Summary Documentation for the 100XS Neutron Cross Section Library (Release 1.0)

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Abstract

The 100XS library (Release 1.0) contains continuous-energy neutron cross sections for nine materials for MCNP™.[1] The nine materials are ^{9}Be, ^{12}C, ^{16}O, ^{27}Al, Si, ^{40}Ca, Fe, W, and ^{238}U. The incident neutron energy range for these cross-section tables is extended beyond the traditional upper limit of 20 MeV to a limit of 100 MeV. ENDF6 format[2] evaluations have been processed with the NJOY nuclear data processing system.[3] Some further modifications have been made to increase the robustness of the resulting MCNP data sets. The library has undergone fairly significant QA and limited data testing. ZAIDs assigned to the final data sets all end in "21c." The library is compatible with MCNP Version 4A with the exception of the ^{238}U data set, which requires an enhancement to 4A. Heating numbers on the library are known to be incorrect, overestimating the energy deposition. The library is currently available only to XTM sponsors and LARAMIE (Los Alamos Radiation Modeling Interactive Environment) customers.

Nuclear Data Evaluations

The nuclear-data evaluations upon which the 100XS library is based were the result of pioneering work performed in the Nuclear Theory and Applications group at Los Alamos. Extensive model and model code developments, as well as improved phenomenological data representations, were required in order to prepare the 100-MeV evaluations. All model improvements were incorporated into the GNASH statistical/preequilibrium/fission theory computer code system.[4] Full details of the theoretical work may be found in Ref. 5. The resulting evaluations were among the first to fully exercise the new features and capabilities of ENDF6.

The starting points for the present work were the Los Alamos CFS files listed in Table I.

Table 1: Initial ENDF6 Evaluations

Material	ENDF/B MAT	CFS Node	Date Last Written
Be-9	409	/T2/PGYC/EVAL/LA100N/BE100N2	01/27/89
C-12	612	/T2/PGYC/EVAL/LA100N/C100N6	12/21/89
O-16	816	/T2/PGYC/EVAL/LA100N/O100N6	12/21/89
Al-27	1327	/T2/PGYC/EVAL/LA100N/AL100N6	12/21/89
Si	1428	/T2/PGYC/EVAL/LA100N/SI100N6	12/21/89
Ca-40	2040	/ENDF/100U/NEUTRON/CA	07/01/93
Fe	260	/T2/PGYC/EVAL/LA100N/FE100N6	12/21/89
W	7400	/T2/PGYC/EVAL/LA100N/W100N4	12/21/89

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Table 1: Initial ENDF6 Evaluations

U-238	9238	/T2/PGYC/EVAL/LA100N/U100N2	01/11/89

These files represent the most recent ENDF6 format evaluations from P.G. Young. (In the instance of ^{40}Ca, Young's file [/T2/PGYC/EVAL/LA100N/CA100N4, last written 02/17/88] was modified by R.E. MacFarlane for consistency with format requirements of ENDF MF=1.)

Processing Code

The version of NJOY employed in this work was vers.94.10. The UNICOS executable used is archived on CFS as NJOY94/XNJOY in the tar file /NJOY/94/TAR10R (last written 7/22/95).

Several modules of NJOY were executed: MODER, RECONR, BROADR, HEATR, and ACER. The processing strategy followed closely that devised by R.E.MacFarlane for preliminary processing of these evaluations. A representative INPUT file for NJOY (for ^{16}O) follows:

```
 0
 6
moder
 20 -21
reconr
 -21 -22
 *pendf tape for 100 mev o-16 from o100n6*/
 816 2/
 .002/
 *8-o-16 from lanl 100 mev library (o100n6)*/
 *processed with the njoy system (njoy/94/xnjoynr)*/
 0/
broadr
 -22 -23
 816 1/
 .002/
 300/
 0/
heatr
 -21 -23 -24 /
 816 /
acer
 -21 -24 0 31 32
 1 1 1/
 *8-o-16 from pgy 100 mev library (o100n6)*/
 816 300./
 .01/
  /
stop
```

The original ENDF/B evaluation is TAPE20. TAPE31 is the processed Type-1 MCNP ACE file.

Some of the key parameters are: the fractional reconstruction tolerance in RECONR is 0.002 (0.2%); the fractional tolerance for thinning in BROADR is 0.002; there is no cross-section energy grid thinning in ACER; and the tolerance for thinning secondary distributions in ACER is 0.01.

ZAIDs for MCNP

The MCNP ZAID identifiers for the materials on 100XS have all been selected to end with "21C." All tables were processed at 300°K. The nine tables have been combined onto one Type 1 library called 100XS1. A nine-line directory file, 100DIR1, contains the information required by MCNP to access 100XS1. The nine lines must be added to the appropriate directory section of an existing XSDIR. The access route for 100XS1 is currently entered as a '0' in 100DIR1. The access route may be changed as appropriate once the library is installed on specific systems (of course, one may first use MAKXSF to convert 100XS1 to more compact Type-2 format). Table 2 provides information for each data table of the sort given in Appendix G of Ref. 1.

Table 2: Information About 100XS Data Tables

Material	ZAID	Atomic Weight Ratio	Temperature (°K)	Number of Energy Points	Total File Size	Photon Production Data	Fission Nubar
Be-9	4009.21c	8.934761	300	316	28,964	Yes	No
C-12	6012.21c	11.89691	300	919	28,809	Yes	No
O-16	8016.21c	15.85751	300	1427	45,016	Yes	No
Al-27	13027.21c	26.74975	300	1473	35,022	Yes	No
Si	14000.21c	27.844	300	2883	76,399	Yes	No
Ca-40	20040.21c	39.61929	300	2718	53,013	Yes	No
Fe	26000.21c	55.365	300	15,598	149,855	Yes	No
W	74000.21c	182.2706	300	21,386	194,513	Yes	No
U-238	92238.21c	236.006	300	30,911	279,245	Yes	Both

Caveats

The major known flaw with the processed library involves neutron heating numbers. The heating numbers are known to be too large in certain energy ranges. Why is this so? The difficulty traces back to sophisticated use of a new ENDF6 feature in the evaluations. MT=5 is used (particularly

at higher energies) as a sort of “catch-all” reaction; multiple reaction channels are all lumped into MT=5 in an attempt to economize on the length and complexity of the evaluation. However, it is clearly impossible to define a single Q-value to represent all of the channels over the entire energy range. Instead, the Q-value for MT=5 has been given in the evaluations as either 0 or the Q-value of the lowest threshold reaction channel to be included in MT=5; in any event the absolute magnitude of Q is lower than it should be. NJOY attempts to calculate neutron heating via the “energy-balance” method (see the HEATR chapter of Ref. 3 for a detailed discussion). Namely, the heating (for a particular reaction) is obtained (as a function of neutron energy) by adding the Q-value to the incident energy and subtracting the average total secondary neutron and photon energy. By using the given Q-value for MT=5 the calculated heating is too high. [Note: For ^{238}U, with fission being one of the channels included in MT=5, the problem may be the reverse. Namely, the Q-value may be too small and therefore the heating numbers too low.]

There are (at least) three ways to remedy the problem. All are well outside the scope of this work. The first is to theoretically determine the average Q-value as a function of neutron energy and then to enter this information as allowed by the HEATR module of NJOY. The second is to include data in MF=6, MT=5 so that multiplicities and average energies of all residual reaction products, specifically including the target residuals, could be obtained. Then, NJOY could calculate heating as the summation of the average energies of all charged particles and recoil nuclei (referred to as the “direct method” in Ref. 3). Finally, MT=5 could be abandoned in favor of the brute-force method of including data for each reaction channel individually in the evaluations.

How high are the heating numbers found on 100XS? Preliminary assessments indicate that they may range up to factors of 2-4 too high as the neutron energy approaches 100 MeV. *Users should clearly be very careful if using heating numbers from this library.*

At the other extreme, there are modest problems with negative heating numbers for a few materials: Si (~3-6 MeV), Fe (~3-4 MeV), and W (~0.7-2 MeV).

Overview of Data Content

For the sake of brevity, we begin this section by simply listing the reactions included for each data table. We will then include a very small sample of representative cross-section plots.

A. Neutron Reactions
A quick reference guide to interpreting the MT values is given in Table 3. All of the MTs listed below may be used with the FM feature of MCNP to obtain reaction rates.

Table 3: Quick Reference to MT Values

MT(s)	Description
2	elastic scattering
3	nonelastic [redundant]

Table 3: Quick Reference to MT Values

4	total inelastic [redundant]
5	(n,anything) [“catch-all” reaction]
6-9, 46-49	(n,2n) for ^{9}Be
16, 17	(n,2n) and (n,3n)
19, 20, 21, 38	first, second, third, and fourth-chance fission
51-90	inelastic scattering to discrete levels
91	continuum inelastic scattering
102	radiative capture (n,γ)
103	(n,p)
104	(n,d)
105	(n,t)
107	(n,α)

^{9}Be: MT = 2, 5, 6-9, 46-49, 51-56, 102-105,and 107.
^{12}C: MT = 2, 5, 51, and 102.
^{16}O: MT = 2, 5, 51-68, and 102.
^{27}Al: MT = 2, 5, 51-56, and 102.
Si: MT = 2, 5, 51-72, and 102.
^{40}Ca: MT = 2, 5, 51-82, and 102.
Fe: MT = 2, 5, and 102.
W: MT = 2, 5, 51-90, and 102.
^{238}U: MT = 2, 5, 16, 17, 19-21, 38, 51-77, 91, and 102.

B. Photon-Production Reactions
The MCNP scheme for identifying photon-production MTs is as follows: the first photon produced by neutron reaction MT=n has photon-production MT=1000*n+1, the second has photon-production MT=1000*n+2, etc. Thus, for example, the evaluators have included 89 different photons from ^{27}Al radiative capture, each with its own energy-dependent cross section. All of the MTs listed below may also be used with the FM feature of MCNP to obtain information about the production of specific photons.

^{9}Be: MT = 5001, 102001, and 105001.
^{12}C: MT = 5001, 51001, and 102001-102003.
^{16}O: MT = 4001-4013, 5001, 22001, 102001-102004, 103001-103003, and 107001-107006.

^{27}Al: MT = 4001-4009, 5001, and 102001-102089.
Si: MT = 4001-4007, 5001, and 102001-102042.
^{40}Ca: MT = 5001 and 102001.
Fe: MT = 5001 and 102001.
W: MT = 4001, 5001, and 102001.
^{238}U: MT = 3001-3004, 5001, 18001, and 102001.

C. Cross-Section Plots
Four representative cross-section plots of data from 100XS are included at the end of this report. Fig. 1 and Fig. 2 are plots of the neutron reaction cross sections for ^{12}C and Fe respectively from 1 eV to 100 MeV. Fig. 3 compares the neutron total cross section for six of the materials on 100XS over the energy range from 1 to 100 MeV. Fig. 4 shows the total photon-production cross section for the same materials over the same energy range. (Note: In both Figs. 3 and 4, the higher solid curve is W, the lower solid curve is ^{9}Be.)

MCNP Compatibility

The 100XS library is designed to take advantage of new ENDF6 capabilities that were included in MCNP Version 4A. As such, with the exception of ^{238}U, the library is completely compatible with MCNP4A.

In the case of ^{238}U, neutron upscattering ($E_{scattered} > E_{incident}$) is allowed in MT=5. This upscattering can be correct physically, because the evaluators have included fission (a positive Q-value reaction) as one of the reactions lumped into MT=5. When such upscattering is sampled in MCNP4A, a fatal error will result and the calculation will be terminated. J.S. Hendricks has written a patch to MCNP4A (included first in intermediate version MCNP4XL[6]) that allows neutron upscatter in certain cases such as when fission is included in MT=5. Those users having access to intermediate version 4XL or later thus have a version of MCNP that is completely compatible with 100XS. The Hendricks patch is proposed for MCNP4B. Final code for MCNP4B may be different. Availability of the patch is described below under ‘Library Availability.’

Library Availability

The 100XS library is stored in Type 1 format on CFS as /X6DATA/CE/SPECIAL/HIENERGY/100XS1 (both open and secure). The corresponding directory file 100DIR1 and the patch to MCNP4A needed to use ^{238}U are stored under the same directory as 100DIR1 and UPPATCH respectively. All files were last written on 10/18/95 and are currently available only to certain XTM customers, sponsors, and collaborators. We would anticipate general release to RSIC at some time in the future.

Related Libraries

Users of the 100XS library may be interested in other MCNP data sets that extend to neutron energies greater than 20 MeV. The ENDF60 library[7] includes several such sets. Information is

given in Table 4.

Table 4: Other MCNP Data Tables with E_n > 20 MeV

Material	ZAID	Upper Energy (MeV)
H-1	1001.60C	100
C	6000.60C	32
I-127	53127.60C	30
Ho-165	67165.60C	30
Au-197	79197.60C	30
Am-241	95241.60C	30

The 100-MeV evaluation upon which ZAID=1001.60C on ENDF60 is based was actually performed by the Nuclear Theory and Applications group at Los Alamos at the same time as the other 100-MeV evaluations upon which the 100XS library is based.

We should also point out that the evaluations upon which the 100XS library is based are most often built upon ENDF/B-V Revision 2 evaluations up to an energy that is material-dependent. Thus, there is significant overlap with ".50c" data tables at low energies. See Ref. 5 for specific energy ranges that are identical to ENDF/B-V.

Quality Assurance

Several tools were used to QA the 100XS library. All of the modifications discussed below resulted from issues discovered in the QA process. For brevity, we will only list here the types of tools used in our QA.

- NJOY performs several consistency checks in ACER. The code checks several attributes of reaction thresholds, energy grids, and secondary energy and angular distributions. It flags anything known to be wrong or considered to be unreasonable.
- The XDATAP code[8] was used to coplot all cross sections from the processed files against cross sections from the original evaluations.
- Average cross sections in many energy ranges were calculated for each reaction.[9] Comparisons were made between the average cross sections from the processed files and those from the original evaluations. Comparisons were also made between the newly-processed results and a previous version of the processed library.
- MF=1 information for each evaluation was studied. Spot checks of the remainder of the evaluations were made as necessary to compare with the detailed outputs from NJOY.
- A host of small, special-purpose checking codes were written, primarily to identify issues on the processed files relating to new ENDF6 features.
- Generic sample MCNP problems were run for each material. The goals were to exercise as much of the data sets as possible and to check for proper flow and reasonableness of results. Also,

a million history, 20-million collision problem was run for 6 hours on a Sun IPX workstation to ensure compatibility with 32-bit machines.

Modifications

As a result of the QA process described above, several modifications were made to either the original evaluations or the processed ACE files. These modifications were largely necessitated by stress imposed on the evaluations, NJOY, and MCNP by the significant use of advanced ENDF6 features. The modifications can be summarized in the following seven categories.

1. Both ^{12}C and ^{16}O evaluations include anisotropic angular distributions for some photons produced in neutron reactions. In particular, the ^{12}C evaluation specifies that photons from the first discrete inelastic level (MT=51, 4.439 MeV) are anisotropic, and the ^{16}O evaluation specifies that photons from two inelastic levels (at 6.131 MeV and 6.917 MeV) are anisotropic. The distributions specified can be quite anisotropic, especially for ^{12}C at neutron energies near the reaction threshold.

   NJOY ver.94.10 does not carry forward information about anisotropic neutron-induced photons to ACE files. Therefore, it was necessary to add this information to the NJOY-processed ACE files for ^{12}C and ^{16}O. The angular distributions given in the new evaluations were unchanged (except for the incident neutron energy grid being extended to 100 MeV) from those given in ENDF/B-V. Therefore, we obtained the appropriate data from the corresponding ENDF/B-V ACE files (ZAID=6012.50C and ZAID=8016.50C) and added it to 100XS.

2. Four of the evaluations (^{12}C, ^{16}O, Si, and ^{40}Ca) included negative probabilities of scattering for certain combinations of incident and exiting neutron energies. In all cases, the reaction in question was MT=5 and the scattering data were provided in terms of Law=1, LANG=2 (Kalbach-87) in MF=6.

   The absolute values of all offending probabilities were relatively small. Therefore, in consultation with P.G.Young, it was determined that we would simply set the probabilities to zero. This was accomplished by making the appropriate corrections to the ACE files themselves, rather than to the evaluations. The modifications, of course, necessitated that the entire probability density function and cumulative density function be renormalized at incident energies having this problem.

3. All nine evaluations included energy distributions that allow neutrons to be upscattered. This was found most frequently for MT=5, with scattering data provided in terms of Law=1, LANG=2 in MF=6. The circumstance was also found for W for MT=91 where the distributions were specified in the more traditional form of an arbitrary tabulated distribution (LF=1) in MF=5. The frequency with which neutrons would upscatter varied considerably among the materials; for W (MT=5) it was greater than one in a thousand at some incident neutron energies.

   For all materials except ^{238}U, it was decided to truncate the energy distributions such that non-

physical upscatter would not occur. Again, this was accomplished by making the appropriate corrections to the ACE files themselves, rather than to the evaluations. The modifications, of course, necessitated that the entire probability density function and cumulative density function be renormalized at incident energies having this problem. When energy distributions were given in the center of mass (COM) the maximum allowable COM energy was determined as that energy for which the laboratory scattering energy equaled the incident energy using $\mu_{COM}=1$.

^{238}U was not modified. See the discussion under 'MCNP Compatibility' for an explanation.

4. For ^{9}Be, the evaluators employed a radical shift in specified reactions at 20 MeV. MTs 6-9, 46-49, 102-105, and 107 were given below 20 MeV; MTs 5 and 51-56 were given above 20 MeV. A transition was accomplished in the evaluation by having the cross section for every reaction (except elastic scattering) be either zero at 20.0 MeV and non-zero at 20.00001 MeV or non-zero at 20.0 MeV and zero at 20.00001 MeV. Such a transition should be fine. Unfortunately, however, the processed energy grid did not include both 20.0 and 20.00001 MeV (the 20 MeV point was discarded). This leads to a rather severe discontinuity in the total cross section at 20 MeV.

   The solution implemented was to change all occurrences of 20.0 MeV in the original evaluation (in MF=3,6,12) to 19.99999 MeV. The modified evaluation was then completely reprocessed with NJOY. Both 19.99999 and 20.00001 MeV were retained in the processed energy grid, thus successfully implementing the evaluators' transition. The modified evaluation is stored on the open CFS as /090895/HIENERGY/BE100N2_NEW (last written 09/25/95).

5. In the Si evaluation, at neutron energies greater than 3 MeV, the dominant neutron reaction for producing photons is MT=5. The original evaluation led to a processed photon-production cross section from MT=5 several thousand times greater than intended over a limited neutron energy range near the reaction threshold. The origin of the anomaly was traced to an artifact of interpolation. The photon-production cross section from MT=5 is equal to the product of the MT=5 neutron interaction cross section times the MT=5 photon multiplicity. Both quantities are dependent on the neutron energy. It turns out that the evaluated quantities vary extremely rapidly (particularly from 3.75 to 4.0 MeV); so rapidly that the product of the quantities (at interpolated energies) was very ill-behaved.

   The solution, arrived at in consultation with P.G.Young, was to add many more points to the photon multiplicity energy grid between threshold and 6 MeV. Multiplicities at the energy points added were chosen so as to preserve the interpolated product of cross section and multiplicity. To further improve the results, the interpolation scheme specified for a portion of the energy range in the multiplicity table was changed form linear-linear to log-log. After these changes were made, the modified evaluation was then completely reprocessed with NJOY. The resulting behavior of the photon-production cross section from MT=5 was judged to be acceptable. The modified evaluation is stored on the open CFS as /090895/HIENERGY/SI100N6_NEW (last written 09/28/95).

6. The ENDF6 format allows secondary energy distributions to be a combination of discrete ener-

gies and a continuous distribution. This capability has been heavily used by the evaluators in this work to describe secondary photons. A complication arises downstream in MCNP in certain circumstances. MCNP would like to use this data in as sophisticated a manner as possible. One aspect of accomplishing this is to sample a secondary photon energy by interpolating between adjacent (in neutron energy) distributions. This becomes a nightmare to code unless one assumes that the number of discrete photon energies is constant (and furthermore, that there is a direct one-to-one correspondence) at adjacent incident neutron energies. Such was not the case for evaluations of ^{16}O, ^{27}Al, ^{40}Ca, Fe, and W.

Rather than complicate MCNP unnecessarily, the approach taken was to modify the processed files (not the evaluations) to ensure that the number of discrete photons was constant for a particular reaction as a function of neutron energy (and that the discrete energies were also identical). All probability densities for energies added to the secondary grids as a result of this modification were zero. The net result is data files that are modestly longer and somewhat less efficient; the plus side is simpler code in MCNP and more robust data libraries.

7. An examination of differential cross-section plots for W led to the obvious conclusion that something had gone wrong in the neutron energy range from 0.02 to 0.1 MeV. After reviewing the details of the evaluation in this energy range, the author incorrectly concluded that the processing code was having difficulty in the unresolved energy region. As later pointed out by R.E.MacFarlane, however, the actual root cause of the problem was that the evaluators had failed to include double-valued energy points in MF=3 at boundaries of various resonance regions. This ultimately caused the processing code to interpolate over a portion of the unresolved resonance region differently than the evaluators intended. MacFarlane's solution, therefore, was to modify the evaluation to include the necessary double-valued energy points in MF=3. Rigorously, this is the correct solution. We had already embarked on a different path, however, and chose not to change directions at the last minute.

   We instead relied on two facts. The first was that the new W evaluation is documented to be the same as ENDF/B-V Rev. 2 up to 6 MeV. The second was that we already had well-behaved processed cross sections from ENDF/B-V Rev. 2 W in the energy range of question. We therefore decided to extract the necessary data from ZAID=74000.55C and use this to overwrite the newly-processed data in the energy range from 0.02 to 0.1 MeV. The results are more than adequate to correctly represent the intent of the evaluators.

Data Testing

Only limited data testing was performed to compare calculated results with measurements.

Calculations of high-energy neutron transmission through various thicknesses of concrete were reported in Ref. 10 using a very early version of these cross sections. All calculations associated with that work were repeated with 100XS. Major differences (for example, in unpublished results for induced photons) were at least qualitatively explained by improvements made over the years.

Also, G.P. Estes ran an MCNP calculation of a water-phantom experiment performed by a collaborator of his at the University of Washington. The experiment was designed to be relevant to fast

neutron therapy. Once again, differences between new calculations and Estes' previous results were qualitatively understood.

Acknowledgments

It is a pleasure to acknowledge the invaluable assistance of several colleagues. Phil Young provided much information about the evaluations as well as the strategy to fix the Si photon-production problem. Bob MacFarlane was the source of NJOY facts and guidance, and provided valuable discussions about processed results and subsequent use in MCNP. Stephanie Frankle assisted in many ways and actually performed some of the initial work on this project. John Hendricks provided patches to MCNP and consulting on code strategy. Guy Estes helped by using the new library in an MCNP calculation and providing the results for comparison with those obtained using previous cross-section sets.

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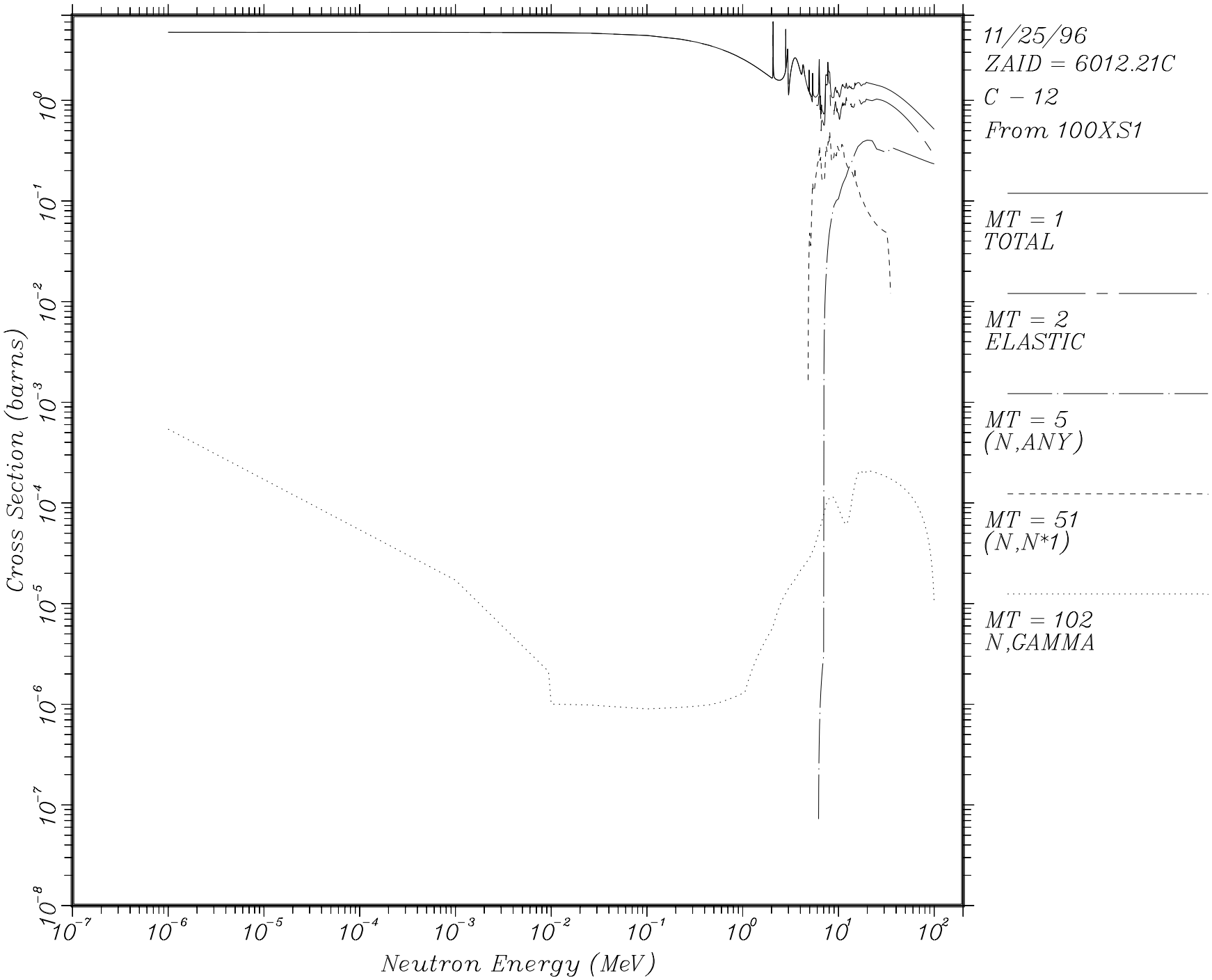
11/25/96
ZAID = 6012.21C
C − 12
From 100XS1
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TOTAL
MT = 2
ELASTIC
MT = 5
(N,ANY)
MT = 51
(N,N*1)
MT = 102
N,GAMMA
Cross Section (barns)
Neutron Energy (MeV)
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
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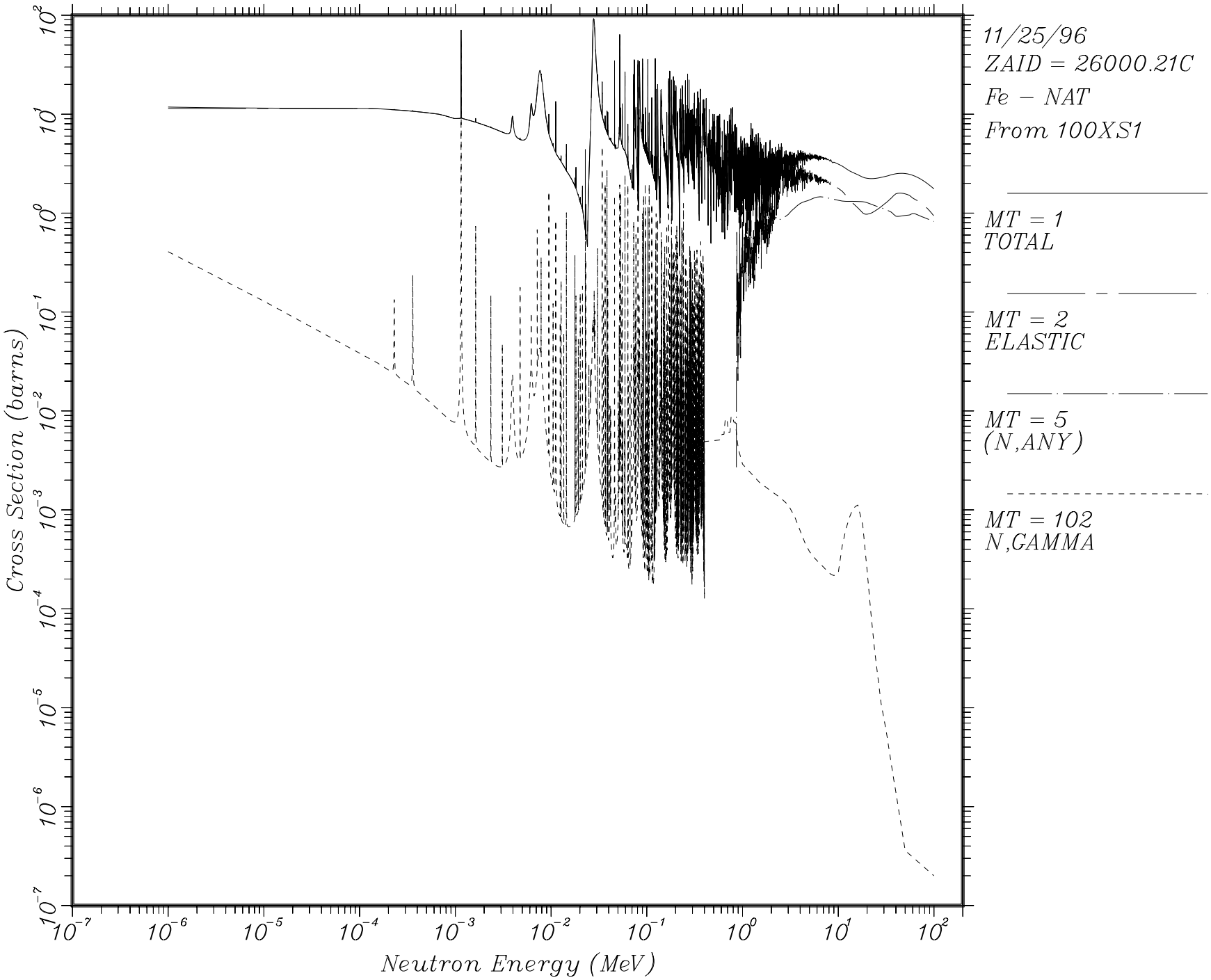
10^{1}
10^{2}


11/25/96
ZAID = 26000.21C
Fe − NAT
From 100XS1
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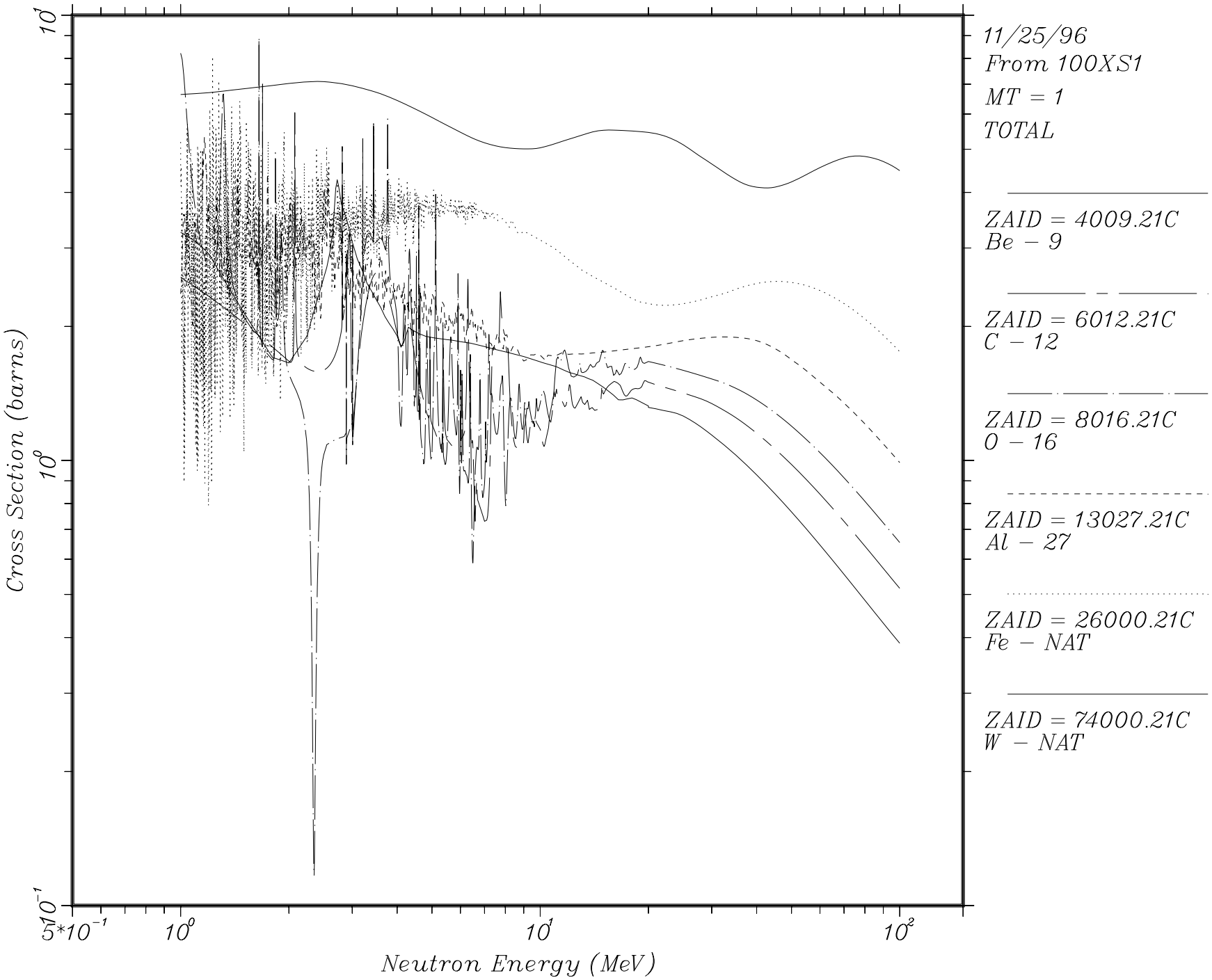
TOTAL
MT = 2
ELASTIC
MT = 5
(N,ANY)
MT = 102
N,GAMMA
Cross Section (barns)
Neutron Energy (MeV)


11/25/96
From 100XS1
MT = 1
TOTAL
ZAID = 4009.21C
Be − 9
ZAID = 6012.21C
C − 12
ZAID = 8016.21C
O − 16
ZAID = 13027.21C
Al − 27
ZAID = 26000.21C
Fe − NAT
ZAID = 74000.21C
W − NAT
Cross Section (barns)
Neutron Energy (MeV)
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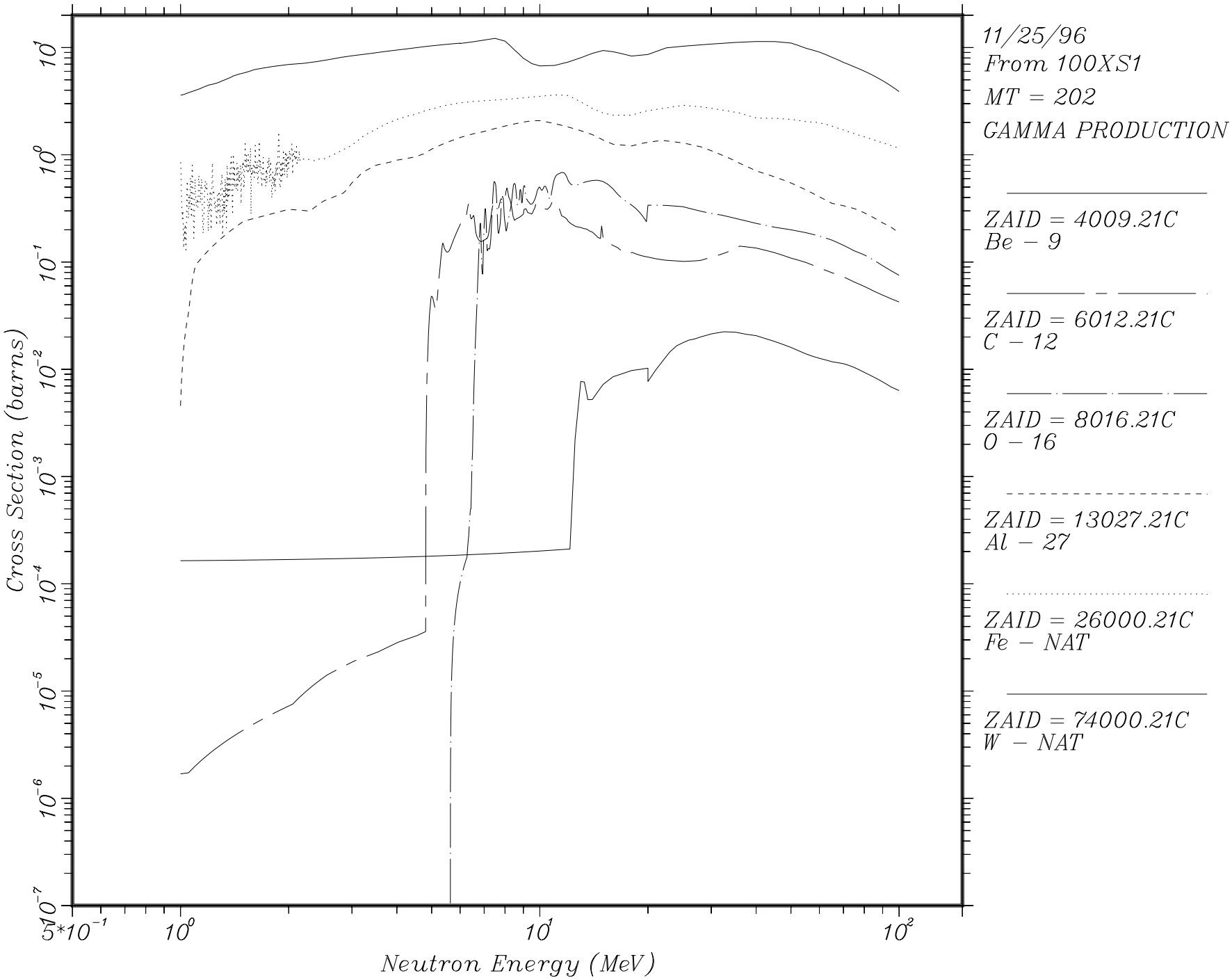
10^{-1}
$5*10^{-1}$
10^0
10^1
10^2


11/25/96
From 100XS1
MT = 202
GAMMA PRODUCTION
ZAID = 4009.21C
Be − 9
ZAID = 6012.21C
C − 12
ZAID = 8016.21C
O − 16
ZAID = 13027.21C
Al − 27
ZAID = 26000.21C
Fe − NAT
ZAID = 74000.21C
W − NAT
Cross Section (barns)
Neutron Energy (MeV)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
$5*10^{-1}$
10^{0}
10^{1}
10^{2}