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===== Sixpak
PROGRAM SIXPAK Sixpak
===== Sixpak
VERSION 92-1 (JANUARY 1992) Sixpak
VERSION 92-2 (FEBRUARY 1992) *INCREASED CORE ALLOCATION TO ACCOMMODATE JEF AND EFF EVALUATIONS. Sixpak
VERSION 92-3 (APRIL 1992) *ADDED ADDITIONAL DATA TESTS. Sixpak
VERSION 92-4 (SEPT. 1992) *CORRECTED KALBACH-MANN CALCULATIONS. Sixpak
*FOR PHOTON PRODUCTION OUTPUT MF=12 Sixpak
(MULTIPLICITY), MF=14 (ISOTROPIC Sixpak
ANGULAR DISTRIBUTIONS) AND MF=15 Sixpak
(SPECTRA) - PREVIOUSLY ONLY MF=15. Sixpak
*FIRST ORDER CORRECTIONS TRANSFORMING Sixpak
CENTER-OF-MASS SPECTRA TO LAB SYSTEM Sixpak
FOR OUTPUT IN MF=5 Sixpak
*CORRECTED ISOTROPIC ANGULAR Sixpak
DISTRIBUTION FLAG (LI) Sixpak
VERSION 94-1 (JANUARY 1994) *VARIABLE ENDF/B INPUT DATA FILENAME TO ALLOW ACCESS TO FILE STRUCTURES (WARNING - INPUT PARAMETER FORMAT HAS BEEN CHANGED) Sixpak
*CLOSE ALL FILES BEFORE TERMINATING (SEE, SUBROUTINE ENDIT) Sixpak
*INCREASED MAXIMUM TABLE SIZE FROM 2000 TO 6000. Sixpak
VERSION 96-1 (JANUARY 1996) *COMPLETE RE-WRITE Sixpak
*IMPROVED COMPUTER INDEPENDENCE Sixpak
*ALL DOUBLE PRECISION Sixpak
*ON SCREEN OUTPUT Sixpak
*UNIFORM TREATMENT OF ENDF/B I/O Sixpak
*IMPROVED OUTPUT PRECISION Sixpak
VERSION 99-1 (MARCH 1999) *CORRECTED CHARACTER TO FLOATING POINT READ FOR MORE DIGITS Sixpak
*UPDATED TEST FOR ENDF/B FORMAT Sixpak
VERSION BASED ON RECENT FORMAT CHANGE Sixpak
*GENERAL IMPROVEMENTS BASED ON USER FEEDBACK Sixpak
VERSION 99-2 (JUNE 1999) *ASSUME ENDF/B-VI, NOT V, IF MISSING MF=1, MT-451. Sixpak
VERS. 2000-1 (FEBRUARY 2000) *GENERAL IMPROVEMENTS BASED ON USER FEEDBACK Sixpak
VERS. 2002-1 (JANUARY 2002) *CORRECTED ANGULAR DISTRIBUTION (MF=4) OUTPUT TO INSURE USED FIELDS ARE 0 Sixpak
(MAY 2002) *OPTIONAL INPUT PARAMETERS Sixpak
(NOV. 2002) *EXTENDED TO ALLOW CHARGED PARTICLE ANGULAR DISTRIBUTION IN MF=4 - Sixpak
WARNING - STRICTLY SPEAKING THIS IS NOT LEGAL, SINCE MF=4 IS SUPPOSED TO BE USED ONLY FOR NEUTRON ANGULAR DISTRIBUTIONS - BUT WHERE MT MAKES IT OBVIOUS THAT THE OUTGOING PARTICLE IS NOT A NEUTRON HOPEFULLY IT WILL NOT CAUSE A PROBLEM IF MF=4 IS USED FOR CHARGED PARTICLES. Sixpak
VERS. 2004-1 (MARCH 2004) *ADDED INCLUDE FOR COMMON Sixpak
*INCREASED MAXIMUM TABLE SIZE FROM 6,000 TO 12,000. Sixpak
*ADDED DUMMY A FOR ELEMENTS Sixpak
*CORRECTED OUTPUT INTERPOLATION LAWS Sixpak
VERS. 2007-1 (JAN. 2007) *CHECKED AGAINST ALL ENDF/B-VII. Sixpak
*INCREASED MAXIMUM TABLE SIZE FROM 12,000 TO 120,000. Sixpak
VERS. 2007-2 (DEC. 2007) *72 CHARACTER FILE NAMES. Sixpak
VERS. 2010-1 (Apr. 2010) *General update based on user feedback Sixpak
VERS. 2011-1 (May 2011) *Added MF/MT=9/5 yield output starting from MF/MT=6/5 distributions. Sixpak
*Increased maximum Legendre order from 30 to 1,000 - WARNING - using more than 30 results in NONSENSE = NOISE!! Sixpak
VERS. 2012-1 (Oct. 2012) *Increased max. point count to 500,000 Sixpak

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EXACTLY THE FORM NEEDED FOR USE IN PROCESSING CODES. Sixpak
Sixpak
THE AUTHOR THANKS CHRIS DEAN (WINFRITH) FOR POINTING OUT ERRORS Sixpak
IN THE EARLIER TREATMENT OF THE KALBACH-MANN FORMALISM AND IN Sixpak
THE DEFINITION OF THE ISOTROPIC ANGULAR DISTRIBUTION FLAG (LI). Sixpak
Sixpak
AUTHORS MESSAGE Sixpak
===== Sixpak
THE COMMENTS BELOW SHOULD BE CONSIDERED THE LATEST DOCUMENTATION Sixpak
INCLUDING ALL RECENT IMPROVEMENTS. PLEASE READ ALL OF THESE Sixpak
COMMENTS BEFORE IMPLEMENTING AND USING THESE CODES. Sixpak
Sixpak
AT THE PRESENT TIME WE ARE ATTEMPTING TO DEVELOP A SET OF COMPUTER Sixpak
INDEPENDENT PROGRAMS THAT CAN EASILY BE IMPLEMENTED ON ANY ONE Sixpak
OF A WIDE VARIETY OF COMPUTERS. IN ORDER TO ASSIST IN THIS PROJECT Sixpak
IT WOULD BE APPRECIATED IF YOU WOULD NOTIFY THE AUTHOR OF ANY Sixpak
COMPILER DIAGNOSTICS, OPERATING PROBLEMS OR SUGGESTIONS ON HOW TO Sixpak
IMPROVE THIS PROGRAM. HOPEFULLY, IN THIS WAY FUTURE VERSIONS OF Sixpak
THIS PROGRAM WILL BE COMPLETELY COMPATIBLE FOR USE ON YOUR Sixpak
COMPUTER. Sixpak
Sixpak
PURPOSE Sixpak
===== Sixpak
1) CHECK ALL DOUBLE-DIFFERENTIAL DATA (MF=6) Sixpak
Sixpak
2) OUTPUT EQUIVALENT MF = 4, 5, 12, 14 AND 15 DATA. Sixpak
Sixpak
DATA CHECKING Sixpak
===== Sixpak
ALL OF THE ENDF/B-VI MF=6 DATA IS CHECKED - FOR DETAILS SEE BELOW. Sixpak
Sixpak
THE MF=6 DATA IS NOT CORRECTED AND OUTPUT IN THE ENDF/B FORMAT. Sixpak
IT IS MERELY CHECKED. IF ERRORS ARE FOUND IT IS UP TO THE USER Sixpak
TO TAKE CORRECTIVE ACTION ON THE MF=6 DATA. Sixpak
Sixpak
IN CONTRAST WHEN PROBLEMS ARE FOUND IN DATA WHICH WILL BE OUTPUT Sixpak
IN THE ENDF/B FORMAT (MF=4, 5, 12, 14 AND 15), WHENEVER POSSIBLE Sixpak
CORRECTIVE ACTION WILL BE TAKEN. Sixpak
Sixpak
FURTHER CHECKS AND CORRECTIONS Sixpak
===== Sixpak
ONCE THE DATA HAS BEEN OUTPUT IN MF = 4, 5, 12, 14 AND 15 FORMATS Sixpak
FURTHER CORRECTIVE ACTION CAN BE TAKEN AS FOLLOWS, Sixpak
Sixpak
PROGRAM LEGEND Sixpak
===== Sixpak
CAN BE USED TO CORRECT ANGULAR DISTRIBUTIONS WHICH ARE NEGATIVE, Sixpak
TO CONVERT FROM LEGENDRE COEFFICIENTS TO TABULATED ANGULAR Sixpak
DISTRIBUTIONS AND GENERALLY PERFORM MORE EXTENSIVE TESTS OF Sixpak
ALL MF=4 DATA. Sixpak
Sixpak
PROGRAM EVALPLOT Sixpak
===== Sixpak
VERSION 92-1 AND LATER VERSIONS CAN PLOT ALL OF THE MF=4, 5 AND 15 Sixpak
DATA OUTPUT BY THIS CODE. EARLIER VERSIONS CAN PLOT MF=4 AND 5. Sixpak
GRAPHICS IS AN EXCELLENT WAY TO CHECK THIS DATA. Sixpak
Sixpak
PROGRAM PLOTTAB Sixpak
===== Sixpak
THIS IS A GENERAL PLOTTING PROGRAM AND THERE IS AN INTERFACE IN Sixpak
THIS CODE TO PRODUCE OUTPUT FOR ANY MF=6 DATA IN THE PLOTTAB Sixpak
INPUT FORMAT. THIS PROGRAM CAN BE USED TO CHECK ALL OF THE MF=6 Sixpak
DATA AS WELL AS THE EQUIVALENT MF=4, 5, 12, 14 AND 15 DATA - AS Sixpak
WELL AS COMPARING THE ORIGINAL MF=6 AND EQUIVALENT DATA. Sixpak
Sixpak
DATA OUTPUT Sixpak
===== Sixpak
THE ENDF/B MF=4, 5, 12, 14 AND 15 FORMATS ONLY ALLOW FOR NEUTRONS Sixpak
INCIDENTS Sixpak
Sixpak
THE ENDF/B MF=4 AND 5 FORMATS ONLY ALLOW FOR NEUTRONS OUTGOING. Sixpak
Sixpak

BY INTEGRATING $G_0(E,EP)*F(E,EP,COS)$ OVER SECONDARY ENERGY (EP) TO DEFINE AN AVERAGE ANGULAR DISTRIBUTION, $F_0(E,COS)$.

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WHAT IS LOST IN THIS PROCESS IS THE CORRELATION BETWEEN EP AND COS SO THAT IN A TRANSPORT CALCULATION ALL MOMENTS OF THE FLUX WILL HAVE THE SAME SPECTRUM, $G_0(E,EP)$ AND EACH WILL BE EFFECTED BY THE AVERAGE ANGULAR DISTRIBUTION.

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FOR APPLICATIONS TO HIGH ENERGY FUSION APPLICATIONS CORRELATED DATA SHOULD BE USED. HOWEVER, FOR LOWER ENERGY APPLICATIONS, SUCH AS FISSION REACTORS, IT SHOULD BE ADEQUATE TO USE THE UNCORRELATED DATA - IN THIS CASE THE MOST IMPORTANT EFFECT WILL BE THE OVERALL NEUTRON MULTIPLICATION AND SPECTRUM.

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AN IMPORTANT CONSIDERATION IN DESIGNING THIS PROGRAM IS THAT MANY COMPUTER CODES - DATA PROCESSING AND TRANSPORT CODES - CANNOT USE THE CORRELATED (MF=6) DATA - NOR ARE THEY INTENDED FOR HIGH ENERGY USE. FOR THESE CODES THE UNCORRELATED DATA PRODUCED BY THIS CODE SHOULD BE ADEQUATE TO MEET THEIR NEEDS.

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WARNING - IT CANNOT BE STRESSED ENOUGH THAT THE OUTPUT OF THIS CODE SHOULD ONLY BE USED FOR LOW ENERGY APPLICATIONS - FAILURE TO HEED THIS WARNING CAN LEAD TO COMPLETELY UNRELIABLE RESULTS.

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ENDF/B FORMAT

THIS PROGRAM ONLY USES THE ENDF/B BCD OR CARD IMAGE FORMAT (AS OPPOSED TO THE BINARY FORMAT) AND CAN HANDLE DATA IN ANY VERSION OF THE ENDF/B FORMAT (I.E., ENDF/B-I, II, III, IV, V OR VI FORMAT).

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IT IS ASSUMED THAT THE DATA IS CORRECTLY CODED IN THE ENDF/B FORMAT AND NO ERROR CHECKING IS PERFORMED. IN PARTICULAR IT IS ASSUMED THAT THE MAT, MF AND MT ON EACH LINE IS CORRECT. SEQUENCE NUMBERS (COLUMNS 76-80) ARE IGNORED ON INPUT, BUT WILL BE CORRECTLY OUTPUT ON ALL LINES. THE FORMAT OF SECTION MF=1, MT=451 AND ALL SECTIONS OF MF=6 MUST BE CORRECT. THE PROGRAM SKIPS ALL OTHER SECTIONS OF DATA AND AS SUCH IS INSENSITIVE TO THE FORMAT OF ALL OTHER SECTIONS.

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CONTENTS OF OUTPUT

5 ENDF/B FORMATTED OUTPUT FILES ARE PRODUCED FOR NEUTRON INCIDENT DATA,

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- 1) ENDFB.MF4 - ANGULAR DISTRIBUTIONS AND LEGENDRE COEFFICIENTS FOR NEUTRONS
- 2) ENDFB.MF5 - TABULATED NEUTRON ENERGY SPECTRA
- 3) ENDFB.M12 - PHOTON EMISSION MULTIPLICITY
- 4) ENDFB.M14 - PHOTON EMISSION ANGULAR DISTRIBUTIONS (ALWAYS ISOTROPIC)
- 5) ENDFB.M15 - TABULATED PHOTON EMISSION SPECTRA

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EMITTED PARTICLE YIELD

NEUTRONS

IN MF=6 THE YIELD FOR EACH REACTION IS THE ACTUAL MULTIPLICITY OF THE REACTION, E.G., $(N,2N) = 2$. IN USING MF=4 AND 5 DATA THE ENDF/B CONVENTION IS THAT THE MULTIPLICITY IS IMPLIED BY THE MT NUMBER, E.G., $MT=16 = (N,2N) = 2$.

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THE ONLY EXCEPTION IN ENDF/B-VI IS $MT=201 =$ TOTAL NEUTRON PRODUCTION WHERE AN ACTUAL ENERGY DEPENDENT YIELD IS INCLUDED IN MF=6. HOWEVER, IN THIS CASE THE MF=3 CROSS SECTION INCLUDES THE MULTIPLICITY (S. PEARLSTEIN, PRIVATE COMMUNICATION, JAN. 1992), $SIG(MT=201) = 2*SIG(N,2N) + 3*SIG(N,3N) \dots$ ETC.

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SO THAT FOR ALL ENDF/B-VI DATA AS OF JANUARY 1992 THE MF=4 AND 5 DATA OUTPUT BY THIS CODE CAN BE USED IN CONJUNCTION WITH THE MF=3 CROSS SECTIONS - WITHOUT ANY REFERENCE TO THE MF=6 YIELD.

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$V(LAB) * \cos(LAB) = V(MM) + V(CM) * \cos(CM)$

$\cos(LAB) = [V(MM) + V(CM) * \cos(CM)] / V(LAB)$

$\cos(LAB) = \frac{[V(MM) + V(CM) * \cos(CM)]}{\sqrt{V(MM)^2 + V(CM)^2 + 2 * \cos(CM) * V(MM) * V(CM)}}$

OR COS(CM) FROM THE RELATIONSHIP,

$V(CM) * \cos(CM) = V(LAB) * \cos(LAB) - V(MM)$

$\cos(CM) = [V(LAB) * \cos(LAB) - V(MM)] / V(CM)$

$\cos(CM) = \frac{[V(LAB) * \cos(LAB) - V(MM)]}{\sqrt{V(LAB)^2 + V(CM)^2 - 2 * \cos(LAB) * V(LAB) * V(MM)}}$

THE JACOBIAN CAN BE DEFINED FROM,

$V(LAB) * \cos(LAB) = V(MM) + V(CM) * \cos(CM)$

$J = D[\cos(CM)] / D[\cos(LAB)] = V(LAB) / V(CM)$
 $= \sqrt{EP(LAB)} / EP(CM)$

WITH THESE DEFINITIONS OF EP(LAB) AND COS(LAB) IN TERMS OF E(MM), EP(CM) AND COS(CM) IT IS POSSIBLE TO PERFORM A POINT-BY-POINT TRANSFORMATION OF DISTRIBUTIONS FROM THE CM TO LAB SYSTEM USING THESE DEFINITIONS - OR IF WE WISHED WE COULD PERFORM THE REVERSE TRANSFORMATION USING THE ABOVE RELATIONSHIPS AND THE IDENTITY,

$F(E, EP(LAB), \cos(LAB)) * D(\cos(LAB)) = F(E, EP(CM), \cos(CM)) * D(\cos(CM))$

THIS IS NOT WHAT WILL BE DONE HERE, SINCE WE WILL ONLY BE INTERESTED IN THE ZEROth ORDER MOMENTS OF THESE DISTRIBUTIONS, BUT WE WILL BE INTERESTED IN DEFINING THOSE MOMENTS IN THE LAB SYSTEM IN TERMS OF MF=6 SPECTRA GIVEN IN THE CM SYSTEM USING,

$F(E, EP(LAB), \cos(LAB)) = F(E, EP(CM), \cos(CM)) * J$

THE LIMITS OF EP(LAB) ARE DEFINED BY SETTING COS(CM) = +1 OR -1,

$EP(LAB) = (\sqrt{EP(CM)} + \sqrt{E(MM)})^2$ FOR COS(CM) = +1
 $= (\sqrt{EP(CM)} - \sqrt{E(MM)})^2$ FOR COS(CM) = -1

IN THIS FORM WE CAN SEE THAT AS LONG AS THE SECONDARY ENERGY IN THE CENTER-OF-MASS SYSTEM, EP(CM), IS MUCH LARGER THAN THE ENERGY OF THE CENTER-OF-MASS, E(MM), THE CENTER-OF-MASS AND LAB ENERGIES WILL BE ALMOST EQUAL - SIMILARLY FOR THE COSINE, IN THIS CASE COS(LAB) AND COS(CM) WILL BE ALMOST EQUAL - HOWEVER, FOR THE MF=6 DATA WE CANNOT ASSUME THAT THIS IS TRUE.

TO FIRST ORDER THE ANGULAR DEPENDENCE CAN BE IGNORED,

$EP(LAB) = E(MM) + EP(CM)$

ALL THIS SAYS IS THAT TO FIRST ORDER THE EFFECT OF TRANSFORMING FROM THE CM TO LAB SYSTEM IS TO INCREASE THE ENERGY OF THE EMITTED PARTICLE IN THE CENTER-OF-MASS SYSTEM BY THE ENERGY OF THE CENTER-OF-MASS TO DEFINE THE LAB ENERGY.

NOT ONLY THE ENERGY, BUT ALSO THE SPECTRA MUST BE TRANSFORMED. STARTING FROM THE DOUBLE DIFFERENTIAL DATA IN THE LAB SYSTEM, $F(E, EP, \cos(LAB))$, WE CAN DEFINE THE LAB SCALAR SPECTRUM AS,

$G_0(E, EP) = \int F(E, EP, \cos(LAB)) * D(\cos(LAB))$

THIS IS THE NORMAL CALCULATION DEFINED ABOVE AND USED FOR DATA GIVEN IN THE LAB SYSTEM.

STARTING FROM DATA IN THE CENTER OF MASS SYSTEM $F(E, EP, \cos(CM))$,

OUTPUT FILES		Sixpak
=====		Sixpak
UNIT DESCRIPTION		Sixpak
-----		Sixpak
3 OUTPUT REPORT (BCD - 120 CHARACTERS/RECORD)		Sixpak
11 ENDF/B DATA MF=4 (BCD - 80 CHARACTERS/RECORD)		Sixpak
12 ENDF/B DATA MF=5 (BCD - 80 CHARACTERS/RECORD)		Sixpak
14 ENDF/B DATA MF=15 (BCD - 80 CHARACTERS/RECORD)		Sixpak
17 ENDF/B DATA MF=12 (BCD - 80 CHARACTERS/RECORD)		Sixpak
18 ENDF/B DATA MF=14 (BCD - 80 CHARACTERS/RECORD)		Sixpak
15 PLOTTAB INPUT PARAMETERS (BCD - 80 CHARACTERS/RECORD)		Sixpak
16 PLOTTAB FORMATTED OUTPUT (BCD - 80 CHARACTERS/RECORD)		Sixpak
SCRATCH FILES		Sixpak
=====		Sixpak
NONE		Sixpak
OPTIONAL STANDARD FILE NAMES (SEE SUBROUTINE FILIO1 AND FILIO2)		Sixpak
=====		Sixpak
UNIT FILE NAME		Sixpak
-----		Sixpak
2 SIXPAK.INP		Sixpak
3 SIXPAK.LST		Sixpak
10 ENDFB.IN		Sixpak
11 ENDFB.MF4		Sixpak
12 ENDFB.MF5		Sixpak
14 ENDFB.M15		Sixpak
17 ENDFB.M12		Sixpak
18 ENDFB.M14		Sixpak
15 PLOTTAB.INP		Sixpak
16 PLOTTAB.CUR		Sixpak
INPUT PARAMETERS		Sixpak
=====		Sixpak
LINE COLS. DESCRIPTION		Sixpak
-----		Sixpak
1 1-72 ENDF/B INPUT DATA FILENAME		Sixpak
(STANDARD OPTION = ENDFB.IN)		Sixpak
2-N 1-6 MINIMUM MAT FOR REQUESTED RANGE		Sixpak
9-11 MINIMUM MT FOR REQUESTED RANGE		Sixpak
12-17 MAXIMUM MAT FOR REQUESTED RANGE		Sixpak
20-22 MAXIMUM MT FOR REQUESTED RANGE		Sixpak
LEAVE THE DEFINITION OF THE FILENAME BLANK - THE PROGRAM WILL		Sixpak
THEN USE THE STANDARD FILENAME (ENDFB.IN).		Sixpak
UP TO 100 MAT/MT RANGES MAY BE SPECIFIED. THE LIST OF RANGES IS		Sixpak
TERMINATED BY A BLANK LINE. IF THE FIRST INPUT LINE IS COMPLETELY		Sixpak
BLANK ALL DATA WILL BE PROCESSED.		Sixpak
EXAMPLE INPUT NO. 1		Sixpak
-----		Sixpak
PROCESS ALL MF=6 DATA ON AN ENDF/B TAPE. USE THE STANDARD INPUT		Sixpak
DATA FILENAME ENDFB.IN IN THIS CASE THE USER CAN EITHER EXPLICITLY		Sixpak
SPECIFY THE FILENAME AND MAT/MT RANGE BY THE FOLLOWING 2 INPUT		Sixpak
LINES,		Sixpak
ENDFB.IN		Sixpak
1 1 9999 999		Sixpak
(BLANK LINE, TERMINATES REQUEST LIST)		Sixpak
OR BY INPUTTING 2 BLANK LINE = PROCESS EVERYTHING.		Sixpak
EXAMPLE INPUT NO. 2		Sixpak
-----		Sixpak
PROCESS BE-9, MAT=425, MT=16. READ THE DATA FROM ENDFB6\BE9.		Sixpak
IN THIS CASE THE FOLLOWING 3 INPUT LINES ARE REQUIRED,		Sixpak
ENDFB6\BE9		Sixpak

425 16 425 16

(BLANK LINE, TERMINATES REQUEST LIST)

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EXAMPLE INPUT NO. 3

PROCESS ALL MT=16 (N,2N) DATA. THIS CAN BE DONE BY SPECIFYING THE
MAXIMUM MAT RANGE = 1 TO 9999, AND MT=16 FOR THE MINIMUM AND
MAXIMUM MT RANGE. READ THE DATA FROM ENDFB6\K300. IN THIS CASE
CASE THE FOLLOWING 3 INPUT LINES ARE REQUIRED,

ENDFB6\K300

1 16 9999 16

(BLANK LINE, TERMINATES REQUEST LIST)

=====