IN ORDER OF ASCENDING ENERGY
 CARD NO. ENERGY
 9 75.790
 10 75.050

ERROR NO.10: THE BLANK CARD THAT SHOULD SEPARATE THE INPUT DATA DECKS IS MISSING
 THIS IS NOT FATAL TO EXECUTION

8 FATAL ERROR(S) IN INPUT DATA

*** EXECUTION TERMINATED ***

3.2 OUTPUT SECTION 2—CALCULATION OF THE "BEST" ENERGY VALUES OF THE EXCITED STATES AND INTENSITY BALANCE/FRACTIONAL BETA FEEDING

In Sec. 2 of the printed output, the results of the least-squares fit of the energies of the excited states to the assigned γ rays is presented. Tables 10A and 10B show the results of a calculation made with the data shown in Table 7. The levels appear in order of ascending energy regardless of the integer identification labels that have been assigned by the user.

For example, in the case presented in Table 10, the capture state at 6374.654 keV was given the identification "1" but since the level has the highest energy, it appears last in the list.

TABLE 10A

Results of the least-squares and intensity-balance calculations.

SECTION 2 PROGRAM STATEFIT-OUTPUT RESULTS

TITLE STATEFIT RUN FOR DISPLAY IN REPORT

7 EXCITED STATES 23 INPUT GAMMA RAYS 11 ASSIGNED GAMMA RAYS

CHI SQUARE PER DEGREE FREEDOM = 1.265 TOTAL UNOBSERVED FEEDING TO ALL EXCITED STATES= 1207.3450

EXCITED STATES (IN ORDER OF LEVEL ENERGY)

NOTES-- SCATTER ERROR = STATISTICAL ERROR MULTIPLIED BY THE SQ. RT. OF CHI SQUARE PER DEGREE FREEDOM

-- FRACTIONAL BETA FEEDING/INTENSITY BALANCE VALUES ARE INVALID UNLESS

GAMMA RAY INTENSITIES ARE CORRECTED FOR INTERNAL CONVERSION

LEVEL NUMBER	CALCULATED LEVEL ENERGY	STATISTICAL ERROR	SCATTER ERROR	INTENSITY BALANCE	DEPOPULATING TRANSITIONS	POPULATING TRANSITIONS
63	63.61362	0.11442	0.12866	974.32300	1	3
105	105.28246	0.18702	0.21030	-35.50000	0	2
133	133.40781	0.24195	0.27207	-14.35000	0	2
138	138.25035	0.14020	0.15765	209.68200	2	0
139	139.26956	0.14163	0.15926	44.51000	1	1
156	156.57260	0.14224	0.15995	19.74000	2	1
1	6374.65403	0.16671	0.18747	8.94000	5	0

TABLE 10B

Results of the least-squares and FRACTIONAL BETA FEEDING calculations with IBETA = 1. This option has been improperly exercised here since the control parameter IBETA should only be set equal to one if the data are derived from a radioactive source, but the calculation has been made on the same neutron-capture data used in Table 10A so that the effect of the alternate choices could be compared directly.

SECTION 2 PROGRAM STATEFIT-OUTPUT RESULTS

TITLE STATEFIT RUN FOR DISPLAY IN REPORT

7 EXCITED STATES 23 INPUT GAMMA RAYS 11 ASSIGNED GAMMA RAYS

CHI SQUARE PER DEGREE FREEDOM = 1.265 TOTAL UNOBSERVED FEEDING TO ALL EXCITED STATES= 1207.3450

EXCITED STATES (IN ORDER OF LEVEL ENERGY)

NOTES-- SCATTER ERROR = STATISTICAL ERROR MULTIPLIED BY THE SQ. RT. OF CHI SQUARE PER DEGREE FREEDOM

-- FRACTIONAL BETA FEEDING/INTENSITY BALANCE VALUES ARE INVALID UNLESS

GAMMA RAY INTENSITIES ARE CORRECTED FOR INTERNAL CONVERSION

LEVEL NUMBER	CALCULATED LEVEL ENERGY	STATISTICAL ERROR	SCATTER ERROR	FRACTIONAL BETA FEEDING	DEPOPULATING TRANSITIONS	POPULATING TRANSITIONS
63	63.61362	0.11442	0.12866	0.80700	1	3
105	105.28246	0.18702	0.21030	-0.02940	0	2
133	133.40781	0.24195	0.27207	-0.01189	0	2
138	138.25035	0.14020	0.15765	0.17367	2	0
139	139.26956	0.14163	0.15926	0.03687	1	1
156	156.57260	0.14224	0.15995	0.01635	2	1
1	6374.65403	0.16671	0.18747	0.00740	5	0

3.2.1 Goodness of fit. As in any least-squares calculation, the reliability of the results and the significance of the computed χ^2 depend critically upon (1) that the function being fitted to the data accurately describe the experimental measurements in the extreme limit of infinitely precise measurements and (2) that the experimental weights associated with each of the data points be truly statistical errors that follow a normal distribution.

In the present calculation, the correctness of the function depends upon the reality or spuriousness of each of the postulated energy levels to which the gamma rays are assigned, i. e., if a level has been entered into the decay scheme as the result of an "accidental" coincidence of one or more γ -ray energy differences or sums, the function will be incorrect to that extent. Also, if a γ ray is incorrectly assigned between a pair of states it is not a true observation of the difference between these two parameters. If we assume that neither of these errors has been made, then the usual statistical significance can be attached to the calculation provided the errors associated with the γ -ray energies are truly statistical. For this reason, one should exercise extreme caution in assigning weights to the γ -ray energies.

For a large number of degrees of freedom the value of χ^2 per degree of freedom should approach unity. The column labeled STATISTICAL ERROR (Table 10) contains the errors in the states as computed with the experimental uncertainties given the assigned γ rays (Sec. 2.4). If for some reason the assigned weights are systematically too high, or too low, it can be shown that multiplication by $\sqrt{\chi^2_{pdf}}$ will normalize the computed errors in such a way as to compensate this kind of deviation in the data. In the column headed SCATTER ERROR, the statistical errors have been adjusted in this manner. On the other hand, this correction will not compensate for an experimenter's selective bias, i. e., if the data have been "culled." The χ^2 should not ordinarily be interpreted in the customary sense, because in the early stages of developing the decay scheme, the assignment of γ rays will be made with caution. For example, if one arbitrarily requires that the experimental uncertainty of any assigned gamma-ray energy must not exceed the residual, i. e., $\Delta G_k \leq |G_k - T_k|$, the χ^2 per degree of freedom will naturally be significantly "too" low. Under this constraint, the χ^2 will approach the value 0.3 for a large number of assigned γ rays.

The confidence that the user has in the actual existence of each state is usually influenced by the number of populating and depopulating

γ rays that can be assigned to it. As a convenience, the total number of populations and depopulations assigned to each state are printed.

3.2.2. Relative intensity. Before they are used to compute the INTENSITY BALANCE (or FRACTIONAL BETA FEEDING), the γ -ray intensity values are corrected for internal conversion by a simple multiplication by the quantity $(1 + \alpha)$. If the coefficients are not provided, the intensity values are used as they are inputted.

3.2.3. Intensity balance/fractional beta feeding. Consideration of the nuclear physics involved dictates that, when the decay scheme is complete, the intensity balance of each state must either be zero or positive (within experimental uncertainties).

The information printed in the fifth column of Sec. 2 of the output depends upon the option exercised by the user when the constant IBETA is entered on the control card. The choice is also reflected in the heading that will be printed above the column. If the value of IBETA is zero (or blank on the card), the heading will appear "INTENSITY BALANCE" (Table 10-A) and if the constant is entered as 1, the column will be headed "FRACTIONAL BETA FEEDING" (Table 10-B). In the case of neutron capture γ -ray data, the INTENSITY BALANCE is in γ -ray intensity units (see Sec. 2.5.1) and can be interpreted as feeding of the states by unobserved secondary γ rays. Negative values indicate an excess of population over depopulation. This may result from errors in the internal-conversion corrections, a misplaced populating γ ray, or a missing depopulating γ ray.

Calculation of the Fractional Beta Feeding is described in Sec. 2.5.2 and is applicable if the data refer to radioactive sources.

In either case, the total unobserved feeding is printed at the beginning of the section. If the "INTENSITY BALANCE" has been computed, the "Fractional Beta Feeding" can be calculated by merely dividing the entries in the column by the total unobserved feeding.

3.3. OUTPUT SECTION 3—REVIEW OF THE ASSIGNED γ RAYS

After the least-squares computation of the level energies, a systematic comparison is made in Section 3 of the program between each of the assigned gamma rays and the calculated transition it is presumed to represent. Table 11 shows this information for the level scheme depicted in Fig. 1. The assigned γ rays are listed in order of ascending energy together with the initial and final level numbers. Since they are not usually arranged monotonically in the data deck, the sequence number (CARD NUMBER) is also given.

TABLE 11

Comparison between the assigned gamma rays and the corresponding computed transition energies.

SECTION 3 ASSIGNED GAMMA RAYS									
NOTE-- MULTI INDICATES GAMMA RAY HAS BEEN ASSIGNED TO MORE THAN 1 PAIR OF ENERGY LEVELS									
-- IF CHI EXCEEDS 100.0, THE ENTRY "GT 99.999" WILL APPEAR.									
ERROR NOTES	CARD NUMBER	INITIAL LEVEL	FINAL LEVEL	GAMMA RAY ENERGY	GAMMA RAY ERROR	CALCULATED TRANSITION	ENERGY DIFFERENCE	CHI	TRANSITION INTENSITY
	6	156	133	23.00000	0.30000	23.16479	-0.165	-0.549	12.17000
	9	138	105	33.02000	0.15000	32.96789	0.052	0.347	33.45000
	7	63	0	63.58000	0.12000	63.61362	-0.034	-0.286	1207.12500
	10	138	63	74.62000	0.08500	74.63673	-0.017	-0.197	176.23200
	11	139	63	75.61000	0.09000	75.65594	-0.046	-0.510	46.00000
	8	156	63	93.01000	0.09500	92.95898	0.051	0.537	10.57000
	5	1	156	6218.25000	0.21000	6218.08144	0.169	0.803	3.00000
	2	1	139	6235.03000	0.25000	6235.38448	-0.354	-1.418	1.49000
	1	1	133	6241.37000	0.26000	6241.28623	0.124	0.476	2.18000
	4	1	105	6269.19000	0.28000	6269.37157	-0.182	-0.648	2.05000
	3	1	0	6374.94000	0.35000	6374.65403	0.286	0.817	0.22000

Assignment of the same γ ray to two different places in the decay scheme may or may not be an inadvertent error. If the user believes that two different pairs of states have nearly exactly the same energy difference, he may feel it advisable to make the assignment to both transitions during the early stages of development of the decay scheme. A unique decision must be made before the final calculation is carried out, otherwise the least-squares computation will be in error. To keep the user alerted to the fact that there are multiple assignments in the fit, the entry "MULTI" is made in the column headed ERROR NOTES ahead of each γ ray that appears more than once in the list of assigned γ rays. The data presented in Table 12 were specifically prepared to demonstrate this feature of the program. If the multiple assignment has been inadvertent, the appropriate correction can be made; if it has been made intentionally,

the user will be reminded to resolve the ambiguity before making the final calculation.

TABLE 12

Demonstration of the error flags that appear when multiple assignments are made and when there is an excessive discrepancy between the gamma-ray energy and its corresponding transition energy.

SECTION 3 ASSIGNED GAMMA RAYS

NOTE-- MULTI INDICATES GAMMA RAY HAS BEEN ASSIGNED TO MORE THAN 1 PAIR OF ENERGY LEVELS
-- IF CHI EXCEEDS 100.0, THE ENTRY "GT 99.999" WILL APPEAR.

ERROR NOTES	CARD NUMBER	INITIAL LEVEL	FINAL LEVEL	GAMMA RAY ENERGY	GAMMA RAY ERROR	CALCULATED TRANSITION	ENERGY DIFFERENCE	CHI	NORMALIZED INTENSITY
	3	138	105	33.15900	0.00100	33.15876	0.000	0.238	0.05101
	4	63	0	63.68600	0.00200	63.68695	-0.001	-0.477	0.84080
MULTI	6	213	138	75.05000	0.00200	75.05000	-0.000	-0.000	0.15918
MULTI	2	75	0	75.05000	0.00200	75.05000	-0.000	-0.000	0.15918
MULTI	5	138	63	75.05000	0.00200	75.05095	-0.001	-0.477	0.15918
	7	150	0	150.10000	0.02000	150.10000	-0.000	-0.000	0.00002
	1	1	105	6180.00000	0.38000	6214.42825	-34.428	-90.601	0.00003
	8	1	0	6374.94000	0.48000	6320.00739	54.933	GT 99.999	0.00000

The CALCULATED TRANSITION is the transition energy T_k derived from the "best" level energies determined in the least-squares fit. The residual (ENERGY DIFFERENCE) is the difference in energy between the assigned γ ray and the calculated transition, i. e. ,

$$\text{ENERGY DIFFERENCE} = G_j - T_{m,m'} \quad (3.3.1)$$

The algebraic sign of the residual indicates whether the γ -ray energy is greater or less than the transition energy.

The relative deviation CHI, i. e. ,

$$\text{CHI} = (G_k - T_k) / \Delta G_k, \quad (3.3.2)$$

is also calculated. The square of each value of CHI is the contribution made by the particular assignment to the total χ^2 shown in Sec. 2. When the total χ^2 per degree of freedom appears excessive, one can usually locate the assigned γ ray that is causing the deviation by reviewing the CHI values. An inordinately high value may indicate that a wrong gamma-ray assignment has been made, or that an error has been made in punching the index numbers on a card. Any fit containing such a defect should be rejected. The actual value of any extremely high CHI is not considered to be significant; instead of printing the value itself, an error flag "GT $\pm$ 99.999" appears (see Table 12).

Considered together with the GAMMA RAY ERROR, the ENERGY DIFFERENCE and the relative deviation CHI, are of value in deciding whether or not the assignment is a "good" one. Periodic review of these columns gives the user an overall feeling for the scatter in the match between the data and the computed energies of the states.

The intensity of each assigned γ ray is printed in the last column. If the data are not associated with a radioactive sample and the control constant IBETA has been set equal to zero, the intensities appear corrected only for internal conversion and the column heading TRANSITION INTENSITY is used. If the alternative option IBETA=1 has been invoked, the corrected intensities are divided by the total feeding and appear under the heading "NORMALIZED INTENSITY." For purposes of display, the choice IBETA=0 was used for the calculation presented in Table 11 and the alternative, IBETA=1 was used for Table 12.

3.4. OUTPUT SECTION 4—TABULATION OF DEPOPULATING TRANSITIONS AND SEARCH FOR UNASSIGNED γ RAYS

In Section 4 of the program, a systematic search of the data is made to prepare a table of which γ rays have been assigned and which ones might be assigned provided they satisfy a standard of acceptance prescribed by the user. Each entry in the total list of γ rays is subject to a "window test"; the parameter "WIDE"(W) is selected by the user to control the stringency with which the selection test will be imposed. It is defined in the equation:

3.4.1. Window test. A γ ray with energy G_j will be selected as eligible for assignment if

$$|G_j - T_{m,m'}| \leq W \sqrt{\Delta G_j^2 + \Delta e_m^2 + \Delta e_{m'}^2},$$

where

$$T_{m,m'} = |e_m - e_{m'}|.$$

3.4.2. Classification of gamma-ray assignments. If there are M excited states, there are $\frac{1}{2}M(M+1)$ possible transitions between them when the ground state is taken into account. In output Sec. 4, the levels are considered one at a time in order of increasing energy. All of the possible transitions to lower states are calculated and grouped into one paragraph (Table 13). For each of these depopulating transitions $T_{m,m'}$, the list of assigned γ rays is searched on the basis of level numbers to ascertain if any have already been assigned to the particular transition. If one is found, this fact is noted and the list of assigned γ rays then scanned again, but this time on the basis of energy equivalence instead of level numbers, to determine whether the particular γ ray might also have been assigned elsewhere. The "window test" (3.4.1) is then invoked and the complete list of observed γ rays is searched to find any members which might be

TABLE 13

Classification of all possible transitions in terms of assigned γ rays and potential assignments (notation used in program sec. 4 and sec. 5).
The data used to generate the table were simulated for purposes of the demonstration and have no physical meaning.

SECTION 4 DEPOPULATING TRANSITIONS												
COMMENTS: (1) ASSIGNED HERE/ALSO ASSIGNED TO A,B: THIS ASSIGNMENT HAS BEEN MADE/ALSO ELSEWHERE (2) UNASSIGNED: THIS GAMMA RAY SATISFIES ACCEPTANCE TEST BUT HAS NOT BEEN ASSIGNED (3) NOT ASSIGNED HERE/ASSIGNED TO/ALSO ASSIGNED TO: GAMMA RAY SATISFIES TEST BUT IS ASSIGNED ELSEWHERE (4) NONE FOUND: NO GAMMA RAY FOUND THAT SATISFIES ACCEPTANCE TEST												
INITIAL LEVEL NUMBER	FINAL LEVEL NUMBER	INITIAL ENERGY	FINAL ENERGY	TRANSITION ENERGY	TRANSITION ERROR	GAMMA RAY ENERGY	GAMMA RAY ERROR	ENERGY DIFFERENCE	KEY	COMMENTS	GAMMA RAY CONFIDENCE LEVELS I.D.	
63	0	63.686	0.0	63.686	0.002	63.686	0.002	-0.000	-0.000	ASSIGNED HERE	A	
75	0	75.050	0.0	75.050	0.002	75.050	0.002	-0.000	-0.000	ASSIGNED HERE	D	
75	0	75.050	0.0	75.050	0.002	75.050	0.002	-0.000	-0.000	ALSO ASSIGNED TO 138 63		
75	63	75.050	63.686	11.364	0.003	75.049	0.200	-0.001	-0.005	UNASSIGNED	TEST GAMMA	
105	0	105.577	0.0	105.577	0.003	NONE FOUND						
105	63	105.577	63.686	41.891	0.004	41.890	0.001	-0.001	-0.267	UNASSIGNED	E	
105	75	105.577	75.050	30.527	0.004	NONE FOUND						
138	0	138.736	0.0	138.736	0.003	NONE FOUND						
138	63	138.736	63.686	75.050	0.003	75.050	0.002	-0.000	-0.000	ASSIGNED HERE	D	
138	63	138.736	63.686	75.050	0.003	75.050	0.002	-0.000	-0.000	ALSO ASSIGNED TO 75 0		
138	75	138.736	75.050	63.686	0.003	75.049	0.200	-0.001	-0.005	UNASSIGNED	TEST GAMMA	
138	75	138.736	75.050	63.686	0.003	63.686	0.002	-0.000	-0.000	NOT ASSIGNED HERE	A	
138	105	138.736	105.577	33.159	0.004	33.159	0.001	0.000	0.000	ASSIGNED HERE	C	
150	0	150.100	0.0	150.100	0.020	150.100	0.020	-0.000	-0.000	ASSIGNED HERE	TEST GAMMA	
150	63	150.100	63.686	86.414	0.020	NONE FOUND						
150	75	150.100	75.050	75.050	0.020	75.050	0.002	-0.000	-0.000	NOT ASSIGNED HERE	D	
150	75	150.100	75.050	75.050	0.020	75.050	0.002	-0.000	-0.000	ASSIGNED TO 75 0		
150	75	150.100	75.050	75.050	0.020	75.050	0.002	-0.000	-0.000	ALSO ASSIGNED TO 138 63		
150	138	150.100	138.736	11.364	0.020	75.049	0.200	-0.001	-0.005	UNASSIGNED	TEST GAMMA	
213	0	213.786	0.0	213.786	0.003	NONE FOUND						
213	63	213.786	63.686	150.100	0.004	150.100	0.020	-0.000	-0.000	NOT ASSIGNED HERE	TEST GAMMA	
213	75	213.786	75.050	138.736	0.004	150.100				ASSIGNED TO 150 0		
213	105	213.786	105.577	108.209	0.005	NONE FOUND						
213	138	213.786	138.736	75.050	0.004	75.050	0.002	0.000	0.000	ASSIGNED HERE	D	
213	138	213.786	138.736	75.050	0.004	75.050	0.002	0.000	0.000	ALSO ASSIGNED TO 75 0		
213	150	213.786	150.100	63.686	0.020	75.049	0.200	-0.001	-0.005	UNASSIGNED	TEST GAMMA	
213	150	213.786	150.100	63.686	0.020	63.686	0.002	-0.000	-0.000	NOT ASSIGNED HERE	A	
213	150	213.786	150.100	63.686	0.020	63.686	0.002	-0.000	-0.000	ASSIGNED TO 63 0		
1	0	6374.940	0.0	6374.940	0.480	6374.940	0.480	0.0	0.0	ASSIGNED HERE	C	
1	63	6374.940	63.686	6311.254	0.480	6311.140	0.400	-0.114	-0.182	UNASSIGNED	A	
1	75	6374.940	75.050	6299.890	0.480	NONE FOUND						
1	105	6374.940	105.577	6269.363	0.480	6269.190	0.380	-0.173	-0.283	UNASSIGNED	A	
1	138	6374.940	138.736	6236.204	0.480	NONE FOUND						
1	150	6374.940	150.100	6224.840	0.480	NONE FOUND						
1	213	6374.940	213.786	6161.154	0.480	NONE FOUND						

assigned to the transition. The results of the study made of each possible transition are described with the use of one or more of six comments entered in the "COMMENTS" column of the printed output as follows:

(1) ASSIGNED HERE: For every member in the list of assigned γ rays, the γ -ray energy, together with the other pertinent information, is printed alongside the transition and followed by the words ASSIGNED HERE in the COMMENT column.

(2) ALSO ASSIGNED TO A, B: When a γ ray is found to have been assigned to the transition under investigation and marked "ASSIGNED HERE", a second search of the assignment list based on energy equivalence is then carried out to determine whether the same γ ray has also been assigned elsewhere. If such an event is found, the γ -ray energy alone is printed again on the next line along with the comment "ALSO ASSIGNED TO A, B". This process continues until the list is exhausted and all the multiple assignments have been noted. Such multiple assignments are also marked in section 3 of the output (see Sec. 3.3).

(3) UNASSIGNED: After the list of assigned γ rays has been searched, the "window test" is then invoked and the complete list of observed γ rays is scanned to find members that satisfy the acceptance criterion (this procedure is followed whether or not any assigned γ rays were found). When an acceptable candidate for assignment has been located, and before any printing is done, the list of assignments is first searched to determine whether the candidate has been assigned between any other levels. If the γ ray has not been previously assigned elsewhere, its energy is written alongside the transition and the word "UNASSIGNED" entered in the comment column. These are the entries that should be given primary consideration for assignment in the next fit.

(4) NOT ASSIGNED HERE: If, in the search of the observed γ rays a candidate for assignment is located, but found to have already been assigned elsewhere, its energy is written alongside the transition and the words "NOT ASSIGNED HERE" are entered in the comment column. This notation is used to emphasize the fact that, although the γ -ray satisfies

the acceptance test, it has already been placed between two other levels. A choice may then be made as to whether the earlier assignment should be retained or abandoned in favor of this new possibility.

(5) ASSIGNED TO A, B/ALSO ASSIGNED TO C, D: After the entry "NOT ASSIGNED HERE" has been made alongside the transition, the existing assignment will be noted on the next line with the notation "ASSIGNED TO A, B". If any further previous assignments are found they are printed on succeeding lines followed by the words "ALSO ASSIGNED TO C, D" etc.

(6) NONE FOUND: If no γ ray was found to have been assigned to the transition and upon completion of the search of the complete list, no members were found to satisfy the "window test", the words "NONE FOUND" are entered alongside the transition in the column where the γ -ray energy is normally written.

The various ways in which each possible transition may be processed is shown in Table 13. The input data have been synthesized to provide this output for demonstration purposes and the content of the table has no physical meaning. The 75.050-keV γ ray has been assigned between three different pairs of states and a fourth place where it might be assigned has also been provided. Note that for the three cases in which the γ ray was assigned, 75-0, 138-63, and 212-138, the output shows this fact with the transitions merely permuted. Note that in the instance where the 75.050-keV γ ray satisfied the "window test" but the assignment, 150-75 had not been made, the words "NOT ASSIGNED HERE" alerts the user to the fact that, although the γ ray is an acceptable candidate, it has already been assigned elsewhere; the other assignments then appear conveniently on the next three lines. To further demonstrate the cataloging routine, a "test" γ ray differing only slightly from the 75.050-keV component, i. e., 75.049 keV was introduced into the list of observed γ rays. Note that in all four cases where this γ ray met the window test, it appears adjacent to the data concerning the assigned 75.050 member.

Table 14 is the Sec. 4 computer output resulting from the fit made with the data in Table 7 and representing the decay scheme in Fig. 1. Note that all of the assigned γ rays appearing in Table 7 (program Sec. 1-B) appear marked "ASSIGNED HERE". The three γ rays shown in dotted lines in Fig. 1, i. e., the 51.2-, 41.9-, and the 6311-keV transitions have been selected by the window test and are noted "UNASSIGNED". The remaining transitions are all marked "NONE FOUND" which indicates that none of the γ rays in the observed data fit any of these transitions. It is not sufficient to conclude from these results that all of the possibilities have been exhausted. When another fit, including the three unassigned γ rays is made, the levels can be expected to shift slightly, and this may reveal more candidates for assignment.

TABLE 14

Results of the data search made following the least-squares fit shown in Table 10A and represented by the decay scheme in fig. 1. Program sec. 4 classifies all possible transitions according to depopulations.

SECTION 4 DEPOPULATING TRANSITIONS

COMMENTS: (1) ASSIGNED HERE/ALSO ASSIGNED TO A,B: THIS ASSIGNMENT HAS BEEN MADE/ALSO ELSEWHERE
(2) UNASSIGNED: THIS GAMMA RAY SATISFYS ACCEPTANCE TEST BUT HAS NOT BEEN ASSIGNED
(3) NOT ASSIGNED HERE/ALSO ASSIGNED TO: GAMMA RAY SATISFYS TEST BUT IS ASSIGNED ELSEWHERE
(4) NONE FOUND: NO GAMMA RAY FOUND THAT SATISFYS ACCEPTANCE TEST

INITIAL LEVEL NUMBER	FINAL LEVEL NUMBER	INITIAL ENERGY	FINAL ENERGY	TRANSITION ENERGY	TRANSITION ERROR	GAMMA RAY ENERGY	GAMMA RAY ERROR	ENERGY DIFFERENCE	KEY	COMMENTS	GAMMA RAY CONFIDENCE LEVEL(I.D.)
63	0	63.614	0.0	63.614	0.114	63.580	0.120	-0.034	-0.203	ASSIGNED HERE	A
105	0	105.282	0.0	105.282	0.187	NONE FOUND					
105	63	105.282	63.614	41.669	0.219	41.890	0.075	0.221	0.954	UNASSIGNED	E
133	0	133.408	0.0	133.408	0.242	NONE FOUND					
133	63	133.408	63.614	69.794	0.268	NONE FOUND					
133	105	133.408	105.282	28.125	0.306	NONE FOUND					
138	0	138.250	0.0	138.250	0.140	NONE FOUND					
138	63	138.250	63.614	74.637	0.181	74.620	0.085	-0.017	-0.084	ASSIGNED HERE	D
138	105	138.250	105.282	32.968	0.234	33.020	0.150	0.052	0.188	ASSIGNED HERE	C
138	133	138.250	133.408	4.843	0.280	NONE FOUND					
139	0	139.270	0.0	139.270	0.182	NONE FOUND					
139	63	139.270	63.614	75.656	0.182	75.610	0.090	-0.046	-0.226	ASSIGNED HERE	D
139	105	139.270	105.282	33.987	0.235	NONE FOUND					
139	133	139.270	133.408	5.862	0.280	NONE FOUND					
139	138	139.270	138.250	1.019	0.199	NONE FOUND					
156	0	156.573	0.0	156.573	0.102	NONE FOUND					
156	63	156.573	63.614	92.959	0.183	93.010	0.095	0.051	0.248	ASSIGNED HERE	C
156	105	156.573	105.282	51.290	0.235	51.219	0.090	-0.071	-0.283	UNASSIGNED	D
156	133	156.573	133.408	23.165	0.281	23.000	0.300	-0.165	-0.401	ASSIGNED HERE	B
156	138	156.573	138.250	18.322	0.200	NONE FOUND					
156	139	156.573	139.270	17.303	0.201	NONE FOUND					
1	0	6374.654	0.0	6374.654	0.167	6374.940	0.350	0.286	0.738	ASSIGNED HERE	C
1	63	6374.654	63.614	6311.040	0.202	6311.140	0.260	0.100	0.302	UNASSIGNED	A
1	105	6374.654	105.282	6269.372	0.251	6269.190	0.280	-0.182	-0.483	ASSIGNED HERE	A
1	133	6374.654	133.408	6241.246	0.294	6241.370	0.260	0.124	0.315	ASSIGNED HERE	B
1	138	6374.654	138.250	6236.404	0.218	NONE FOUND					
1	139	6374.654	139.270	6235.384	0.219	6235.030	0.250	-0.354	-1.067	ASSIGNED HERE	B
1	156	6374.654	156.573	6218.081	0.219	6218.250	0.210	0.169	0.555	ASSIGNED HERE	C

3.4.3. Merit of the assignments. For every γ ray that is assigned, or that is a candidate for assignment, two additional numbers are calculated to aid the user in deciding what action to take when he reviews the output. In the column headed ENERGY DIFFERENCE, the residual, i. e., the

difference in energy between the γ ray and the computed transition is written (see Sec. 3.3.1). The algebraic sign of the difference is retained so that it is immediately apparent whether the γ ray is too high or too low in energy and by what amount. This number can be related directly to the errors in both the transition and the γ ray.

The relative error KEY, that is, the ratio between the difference in energy and the computed statistical uncertainty, is calculated and is a measure of what contribution the assignment does or will make to the total goodness of fit of the calculation.

$$\text{KEY} = \frac{G_j - T_{m,m'}}{\sqrt{\Delta G_j^2 + \Delta T_{m,m'}^2}} \quad (3.4.3.1)$$

Finally, the experimenter's rank or "confidence level" associated with the γ ray in question is printed for every γ ray that is assigned or selected for possible assignment. In the system used by the authors, the letters range from A through F in order of diminishing confidence.

3.5. OUTPUT SECTION 5—TABULATION OF POPULATING TRANSITIONS AND SEARCH FOR UNASSIGNED GAMMA RAYS

As in output Sec. 4, each of the levels is again considered in order of ascending energy; the search routine used is identical. However, in this section, all of the possible transitions from higher-lying states are computed and grouped into one paragraph (Table 15). The information presented is, of course, a repetition of that in Sec. 4 but differently distributed. If one wishes to review the status of a particular state, he need only consult at the same time the paragraph in Sec. 4 containing the depopulating transitions and the corresponding paragraph in Sec. 5 containing all the populating transitions to that state. The two associated paragraphs are readily identified by the fact that in Sec. 4, the identification of the state from which all the depopulations are grouped is repeated throughout the paragraph in the first column headed INITIAL LEVEL NUMBER, while in

Sec. 5, the state identification is common in the second column, FINAL LEVEL NUMBER. If one wishes to review the entire set of assignments without reference to a particular state, either section is equally applicable. Table 15 is a typical example of the output of Section 5 of the program. It contains the same information shown in Table 14 for Sec. 4.

TABLE 15

Results of the data search made following the least-squares fit shown in Table 10A represented by the decay scheme in fig. 1. Program sec. 5 classifies all possible transitions according to populations. (The informational content of the table is redundant with that in program sec. 4 (Table 14).

SECTION 5 POPULATING TRANSITIONS											
COMMENTS: (1) ASSIGNED HERE/ALSO ASSIGNED TO A,R: THIS ASSIGNMENT HAS BEEN MADE/ALSO ELSEWHERE (2) UNASSIGNED: THIS GAMMA RAY SATISFIES ACCEPTANCE TEST BUT HAS NOT BEEN ASSIGNED (3) NOT ASSIGNED HERE/ALSO ASSIGNED TO: GAMMA RAY SATISFIES TEST BUT IS ASSIGNED ELSEWHERE (4) NONE FOUND: NO GAMMA RAY FOUND THAT SATISFIES ACCEPTANCE TEST											
INITIAL LEVEL NUMBER	FINAL LEVEL NUMBER	INITIAL ENERGY	FINAL ENERGY	TRANSITION ENERGY	TRANSITION ERROR	GAMMA RAY ENERGY	GAMMA RAY ERROR	ENERGY DIFFERENCE	KEY	COMMENTS	GAMMA RAY CONFIDENCE LEVEL(1.D.)
63	0	63.614	0.0	63.614	0.114	63.580	0.120	-0.034	-0.203	ASSIGNED HERE	A
105	0	105.282	0.0	105.282	0.187	NONE FOUND					
133	0	133.408	0.0	133.408	0.242	NONE FOUND					
138	0	138.250	0.0	138.250	0.140	NONE FOUND					
139	0	139.270	0.0	139.270	0.142	NONE FOUND					
156	0	156.573	0.0	156.573	0.142	NONE FOUND					
1	0	6374.654	0.0	6374.654	0.167	6374.940	0.350	0.286	0.738	ASSIGNED HERE	C
105	63	105.282	63.614	41.669	0.219	41.890	0.075	0.221	0.954	UNASSIGNED	E
133	63	133.408	63.614	69.794	0.268	NONE FOUND					
138	63	138.250	63.614	74.637	0.181	74.620	0.085	-0.017	-0.084	ASSIGNED HERE	D
139	63	139.270	63.614	75.656	0.182	75.610	0.090	-0.046	-0.226	ASSIGNED HERE	D
156	63	156.573	63.614	92.959	0.183	93.010	0.095	0.051	0.248	ASSIGNED HERE	C
1	63	6374.654	63.614	6311.040	0.202	6311.140	0.260	0.100	0.302	UNASSIGNED	A
133	105	133.408	105.282	28.125	0.306	NONE FOUND					
138	105	138.250	105.282	32.968	0.234	33.020	0.150	0.052	0.188	ASSIGNED HERE	C
139	105	139.270	105.282	33.987	0.235	NONE FOUND					
156	105	156.573	105.282	51.290	0.235	51.219	0.090	-0.071	-0.283	UNASSIGNED	D
1	105	6374.654	105.282	6269.372	0.251	6269.190	0.280	-0.182	-0.483	ASSIGNED HERE	A
138	133	138.250	133.408	4.843	0.280	NONE FOUND					
139	133	139.270	133.408	5.862	0.290	NONE FOUND					
156	133	156.573	133.408	23.165	0.281	23.000	0.300	-0.165	-0.401	ASSIGNED HERE	B
1	133	6374.654	133.408	6241.246	0.294	6241.370	0.260	0.124	0.315	ASSIGNED HERE	B
139	138	139.270	138.250	1.019	0.199	NONE FOUND					
156	138	156.573	138.250	18.322	0.200	NONE FOUND					
1	138	6374.654	138.250	6236.404	0.218	NONE FOUND					
156	139	156.573	139.270	17.303	0.201	NONE FOUND					
1	139	6374.654	139.270	6235.384	0.219	6235.030	0.250	-0.354	-1.067	ASSIGNED HERE	B
1	156	6374.654	156.573	6218.081	0.219	6218.250	0.210	0.169	0.555	ASSIGNED HERE	C

3.6. OUTPUT SECTION 6—COMPLETE LIST OF POSSIBLE TRANSITIONS IN ORDER OF ENERGY

One sometimes wishes to know where a particular γ ray might be fitted into the level system. A monotonically ordered list of all possible transitions is useful for this purpose. The energies of the levels between each transition occurs is also listed. If a γ ray has been assigned to a particular transition, the transition is marked by a row of asterisks (see Table 16). The specific assigned γ ray may be identified by consulting either output section 3 or section 7.

TABLE 16

Monotonically ordered list of all possible transition energies (for the decay scheme shown in fig. 1.)

SECTION 6 COMPUTED LIST OF ALL POSSIBLE TRANSITION ENERGIES
NOTE-- ***** INDICATES ASSIGNED GAMMA RAY

TRANSITION ENERGY	INITIAL ENERGY	FINAL ENERGY
1.01921	139.270	138.250
4.84254	138.250	133.408
5.86175	139.270	133.408
17.30304	156.573	139.270
18.32225	156.573	138.250
23.16479 *****	156.573	133.408
28.12535	133.408	105.282
32.96789 *****	138.250	105.282
33.98710	139.270	105.282
41.66884	105.282	63.614
51.29014	156.573	105.282
63.61362 *****	63.614	0.0
69.79419	133.408	63.614
74.63673 *****	138.250	63.614
75.65594 *****	139.270	63.614
92.95898 *****	156.573	63.614
105.28246	105.282	0.0
133.40781	133.408	0.0
138.25035	138.250	0.0
139.26956	139.270	0.0
156.57260	156.573	0.0
6218.08144 *****	6374.654	156.573
6235.38448 *****	6374.654	139.270
6236.40368	6374.654	138.250
6241.24623 *****	6374.654	133.408
6269.37157 *****	6374.654	105.282
6311.04042	6374.654	63.614
6374.65403 *****	6374.654	0.0

3.7. OUTPUT SECTION 7—COMPLETE LIST OF OBSERVED γ -RAY ENERGIES INCLUDING ASSIGNED TRANSITIONS

In Sec. 7, the complete block of input data is reviewed (Table 17). Construction of the decay scheme will usually commence before final detailed analysis of the spectroscopic data has been completed, so this list of γ rays can be expected to change from time to time as new γ rays are resolved and others deleted. The list of observed γ rays is presented in order of increasing energy. For convenience, the number of the associated cards in the data deck is noted. Instead of listing the γ -ray intensity as it was introduced, the intensity is printed as "TRANSITION INTENSITY", which indicates that correction has been made for internal conversion.

TABLE 17

Review of the input data - the assignment information is combined with the complete list of experimentally observed gamma rays.

SECTION 7 COMPLETE LIST OF OBSERVED GAMMA RAY ENERGIES (INCLUDING ASSIGNED TRANSITIONS)

GAMMA NUMBER	CARD NUMBER	GAMMA RAY ENERGY	GAMMA RAY ERROR	TRANSITION INTENSITY	INTENSITY ERROR	INITIAL ENERGY	FINAL ENERGY	CONFIDENCE LEVEL
1	1	23.000	0.300	12.170	9.13	156.6	133.4	B
2	2	33.020	0.150	33.450	2.68	138.3	105.3	C
3	3	39.100	0.800	36.500	21.17			D
4	4	41.890	0.075	450.576	45.04			E
5	5	51.219	0.090	584.400	17.55			D
6	6	63.580	0.120	1207.125	12.04	63.6	0.0	A
7	7	68.402	0.105	2.810	0.17			C
8	8	74.620	0.085	176.232	26.44	138.3	63.6	D
9	9	75.610	0.090	46.000	11.50	139.3	63.6	D
10	10	83.894	0.078	4.060	0.89			C
11	11	93.010	0.095	10.570	0.21	156.6	63.6	C
12	12	101.066	0.076	1.330	0.05			C
13	13	117.956	0.095	1.430	0.09			A
14	14	129.120	0.180	0.520	0.05			
15	15	6152.120	0.420	0.050	0.01			D
16	16	6173.650	0.230	0.200	0.02			B
17	17	6217.400	0.220	8.410	0.17			A
18	18	6218.250	0.210	3.000	0.30	6374.7	156.6	C
19	19	6235.030	0.250	1.490	0.05	6374.7	139.3	B
20	20	6241.370	0.260	2.180	0.06	6374.7	133.4	B
21	21	6269.190	0.280	2.050	0.05	6374.7	105.3	A
22	22	6311.140	0.260	2.010	0.03			A
23	23	6374.940	0.350	0.220	0.04	6374.7	0.0	C

As each entry is made in the list, the assignments are searched to determine whether that γ ray has been assigned. If it is assigned, this fact is shown by printing the energies of the associated initial and final levels. One can thus review the entire input data and see at a glance which γ rays have been assigned and between which levels.

Acknowledgments

In its present form, the program STATEFIT incorporates a large number of modifications and improvements that were made over a period of years. The authors wish to thank a number of students who worked and studied with our group under the Argonne Undergraduate Honors Research Program. Much of the detailed coding was done and many useful suggestions were made by them. In particular we wish to mention the following:

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Thomas E. Main (Spring 1970) Knox College, Galesburg, Illinois.

Clemence J. Rachel (Spring 1974) St. Josephs College, Collegeville,
Indiana.

Gregory M. Swider (Summer-Fall 1974) Knox College, Galesburg,
Illinois.

Reference

- ¹ S. B. Burson, P. J. Daly, P. F. A. Goudsmit, and A. A. C. Klaasse, Nucl. Phys. A204 (1973) 337.

FORTRAN Listing of Program STATEFIT

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C PROGRAM STATEFIT
 C DIVISION ARGONNE NATIONAL LABORATORY, 9700 S. CASS AVE., ARGONNE, ILL.60439
 C REQUIRED INPUT DATA:
 C (1) COMPLETE LIST OF EXPERIMENTAL GAMMA-RAY ENERGIES:
 C THIS LIST CONTAINS ALL OF THE AVAILABLE DATA INCLUDING THE EXPERIMENTALLY
 C DETERMINED GAMMA-RAY ENERGY VALUES TOGETHER WITH ASSOCIATED UNCERTAINTIES,
 C RELATIVE INTENSITIES, ERRORS IN INTENSITY, A CONFIDENCE RATING, AND THE
 C TOTAL CONVERSION COEFFICIENT (K+L+M) IF KNOWN.
 C (2) LIST OF EXPERIMENTALLY DETERMINED GAMMA-RAY ENERGY VALUES THAT ARE
 C ASSIGNED BETWEEN A SET OF ENERGY LEVELS PRESUMED TO EXIST. THE LEVELS ARE
 C IDENTIFIED BY INTEGERS (NO INPUT ESTIMATES OF LEVEL ENERGIES NEED
 C BE SUPPLIED).
 C CALCULATION:
 C (A) --CALCULATES TRANSITION INTENSITY BY MULTIPLYING THE RELATIVE INTENSITY
 C BY (1+ TOTAL CONVERSION COEFFICIENT) FOR TRANSITIONS WHERE COEFF. IS KNOWN.
 C (B) --MAKES LEAST SQUARES FIT OF ASSIGNED TRANSITIONS IN LIST (2) TO
 C DETERMINE BEST ENERGIES FOR STATES.
 C
 C (C) --COMPUTES RELATIVE FEEDING OF EACH STATE.
 C (D) --CALCULATES ENERGIES OF ALL POSSIBLE TRANSITIONS WHICH COULD OCCUR
 C BETWEEN THE FITTED STATES
 C (E) --COMPUTES CHI-SQD PER DEG FREEDOM FROM THE INPUT DATA IN LIST (2) AND THE
 C BEST VALUES DETERMINED IN (D).
 C
 C FIRST CARD -- TITLE CARD
 C SECOND CARD: CONTROL CARD WIDE, IBETA FORMAT (F6.0, I6)
 C WIDE DETERMINES WINDOW WIDTH TO TEST UNASSIGNED GAMMA
 C RAYS. IBETA SHOULD BE 1 FOR BETA ACTIVE SAMPLES, AND
 C OTHERWISE LEFT BLANK (ALTERS BETA FEEDING NORMALIZATION SECT. 2)
 C NEXT LISTG CARDS TOTAL LIST OF OBSERVED GAMMA RAYS
 C GAMMA-RAYS.
 C FORMAT (4F12.0, 1A12, 1E12.0)
 C GAMMA ENERGY (CEN), ERROR (DEL CEN), RELATIVE INTENSITY (INT), ERROR (DINT),
 C CONFIDENCE LEVEL (CONF), CONVERSION COEFFICIENT (ALPHA).
 C BLANK CARD MUST FOLLOW THE LAST CARD OF THE LIST OF LISTG GAMMA RAYS
 C NEXT NGAM CARDS - THOSE GAMMA RAYS THAT HAVE BEEN ASSIGNED BETWEEN
 C ANY TWO STATES
 C FORMAT (1F12.0, 2I6)
 C GAMMA ENERGY (EG), (FORMAT F12.0)
 C THE 2I6 FORMAT IS FOR THE INTEGERS THAT IDENTIFY THE INITIAL AND FINAL
 C STATES CONNECTED BY THE TRANSITION. THE GROUND STATE MUST BE IDENTIFIED BY
 C THE INTEGER 0 (ZERO).
 C BLANK CARD MUST FOLLOW THE LAST CARD OF THE NGAM ASSIGNED GAMMA RAYS
 C
 C
 C IF ONE DESIRES TO PRINT THE MATRICIES IN THE LEAST-SQUARES CALCULATION,
 C THE LOGICAL VARIABLE 'PRTLS' SHOULD BE TRUE. TO ACCOMPLISH THIS, REMOVE
 C THE 'C' FROM THE APPROPRIATE COMMENT CARDS BRACKETED BY THE FOLLOWING
 C TWO CARDS IN BOTH THE MAIN PROGRAM AND IN "LEASQE".
 C THERE IS ONE SET OF THESE CARDS IN THE MAIN PROGRAM AND
 C THERE ARE FIVE SETS IN "LEASQE"

```

C
C *****
C EXAMPLE OF HOW SUCH CARDS ARE SEPERATED FROM OTHERS.
C THE PLUSES AND MINUSES MARK SUCH CARDS.
C -----
C
C IMPLICIT REAL*8 (A-H,O-Z)
C INTEGER*2 JU,JL,NU,NL,ICEN,NA,MC,KAY,IE,NES,INES,JNES,IDELOR,F
C LOGICAL PRTLS,IBETA,LOGICL
C
C DIMENSION TITLE(10)
C
C *****
C
C THE DIMENSION OF THE ARRAYS IN THE PROGRAM ARE SPECIFIED BY THE FOLLOWING
C CONSTANTS
C THE CONSTANT 'NDIMA' SPECIFIES THE MAXIMUM NUMBER OF ASSIGNED
C GAMMA RAYS THAT THE PROGRAM WILL ACCOMODATE.
C THE CONSTANT 'NDIMB' SPECIFIES THE MAXIMUM NUMBER OF OBSERVED
C GAMMA RAYS THAT THE PROGRAM WILL ACCOMODATE.
C THE CONSTANT 'NDIMC' SPECIFIES THE MAXIMUM NUMBER OF EXCITED
C STATES THAT CAN BE PROCESSED.
C THE CONSTANTS 'NDIMAF' AND 'NDIMCF' SPECIFY THE SIZE OF THE OBSERVATION
C MATRIX 'F'. 'NDIMAF' MUST BE EQUAL TO OR LESS THAN 'NDIMA';
C 'NDIMCF' MUST BE LESS THAN OR EQUAL TO 'NDIMC'.
C THE CONSTANT 'NDIMD' SPECIFIES THE MAXIMUM NUMBER OF TRANSITIONS THAT
C CAN OCCUR BETWEEN THE NDIMC EXCITED STATES (PLUS THE GROUND STATE).
C 'NDIMD' MUST BE COMPUTED AFTER 'NDIMCF' HAS BEEN DETERMINED;
C NDIMD = NDIMCF*(NDIMCF+1)/2
C
C CORE STORAGE DEMAND IN PROGRAM CONTROL CARDS SHOULD BE VARIED WITH
C DIMENSIONS OF ARRAYS.
C
C 'LEASQE' MUST BE DIMENSIONED TO NDIMCF BY NDIMCF
C TO CHANGE PROGRAM DIMENSIONS, ARRAYS ON LINES 5516 & 5517 IN SUBROUTINE
C
C TO CHANGE PROGRAM DIMENSIONS, MODIFY THE FOLLOWING CARDS
C
C *****
C
C 5100 NDIMA = 50
C 5200 NDIMB = 100
C 5300 NDIMC = 20
C 5400 NDIMD = 210
C 5500 NDIMAF = 50
C 5510 NDIMCF = 20
C
C THE FOLLOWING CARDS CONTAIN ARRAYS DIMENSIONED TO NDIMA
C 5101 DIMENSION EG( 50),EEG( 50),JU( 50),JL( 50),NU( 50),NL( 50)
C 5102 DIMENSION CHI( 50),DELTA( 50),EGCALC( 50)

```


5103 DIMENSION RINTEN(50),RARE(50),AINTEN(50)

5104 DIMENSION MA(50),KAY(50),MC(50)

C

C THE FOLLOWING CARDS CONTAIN ARRAYS DIMENSIONED TO NDIMB

5201 DIMENSION CEN(100),DELCEN(100),RINT(100),DINT(100)

5202 DIMENSION CONF(100),COM(100),ALPHA(100),ICEN(100)

C

C THE FOLLOWING CARDS CONTAIN ARRAYS DIMENSIONED TO NDIMC

5301 DIMENSION E(20),EE1(20),EE2(20),EE1S(20),ES(20),IE(20)

5302 DIMENSION NES(20),JNES(20),XTFEED(20),V(20),B(20),SCALE(20)

5303 COMMON A(20, 20)

C

C THE FOLLOWING CARDS CONTAIN ARRAYS DIMENSIONED TO NDIMD

5401 DIMENSION DELOR(210),IDELOR(210)

C

C THE DIMENSIONS OF THE 'F' MATRIX ARE NDIMCF BY NDIMAF

5501 DIMENSION F(20,50)

C

C

C

C

XXXXXX XXXXX XXXXX XXXXX XXXXX XXXXX XXXXX

C

ADD OR REMOVE THE APPROPRIATE C'S WHEN YOU WANT TO DISABLE OR
USE THIS PART OF THE PROGRAM.

C

THE EQUIVALENCE STATEMENT BELOW IS FOR STORAGE SAVING ONLY;

IT MAY BE DISABLED OR DELETED WITHOUT HARM TO THE PROGRAM

(IF SUFFICIENT STORAGE IS REQUESTED IN JCL-SEE JOB CARD).

OTHERWISE, WHEN YOU CHANGE ARRAY SIZES, THE EQUIVALENCE STATEMENT

MAY HAVE TO BE CHANGED. WHEN MAKING THESE CHANGES, REMEMBER TO

CONSIDER THE DIFFERING PRECISION(# OF BYTES) OF THE INDIVIDUAL ARRAYS.

C

C5600 EQUIVALENCE (F(1),XTFEED(1)),(F(481),AINTIN(1)),

C *(F(2481),DELTA(1)),(F(4481),ES(1)),

C *(F(4961),CHI(1)),(F(6961),EE1S(1)),

C *(F(7481),IDELOR(1)),(A(1),DELOR(1)),

C *(A(7261),MA(1)),(A(7401),KAY(1)),(A(7601),MC(1))

C

XXXXXX XXXXX XXXXX XXXXX XXXXX XXXXX XXXXX

C

CLEARING ALL ARRAYS BEFORE THEY ARE USED

C

C

DO 5000 I=1,NDIMA

EG(I)=0

EEG(I)=0

JU(I)=0

JL(I)=0

NU(I)=0

NL(I)=0

EGCALC(I)=0

```

      RINTEN(I)=0
      RARE(I)=0
5000  CONTINUE
      DO 5005 I=1,NDIMB
      CEN(I)=0
      DELCEN(I)=0
      RINT(I)=0
      DINT(I)=0
      CONF(I)=0
      COM(I)=0
      ALPHA(I)=0
      ICEN(I)=0
5005  CONTINUE
      DO 5010 I=1,NDIMC
      E(I)=0
      EE1(I)=0
      EE2(I)=0
      IE(I)=0
      NES(I)=0
      JNES(I)=0
5010  CONTINUE
      DO 5015 I=1,NDIMCF
      DO 5015 J=1,NDIMAF
      F(I,J)=0
5015  CONTINUE
C
C
      1 READ(5,2,END=999) TITLE
      2 FORMAT(10A8)
C
C
      THIS 8000 SECTION PRINTS OPERATING INSTRUCTIONS
C
      NSECT = 0
      NTPAGE = 1
      PRINT 1110,NSECT,NTPAGE
1110  FORMAT (1H1, 48X,'SECT.',I2,3X,'PAGE',I4)
8000  PRINT 8001
8001  FORMAT ( 25X,'PROGRAM STATEFIT'//
*28X,'WRITTEN BY'/27X,'S. B. BURSON'/27X,'G. T. WOOD, AND'/
*27X,'C. H. BATSON',//,25X,'PHYSICS DIVISION',/,20X,
*'ARGONNE NATIONAL LABORATORY'/25X,'ARGONNE, ILLINOIS'/)
8002  PRINT 8003,TITLE
8003  FORMAT(X,'JOB TITLE:',2X,6A8,'-',/,13X,4A8,/)
8004  PRINT 8005
8005  FORMAT (22X,'OPERATING INSTRUCTIONS'//22X, 'DATA DFCK ORGANIZATI
*ON'//)
8006  PRINT 8007
8007  FORMAT(/,X,'FIRST CARD:  TITLE CARD, (ANY 80 CHARACTERS.)',/,
*5X,'FORMAT(10A8) ')
8008  PRINT 8009
8009  FORMAT(/,X,'SECOND CARD:  WIDE, IBETA',/,5X,'FORMAT(F6.0,I6)',/,
*9X,' WIDE DETERMINES WIDTH OF WINDOW USED TO SEARCH COMPLETE',/,
*10X,'LIST OF OBSERVED GAMMA RAYS (SECTION 1-A) FOR POSSIBLE',/,

```



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*10X,'ASSIGNMENTS.',/,10X,'E(T) = CALCULATED TRANSITION ENERGY =',
*' E(JU) - E(JL)',/,
*10X,'DEITA = ABS(E(T) - E(GAMMA))',/,
*10X,'ERR(DELTA) = COMPUTED STATISTICAL ERROR IN DELTA',/,
*10X,'A GAMMA RAY IS SELECTED FROM THE COMPLETE LIST',/,
*10X,'(SECTION 1-A) IF: DELTA < WIDE*ERR(DELTA).',/,
*10X,'WIDE IS NORMALLY SET EQUAL TO 1 OR APPROXIMATELY SO '///
*9X,' IBETA MAY EQUAL ONE OR ZERO. IF IBETA=0, THE INTENSITY'/10X,
*'BALANCE(OF EACH STATE) IS:'/'10X,
*'XTFEED = TOTAL DEPOPULATING INTENSITY - TOTAL POPULATING'/10X,
*'INTENSITY.'/'10X,
*'IF IBETA=1(FOR RADIOACTIVE SAMPLES), XTFEED'/10X
*'FOR EACH STATE IS DIVIDED BY THE TOTAL BETA'/10X
*'FEEDING TO ALL EXCITED STATES.'/)
8016 PRINT 8017
8017 FORMAT (/X,'NEXT LISTG CARDS: CEN,DELCE, RINT,DINT,CONF,COM,ALPHA'
*/5X,'FORMAT (4F12.0,A4,A8,E12.0) ' /
*9X,'(THESE LISTG CARDS ARE THE EXPERIMENTALLY OBSERVED GAMMA',/,
*10X,'RAYS (SECTION 1-A), 1 GAMMA RAY PER CARD. LISTG IS NOT',/,
*10X,'TO EXCEED THE PROGRAM CONSTANT "NDIME", 5000 SERIES LINE'/10X
*,'NUMBERS) ' /
*9X,'(CEN = EXPERIMENTALLY OBSERVED GAMMA RAY ENERGY IN KEV.)',/,
*10X,'WARNING! THE ENERGY VALUE EG OF ANY ASSIGNED GAMMA RAY',/,
*10X,'MUST BE IDENTICALLY EQUAL TO THE CORRESPONDING ENERGY',/,
*10X,'VALUE CEN IN THIS LIST OF OBSERVED GAMMA RAYS OF EXECUTION',/
*,'10X,'WILL TERMINATE.',/,
*9X,'(DELCE = EXPERIMENTAL ERROR IN CEN.)' /,
*9X,'(RINT = RELATIVE INTENSITY OF THE GAMMA RAY IN ARBITRARY',/,
*10X,'UNITS.)',/,9X,'(DINT = EXPERIMENTAL ERROR IN RINT.)',/,
*9X,'(CONF+COM=CONFIDENCE RATING OF OBSERVED GAMMA'/10X,
*'RAY (OR COMMENT) ARBITRARILY ASSIGNED BY EXPERIMENTER.)' /,
*9X,'(ALPHA = THE TOTAL INTERNAL CONVERSION COEFFICIENT.)')
NTPAGE = 2
PRINT 1110,NSECT,NTPAGE
8020 PRINT 8021
8021 FORMAT (/5X,'(OPERATING INSTRUCTIONS CONTINUED) ' /)
8014 PRINT 8015
8015 FORMAT (/X,'NEXT CARD: BLANK CARD; THIS CARD IS OPTIONAL AND IS
*USED',/,26X,'TO SEPERATE THE DATA DECKS. OMISSION',/,
*26X,'WILL NOT CAUSE PROGRAM TO TERMINATE.',/)
8010 PRINT 8011
8011 FORMAT (/X,'NEXT NGAM CARDS: EG, JU, JL',/,
*5X,'FORMAT(1F12.0,2I6) ' ,/,
*9X,'(THESE NGAM CARDS ARE ASSIGNED GAMMA RAYS (SECTION 1-B)',/,
*10X,'1 GAMMA RAY PER CARD. NGAM IS NOT TO EXCEED THE PROGRAM'/10X
*,'CONSTANT "NDIMA" IN THE 5000 SERIES LINE NUMBERS) ' /
*9X,'(EG IS GAMMA RAY ENERGY IN KEV. WARNING! EG MUST BE',/,
*10X,'IDENTICALLY EQUAL TO CORRESPONDING ENERGY VALUE CEN',/,
*10X,'IN COMPLETE LIST OF OBSERVED GAMMA RAYS.)')
8012 PRINT 8013
8013 FORMAT (9X,'(JU AND JL ARE THE INTEGER INDEX NUMBERS OF THE',/,
*10X,'UPPER AND LOWER EXCITED STATES, WHICH NEED NOT BE CONSECUTIVE
*'/10X,'INTEGERS AND NEED NOT BE ASSIGNED IN ASCENDING ENERGY ORDER
*)' / 9X,'(RESTRICTIONS: FOR THE GROUND STATE,'/'10X,
*'JL=0; ALL JU VALUES MUST BE NON ZERO) ' /)

```

```

8018 PRINT 8019
8019 FORMAT (/,X,'LAST CARD:  BLANK CARD;  THIS CARD SIGNALS END OF DATA
*DECK, '/26X,'COMMISSION WILL CAUSE ABNORMAL TERMINATION.')
```

PRINT 8024

```

8024 FORMAT (//22X,'PROGRAM ALTERATIONS'//)
PRINT 8025
8025 FORMAT ( 1X,'SET NDIMA (LINE 5100)=MAXIMUM NGAM EXPECTED.'//,
* 1X,'SET NDIMB (LINE 5200)=MAXIMUM LISTG EXPECTED.'//,
* 1X,'SET NDIMC (LINE 5300)=MAXIMUM NLEV EXPECTED(NO.LEVELS TO BE FI
*TTED).',//,
* 1X,'SET MATRIX GAMMA AXIS NDIMAF (LINE 5500) EQ/LT NDIMA',//,
* 1X,'SET MATRIX EXCITED-STATE AXIS NDIMCF (LINE 5510) EQ/LT NDIMC'//,
* 1X,'SET NDIMD (LINE 5400)=NDIMCF*(NDIMCF+1)/2',//,
* 5X,'NDIMD=TOTAL TRANSITIONS BETWEEN NDIMCF EXCITED STATES',//,
*11X,'(INCLUDING GROUND STATE)')
```

PRINT 8026

```

8026 FORMAT (X,'REDIMENSIONING ARRAYS - REFER TO 5000 SERIES LINE NUMBE
*RS'/
*10X,'SET DIMENSIONS IN LINES 5101-5104 TO NDIMA'//,
*10X,'SET DIMENSIONS IN LINES 5201&5202 TO NDIMB'//,
*10X,'SET DIMENSIONS IN LINES 5301-5303 TO NDIMC'//,
*10X,'SET DIMENSIONS IN LINE 5401 TO NDIMD'//,
*10X,'SET DIMENSIONS IN LINE 5501 TO NDIMCF BY NDIMAF'//,
*10X,'SET DIMENSIONS IN LINES 5516&5517 TO NDIMCF BY NDIMCF'//,
*25X,'THESE LINES ARE IN SUBROUTINE LEASQE'//)
PRINT 8234
8234 FORMAT (//19X,'(END OF OPERATING INSTRUCTIONS)')
NTPAGE = 3
NSECT = 1
PRINT 1110,NSECT,NTPAGE
9000 PRINT 9001
9001 FORMAT (//25X,'PROGRAM STATEFIT'//25X,'INPUT INFORMATION'//)
80021 PRINT 80031,TITLE
80031 FORMAT (X,'JOB TITLE:',2X,6A8,'-' /13X,4A8//)
80041 PRINT 9004
9004 FORMAT (X,'NOTE!  IF EXECUTION TERMINATES AT THIS POINT, CHECK ',
*'FOR ERRORS',/,8X,'IN DATA DECK.  BLANK CARD OR EOF CARD MAY ',
*'BE MISSING',/,8X,'AT END OF DATA.',//)
3 READ 4,WIDE,IBETA
4 FORMAT (F6.0,I6)
PRINT 9005,WIDE,IBETA
9005 FORMAT (X,'CONTROL CARD:  WIDE =',F6.0,2X,5X,'IBETA =',I6//)
PRINT 3800,NDIMA,NDIMB,NDIMC,NDIMCF,NDIMAF,NDIMD
3800 FORMAT (/10X,'PROGRAM DIMENSIONS'//3X,'ASSIGNED GAMMA RAYS (NDIMA)
*   = ',I4/3X,'OBSERVED GAMMA RAYS (NDIMB)   = ',I4/3X,'NO. OF EXCI
*TED STATES (NDIMC) = ',I4//,
*7X,'F MATRIX (NDIMCF BY NDIMAF)',//,
*3X,'EXCITED STATE AXIS:  (NDIMCF) = ',I4//,
*3X,'ASSIGNED GAMMA AXIS: (NDIMAF) = ',I4//,
*3X,'NO. POSSIBLE TRANSITIONS: (NDIMD) = ',I4,/)
C
KK = 0
I = 1
K=1
IIA = 0
```



```

IIB = 0
IIC = 0
IIAF = 0
IICF = 0
NLEV=1
LOGICL = .FALSE.

```

C

```

5 READ 10000,AA,BB,CC,DD,EE,FF,GG
10000 FORMAT (4F12.0,A4,A8,E12.0)
IF (AA.EQ.0.0) GO TO 7
IF (BB.GT.10000) GO TO 90999
CEN(L) = AA
DELCEN(L) = BB
RINT(L) = CC
DINT(L) = DD
CONF(L) = EE
COM(L) = FF
ALPHA(L) = GG
L = L + 1
IF (L.LE.NDIMB) GO TO 5
IIB = 1
12 READ 10000,AA,BB,CC,DD,EE,FF,GG
L = L + 1
IF (AA.NE.0.0) GO TO 12
GO TO 7
90999 EG(1) = AA
JU(1) = BB/1000000.
JL(1) = BB - JU(1)*1000000
LOGICL = .TRUE.
K = 2
7 READ 10101,EG(K),JU(K),JL(K)
10101 FORMAT (F12.0,2I6)
IF (EG(K).EQ.0.0) GO TO 8
K = K + 1
IF (K.LE.NDIMA) GO TO 7
IIA = 1
13 READ 10101,AA,IXXI,IXII
KK = KK + 1
IF (AA.NE.0.0) GO TO 13
8 NGAM = K + KK - 1
LISTG = L - 1
IF (NGAM.GT.NDIMA) IIA = 1
IF (LISTG.GT.NDIMB) IIB = 1

```

C

C

C

FROM HERE TO STATEMENT 19, THE TOTAL NUMBER OF LEVELS IS DETERMINED

```

NU(1)=1
NES(1)=JU(1)
IF(JL(1).EQ.0)GO TO 7060
NES(2)=JL(1)
NL(1)=2
M=2
GO TO 7070
7060 NL(1)=0
M=1

```


C NGAM EQUALS TOT
C
C
C THIS SECTION
C AND EXCITE
C HERE, AND
C
C
C
3802 PRINT 3803, N
3803 FORMAT (//3
*', 11X,

3802 PRINT 3803,N
3803 FORMAT (//3
* , 11X,

```
3802 PRINT 3803,NDIMA,NDIMB,NDIMC
3803 FORMAT (///30X,'PROGRAM UTILIZATION'//21X,'ASSIGNED',12X,'OBSERVED
*,11X,
* 'EXCITED'/20X,'GAMMA RAYS',10X,'GAMMA RAYS',10X,'STATES'/' STORA
*GE CAPACITY',5X,I4,16X,I4,15X,I4/' STORAGE NEEDED')
```

```

      PRINT 3811,NGAM,LISTG,NLEV
3811  FORMAT ('+',21X,I4,16X,I4,15X,I4//)
      IF (NLEV.GT.NDIMC)  IIC = 1
      IF (NLEV.GT.NDIMCF) IICF = 1
      IF (NGAM.GT.NDIMAF) IIAF = 1
      IF (IIA.GT.0) PRINT 3807
3807  FORMAT ('+',20X,'EXCEEDED')
      IF (IIB.GT.0) PRINT 3815
3815  FORMAT ('+',38X,'EXCEEDED')
      IF (IIC.GT.0) PRINT 3812
3812  FORMAT ('+',60X,'EXCEEDED')
      IF (IICF.GT.0) PRINT 3698,NDIMCF,NLEV
      IF (IIAF.GT.0) PRINT 3666,NDIMAF,NGAM
3698  FORMAT (//16X,'MATRIX DIMENSIONS ARE TOO SMALL FOR INPUT DATA'/16X
*,'"NDIMCF" = ',I4,5X,'"NLEV" = ',I4)
3666  FORMAT (///16X,'MATRIX DIMENSIONS TOO SMALL FOR INPUT DATA'/16X,
*,'"NDIMAF" = ',I4,5X,'"NGAM" = ',I4)
      IF (IIA.EQ.0.AND.IIB.EQ.0.AND.IIC.EQ.0.AND.IIAF.EQ.0.AND.IICF.EQ.0
*) GO TO 3888
      PRINT 3819
3819  FORMAT (//5X,'INPUT TOO GREAT FOR STORAGE SIZES ALLOTTED'/5X,'EXEC
*UTION TERMINATED')
3888  CONTINUE

```

C
C
C
C
C
C
C
C

THIS 9000 SECTION PRINTS OUT THE INPUT DATA VERBATUM AND
CHECKS THE INPUT FOR ERRORS FATAL TO PROPER PROGRAM EXECUTION

PRINT SECTION 1-A

```

      NTPAGE = 4
      PRINT 1111,NSECT,NTPAGE
1111  FORMAT (1H1,102X,'SECT.',I2,3X,'PAGE',I4)
      PRINT 90339
      PRINT 9025
9025  FORMAT (//10X'SECTION 1-A'14X 'COMPLETE INPUT LIST OF OBSERVED GAMM
*A RAY ENERGIES')
      PRINT 9026
9026  FORMAT (/,7X,'CARD'10X'GAMMA RAY'6X'GAMMA RAY'5X'  RELATIVE',6X,
*, 'INTENSITY'5X'CONFIDENCE'4X'CONVERSION')
      PRINT 9027
9027  FORMAT (6X,'NUMBER',11X,'ENERGY'9X'ERROR'8X'INTENSITY'8X'ERROR'7X'L
*EVEL&I.D.'4X'COEFFICIENT')
      LINCT = 7
      DO 9035 K3=1,LISTG
      LINCT = LINCT + 1
      IF (LINCT.LE.60) GO TO 9035
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9025
      PRINT 9033
9033  FORMAT ('+',86X,'-CONTINUED')
      PRINT 9026

```

```

      PRINT 9027
      LINCT = 9
9035 PRINT 9029, K3,CEN(K3),DELCEN(K3),RINT(K3),DINT(K3),CONF(K3),COM(K
      *3),ALPHA(K3)
9029 FORMAT(6X,I4,5X,4F15.3,3X,1A4,1A8,1P1D12.2)
C
C
C      PRINT SECTION 1-B
C
C      IF(LISTG.LT.1) GO TO 9501
C
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9010
9010 FORMAT (10X,'SECTION 1-B:'17X 'LIST OF ASSIGNED GAMMA RAYS'//)
      PRINT 9012
9012 FORMAT (7X,'CARD'10X'GAMMA RAY'11X'INITIAL'9X'FINAL')
      PRINT 9013
9013 FORMAT(6X,'NUMBER'11X'ENERGY'13X'LEVEL'10X'LEVEL',/)
      LINCT = 9
      DO 9015 K2=1,NGAM
      LINCT = LINCT + 1
      IF (LINCT.LE.60) GO TO 9015
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 90339
      PRINT 90109
90109 FORMAT (20X,'SECTION 1-B:',7X,'LIST OF ASSIGNED GAMMA RAYS - CONTI
      *NUED'//)
      PRINT 9012
      PRINT 9013
      LINCT = 7
9015 PRINT 9017, K2,EG(K2),JU(K2),JL(K2)
9017 FORMAT(6X,I4,5X,1F15.3,5I15)
C
C      THE REST OF SECTION 1 SEARCHES THE DATA TO DETECT ANY ERRORS THAT
C      WOULD PREVENT PROPER EXECUTION OF THE PROGRAM. SEVEN ERRORS CAN BE
C      DETECTED; NOS. 1-6 CAUSE TERMINATION OF PROGRAM AFTER ALL THE ERRORS
C      HAVE BEEN FOUND; NO. 7 IS DETECTED, BUT IT ALONE WILL NOT TERMINATE.
C
C
9501 NTPAGE = NTPAGE + 1
      ERCARD = 0.
      PRINT 1111,NSECT,NTPAGE
      PRINT 9504
9504 FORMAT (///46X,'TESTS MADE IN SECTION 1')
      PRINT 90339
90339 FORMAT (2(1H ))
9505 PRINT 9506
9506 FORMAT(X,'ERROR NO.1: THE SAME INDEX NUMBER MUST NOT BE USED TO ID
      *ENTIFY BOTH UPPER AND LOWER LEVELS ON AN ASSIGNED GAMMA RAY CARD.'
      *)
9507 PRINT 9508
9508 FORMAT(X,'ERROR NO.2: FOR EVERY ASSIGNED GAMMA RAY, THERE MUST BE
      *A CORRESPONDING CARD IN THE COMPLETE LIST OF OBSERVED GAMMA RAYS',

```



```

      *//,13X,'(SECTION 1-A). THE TWO ENERGY VALUES MUST BE IDENTICALLY E
      *QUAL.')
```

9601 PRINT 9602

9602 FORMAT (X,'ERROR NO.3: TOTAL LIST OF OBSERVED GAMMA RAYS IS CHECKE
 *D TO SEE IF ERRORS HAVE BEEN ASSIGNED TO ALL ENERGY VALUES.'/14X,
 *'(DOES NOT CAUSE TERMINATION UNLESS GAMMA RAY IS ASSIGNED.)')

3201 PRINT 3201

3201 FORMAT (X,'ERROR NO.4: TWO DIFFERENT GAMMA RAYS CANNOT BE ASSIGNED
 * TO THE SAME TRANSITION,.'/,14X,'NOR CAN A SINGLE GAMMA RAY ASSIGNE
 *D TO ONE TRANSITION BE LISTED TWICE.')

3988 PRINT 3988

3988 FORMAT (X,'ERROR NO.5: TWO OBSERVED GAMMA RAYS SHOULD NOT HAVE THE
 * SAME ENERGY')

95022 PRINT 95022

95022 FORMAT (X,'ERROR NO.6: AN ASSIGNED GAMMA RAY HAS BEEN GIVEN AN UPP
 *PER LEVEL OF ZERO.')

62 PRINT 62

62 FORMAT (X,'ERROR NO.7: AT LEAST ONE TRANSITION MUST POPULATE THE G
 *ROUND STATE')

63 PRINT 63

63 FORMAT (X,'ERROR NO.8: THE ARRAY SPACE PROVIDED HAS BEEN EXCEEDED
 *BY THE INPUT'/14X,'EXCESS IS IGNORED AND EXECUTION TERMINATED')

9503 PRINT 9503

9503 FORMAT (X,'ERROR NO.9: THE LIST OF OBSERVED GAMMA RAYS SHOULD BE O
 *RDERED BY INCREASING ENERGY; IF NOT, AN ERROR MESSAGE WILL'/14X,'
 *BE PRINTED, BUT EXECUTION WILL CONTINUE.')

90909 PRINT 90909

90909 FORMAT (X,'ERROR NO.10: A BLANK CARD BETWEEN THE DATA DECKS IS MIS
 *SING.')

8999 PRINT 8999

8999 FORMAT(/14X,'OCCURRENCE OF ANY ERROR EXCEPT 9 AND 10 TERMINATES EX
 *ECUTION OF PROGRAM'////48X,'ERRORS FOUND'/)
 LINCT = 32

C
 C TEST FOR ERROR NO. 1
 C THIS SECTION TESTS THE DATA TO INSURE THAT THE SAME NUMBER HAS NOT
 C BEEN USED FOR THE UPPER AND LOWER LEVELS OF THE TRANSITIONS WITH
 C ASSIGNED GAMMA RAYS.
 C

9061 DO 9065 K2=1,NGAM
 IF(JU(K2).EQ.JL(K2)) GO TO 9063
 GO TO 9065

9063 PRINT 9064,K2,EG(K2),JU(K2),JL(K2)

9064 FORMAT(X,'ERROR NO.1: ASSIGNED GAMMA RAY HAS THE SAME UPPER AND LO
 *WER LEVEL NUMBER.'/,13X,
 *'ASSIGNMENT CARD',I5,':',5X,1P15.3,2I15)
 ERCARD=ERCARD+1
 LINCT = LINCT + 2
 IF (LINCT.LE.60) GO TO 9065
 NTPAGE = NTPAGE + 1
 PRINT 1111,NSECT,NTPAGE
 PRINT 9502

9502 FORMAT (///46X,'TESTS MADE IN SECTION 1',/,50X,'ERRORS FOUND')
 PRINT 90333

90333 FORMAT ('+',70X,'-CONTINUED')

```

      PRINT 90339
      LINCT = 6
9065  CONTINUE
C
C   TEST FOR ERROR NO. 2
C   THIS SECTION (90350 TO 9043) CHECKS TO SEE IF THE ASSIGNED GAMMA
C   RAYS ARE ALL IN THE TOTAL LIST OF OBSERVED GAMMA RAYS. IF NOT, EACH
C   DISCREPANCY IS NOTED IN THE LISTING. THE NUMBER OF ERRORS FATAL
C   TO EXECUTION ARE COUNTED (ERCARD) AND PRINTED OUT. THEN EXECUTION
C   IS TERMINATED.
C
C
90350 DO 90360 K4=1,NGAM
      DO 90355 K5=1,LISTG
      IF (DABS(EG(K4)-CEN(K5)) - 0.00001) 90360,90360,90355
90355  CCNTINUE
      PRINT 90356, K4,EG(K4),JU(K4),JL(K4)
90356  FORMAT(/,X,'ERROR NO.2: ASSIGNED GAMMA RAY NOT FOUND IN LIST OF OB
      *SERVED GAMMA RAYS.',/,13X,
      *'ASSIGNMENT CARD',I5,':',5X,1F15.3,2I15,/)
      ERCARD=ERCARD+1
      LINCT = LINCT + 5
      IF (LINCT.LE.60) GO TO 90360
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9502
      PRINT 90333
      PRINT 90339
      LINCT = 6
90360  CONTINUE
C
C   TEST FOR ERROR NO.3
C   THIS SECTION CHECKS TO SEE THAT EACH GAMMA RAY HAS AN UNCERTAINTY
C   IN ITS ENERGY DETERMINATION ASSIGNED TO IT.
C
9650  DO 9654 K=1,LISTG
      IF (DELCEN(K).EQ.0) GO TO 9651
      GO TO 9654
9651  DO 96515 J=1,NGAM
      IF (DABS(EG(J)-CEN(K)) - 0.00001) 96516,96516,96515
96515  CONTINUE
      PRINT 9652,K,CEN(K),DELCEN(K),RINT(K),DINT(K),CONF(K),COM(K),
      *ALPHA(K)
9652  FORMAT (X,'ERROR NO.3: A MEMBER OF THE LIST OF OBSERVED GAMMA RAY
      *S DOES NOT HAVE AN ERROR ASSIGNED TO THE ENERGY.',/,13X,
      *'OBSERVED CARD',I5,':',5X,4F15.3,1A4,1A8,1D15.2,/)
      GO TO 96518
96516 PRINT 96519,K,CEN(K),DELCEN(K),RINT(K),DINT(K),CONF(K),COM(K),
      *ALPHA(K),J,EG(J),JU(J),JL(J)
96519 FORMAT(X,'ERROR NO.3: ASSIGNED GAMMA RAY DOES NOT HAVE AN ENERGY E
      *RROR',/,8X,
      *'OBSERVED CARD',I5,':',5X,4F15.3,1A4,1A8,1D15.2,/,
      *8X,'ASSIGNED CARD',I5,':',5X,F15.3,2I15,/)
      ERCARD = ERCARD + 1
96518 LINCT = LINCT + 4

```



```

IF (LINCT.LE.60) GO TO 9654
NTPAGE = NTPAGE + 1
PRINT 1111,NSECT,NTPAGE
PRINT 9502
PRINT 90333
PRINT 90339
LINCT = 6

```

```

9654 CONTINUE

```

```

C
C TEST FOR ERROR NO. 4
C THIS SECTION CHECKS TO SEE THAT NO TRANSITION HAS TWO GAMMA RAYS
C ASSIGNED TO IT, OR THAT NO ASSIGNED GAMMA RAY IS LISTED TWICE.
C

```

```

NGAM1 = NGAM-1
DO 3100 KK = 1,NGAM1
KK1 = KK+1
DO 3101 LL= KK1,NGAM
IF (JU(KK).NE.JU(LL).OR.JL(KK).NE.JL(LL)) GOTO 3101
3105 PRINT 3205, KK,EG(KK),JU(KK),JL(KK),LL,EG(LL),JU(LL),JL(LL)
3205 FORMAT (X,'ERROR NO. 4: TWO ASSIGNED GAMMA RAYS HAVE THE SAME INIT
*IAL AND FINAL LEVEL NUMBERS.',/,14X,
*'ASSIGNMENT CARD',I5,':',5X,F15.3,2I15,/,14X,
*'ASSIGNMENT CARD',I5,':',5X,F15.3,2I15,/)
ERCARD = ERCARD + 1
LINCT = LINCT + 4
IF (LINCT.LE.60) GO TO 3101
NTPAGE = NTPAGE + 1
PRINT 1111,NSECT,NTPAGE
PRINT 9502
PRINT 90333
PRINT 90339
LINCT = 6

```

```

3101 CONTINUE

```

```

3100 CONTINUE

```

```

C
C TEST FOR ERROR NO. 5
C THIS SECTION SEARCHES THE OBSERVED GAMMA RAY LIST TO SEE IF ANY
C ARE LISTED TWICE,I.E. IF TWO GAMMA RAYS HAVE THE SAME ENERGY.
C

```

```

LISTG1 = LISTG - 1
DO 3993 LIL = 1,LISTG1
LILY = LIL + 1
DO 3992 LUL = LILY,LISTG
IF (CEN(LIL).EQ.CEN(LUL)) GO TO 3990
3992 CONTINUE
3993 CONTINUE
GO TO 9040
3990 PRINT 3989,LIL,CEN(LIL),LUL,CEN(LUL)
3989 FORMAT (X,'ERROR NO.5: TWO OBSERVED GAMMA RAYS HAVE THE SAME ENERG
*Y.',/,14X,'OBSERVED CARD',I5,':',5X,1F15.3,/,
*14X,'OBSERVED CARD',I5,':',5X,1F15.3,/)
ERCARD = ERCARD + 1
LINCT = LINCT + 4
IF (LINCT.LE.60) GO TO 3992
NTPAGE = NTPAGE + 1

```

```

PRINT 1111,NSECT,NTPAGE
PRINT 9502
PRINT 90333
PRINT 90339
LINCT = 6
GO TO 3992

```

C
C
C
C
C
C
C
C

TEST FOR ERROR NO.6

THE FOLLOWING STEPS TEST THE DATA TO DETERMINE IF AN ASSIGNED
GAMMA RAY HAS A ZERO FOR ITS UPPER LEVEL. THIS CONTRADICTS THE
PHYSICS INVOLVED, AND SO IT IS FATAL

```

9040 DO 8888 NUN = 1,NGAM
      IF (JU(NUN).NE.0) GO TO 8888
      PRINT 3605,NUN,EG(NUN),JU(NUN),JI(NUN)
3605 FORMAT (/X,'ERROR NO.6: A GAMMA RAY HAS BEEN ASSIGNED WITH AN UPP
      *ER LEVEL OF ZERO',
      */,10X,'ASSIGNMENT CARD',I5,':',5X,F15.3,2I15,/)
      LINCT = LINCT + 3
      IF (LINCT.LE.60) GO TO 8888
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9502
      PRINT 90333
      PRINT 90339
      LINCT = 6
8888 CONTINUE

```

C
C
C
C
C
C
C

TEST FOR ERROR NO. 7

THIS SECTION CHECKS ALL GAMMA RAYS TO INSURE THAT AT LEAST
ONE OF THEM TERMINATES AT THE GROUND STATE

```

      LUST = 0
      DO 6565 LOL = 1,NGAM
      IF (JL(LOL).EQ.0.AND.JU(LOL).EQ.0) GO TO 6565
      IF (JL(LOL).EQ.0) LUST = 1
6565 CONTINUE
      IF (LUST.EQ.1) GO TO 67
      LINCT = LINCT + 2
      IF (LINCT.LE.60) GO TO 61
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9502
      PRINT 90333
      PRINT 90339
      LINCT = 6
61 PRINT 66
66 FORMAT ('0ERROR NO.7: NO GAMMA RAYS POPULATE THE GROUND STATE')
      ERCARD = ERCARD + 1.
67 CONTINUE

```

C
C

```

C      TEST FOR ERROR NO.8
C      THIS SECTION TELLS THE USER IF HE HAS TRIED TO INPUT TOO MUCH
C      DATA FOR THE ARRAY DIMENSIONS.
C      SUCH INFORMATION HAS ALREADY BEEN DISPLAYED EARLIER.
C
      CRAP = IIA+IIB+IIC+IIAF+IICF
      IF (CRAP.EQ.0) GO TO 83
      LINCT = LINCT + 2
      IF (LINCT .LE.60) GO TO 81
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9502
      PRINT 90333
      PRINT 90339
      LINCT = 8
81 PRINT 97
97 FORMAT (1X,'ERROR NO.8: THE DIMENSION OF AT LEAST ONE ARRAY HAS BE
*EN EXCEEDED BY AN EXCESSIVE AMOUNT OF INPUT DATA',/)
      IF (IIA.EQ.0) GO TO 9696
      ERCARD = ERCARD + 1.
      PRINT 95,NDIMA,NGAM
95 FORMAT (5X,'ARRAY DIMENSIONS ALLOW NO MORE THAN',I4,' ASSIGNED GAM
*MA RAYS, BUT THE INPUT DATA REQUIRE SPACE FOR AT LEAST',I4,/)
      LINCT = LINCT + 2
9696 IF (IIB.EQ.0) GO TO 94
      ERCARD = ERCARD + 1.
      PRINT 93,NDIMB,LISTG
93 FORMAT (5X,'ARRAY DIMENSIONS ALLOW NO MORE THAN',I4,' OBSERVED GAM
*MA RAYS, BUT THE INPUT DATA REQUIRE SPACE FOR AT LEAST',I4,/)
      LINCT = LINCT + 2
94 IF (IIC.EQ.0) GO TO 9292
      ERCARD = ERCARD + 1.
      PRINT 91091,NDIMC,NLEV
91091 FORMAT (5X,'ARRAY DIMENSIONS ALLOW NO MORE THAN',I4,' EXCITED STAT
*ES, BUT THE INPUT DATA REQUIRE SPACE FOR AT LEAST',I4,/)
      LINCT = LINCT + 2
9292 IF (IIAF.EQ.0.AND.IICF.EQ.0) GO TO 83
      ERCARD = ERCARD + 1.
      PRINT 82,NDIMCF,NDIMAF,NLEV,NGAM
82 FORMAT (5X,'THE OBSERVATION MATRIX "F" HAS MAXIMUM DIMENSIONS OF',
*I4,' BY',I4/6X,'BUT THE INPUT DATA REQUIRE AT LEAST',I4,' BY',I4)
      LINCT = LINCT + 2
83 CONTINUE

C
C
C      TEST FOR ERROR NO.9
C      LIST OF OBSERVED GAMMA RAYS IS CHECKED TO SEE IF IT IS IN ORDER OF
C      INCREASING ENERGIES. DETECTION OF THIS ERROR ALONE WILL NOT CAUSE
C      PROGRAM TO TERMINATE EXECUTION.
C
      ISH = 0
      LINCT = LINCT + 3
      DO 785 K=2,LISTG
      IF (CEN(K).GE.CEN(K-1)) GO TO 785
      IF (ISH.EQ.0) PRINT 787

```



```

787 FORMAT (' ERROR NO.9: THE INPUT DECK OF OBSERVED GAMMA RAYS IS NO
      *T IN ORDER OF ASCENDING ENERGY'/20X,'CARD NO.',10X,'ENERGY'/)
      K1 = K-1
      PRINT 786,K1,CEN(K1),K,CEN(K)
786 FORMAT (2(22X,I4,10X,F8.3/))
      ISH = ISH + 1
      LINCT = LINCT + 4
      IF (LINCT.LE.60) GO TO 785
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 9502
      PRINT 90333
      PRINT 90339
      LINCT = 6
785 CONTINUE

C
C
C      TEST FOR ERROR NO.10
C      THIS SECTION INFORMS THE USER IF THE BLANK CARD THAT SEPARATES
C      THE TWO DATA DECKS IS MISSING.  (NOT FATAL TO EXECUTION)
C
      IF (LOGIC1) PRINT 91919
91919 FORMAT ('ERROR NO.10: THE BLANK CARD THAT SHOULD SEPARATE THE INP
      *UT DATA DECKS IS MISSING'/8X,'THIS IS NOT FATAL TO EXECUTION')

C
C
C      IN THIS SECTION , EXECUTION IS TERMINATED IF ANY FATAL INPUT ERRORS
C      HAVE BEEN FOUND.
C
C
943 IF (ERCARD.EQ.0.0) GO TO 9043
      NERCARD = ERCARD
      PRINT 9041,NERCARD
9041 FORMAT(//,5X,I3,' FATAL ERROR(S) IN INPUT DATA',
      *15X,' *** EXECUTION TERMINATED ***')
      GO TO 1
9043 CONTINUE
9050 CONTINUE

C
C
C      THE TESTING FOR INPUT ERRORS IS COMPLETED.
C
C
C      FROM HERE TO 9051 THE EXPERIMENTALLY DETERMINED RELATIVE INTENSITY
C      (RINT) VALUES ARE CONVERTED TO TRANSITION INTENSITIES BY MULTIPLICATION
C      BY (1+ALPHA) WHERE ALPHA IS THE K+L+M CONVERSION COEFFICIENT.
C
      DO 9051 K4=1,LISTG
      RINT(K4)=RINT(K4)*(1+ALPHA(K4))
9051 DINT(K4)=DINT(K4)*(1+ALPHA(K4))

C
C
C      FROM HERE TO 9060 THE DATA FROM THE TOTAL LIST OF GAMMA RAYS IS IN
C      SERTED IN THE APPROPRIATE ASSIGNED GAMMA RAY INFORMATION ARRAY.
C      I.E. THE ERROR IN THE ENERGY, THE TRANSITION INTENSITY, AND ITS ERROR.

```

```

C
DO 9060 KK=1,NGAM
DO 9060 LL=1,LISTG
IF (DABS(EG(KK)-CEN(LL)) - 0.00001) 9062,9062,9060
9062 EEG(KK) = DELCEN(LL)
RINTEN(KK)=RINT(LL)
RARE(KK)=DINT(LL)
9060 CONTINUE
C
C
C CALCULATE OBSERVATION MATRIX
C
DO 21 K=1,NGAM
DO 22 I=1,NLEV
22 F(I,K)=0
IU=NU(K)
IL=NL(K)
IF(IL.NE.0) F(IL,K)=-1
21 F(IU,K)=1
C
C
C
PRTLS = .FALSE.
C
C
C *****
C
C REMOVE THE "C" FROM THE FOLLOWING CARDS, AND FROM ALL CARDS IN THE
C THE SUBROUTINE "LEASQE" SURROUNDED BY THE "+" AND "-" CARDS
C IN ORDER TO HAVE ALL THE MATRICES USED IN THE ENERGY LEVEL
C CALCULATION PRINTED OUT.
C PRTLS = .TRUE.
C
C -----
C
C CALL LEASQE(EG,EEG,NGAM,300,F,NLEV,NDIMCF,E,EE1,EE2,CSQPDF,EGCALC,
C *PRTLS,V,E,SCALE)
C
C
C THE FOLLOWING STATEMENTS CLEAR THE EQUIVALENCED ARRAYS
C
DO 5701 I=1,NDIMA
MC(I)=0
KAY(I)=0
MA(I)=0
DELTA(I)=0
CHI(I)=0
AINTEN(I)=0
5701 CONTINUE
DO 5703 I=1,NDIMC
XTFEED(I)=0
ES(I)=0
EE1S(I)=0
5703 CONTINUE
DO 5020 I = 1,NDIMD

```

```

        DELOR(I)=0
        IDELOR(I)=0
5020 CONTINUE
C
C
C CALCULATE FRACTIONAL FEEDING AND RELATIVE INTENSITIES
C
C
        DO 50 I=1,NLEV
        XTFEED(I)=0
        DO 50 J=1,NGAM
        IF (NU(J).EQ.I) XTFEED(I)=XTFEED(I)+RINTEN(J)
        IF (NL(J).EQ.I) XTFEED(I)=XTFEED(I)-RINTEN(J)
50 CONTINUE
        SUM=0
        DO 6161 I=1,NGAM
6161 AINTEN(I)=RINTEN(I)
        DO 51 I=1,NLEV
        SUM=SUM+XTFEED(I)
51 CONTINUE
        IF (IBETA) GO TO 59
        GO TO 54
59 DO 52 I=1,NLEV
52 XTFEED(I)=XTFEED(I)/SUM
        DO 53 I=1,NGAM
53 RINTEN(I)=RINTEN(I)/SUM
54 CONTINUE
C
C BEGINNING WITH THIS SECTION, THE COMPUTED RESULTS ARE PRINTED.
C
C
        NSECT = 2
        NTPAGE = NTPAGE + 1
        PRINT 1111,NSECT,NTPAGE
        PRINT 722
722 FORMAT (//10X,'SECTION 2',17X,'PROGRAM STATEFIT-OUTPUT RESULTS')
        PRINT 201,TITLE
201 FORMAT (/' TITLE',3X,10A8)
        PRINT 113,NLEV,LISTG,NGAM
113 FORMAT (/,I6,16H EXCITED STATES ,I4,18H INPUT GAMMA RAYS ,I4,20H AS
        *SIGNED GAMMA RAYS)
        IF ((NLEV-NGAM).EQ.0.0) GO TO 767
        PRINT 100,CSQPDF,SUM
100 FORMAT (//,1X'CHI SQUARE PER DEGREE FREEDOM = ',F12.3,5X,'TOTAL UNO
        *BSERVED FEEDING TO ALL EXCITED STATES= ',F15.4)
        GO TO 769
767 PRINT 102,SUM
102 FORMAT (//,' CHI SQUARE PER DEGREE FREEDOM = UNDEFINED (ZERO DEGREE
        *S OF FREEDOM)'/10X,'TOTAL UNOBSERVED FEEDING TO ALL EXCITED STATES
        * = 'F15.4)
769 CONTINUE
        DO 99 I=1,NLEV
99 ES(I)=E(I)

```

C
C


```

C      PRINT SECTION 2
C
C      SECTION 2 LISTS ALL THE EXCITED STATES IN ORDER OF INCREASING
C      ENERGY.
C
C      ORDER ENERGY LEVELS (BY ENERGIES)
C
C      CALL CRDEFA(ES,IE,NLEV,.00007D0)
C
C
      LINCT = 23
      PRINT 705
705  FORMAT(////22X,'EXCITED STATES (IN ORDER OF LEVEL ENERGY)'/)
      PRINT 765
765  FORMAT(' NOTES-- SCATTER ERROR = STATISTICAL ERROR MULTIPLIED BY T
1HE SQ. RT. OF CHI SQUARE PER DEGREE FREEDOM')
      PRINT 766
766  FORMAT(6X'-- FRACTIONAL BETA FEEDING/INTENSITY BALANCE VALUES ARE
*INVALID UNLESS',9X,'GAMMA RAY INTENSITIES ARE CORRECTED FOR INTER
*NAL CONVERSION'/)
      IF(IBETA.EQ.0) PRINT 103
103  FORMAT(7X,'LEVEL'8X'CALCULATED'7X'STATISTICAL'10X'SCATTER'8X'INTEN
*SITY'9X'DEPOPULATING'8X'POPULATING')
      IF(IBETA.EQ.1) PRINT 104
104  FORMAT(7X,'LEVEL'8X'CALCULATED'7X'STATISTICAL'10X'SCATTER' 8X'FRACT
*IONAL'8X'DEPOPULATING'8X'POPULATING')
      IF(IBETA.EQ.0) PRINT 105
105  FORMAT(7X'NUMBER'6X'LEVEL ENERGY'9X'ERROR'14X'ERROR'10X'BALANCE'10
*X'TRANSITIONS'9X'TRANSITIONS'/)
      IF(IBETA.EQ.1) PRINT 752
752  FORMAT(7X'NUMBER'6X'LEVEL ENERGY' 9X'ERROR'14X'ERROR' 8X'BETA FEED
*ING'7X'TRANSITIONS'9X'TRANSITIONS'/)
      DO 107 I=1,NLEV
      K=IE(I)
      J=NES(IE(I))
      NUMUP = 0
      NUMLO = 0
      DO 1088 L=1,NGAM
      IF (JL(L).EQ.J) NUMLO = NUMLO + 1
      IF (JU(L).EQ.J) NUMUP = NUMUP + 1
1088  CONTINUE
      PRINT 110,I,ES(I),EE1(K),EE2(K),XTFEED(K),NUMUP,NUMLO
110  FORMAT (I10,6X,F14.5,7X,F9.5,10X,F9.5,7X,F14.5, 9X,I3,18X,I3)
      LINCT = LINCT + 1
      IF (LINCT.LE.60) GO TO 107
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 705
      IF(IBETA.EQ.0) PRINT 103
      IF(IBETA.EQ.1) PRINT 104
      IF(IBETA.EQ.0) PRINT 105
      IF(IBETA.EQ.1) PRINT 752
      LINCT = 10

```

```

107 CONTINUE
C
C   BEGIN SECTION 3
C CALCULATE CHI
C
      NSECT = 3
      NTPAGE = NTPAGE + 1
      DO 729 I=1,NGAM
        DELTA(I)=EG(I)-EGCALC(I)
        CHI(I)=DELTA(I) /EEG(I)
729 CONTINUE
C
C
C PRINT SECTION 3
C
      SECTION 3 PRINTS A TABLE OF ALL THE ALREADY ASSIGNED GAMMA RAYS.
C
      PRINT 1111,NSECT,NTPAGE
      PRINT 711
711 FORMAT (///10X,'SECTION 3 ASSIGNED GAMMA RAYS')
      PRINT 761
761 FORMAT (/,2X,'NOTE-- MULTI INDICATES GAMMA RAY HAS BEEN ASSIGNED TO
* MORE THAN 1 PAIR OF ENERGY LEVELS')
      PRINT 762
762 FORMAT (6X,'-- IF CHI EXCEEDS 100.0, THE ENTRY"GT 99.999"WILL APPEA
*R.')
      IF (IBETA.EQ.0) PRINT 300
300 FORMAT (//5X'ERROR'3X'CARD' 5X'INITIAL'3X'FINAL'3X'GAMMA RAY'5X'GAM
1MA RAY'5X'CALCULATED'5X'ENERGY'7X'CHI'6X'TRANSITION')
      IF (IBETA.EQ.1) PRINT 301
301 FORMAT (//5X'ERROR'3X'CARD' 5X'INITIAL'3X'FINAL'3X'GAMMA RAY'5X'GAM
1MA RAY'5X'CALCULATED'5X'ENERGY'7X'CHI'6X'NORMALIZED')
      PRINT 716
716 FORMAT (5X'NOTES'3X'NUMBER'4X'LEVEL'4X'LEVEL'4X'ENERGY'9X'ERROR'7X'
1TRANSITION'3X'DIFFERENCE'14X'INTENSITY'/)
C
      DO 725 K=1,NGAM
        MA(K)=0
        DO 726 J=1,NGAM
          IF (DABS(EG(K)-EG(J))-.00001) 727,727,726
727 MA(K)=MA(K)+1
726 CONTINUE
781 MC(K) = 0
          IF (DABS(CHI(K))-100.0) 725,735,735
735 MC(K)=1
          CHI(K)=99.999*DABS(CHI(K))/CHI(K)
725 CONTINUE
        DO 7025 I=1,NGAM
          K=NU(I)
          NU(I)=JU(I)
          JU(I)=K
          K=NL(I)
          NL(I)=JL(I)
          JL(I)=K

```

```

7025 CONTINUE
C
    LINCT = 14
C
C    ORDER EG IN ASSFNDING ENERGY SEQUENCE FOR CONVIENENCE IN SECTION 3
C
    CALL ORDERA(EG,KAY,NGAM,.00007D0)
    DO 736 J=1,NGAM
    K=KAY(J)
    LINCT = LINCT + 1
    IF (LINCT.LE.60) GO TO 70255
    NTPAGE = NTPAGE + 1
    PRINT 1111,NSECT,NTPAGE
    PRINT 711
    PRINT 300
    PRINT 716
    LINCT = 10
70255 IF (MA(K).GT.1) GO TO 737
    IF (MC(K).GT.0) GO TO 739
C
    PRINT 91,KAY(J),NU(K),NL(K),EG(J),EEG(K),EGCALC(K),DELTA(K),CHI(K)
    1,RINTEN(K)
    91 FORMAT(I16,I10,I9,3F14.5,4X,F8.3,3X,2X,F7.3,2X,F12.5)
    GO TO 736
739 PRINT 92,KAY(J),NU(K),NL(K),EG(J),EEG(K),EGCALC(K),DELTA(K),CHI(K)
    1,RINTEN(K)
    92 FORMAT(I16,I10,I9,3F14.5,4X,F8.3,3X,2HGT,F7.3,2X,F12.5)
    GO TO 736
737 IF (MC(K).GT.0) GO TO 743
    PRINT 96,KAY(J),NU(K),NL(K),EG(J),EEG(K),EGCALC(K),DELTA(K),CHI(K)
    1,RINTEN(K)
    96 FORMAT(5X'MULTI'I6,I10,I9,3F14.5,4X,F8.3,5X,F7.3,2X,F12.5)
    GO TO 736
743 PRINT 742,KAY(J),NU(K),NL(K),EG(J),EEG(K),EGCALC(K),DELTA(K),CHI(K)
    1,RINTEN(K)
    742 FORMAT(5X'MULTI'I6,I10,I9,3F14.5,4X,F8.3,3X,2HGT,F7.3,2X,F12.5)
736 CONTINUE
C
C    PUT EG BACK IN ORIGIONAL SEQUENCE (SAME ORDER AS THE INPUT CARDS)
C
    DO 760 L=1,NGAM
    SAM=EG(I)
    DO 700 LL=1,NGAM
    IF (KAY(LL).NE.L) GO TO 700
    EG(L)=EG(LL)
    EG(LL)=SAM
    KAY(LL)=KAY(L)
    KAY(L)=I
    GO TO 760
700 CONTINUE
760 CONTINUE
C
C    PRINT SECTION 4
C
C    SECTION 4 LISTS ALL THE GAMMA RAYS THAT HAVE BEEN ASSIGNED OR

```



```

C      MIGHT BE ASSIGNED TO A TRANSITION; GROUPING IS BY LEVEL DEPOPULATED.
C
C
      NSECT = 4
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 712
712  FORMAT ( 10X,'SECTION 4 DEPOPULATING TRANSITIONS'/)
      PRINT 1331
1331  FORMAT(1X,'COMMENTS: (1) ASSIGNED HERE/ALSO ASSIGNED TO A,B: THIS AS
      *SIGNMENT HAS BEEN MADE/ALSO ELSEWHERE')
      PRINT 1332
1332  FORMAT( 10X,'(2) UNASSIGNED: THIS GAMMA RAY SATISFY'S ACCEPTANCE TEST
      * BUT HAS NOT BEEN ASSIGNED')
      PRINT 1333
1333  FORMAT(10X,'(3) NOT ASSIGNED HERE/ASSIGNED TO/ALSO ASSIGNED TO: GAM
      *MA RAY SATISFY'S TEST BUT IS ASSIGNED ELSEWHERE')
      PRINT 1334
1334  FORMAT( 10X,'(4) NONE FOUND: NO GAMMA RAY FOUND THAT SATISFY'S ACCEP
      *TANCE TEST')
      PRINT 720
720  FORMAT(/' INITIAL',2X,'FINAL',3X,'INITIAL',2X,'FINAL',3X,'TRANSITI
      *ON',2X,'TRANSITION',2X,'GAMMA RAY',2X,'GAMMA RAY',2X,'ENERGY',3X
      *, 'KEY',5X,'COMMENTS',14X,'GAMMA RAY')
      PRINT 721
721  FORMAT (' LEVEL',3X,'LEVEL',3X,'ENERGY',3X,'ENERGY',4X,'ENERGY',
      *6X,'ERRCR',6X,'ENERGY',6X,'ERROR',3X,'DIFFERENCE',30X,'CONFIDENCE
      * ')
      PRINT 1336
1336  FORMAT (' NUMBER',3X,'NUMBER',104X,'LEVEL&I.D.')
      YCAL=0.0
      DO 98 I=1,NLEV
      K=IE(I)
      98  EE1S(I)=EE1(K)
      LLEV=NLEV+1

C
C MOVE ALL LEVEL ENERGIES UPWARD ONE NOTCH AND INSERT 0.0 FOR THE
C GROUND STATE ENERGY IN POSITION ONE
C
      FRED=ES(1)
      FRAN=EE1S(1)
      ES(1)=0.0
      EE1S(1)=0.0
      DO 65 IS=1,NLEV
      IT=IS+1
      EOB=ES(IT)
      BILL=EE1S(IT)
      ES(IT)=FRED
      EE1S(IT)=FRAN
      FRED=EOB
65  FRAN=BILL

C
C CALCULATE EACH POSSIBLE TRANSITION ENERGY AND ITS ERROR
C
      INK=0

```

```

ICOUNT=0
IPAGE=0
C
DO 60 I=2,LLEV
II=I-1
PRINT 64
64 FORMAT(1H )
ICOUNT=ICOUNT+1
DO 60 J=1,II
INK=INK+1
DELE=ES(I)-ES(J)
DELOK(INK)=DABS(DELE)
EDEL=DSQRT(EE1S(I)**2+EE1S(J)**2)
IW=NES(IE(I-1))
IF (J.EQ.1) GO TO 1001
JF=NES(IE(J-1))
GO TO 1002
1001 JF=0
1002 MULTI=0
C
C SEARCH LIST OF ASSIGNED GAMMA RAYS TO SEE IF ANY HAVE BEEN
C ASSIGNED TO THIS TRANSITION
C
NCHEK = 0
DO 3001 MY = 1,NGAM
IF (IW.NE.NU(MY).OR.JF.NE.NL(MY)) GO TO 3001
DO 3995 IK = 1,LISTG
IF (DABS(EG(MY)-CEN(IK)) - 0.00001) 3994,3994,3995
3995 CONTINUE
3994 NCHEK = IK
RKONF = CONF(NCHEK)
RKOM = COM(NCHEK)
DELCE = DELCEN(NCHEK)
REZID = EG(MY) - DELE
CHIB = REZID/(DSQRT(EE1S(I)**2. + EE1S(J)**2. + DELCE**2.))
PRINT 718,IW,JF,ES(I),ES(J),DELE,EDEL,EG(MY),DELCE,REZID,CHIB,
* RKONF,RKOM
718 FORMAT (' ',I5,3X,I5,3X,F8.3,1X,F8.3,2X,F8.3,4X,F8.3,3X,F8.3,3X,
* F8.3,3X,F6.3,2X,F6.3,2X,'ASSIGNED HERE', 9X,A4,A8)
ICOUNT = ICOUNT + 1
DO 215 K=1,NGAM
IF(K.EQ.MY) GO TO 215
IF(DABS(CEN(NCHEK)-EG(K))-0.00001) 211,211,215
211 IF(ICOUNT-(IPAGE*50).LT.50) GO TO 212
IPAGE=IPAGE+1
NTPAGE = NTPAGE + 1
PRINT 1111,NSECT,NTPAGE
PRINT 712
PRINT 720
PRINT 721
PRINT 1336
212 PRINT 213,EG(K),NU(K),NL(K)
213 FORMAT( 59X,F8.3,24X,'ALSO ASSIGNED TO',215)
ICOUNT=ICOUNT+1
215 CONTINUE

```



```

      GO TO 30011
3001 CONTINUE
C
C SEARCH TOTAL LIST OF GAMMA RAYS TO SEE IF ANY FIT THE COMPUTED
C TRANSITION
C WIDE IS THE BANDWIDTH OF THE SELECTION TEST
C
30011 DO 55 I=1,LISTG
      IF (NCHEK.EQ.L) GO TO 55
      MAD=0
      MUD=0
      IF (DABS(DABS(DELE)-CEN(L))-WIDE*DSQRT(DELCEN(L)**2+EDEL**2)) 57,5
17,55
57 MULTI=MULTI+1
   REZID = CEN(L) - DELE
   CHIB = REZID/(DSQRT(EE1S(I)**2. + EE1S(J)**2. + DELCEN(L)**2.))
   DO 202 MY=1,NGAM
   IF (DABS(CEN(L)-EG(MY))-0.00001) 232,232,202
232 MUD=MUD+1
   IF (MUD.GT.1) GO TO 298
   PRINT 291,IW,JF,ES(I),ES(J),DELE,EDEL,CEN(L),DELCEN(L),REZID,
   *CHIB,CONF(L),COM(L)
291 FORMAT (' ',I5,3X,I5,3X,F8.3,1X,F8.3,2X,F8.3,4X,F8.3,3X,F8.3,3X,
   * F8.3,3X,F6.3,2X,F6.3,2X,'NOT ASSIGNED HERE',5X,A4,A8)
   ICCOUNT=ICOUNT+1
   IF (ICOUNT-(IPAGE*50).LT.50) GO TO 292
   IPAGE=IPAGE+1
   NTPAGE = NTPAGE + 1
   PRINT 1111,NSECT,NTPAGE
   PRINT 712
   PRINT 720
   PRINT 721
   PRINT 1336
292 PRINT 293, EG(MY),NU(MY),NL(MY)
293 FORMAT( ' 59X,F8.3,30X,'ASSIGNED TO',2I5)
   ICCOUNT=ICOUNT+1
   GO TO 202
298 IF (ICOUNT-(IPAGE*50).LT.50) GO TO 299
   IPAGE=IPAGE+1
   NTPAGE = NTPAGE + 1
   PRINT 1111,NSECT,NTPAGE
   PRINT 712
   PRINT 720
   PRINT 721
   PRINT 1336
299 PRINT 213, EG(MY),NU(MY),NL(MY)
   ICCOUNT=ICOUNT+1
202 CONTINUE
   IF (MUD.NE.0) GO TO 55
205 PRINT 719,IW,JF,ES(I),ES(J),DELE,EDEL,CEN(L),DELCEN(L),REZID,
   * CHIB,CONF(L),COM(L)
719 FORMAT (' ',I5,3X,I5,3X,F8.3,1X,F8.3,2X,F8.3,4X,F8.3,3X,F8.3,3X,
   * F8.3,3X, F6.3,2X,F6.3,2X,'UNASSIGNED',12X,A4,A8)
   ICCOUNT=ICOUNT+1
55 CONTINUE

```

```

C      IF(MULTI) 58,56,58
56  IF (NCHEK.NE.0) GO TO 58
    PRINT 717,TW,JF,ES(I),ES(J),DELE,EDEL
717  FORMAT (' ',I5,3X,I5,3X,F8.3,1X,F8.3,2X,F8.3,4X,F8.3,7X,'NONE FOUN
    *D')
    ICOUNT=ICOUNT+1
58  IF(J.LT.II) GO TO 758
    IF(I.EQ.LLEV.AND.J.EQ.II) GO TO 60
    IF((ICOUNT-IPAGE*50)-49) 60,757,759
757  ICOUNT=ICOUNT+1
    GO TO 759
758  IF(ICOUNT-(IPAGE*50).LT.50) GO TO 60
759  IPAGE=IPAGE+1
    NTPAGE = NTPAGE + 1
    PRINT 1111,NSECT,NTPAGE
    PRINT 712
    PRINT 720
    PRINT 721
    PRINT 1336
60  CONTINUE

C
C
C PRINT SECTION 5
C
C SECTION 5 LISTS ALL THE GAMMA RAYS THAT HAVE BEEN ASSIGNED OR MIGHT
C BE ASSIGNED; GROUPING IS BY THE ENERGY LEVEL POPULATED.
C
C
C      NSECT = 5
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 713
713  FORMAT ( 10X,'SECTION 5 POPULATING TRANSITIONS'/)
      PRINT 1331
      PRINT 1332
      PRINT 1333
      PRINT 1334
      PRINT 720
      PRINT 721
      PRINT 1336
      KPAGE=0
      KOUNT=0

C
DO 80 I=1,NLEV
PRINT 68
68  FORMAT(1H )
    KOUNT=KOUNT+1
    IXI=I+1
    DO 80 J=IXI,LLEV
    DELEA=ES(J)-ES(I)
    EDELA=DSQRT(EE1S(I)**2+EE1S(J)**2)
    JF=NES(IE(J-1))
    IF (I.EQ.1) GO TO 2001
    IW=NES(IE(I-1))

```

```

GO TO 2002
2001 IW=0
2002 MULTI=0
NCHEK = 0
DO 3202 MY = 1,NGAM
IF (JF.NE.NU(MY).OR.IW.NE.NL(MY)) GO TO 3202
DO 3997 IK = 1,LISTG
IF (DABS(EG(MY)-CEN(IK)) - 0.00001) 3996,3996,3997
3997 CONTINUE
3996 NCHEK = IK
RKONF = CONF(NCHEK)
RKCM = COM(NCHEK)
NCHEK2 = IK
DELCE = DELCEN(NCHEK)
REZID = EG(MY) - DELEA
CHIB = REZID/(DSQRT(EE1S(I)**2. + EE1S(J)**2. + DELCE**2.))
PRINT 718,JF,IW,ES(J),ES(I),DELEA,EDELA,EG(MY),DELCE,REZID,CHIB,
* RKONF,RKCM
KOUNT = KOUNT + 1
DO 220 K=1,NGAM
IF(K.EQ.MY) GO TO 220
IF(DABS(CEN(NCHEK)-EG(K))-0.00001) 216,216,220
216 IF((KOUNT-KPAGE*50).LT.50) GO TO 217
KPAGE=KPAGE+1
NTPAGE = NTPAGE + 1
PRINT 1111,NSECT,NTPAGE
PRINT 713
PRINT 720
PRINT 721
PRINT 1336
217 PRINT 218,EG(K),NU(K),NL(K)
218 FORMAT( 59X,F8.3,24X,'ALSO ASSIGNED TO',2I5)
KOUNT=KOUNT+1
220 CONTINUE
GO TO 32025
3202 CONTINUE
C
C
32025 DO 71 L=1,LISTG
IF (NCHEK.EQ.L) GO TO 71
MUD=0
MAD=0
IF(DABS(DABS(DELEA)-CEN(L))-WIDE*DSQRT(DELCEN(L)**2+EDELA**2)) 73,
*73,71
73 MULTI=MULTI+1
REZID = CEN(L) - DELEA
CHIB = REZID/(DSQRT(EE1S(I)**2. + EE1S(J)**2. + DELCEN(L)**2.))
DO 75 MY=1,NGAM
IF (DABS(CEN(L)-EG(MY))-0.00001) 235,235,75
235 MUD=MUD+1
IF(MUD.GT.1) GO TO 398
PRINT 291,JF,IW,ES(J),ES(I),DELEA,EDELA,CEN(L),DELCEN(L),REZID,
*CHIB,CONF(L),COM(L)
KOUNT=KOUNT+1
IF((KOUNT-KPAGE*50).LT.50) GO TO 392

```



```

    KPAGE=KPAGE+1
    NTPAGE = NTPAGE + 1
    PRINT 1111,NSECT,NTPAGE
    PRINT 713
    PRINT 720
    PRINT 721
    PRINT 1336
392 PRINT 293,EG(MY),NU(MY),NL(MY)
    KOUNT=KOUNT+1
    GO TO 75
398 IF((KOUNT-KPAGE*50).LT.50) GO TO 399
    KPAGE=KPAGE+1
    NTPAGE = NTPAGE + 1
    PRINT 1111,NSECT,NTPAGE
    PRINT 713
    PRINT 720
    PRINT 721
    PRINT 1336
399 PRINT 213, EG(MY),NU(MY),NL(MY)
    KOUNT=KOUNT+1
    75 CONTINUE
    IF (MUD.NE.0) GO TO 71
78 PRINT 719,JF,IW,ES(J),ES(I),DELEA,EDELA,CEN(L),DELCEN(L),REZID,
    * CHIB,CCNF(L),COM(L)
    KOUNT=KOUNT+1
71 CONTINUE

```

C

```

    IF(MULTI) 79,72,79
72 IF (NCHEK.NE.0) GO TO 79
    PRINT 717,JF,IW,ES(J),ES(I),DELEA,EDELA
    KOUNT=KOUNT+1
79 IF(J.LT.LLEV) GO TO 779
    IF(I.EQ.NLEV.AND.J.EQ.LLEV) GO TO 80
    IF((KOUNT-KPAGE*50)-49) 80,777,780
777 KOUNT=KOUNT+1
    GO TO 780
779 IF((KOUNT-KPAGE*50).LT.50) GO TO 80
780 KPAGE=KPAGE+1
    NTPAGE = NTPAGE + 1
    PRINT 1111,NSECT,NTPAGE
    PRINT 713
    PRINT 720
    PRINT 721
    PRINT 1336
80 CONTINUE

```

C

C ORDER TRANSITION ENERGIES

C

```

    CALL ORDERA(DELOR,IDELOR,INK,.00007)
    JAM = INK/110
    JIM=JAM+1
    JET=0
    DO 655 JOE=1,JIM

```

C

C

C PRINT SECTION 6

C
C
C
C
C

SECTION 6 LISTS ALL POSSIBLE TRANSITIONS, BOTH WITH ASSIGNED GAMMA
RAYS AND WITHOUT.

NSECT = 6
NTPAGE = NTPAGE + 1
PRINT 1111, NSECT, NTPAGE
PRINT 714

714 FORMAT (10X, 'SECTION 6 COMPUTED LIST OF ALL POSSIBLE TRANSITION E
*NERGIES')

PRINT 755

755 FORMAT (44H NOTE-- ***** INDICATES ASSIGNED GAMMA RAY)

PRINT 891

891 FORMAT (/, 2 (5X, 10HTRANSITION, 16X, 7HINITIAL, 5X, 5HFINAL, 11X))

PRINT 892

892 FORMAT (1H , 2 (6X, 6HENERGY, 19X, 6HENERGY, 5X, 6HENERGY, 11X) /)

C

DO 650 JEB=1, 55
JIB = JET + JEB
NUT=JIB+55
KIB=IDELOR(JIB)
IF (KIB.EQ.0) GO TO 650
894 DO 900 IN=2, LLEV
IF (KIB-IN*(IN-1)/2) 901, 901, 900
900 CONTINUE
901 LI=IN
IF=KIB- (LI-2) * (LI-1) / 2
LIA=NES (IE (LI-1))

C
C
C

GROUND STATE ASSIGNMENTS SHOULD NOW PRINT OUT.

IF (LF-1) 2005, 2005, 2000
2000 LFA=NES (IE (LF-1))
GO TO 2010
2005 LFA = 0
2010 RLIE = ES (LI)
RLFE = ES (LF)
DO 903 NY=1, NGAM
IF (LIA.EQ.NU (NY) .AND. LFA.EQ. NL (NY)) GO TO 905
902 IF (LIA.EQ. NL (NY) .AND. LFA.EQ. NU (NY)) GO TO 905
903 CONTINUE
JIBT=0
GO TO 906
905 JIBT=1
906 KUT=IDELOR (NUT)
IF (KUT.EQ.0) GO TO 920
893 DO 907 IN=2, LLEV
IF (KUT-IN*(IN-1)/2) 908, 908, 907
907 CONTINUE
908 LLI=IN
LLF=KUT- (LLI-2) * (LLI-1) / 2
LLIA=NES (IE (LLI-1))
IF (LLF-1) 2020, 2020, 2015

2015 LLFA=NES(IE(LLF-1))

GO TO 2025

2020 LLFA=0

2025 RLLIE = ES(LLI)

RLLFE = ES(LLF)

DO 910 NY=1,NGAM

IF (LLIA.EQ.NU(NY).AND.LLFA.EQ.NL(NY)) GO TO 915

909 IF (LLIA.EQ.NL(NY).AND.LLFA.EQ.NU(NY)) GO TO 915

910 CONTINUE

IF (JIBT.NE.0) GO TO 913

C

911 PRINT 912,DELOR(JIB),RLIE,RLFE,DELOR(NUT),RLLIE,RLLPF

912 FORMAT (2(F15.5,15X,F8.3,3X,F8.3,10X))

GO TO 650

913 PRINT 914,DELOR(JIB),RLIE,RLFE,DELOR(NUT),RLLIE,RLLFE

914 FORMAT (F15.5,6H *****,9X,F8.3,3X,F8.3,10X,F15.5,15X,F8.3,3X,F8.3)

GO TO 650

915 IF (JIBT.NE.0) GO TO 918

916 PRINT 917,DELOR(JIB),RLIE,RLFE,DELOR(NUT),RLLIE,RLLFE

917 FORMAT (F15.5,15X,F8.3,3X,F8.3,10X,F15.5,6H *****,9X,F8.3,3X,F8.3)

GO TO 650

918 PRINT 919,DELOR(JIB),RLIE,RLFE,DELOR(NUT),RLLIE,RLLFE

919 FORMAT (2(F15.5,6H *****,9X,F8.3,3X,F8.3,10X))

GO TO 650

920 IF (JIBT.NE.0) GO TO 922

921 PRINT 912,DELOR(JIB),RLIE,RLFE

GO TO 650

922 PRINT 914,DELOR(JIB),RLIE,RLFE

650 CONTINUE

JET = JET + 110

655 CONTINUE

C

C

C

PRINT SECTION 7

C

C

SECTION 7 LISTS ALL THE OBSERVED GAMMA RAYS,THOSE THAT ARE ASSIGNED
TO A TRANSITION, AND THOSE THAT ARE NOT.

C

C

C

ORDER LIST GAMMA RAYS

C

CALL ORDERA(CEN,ICEN,LISTG,.7D-3)

C

C

NSECT = 7

NTPAGE = NTPAGE + 1

ZERO = 0.0

PRINT 1111,NSECT,NTPAGE

PRINT 715

715 FORMAT (/10X,'SECTION 7 COMPLETE LIST OF OBSERVED GAMMA RAY ENERGI
*ES (INCLUDING ASSIGNED TRANSITIONS)')

LPREV = 7

PRINT 923

923 FORMAT (/7H GAMMA ,5X,'CARD',5X,'GAMMA RAY',4X,'GAMMA RAY',4X,'TRAN
*SITION',4X,'INTENSITY',4X,'INITIAL',4X,'FINAL',5X,'CONFIDENCE')


```

      PRINT 924
924  FORMAT (7H NUMBER,4X,'NUMBER',5X,'ENERGY',8X,'ERROR',6X,'INTENSITY
      *',7X,'ERROR',7X,'ENERGY',4X,'ENERGY',6X,'LEVEL'/)
      NEIN=0
      LINCT = LPREV
      DO 950 J=1,LISTG
      MCHK = 0
      KOP=ICEN(J)
      DO 926 I=1,NGAM
      IF (DABS(CEN(J)-EG(I))-0.0007) 931,931,926
926  CONTINUE
C
      IF (MCHK.EQ.1) GO TO 950
      NEIN=NEIN+1
      PRINT 930,J,KOP,CEN(J),DELCEN(KOP),RINT(KOP),DINT(KOP),CONF(KOP),
      *CCM(KOP)
      LINCT = LINCT + 1
      IF (LINCT.LE.60) GO TO 950
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 715
      PRINT95055
      PRINT 923
      PRINT 924
      LINCT = LPREV
      GO TO 950
931  LAU=JU(I)
      MCHK = 1
      LAL=JL(I)
      KUP=E(LAU)+0.5
      KLO=E(LAL)+0.5
      IF (LAL.EQ.0) KLO = 0
      IF (LAL.NE.0) GO TO 93305
      PRINT 933,J,KOP,CEN(J),DELCEN(KOP),AINTEN(I),RARE(I),E(LAU),ZERO
      1,CONF(KOP),COM(KOP)
      GO TO 93306
93305 PRINT 933,J,KOP,CEN(J),DELCEN(KOP),AINTEN(I),RARE(I),E(LAU),E(LAL)
      1,CONF(KOP),COM(KOP)
933  FORMAT (' ',I4,6X,I4,5X,F8.3,7X,F6.3,4X,F10.3,5X,F8.2,5X,F6.1,5X,
      1F6.1,4X,A4,A8)
930  FORMAT (' ',I4,6X,I4,5X,F8.3,7X,F6.3,4X,F10.3,5X,F8.2,26X,A4,A8)
93306 LINCT = LINCT + 1
      IF (LINCT.LE.60) GO TO 926
      NTPAGE = NTPAGE + 1
      PRINT 1111,NSECT,NTPAGE
      PRINT 715
      PRINT 95055
95055 FORMAT ('+',99X,' -CONTINUED')
      PRINT 923
      PRINT 924
      LINCT = LPREV
      GO TO 926
950  CONTINUE

```

C
C

C
999 CALL EXIT
1000 RETURN
END

C

SUBROUTINE ORDERA (DIF, IDIF, NDIF, ACC)

C

```
IMPLICIT REAL*8 (A-H,O-Z)
INTEGER*2 IDIF
DC 800 NA=1,NDIF
DIMENSION DIF(NDIF),IDIF(NDIF)
IF(DIF(NA)) 800,800,780
780 BOB=DIF(NA)
DIF(NA)=0
NC=NA
798 NO=1
DO 790 NB=1,NDIF
IF(DIF(NB)) 791,790,791
791 IF(DABS(DIF(NB))-BOB+ACC) 792,790,790
792 NO = NC + 1
790 CONTINUE
782 IF(DIF(NO)) 784,786,786
784 KC=NC+1
GO TO 782
786 BILL=BCE
BOB=DIF(NO)
DIF(NO)=-BILL
IDIF(NO)=NC
IF(BOB) 800,800,799
799 KC=NO
GO TO 798
800 CONTINUE
DC 810 IK=1,NDIF
810 DIF(IK)=DABS(DIF(IK))
820 RETURN
END
```

SUBROUTINE LEASQE(Y,EY,NY,IY,F,NF,IF,C,EYC,ERC,CSQPDF,YCALC,PRT,
*V,B,SCALE)

C
C CHANGES MADE IN LEASQE FOR 3600/360 CONVERSION, APRIL 1970, BY C. BATSON
C

IMPLICIT REAL*8 (A-H,O-Z)
INTEGER*2 F
DIMENSION Y(1),EY(1),F(1),C(1),EYC(1),ERC(1),YCALC(1)
DIMENSION V(IF),B(IF),SCALE(IF)

C
C *****
C

C ALL COMMENT CARDS BELOW WITH EXECUTABLE STATEMENTS ARE STEPS IN
C THE SUBROUTINE THAT HAVE BEEN DELETED TO SAVE CORE DEMAND.
C THEY SERVE TO PRINT OUT THE ERROR MATRICES AND ARRAYS
C WHEN THE "A" MATRIX IS NON-INVERTIBLE.
C TO USE, SIMPLY REMOVE THE "C" FROM EACH, AND ALSO
C REMOVE SIMILARLY NUMBERED "CONTINUE" CARDS.
C
C -----

C THE FOLLOWING MATRICES ARE SQUARE WITH DIMENSION NDMCF BY NDMCF
5516 COMMON A(20, 20)

C *****

C5517 DIMENSION D(20, 20),E(20, 20)

C
C -----
C

	LOGICAL PRT,MODE,CAC	6
C	IF CSQPDF=-2,USE EXISTING INVERSE MATRIX IN MEMORY TO DETERMINE SOLUTI	6
C	IF CSQPDF=-1 USE PREV CALC SOL VEC AND F TO CALC CSQPDF AND YCALC	6
	CAC=CSQPDF.EQ.-2.	7
	MODE=CSQPDF.EQ.-1.	8
	IF(EY(1)) 1,3,1	9
3	DO 2 I=1,NY	10
2	EY(I)=1.	11
1	IF(CAC)GO TO 60	
	IF(MODE.AND.PRT)GO TO 200	
	IF(MODE)GO TO 500	
C	CALCULATE SCALING FACTORS	17
C	CALCULATE DIAGONAL ELEMENTS	17
	DO 54 I=1,NF	
	SC=0.	19
	DO 56 K=1,NY	20
	L=IF*(K-1)+I	21
56	SC=SC+(F(L)/EY(K))**2	22
	IF(SC.EQ.0.)GO TO 11	23
	SCALE(I)=DSQRT(SC)	
	A(I,I)=1.	26
	GO TO 12	27
11	A(I,I)=0.	28

```

      SCALE(I)=0.
C
C      +++++ +++++ +++++
C
C      12 E(I,I)=0.
C      54 D(I,I)=A(I,I)
C
C      -----
C
C      12 CONTINUE
C      54 CONTINUE
C      CALCULATE OFF DIAGONAL ELEMENTS
C      DO 5 I=2,NF
C      M=I-1
C      DO 5 J=1,M
C      AA=0.0
C      IF (SCALE(I).EQ.0..OR.SCALE(J).EQ.0.) GO TO 13
C      DO 4 K=1,NY
C      IK=IF*(K-1)
C      L=IK+I
C      LL=IK+J
C      4 AA=AA+F(L)*F(LL)/(EY(K)*EY(K)*SCALE(I)*SCALE(J))
C
C      +++++ +++++ +++++
C
C      13 E(I,J)=AA
C      D(J,I)=AA
C      E(J,I)=0.
C
C      -----
C
C      13 CONTINUE
C      A(I,J)=AA
C      5 A(J,I)=AA
C      CALC CONSTANT VECTOR
C      60 DO 10 I=1,NF
C      CV=0.0
C      DO 9 K=1,NY
C      L=IF*(K-1)+I
C      9 CV=CV+Y(K)*F(L)/(SCALE(I)*EY(K)**2)
C      10 V(I)=CV
C      IF(CAC) GO TO 61
C      IF(PRT) GO TO 200
C      CALC INVERSE OF AMATRIX
C      DET=1.
C
C
C      50 CALL MATINV(A,NF,B,0,DET,IF)
C
C      IF(DET.NE.0.)GO TO 51
C      PRINT 499
C      499 FORMAT(24H0INVERSE MATRIX SINGULAR)
C      51 DO 420 I=1,NF
C      DO 420 J=1,NF

```

```

      EE=0.
C      DO 419 K=1,NF
C
C      +++++ +++++ +++++
C
C 419 EE=EE+A(I,K)*D(K,J)
C 420 E(I,J)=EE
C
C      -----
C
C 420 CONTINUE
C CALC COEFFICIENTS OF EXPANSION
  61 DO 15 I=1,NF
    CC=0.0
    DO 14 J=1,NF
      14 CC=CC+A(I,J)*V(J)
      15 C(I)=CC/SCALE(I)
      IF(PRT) GO TO 210
500 CSQ=0.0
    DO 20 I=1,NY
      YCAL=0.0
      DO 19 J=1,NF
        L=IF*(I-1)+J
        19 YCAL=YCAL+C(J)*F(L)
        YCALC(I)=YCAL
      20 CSQ=CSQ+((Y(I)-YCAL)/EY(I))**2
      CSQPDF=CSQ/DFLOAT(NY-NF)
      IF(PRT) PRINT 250,CSQPDF
250 FORMAT(23H0CHI SQ DEGREE FREEDOM=,F15.5)
      IF(CAC) RETURN
      IF(MODE) RETURN
      DO 25 I=1,NF
        EYC(I)=DSQRT(A(I,I))/SCALE(I)
        25 ERC(I)=EYC(I)*DSQRT(CSQPDF)
      RETURN
200 PRINT 123
123 FORMAT(17H0 FUNCTION MATRIX)
    DO 90 J=1,NY
      IJ=IF*(J-1)
      IJ1=IJ+1
      IJ2=IJ+NF
      90 PRINT 103,(F(LLL),LIL=IJ1,IJ2)
      IF(MODE) GO TO 500
      PRINT 111
111 FORMAT(10H0 A-MATRIX)
    DO 8 II=1,NF
      8 PRINT 103,(A(II,JJ),JJ=1,NF)
103 FORMAT(X,8E15.7)
    PRINT 113
113 FORMAT(16H0CONSTANT VECTOR)
    PRINT 103,(V(I),I=1,NF)
    GO TO 50
210 PRINT 112
112 FORMAT(17H0INVERSE A-MATRIX)
    DO 7 II=1,NF

```



```

      7 PRINT 103, (A(II,JJ),JJ=1,NF)
C
C      +++++ +++++ +++++
C
C      PRINT 116
C 116 FORMAT(18HOCHECK UNIT MATRIX)
C      DO 53 II=1,NF
C 53 PRINT 103, (E(II,JJ),JJ=1,NF)
C
C      -----
C
C      PRINT 114
C 114 FORMAT(16HOSOLUTION VECTOR)
C      PRINT 103, (C(I),I=1,NF)
C      GO TO 500
2000 RETURN
      END

```

```

      SUBROUTINE MATINV† (A,N,B,M,DETERM,NMAX)
C
C   MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
C
C**** REMOVE NEXT STATEMENT IN SINGLE PRECISION VERSION
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PIVOT
      DIMENSION A(NMAX,N), B(NMAX,M)
      DIMENSION PIVOT(120),INDEX(120)
C
C   INITIALIZE DETERMINANT AND PIVOT ELEMENT ARRAY
C
      DETERM=1.0
      DO 20 I=1,N
      PIVOT(I)=0.0
20    INDEX(I)=0.0
C
C   PERFORM SUCCESSIVE PIVOT OPERATIONS (GRAND LOOP)
C
      DO 550 I=1,N
C
C   SEARCH FOR PIVOT ELEMENT AND EXTEND DETERMINANT PARTIAL PRODUCT
C
      AMAX=0.0
      DO 105 J=1,N
      IF (PIVOT(J).NE.0.0) GO TO 105
      DO 100 K=1,N
      IF (PIVOT(K).NE.0.0) GO TO 100
      TEMP=DAES(A(J,K))
      IF (TEMP.LT.AMAX) GO TO 100
      IROW=J
      ICOLUM=K
      AMAX=TEMP
100    CONTINUE
105    CONTINUE
      INDEX(I)=4096*IROW+ICOLUM
      J=IROW
      AMAX=A(J,ICOLUM)
      DETERM=AMAX*DETERM
C
C   RETURN IF MATRIX IS SINGULAR (ZERO PIVOT) AFTER COLUMN INTERCHANGE
C
      IF (DETERM.EQ.0.0) GO TO 600
C
      PIVOT(ICOLUM)=AMAX
C
C   INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
      IF (IROW.EQ.ICOLUM) GO TO 260
      DETERM=-DETERM
      DO 200 K=1,N
      SWAP=A(J,K)
      A(J,K)=A(ICOLUM,K)

```

[†]"ANL F402S, Matrix Inversion with Accompanying Solution of Linear Equations", Argonne National Laboratory, Applied Mathematics Division, System/360 Library Subroutine.

```

      A(ICOLUM,K)=SWAP
200  CONTINUE
      IF (M.LE.0) GO TO 260
      DO 250 K=1,M
      SWAP=B(J,K)
      B(J,K)=B(ICOLUM,K)
      B(ICOLUM,K)=SWAP
250  CONTINUE
C
C      DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
260  K=ICOLUM
      A(ICOLUM,K)=1.0
      DO 350 K=1,N
      A(ICOLUM,K)=A(ICOLUM,K)/AMAX
350  CONTINUE
      IF (M.LE.0) GO TO 380
      DO 370 K=1,M
      B(ICOLUM,K)=B(ICOLUM,K)/AMAX
370  CONTINUE
C
C      REDUCE NON-PIVOT ROWS
C
380  DO 550 J=1,N
      IF (J.EQ.ICOLUM) GO TO 550
      T=A(J,ICOLUM)
      A(J,ICOLUM)=0.0
      DO 450 K=1,N
      A(J,K)=A(J,K)-A(ICOLUM,K)*T
450  CONTINUE
      IF (M.LE.0) GO TO 550
      DO 500 K=1,M
      B(J,K)=B(J,K)-B(ICOLUM,K)*T
500  CONTINUE
550  CONTINUE
C
C      INTERCHANGE COLUMNS AFTER ALL PIVOT OPERATIONS HAVE BEEN PERFORMED
C
600  DO 710 I=1,N
      I1=N+1-I
      K=INDEX(I1)/4096
      ICOLUM=INDEX(I1)-4096*K
      IF (K.EQ.ICOLUM) GO TO 710
      DO 705 J=1,N
      SWAP=A(J,K)
      A(J,K)=A(J,ICOLUM)
      A(J,ICOLUM)=SWAP
705  CONTINUE
710  CONTINUE
C
      RETURN
      END

```