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The NIRA Computer Program Package (Photonuclear Data Center)

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The NIRA Computer Program Package (Photonuclear Data Center)

+ Technical note no, 103,

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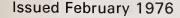
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Preface

The Photonuclear Data Center, a part of the Center for Radiation Research, is one of many data centers within the National Standard Reference Data System receiving support from the National Bureau of Standards' Office of Standard Reference Data. Its function is to collect, abstract, index, and evaluate experimental data published in the world's technical literature relating to the interaction of electromagnetic radiation with nuclei. It provides information-center services for the technological and scientific communities concerned with photonuclear reactions. Ever since its creation in 1963, the Data Center has made considerable use of computer-compatible index, bibliographic, and data files. These are used with the central computer facilities at the National Bureau of Standards to retrieve specific types of information; to prepare camera-ready copy for publication of tabular, bibliographical and graphical information; and, to carry out various manipulations of digital data sets germane to their evaluation.

This Technical Note is the first of several being written to describe all aspects of the computer-based operations of the Photonuclear Data Center. These notes are meant both to document the procedures used in the Data Center as well as to serve as 'user's manuals' for individuals having a need to make use of the Data Center's files. The program library described in this Note has been designed for use with the particular central computer facilities available at the National Bureau of Standards. No attempt has been made to write the various programs in a completely general form (facilityindependent). For those desiring to have it, the complete program library (in symbolic form) is available from the Photonuclear Data Center.

Everett G. Fuller

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The NIRA Computer Program Package (Photonuclear Data Center)

H. J. Vander Molen and Henry M. Gerstenberg

The Photonuclear Data Center's NIRA library of programs, executable from mass storage on the National Bureau of Standards' central computer facility, is described. Detailed instructions are given (with examples), for the use of the library to analyze, evaluate, synthesize, and produce for publication, camera-ready tabular and graphical presentations of digital photonuclear reaction cross-section data. NIRA is the acronym for Nuclear Information Research Associate.

1. Introduction

There are two aspects of the Photonuclear Data Center's operations which make use of the NBS computer facilities. The first is related to the abstracting and indexing of experimental papers published in the world's technical literature. This provides the input both for the Center's computer-searchable index to the available experimental data for the field of photonuclear physics, as well as the annotated bibliographies or data indexes which the Center regularly publishes and updates [1].¹

The second computer-oriented activity of the Center relates to its library of digital cross section data and the systematic evaluations being made of these data. To do this, it has been necessary to generate procedures for handling, storing, classifying, evaluating, and presenting data. The program library described here is an implementation of these objectives on the National Bureau of Standards' main computer facility, a UNIVAC 1108 computer operating under the EXEC-8 system.²

2. Description of the Library

The NIRA program library consists primarily of programs which handle <u>data</u>,

rather than index or bibliographic information. Most of these programs are quite simple, both conceptually and in implementation. All can be executed from a demand terminal, although ordinary batch usage was the primary intention. All are mutually compatible; data processed by any program can be read by any other program without human manipulation. It is likely that, in the future, need will arise for even more programs. However, the basic operations described here should suffice for most procedures.

The programs reside, as addressable elements, in a file called "NIRA*PROGM.". (The asterisk and period are essential parts of the name.) This file is stored as a "read-only" file. It is therefore not possible to alter it by any error in normal use. (It is possible to delete it, however, so be cautious when using DELETE statements.) Two or more runs may simultaneously access this file. As a backup, the entire program library (in symbolic form), as well as a complete listing, is kept in the Photonuclear Data Center. At present, this library deck consists of more than 3,000 punched cards with control cards in place for reloading to mass storage.

Most of the individual programs are designed to operate on a deck of punched cards which define a "data set". Similarly, most of the programs output either real or

¹Figures in brackets indicate the literature references given on p. 6.

²Use of brand names in this r-port is for identification purposes only and is not to be construed as a recommendation of a particular product or company.

virtual punched cards. In all such cases, the program adds a comment card to the deck which states what the program has done to the data. This card is listed on the user's printout for the run in which the program is called. For reasons of economy (i.e., to limit the amount of the computer's memory used), most of the programs will accept a maximum of 500 data points and 100 comment cards. This can be changed without great difficulty, but this quantity of memory has been more than sufficient thus far.

As defined by the Photonuclear Data Center, a "data set" consists of the results of the measurement of an excitation function, angular distribution, or reaction product spectrum under specified conditions for a single target. The set consists of a <u>Header Card</u> which contains the acquisition number, number of data points, reference, nucleus, and reaction, plus some data source information; two <u>Label Cards</u> which give the axis labels, usually "Photon Energy (MeV)" and "Cross Section (mb)"; an arbitrary number of <u>Comment Cards</u>; and then <u>Data Cards</u> in Fortran format (7(E9.4,','), E9.4,1X).

3. Use of the Program Library

To use the library, it is necessary to assign the library file to a particular computer name. To do this, use the two EXEC-8 control cards [2]:

@ASG,A NIRA*PROGM.

@USE PF.,NIRA*PROGM.

The "commercial at" sign is represented by a 7/8 punch on the card punch, and by "@" on the Teletype.

As indicated in the individual descriptions given in the Appendix, most of the programs are called by entering three cards For example: SORT is called by:

@MAP, INX MAPR, SORT

IN PF.SORT

@XQT SORT

Similarly, SMOOTH is called by:

@MAP, INX MAPR, SMOOTH

IN PF.SMOOTH

@XQT SMOOTH

A few programs require more elaborate control cards than this MAP-IN-XQT sequence. These have been combined with the appropriate individual programs into what in the following discussion are referred to as "job-control decks". Each deck is named, and only one card need be entered to call a deck; e.g., PPLOT is called by:

@ADD,P PF.PPLOT

The individual writeups give the exact cards to use. (Do not forget the ASG-USE sequence at the beginning of your run, however!) Note that the run cards, tape identification labels, etc., that are used in a number of the examples, are given for purposes of illustration only, and that in making use of the library, the user should be sure to use the appropriate number and designation associated with his computer account. Throughout the listings, square brackets, i.e., [], are used to designate cards containing information germane to particular runs only. Brackets are not used in entering information unless specifically called for in the program description.

4. Qualitative Description of the Programs and Their Use

A brief description of the purpose of the various programs is given here. The individual descriptions should be consulted before they are used.

4.1. Programs Which Create Data Sets

DIGIT is a job-control deck that takes data from a tape made by the sonic delayline digitizer, converts it to data-library format, operates on it with CLEAN, provides punched cards for the data library, and/or leaves the data in a computer file element called DIGOUT for use by other programs.

HIST converts a normal data set into a histogram.

UNHIST converts a histogram into a normal data set.

4.2. Programs Which "Dress-Up" Data

SMOOTH performs a normal vertical smoothing on raw data.

STIFF is used to "dress-up" digital data so that it may be used as input to obtain computer-drawn, smooth, continuous cross section curves.

AVRG smooths raw data over a pre-set energy interval.

INTERP parabolically interpolates smoothed data to give points at "nice" energies.

SQUARE squares up histograms.

4.3. Programs Which Manipulate Data

COMBIN algebraically adds two cross sections. It will read a (γ,n) and a $(\gamma,2n)$ cross section, and punch a (γ,xn) cross section, for example.

DBAL reverses a cross section by means of the principle of detailed balance.

CALC renormalizes data sets.

UNSTAT removes the statistical theory's multiplicity correction from a (γ, sn) cross section.

4.4. "Housekeeping" Programs

CLEAN checks data for format and makes several computer-oriented (non-manipulative) corrections. A data set which has passed through CLEAN should give no problems when read by the other programs.

MONO forces energies to increase monotonically.

SORT sorts data points by energy.

TRUNC picks out a subset of a data set.

CONCAT joins together several data sets covering different energy ranges.

4.5. Programs Which Produce Final Copy

YIELD⁴ is used to print a column-wise table of cross sections. It is also used to calculate σ_{-1} at 10, 15, 20, 25, and 30 MeV. SPCDST is a deck used to print an index table of spectral and angular distribution data.

LIST is used to produce camera-ready copy of tables made by either YIELD4 or SPCDST.

PPLOT is a plotting job-control deck. It produces plots which are suitable for mounting on reduction paper.

GDR calculates the integral moments σ_0 , σ_{-1} , and σ_{-2} of the cross section, and estimates the giant resonance parameters E_m , σ_m , and Γ . See Ref. [1] for definitions.

4.6. Use of Programs

The use of the programs is completely flexible. Nevertheless, there is a "normal" or "usual" sequence of steps through which data pass from journal article to final copy.

(1) The data are digitized and assigned an acquisition number. The data set is then run through DIGIT. If the data already exist in digital form, they are punched and run through CLEAN. UNHIST may also be used if the data are given as a histogram.

(2) If CLEAN indicates monotonicity problems with the data, SORT and/or MONO may be used to correct the trouble.

(3) The data set is manipulated, if appropriate, to get it into the proper units and form for comparison. COMBIN, DBAL, UNSTAT, TRUNC, and CALC are provided for such manipulation.

(4) The data are plotted, using the CPLOT mode of PPLOT. Comparisons are made, and the best data are selected.

(5) The selected data, if a (γ ,sn), (γ ,xn), or (γ , μ_t), are run through GDR to calculate σ_0 , σ_{-1} , and σ_{-2} . This program also gives estimated values for E_m , σ_m , and Γ .

(6) The selected data are used to create a smoothed cross section curve. This smooth curve is the source of the evaluated data set. The curve is usually drawn by hand. SMOOTH and AVRG are sometimes used in conjunction with, or even in place of, the manual drawing. (SQUARE is used to dress up histograms.) If the manual method is used, the hand-drawn line is digitized, run through DIGIT and MONO, and then run through STIFF to smooth out the hand-induced irregularities. If the hand-drawn line was digitized in sections, CONCAT is used to join the sections together before STIFF is used.

(7) The evaluated data are then run through INTERP to obtain a compact representation with cross-section values given at specified energy intervals. Occasionally, MONO is needed between STIFF and INTERP. The output of INTERP is filed as the final form of the "evaluated" cross section.

(8) The yields are calculated from the selected (not evaluated) data using the YIELD aspects of YIELD4.

(9) The evaluated cross sections, as well as the selected data set, are plotted using PPLOT.

(10) The evaluated cross sections are tabulated using YIELD4 and LIST.

(11) The index to supplementary data is tabulated using SPCDST.

5. Some Notes on Efficient Use

Almost all of the programs described in the preceding pages read cards for input and punch cards for output. It is not necessary to execute just one program per computer run. There are several "tricks" which enable the user to perform a sizable amount of work in one computer run.

5.1. Multiple Execution

Most of the programs are called in the following manner:

- @MAP, INX MAPR, GDR
- IN PF.GDR
- @XQT GDR

The first two cards direct the MAP processor to transform the relocatable element PF.GDR into the absolute (executable) element GDR. Even after execution, the absolute element GDR is still in the run's temporary program file (TPF\$.). It can be re-executed with another XQT card: @MAP,INX MAPR,GDR IN PF.GDR @XQT GDR [lst data set] @XQT GDR [2nd data set] @QXT GDR [3rd data set] etc.

5.2. Temporary File

A temporary file is useful when the same data set is needed for input to more than one program. The file is created by:

- e 1 0

E 224 - 37 C

@ASG,T TF.

Data are then put into the file element by element. The file elements are fed to the processing programs by ADD.

Example: Suppose one started out with a $(\gamma,n+np)$ and a $(\gamma,2n)$ data set. It is desired to calculate a (γ,sn) and a (γ,xn) data set. The cards would be:

@ASG,T TF. @ELT,IS TF.1 [(γ,n+np) data] @ELT,IS TF.2 [(γ,2n) data] @MAP,INX MAPR,COMBIN IN PF.COMBIN @XQT COMBIN 0,0,1.,1., @ADD,P TF.1 @ADD,P TF.2 @XQT COMBIN 0,0,1.,2., @ADD,P TF.1 @ADD,P TF.2 5.3. Breakpoint File

A breakpoint file is useful when it is desired to feed the output of one program into the input of another program. The file is created by:

@ASG,T BF.

The punched output of a program is diverted to the breakpoint file by:

@BRKPT PUNCH\$/BF (Note no punctuation!)

Then the first program is executed. After the last data card of the first program, the punch channel is re-activated by:

@BRKPT PUNCH\$

Now the contents of the breakpoint file can be fed into the 2nd program by means of:

@ADD,P BF.

Example: Suppose it is desired to calculate a (γ, xn) total neutron yield. The starting data are a (γ, sn) data set measured via a BF3 detector and a statistical multiplicity correction. It is necessary to first call UNSTAT to transform the (γ, sn) data set into a (γ, xn) data set, then to call YIELD4 to calculate the yield.

> @ASG,T BF. @MAP,INX MAPR,UNSTAT IN PF.UNSTAT @BRKPT PUNCH\$/BF @XQT UNSTAT [parameter card] [(γ,sn) data] @BRKPT PUNCH\$ @MAP,INX MAPR,YIELD4 IN PF.YIELD4 @XQT YIELD4 (NONE) YIELD @ADD,P BF.

The breakpoint file is erased whenever new @BRKPT PUNCH\$/BF card is encountered. sides adding data with an @ADD statement, he contents of the breakpoint file can be isted by entering:

@ADD, P PF.LIST

as can be seen in the description of SPCDST. The breakpoint file can also be punched by:

> QELT, ID PUNCH CADD, D BF. QEND QPCH, S PUNCH

(The SYM processor of EXEC-8 will also punch BF, but requires cataloging. This had led to interference between runs.)

The breakpoint file is an extremely powerful tool when used in conjunction with a temporary file. The following example begins with a (p,γ_0) data set. The data set is inverted and plotted. Simultaneously, a smoothed form of the same cross section is digitized, smoothed, punched, inverted, plotted, and tabulated.

@RUN, M/NR VAND41, 30850-VANDER, NIRA, 1, 50/1000 @ASG,A NIRA*PROGM. @USE PF.,NIRA*PROGM. @ASG,T BF. @ASG,T TF. @MAP, INX MAPR, DBAL IN PF.DBAL **@BRKPT PUNCH\$/BF** @XQT DBAL [parameter card] $[(p, \gamma_0) data]$ **@BRKPT** PUNCH\$ @ELT.IS TF.1 @ADD,P BF. @ELT,IS DIGIN [digitizer control cards] @ASG,LJO IN.,8C,VANO2 @SETC 1 @ADD,P PF.DIGIT @MAP, INX MAPR, MONO IN PF.MONO @BRKPT PUNCH\$/BF @XQT MONO @ADD,P DIGOUT **@BRKPT** PUNCH\$ @ELT,IS TF.2

@ADD, P BF. @ELT, IS TF.2 @ADD,P BF. @MAP, INX MAPR, STIFF IN PF.STIFF @PCH.S TF.2 @BRKPT PUNCH\$/BF @MAP, INX MAPR, YIELD4 @XQT STIFF IN PF.YIELD4 @BRKPT PUNCH\$/BF [parameter card] @ADD,P TF.2 @XQT YIELD4 @BRKPT PUNCH\$ [blank card] @ELT, IS TF.2 @ADD,P TF.2 @ADD,P BF. @BRKPT PUNCH\$ @BRKPT PUNCH\$/BF @ADD,P PF.LIST @XQT DBAL @ADD,P PF.PPLOT [parameter card] @ADD,P TF.1 @ADD,P TF.2 \$CURVE @BRKPT PUNCH\$ @ADD,P TF.2 @ELT,IS TF.2 \$PPLOT @ADD,P BF. @ADD.P PF.PRINTR @MSG,W 30850-VANDER,WRITE ENABLE REEL VANO3 @MAP, INX MAPR, INTERP IN PF.INTERP @ASG,TMJ 9.,8C,VANO3W @BRKPT PUNCH\$/BF @CLOSE 9. @XQT INTERP @XQT NBS*CALCMP. @ADD,P TF.2 **@BRKPT PUNCH\$** @FIN

References

- [1] E. G. Fuller, H. M. Gerstenberg, H. Vander Molen, and T. C. Dunn, <u>Photonuclear</u> <u>Reaction Data, 1973</u>, Nat. Bur. Stand. (U.S.), Spec. Publ. 380, 125 pages (March 1973).
- UNIVAC 1100 Series, EXEC-8 Hardware/Software Summary UP-7824 Rev. 1 (1971-1974) Sperry Rand Corporation, New York, N. Y.

6. Appendix; NIRA Listings

6.1. Programs

AVRG

AVRG is a means of smoothing a data set. The cross section at each energy, E is replaced by the average value over a specified energy interval, ε . (This is in contrast to SMOOTH which averages over 3 points regardless of spacing.) The averaged data set is then punched. The formula used is:

$$\sigma(E_{i}) = \frac{1}{\varepsilon} \qquad \int_{E_{i}^{-}}^{E_{i}^{+}} \frac{\varepsilon/2}{\sigma(E)dE} dE_{i}$$

The integration is rectangular. The averaging interval " ϵ " is constant except at the low energy end. If $E_i - E_l < \epsilon/2$, $\epsilon = 2(E_i - E_l)$.

The averaging interval " ε " is punched as a floating point number in free form, followed by a comma, on a parameter card immediately preceding the data set. If the card is omitted, $\varepsilon = 1$ MeV. Any number of data sets may be entered. The value given to epsilon remains in force until a new parameter card is encountered.

@MAP,INX MAPR,AVRG IN PF.AVRG @XQT AVRG [parameter card] [data set]

CALC

CALC manipulates a data set by the formulas: $E_1 = A_1E_1 + A_2$ and $\sigma_1 = B_1\sigma_1 + B_2$. The first card read by CALC must contain A_1 , A_2 , B_1 , B_2 , and the new acquisition number. If zero is entered for the new acquisition number, the old acquisition number will be used. The program will read only one data set.

Example: If it is desired to change a data set scale from millibarns to microbarns, the parameter card would be: 1.,0.,1000.,0.,0

```
@MAP,INX MAPR,CALC
IN PF.CALC
@XQT CALC
[parameter card]
[data set]
```

CLEAN

CLEAN reads a data set and checks it for format. It will automatically modify the set as follows:

- (1) If the label cards are missing, "PHOION ENERGY (MEV)" and "CROSS SECTION (MB)" are inserted.
- (2) If the number of data points is missing or incorrect, the correct number is inserted.
- (3) If the header card is missing, one is inserted.
- (4) If two adjacent data points have the same energy, the second energy is increased one part per thousand.
- (5) If the data are non-monotonic, except for the case above, a warning is printed.
- (6) If a blank card is encountered, it is skipped over.
- (7) If two points have identical x- and y-coordinates (e.g., due to double-sparking of digitizer), the second point of the doublet is deleted.

This routine can read any "free" format. A warning is printed if the data are not in the standard "(7(E9.4,','),E9.4,1X)" Data Center format. The monotonicity and double-sparking tests are bypassed if the acquisition number is negative (i.e., special test data).

A data set punched by CLEAN can be handled by all the other programs without problems.

@MAP,INX MAPR,CLEAN IN PF.CLEAN @XQT CLEAN

COMBIN

COMBIN is used to algebraically add two cross sections and punch a new data set. The formula is:

$$\sigma' = \alpha \sigma_a + \beta \sigma_b ,$$

where α and β can be any positive or negative floating point number. The two data sets must be preceded by a parameter card containing NA, NB, α , and β in free field format. NA and NB must be fixed-point positive or negative integers, and α and β are floating-point numbers. The maximum energy in the new data set will be the larger of that in the two sets combined if NA = 0. Setting NA = -1 results in the maximum energy being the lesser of that in the two sets. In both cases, NB is the acquisition number for the new data set.

Only two data sets may be entered. The set with the best resolution should be the second data set. If the resolution differs greatly between the two sets, then the programs AVRG or SMOOTH should be used to obtain comparable resolution before using COMBIN.

The program makes the resolution of output data similar to that of the first data set. For the region where the data sets overlap in energy, the second set is linearly interpolated to match exactly the energies of the first data set. For the regions where there is no overlap and data exist only in the second set, then the resolution of the first set is averaged over ten data points nearest the region of interest. This average energy resolution is then used in the linear interpolation of the second data set to obtain output data points of the second data set having a resolution similar to that of the first data set.

> @MAP,INX MAPR,COMBIN IN PF.COMBIN @XQT COMBIN [parameter card] [data set A] [data set B]

CONCAT

This program reads an arbitrary number of data sets, and punches one data set which is a simple concatenation (i.e., joining together) of the input data sets. The header and label cards of the output are, except for the number of points, copied from those of the first data set read. The total number of points must not exceed 500. Generally, it is wise to feed the output of CONCAT into SORT.

```
@MAP,INX MAPR,CONCAT
IN PF.CONCAT
@XQT CONCAT
[data sets]
```

DBAL

DBAL reverses a cross section via the principle of detailed balance. It reads a parameter card and a data set.

For reactions of the type A+ $\gamma \rightarrow$ B+b, the equations used are:

$$\sigma(\gamma, b_0) = f(A, E_0) \sigma(b, \gamma_0)$$
 where,

$$f(A,E_{e}) = \frac{(2J_{B}+1)(2s+1)}{(2J_{A}+1)} \frac{m}{M_{B}+m} \frac{M_{B}}{(2E_{e}-BE)}$$
 with

$$E_{e} = \frac{M_{B}}{M_{B}+m} E_{b}+BE \quad \text{or} \quad E_{e} = E_{\gamma} - \frac{E_{\gamma}^{2}}{2(M_{A}c^{2}+E_{\gamma})}$$

The parameters are:

q = flag to indicate direction of change m = mass of particle b s = spin of particle b M_A = mass of nucleus A M_B = mass of nucleus B J_A = spin of nucleus A J_B = spin of nucleus B BE = binding energy of b in A

To turn a ground-state capture cross section into the related photodisintegration cross section, the parameter card is:

1, m, s,
$$M_B$$
, J_B , M_A , J_A , BE

Similarly, for the reverse transformation, the card should read:

0., m, s, M_B , J_B , M_A , J_A , BE

Any number of data sets may be entered, but each must have a parameter card.

@MAP,INX MAPR,DBAL
IN PF.DBAL
@XQT DBAL
[parameter card]
[data set]

GDR

GDR reads a data set, calculates σ_0 , σ_{-1} , and σ_{-2} , and estimates E_0 , σ_{max} , and the width. Only one data set may be entered.

The integration is done by the trapezoidal rule. The upper limit of integration is the greatest integer which is less than the max energy of the data set. The value of E_0 is a calculated mean energy. The estimates of σ_{max} and width are, in practice, almost worthless. A better job can be done by eye.

The data set is repunched with the calculated giant resonance parameters given on a comment card.

@MAP,INX MAPR,GDR IN PF.GDR @XQT GDR [data set]

HIST

This program converts a normal data set into a histogram. Vertical bars are placed midway between every two points of the input data set. A slight inclination of the verticals is introduced to preserve monotonicity. Any number of data sets may be entered. <u>CAUTION</u> - The output may look strange if the input is not approximately evenly spaced in energy.

@MAP,INX MAPR,HIST IN PF.HIST @XQT HIST [data sets]

INTERP

INTERP reads a data set and punches a parabolic interpolation of the input. The output, except for the first and last points, is given at every tenth, fifth, or half MeV, depending on local curvature.

The output is suitable for input into PPLOT and YIELD4. Any number of data sets may be entered.

@MAP,INX MAPR,INTERP
IN PF.INTERP
@XQT INTERP
[data sets]

MONO

MONO is a program that corrects monotonicity problems which result from roundoff errors in going from the raw digitized data to the Data Center's data card format. The <u>order</u> of the points is maintained, but energies are adjusted upwards such that they monotonically increase. (This is not always the appropriate correction - see SORT.)

If more than one data set is entered, each one will be checked, corrected if necessary, and punched.

@MAP,INX MAPR,MONO
IN PF.MONO
@XQT MONO
[data sets]

SMOOTH

SMOOTH performs one pass of a normal vertical smoothing on a data set. Any number of data sets may be entered. The energies do not need to be equally-spaced. The algorithm used is:

 $\sigma_{i} = \frac{1}{2} \left[\sigma_{i} + \frac{\sigma_{i+1} - \sigma_{i-1}}{E_{i+1} - E_{i-1}} (E_{i} - E_{i-1}) + \sigma_{i-1} \right]$

In the special case of equally-spaced energies, this reduces to the familiar form:

$$\sigma_{i} = \frac{1}{4} \sigma_{i-1} + \frac{1}{2} \sigma_{i} + \frac{1}{4} \sigma_{i+1}$$

@MAP,INX MAPR,SMOOTH
IN PF.SMOOTH
@XQT SMOOTH
[data sets]

SORT

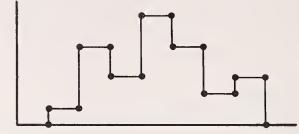
This program sorts the points of a data set by energy. Its primary uses are: (1) removing monotonicity problems caused by digitizing data in a region of high-point count density, and (2) fixing a deck of cards someone dropped on the floor. Note that <u>SORT</u> and <u>MONO</u> have the same goal but accomplish it in different ways; <u>SORT</u> changes the order of the points, while MONO changes the value of the points.

If more than one data set is entered, the program will sort each data set.

@MAP,INX MAPR,SORT IN PF.SORT @XQT SORT [data sets]

SQUARE

This program is used to "dress up" a histogram-type bar graph. (We use "histogram" to denote a bar graph, not in the strict statistical sense.) If the "corner points" of a histogram are digitized:



then, in general, the output of the digitizer program will give a graph in which the horizontal and vertical lines are not truly parallel to the axes.

SQUARE reads such a "raw" data set, and adjusts the points such that horizontal lines are truly horizontal. Vertical lines are inclined very slightly (one part per thousand) to avoid monotonicity problems.

The height of each "squared" horizontal is the average of the heights of the two raw points defining it, and similarly for the verticals. Any number of data sets may be entered.

@MAP,INX MAPR,SQUARE
IN PF.SQUARE
@XQT SQUARE
[data sets]

STIFF

STIFF performs one pass of a non-vertical smoothing routine. This means that energies are also adjusted to smooth the data. Such smoothing is the appropriate treatment for digitized curves where errors are both vertical and horizontal.

The program is used to smooth digital data which has been generated from "smooth" curves drawn by hand through actual data points. The resulting "smooth" data are used to generate computer-drawn curves which approximate the actual data presented in graphical form. They are also used to generate the tables of "smoothed" cross section data.

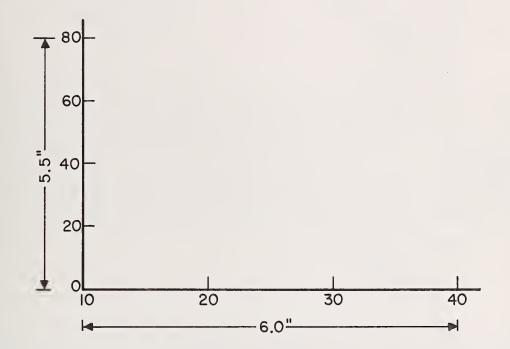
The smoothing is carried out by averaging over three successive data points, i, j, and k, when their coordinates are expressed in inches. The program first uses points i and k to determine a straight line. The coordinate axes are then rotated to establish an x'-axis which is parallel to this line, and the average y'-coordinate of the point j is determined from:

 $\overline{y}'(j) = \frac{1}{4} y'(i) + \frac{1}{2} y'(j) + \frac{1}{4} y'(k).$

The coordinates of the point j, x'(j), $\overline{y'}(j)$ are then referred back to the original unrotated system to obtain the "smoothed" coordinates of the point j.

Since the program must work with the coordinates of each point expressed in actual linear dimensions, the first card must contain XLNGTH and YLNGTH (in inches), and the three fiduciary points of the plot from which the data were digitized.

Example:



The parameter card is then:

6.,5.5,10.,0.,40.,0.,10.,80.

More than one data set may be entered. If new parameter cards are not entered along with the new data sets, the old parameters will remain in effect.

The primary use of STIFF is to "dress up" a smooth curve by reducing the small pointto-point irregularities introduced by hand-digitizing. The output is suitable for input into INTERP.

@MAP,INX MAPR,STIFF
IN PF.STIFF
@XQT STIFF
[parameter card]
[data sets]

TRUNC

This program reads a data set and punches a truncated data set consisting of data points which fall within a selected energy interval. The upper and lower limits are entered on a parameter card as floating point numbers in free format. The energy interval is inclusive of the end points. Any number of data sets may be entered. If no new energy limits are entered, the old limits remain in force. If no limits are entered [0.,30.,] is assumed.

```
@MAP, INX MAPR, TRUNC
 IN PF.TRUNC
@XQT TRUNC
[E<sub>lower</sub>, E<sub>upper</sub>]
[data sets]
```

UNHIST

This program reads a histogram (either "squared" or "raw") and converts it into a normal data set.

Output points are placed in the center of the horizontal bars, except when multiple bins are detected. No problem should occur if (as is almost always the case) the input bins are of approximately equal width. Any number of data sets may be entered.

> @MAP, INX MAPR, UNHIST IN PF.UNHIST @XQT UNHIST [data sets]

UNSTAT

UNSTAT reads a (γ, sn) cross section, and calculates a (γ, xn) cross section via the statistical model. Its primary use is to strip out the statistical multiplicity correction used by many experimenters with Halpern detectors. The relations used, taken from T. K. Deague, E. G. Muirhead, and B. M. Spicer, Nucl. Phys. A139, 501 (1969), are:

 $\sigma(sn) = \sigma(xn) F(E)$

$$F(E) = \frac{1}{1 + (1 - x)[1 - (1 - f(E))exp - f(E)]}$$

f(E) = (E-E2) (a/(E-E1))^{1/2}, where

(a/(c-ci)) •

x = direct de-excitation fraction

a = level density (in MeV^{-1})

El = the (γ, n) threshold (in MeV)

 $E2 = the (\gamma, 2n) threshold (in MeV)$

The first card must contain floating-point numbers for x, a, El, and E2 in free format.

Any number of data sets may be entered. If new parameter cards are not entered along with the new data sets, the old parameters will remain in effect.

@MAP,INX MAPR,UNSTAT IN PF.UNSTAT @XQT UNSTAT [parameter card] [data sets]

YIELD4

The program YIELD4 is designed to operate on a number of data sets and calculate: (1) a cross-section table with values for each of the reactions entered being given at evenly-spaced energy intervals (usually, every half MeV), and/or (2) values of σ_{-1} for upper-energy integration limits of 10, 15, 20, 25, and 30 MeV for each of the reactions entered. A linear interpolation is used to calculate values at specified energy values. This program is a version of YIELD3 which operates on a single data set to produce a printout in which for each energy E_{1} in the set the following quantities are given:

$$\mathbf{E}_{\mathbf{i}} \quad \boldsymbol{\sigma}_{\mathbf{i}} \quad \boldsymbol{\sigma}_{\mathbf{i}} / \mathbf{E}_{\mathbf{i}} \quad \boldsymbol{\sigma}_{\mathbf{i}} / \mathbf{E}_{\mathbf{i}}^{2} \qquad \sum_{\mathbf{l}}^{\mathbf{i}} \boldsymbol{\sigma}_{\mathbf{j}} \qquad \sum_{\mathbf{l}}^{\mathbf{i}} \boldsymbol{\sigma}_{\mathbf{j}} / \mathbf{E}_{\mathbf{j}} \qquad \sum_{\mathbf{l}}^{\mathbf{l}} \boldsymbol{\sigma}_{\mathbf{j}} / \mathbf{E}_{\mathbf{j}}$$

The operations carried out by YIELD4 are determined by entries punched on a parameter card. These entries must be separated by at least one, and no more than five, blank spaces. There must be <u>no</u> blanks within an entry, and commas must <u>not</u> be used to separate entries. This parameter card must be provided even if no entries are punched on it. In its normal state, the program calculates a cross-section table at half-MeV intervals. The following entries may be made:

DELTA=XXXXXX	If an interval other than 0.5 MeV is desired, replace the six X's with a floating-point number giving the interval. When the normal DELTA is not used, this <u>must</u> be the first par- ameter on the card.
(G,XN)	To skip a particular reaction in building the table, enter the reaction with parentheses.
62Ful	To skip a particular reference in building the cross-section table, enter the reference number.
PUNCH	The output is listed in the normal Data Center cross-section library format, i.e., Energy, Cross Section, Energy, Cross Sectionetc. <u>Note</u> : "PUNCH" and "YIELD" are mutually exclusive.
(NONE)	No cross-section table is desired.

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YIELD	The yield table is calculated, i.e., σ_{-1} values
	at 10, 15, 20, 25, and 30 MeV.
	Note: "PUNCH" and "YIELD" are mutually exclusive.
PRINT	Gives a full printout of YIELD3 for each data set
	entered. See above discussion.

The cross-section table is punched in the proper format to be listed by LIST. See the description of LIST for more details. <u>Note</u>: The cross-section table can hold a maximum of 200 energies and 13 reactions.

@MAP,INX MAPR,YIELD4
IN PF.YIELD4
@XQT YIELD4
[parameter card] This card must be here, even if blank.
[data sets]

6.2. Control Decks

The following are decks of UNIVAC job-control statements each identified by a specific name. These control decks perform various functions primarily related to the formating of data for various final output modes (plots, tables, etc.). From the user's point of view, they differ from the programs described above primarily in the way they are called from mass storage and executed.

DIGIT

DIGIT is a deck of UNIVAC job-control statements, stored as mass storage, which:

- (1) executes the digitizer program;
- (2) takes the output of the digitizer program and inputs it into CLEAN;
- (3) executes CLEAN;
- (4) punches the output of CLEAN complete with headers and labels (<u>Caution</u>: The labels are always "PHOTON ENERGY (MEV)" and "CROSS SECTION (MB)");
- (5) leaves the output in an element called DIGOUT for use in other programs.

The use of DIGIT is best illustrated by a skeletal example:

@ELT, IS DIGIN

[digitizer control cards] @ASG,LJO IN.,8C,[user's tape number] @ADD,P PF.DIGIT

The data in the element DIGOUT may be accessed immediately in the same job by the statement:

@ADD,P DIGOUT

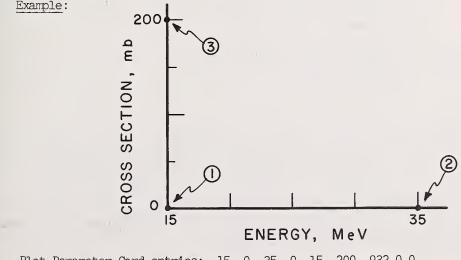
If it is desired to use the data in the same job and <u>not</u> punch the output of CLEAN, precede the @ADD,P PF.DIGIT card with:

esetc 1

Two digitizer control cards must be given for each curve recorded on the tape. The order of these pairs of cards must correspond to the order of the data on the tape. The first card of each pair is a Header Card; the second a Plot Parameter Card. The <u>Header</u> Card gives the acquisition number of the data set, the reference number, the nuclide, the reaction, and any pertinent comments in the following format:

Position	Quantity
1 - 5	Acquisition number, right adjust
6	Blank
7 –11	Number of data points (to be provided
	by program)
12	Blank
13 –18	Data Center reference number
19 –23	Blank
24 -30	Nuclide/Element identification
	25,25 Z, right adjust
	26,27 Symbol, left adjust
	28-30 A, left adjust
31	Blank
32 -43	Reaction with (), left adjust
44	Blank
45	Source flag: blank if digitized at Data
	Center; or, 1 if digital data was supplied
	by original source
52 -80	Available for comments if needed

The <u>Plot Parameter Card</u> must contain nine numbers separated by commas. The first six, in floating-point notation, give the coordinates of the three fiducial points used to establish the axis scales for the digitizer programs. The last three numbers in fixed-point notation give the acquisition number for the plot, an x-axis flag, and a y-axis flag. For a linear scale the flag is 0; setting the flag equal to 1 indicates that the corresponding axis scale is logarithmic.



Plot Parameter Card entries: 15.,0.,35.,0.,15.,200.,932,0,0,

LIST

LIST is a combination of job-control statements (in PF.LIST) and a simple program (in PF.LISTR) which lists data in the breakpoint file (BF.) on the slow printer. It is designed to produce camera-ready copy. Each line is printed twice to ensure dark type.

Whenever a card with "\$PAGE" (starting in column one) is encountered, the program skips to the top of the next page in the printer. The \$PAGE card is, of course, not printed.

Lines longer than 80 characters may be printed with this program. The first 80 characters of the long line are entered on an 80-column card in the normal fashion. The rest of the line is entered in columns 7-46 of a continuation card immediately following the primary card. The continuation card must have "\$MORE" punched in columns 1-5. A maximum of 120 characters may be printed on one line. The primary use of LIST is to build tables in formats suitable for mounting on 40% reduction paper. The long linelength required by such forms precludes the use of simple 80-80 listing.

There are two uses for LIST:

(1) to list a deck of cards:

@ASG,T BF. @DATA,I BF.,,LISTR [card deck to be listed] @END LISTR @ADD,P PF.LIST

(2) to list an already-existing breakpoint file called BF:

@ADD,P PF.LIST

Example: LIST may be used to immediately print the output of YIELD4:

@ASG,T BF.

@MAP,INX MAPR,YIELD4
IN PF.YIELD4
@BRKPT PUNCH\$/BF
@XQT YIELD4
[parameter card]
[data sets]
@BRKPT PUNCH\$
@ADD,P PF.LIST

PPLOT

PPLOT is a production plotting job-control deck. It will plot points, smooth curves, or zigzag lines. As written, the program produces point plots in a standard format. Normally, the nuclide symbol is drawn above the plot. Also, whenever a data set is plotted in POINT mode, the reaction and reference are drawn in the upper right-hand corner of the plot. Two control cards are provided for altering the legend. Provisions are made, however, to modify this format both through the use of plot control cards as well as by entering the desired changes for specific plot parameters which control the format used for a given plot. An arbitrary number of data sets may be plotted. Plotting may be done on the printer, the SC 4020, or the Calcomp. It is recommended that a printer plot be made on the slow printer.

A. Program Calling and Post-Processors

The plot program is called by the statement:

@ADD,P PF.PPLOT

A printer plot may be created on the slow printer by also calling:

@ADD,P PF.PRINTR

The normal sequence of cards is:

@ADD,P PF.PPLOT
[control cards]
\$\$PARMS
\$ Parameter Specifications
{ (only if needed)
\$\$END
[data sets]
@ADD,P PF.PRINTR (if printer plot is desired)
@MSG,W [user's account number], WRITE ENABLE REEL [user's reel number]
@ASG,TMJ 9.,8C,[user's reel number]W
@CLOSE 9.
@XQT NBS*CALCMP.

B. Plot Control Cards

General

PPLOT is controlled by a set of control cards. On all of these cards, a dollar sign must appear in column one. The control cards include:

Controls	
\$CURVE	The program normally plots data points. This card switches to a curve-tracing mode.
\$LINES	This card switches to a zigzag line tracing mode. (This is also useful for drawing histogram bar graphs.)
\$POINT	This card returns the program to point plotting mode.
\$CPLOT	The program will stay in CPLOT mode until a \$FRAME card is encountered. While in CPLOT mode:
	-plots are 12" x 9.5"
	-the nuclide ID is suppressed
	-each data set is plotted on a new frame
,	-all these frames are drawn to the same scale
	-the data sets are plotted as points connected by zigzag lines

\$SMALL

A special control card to plot small frames. This card causes a 4 x 2.5 in. frame to be plotted. Two such small frames will fit side-by-side on 40% reduction paper. Or, a small frame may be pasted onto a regular frame as an insert. The effect of SMALL persists until a FRAME card is encountered.

\$FRAME

This card marks the beginning of a new frame. The program returns to POINT mode.

Legend Controls

\$LABEL

\$PPLOT

Anything punched in card columns 7 through 24 of this card is written as a single line into the plot legend.

This card causes the current frame to be repeated (re-drawn) without any annotation. The primary use of this card is to plot graphs to be sent to a draftsman for lettering. If entered as the first card of a frame, \$PPLOT will cause a "stripped" frame to be plotted. If entered as the last control card of a frame, two plots will be drawn, one with annotation and one without.

Data Modification Controls

The energies and/or cross section values of data sets may be renormalized by the control cards:

by the given value.

\$MUL E[value]	Multiplies the energies of the next data set by the given floating-point value.	
\$MUL S[value]	Multiplies the cross sections of the next data set	

Similarly, offsets can be added to the data by:

\$ADD	E[value]		Adds	the	value	to	the	energi	ies	of	the	next	data	set.
\$ADD	S[value]	•	Adds set.	the	value	to	the	cross	sec	tiò	ns •	of th	e nex	t [.] data

All four of the above manipulate only the next data set. If used in combination, the multiplication is done first. All values are given as floating-point numbers which must start immediately after the E or S (i.e., no space).

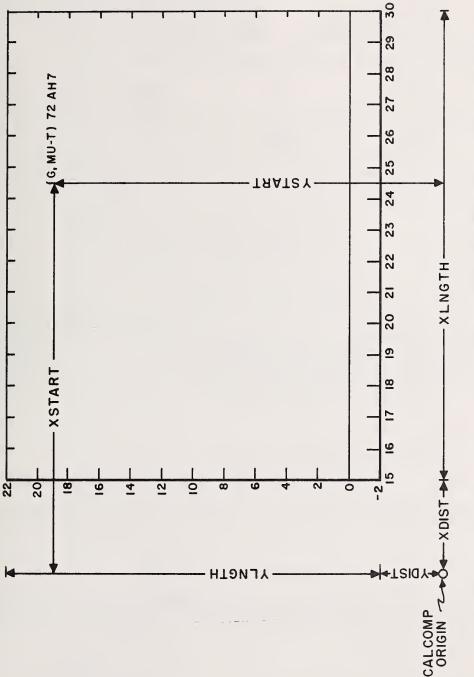
C. Parameters and Defaults

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PPLOT does not require any plot parameters to be specified. The normal plot constants are:

XDIST = 1.25 YDIST = 1.25 XLNGTH = 9.25 YLNGTH = 6.00 FONTB = .09375

-FONT is plot symbol size. .09375 = 3/32 in.



Definition of Plot Parameters and Variables. All distances are measured in inches from an origin on the plotter. XDECPL and YDECPL give the number of places after the decimal point to be carried on the axis labels. SYMBOL is used to specify a particular CALCOMP font used to represent data points on the graph. For the graph above, the other plot variables have the following values: XDOWN=15., XUP=30., XDIV=15., XDECPL=0., YDOWN=-2., YUP=22., YDIV=12., and YDECPL=0.

FONTH = .09375	
CHARB = 0.1875	-CHAR is legend and numeric symbol size.
CHARH = 0.1875	0.1875 = 3/16 in.
SCALB = 0.15625	-SCAL is axis label symbol size.
SCALH = 0.15625	0.15625 = 5/32 in.
XLBL = PHOTON ENERGY (MEV)	-If only one data set is plotted, XLBL and
YLBL = CROSS SECTION (MB)	YLBL are copied from the label cards of the data set.

The plot variables are normally calculated from the data. They include

XDOWN	YDOWN	SYMBOL
XUP	YUP	XSTART
XDIV	YDIV	YSTART
XDECPL	YDECPL	

The various plot parameters and variables are defined in the figure given on p. 21.

The plot control switches, and defaults, are:

RULE = 1	Set to zero to inhibit upper right legend.
NIOP = 1	Set to zero to inhibit nuclide ID.
MOVE = 1	Set to zero to inhibit frame advance.
RECALC = 0	Set to 1 to re-calculate XDIV, YDIV, XDECPL, YDECPL, XSTART, and YSTART.

Any and all of these parameters (in fact, the entire SPECS array) can be modified by means of the \$\$PARMS cards. The constants and variables are meant to be changed. However, it is recommended that the casual user leave the plot switches alone.

Parameters are entered in FORTRAN "NAMELIST" format. That is, you punch the parameter name, an equals sign, the numeric value, and a comma.

Example:

\$\$PARMS
\$ XDOWN=10.,XUP=40.,XDIV=4.,XDECPL=0.,
\$\$END

Don't forget the dollar signs in column one! All parameters return to their default values when "\$FRAME" is encountered.

D. Examples:

Actual use of PPLOT is best illustrated by a few examples.

1. To plot a $(\gamma, sn),$ $(\gamma, 2n),$ and (γ, p) graph in a form ready for the draftsman, use:

@ADD,P PF.PPLOT
[(γ ,sn) data]
[(γ ,2n) data]
[(γ ,p) data]

\$CURVE
[(γ,sn) curve]
[(γ,2n) curve]
[(γ,p) curve]
\$PPLOT
@ADD,P PF.PRINTR
@MSG,W [user's account number], WRITE ENABLE REEL [user's reel number]
@ASG,TMJ 9.,8C,[user's reel number]W
@CLOSE 9.
@XQT NBS*CALCMP.

This will give both a printer plot and a tape for the Calcomp. To do the same thing, but with a nine-inch, rather than a six-inch plot height, use:

```
@ADD,P PF.PPLOT
$$PARMS
$ YLNGTH=9.,
$$END
[(\gamma,sn), (\gamma,2n), and (\gamma,p) data sets]
$CURVE
[(\gamma,sn), (\gamma,2n), and (\gamma,p) curves]
$PPLOT
@ADD,P PF.PRINTR
etc.
```

2. To plot a $(\gamma, \mathbf{x}n)$ cross section and a (γ, p) cross section on separate frames, use:

```
@ADD,P PF.PPLOT
[(\gamma, xn) points]
$CURVE
[(\gamma, xn) curve]
$FRAME
[(\gamma, p) points]
$CURVE
[(\gamma, p) curve]
@ADD,P PF.PRINTR
etc.
```

3. To plot a (γ, p) cross section and a (γ, μ_t) cross section on separate frames, with the intention of pasting the (γ, μ_t) graph in the upper right-hand corner of the (γ, p) graph as an insert, and also assuming the (γ, μ_t) data consist of bar graph corners, use:

@ADD,P PF.PPLOT
\$\$PARMS
\$ XSTART=1.5, (this moves the legend to the upper left corner)
\$\$END

```
[(γ,p) points]

$CURVE

[(γ,p) curve]

$PPLOT

$FRAME

$SMALL

$LABEL (G,MU-T) 64ER2

$LINES

[(γ,μ<sub>t</sub>) data]

$PPLOT

@ADD,P PF.PRINTR

etc.
```

4. To obtain a set of comparison plots, use:

```
@ADD,P PF.PPLOT

$CPLOT

[all (\gamma,n), (\gamma,sn), (\gamma,xn), (\gamma,\mu_{t}) data]

$FRAME

$CPLOT

[all (\gamma,p) and (\gamma,xp) data]

$FRAME

$CPLOT

[all (\gamma,\mu_{t}) data]

$FRAME

$CPLOT

[all (\gamma,\alpha) data]

etc.
```

SPCDST

This deck creates an index table of spectrum and angular distribution papers. Use is made of the Photonuclear Data Index which must be in mass storage in a file called "DC*INDEX.". The output table is placed in a file called "BF.", where it can be listed by LIST. The user enters:

- 1) the nuclide
- 2) the references and reactions of SPC entries
- 3) DST
- 4) the references and reactions of DST entries
- 5) @EOF

The references must start in Column 1. The user should leave at least one space after the reference as a separator. The reactions do not need parentheses.

Calling sequences and example:

 @ASG,T
 BF.

 @ADD,P
 PF.SPCDST

 5B
 10

 68SH6
 G,P

 DST

 68SH6
 G,P

 63FU3
 P,G

 65PA1
 HE,G

 68L11
 HE,G

 @EOF

 @ADD,P
 PF.LIST

NBS-114A (REV. 7-73)				
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4. TITLE AND SUBTITLE			5. Publicatio	on Date
The NIDA Comp	Febru	ary 1976		
(Photonuclear	iter Program Package Data Center)		6. Performin	g Organization Code
7. AUTHÓR(S) H. J. Vander M	folen and Henry M. Gerstenbe	erg	8. Performing	g Organ, Report No.
9. PERFORMING ORGANIZAT				Task/Work Unit No. 410232
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	nce Foundation through the N Lences-National Research Com		F	inal
-	Nuclear Science	·····,	14. Sponsorin	ng Agency Code
15. SUPPLEMENTARY NOTES			<u> </u>	
bibliography or literature su The Photonucle mass storage on the described. Detaile library to analyze, tabular and graphic data. NIRA is the	ear Data Center's NIRA libra e National Bureau of Standan ed instructions are given (w , evaluate, synthesize, and cal presentations of digital acronym for Nuclear Informa	ary of programs, cd's central com with examples), produce for pub l photonuclear re ation Research As	executabl puter faci for the us lication, eaction cr ssociate.	e from lity, is e of the camera-ready oss-section
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DIMENSIONS/NBS (formerly Technical News Bulletin)—This monthly magazine is published to inform scientists, engineers, businessmen, industry, teachers, students, and consumers of the latest advances in science and technology, with primary emphasis on the work at NBS. The magazine highlights and reviews such issues as energy research, fire protection, building technology, metric conversion, pollution abatement, health and safety, and consumer product performance. In addition, it reports the results of Bureau programs in measurement standards and techniques, properties of matter and materials, engineering standards and services, instrumentation, and automatic data processing.

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Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

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NOTE: At present the principal publication outlet for these data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St. N. W., Wash. D. C. 20056.

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