

NJOY/PANINI-04  
19 May 1994

To: NJOY Users

Please find enclosed herewith a few notes on NJOY and SMILER as provided by Gian-carlo Panini, ENEA Bologna. These are provided to you so that you are aware of some problems he has encountered and the corrective actions he is proposing. The corrections proposed are NOT OFFICIAL and are sent to you for information only.

Best regards

Enrico Sartori

#####

MAIL FROM:<BPANI1@IBOENEA.BITNET>  
RCPT TO:<jew@ornl.gov>  
DATE: May 18,1993  
TO:<jew@ornl.gov>  
FROM:<BPANI1@IBOENEA.BITNET>

Copy of message to R.McFarlane

SUBJECT: Problem with photon production matrices with constant spectrum at low energy groups.

Dear Bob,

I confirm that the discrepancy I observed in the output of NJOY 91.38 disappears in the 91.91 version. I recall you here the terms of the problem as I mentioned yesterday by telephone.

I processed MAT 2425 Cr-50 from JEF 2.2 in the standard VITAMIN-J 175n+42g groups, I got no errors and I translated it to AMPX Master Interface Library by means of SMILER (included in AMPX-77). By means of a RADE run I found an error in SMILER in that it does not recognize the constant spectrum feature - described in Section F of GROUPE report - with the format described on page 38 of the same report. I corrected the error - and I am being to send the correction to John White at RSIC - and RADE then revealed an inconsistency in GENDF that you may check by yourself. Look at the following and note the cross section value of MT=102 for the first group (1.489E+01):

THIS IS THE OUTPUT FOR MT=102 - SAME RESULTS FOR BOTH VERSIONS! 139.5S  
=====139.5S  
GROUP CONSTANTS AT T=2.936E+02 DEG K 138.5S  
FOR MF 3 AND MT102 (N,G) CROSS SECTION.

ENRGY GROUP CONSTANTS AT  
GROUP INFINITE DILUTION

1 1.489E+01  
2 7.144E+00  
3 3.709E+00  
4 3.272E+00  
5 2.887E+00  
.....

Note the value of the yield from MF=12, MT=102 of the source JEF data below 1 keV, i.e. 2.822610+0

THIS IS MF=12, MT=102 FOR CR-50 MAT=2425 FROM JEF 2.2 0 0  
=====139.5S  
2.405000+4 4.951690+1 1 0 1 0242512102 2121  
0.000000+0 0.000000+0 0 1 1 69242512102 2122  
69 2 242512102 2123  
1.000000-5 2.822610+0 1.000000+3 2.822610+0 3.000000+3 2.803220+0242512102 2124  
5.000000+3 2.789470+0 8.000000+3 2.774120+0 1.000000+4 2.767620+0242512102 2125  
3.000000+4 2.734600+0 5.000000+4 2.713920+0 7.999990+4 2.701220+0242512102 2126

1.000000+5	2.699130+0	2.000000+5	2.705360+0	3.000000+5	2.716210+0242512102	2127
4.000000+5	2.727170+0	5.000000+5	2.738600+0	6.000000+5	2.749810+0242512102	2128
7.000000+5	2.759920+0	8.000000+5	2.771600+0	9.000000+5	2.787510+0242512102	2129
1.000000+6	2.803590+0	1.300000+6	2.837350+0	1.500000+6	2.858890+0242512102	2130
1.800000+6	2.887070+0	2.000000+6	2.909490+0	2.300000+6	2.939210+0242512102	2131
2.420000+6	2.951110+0	2.500000+6	2.960500+0	2.700000+6	2.976460+0242512102	2132
2.800000+6	2.977740+0	2.983600+6	2.992290+0	3.000000+6	2.995000+0242512102	2133
3.180000+6	3.011970+0	3.225000+6	3.016380+0	3.230000+6	3.015790+0242512102	2134
3.500000+6	3.040600+0	3.667000+6	3.054370+0	3.668000+6	3.054810+0242512102	2135
3.690000+6	3.057680+0	3.703400+6	3.058970+0	3.770000+6	3.063160+0242512102	2136
3.930000+6	3.069720+0	3.980000+6	3.072740+0	4.000000+6	3.073030+0242512102	2137
4.017500+6	3.075490+0	4.120000+6	3.081730+0	4.500000+6	3.076990+0242512102	2138
4.850000+6	3.092400+0	5.000000+6	3.098630+0	5.500000+6	3.117720+0242512102	2139
5.800000+6	3.111750+0	6.000000+6	3.120180+0	6.200000+6	3.127370+0242512102	2140
6.500000+6	3.105690+0	7.000000+6	3.113800+0	7.500000+6	3.123410+0242512102	2141
8.000000+6	3.130180+0	9.000000+6	3.195450+0	1.000000+7	3.225010+0242512102	2142
1.050000+7	3.267080+0	1.100000+7	3.314150+0	1.150000+7	3.354190+0242512102	2143
1.200000+7	3.389510+0	1.300000+7	3.481230+0	1.400000+7	3.554330+0242512102	2144
1.470000+7	3.593830+0	1.600000+7	3.702970+0	1.700000+7	3.793380+0242512102	2145
1.800000+7	3.893920+0	1.900000+7	3.990470+0	2.000000+7	4.031910+0242512102	2146
					242512 0	2147
					2425 0 0	2148

Note also the yield from MF=15, MT=102 is constant and is 1

THIS IS MF=15, MT=102 FOR CR-50 MAT=2425 FROM JEF 2.2 0 0  
 THE TWO LOWER ENERGY SPECTRUM ARE ONLY SHOWN AND ARE EQUAL. 0 0

=====139.5S					
2.405000+4	4.951690+1	0	0	1	0242515102 3038
0.000000+0	0.000000+0	0	1	1	2242515102 3039
2	2				242515102 3040
1.000000-5	1.000000+0	2.000000+7	1.000000+0		242515102 3041
0.000000+0	0.000000+0	0	0	1	69242515102 3042
69	2				242515102 3043
0.000000+0	1.000000-5	0	0	1	51242515102 3044
51	2				242515102 3045
0.000000+0	3.775280-7	2.500000+5	3.775280-7	2.500000+5	4.197450-9242515102 3046
5.000000+5	4.197450-9	5.000000+5	1.066750-6	7.500000+5	1.066750-6242515102 3047
7.500000+5	7.958490-8	1.000000+6	7.958490-8	1.000000+6	6.092720-8242515102 3048
1.250000+6	6.092720-8	1.250000+6	4.794600-8	1.500000+6	4.794600-8242515102 3049
1.500000+6	2.487690-8	1.750000+6	2.487690-8	1.750000+6	1.733470-7242515102 3050
2.000000+6	1.733470-7	2.000000+6	1.544260-7	2.250000+6	1.544260-7242515102 3051
2.250000+6	1.241210-7	2.500000+6	1.241210-7	2.500000+6	3.654580-8242515102 3052
2.750000+6	3.654580-8	2.750000+6	1.651780-7	3.000000+6	1.651780-7242515102 3053
3.000000+6	8.137690-8	3.250000+6	8.137690-8	3.250000+6	3.909670-8242515102 3054
3.500000+6	3.909670-8	3.500000+6	1.387200-7	3.750000+6	1.387200-7242515102 3055
3.750000+6	4.535810-8	4.000000+6	4.535810-8	4.000000+6	9.708300-8242515102 3056
4.250000+6	9.708300-8	4.250000+6	6.551260-8	4.500000+6	6.551260-8242515102 3057
4.500000+6	4.589570-8	4.750000+6	4.589570-8	4.750000+6	9.745200-8242515102 3058
5.000000+6	9.745200-8	5.000000+6	3.439020-8	6.000000+6	3.439020-8242515102 3059
6.000000+6	6.480110-8	7.000000+6	6.480110-8	7.000000+6	3.615580-8242515102 3060
8.000000+6	3.615580-8	8.000000+6	1.320270-7	9.000000+6	1.320270-7242515102 3061
9.000000+6	4.371820-9	9.262000+6	4.371820-9	9.262000+6	0.000000+0242515102 3062
0.000000+0	1.000000+3	0	0	1	51242515102 3063
51	2				242515102 3064
0.000000+0	3.775280-7	2.500000+5	3.775280-7	2.500000+5	4.197450-9242515102 3065
5.000000+5	4.197450-9	5.000000+5	1.066750-6	7.500000+5	1.066750-6242515102 3066
7.500000+5	7.958490-8	1.000000+6	7.958490-8	1.000000+6	6.092720-8242515102 3067
1.250000+6	6.092720-8	1.250000+6	4.794600-8	1.500000+6	4.794600-8242515102 3068
1.500000+6	2.487690-8	1.750000+6	2.487690-8	1.750000+6	1.733470-7242515102 3069
2.000000+6	1.733470-7	2.000000+6	1.544260-7	2.250000+6	1.544260-7242515102 3070
2.250000+6	1.241210-7	2.500000+6	1.241210-7	2.500000+6	3.654580-8242515102 3071
2.750000+6	3.654580-8	2.750000+6	1.651780-7	3.000000+6	1.651780-7242515102 3072
3.000000+6	8.137690-8	3.250000+6	8.137690-8	3.250000+6	3.909670-8242515102 3073
3.500000+6	3.909670-8	3.500000+6	1.387200-7	3.750000+6	1.387200-7242515102 3074
3.750000+6	4.535810-8	4.000000+6	4.535810-8	4.000000+6	9.708300-8242515102 3075
4.250000+6	9.708300-8	4.250000+6	6.551260-8	4.500000+6	6.551260-8242515102 3076
4.500000+6	4.589570-8	4.750000+6	4.589570-8	4.750000+6	9.745200-8242515102 3077

5.000000+6 9.745200-8 5.000000+6 3.439020-8 6.000000+6 3.439020-8242515102 3078  
 6.000000+6 6.480110-8 7.000000+6 6.480110-8 7.000000+6 3.615580-8242515102 3079  
 8.000000+6 3.615580-8 8.000000+6 1.320270-7 9.000000+6 1.320270-7242515102 3080  
 9.000000+6 4.371820-9 9.262000+6 4.371820-9 9.262000+6 0.000000+0242515102 3081  
 .....

The multiplication of MF=12 yield times the cross section gives exactly the first value appearing in the list called PROD (4.203E+01) in both versions (see below): and this is OK.

What is wrong is the list called SPEC (the constant spectrum): if you perform the ratio of the 91.38 values to the 91.91 values (e.g. 1.066E-02/3.775E-03) the result is 2.823..., i.e. the MF=12 yield - I 139.5S  
 made the same computation from GENDF output from which I got a higher 139.5S  
 number of significant figures. This has been revealed by RADE which 139.5S  
 for groups 1 to 33 (143 to 175 in reverse order) produced an estimated  
 binding energy 2.823... times higher than the one given in the BNL for  
 Cr-50.

Now with the correction in SMILER and with the 91.91 version the resulting binding in RADE is about 9.29 which the correct value.

THIS IS THE NJOY 91.38 OUTPUT 139.5S  
 =====139.5S  
 GROUP CONSTANTS AT T=2.936E+02 DEG K 139.5S  
 FOR MF16 AND MT102 (N,G) GAMMA MATRIX.

SPECTRUM CONSTANT BELOW 9.6112E+02 EV ( 33 GROUPS)

INITL GROUP	FINAL GROUP	ISOTROPIC +0	MATRIX +1	VS +2	FINAL +3	GROUP	
SPEC	1	1.066E-02	1.066E-02	1.066E-02	1.598E-02	1.598E-02	1.066E-02
SPEC	7	5.328E-03	2.664E-02	5.328E-02	5.328E-02	5.387E-02	1.185E-03
SPEC	13	5.924E-04	3.070E-02	6.022E-03	2.650E-01	3.011E-01	1.618E-01
SPEC	19	4.493E-02	5.382E-02	1.353E-03	2.165E-02	1.123E-02	1.286E-01
SPEC	25	1.966E-01	1.423E-01	8.501E-02	1.299E-01	1.147E-01	1.012E-01
SPEC	31	4.854E-02	4.854E-02	9.145E-02	9.145E-02	5.103E-02	5.103E-02
SPEC	37	3.759E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	PROD	4.203E+01	2.016E+01	1.047E+01	9.236E+00	8.148E+00	7.189E+00
7	PROD	6.341E+00	5.593E+00	4.932E+00	4.348E+00	3.833E+00	3.377E+00
13	PROD	2.974E+00	2.618E+00	2.304E+00	2.025E+00	1.778E+00	1.559E+00
19	PROD	1.365E+00	1.193E+00	1.040E+00	9.043E-01	7.841E-01	6.777E-01
25	PROD	5.842E-01	5.024E-01	4.315E-01	3.710E-01	3.202E-01	2.784E-01
31	PROD	2.451E-01	2.198E-01	2.020E-01			
34	1	7.197E-04	7.197E-04	7.197E-04	1.079E-03	1.079E-03	7.197E-04
34	7	3.598E-04	1.799E-03	3.598E-03	3.598E-03	3.639E-03	8.051E-05

THIS IS THE NJOY 91.91 OUTPUT 139.5S  
 =====139.5S  
 GROUP CONSTANTS AT T=2.936E+02 DEG K 139.5S  
 FOR MF16 AND MT102 (N,G) GAMMA MATRIX.

SPECTRUM CONSTANT BELOW 9.6112E+02 EV ( 33 GROUPS)

INITL GROUP	FINAL GROUP	ISOTROPIC +0	MATRIX +1	VS +2	FINAL +3	GROUP	
SPEC	1	3.775E-03	3.775E-03	3.775E-03	5.663E-03	5.663E-03	3.775E-03
SPEC	7	1.888E-03	9.438E-03	1.888E-02	1.888E-02	1.909E-02	4.197E-04
SPEC	13	2.099E-04	1.088E-02	2.133E-03	9.387E-02	1.067E-01	5.732E-02
SPEC	19	1.592E-02	1.907E-02	4.795E-04	7.671E-03	3.980E-03	4.558E-02
SPEC	25	6.964E-02	5.043E-02	3.012E-02	4.602E-02	4.065E-02	3.584E-02
SPEC	31	1.720E-02	1.720E-02	3.240E-02	3.240E-02	1.808E-02	1.808E-02
SPEC	37	1.332E-01					
1	PROD	4.203E+01	2.016E+01	1.047E+01	9.236E+00	8.148E+00	7.189E+00
7	PROD	6.341E+00	5.593E+00	4.932E+00	4.348E+00	3.833E+00	3.377E+00

13	PROD	2.974E+00	2.618E+00	2.304E+00	2.025E+00	1.778E+00	1.559E+00
19	PROD	1.365E+00	1.193E+00	1.040E+00	9.043E-01	7.841E-01	6.777E-01
25	PROD	5.842E-01	5.024E-01	4.315E-01	3.710E-01	3.202E-01	2.784E-01
31	PROD	2.451E-01	2.198E-01	2.020E-01			
34	1	7.197E-04	7.197E-04	7.197E-04	1.079E-03	1.079E-03	7.197E-04
34	7	3.598E-04	1.799E-03	3.598E-03	3.598E-03	3.639E-03	8.051E-05

THIS IS THE INPUT STREAM USED FOR BOTH VERSIONS

0 0

=====139.5S

```

0
6
*MODER*
20 -21
*RECONR*
-21 -22
*JEF-2.2*/
2425 1/
0.001 0 7/
*CR-50 JEF-2.2 MAT=2425*/
0/
*BROADR*
-22 -23
2425 1/
.001/
293.6
0/
*GROU*
-21 -23 0 -25
2425 17 10 12 1 1 1 1
*CR-50 JEF-2.2 MAT=2425*/
293.6
1.E10
3/
16/
0/
0/
*MODER*
-25 31
*STOP*

```

Let me shortly to comment this results:

- 1-it is necessary to check the data being produced at each step of their life - compilation, evaluation, processing and final utilization;
- 2-since the NJOY System has a lack at its own point - it is no possible to check GENDF for consistency - the way suggested by J.White - use SMILER and RADE - is for the present time the best possible and should be encouraged;
- 3-when a user library is completed, then, and only then, it must be completely re-processed.

Thank you for your attention.

Ciao.

Gian Carlo

ENEA Bologna, 940518 at 16:50 CET

cc: J.White, RSIC

cc: E.Sartori, NEA DB

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MAIL FROM:<BPANI1@IBOENEA>

RCPT TO:<jew@ornl.gov>

DATE: May, 19, 1994

TO:<jew@ornl.gov>

FROM:<BPANI1@IBOENEA>

SUBJECT: Corrections to SMILER

Dear John,

referring to the e.mail to Bob McFarlane of which you should have received a copy I am sending herewith enclosed the corrections to SMILER I mentioned thereby.

=====  
Corrections to SMILER to make it to accept the constant spectrum feature of low energy group gamma production matrix for MT=18 and MT=102.

In SUBROUTINE MILER REPLACE record labeled 390:

LNEXT=LT +NMAX

with the following sequence:

LCSP =LT +NMAX

LNEXT =LCSP +NMAX

In SUBROUTINE MILER REPLACE record labeled 670:

\* IDC,LIMIT,NR9,N9,N6)

0000

with the following:

\* IDC,LIMIT,NR9,N9,N6,D(LCSP))

In SUBROUTINE MILER REPLACE record labeled 770:

\* IDC,LIMIT,NR9,N9,N6)

0000

with the following:

\* IDC,LIMIT,NR9,N9,N6,D(LCSP))

In SUBROUTINE MILER REPLACE record labeled 870:

\* IDC,LIMIT,NR9,N9,N6)

0000

with the following:

\* IDC,LIMIT,NR9,N9,N6,D(LCSP))

In SUBROUTINE RGENDF REPLACE record labeled 30:

\* IFTG, IDC, LIMIT, NR9, N9, N6)

0000

with the following:

\* IFTG, IDC, LIMIT, NR9, N9, N6, SPEC)

In SUBROUTINE RGENDF INSERT after record labeled 100:

DIMENSION T(NMAX),D(LIMIT)

0000

the following:

DIMENSION SPEC(NMAX)

In SUBROUTINE RGENDF INSERT after record labeled 1980:

ENDIF

0000

the following sequence:

C-----THIS SECTION TO ALLOW THE READING  
C-----OF REDUCED MATRIX WHEN CONSTANT  
C-----SPECTRUM IS GIVEN AT LOW  
C-----ENERGIES - IT APPLIES ONLY FOR  
C-----MT=18, MT=102

IF(MF.EQ.16.OR.MF.EQ.17) THEN

C-----SAVE CONSTANT SPECTRUM

IF(IG.EQ.0) THEN

JNG2 = NG2

JIG2LO= IG2LO

JNW = NW

DO I=1,JNW

SPEC(I)=D(LA+I-1)

ENDDO

C-----ELIMINATE TRAILING ZERO

DO I=1,JNW

IF (SPEC(JNW-I+1).GT.0.0) GOTO 3999

ENDDO

I=1

3999 JNW=JNW-I+1

GO TO 3000

ELSE

IF(IG2LO.EQ.0) THEN

C-----RECONSTRUCT MATRIX ROW

FACT=D(LA+1)

```
DO I=1,JNW
D(LA+I)=SPEC(I)*FACT
ENDDO
NG2 = JNG2+1
IG2LO= JIG2LO
NW = JNW+1
ENDIF
ENDIF
ENDIF
```

C-----LAST RECORD OF AMENDEMENTS-----

This completes the corrections in SMILER.  
Ciao  
Gian Carlo Panini  
ENEA Bologna, 940519 at 14:35  
cc:E.Sartori, NEA DB