ANL Physics Division Informal Report

PHY-1970 B

(Revision 1)

The original report PHY-1970 B is no longer in stock. The attached set contains additions and changes made in 1971. Also attached is Section VII (only), Program AUTOFIT, from the original report.

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The attached set of pages are additions and changes to the Manual of Data-Analysis Programs for Charged-Particle Reactions. A few previous errors are corrected. However, most of the sheets relate to improvements in the programs. Compatability with previous conventions and data organization has been maintained.

The most significant changes are the following.

1. Addition of a target-thickness correction subroutine package.
2. In Program SUBTBACK, a new option to punch a Standard Spectrum Data Set of the background, the residual spectrum, or both.
3. In Program AUTOFIT,
    a. A simplified treatment of the option NREF = 0;
    b. An option to constrain the separation of overlapping peaks to a prescribed value;
    c. Use of the centroids of peaks for the position in multichannel data; and
    d. A printing of chi-squared values.

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CARDS FOR STANDARD SPECTRUM DATA SET

Column	Variable		Value	Usage
CARD 1.	Reaction Identification Card			
	RUNID, ISPECT, ICAL, NOFTEN, IFMT, II, IJ, AM2, E1, ANG, FREQ, THE, TLE			
	FORMAT (A8, A1, I1, 2I2, 4X2I1, 4F10.5, 2F5.0)			
1—8	RUNID	=	Alphanumeric spectrum identification. (Should be present.)	
9	ISPECT	=	A	MCA data.
		=	T	Tandem split-pole spectrograph data.
		=	C	Cyclotron split-pole spectrograph data.
		=	B	Tandem Browne-Buechner spectrograph data.
10	ICAL	=	n, $0 \leq n \leq 9$ (MCA data only), where n is the number of calibration coefficients of a polynomial of degree n - 1 used to calculate particle energy (MeV) from channel number. If n = 0, no coefficients will be read in and channel number cannot be converted to particle energy (or Q value).	
	or	=	Spectrograph calibration number.	
		= (T) 1	Calibration date	5-23-69
		= (C) 1		3-9-70
		= (B) 1		10-31-63
		= (B) 2		7-9-64
		= (B) 3		5-20-65
		= (B) 4		1-5-67
11—12	NOFTEN	=	0	MCA data. (This also sets ISPECT = A.)
			n, $1 \leq n \leq 99$ (Spectrograph data only.)	
			Tracks in the emulsion are counted in intervals of 1/n millimeters along the plate. For example, n = 2 signifies 0.5 mm intervals.	
14	IFMT	=	n, $0 \leq n \leq 5$	
			The format control for the spectrum cards (Cards 3).	
			n = 0	Default format. IFMT = 1 or 3 for spectrograph and MCA data, respectively.

		= 1	Format (10F6.0, F6.3) Automatic plate scanner.
		= 2	Format (F6.0, 9F7.0, F6.1) Spectrograph format.
		= 3	Format (F6.0, 9F7.0, 8XF3.0) DIDJ MCA cards.
		= 4	Format (F6.0, 9F7.0, 8XF3.0) Cyclotron MCA cards.
		= 5	Format (F6.0, 9F7.0, 8XF2.0) Fast Dump MCA cards.

19,20 II, IJ = Mass identification numbers of incident and outgoing particles, respectively.

= 0	Read in masses on separate Card 2.	
= 1	p (proton)	Mass = 1.007276
= 2	d (deuteron)	2.013554
= 3	t (triton)	3.015501
= 4	$^{3}He^{+}$	3.015481
= 5	$^{3}He^{++}$	3.014932
= 6	$^{4}He^{++}$ (alpha)	4.001506
= 7	$^{6}Li^{+++}$	6.013479
= 8	$^{7}Li^{+++}$	7.014358

21—30 AM2 = Mass of target nucleus (^{12}C scale).

31—40 E1 = Laboratory energy of incident particle (MeV).

41—50 ANG = Laboratory scattering angle (degrees).

51—60 FREQ > 0 NMR frequency (MHz)

< 0 |FREQ| = Magnetic field of spectrograph (kG).

61—65 THE = Setting of high-energy screw on Enge split pole.

66—70 TLE = Setting of low-energy screw on Enge split pole.

CARD 2. Reaction Mass Card. (Use only if II or IJ = 0).

AM1, AM3, Z3, Z1

FORMAT (2F10.5, 2F5.0)

1—10 AM1 = Mass of incident particle (electron mass subtracted).

11—20 AM3 = Mass of outgoing particle (electron mass subtracted).

21—25 Z3 = Charge number of outgoing particle.
If left blank, a value Z3 = 1.0 is assumed.

26—30 Z1 = Charge number of incident particle.
If left blank, a value Z1 = 1.0 is assumed.

NOTE: If this card is present, values for both AM1 and AM3 must be given.

CARD 3. Raw Data Cards

(Y(I), I = 1, 10), D

FORMAT: See IFMT, Card 1.

Y(I) = Number of counts for the Ith channel of the card.

D = Plate distance (cm) or channel number of the first channel of data on the card. (See Note 4.)

NOTE 1: These cards are normally prepared on auxiliary computers without decimal points. The formats assume standard production.

NOTE 2: The cards may be in any order (EXCEPT that the first card must have the lowest value of D), and regions may be omitted.

NOTE 3: For MCA cards, the value of D is multiplied by 10 since the value read is usually a card-count number.

NOTE 4: For MCA data, the first channel of the analyzer is defined as channel zero. For IFMT = 3 and 5, channel zero is assumed to be the first entry on card count 0; for IFMT = 4, channel zero is the first entry on card count 1.

NOTE 5: For IFMT = 5, D must be in the range $0 \leq D \leq 99$; i.e., there cannot be more than 100 cards (1000 channels).

CARD 4. Raw Data Termination Card.

1—2 ICARD = -1 This terminates input of Cards 3.

COMMON BLOCK /TARGET/

COMMON /TARGET/ XF, XG, P, WTMOLG, GCLCST, DEL, AWMF, ZMF, AWMG, ZMG, ZF (10), WF (10), ATFRF (10), ZG (10), WG (10), ATFRG (10), Z1, PHI, RPHI, RANG, NTARF, NTARG, ITARG

XF = The total effective thickness of the solid target or the gas cell window (mg/cm^2).

XG = One half the total effective thickness of the gas (mg/cm^2).

P = The gas pressure, in units of Torrs for the default gas-cell constant.

WTMOLG = The total molecular weight of the gas (gm/mole).

GCLCST = The gas-cell constant which relates the gas thickness XG to its pressure and molecular weight. The relationship is XG = WTMOLG*P*GCLCST where the default GCLCST is $(273.16 \times 2.54)/(760. \times 298. \times 22.414) = 1.3668 \times 10^{-4}$. The gas cell is assumed to be two inches in diameter.

DEL = A convergence criterion for iterating energies (MeV). The default value is 0.0001 MeV.

AWMF = The effective molecular weight of the foil (gm/mole).

ZMF = The effective atomic charge for the foil.

AWMG = The effective molecular weight of the gas (gm/mole).

ZMG = The effective atomic charge of the gas.

ZF = The array of charges for each element of the foil material.

WF = The array of atomic weights (u) for each element of the foil material.

ATFRF = The array of the number of atoms of each element which makes up the molecule of the foil material. This is later converted to a fraction.

ZG = Same as ZF for the gas material.

WG = Same as WF for the gas material.

ATFRG = Same as ATFRF for the gas material.

Z1 = The charge number of the incident particle in the reaction.

PHI = The angle that the normal to the solid target makes with the beam direction (degrees).

RPHI = The value of PHI in radians.

RANG = The value of ANG (the reaction angle) in radians.

NTARF = The number of separate elements which make up a molecule of the foil material (≤ 10).

NTARG = Same as NTARF for the gas material.

ITARG = A code for identifying the type of target.

- = 0 No target-thickness corrections.
- ≥ 1 Make corrections for an enclosed, circular gas cell.
- ≤ -1 Make corrections for a solid target.

SUBROUTINE SPCTRM

Purpose: Controls the reading of a Standard Spectrum Data Set from data cards in the normal input stream.

Calling Sequence: CALL SPCTRM

Common Blocks:

/DATA/ Input: IERR = 0

Output: RUNID, FREQ, NOFTEN, II, IJ, ISPECT, IFMT

/QVAL/ Input: None

Output: E1, ANG, AM2, INX = 0

/YOKE/ Input: None

Output: THE, TLE, ITRN = 0

Subroutine Calls: GETMAS, CHKINP, XYINP

Operation:

(1) Reads the Reaction Identification Card.

(2) Calls GETMAS and CHKINP.

(3) If no errors have occurred (IERR = 0) it calls XYINP and sets INX = 0 and ITRN = 0.

Error Conditions: IERR should be checked after the call to SPCTRM for errors in GETMAS or CHKINP. Should an error occur, the reading of the Standard Spectrum Data Set will be incomplete.

SUBROUTINE GETMAS

Purpose: Interprets the reaction codes and sets values for the masses of the incident and outgoing particles.

Calling Sequence: CALL GETMAS

Common Blocks:

/DATA/ Input: II, IJ
Output: Same as input

/QVAL/ Input: None
Output: AM1, AM3, Z3

/TARGET/ Input: None
Output: Z1

Subroutine Calls: None

Operation: Sets values for particle masses and charges in accordance with the following table.

Code	Mass	Charge	Particle	
0	Reads AM1, AM3, Z3, and Z1 from separate card.			
1	1.007276	1	p	(proton)
2	2.013554	1	d	(deuteron)
3	3.015501	1	t	(triton)
4	3.015481	1	$^{3}He^{+}$	
5	3.014932	2	$^{3}He^{++}$	
6	4.001506	2	$^{4}He^{++}$	(alpha)
7	6.013479	3	$^{6}Li^{+++}$	
8	7.014358	3	$^{7}Li^{+++}$	
9	Error. Sets IERR = 1.			

SUBROUTINE XYINP

Purpose: Reads the Spectrum Data Cards, checks for errors, and creates the arrays of counts and distance values.

Calling Sequence: CALL XYINP

Common Blocks: /DATA/

Input: OFTEN, IFMT

Output: Same as input, plus DIST, COUNTS, NCHANN, IERR

Subroutine Calls: None

Operation:

(1) Sets the array COUNTS to zero.

(2) Selects the appropriate format statement for reading the data cards.

(3) Reads the data cards and stores the information in the proper locations of the array COUNTS.

(4) Evaluates the total number of channels spanned by the data.

(5) Checks for error conditions.

(6) Creates the array DIST.

Error Conditions: Processing terminates, the program sets IERR = 1 and prints an error message if either of the following conditions occur:

(1) "D = xxxx LESS THAN D1 = yyyy"

The cards are out of order so that the lowest value of D is not on the first card.

(2) "NCHANN = xxxx GREATER THAN 4100"

The data exceed 4100 channels.

SUBROUTINE PDSINP

Purpose: Controls the reading of a Standard Spectrum Data Set from a member of a partitioned data set (S/360 only).

Calling Sequence: CALL PDSINP (IOVRD)

Common Blocks:

/DATA/ Input: RUNID, IERR = 0

Output: Same as input, plus DIST, COUNTS FREQ, OFTEN, NOFTEN, NCHANN, II, IJ, ISPECT, IFMT

/QVAL/ Input: None

Output: E1, H, ANG, AM1, AM2, AM3, Z3, JDATA, ICAL, INX = 0

/YOKE/ Input: None

Output: THE, TLE, ITRN = 0

/TARGET/ Input: None

Output: Z1

Namelist: /OVRID/ ICAL, NOFTEN, AM1, AM2, AM3, Z3, E1, ANG, FREQ, THE, TLE

Subroutine Calls: GETMAS, CHKINP, FTNIOPDS package

Argument List: IOVRD = Control for overriding the reaction identification card,

- ≤ 0 Do not override
- ≥ 1 Override.

Operation: The general operation is nearly identical with those of Subroutines SPCTRM and XYINP, except that a facility is available for overriding the information on the Reaction Identification Card and the Reaction Mass Card.

SUBROUTINE PACKAGE TARCOR

Purpose: Adjusts the energies of the incident and outgoing reactant particles to account for their energy loss in unbacked solid targets or in enclosed gas cells.

Subroutine Names: TARCOR, E1FIX, E3FIX, ELOSS, DEDX

Calling Sequences:
CALL TARCOR
CALL E1FIX
CALL E3FIX

Common Block:

/TARGET/	Input:	Z1, ITARG
	Output:	All variables
/QVAL/	Input:	E1, ANG, AM1, AM3, Z3, E3
	Output:	Same as input

Subroutine Calls: None outside the package

Operation:

(1) TARCOR reads in and initializes data. It must be called before other routines.

(2) E1FIX subtracts from the bombarding energy the energy loss of the incident particle in one half the thickness of the solid target, or in the entrance window and one half the thickness of the gas.

(3) E3FIX evaluates by iteration the energy of the outgoing particle at the center of the target which will result in the observed energy of the particle. The material is either one half the thickness of the solid target or the exit window and one half the thickness of the gas.

(4) ELOSS integrates by Simpson's rule dE/dx through the material.

(5) DEDX evaluates dE/dx in units MeV per gm/cm^2. The formalism of Williamson et al.[1] is used.

Data Input: Special input is required by Subroutine TARCOR. See page IV. M. 3.

Error Conditions: If either NTARF or NTARG is greater than 10, a message is issued and the program stops.

Description: The TARCOR package was principally written to make energy loss corrections for reactions that take place in enclosed, circular gas cells. An option also allows the treatment of unbacked solid targets. It is assumed that the reaction takes place at the center of the target so that straggling corrections are not included. The dE/dx formulas of Williamson et al.[1] are used. The package handles the reading of special data and the logic for computing the energy losses.

For solid targets, the thickness is compensated for angle effects—that the target is not normal to the particle directions. Let t be the target thickness, θ be the scattering angle, and ϕ be the angle of the target normal to the beam direction. Then the incident particle travels a distance $a = t/2\cos\phi$ and the outgoing particle travels a distance $b = t/2\cos|\theta - \phi|$.

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[1] C. F. Williamson, J.-P. Boujot, and J. Picard, Report CEA-R3042, Saclay, 1966 (unpublished).

INPUT CARDS FOR SUBROUTINE TARCOR

Column	Variable		Value	Usage
CARD 1.	Foil Control Card			
	XF, PHI, DEL, NTARF			
	FORMAT (3F10.5, I5)			
1—10	XF	=		The total effective thickness of the solid foil or gas cell window (mg/cm^2).
11—20	PHI	=		The angle that the normal to the target makes with the beam direction (degrees).
21—30	DEL	=		The convergence criterion in the iteration for the energy of the outgoing particle (MeV). If left blank, DEL will be set to 0.0001.
31—35	NTARF	=		The number of elements which comprise the foil material ($1 \leq NTARF \leq 10$).

There are to be NTARF Cards 2.

CARD 2.	Foil Element Card			
	ATARF (N), ZF (N), WF (N)			
	FORMAT (2F5.0, F10.5)			
1—5	ATARF (N)	=		The number of atoms for the Nth element in a molecule of the foil material.
6—10	ZF (N)	=		The atomic charge of the Nth element.
11—20	WF (N)	=		The atomic mass (u) of the Nth element.

For solid targets ($ITARG \leq -1$) do not include any more cards here.

For gas cells, include the following cards.

CARD 3. Gas Cell Control Card

WTMOLG, P, GCLCST, NTARG

FORMAT (3F10.5, I5)

1—10	WTMOLG	=	The total molecular weight of the gas (gm/mole).
11—20	P	=	The pressure of the gas. Standard units are Torr for the default value of GCLCST.
21—30	GCLCST	=	The gas cell constant (see Common Block TARGET). If left blank, GCLCST will be set to 1.3668×10^{-4}.
31—35	NTARG	=	The number of elements which comprise the gas material ($1 \leq$ NTARG ≤ 10).

There are to be NTARG Cards 4.

CARD 4. Gas Element Card

ATARG (N), ZG (N), WG (N)

FORMAT (2F5.0, F10.5)

NOTE: This card is identical to Card 2, except that it treats the elements in the gas.

21—25 THE = The setting of the high-energy screw on the Enge split-pole spectrograph.

26—30 TLE = The setting of the low-energy screw on the Enge split-pole spectrograph.

Note: If values are not specified for THE and TLE, they will be evaluated by the program for the first state of the first reaction. The values will apply for all calculations at the same angle.

NOTE: There must be NANG Cards 3.

CARD 3a. MCA Calibration Card (Use only if ISPECT = A and ICAL > 0.)

CALCOF (I), I = 1, ICAL

FORMAT (4E15.8)

1—15 CALCOF (I) = The Ith coefficient of a polynomial relating particle energy and channel number.

16—30, etc.

There are to be NREACT sets of the following cards 4—6.

CARD 4. Reaction Identification Card

II, IJ, QZ, AM2, N

FORMAT (2I1, F8.4, F10.6, I5)

1—2 II, IJ = Mass identification numbers of the incident and outgoing particles, respectively.

= 0	Read in mass on separate Card 5.	
= 1	p (proton)	Mass = 1.007276
= 2	d (deuteron)	2.013554
= 3	t (triton)	3.015501
= 4	$^{3}He^{+}$	3.015481
= 5	$^{3}He^{++}$	3.014932
= 6	$^{4}He^{++}$ (alpha)	4.001506
= 7	$^{6}Li^{+++}$	6.013479
= 8	$^{7}Li^{+++}$	7.014358

3—10	QZ	=	The Q-value (MeV) for the ground-state transition for the reaction.
11—20	AM2	=	The mass (u) of the target nucleus.
21—25	N	=	The number of states for which calculations will be done.

CARD 5. Reaction Mass Card (Use only if II or IJ = 0.)

AM1, AM3, Z3

FORMAT (3F10.5)

1—10	AM1	=	The mass (u) of the incident particle.
11—20	AM3	=	The mass (u) of the outgoing particle.
21—30	Z3	=	The charge number of the outgoing particle. If left blank, a value Z3 = 1.0 is assumed.

CARD 6. Excitation Energy Card

ST (I), I = 1, N

FORMAT (9F8.4)

1—8 9—16, etc.	ST (I)	=	The Ith excitation energy (MeV) of the residual nucleus.

The program will process a new set of cards, beginning with Card 1.

INPUT CARDS FOR PROGRAM RUTHFORD

Column	Variable		Usage
CARD 1.	Energy and Mass Card		
	ELAB, AM2, Z2, IMS, AM1, Z1, ISPN		
	FORMAT (2F10.5, F5.0, 4XI1, F10.5, F5.0, 3XI2)		
1—10	ELAB	=	Laboratory energy of the incident particle (MeV).
11—20	AM2	=	The mass of the target nucleus in mass units (u).
21—25	Z2	=	The charge of the target nucleus.
30	IMS	=	The projectile mass identification,

= blank or 0; AM1 and Z1 must be punched

= 1	p (proton)	Mass =	1.007276
= 2	d (deuteron)		2.013554
= 3	t (triton)		3.015501
= 4	$^{3}He^{+}$		3.015481
= 5	$^{3}He^{++}$		3.014932
= 6	$^{4}He^{++}$		4.001506
= 7	$^{6}Li^{+++}$		6.013479
= 8	$^{7}Li^{+++}$		7.014358

= 9 Identical Particles: AM1 and Z1 set equal to AM2 and Z2.

31—40	AM1	=	The mass of the projectile in mass units (u); required if IMS = 0.
41—45	Z1	=	The charge number of the projectile; required if IMS = 0. But note that if Z1 is left blank, the program sets Z1 = 1.0.
49—50	ISPN	=	Twice the spin value of the projectile or target nucleus; required only if IMS = 9.

CARD 2. Angle Control Card.

NANG, ANGI, ANGF, DELANG

FORMAT (I3, F7.2, 2F10.5)

1—3	NANG	=	The number of angles whose values will be read in on Cards 3. If NANG > 0, the rest of Card 2 is ignored.
	Note:	NANG ≤ 200.	
4—10	ANGI	=	The smallest laboratory angle for which calculations are desired. If left blank, the program sets ANGI = 0.0.
11—20	ANGF	=	The largest laboratory angle for which calculations are desired. If left blank, the program sets ANGF = 180.0.
21—30	DELANG	=	The increment (laboratory degrees) between angles in the calculation. If left blank, the program sets DELANG = 5.0.

NOTE: The program will calculate values only for 200 angles. If more than 200 angles are requested, calculations will be done only for the first 200 angles. ANGI, ANGF, and DELANG must be set accordingly.

CARD 3. Angle Values Card (Use only if NANG > 0.)

ANG(I), I = 1, NANG

FORMAT (16F5.2)

1—5	ANG(I)	=	The Ith angle for which calculations are desired. These angles need not be evenly spaced, but there cannot be more than 200 such values.

The program will process a new set of data, beginning with Card 1.

INPUT CARDS FOR PROGRAM SUBTBACK

Column	Variable	Value	Usage

CARD 1. Title Card

TITLE (I), I = 1, 20

FORMAT (20A4)

1—80 TITLE = Any alphanumeric string.

NOTE: If columns 1—4 are blank, the program terminates. The program also terminates on an end-of-file card (7—8 punch in col. 1 for CDC 3600, /* for S/360).

CARD 2. Control Card.

NJ, DSCALE, ITYP

FORMAT (I2, F8.4)

1—2 NJ = The number of background data points. X and Y coordinates for NJ background points will be read in.

Note: $NJ \leq 50$

3—10 DSCALE = The number of points per inch of graph, the horizontal scale factor.

Note: If left blank (standard), the program sets DSCALE = 20.

14—15 ITYP = Control number for punching spectra.
- < 0 Punch background only.
- $= 0$ Punch new spectrum only without background.
- > 0 Punch both.

CARD 3. Background Values Card

DB (I), BVAL (I), I = 1, NJ

FORMAT (16F5.0)

1—5 11—15, etc.	DB (I)	=	The Ith plate distance (cm) or channel number at which a background value is to be specified.
6—10 16—20, etc.	BVAL (I)	=	The value of the background for the Ith background position.

CARD 4. Spectrum Control Card

RUNID, IOVRD, YMAX

FORMAT (A8, 1XI1, F10.5)

1—8	RUNID	=	Blank	A Standard Spectrum Data Set will be placed immediately after this card. (On CDC 3600, an entry may be present.)
		=	Membname	For the S/360, the program will search for the Standard Spectrum Data Set in the system storage devices. Membname identifies the member name of the Data Set in the P. D. S. file. The name must be left adjusted.
10	IOVRD	=	Reaction identification override control (S/360 only).	
			= 0 or blank	Do not override the reaction ID's stored in the system P. D. S.
			≥ 1	Override the reaction ID's.
11—20	YMAX	=	The maximum counts to be plotted for this spectrum. Values larger than YMAX will be truncated to YMAX.	
	Note:		If left blank, the program will compute its own YMAX.	

CARD 5. Standard Spectrum Data Set.

For RUNID = Blank, or for the CDC 3600, enclose a Standard Spectrum Data Set at this point.

CARD 6. Override Card (Present only for S/360, and only if IOVRD $\geq$ 1.)

See the discussion of the Subroutine PDSINP for a description of this card.

The program will process a new set of data, beginning with Card 1.

INPUT CARDS FOR PROGRAM QPLOT

Column	Variable		Value	Usage
CARD 1.	Title Card			
	TITLE (I), I = 1, 20			
	FORMAT (20A4)			
1—80	TITLE	=	Any alphanumeric string.	

NOTE: If columns 1—4 are blank, the program terminates. The program also terminates on an end-of-file card (7-8 punch in col. 1 for CDC 3600/* for S/360).

CARD 2. Plot Control Card

NSET, NSP, IDQ, IPL, QSCALE, DSCALE, TMASS

FORMAT (2I2, 4X2A1, 3F10.5)

1—2	NSET	=	The number of sets of data (spectra) to follow for this calculation.
4	NSP	=	The number of spectra to be plotted across 10 in. of Calcomp paper, $1 \leq NSP \leq 6$. NSET will be divided into groups with NSP spectra in each group.

Note 1: If left blank, NSP will be set to 4.

Note 2: If NSP is specified > 6, it will be reduced to 6.

9	IDQ	=	Blank	Both Q and D plots.
		=	Q	Q plots only.
		=	D	D plots only.
		=	E	Excitation-energy plots only.
		=	F	Both excitation-energy and D plots.

Note: For MCA data without calibration coefficients (Calib. A0 in the Standard Spectrum Data Set), the program will automatically set IDQ = D.

10	IPL	=	Blank or L	Line plots only.
		=	P	Point plots only.
		=	B	Both line and point plots.

11—20 QSCALE = The number of MeV per inch of graph, the horizontal scale factor for Q and E_x plots.

Note: If left blank, QSCALE will be set to 0.20.

21—30 DSCALE = The number of points per inch of graph, the horizontal scale factor for D plots.

Note: If left blank (standard), DSCALE will be set to 20.

31—40 TMASS = The mass of the target in mass units (u), normally left blank. If TMASS $>$ 0, this value overrides all the target masses in the Standard Spectrum Data Sets.

There are to be NSET sets of the following Cards 3—6.

CARD 3. Spectrum Control Card

RUNID, IOVRD, YMAX, QZ, ITARG

FORMAT (A8, 1XI1, 2F10.5, 3XI2)

1—8	RUNID	=	Blank	A Standard Spectrum-Data Set will be placed immediately after this card. (On the CDC 3600, an entry may be present.)
		=	Membname	For the S/360, the program will search for the Standard Spectrum Data Set in the system storage devices. Membname identifies the member name of the Data Set in the P.D.S. file. The name must be left adjusted.
10	IOVRD	=	Reaction identification override control (S/360 only).	
		=	0 or blank	Do not override the reaction identifications stored in the system P.D.S.
		$\geq$	1	Override the reaction ID's.

11—20 YMAX = The maximum counts to be plotted for this spectrum. Values larger than YMAX will be truncated to YMAX.

Note: If left blank, the program will compute its own YMAX.

21—30 QZ = The ground-state Q value of the reaction, used to compute excitation energies (IDQ = E or F only).

34—35 ITARG = Target thickness correction control.

= 0 No corrections for target thickness.
≥ 1 Make corrections for gas cell.
≤ -1 Make corrections for a solid, unbacked target.

CARD 4. Standard Spectrum Data Set.

For RUNID = Blank, or for the CDC 3600, enclose a Standard Spectrum Data Set at this point.

CARD 5. Override Card (Present only for S/360, and only if IOVRD ≥ 1.)

See the discussion of the Subroutine PDSINP for a description of this card.

CARD 6. Target-thickness correction cards. See the discussion for the Subroutine Package TARCOR, page IV. M. 1.

CARD 7. MCA Calibration Card (Use only if ISPECT = A and ICAL > 0.)

CALCOF (I), I = 1, ICAL

FORMAT (4E15.8)

1—15 CALCOF (I) = The Ith coefficient of a polynomial relating particle energy and channel number.

16—30 etc.

The program will process a new set of data, beginning with Card 1.

modified. It is treated as a table of values regardless of the units of the abscissa. However, if the reference peak is to be selected from the spectrum, the shape parameters are converted to the appropriate units and the peak is extracted from the new interpolated spectrum.

D. Subroutine REFPEK

The reference peak shape is not obtained from an analytic function but is expressed as a table of values specifying the shape, channel by channel, of the peaks in the spectrum, with linear interpolation assumed between channels. Thus, any experimentally-defined shape can be used.

The reference peak shape can be selected from an internally-stored table of shapes, or it can be given explicitly in the input. It can also be selected directly from the spectrum, provided that information about its location is given in the input.

Subroutine REFPEK obtains the reference peak and evaluates the parameters which characterize its width and shape. Specifically, these parameters are the total width in channels, and the distances Δ_1, Δ_2, and Δ_3, as shown schematically in Fig. VII.2. By convention, the position of a peak for spectrograph data is defined as the position of its "third-height" point, i.e., the abscissa of the point on the high-energy (larger distance) side of the peak where the height is one third the height at the maximum. For MCA data, peak positions are defined as the position of the centroid.

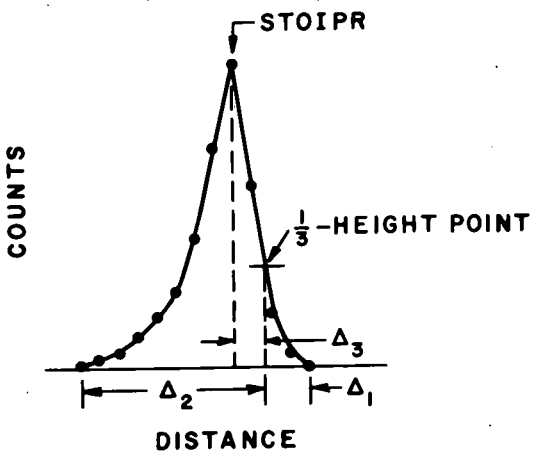

Fig. VII.2

E. Subroutine PEKPIC

Peaks are identified in the spectrum by a routine that

inquires whether a sequence of ordinate values has the same shape as the reference peak. This is accomplished quantitatively by calculating a linear-regression correlation coefficient and testing this against a prescribed value.

The reference peak is moved through the spectrum in one-channel steps. The data within the range of the reference peak are used to obtain the correlation coefficient, defined as

$$\rho = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\left[\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2\right]^{1/2}} .$$

The values x_i represent the set $\{x\}$ of ordinates of the reference peak, with mean value $\bar{x}$, and the values y_i represent the set $\{y\}$ of ordinates of the data, with mean value $\bar{y}$. The sum extends over all channels of the reference peak.

The correlation coefficient is in the range $-1 \leq \rho \leq 1$. The value $\rho = +1$ represents perfect correlation and $\rho = 0$ represents no correlation. A peak is declared to exist at a certain channel if the value of ρ at that channel exceeds a test value β. In practice, if $\rho > \beta$ for more than one of four consecutive channels, a peak is defined only for the channel at which ρ is a maximum. Several criteria preclude the identification of peaks with very small areas, as these are usually spurious.

If the background has already been removed from the spectrum, the set of peaks thus selected is subtracted from the spectrum. The reference peak defines the peak shape and it is normalized to the data by equating the area (number of counts) of the reference peak to the area of the peak in the data. The ordinates in the revised spectrum are not allowed to be negative. Then a second

execute the procedure. These also use Subroutine MATMPY.

K. Subroutine ORDER

ORDER is a special addition to the variable-metric package. It reorders the peaks into ascending order of x_ℓ so that the printout in Subroutine RESLTS will be done properly.

L. Subroutine FCN

Subroutine FCN controls the minimization of the function F with respect to the a_ℓ's. It sets up the linear equations formed from the requirement $\partial F/\partial a_\ell = 0$ and calls MATINV[5] to obtain the inverse matrix. It also requests the derivatives $\partial F/\partial x_\ell$ and requests the relocation of the reference peak at new locations x_ℓ.

M. Subroutine DERIVP

The numerical derivatives $\partial F/\partial x_\ell$ are calculated in DERIVP by shifting a peak 0.1 channels in each direction and requesting a new value of F at each of the new positions.

N. Subroutine SHIFT

The reference peak is placed at a position x_ℓ by use of the routine SHIFT. Linear interpolation is used between points in the reference peak if the shift involves fractions of a channel.

O. Subroutine FUN

The array {E} and the value of F are calculated in Subroutine FUN.

P. Peak Constraints (New Option)

A recent addition to the variable-metric package allows constraints to be placed on relative peak separations. If estimates of peak positions are read in as data, and if adjacent overlapping peaks in a subgroup are properly flagged, the program will adjust their absolute positions for a good fit but will keep their initial separations constant. This is particularly convenient if the peak positions are given in units of Q value.

---

[1] P. Spink and J. R. Erskine, ANL Physics Division Informal Report PHY-1965B, 1965 (unpublished).

[2] D. R. Hartree, Numerical Analysis, 2nd Ed. (Clarendon Press, Oxford, 1958).

[3] Applied Mathematics Division Program Library Report E206S. The routine LSQPOL used in AUTOFIT is a slight revision of the routine described in this report.

[4] W. C. Davidon, Argonne National Laboratory Report ANL-5990 (Rev. 2), 1966 (unpublished).

[5] App. Math. Div. Program Library Report F402S.

III. RECOMMENDATIONS FOR INPUT

The following suggestions are intended to aid the user in setting up the input card decks to AUTOFIT. The user should refer to the list of input cards (Sec. V).

A. Conversion to Q-Space

The conversion of the spectrum to Q-space (NCALC = 1) will in general not be necessary. If the data of interest cover a range larger than 50 cm of spectrograph plate distance, the user may wish to make corrections for the variable dispersion. The conversion is also useful for MCA data if the calibration is not linear.

B. Backgrounds

The automatic option is sometimes capable of providing a reasonable estimate of the background, but it can also produce very unrealistic results. Its use is not recommended if high-quality results are desired. Background option 1 (NBACK $>$ 0) gives the user the maximum control over the background curve. If enough points are specified, the background can be tailored to any specification.

Constant backgrounds can be entered with option 2 (NBACK = -1). Option 1 can also be used with NBACK = +1 if DB(1) specifies any abscissa in the middle of the spectrum and BACK(1) specifies the background value.

C. Reference Peak

The option with NREF = 0 is generally not recommended. It is convenient to use but normally gives inferior results. A much better procedure is: (1) select a peak from the spectrum, remove the background, and plot the points; (2) approximate the data points with

a smooth curve; (3) extract new values for the shape of the peak from the curve; and (4) enter the new peak shape with the option NREF = -1.

In establishing the shape of the reference peak, it is better to require that the top of the peak occur at an integral channel number, not between channels.

Typically, if a number of spectra are obtained under nearly identical conditions (except possibly for the detection angle), it will be possible to use a single reference peak shape for all spectra, not a separate shape for each spectrum.

By design, the reference peak shape is not modified if the spectrum is converted to Q-space. (For NREF = 0, the reference peak is selected from the converted spectrum). However, a peak near the middle of the spectrum will have the same width (in units of channels) and shape in the converted spectrum as it had in the original. If necessary, a peak shape for a later pass can be selected from the printout of the converted spectrum.

D. Peak Selection

The automatic peak-selection option is useful if one does not wish to examine a spectrum closely or to punch cards for many peak positions. The punched output is easily edited, and these cards can be used for specifying peak positions on a subsequent pass.

If several spectra (taken at different angles) of a single reaction are being processed together, it is convenient to give peak positions in units of Q-values. These can also be read directly from a Q-plot of the data.

Estimates of peak positions need not be very precise. An accuracy of 1—2 channels is often sufficient.

The option that requests the program to hold the positions of peaks fixed while obtaining their areas is not generally recommended. It is useful if the program has troubles in separating closely-spaced

or too few peaks are specified. One should revise the estimates of the peak positions and rerun the program.

B. Results of the Peak-Fitting Analysis

The final printed summary of results should be examined for signs that the calculated fits to the data may not be reliable. If necessary, the input deck can be revised and another pass made.

1. Errors.

One can roughly estimate the errors expected for the final positions and areas of the peaks and compare these with the calculated errors. Large discrepancies require attention. The expected error in the area (NUMB. COUNTS) A is $\sqrt{A}$. The expected error in the peak position is roughly FWHM/(2.5$\sqrt{A}$), where FWHM is the full-width at half maximum of the peak.

Normally, the positions and areas of the peaks will be determined much more precisely than the listed errors would indicate. A large discrepancy between estimated and listed error is thus only a sign that the program experienced difficulties in the analysis, not that the answers are necessarily unreliable. Only if the Calcomp plots (on other printouts) show signs of poor fits is a new analysis required.

2. Negative peaks.

The program sometimes produces peaks with negative areas. This is usually a sign that AUTOFIT has been asked to place too many peaks in a small region. Some should be eliminated and the data should be reanalyzed. If the user intends to have all the peaks he requested, a revised set of estimated peak positions can sometimes eliminate negative peaks.

3. Peaks with Zero Areas and Errors

The printout may show that some peaks have areas and errors which are exactly zero. This results from a spurious condition. During the variable-metric analysis, these peaks have been moved outside the range of the spectrum in the work area (not outside the total spectrum) and therefore have zero amplitudes. The errors are arbitrarily set to zero. The cause is usually the same as for negative peaks and should be treated accordingly.

C. New Messages (September 1971)

1. FBEST = xxx FOR nn PEAKS WITH mm TOTAL CHANNELS

When NSSW2 > 0, the program will print the above message for each subgroup. FBEST is the unnormalized chi-square and the total degrees of freedom is mm - nn.

2. CANNOT OBTAIN REFERENCE PEAK
CHANNEL = nn MAX. HT. = xxx WIDTH = mm

This message may be produced when NREF = 0. The reference peak cannot be selected from the spectrum if (a) the estimated position is below channel 12 or (b) within 5 channels of the last channel; (c) the largest count of the reference peak is not greater than 10 counts; or (d) the width is less than 4 or greater than 40 channels.

Note: For NCALC = 1, the program will require NQPLOT = 1 (or 0), but will plot counts vs Q-value only.

14	NSSW1	=	0	Suppress printed output from variable-metric-minimization routines. (Standard!)
		=	1	Print the v.m.m. calculations.
16	NSSW2	=	0	Suppress printed output of raw data, resolved peaks, and composite spectra.
		=	1	Print the above.
21—30	BETA	=		Parameter that controls the sensitivity of the PEKPIC routine. BETA is the minimum value of an acceptable linear correlation coefficient relating the reference-peak shape with the data.

Note: If left blank (standard option), the program will set BETA = 0.6. Values less than 0.5 are not recommended.

31—40	QSCAL	=	The number of MeV per inch of graph, the horizontal scale factor for Q-plots.

Note: If left blank (standard), the program will select a convenient scale factor based on the value of DSCAL.

41—50	DSCAL	=	The number of points per inch of graph, the horizontal scale factor for D-plots.

Note: If left blank (standard), the program will set DSCAL = 20.

CARD 3. Background Data Cards (Not used for NBACK = 0.)

DB(I), BACK(I), I = 1, |NBACK|

FORMAT (16F5.0)

1—5	DB(I)	=	For NBACK > 0 (option 1):
11—15, etc.			DB(I) is the plate distance (cm) or channel number at which a background value is to be specified.
			For NBACK < 0 (option 2):

DB(I) is the plate distance (cm) or channel number at the lower end of the Ith interval for which a background value is to be specified. DB(1) is supplied by the program and may be left blank.

6—10 BACK(I) = The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK < 0).

NOTE 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).

NOTE 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK (1) for the first channel, and BACK (NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

CARD 4a. Reference Peak Values Card (Use only for NREF ≤ -1.)

N, STOREF (I), I = 1, N

FORMATS (I5, 15F5.0) and (16F5.0)

1—5 N = The number of channels in the reference peak.

Note: N ≤ 40. If N > 40, the program will truncate it to 40.

6—10, 11—15, etc. STOREF(I) = The number of counts in the Ith channel of the reference peak, reading from the back edge (low plate distance) to the front edge (high distance).

Note: STOREF(I) may be continued on successive cards if N > 15, starting in columns 1—5.

CARD 4b. Reference Peak Parameter Card (Use only if NREF = 0.)

STOIPR

FORMAT (F10.5)

1—10	STOIPR	=		The approximate position (within about four channels) of the channel with the maximum count in the reference peak. The units are cm or channel number if NPKRD >0 and MeV (Q value) if NPKRD <0. If NPKRD = 0, the units must agree with the calculation space determined by NCALC.

CARD 5. Spectrum Control Card

RUNID, IGS, IOVRD, YMAX, GSQVAL, ITARG

FORMAT (A8, 2I1, 2F10.5, 3XI2)

1—8	RUNID	=	Blank	A Standard Spectrum Data Set will be placed immediately after this card. (On the CDC 3600, an entry may be present.)
		=	Membname	For the S/360, the program will search for the Standard Spectrum Data Set in the system storage devices. Membname identifies the member name of the Data Set in the P. D. S. file. The name must be left adjusted.
9	IGS	=	0	GSQVAL will specify the ground-state Q-value (MeV) of the reaction. Excitation energies will be calculated if GSQVAL $\neq 0.0$.
		=	1	GSQVAL will specify the location of the ground-state peak. Excitation energies will be calculated if GSQVAL $\neq 0.0$.
		=	2	Special case. This is the same as IGS = 0, but GSQVAL may be zero.
10	IOVRD	=		Control to override the reaction identification (S/360 only).
		=	0 or blank	Do not override the reaction ID's stored in the system P. D. S.
		$\geq$	1	Override the reaction ID's.

11—20 YMAX = The maximum number of counts to be plotted for this spectrum. Values larger than YMAX will be truncated to YMAX.

Note: If YMAX $<$ 100, the program will compute its own YMAX.

21—30 GSQVAL = The ground-state Q-value of the reaction in MeV (IGS = 0), or the approximate "third-height" plate distance (cm) or channel number of the ground-state peak (IGS = 1). This is used for computing excitation energies.

Note: If left blank, no excitation energies will be calculated unless IGS = 2.

34—35 ITARG = Target thickness correction control.

= 0	No corrections for target thickness.
$\geq$ 1	Make corrections for gas cell.
$\leq$ -1	Make corrections for a solid, unbacked target.

CARD 6. Standard Spectrum Data Set

For RUNID = Blank, or for the CDC 3600, enclose a Standard Spectrum Data Set at this point.

CARD 7. Override Card (Present only for S/360, and only if IOVRD $\geq$ 1.) See the discussion of the Subroutine PDSINP for a description of this card.

CARD 8. Target-thickness correction cards. See the discussion for the Subroutine Package TARCOR, page IV.M.1.

CARD 9. MCA Calibration Card (Use only if ISPECT = A and ICAL > 0.)

CALCOF (I), I = 1, ICAL

FORMAT (4E15.8)

1—15 16—30, etc.	CALCOF (I) =	The Ith coefficient of a polynomial relating particle energy and channel number.

CARD 10a. Peak Position Cards (Use only if NPKRD ≥ +1.)

PEKPOS (I), IFIXPK (I)

FORMAT (F9.4, I1)

1—9	PEKPOS (I) =		The estimated third-height location of the Ith peak to be considered by the program, specified in plate distance (cm) or channel number.
10	IFIXPK (I) =	0 or blank	The program will adjust PEKPOS (I) for the best fit to the data. (Standard option.)
	=	1	PEKPOS (I) will be held fixed (F) by the program.
	≥	2	Successive overlapping peaks so flagged will be constrained (C) to have a constant separation.

See notes after Card 10b.

CARD 10b. Peak Position Card (Use only if NPKRD ≤ -1.)

IFIXPK (I), PEKPOS (I)

FORMAT (9XI1, F10.5)

10	IFIXPK (I) =	0 or blank	The program will adjust PEKPOS (I) for the best fit to the data. (Standard option.)
	=	1	PEKPOS (I) will be held fixed (F) by the program.
	≥	2	Successive overlapping peaks so flagged will be constrained (C) to have a constant separation.

11—20	PEKPOS (I) =	The estimated third-height location of the Ith peak to be considered by the program, specified in Q value (MeV).

NOTE 1: No more than 200 cards will be accepted by the program for Cards 10a or 10b.

NOTE 2: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS (I).

CARD 11. Peak Position Termination Card (Use only with Cards 10a or 10b.)

1—2 -1 only.

The program will process a new set of data, beginning with Card 1.

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Informal Report PHY-1970 B
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MANUAL OF DATA-ANALYSIS PROGRAMS FOR CHARGED-PARTICLE REACTIONS*

by

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Section VII only

Program AUTOFIT

A limited number of copies are available for general distribution. Anyone who desires a copy should contact the author directly, or contact J. R. Erskine of the ANL Physics Division. The PHY Informal Reports are not handled through the ANL Technical Publications Department.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

PROGRAM AUTOFIT

I. INTRODUCTION

Program AUTOFIT is a spectrum-decomposition program of wide versatility. Although it is specifically designed for the analysis of spectra obtained from charged-particle reactions, minor revisions can allow it to be applied to many other problems.

The program described here is an extensive revision of another program with the same name.[1] This new version has the same general structure as the original program and does everything its predecessor did. However, through extensive reprogramming, many new features have been added and many of the mathematical algorithms have been improved or changed.

Program AUTOFIT has facilities for removing backgrounds, setting the shape of a reference peak, and obtaining estimates of the locations of the peaks. The user may allow the program to accomplish these tasks automatically, or he may exert greater control over the operations by specifying input parameters in detail. From such information, the program performs a sophisticated least-squares analysis of the data in order to obtain more precise values for locations and areas of the peaks. An analysis of errors is carried out simultaneously. The final results may be printed and punched, with abscissas also expressed in reaction Q-values and excitation energies.

An important feature of AUTOFIT is the graphical display of the original data and all calculated results. The user may thus readily evaluate the performance of the program and, if necessary, prepare the data for a subsequent pass. All scale factors can be selected automatically by the program or specified by the user. A photographic reproduction of a sample plot from AUTOFIT is shown in Fig. VII. 1.

Another available facility is especially applicable to

spectrograph data. The dispersions of the spectrographs are not constant over the entire range of plate distances, and this results in a variable peak shape. The peaks may be wider at one end than at the other. However, to the extent that the widths are dominated by beam-width and target-thickness effects, the widths in units of energy should be nearly constant. Since AUTOFIT utilizes a fixed peak shape for all peaks, the effects of a variable dispersion can be eliminated if the spectrum is expressed as counts per unit energy. The program thus incorporates a subroutine that translates the original spectrum given with an abscissa of plate distance into one whose abscissa is the reaction Q-value.

The automatic features of the program are intended to save labor in the initial stages of analysis. They are not expected to give perfectly acceptable results although, with some data, they have been known to give results of high quality. In general, one should expect that the quality of the answers is almost proportional to the amount of effort expended in setting up the input decks.

The following section briefly describes the operations of the program. Consideration is given to the methods used in evaluating precise peak locations and areas and to the algorithms used for obtaining a reference peak shape, removing backgrounds, selecting peaks from a spectrum, and converting a spectrum from D-space to Q-space. Subsequent sections discuss recommendations for setting up the input decks and guides for interpreting the results.

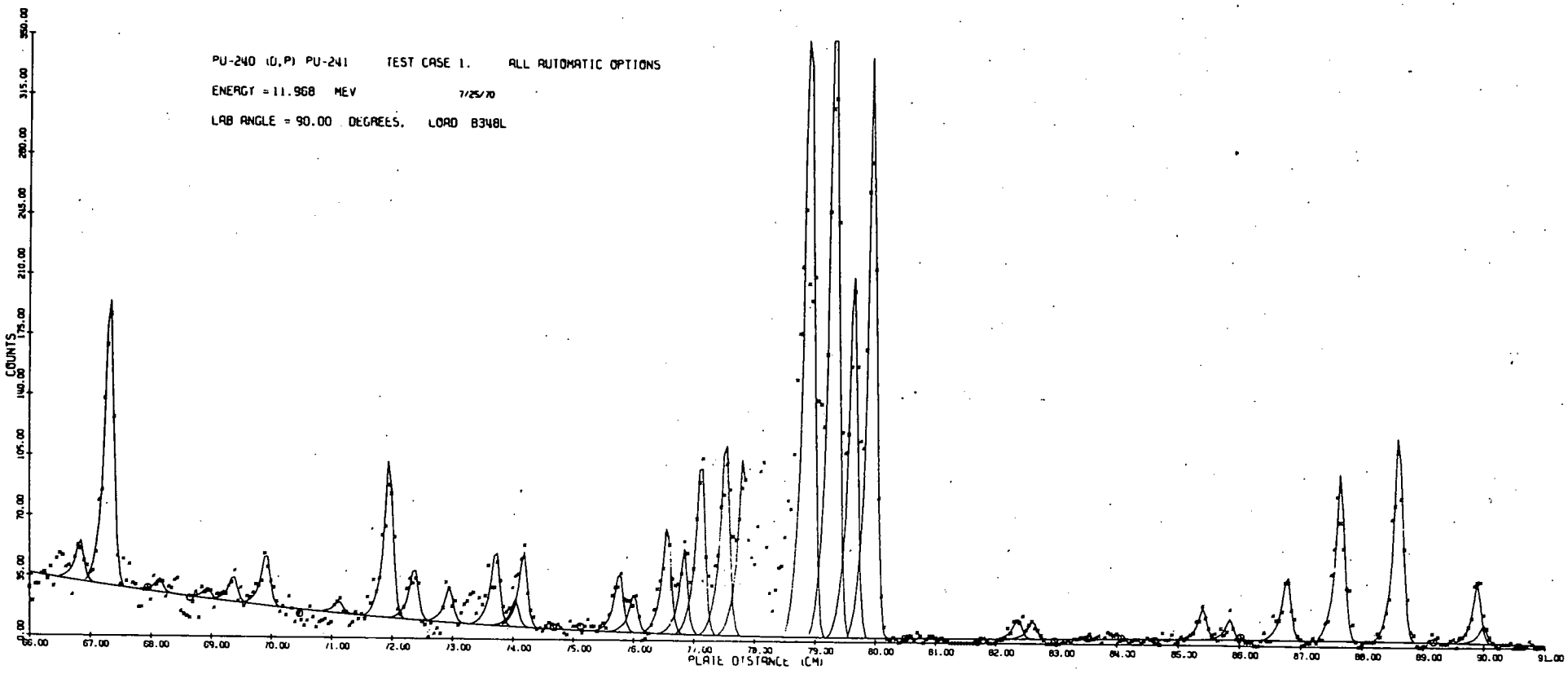

Fig. VII. 1. A representative graphical output from the Program AUTOFIT. The automatic options were used so the results are not optimized.

II. DESCRIPTION OF PROGRAM

A. Program AUTOFIT (MAIN)

The main program controls the reading of the input cards, initializes variables, checks for error conditions and makes corrections if possible, and prepares the data for analysis.

The data cards are read directly by the main program, except for the Standard Spectrum Data Set which is obtained from the subroutine packages SPCTRM or PDSINP. The subroutine ARYODR is called for rearranging the background data points and peak positions into ascending order of abscissas. If the spectrum is to be converted to Q-space, Subroutine INTERP is called.

In preparing the data for analysis, the main program establishes the logic for selecting a reference peak shape, estimating peak positions, and removing backgrounds. The task is simplified if the user does not request the automatic options. Otherwise, the background cannot be calculated until the peak positions are known, and these cannot be established until a reference peak shape is evaluated. A reference peak selected from the spectrum will include the background until such is removed. With all the automatic options in effect, a simple iterative procedure is used to obtain the necessary information. Otherwise the information is calculated from the input variables. The subroutines BGRND, PEKPIC, and REFPEK are called for establishing the backgrounds, peak positions, and reference peak shape, respectively. A new spectrum, with the background subtracted, is computed. The new ordinates are not allowed to be less than zero.

A final check is made to determine whether the estimated peak locations are in the range of the spectrum. Those outside the range are deleted from further processing.

Finally, Subroutine RESLTS is called for processing the data.

B. Subroutine RESLTS

Subroutine RESLTS is, in effect, the second half of the main program. It divides the spectrum into sections and requests the analysis of each section. The results for each section are then printed. When all sections are completed, a tabulated summary of the significant quantities is printed and punched.

Since the analysis routines cannot handle more than twenty peaks simultaneously, RESLTS must divide the spectrum into groups with no more than twenty peaks in each group. These groups are formed in such a nammer than no peak in one group overlaps a peak in a neighboring group. Peaks are considered to overlap if any part of their tails occur in the same channel. In the event that the spectrum contains a group with more than twenty overlapping peaks, this entire group is divided in half and a message is printed. RESLTS transmits the information appropriate for each group to Subroutine PREPAR.

On the return from PREPAR, the normalized fitted peaks are summed to obtain the areas, the errors are converted to appropriate units and stored in arrays. If requested by the user, a printout for the group gives the distance values and original counts, the background, the normalized individual fitted peaks (with backgrounds included), and the composite spectrum of the fitted peaks. The same information can be plotted by calling Subroutine GRAPH.

A final summary page lists the information characterizing the spectrum and tabulates:

(a) peak position (cm or channel number),

(b) Q-value for the peak (MeV),

(c) excitation energy of the peak (MeV),

(d) error in the peak position (keV if Q-values are listed, channels if the data is MCA data without calibration coefficients),

(e) number of counts in the peak,

(f) statistical error in the number of counts computed by the program during the analysis procedures,

(g) sum of the background underneath the peak, and

(h) estimated error in the number of counts; this is the square root of the sum of the number of counts and the background.

C. Subroutine INTERP

If the variable dispersion of the spectrographs (or a nonlinear calibration for MCA data) presents a serious difficulty in the analysis of the data, the spectrum may be converted to Q-space. A direct conversion of the set of plate distances to a set of Q-values is inadequate since the Q-values will not be evenly spaced, in violation of the program requirements. A new interpolated spectrum must be created, with equal increments between channels.

Subroutine INTERP creates a new spectrum from the original data. First, the set of distances $\{D\}$ is converted directly to a set of Q-values $\{Q_D\}$. By design, the new spectrum is to have the same number of channels as the old spectrum. The extreme values of $\{Q_D\}$ in combination with this requirement thus determine the new increment between channels and the array of abscissas for the new spectrum $\{Q\}$ is found. The values of $\{Q\}$ do not in general coincide with the values of $\{Q_D\}$ and interpolation procedures are required for the formation of the new array or ordinates.

Several interpolation formulae were examined and it was concluded that Everett's formula to second-order central differences without throwback[2] was sufficiently fast and reliable. This is equivalent to Lagrange's four-point formula[2] and represents the solution obtained in fitting a cubic equation through four consecutive points.

Let the value of a function f(x) which is calculated at a point x_n be denoted as f_n, and let the values of x_n be equally spaced with the interval h. Then the value of the function at a point x' between x_0 and x_1 is $f(x') = f(x_0 + ph)$, where the fractional distance between x_0 and x_1 is $p = (x' - x_0)/(x_1 - x_0)$. This is evaluated to be

$$f(x') = q\left[f_0 + \frac{1}{3!}(q^2 - 1)\delta^2 f_0 + \ldots\right] +$$

$$+ p\left[f_0 + \frac{1}{3!}(p^2 - 1)\delta^2 f_1 + \ldots\right],$$

where $q = 1 - p$ and the second-order central difference is

$$\delta^2 f_n = f_{n+1} - 2f_n + f_{n-1}.$$

In the case that fourth-order central differences exceed 1000, it is often wise to replace $\delta^2 f_n$ with modified second-order differences

$$\delta_m{}^2 f = \delta^2 f - 0.184\,\delta^4 f,$$

where

$$\delta^4 f_n = f_{n+2} - 4f_{n+1} + 6f_n - 4f_{n-1} + f_{n-2}.$$

Such modification has not been found necessary for physical data and is not included in INTERP.

In Subroutine INTERP, the values x' are obtained from $\{Q\}$ and the values x_n from $\{Q_D\}$. Of course, the values of $\{Q_D\}$ do not have equal spacing h, but this nonlinearity is negligible for four successive points. The values $f(x')$ must also be multiplied by a channel-width factor in order that the areas of the peaks be conserved. This factor is $\Delta Q_{ave}/\Delta Q_i$, where ΔQ_{ave} is the equal spacing between points in the new spectrum and ΔQ_i is the spacing between points in $\{Q_D\}$, evaluated near the proper channel.

If background points and peak positions are given in the input, these distances are also converted to Q values. The background ordinates are also corrected for the channel-width factors.

By intention and design, the reference peak shape is not

modified. It is treated as a table of values regardless of the units of the abscissa. However, if the reference peak is to be selected from the spectrum, the shape parameters are converted to the appropriate units and the peak is extracted from the new interpolated spectrum.

D. Subroutine REFPEK

The reference peak shape is not obtained from an analytic function but is expressed as a table of values specifying the shape, channel by channel, of the peaks in the spectrum, with linear interpolation assumed between channels. Thus, any experimentally-defined shape can be used.

The reference peak shape can be selected from an internally-stored table of shapes, or it can be given explicitly in the input. It can also be selected directly from the spectrum, provided that information about its location is given in the input.

Subroutine REFPEK obtains the reference peak and evaluates the parameters which characterize its width and shape. Specifically, these parameters are the total width in channels, and the distances Δ_1, Δ_2, and Δ_3, as shown schematically in Fig. VII.2. By convention, the position of a peak for spectrograph data is defined as the position of its "third-height" point, i.e., the abscissa of the point on the high-energy (larger distance) side of the peak where the height is one third the height at the maximum. For MCA data, peak positions are defined as the position of the centroid.

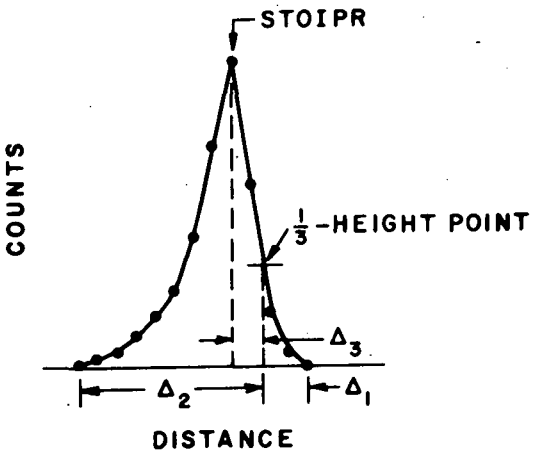

Fig. VII.2

E. Subroutine PEKPIC

Peaks are identified in the spectrum by a routine that

inquires whether a sequence of ordinate values has the same shape as the reference peak. This is accomplished quantitatively by calculating a linear-regression correlation coefficient and testing this against a prescribed value.

The reference peak is moved through the spectrum in one-channel steps. The data within the range of the reference peak are used to obtain the correlation coefficient, defined as

$$\rho = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\left[\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2\right]^{1/2}} .$$

The values x_i represent the set $\{x\}$ of ordinates of the reference peak, with mean value $\bar{x}$, and the values y_i represent the set $\{y\}$ of ordinates of the data, with mean value $\bar{y}$. The sum extends over all channels of the reference peak.

The correlation coefficient is in the range $-1 \leq \rho \leq 1$. The value $\rho = +1$ represents perfect correlation and $\rho = 0$ represents no correlation. A peak is declared to exist at a certain channel if the value of ρ at that channel exceeds a test value β. In practice, if $\rho > \beta$ for more than one of four consecutive channels, a peak is defined only for the channel at which ρ is a maximum. Several criteria preclude the identification of peaks with very small areas, as these are usually spurious.

If the background has already been removed from the spectrum, the set of peaks thus selected is subtracted from the spectrum. The reference peak defines the peak shape and it is normalized to the data by equating the area (number of counts) of the reference peak to the area of the peak in the data. The ordinates in the revised spectrum are not allowed to be negative. Then a second

complete pass is made through the data. This is necessary in order to select peaks that may be only partially resolved from those identified on the first pass. Since this second pass has a tendency to select spurious peaks, the test criterion is tightened by replacing β with $\beta' = (1 + \beta)/2$.

If the total set of peaks is found to contain pairs with separations of one channel, the upper members are rejected. No more than 200 peaks will be selected. If 200 peaks are identified before the routine has finished, a message is issued and the processing is terminated.

The PEKPIC routine is not foolproof, but the method of correlation coefficients has been found to be superior to other methods, such as chi-squares, both in programming and in the quality of the results. The user can exert some control over the performance of PEKPIC by specifying the parameter β. For good data, clearly identifiable peaks frequently have $\beta > 0.9$. However, some good peaks may have β as low as 0.5 and spurious peaks may have $\beta > 0.8$.

F. Subroutines BGRND and LSQPOL

Three options are available for removing backgrounds from the spectrum, one of which is completely automatic. The others require information from the user.

With one option, the spectrum can be divided into sections, with a constant background value in each section. The user supplies the limits of the sections and the background values. This option may be infrequently used, but it is useful, for example, if the user desires a single constant background value for the entire spectrum.

A second option allows the user to specify the coordinates of a set of background points throughout the spectrum. The routine then calculates a continuous line that passes through all these points. Lagrange's three-point interpolation formula[2] is used for the regions between points. The final curve is thus a patchwork of parabolas. Three successive points are used to calculated a curve between the first two

points. The program then drops the first point and uses the next three points to calculate the next section. Although the background line is continuous, its derivative may be discontinuous at each background point. The background is not allowed to be less than zero.

The automatic option requires that estimated peak positions be either supplied by the user or determined by Subroutine PEKPIC. The routine BGRND examines the regions between such peaks and excludes the channels that contain the tails of peaks. If such a region is longer than ten channels, it is divided into subregions of about ten channels each. The abscissa and ordinate of a background point are taken to be the midpoint of the abscissas of the subregion, and the average of the ordinates of the data points in the subregion, respectively.

Since most physical spectra have backgrounds that decrease as plate distance or channel number increases, a constraint is imposed on the background points. The ordinate of each new background point $Y_{B,i}$ is compared with the ordinate of the last background point $Y_{B,i-1}$. If it exceeds the value $Y_{B,i-1} + 2\sqrt{Y_{B,i-1}}$, the point is rejected. No more than fifty points will be selected. The set of background points is then used to compute a polynomial of order not exceeding four. This is done with Subroutine LSQPOL, which uses standard least-square techniques.[3]

G. Subroutine GRAPH

A graphical display of the data and the computed results from the analysis are provided by Subroutine GRAPH. It is designed specifically for 12-in. Calcomp plotters and produces a graph across 10 in. of paper.

In the first call to GRAPH, horizontal and vertical scale factors are established, axes and labels are drawn, and the entire spectrum, background line, and background points are plotted. On subsequent calls, either the individual best-fit computed peaks, or the

composite sum of such peaks, are superimposed on the spectrum.

H. Subroutine PREPAR

The information concerning each group of peaks is received from Subroutine RESLTS by PREPAR and the data are prepared for detailed analysis by the variable-metric-minimization package. All abscissas are converted to channel numbers and the group is divided into subgroups. The peaks within each subgroup overlap with their neighbors in that subgroup, but not with their neighbors in other subgroups. For each subgroup, PREPAR establishes the initial error matrix, the weights for the data points, and a convergence criterion. The weights are defined as $1/\sqrt{Y_i + 10}$, where Y_i is the ordinate of the ith data point. Adding 10 to Y_i slightly increases the relative weighting of the data near the tops of peaks, and prevents divisions by zero. The subgroup is then transmitted to Subroutine DAVIDN, the control routine for the variable-metric minimization package.[4]

Upon the return from DAVIDN, PREPAR establishes the errors in peak positions and produces normalized values of the individual fitted peaks.

I. Detailed Peak Analysis

A complex spectrum can be represented by an array $\{E\}$ which is formed from the sum of a set of resolved components $Z(x)$. Each element of the array can be expressed as

$$E_i = \sum_{\ell=1}^{L} a_\ell Z_i(x_\ell),$$

where $Z_i(x_\ell)$ designates the number of counts in the ith channel of an unnormalized reference peak located at an abscissa x_ℓ, and a_ℓ is a normalization factor. The sum extends over L individual components

in the complex spectrum. If the reference peak located at x_ℓ does not extend to the ith channel, $Z_i(x_\ell)$ is defined as zero. The quantities a_ℓ and x_ℓ are varied until the array $\{E\}$ is closely matched with the array of ordinates $\{Y\}$ of the data. This is accomplished quantitatively by forming a χ^2 function

$$F = \sum_{i=1}^{N} (Y_i - E_i)^2/(\Delta Y_i)^2,$$

summed over all the channels of the data, and minimizing F with respect to a_ℓ and x_ℓ.

Program AUTOFIT separates the minimization with respect to the a_ℓ's and the x_ℓ's. If the x_ℓ's are known, either from the initial estimates of peak position or from the results of the variable-metric calculations,[4] then the a_ℓ's can be obtained by setting $\partial F/\partial a_\ell$. Standard matrix-inversion techniques[5] are then used to extract values of the a_ℓ's from the equations thus formed.

The positions of the peaks are established by a variable-metric minimization procedure[4] coded in a set of subroutines. As the x_ℓ's are varied, the function F is recalculated (each time with a best set of a_ℓ's) and inspected. If the change in F between successive complete iterations is less than a convergence criterion ϵ, the procedure is terminated, a final best set of a_ℓ's is calculated, and the results are transmitted to the calling program.

The weights ΔY_i in the function F are taken to be $\sqrt{Y_i + 10}$ during the minimization procedures. The final best values of the a_ℓ's, however, are obtained with $\Delta Y_i = \sqrt{E_i + 10}$.

J. Subroutines DAVIDN, READY, AIM, FIRE, DRESS, and MATMPY

Subroutine DAVIDN is the control program of the variable-metric package.[4] It calls READY, AIM, FIRE, and DRESS to

execute the procedure. These also use Subroutine MATMPY.

K. Subroutine ORDER

ORDER is a special addition to the variable-metric package. It reorders the peaks into ascending order of x_ℓ so that the printout in Subroutine RESLTS will be done properly.

L. Subroutine FCN

Subroutine FCN controls the minimization of the function F with respect to the a_ℓ's. It sets up the linear equations formed from the requirement $\partial F / \partial a_\ell = 0$ and calls MATINV[5] to obtain the inverse matrix. It also requests the derivatives $\partial F / \partial x_\ell$ and requests the relocation of the reference peak at new locations x_ℓ.

M. Subroutine DERIVP

The numerical derivatives $\partial F / \partial x_\ell$ are calculated in DERIVP by shifting a peak 0.1 channels in each direction and requesting a new value of F at each of the new positions.

N. Subroutine SHIFT

The reference peak is placed at a position x_ℓ by use of the routine SHIFT. Linear interpolation is used between points in the reference peak if the shift involves fractions of a channel.

O. Subroutine FUN

The array {E} and the value of F are calculated in Subroutine FUN.

P. Peak Constraints (New Option)

A recent addition to the variable-metric package allows constraints to be placed on relative peak separations. If estimates of peak positions are read in as data, and if adjacent overlapping peaks in a subgroup are properly flagged, the program will adjust their absolute positions for a good fit but will keep their initial separations constant. This is particularly convenient if the peak positions are given in units of Q value.

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[1] P. Spink and J. R. Erskine, ANL Physics Division Informal Report PHY-1965B, 1965 (unpublished).

[2] D. R. Hartree, Numerical Analysis, 2nd Ed. (Clarendon Press, Oxford, 1958).

[3] Applied Mathematics Division Program Library Report E206S. The routine LSQPOL used in AUTOFIT is a slight revision of the routine described in this report.

[4] W. C. Davidon, Argonne National Laboratory Report ANL-5990 (Rev. 2), 1966 (unpublished).

[5] App. Math. Div. Program Library Report F402S.

III. RECOMMENDATIONS FOR INPUT

The following suggestions are intended to aid the user in setting up the input card decks to AUTOFIT. The user should refer to the list of input cards (Sec. V).

A. Conversion to Q-Space

The conversion of the spectrum to Q-space (NCALC = 1) will in general not be necessary. If the data of interest cover a range larger than 50 cm of spectrograph plate distance, the user may wish to make corrections for the variable dispersion. The conversion is also useful for MCA data if the calibration is not linear.

B. Backgrounds

The automatic option is sometimes capable of providing a reasonable estimate of the background, but it can also produce very unrealistic results. Its use is not recommended if high-quality results are desired. Background option 1 (NBACK $>$ 0) gives the user the maximum control over the background curve. If enough points are specified, the background can be tailored to any specification.

Constant backgrounds can be entered with option 2 (NBACK = -1). Option 1 can also be used with NBACK = +1 if DB(1) specifies any abscissa in the middle of the spectrum and BACK(1) specifies the background value.

C. Reference Peak

The option with NREF = 0 is generally not recommended. It is convenient to use but normally gives inferior results. A much better procedure is: (1) select a peak from the spectrum, remove the background, and plot the points; (2) approximate the data points with

a smooth curve; (3) extract new values for the shape of the peak from the curve; and (4) enter the new peak shape with the option NREF = -1.

In establishing the shape of the reference peak, it is better to require that the top of the peak occur at an integral channel number, not between channels.

Typically, if a number of spectra are obtained under nearly identical conditions (except possibly for the detection angle), it will be possible to use a single reference peak shape for all spectra, not a separate shape for each spectrum.

By design, the reference peak shape is not modified if the spectrum is converted to Q-space. (For NREF = 0, the reference peak is selected from the converted spectrum). However, a peak near the middle of the spectrum will have the same width (in units of channels) and shape in the converted spectrum as it had in the original. If necessary, a peak shape for a later pass can be selected from the printout of the converted spectrum.

D. Peak Selection

The automatic peak-selection option is useful if one does not wish to examine a spectrum closely or to punch cards for many peak positions. The punched output is easily edited, and these cards can be used for specifying peak positions on a subsequent pass.

If several spectra (taken at different angles) of a single reaction are being processed together, it is convenient to give peak positions in units of Q-values. These can also be read directly from a Q-plot of the data.

Estimates of peak positions need not be very precise. An accuracy of 1—2 channels is often sufficient.

The option that requests the program to hold the positions of peaks fixed while obtaining their areas is not generally recommended. It is useful if the program has troubles in separating closely-spaced

peaks whose positions are known in advance. However, the positions of peaks are almost never known a priori. Even if their energy values are precisely known, experimental uncertainties and insufficient yields may make their positions in a spectrum poorly known.

E. Printout Options

The input NSSW1 = 1 produces messages from the variable-metric-minimization package. This is useful for error tracing or debugging. Otherwise, set NSSW1 = 0.

The input NSSW2 = 1 produces a printout of the same information that is given on the Calcomp plots. It is sometimes very useful if the user wishes to make minor corrections to the final results from AUTOFIT by manually summing the counts in a peak.

IV. INTERPRETING THE OUTPUT

A. Special Messages

Most of the printed output is self-explanatory. In addition to the error messages indicating improper data (listed in the descriptions of the utility subroutines), a few other messages can be produced under special conditions.

1. nn PEAKS DELETED

Some of the peak positions that were read in are not in the range of abscissa values. These peaks, nn in number, are not considered in the subsequent analysis.

2. NUMBER OF PEAKS IS GREATER THAN 200

The PEKPIC routine has identified 200 peaks in the spectrum and has not completed its search. Only the 200 peaks identified to this point are processed further.

3. THERE WERE nn PEAKS IN THE GROUP STARTING WITH xxx—DIVIDE IN HALF

A group with more than 20 overlapping peaks, with the first peak located at xxx, was identified. The entire group is divided into two separate groups.

4. EPSILON TOO SMALL—CANNOT CONVERGE FOR PEAKS AT xxx, yyy....

Twenty-five complete iterations have been made by the variable-metric package in an attempt to minimize the function F for the peaks located at the positions listed. Convergence was not achieved and the results of the last iteration are returned to the calling programs. Normally, these are sufficiently accurate. However, this message is sometimes produced if the spectrum is very complex and either too many

or too few peaks are specified. One should revise the estimates of the peak positions and rerun the program.

B. Results of the Peak-Fitting Analysis

The final printed summary of results should be examined for signs that the calculated fits to the data may not be reliable. If necessary, the input deck can be revised and another pass made.

1. Errors.

One can roughly estimate the errors expected for the final positions and areas of the peaks and compare these with the calculated errors. Large discrepancies require attention. The expected error in the area (NUMB. COUNTS) A is $\sqrt{A}$. The expected error in the peak position is roughly FWHM/(2.5$\sqrt{A}$), where FWHM is the full-width at half maximum of the peak.

Normally, the positions and areas of the peaks will be determined much more precisely than the listed errors would indicate. A large discrepancy between estimated and listed error is thus only a sign that the program experienced difficulties in the analysis, not that the answers are necessarily unreliable. Only if the Calcomp plots (on other printouts) show signs of poor fits is a new analysis required.

2. Negative peaks.

The program sometimes produces peaks with negative areas. This is usually a sign that AUTOFIT has been asked to place too many peaks in a small region. Some should be eliminated and the data should be reanalyzed. If the user intends to have all the peaks he requested, a revised set of estimated peak positions can sometimes eliminate negative peaks.

3. Peaks with Zero Areas and Errors

The printout may show that some peaks have areas and errors which are exactly zero. This results from a spurious condition. During the variable-metric analysis, these peaks have been moved outside the range of the spectrum in the work area (not outside the total spectrum) and therefore have zero amplitudes. The errors are arbitrarily set to zero. The cause is usually the same as for negative peaks and should be treated accordingly.

C. New Messages (September 1971)

1. FBEST = xxx FOR nn PEAKS WITH mm TOTAL CHANNELS

When NSSW2 > 0, the program will print the above message for each subgroup. FBEST is the unnormalized chi-square and the total degrees of freedom is mm - nn.

2. CANNOT OBTAIN REFERENCE PEAK
CHANNEL = nn MAX. HT. = xxx WIDTH = mm

This message may be produced when NREF = 0. The reference peak cannot be selected from the spectrum if (a) the estimated position is below channel 12 or (b) within 5 channels of the last channel; (c) the largest count of the reference peak is not greater than 10 counts; or (d) the width is less than 4 or greater than 40 channels.

V. INPUT CARDS FOR PROGRAM AUTOFIT

Column	Variable		Value	Usage
CARD 1.	Title Card			
	TITLE (I), I = 1, 20			
	FORMAT (20A4)			
1—80	TITLE	=	Any alphanumeric string.	
NOTE:	If columns 1—4 are blank, the program terminates. The program also terminates on an end-of-file card (7-8 punch in col. 1 for CDC 3600, /* for S/360).			
CARD 2.	Option Control Card			
	NCALC, NBACK, NPKRD, NREF, NQPLOT, NSSW1, NSSW2, BETA, QSCAL, DSCAL			
	FORMAT (I2, I4, 5I2, 4X3F10.5)			
2	NCALC	=	0	Do calculations in D-space (plate distance or channel number is the abscissa).
		≥	1	Convert spectrum to Q-space by interpolation before doing calculations.
3—6	NBACK	=	0	Background determined automatically by program.
		=	+n	Background option 1. The X and Y coordinates for n background points will be read in; program calculates a curve passing through all points.
		=	-n	Background option 2. n background intervals will be read in (background is a constant between the limits of each interval).
	Note 1: n ≤ 50.			If n > 50, the program will truncate it to 50.
	Note 2: n ≥ 3 for background option 1 (positive sign). But also see note 2 for card 3.			

7—8	NPKRD	=	0	Initial peak positions to be selected by program.
		≥	+1	Initial peak positions to be read, as values of plate distance or channel number.
		≤	-1	Initial peak Q-values to be read.
9—10	NREF	=	0	Reference peak to be selected from spectrum. (This option is generally not recommended.)
		=	-1	Reference peak values to be read from spearate cards.
		=	n, $1 \leq n \leq 10$	Reference peak to be selected from ten internally-stored peak shapes, according to the value of n.

n	Base width	FWHM	Chan. of maximum
1	6	1.2	4
2	7	1.6	5
3	8	1.9	5
4	9	2.3	6
5	10	2.8	7
6	11	3.0	7
7	12	2.5	8
8	13	3.0	9
9	14	4.4	9
10	15	4.6	10

11	(sign)	+		The individual fitted peaks are to be plotted on the graphical output.
		-		The composite spectrum of the fitted peaks is to be plotted.
12	NQPLOT	=	0	No graph will be plotted.
		=	1	Graph of counts vs plate distance (or channel number) will be plotted.
		=	2	Graph of counts vs Q-value will be plotted.

Note: For NCALC = 1, the program will require NQPLOT = 1 (or 0), but will plot counts vs Q-value only.

14	NSSW1	=	0	Suppress printed output from variable-metric-minimization routines. (Standard!)
		=	1	Print the v.m.m. calculations.
16	NSSW2	=	0	Suppress printed output of raw data, resolved peaks, and composite spectra.
		=	1	Print the above.
21—30	BETA	=		Parameter that controls the sensitivity of the PEKPIC routine. BETA is the minimum value of an acceptable linear correlation coefficient relating the reference-peak shape with the data.

Note: If left blank (standard option), the program will set BETA = 0.6. Values less than 0.5 are not recommended.

31—40	QSCAL	=	The number of MeV per inch of graph, the horizontal scale factor for Q-plots.

Note: If left blank (standard), the program will select a convenient scale factor based on the value of DSCAL.

41—50	DSCAL	=	The number of points per inch of graph, the horizontal scale factor for D-plots.

Note: If left blank (standard), the program will set DSCAL = 20.

CARD 3. Background Data Cards (Not used for NBACK = 0.)

DB(I), BACK(I), I = 1, |NBACK|

FORMAT (16F5.0)

1—5	DB(I)	=	For NBACK > 0 (option 1):
11—15, etc.			DB(I) is the plate distance (cm) or channel number at which a background value is to be specified.
			For NBACK < 0 (option 2):

DB(I) is the plate distance (cm) or channel number at the lower end of the Ith interval for which a background value is to be specified. DB(1) is supplied by the program and may be left blank.

6—10 BACK(I) = The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK < 0).

NOTE 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).

NOTE 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK (1) for the first channel, and BACK (NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

CARD 4a. Reference Peak Values Card (Use only for NREF ≤ -1.)

N, STOREF (I), I = 1, N

FORMATS (I5, 15F5.0) and (16F5.0)

1—5 N = The number of channels in the reference peak.

Note: N ≤ 40. If N > 40, the program will truncate it to 40.

6—10, 11—15, etc. STOREF(I) = The number of counts in the Ith channel of the reference peak, reading from the back edge (low plate distance) to the front edge (high distance).

Note: STOREF(I) may be continued on successive cards if N > 15, starting in columns 1—5.

CARD 4b. Reference Peak Parameter Card (Use only if NREF = 0.)

STOIPR, DELTA1, DELTA2, DELTA3

FORMAT (4F10.5)

1—10	STOIPR	=	The plate distance (cm) or channel number of the maximum count in the reference peak.
11—20	DELTA1	=	Distance (cm) or channels from the front (high-energy) edge of the reference peak to the "third-height" position on the front edge.
21—30	DELTA2	=	Distance (cm) or channels from the back (low-energy) edge of the reference peak to the third-height position.
31—40	DELTA3	=	Distance (cm) or channels from STOIPR to the third-height position.

NOTE 1: For MCA operation, the "third-height" position is defined as STOIPR and hence the program sets DELTA3 = 0.0.

NOTE 2: Δ_1, Δ_2, and Δ_3 may be any fraction of a cm, but $(\Delta_1 + \Delta_2)$, $(\Delta_1 + \Delta_3)$, and $(\Delta_2 - \Delta_3)$ must all be exact multiples of the channel interval (usually 0.05 cm).

CARD 5. Spectrum Control Card

RUNID, IGS, ORVRD, YMAX, GSQVAL

FORMAT (A8, 2I1, 2F10.5)

1—8	RUNID	=	Blank	A Standard Spectrum Data Set will be placed immediately after this card. (On the CDC 3600, an entry may be present.)
		=	Membname	For the S/360, the program will search for the Standard Spectrum Data Set in the system storage devices. Membname identifies the member name of the Data Set in the P.D.S. file. The name must be left adjusted.
9	IGS	=	0	GSQVAL will specify the ground-state Q-value (MeV) of the reaction. Excitation energies will be calculated if GSQVAL $\neq$ 0.0.

		=	1	GSQVAL will specify the location of the ground-state peak. Excitation energies will be calculated if GSQVAL $\neq 0.0$.
		=	2	Special case. This is the same as IGS = 0, but GSQVAL may be zero.
10	IOVRD	=	Control to override the reaction identification (S/360 only).	
		=	0 or blank	Do not override the reaction ID's stored in the system P.D.S.
		$\geq$	1	Override the reaction ID's.
11—20	YMAX	=		The maximum number of counts to be plotted for this spectrum. Values larger than YMAX will be truncated to YMAX.

Note: If YMAX < 100, the program will compute its own YMAX.

21—30	GSQVAL	=	The ground-state Q-value of the reaction in MeV (IGS = 0), or the approximate "third-height" plate distance (cm) or channel number of the ground-state peak (IGS = 1). This is used for computing excitation energies.

Note: If left blank, no excitation energies will be calculated unless IGS = 2.

CARD 6. Standard Spectrum Data Set

For RUNID = Blank, or for the CDC 3600, enclose a Standard Spectrum Data Set at this point.

CARD 7. Override Card (Present only for S/360, and only if IOVRD ≥ 1.)

See the discussion of the Subroutine PDSINP for a description of this card.

CARD 8. MCA Calibration Card (Use only if ISPECT = A and ICAL > 0.)

CALCOF(I), I = 1, ICAL

FORMAT (4E15.8)

1—15	CALCOF(I) =	The Ith coefficient of a polynomial relating particle energy and channel number.
16—30, etc.		

CARD 9a. Peak Position Cards (Use only if NPKRD ≥ +1,)

PEKPOS(I), IFIXPK(I)

FORMAT (F9.4, I1)

1—9	PEKPOS(I) =		The estimated third-height location of the Ith peak to be considered by the program, specified in plate distance (cm) or channel number.
10	IFIXPK(I) =	0 or blank	The program will adjust PEKPOS(I) for the best fit to the data. (Standard option.)
	≥	1	PEKPOS(I) will be held fixed by the program.

See notes after Card 9b.

CARD 9b. Peak Position Card (Use only if NPKRD ≤ -1.)

IFIXPK(I), PEKPOS(I)

FORMAT (9XI1, F10.5)

10	IFIXPK(I) =	0 or blank	The program will adjust PEKPOS(I) for the best fit to the data. (Standard option.)
	≥	1	PEKPOS(I) will be held fixed by the program.
11—20	PEKPOS(I) =		The estimated third-height location of the Ith peak to be considered by the program, specified in Q value (MeV).

NOTE 1: No more than 200 cards will be accepted by the program for Cards 9a or 9b.

NOTE 2: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS(I).

CARD 10. Peak Position Termination Card (Use only with Cards 9a or 9b.)

The program will process a new set of data, beginning with Card 1.

VI. PUNCHED OUTPUT

The items printed in the final tabulated summary of the results of AUTOFIT are also punched on cards. The units are the same as for the printed output (page VII.) and the format is given here.

Column	Format	Quantity
CARD 1.	Summary Data Card	
1—9	F9.4	Peak position.
10	blank	
11—20	F10.4	Q value.
21—30	F10.4	Excitation energy.
31—40	F10.2	Number of counts in the peak.
41—50	F10.2	Number of counts in the background underneath the peak.
51—58	F8.2	Error in the peak position.
59—66	F8.1	Error in the number of counts, computed during the minimization procedures.
67—69	blank	
70—75	A6	Spectrum identification code. (Only six characters are available.)
76—80	F5.1	Angle

NOTE: There is a separate card for each peak analyzed by the program.

CARD 2.	Termination Card		
1—2	I2	-1	(Termination code.)