Title:

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Intended for:

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Form 836 (7/06)

Tally Edits for the MCNP6 GENXS Option

Summary

The GENXS option in MCNP6 provides a capability to generate double-differential particle production cross sections and residual nucleus production cross sections from the high-energy nuclear interaction models implemented in MCNP6. The format of the input file required specifying the desired output is described below. Guidance for plotting the results from a MCTAL file is also provided. A sample problem input and output is included, using the currently implemented elastic scattering model.

I. Introduction

Application of the GENXS Option

The GENXS option in MCNP6 allows the application of high-energy nuclear interaction models in a cross section generation mode, without particle transport. A source may be specified inside a medium; each history will consist only of the interaction of the source particle at the source energy with the components of the medium. The tallied outcome from the event consists of the energies and direction cosines of the secondary particles and the recoil nuclei. Although one expects that, in normal applications, the material composition will be a single isotope, averaged results may be obtained for a natural multi-isotopic element or a complex composition. A GENXS calculation is independent of the material density specification.

The option is invoked by specifying "GENXS" or "GENXS *filename*" on the TROPT card. The content and format of the edited output are determined from an auxiliary input file specific to the GENXS option. In the first case, the output tally edit information is read from file INXC; in the second, it is read from the user-specified file *filename*. In any case, the absence of the needed file will produce a fatal error. The format of the INXC file is described below.

Historical Note and Future Development

The motivation for the GENXS option and its associated output capability arises from the need for a verification tool for the future implementation into MCNP6 of complex interaction physics models. Of course, the ability to produce cross sections from any of the interaction models in MCNP6 for validation with physics experiments is also important.

The current GENXS output editor evolved from the existing cross section editor in the LAHET Code System. In the absence of any secondary particle production in MCNP6 at the present

time, the features of the coding have been tested on LAHET3 output. The current MCNP6 implementation is purely a matter of expediency. When a generalized tally structure is defined for future implementation into MCNP6, all the functionality of the current method should be incorporated using "real" MCNP coding and utilizing standard MCNP input specification, as well as plotting from RUNTPE.

Although it is intended that the GENXS editing capability be implemented *before* the nuclear interaction models are inserted into MCNP6, it may be expected that corrections and modifications will need to be applied once testing with real multiple secondary particle emission commences.

Treatment of the K^0 and anti-K^0 require special considerations in a high-energy transport code. Secondary K^0 and anti-K^0 produced by interaction models are transported as either K^0-long or K^0-short with equal probability. Similarly, K^0-long and K^0-short interact with a target isotope as either K^0 or anti-K^0 with equal probability. In the current version of mcnp_particles.F90, only the parameters *k0_short* and *k0_long* are provided to identify these particles. For use of the GENXS option, it is assumed that a secondary K^0 will be assigned particle identifier *k0_short* and that a secondary anti-K^0 will be assigned particle identifier *k0_long*.

Using the GENXS Option

To calculate the inelastic secondary particle production only, turn off the elastic scattering with NESCAT=OFF on the TROPT card. Isotopic elastic scattering cross sections will be set to zero and the total cross section will equal the nonelastic cross section. All histories will sample the nonelastic interaction model. [Note that this applies only to the GENXS option; in a transport calculation, NESCAT=OFF implies a delta-scatter for the elastic process.]

To examine only elastic scattering, use NREACT=ATTEN on the TROPT card. All histories will sample the elastic scattering model and produce results for the scattered projectile and the recoil nucleus. Until the nuclear interaction models are implemented, only nuclear elastic scattering will produce results.

Features of the Allowed Output Options

For a multi-isotopic composition, quoted cross sections are a weighted average of the isotopic cross sections, weighted by the input atom fractions. Thus they represent average cross sections per atom in the composition. Results will reflect the variance introduced by sampling for the target isotope.

Energy- and angle-integrated results are provided as yield as well as cross section. The term "yield" might be better defined as "multiplicity". The nonelastic yield for a given particle type is the number of secondary particles of that type produced *per nonelastic event*. The elastic yield is per elastic event and is always unity. An input option defined below allows single- and double-differential results to be provided as yield rather than cross section, with the above normalization.

II. The INXC Input File

INXC File Structure

Apart from the formatted title cards, all data is entered as *list-directed input*. Repeat counts are allowed. A slash "/" may be used to terminate an input line; unread variables following "/" are assigned the default.

Card 1: 80-character problem title.

Card 2: NCASE   KPLOT   L_RES
  NCASE: The number of double-differential cross section edits. The default is 0.
  KPLOT: If nonzero, write cross section edits to the MCTAL file. The default is 0.
              Note: plotting is available *only* with the MCTAL file.
  L_RES: If nonzero, perform a residual nuclei edit. The default is 0.

For *each* of the NCASE cases, the following cards 3 through 7 are repeated as required.

Card 3: 80-character case title.

Card 4: NERG   NANG   NTYPE   FNORM   IMOM   IYIELD
  NERG: The number of energy (momentum) bin boundaries. The default is 0,
              which will produce only energy-integrated values.
  NANG: |NANG| is the number of angle bin boundaries. For NANG > 0, cosine
              bins are specified; for NANG < 0, degree bins are specified. The default
              is 0, which will produce only angle-integrated values.
  NTYPE: The number of particle types, including elastic scattering as a special case.
              If NTYPE = 0, *all* allowed particle types are included in the tally,
              including elastic scattering and elastic recoil. The default is 0.
  FNORM: A normalization factor for the double-differential cross section edit. Use
              1000.0 to convert output to millibarns. The default is 1.
  IMOM: If nonzero, treat the input energy bins as momentum bins (MeV/c) rather
              than energy bins (MeV). The output double-differential cross section
              edits will be per unit momentum. The default is 0.
  IYIELD: If nonzero, the output will be differential multiplicities or yields rather
              than differential cross sections. Multiplicities for nonelastic reactions are
              defined with respect to the nonelastic cross section; for elastic scattering,
              the differential multiplicity is with respect to the elastic cross section.
              The default is 0.

Card 5: Energy (momentum) bin boundaries (present if NERG > 0). See allowed formats below.

Card 6: Angle bin boundaries (present if NANG ≠ 0). See allowed formats below.

Card 7: Particle types tallied for this case (present if NTYPE > 0). See definitions below.

Options for Energy (Momentum) Bin Boundaries (Card 5)

The following four modes are currently allowed. The values are energy in MeV or, if IMOM ≠ 0, momentum in MeV/c.

1. All bins E_i for i = 1,…,NERG may be specified in increasing order.

2. If only one energy (momentum) value E_1 is entered, then $E_i = iE_1$ for i = 2,…,NERG.

3. If N < NERG bins E_i for i = 1,…,N are entered in increasing order, then $E_i = E_{i-1} + E_N - E_{N-1}$ for i = N+1,…,NERG.

4. If only 2 values V_1 and V_2 are entered, with $V_1 < 0$ and $V_2 > 0$, then $E_{NERG} = V_2$ and $\log_{10}(E_{i-1}/ E_i) = V_1$ for i = 1,…,NERG-1 (equal-lethargy spacing).

Options for Angle Bin Boundaries (Card 6)

For NANG > 0, cosine bins are entered by one of the three following options.

1. Cosine bins μ_i for I = 1,…,NANG are entered in increasing order; μ_{NANG} is always set to 1.

2. If a null record "/" is present, NANG equally spaced cosines $-1 < \mu_i = 1$ are defined with $\mu_{NANG} = 1$.

3. If only **one** value is entered, then the entered value is μ_1 and $\mu_{NANG} = 1$; the remaining cosine boundaries are interpolated uniformly.

4. If **two** (or more) values are entered, then the first entered value is μ_1, the second is μ_{NANG-1}, and $\mu_{NANG} = 1$; the remaining cosine boundaries are interpolated uniformly.

For NANG < 0, degree bins are entered by one of the three following options.

1. Degree bins ϕ_i for I = 1,…,NANG are entered in *decreasing* order; ϕ_{NANG} is always set to 0.

2. If a null record "/" is present, NANG equally spaced degree bins $180 < \phi_i = 0$ are defined with $\phi_{NANG} = 0$.

3. If only **one** value is entered, then the entered value is ϕ_1 and $\phi_{NANG} = 0$; the remaining degree boundaries are interpolated uniformly.

4. If **two** (or more) values are entered, then the first entered value is ϕ_1, the second is ϕ_{NANG-1}, and $\phi_{NANG} = 0$; the remaining cosine boundaries are interpolated uniformly.

Specifying Particle Types (Card 7)

Entries on card 7 are a set of flags K_i for $I = 1,\ldots,$NTYPE which identify the particle types to be included in a single cross section edit case. Negative entries $K_i < 0$ indicate tallies related to elastic scattering. Values of $K_i > 0$ designate the tallying of production of the indicated particle type by nonelastic processes; they are the same as the internal MCNP numbering scheme for particle type (with the proviso for K^0 and anti-K^0 as described above). The full set of allowed flags K_i is:

1	neutron
2	photon
3	electron (e^-)
4	positron (e^+)
5	proton
6	π^+
7	π^-
8	π^0
9	μ^-
10	μ^+
11	ν_e
12	anti-ν_e
13	ν_m
14	anti-ν_m
15	K^+
16	K^-
17	K^0
18	anti-K^0
19	antiproton
20	antineutron
21	deuteron (^{2}H)
22	triton (^{3}H)
23	helion (^{3}He)
24	alpha (^{4}He)
−1	elastic scattered projectile
−2	elastic recoil nucleus

As noted, in the absence of any nonelastic reaction models, only the elastic cases will produce a meaningful tally.

When the default (NTYPE = 0) is taken, all 26 edit types are allowed. Only brief output is produced when no secondaries of a given type occur. The ordering by particle type in the output is: proton, neutron, π^+, π^0, π^-, K^+, K^0, anti-K^0, K^-, antiproton, antineutron, deuteron, triton, helion, alpha, photon, electron, positron, μ^-, μ^+, ν_e, anti-ν_e, ν_m, anti-ν_m , elastic scattered projectile, elastic recoil nucleus .

III. Sample Problem

The sample problem to illustrate a GENXS calculation represents 23.08 GeV protons on natural W. Five cross section edits are specified. In addition, the MCTAL file is written and the residual nucleus edits are performed. The latter are very uninteresting, since there is only elastic

scattering at the present time; however, since natural W is the target material, there are five isotopes to demonstrate the residual nucleus edits.

The INP file is:

```
Test problem: RECOIL2
  1  1   -16.654    -1 2 -3
  2  0             -4 (1:-2:3)
  3  0              4

  1  cz   4.0
  2  pz  -1.0
  3  pz   1.0
  4  so  50.0

  m1    74180 0.001300   74182 0.263000   74183 0.143000
        74184 0.306700   74186 0.286000
  sdef erg = 23080 par = 5 dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 23080
  mode    h
  print 40 110 95
  nps 10000000
  prdmp 2j -1
  tropt genxs nreact atten
```

The INXC file is:

```
Test problem: RECOIL2
5,1,1/
Elastic scattering edit
0,-200,1/
2.0/                       ! 200 bin boundaries, 2 deg to 0 deg
-1/                        ! elastic scattered projectile
Elastic scattering energy edit
125,0,1/
23079,23079.01/           ! 125 10 keV bins above 23.079 GeV
-1/                        ! elastic scattered projectile
Elastic recoil angle edit
0,102,1/
0.0,0.02/                  ! 101 boundaries mu = 0 to 0.02&1.0
-2/                        ! elastic recoil nucleus
Elastic recoil energy edit
125,0,1/
0.01/                      ! 125 10 keV bins below 1.25 MeV
-2/                        ! elastic recoil nucleus
Elastic recoil momentum edit
150,0,1,,1/
5/                         ! 150 5 MeV/c bins below 750 MeV/c
-2/                        ! elastic recoil nucleus
```

The above input specifies 5 cross section edit cases plus the residual nucleus edit and writes a MCTAL file for plotting. Since there is only elastic scattering, all the cases are chosen to be single-differential cross sections only (NERG=0 or NANG=0):

1. $d\sigma/d\Omega$ for the projectile, binned by degrees;
2. $d\sigma/dE$ for the projectile, binned by energy;
3. $d\sigma/d\Omega$ for the recoil nuclei, binned by cosine;
4. $d\sigma/dE$ for the recoil nuclei, binned by energy;
5. $d\sigma/dp$ for the recoil nucleus, binned by momentum.

The output from these cases is illustrated in the accompanying plots.

The actual output listing from the residual nucleus edit is shown here:

```
 Distribution of residual nuclei:


                            Cross Section (b)
     Z = 74   all A      1.11594E+00 0.0000
              A = 180    1.40752E-03 0.0089
              A = 182    2.91615E-01 0.0005
              A = 183    1.59094E-01 0.0008
              A = 184    3.42476E-01 0.0005
              A = 186    3.21350E-01 0.0005


 Summary by charge number:

   Z     Cross Section (b)      Mean Recoil (MeV)
   74    1.11594E+00 0.0000     1.30329E-02 0.0008


 Summary by mass number:

   A     Cross Section (b)      Mean Recoil (MeV)
  180    1.40752E-03 0.0089    1.39919E-02 0.0233
  182    2.91615E-01 0.0005    1.31164E-02 0.0016
  183    1.59094E-01 0.0008    1.30618E-02 0.0021
  184    3.42476E-01 0.0005    1.30351E-02 0.0015
  186    3.21350E-01 0.0005    1.29360E-02 0.0015


 Mean weight of residual nuclei per event   3.97430E-01 0.0000
 Number of residual nuclei outside of table range:      0
```

Since the computation is for only elastic scattering from a composition (natural element), the cross section shown for production of a particular residual nucleus is just $f_i \boldsymbol{s}^e_i$ per atom in the element and the cross section for any residual with charge number Z=74 is

$$\Sigma_{i=1,...,5} \; f_i \boldsymbol{s}^e_i,$$

i.e., the average elastic cross section per atom in the composition. Since the attenuation weighting option was used and every event is an elastic event, the quantity "mean weight of residual nuclei per event" equals the ratio of the mean elastic cross section to the mean total cross section for the element.

IV. Plotting the MCTAL File

Plotting of GENXS output is achieved only by plotting from the MCTAL file. However, the MCTAL file is written with a very specific format and the naming of tallies follows specific rules.

The data written to MCTAL is the same as the printed output, including all the energy and angle bin normalization. Therefore, **use NONORM** when plotting. The energy and angle data are "per steradian" or "per MeV (per MeV/c for momentum)" or both. In all cases, cross sections are in "barns" unless modified by the FNORM entry in the INXC file. Default titles for each plot are supplied to assist the user in identification.

Energy and angle cross sections are plotted using the conventional C (cosine) and E (energy) bin identification, with total bins corresponding to energy- and angle-integrated cross sections. Note that if tallying by degree bins has been specified in the INXC input, then the "cosine" bins on the MCTAL file will be the actual degree bin boundaries. A tally number is defined for each case and particle type in the form *nii,* where *n* is the case number and *ii* is the two-digit formatted particle identifier (01 through 24) as shown above; *ii* = 99 is used for the elastic scattered projectile and *ii* = 98 for the elastic recoil nucleus. Each case will produce a tally for each of the NTYPE particles in that case. The five simple cases in the sample problem above produce tallies 199, 299, 398, 498 and 598 respectively on the MCTAL file and are shown below.

Tally numbers 1 through 5 on the MCTAL file are produced by the residual nucleus edit. For tallies 1 through 4, the specific definitions are:
1. production cross section vs. Z;
2. mean recoil energy vs. Z;
3. production cross section vs. A;
4. mean recoil energy vs. A.

In each case, the discrete bin identifier (Z or A) is represented by the conventional F (cell, surface, or detector) bin array. In the attached examples, tallies 1 through 4 show the "summary" edit information above.

Tally 5 contains the full tabulation of production cross sections as a function of Z and A. It may be used to plot the distribution of residual nuclei as a function of Z for fixed A, or conversely. In this case, the charge number Z uses the conventional F (cell, surface, or detector) bin array and the mass number A is represented by the conventional S (segment) bin array. Both cases are illustrated in the attached plots.

These features are illustrated by the following COMOUT file which was used to produce the attached plots of the sample calculation.

```
rmctal mctal
free f bar
title 1 "RECOIL2: Residual Nucleus Production" &
tally 1 linlin title 2 "Production Cross Section vs. Z" xtitle "Charge Number Z"
ytitle "Cross Section (barns)" xlims 72 76 file
tally 2 linlin title 2 "Mean Recoil Energy vs. Z" ytitle "Recoil Energy (MeV)" &
xlims 72 76 file
tally 3 linlog title 2 "Production Cross Section vs. A" xtitle "Mass Number A" &
ytitle "Cross Section (barns)" xlims 178 188 file
tally 4 linlin title 2 "Mean Recoil Energy vs. A" ytitle "Recoil Energy (MeV)" &
xlims 178 188 file
```

```
free s bar linlog
tally 5 xtitle "Mass Number A" ytitle "Cross Section (barns)" &
fixed f 74 title 2 "Z = 74" xlims 178 188 file
free f bar linlog
tally 5 xtitle "Mass Number Z" ytitle "Cross Section (barns)" &
fixed s 184 title 2 "A = 184" xlims 72 76 file
reset all
nonorm
linlog
tally 199 free c title 1 "RECOIL2: Elastic Scattering" &
title 2 "Angular Distribution" xlims 0 2 ylims 0.001 100000 &
xtitle "angle [degrees]" ytitle "barns/steradian" file
tally 299 free e &
title 2 "Energy Distribution" &
xlims 23079 23080 ylims 0.00001 100 ytitle "barns/MeV" file
tally 398 free c &
title 1 "RECOIL2: Elastic Recoil" title 2 "Angular Distribution" &
xlims 0 0.02 ylims 0.0001 1000 ytitle "barns/steradian" file
tally 498 free e &
title 2 "Energy Distribution" xlims 0 1.25 ylims 0.000001 100 &
ytitle "barns/MeV" file
tally 598 free e &
title 2 "Momentum Distribution" xlims 0 750 ylims 0.00000001 0.1 &
xtitle "momentum (MeV/c)" ytitle "barns/(MeV/c)" file
end
```

V. Summary

The use of the edit and plot options for the MCNP6 GENXS capability will allow the installation of particle interaction models into MCNP6 to proceed with the ability to monitor the model output. As noted above, the present methods should only be the precursor to a complete MCNP-style editor, but they do illustrate the needed features and provide an interim working tool. Although only the simple results from the elastic scattering model are available, the sample case shown demonstrates the general features of the edit and plot options.

RECOIL2: Residual Nucleus Production

Production Cross Section vs. Z
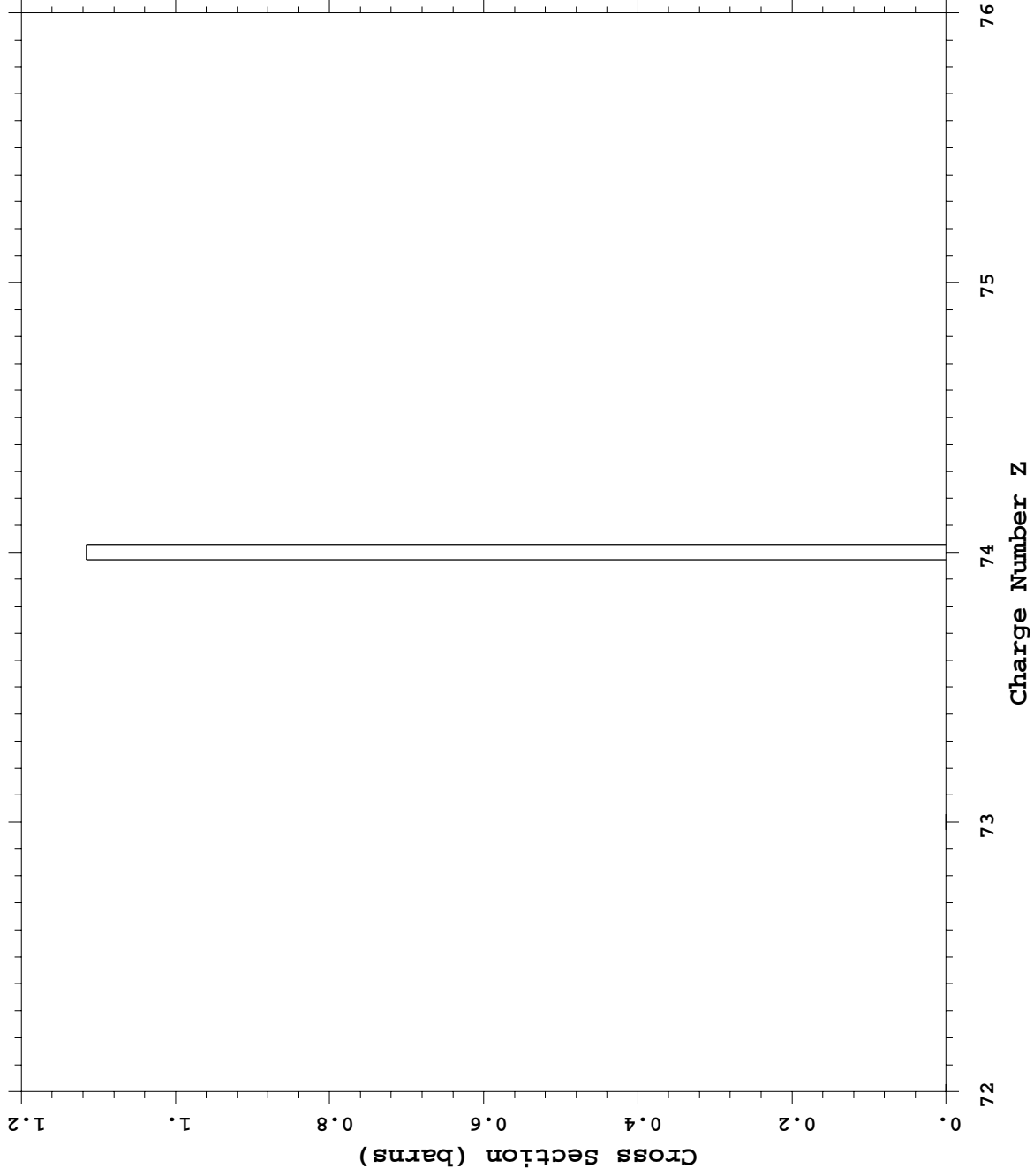
mcnp   6.0
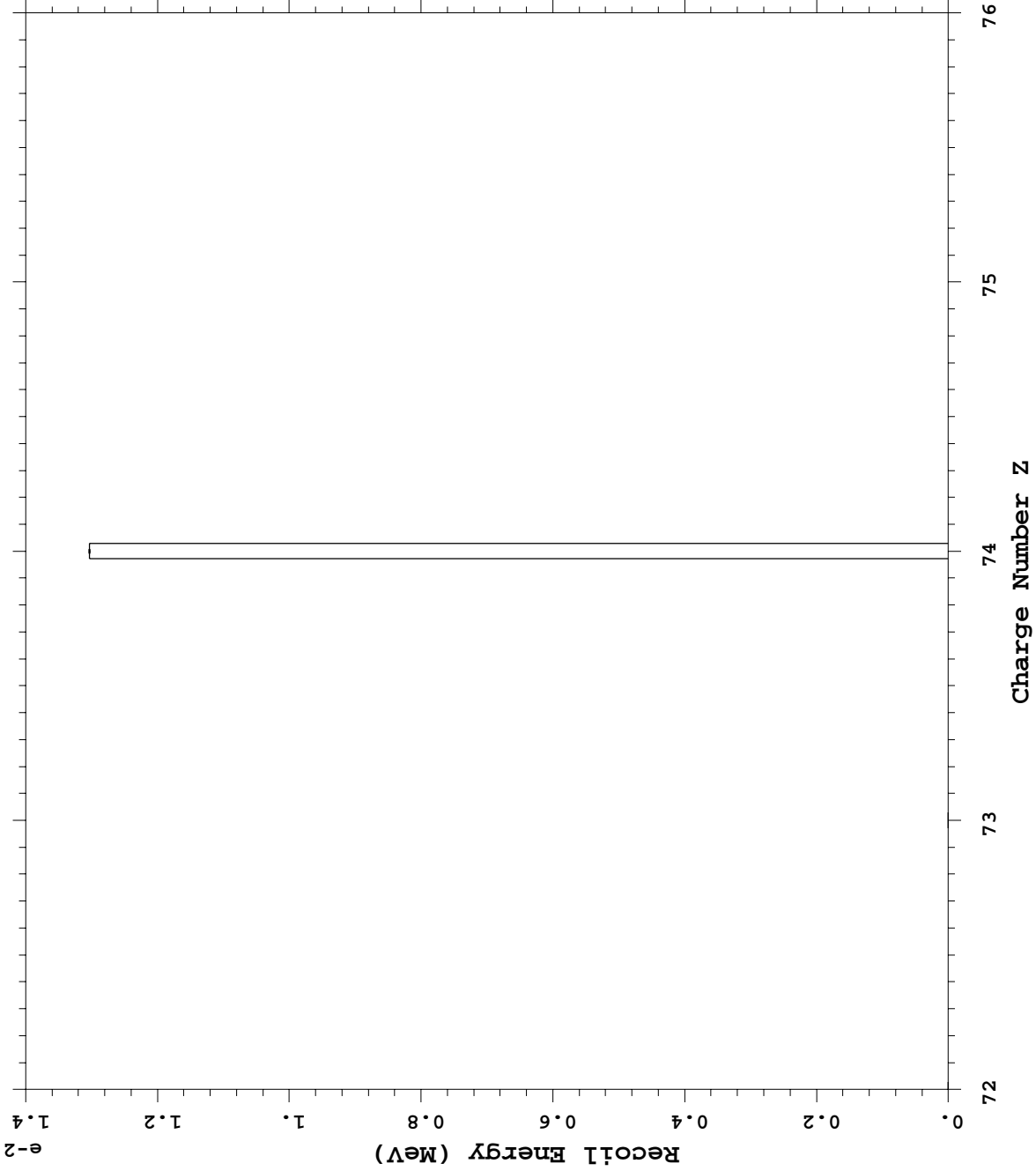
tally   1

nps   10000000
bin normed
mctal = mctal

f   surface   *
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   1
e   energy   1
t   time   1

————— mctal

Charge Number Z

Cross Section (barns)

RECOIL2: Residual Nucleus Production

Mean Recoil Energy vs. Z

mcnp   6.0

tally   2

nps   10000000
bin normed
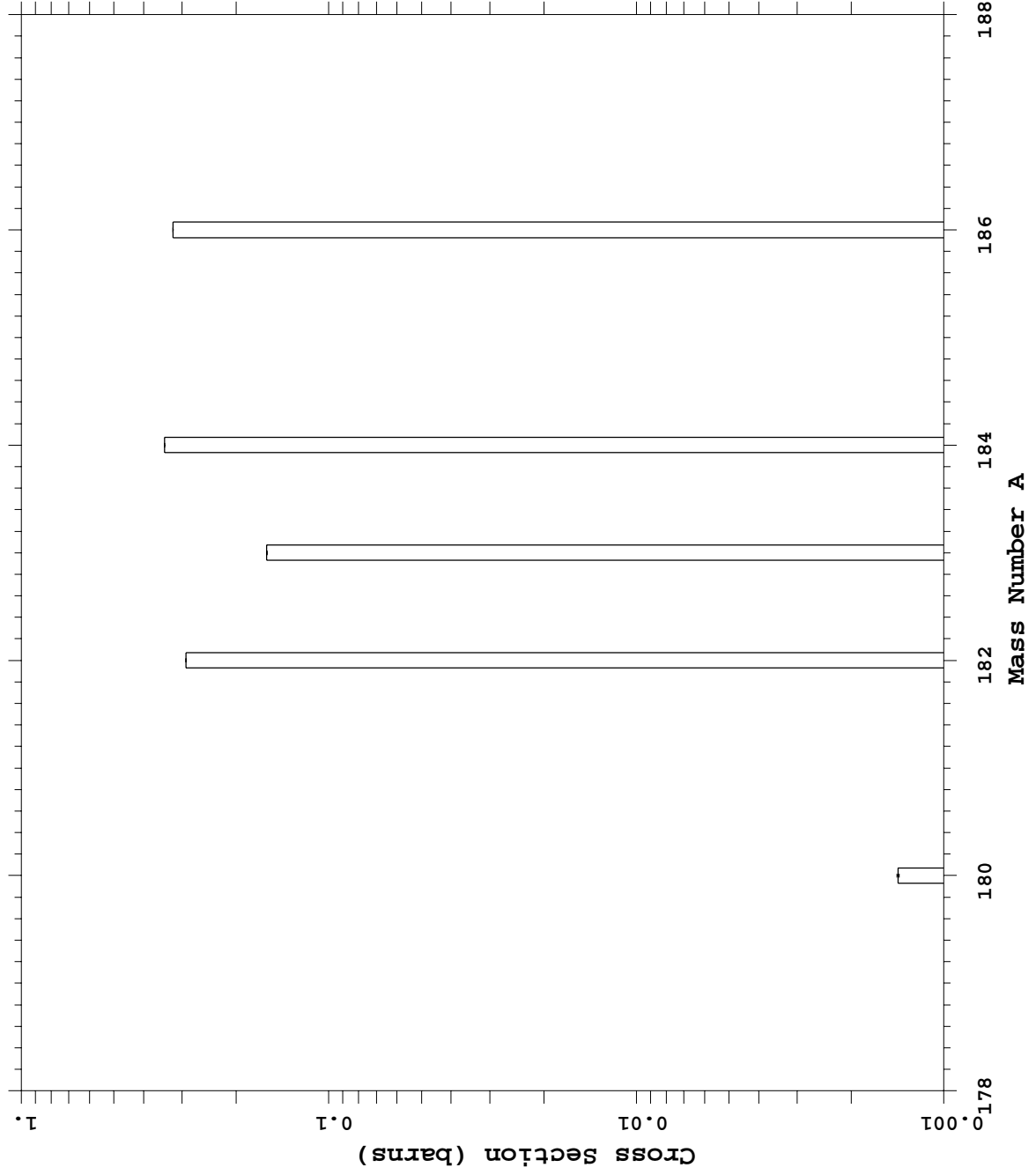mctal = mctal

f   surface   *
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   1
e   energy   1
t   time   1

————   mctal

Recoil Energy (MeV)

e-2

1.4

1.2

1.

0.8

0.6

0.4

0.2

0.

72   73   74   75   76

Charge Number Z

RECOIL2: Residual Nucleus Production

Production Cross Section vs. A

mcnp   6.0

tally   3

nps   10000000
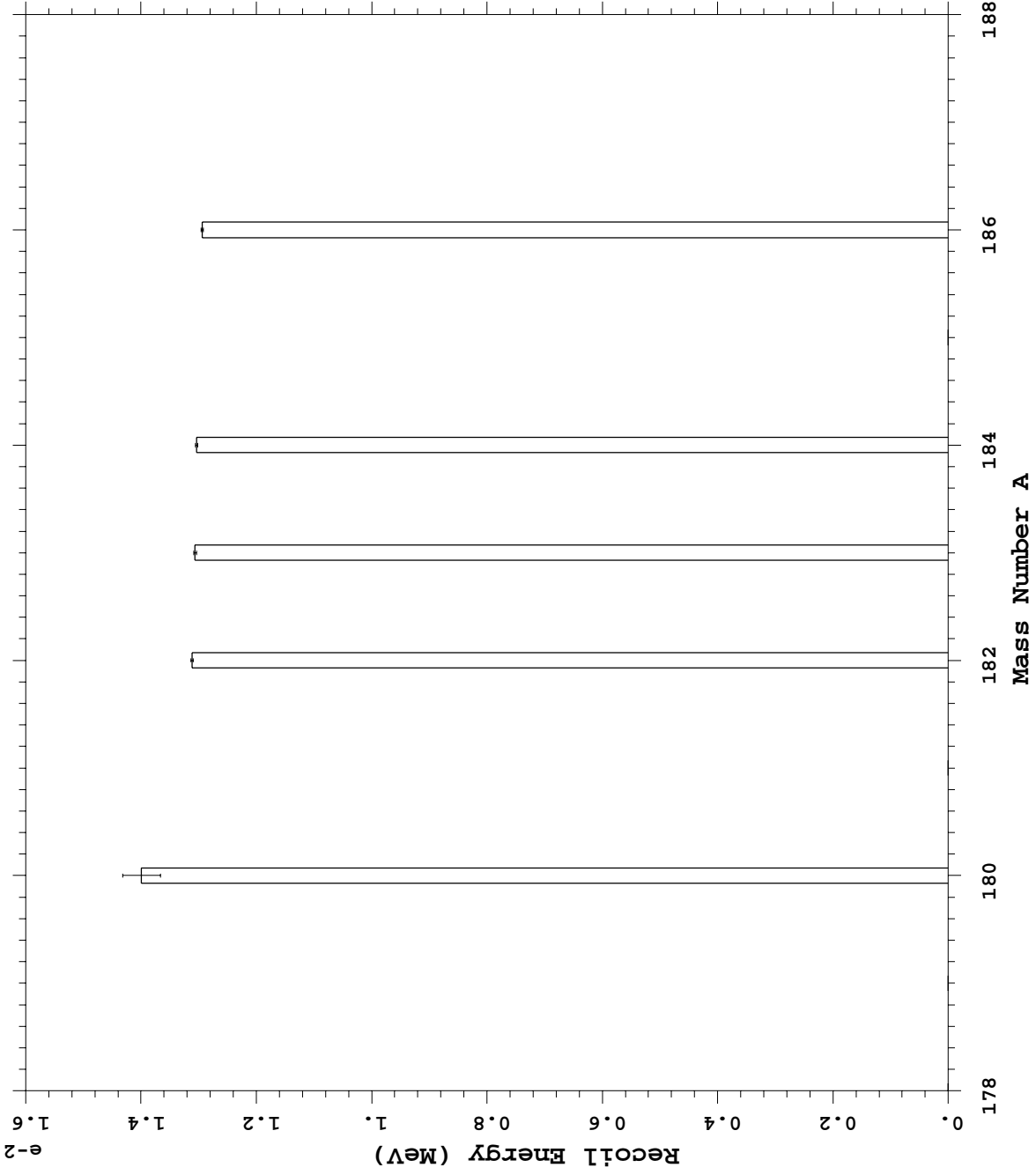bin normed
mctal = mctal

f   surface   *
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   1
e   energy   1
t   time   1

_____ mctal

Mass Number A

Cross Section (barns)

RECOIL2: Residual Nucleus Production

Mean Recoil Energy vs. A

mcnp   6.0

tally   4

nps   10000000
bin normed
mctal = mctal

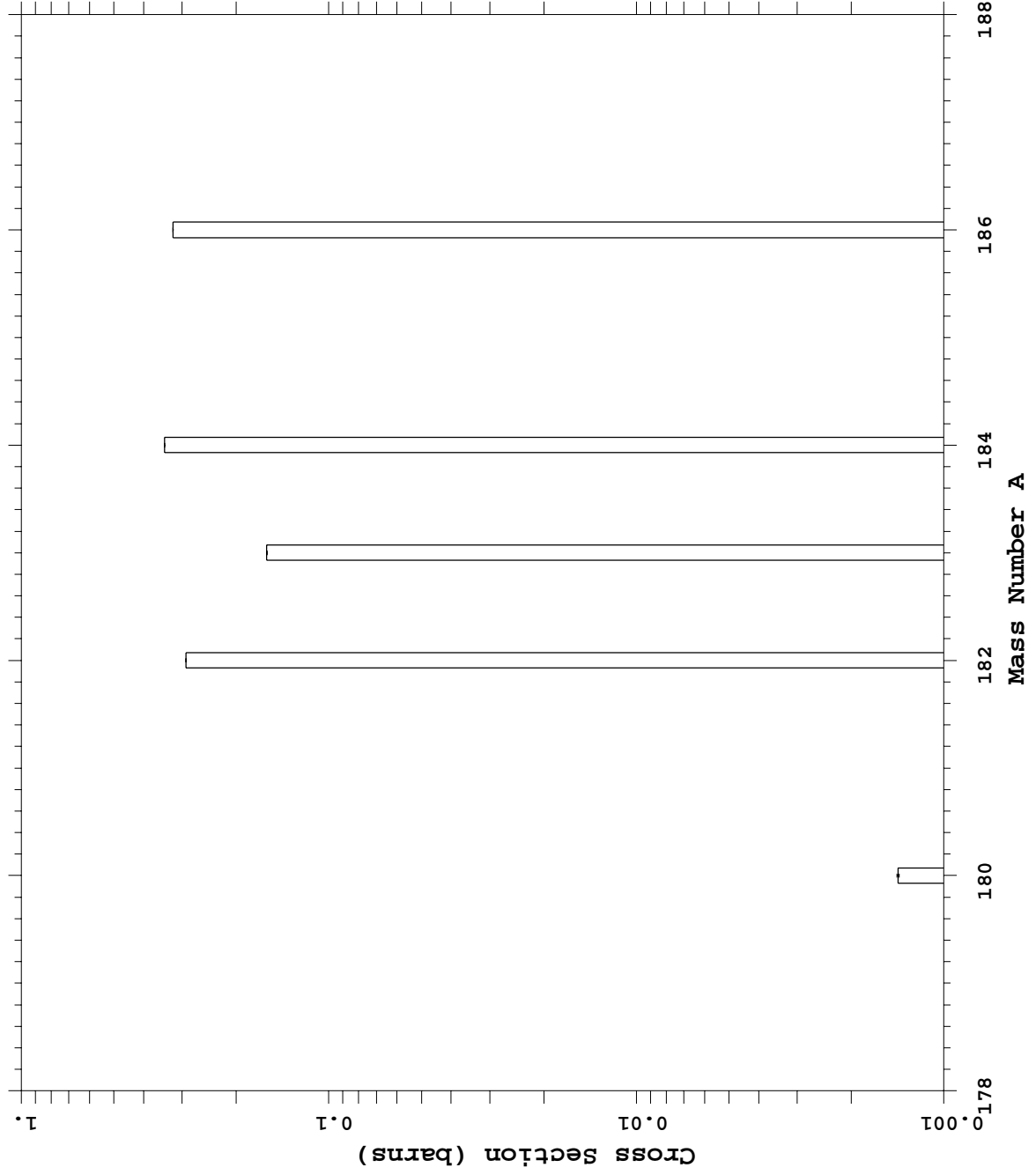f   cell   *
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   1
e   energy   1
t   time   1

—— mctal

Mass Number A

Recoil Energy (MeV)

RECOIL2: Residual Nucleus Production

Z = 74

mcnp   6.0

tally   5

nps   10000000
bin normed
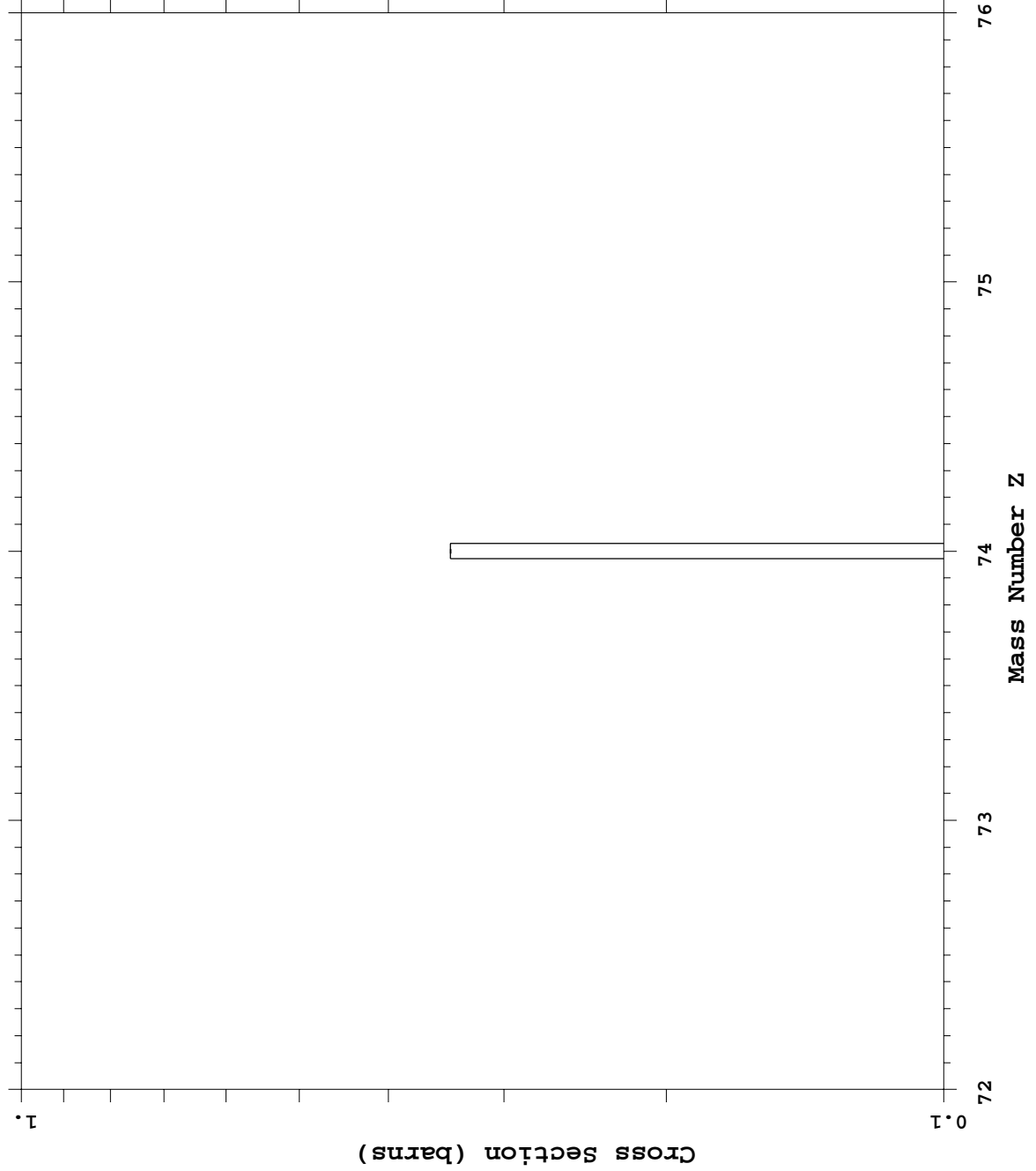mctal = mctal

f   detector   74
d   flag/dir   1
u   user   1
s   segment   *
m   mult   1
c   angle   1
e   energy   1
t   time   1

_____ mctal

Cross Section (barns)

Mass Number A

RECOIL2: Residual Nucleus Production

A = 184

mcnp   6.0

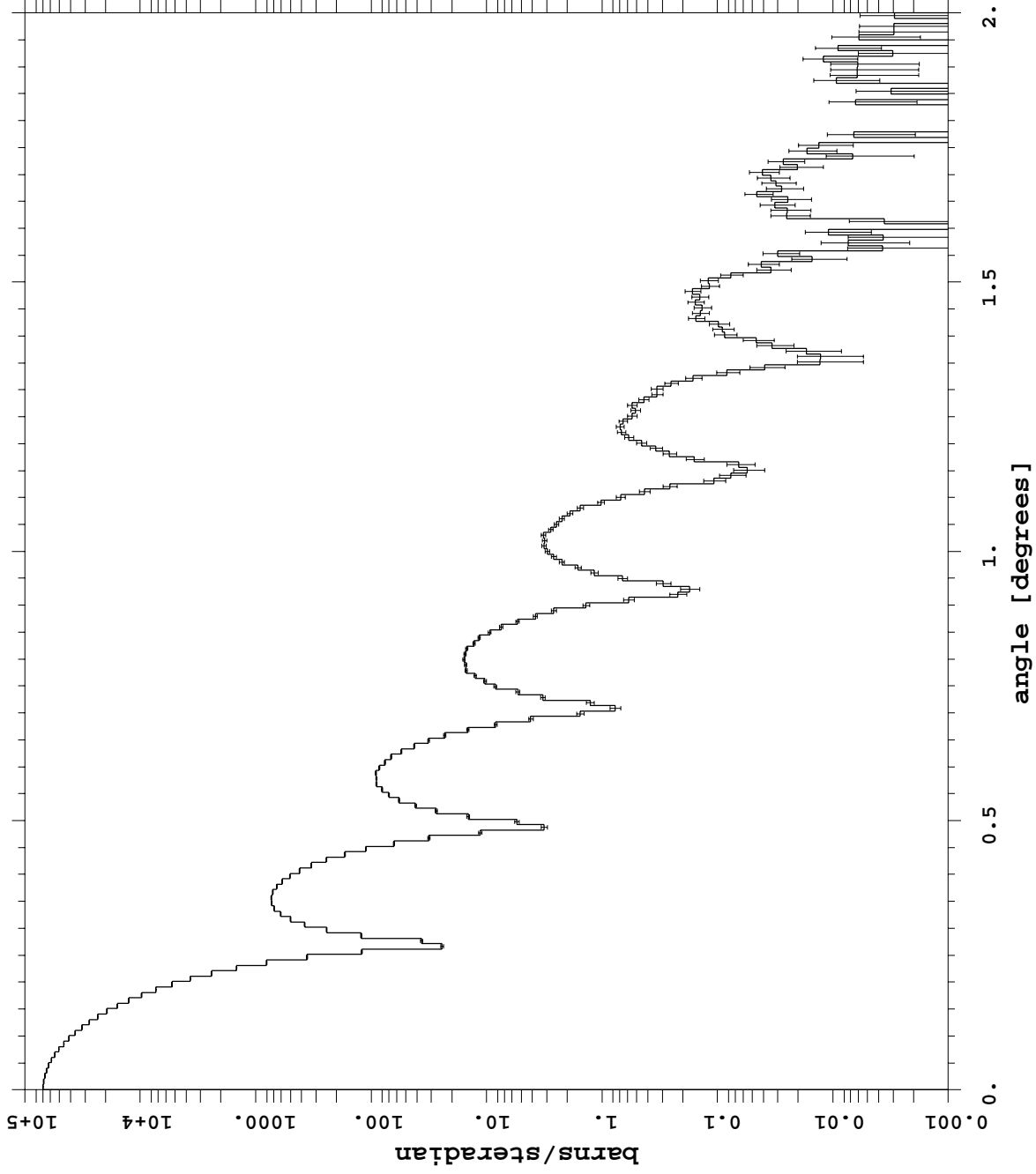tally   5

nps   10000000
bin normed
mctal = mctal

f   detector   *
d   flag/dir   1
u   user   1
s   segment   184
m   mult   1
c   angle   1
e   energy   1
t   time   1

——— mctal

Mass Number Z

Cross Section (barns)

RECOIL2: Elastic Scattering

Angular Distribution

mcnp		6.0
tally	199	
nps	10000000	
mctal = mctal		

f	cell	1
d	flag/dir	1
u	user	1
s	segment	1
m	mult	1
c	angle	*
e	energy	2 t
t	time	1

mctal

angle [degrees]

barns/steradian

RECOIL2: Elastic Scattering
Energy Distribution
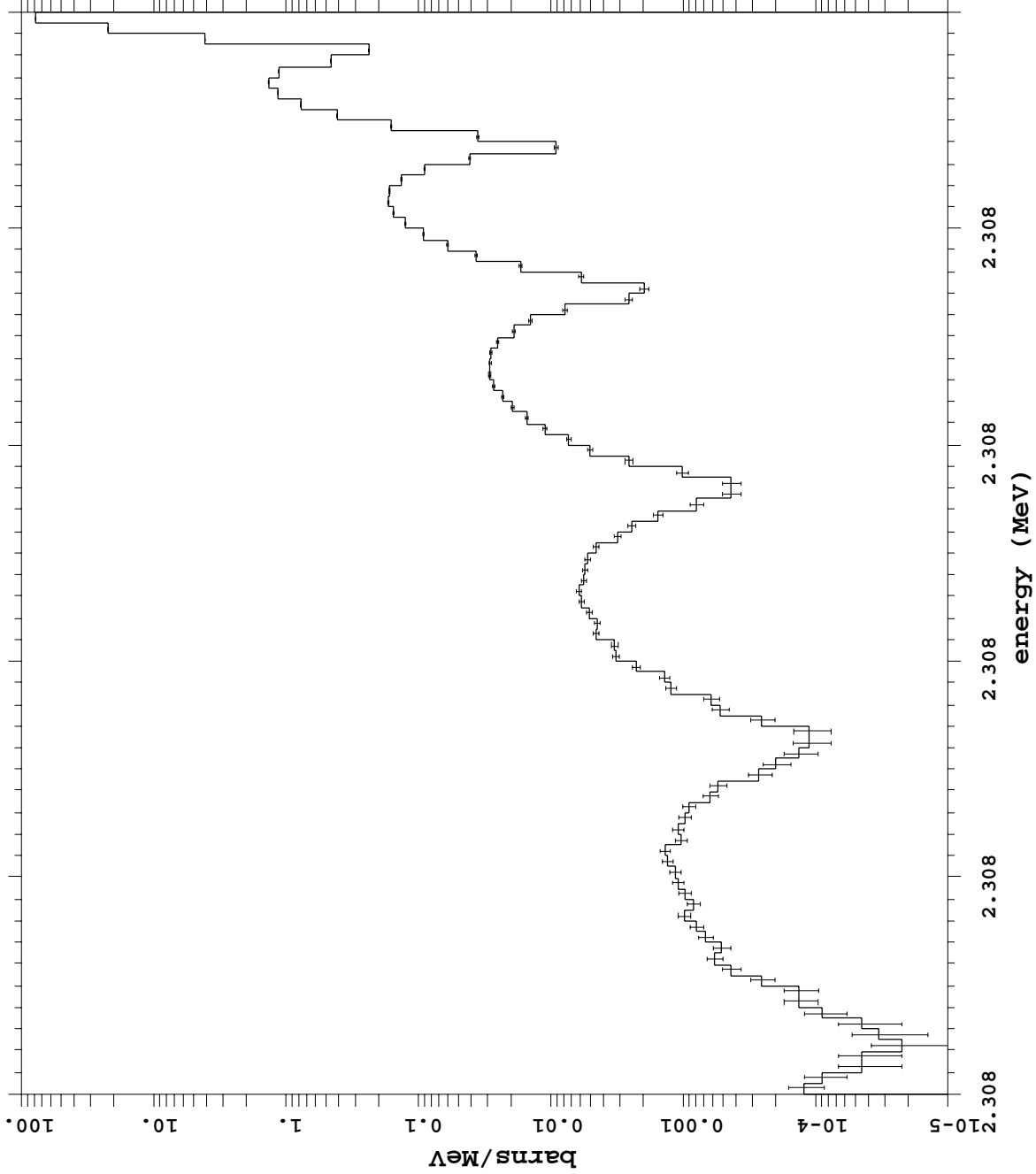
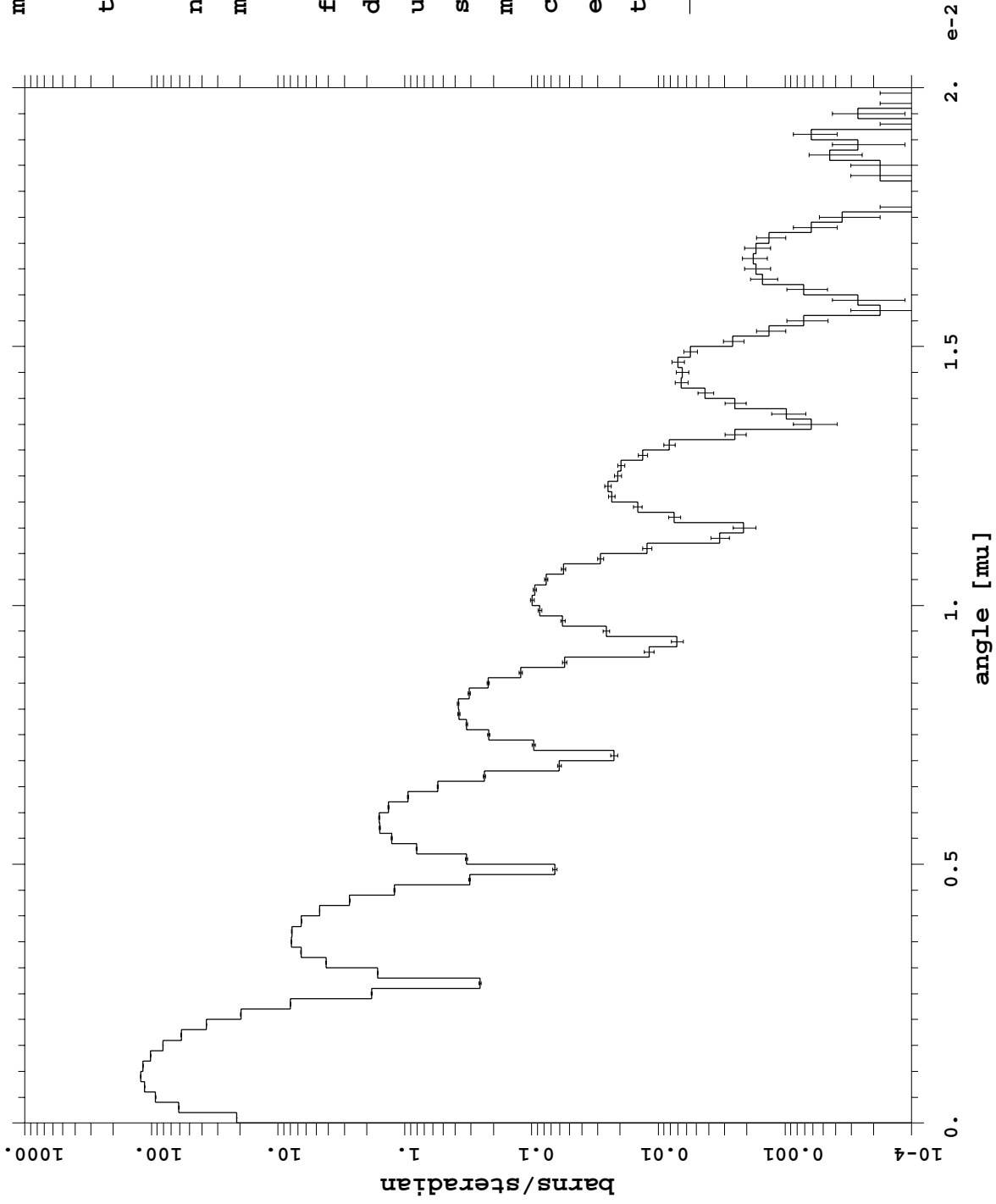mcnp   6.0

tally   299

nps   10000000

mctal = mctal

f   cell   1
d   flag/dir 1
u   user   1
s   segment   1
m   mult   1
c   angle   2   t
e   energy   *
t   time   1

        mctal

barns/MeV

100.
10.
1.
0.1
0.01
0.001
0.0001
10-4
10-5

2.308   2.308   2.308   2.308   2.308   2.308

energy (MeV)

e4

RECOIL2: Elastic Recoil
Angular Distribution

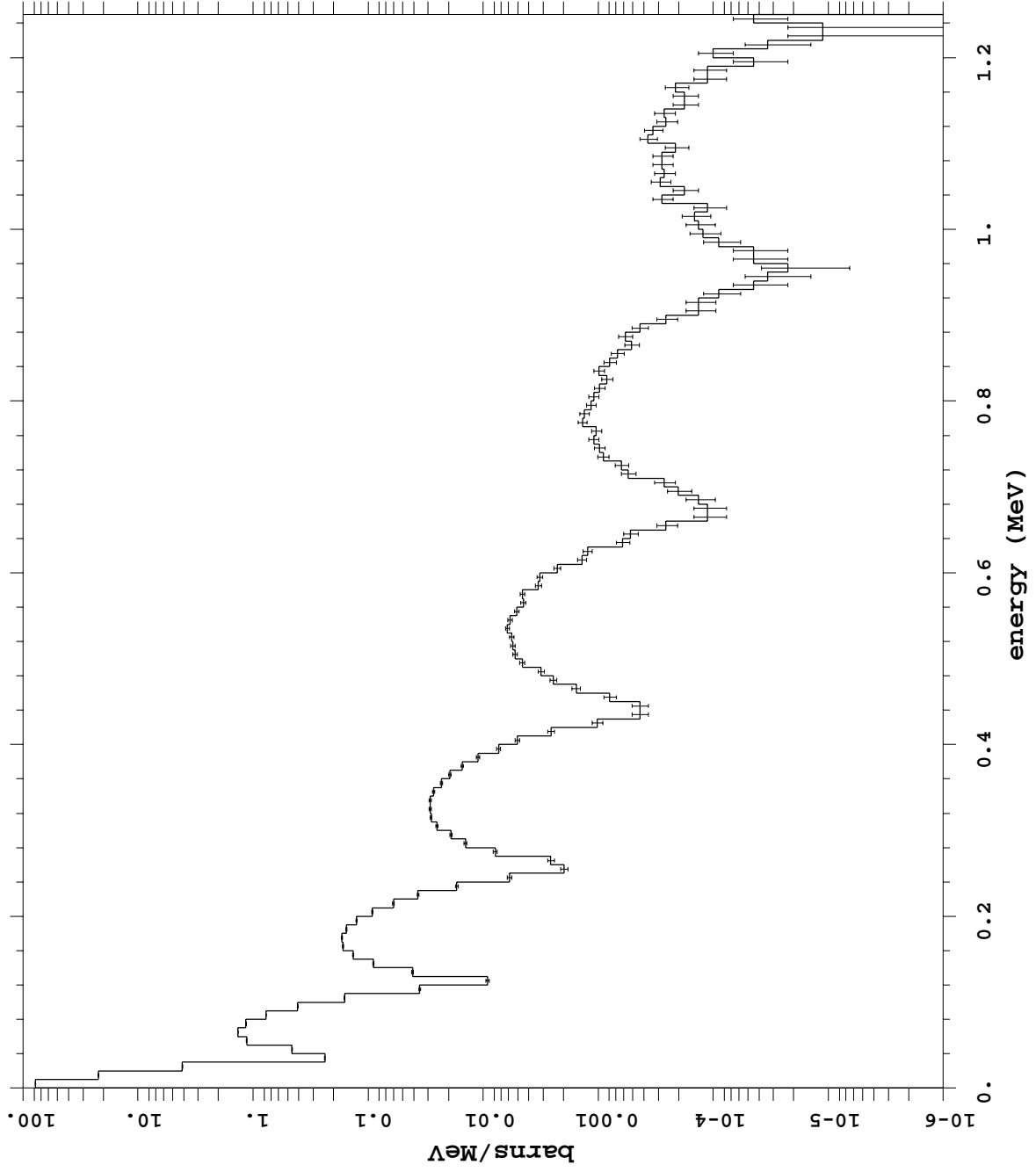mcnp   6.0

tally   398

nps   10000000

mctal = mctal

f   cell   1
d   flag/dir 1
u   user   1
s   segment   1
m   mult   1
c   angle   *
e   energy   2   t
t   time   1

         mctal

barns/steradian

angle [mu]

RECOIL2: Elastic Recoil
Energy Distribution

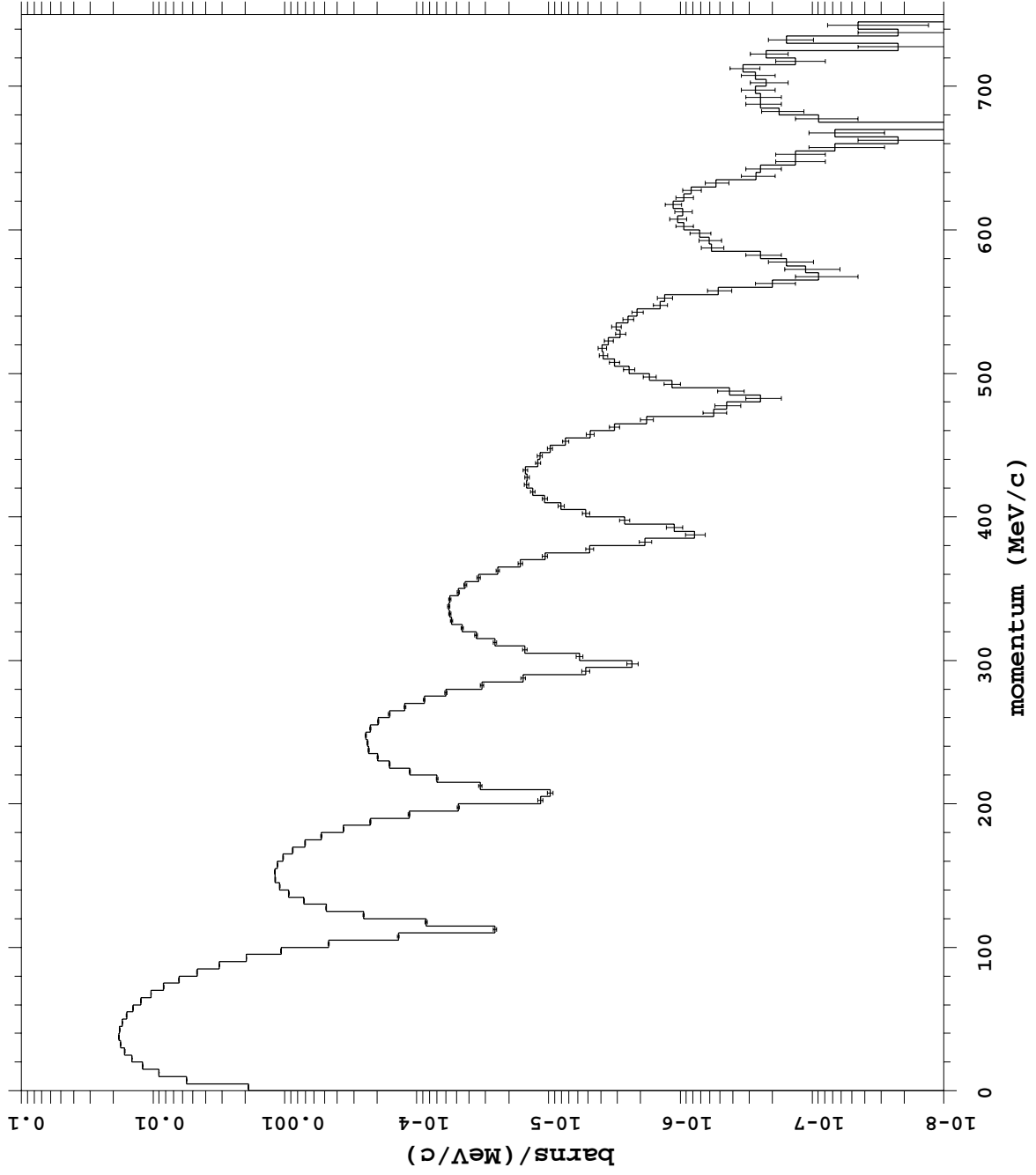mcnp   6.0

tally   498

nps   10000000

mctal = mctal

f   cell   1
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   2   t
e   energy   *
t   time   1

          mctal

energy (MeV)

barns/MeV

RECOIL2: Elastic Recoil

Momentum Distribution

momentum (MeV/c)

barns/(MeV/c)

mcnp   6.0

tally   598

nps   10000000

mctal = mctal

f   cell   1
d   flag/dir   1
u   user   1
s   segment   1
m   mult   1
c   angle   2   t
e   energy   *
t   time   1
    ───── mctal