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Title:	Release of Continuous Representation for S(α, β) ACE Data
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Release of Continuous Representation for S(α, β) ACE Data

D. Kent Parsons and Jeremy Lloyd Conlin

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ATTENTION: This document is long and not intended to be printed. If you do print, please do not print the *many* pages of plots—which begin on page 11—which are best viewed on a computer screen.

1 Background

For low energy neutrons, the default free gas model for scattering cross sections is not always appropriate. Molecular effects or crystalline structure effects can affect the neutron scattering cross sections. These effects are included in the S(α, β) thermal neutron scattering data and are tabulated in `file 7` of the ENDF6 format files. S stands for scattering. α is a momentum transfer variable and β is an energy transfer variable.

The S(α, β) cross sections can include coherent elastic scattering (no E change for the neutron, but specific scattering angles), incoherent elastic scattering (no E change for the neutron, but continuous scattering angles), and inelastic scattering (E change for the neutron, and change in angle as well). Every S(α, β) material will have inelastic scattering and may have either coherent or incoherent elastic scattering (but not both). Coherent elastic scattering cross sections have distinctive jagged-looking Bragg edges, whereas the other cross sections are much smoother.

The evaluated files from the NNDC are processed locally in the `THERMR` module of NJOY. Data can be produced either for continuous energy Monte Carlo codes (using `ACER`) or embedded in multi-group cross sections for deterministic (or even multi-group Monte Carlo) codes (using `GROUPR`).

Currently, the S(α, β) files available for MCNP use discrete energy changes for inelastic scattering. That is, the scattered neutrons can only be emitted at specific energies—rather than across a continuous spectrum of energies. The discrete energies are chosen to preserve the average secondary neutron energy, i.e., in an integral sense, but the discrete treatment does not preserve any differential quantities in energy or angle.

2 New S(α, β) Libraries for MCNP

A new data library for S(α, β) materials for MCNP has been released. It is the first thermal scattering library for MCNP that includes continuous secondary energy data. The new continuous option was processed with the `IWT=2` flag on card `9` of the `ACER` input in NJOY. (The previous discrete representations used `IWT=0` or `1`.) See Appendix B for sample NJOY input decks.

`ACE` files for MCNP have been produced (along with the appropriate entries for the `xsdir` file) for each of the S(α, β) materials and at each of the given temperatures. Version 99.336 of NJOY was used on yellow-rail to process the thermal scattering evaluation files. The new continuous `ACE` files are considerably larger (∼10x) than the previous discrete `ACE` files.

The new library contains all of the same materials as the most recent S(α, β) library [4], `endf70sab`, as well as the latest thermal scattering evaluation addition to ENDF/B-VII.1, SiO_2.

Most of the scattering files are to be used as isotopic replacements in an MCNP run (using the `MT` card). However, two of the $S(\alpha,\beta)$ files (benzene and SiO_2) are to be used as whole material replacements in MCNP.

Most of the $S(\alpha,\beta)$ files have a maximum energy $E_{\max} = 10\,\text{eV}$—which is a `THERMR` input in NJOY. The exceptions are cryogenic materials like liquid and solid methane, para and ortho D and H, or the reactor material, UinUO2. The UinUO2 has a 1 eV maximum—so that the $S(\alpha,\beta)$ does not obscure a low-lying scattering resonance in the uranium at a few eV. MCNP uses the free gas scattering model above E_{max} and $S(\alpha,\beta)$ scattering below it.

The new files have been installed at `/usr/projects/data/nuclear/mc/type1` on the open and secure ICN networks at Los Alamos and should be distributed soon to RSICC with the new version of MCNP 6.

2.1 New Naming Convention for Diatomic $S(\alpha,\beta)$ Materials

A new naming convention has been adopted for the diatomic $S(\alpha,\beta)$ materials. These materials and their new naming scheme are:

- `be-o` beryllium in beryllium oxide,
- `o-be` oxygen in beryllium oxide,
- `h-zr` hydrogen in zirconium hydride,
- `zr-h` zirconium in zirconium hydride,
- `o2-u` oxygen in uranium oxide,
- `u-o2` uranium in uranium oxide.

The new names are reflected in Table 1. The previous convention was to use a slash (/) where now we are using a dash (-). The new naming convention for these materials is intended to avoid filename problems on Unix-like operating systems; i.e., Unix filenames can't have a slash in them.

For this release of the $S(\alpha,\beta)$ data, both the new names (e.g., `o2-u`) and the traditional names (e.g., `o2/u`) will work. Future releases are not guaranteed to include the traditionally named ZAIDs.

In the previous $S(\alpha,\beta)$ data release [4], the ZAID extension for the $S(\alpha,\beta)$ materials were like `1xt` where `x` ranged from 0–8 and represented an evaluated temperature. The new, continuous representation has similar extensions, `2xt`. Both the discrete (`1xt`) and continuous (`2xt`) representations are available in this release. The lone exception is the `sio2` data tables which are only available in the continuous representation.

A complete listing of the $S(\alpha,\beta)$ data tables available for this release is listed in Table 1.

2.2 Cross Section Plots

Cross section plots representative of each set of $S(\alpha,\beta)$ files are given in Appendix D. The `MCPLOT` option of MCNP 5 was used to plot the $S(\alpha,\beta)$ cross sections against the free gas cross sections for the identical isotope or material. A typical `MCPLOT` command would be

```
xs lwtr.10t mt 1 coplot xs 1001.70c mt -3
```

The intention of these plots was to verify that the higher energy $S(\alpha,\beta)$ cross sections asymptote into the free gas cross sections.

3 Testing the New $S(\alpha,\beta)$ Data Files

The deficiencies in the old, discrete $S(\alpha,\beta)$-representation was noted by Cullen, et al. [3]. In their paper they show a series of calculations in what they call the "broomstick" problem to show that the secondary energy and angular distribution is discrete instead of continuous as one would expect.

The broomstick problem consists of a very long (10^5 cm) and very narrow (10^{-8} cm radius) cylinder filled with the scattering material and surrounded by a vacuum. A thermal monoenergetic ($E = 0.0253$ eV) source is placed in the middle of the broomstick. The energy and angular distribution of neutrons are tallied on planes perpendicular to the ends of the broomstick. With this geometry, any neutron that scatters will leave the broomstick and stream until it is tallied on the planes perpendicular to the ends of the cylinder.

As a test of our $S(\alpha, \beta)$ data files we have performed the broomstick calculations for all of our continuous and discrete representations of the $S(\alpha, \beta)$ thermal scattering data. For comparison, we have also performed the broomstick calculation with the thermal scattering treatment turned off; accomplished in MCNP by having no `MT` card. The secondary neutron energy and angular distributions were plotted and are included in Appendix C.

4 Archival Information

All of the files used to create these new $S(\alpha, \beta)$ data tables have been archived in `/hpss/nucldata/mc/type1/endf71sab` If you have need of this data, please contact a member of the Nuclear Data Team at Los Alamos National Laboratory `nucldata@lanl.gov`.

Table 1: $S(\alpha, \beta)$ cross section libraries available in MCNP.

Discrete ZAID	Continuous ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Data
			Aluminum-27 (13027)					
al27.10t	al27.20t	endf70sab	ENDF/B-VII.0	2005	20	20	80	coh
al27.11t	al27.21t	endf70sab	ENDF/B-VII.0	2005	80	20	80	coh
al27.12t	al27.22t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
al27.13t	al27.23t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
al27.14t	al27.24t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh
al27.15t	al27.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh
			Beryllium Metal (4009)					
be.10t	be.20t	endf70sab	ENDF/B-VII.0	1993	293.6	20	80	coh
be.11t	be.21t	endf70sab	ENDF/B-VII.0	1993	400	20	80	coh
be.12t	be.22t	endf70sab	ENDF/B-VII.0	1993	500	20	80	coh
be.13t	be.23t	endf70sab	ENDF/B-VII.0	1993	600	20	80	coh
be.14t	be.24t	endf70sab	ENDF/B-VII.0	1993	700	20	80	coh
be.15t	be.25t	endf70sab	ENDF/B-VII.0	1993	800	20	80	coh
be.16t	be.26t	endf70sab	ENDF/B-VII.0	1993	1000	20	80	coh
be.17t	be.27t	endf70sab	ENDF/B-VII.0	1993	1200	20	80	coh
			Beryllium in Beryllium Oxide (4009)					
be-o.10t	be-o.20t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
be-o.11t	be-o.21t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
be-o.12t	be-o.22t	endf70sab	ENDF/B-VII.0	2005	500	20	80	coh
be-o.13t	be-o.23t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh
be-o.14t	be-o.24t	endf70sab	ENDF/B-VII.0	2005	700	20	80	coh
be-o.15t	be-o.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh

[a] All of the $S(\alpha, \beta)$ data is taken from the ENDF/B-VII.0 [1] release. The lone exception is `sio2` which comes from ENDF/B-VII.1 [2].

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Table 1: S(α, β) cross section libraries available in MCNP (continued).

Discrete ZAID	Continuous ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Data
be-o.16t	be-o.26t	endf70sab	ENDF/B-VII.0	2005	1000	20	80	coh
be-o.17t	be-o.27t	endf70sab	ENDF/B-VII.0	2005	1200	20	80	coh
			Benzene (1001, 6000, 6012)					
benz.10t	benz.20t	endf70sab	ENDF/B-VII.0	1969	293.6	20	80	none
benz.11t	benz.21t	endf70sab	ENDF/B-VII.0	1969	350	20	80	none
benz.12t	benz.22t	endf70sab	ENDF/B-VII.0	1969	400	20	80	none
benz.13t	benz.23t	endf70sab	ENDF/B-VII.0	1969	450	20	80	none
benz.14t	benz.24t	endf70sab	ENDF/B-VII.0	1969	500	20	80	none
benz.15t	benz.25t	endf70sab	ENDF/B-VII.0	1969	600	20	80	none
benz.16t	benz.26t	endf70sab	ENDF/B-VII.0	1969	800	20	80	none
benz.17t	benz.27t	endf70sab	ENDF/B-VII.0	1969	1000	20	80	none
			Ortho Deuterium (1002)					
dortho.10t	dortho.20t	endf70sab	ENDF/B-VII.0	1993	19	20	80	none
			Para Deuterium (1002)					
dpara.10t	dpara.20t	endf70sab	ENDF/B-VII.0	1993	19	20	80	none
			Iron-56 (26056)					
fe56.10t	fe56.20t	endf70sab	ENDF/B-VII.0	2005	20	20	80	coh
fe56.11t	fe56.21t	endf70sab	ENDF/B-VII.0	2005	80	20	80	coh
fe56.12t	fe56.22t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
fe56.13t	fe56.23t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
fe56.14t	fe56.24t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh
fe56.15t	fe56.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh
			Graphite (6000, 6012)					
grph.10t	grph.20t	endf70sab	ENDF/B-VII.0	1993	293.6	20	80	coh
grph.11t	grph.21t	endf70sab	ENDF/B-VII.0	1993	400	20	80	coh
grph.12t	grph.22t	endf70sab	ENDF/B-VII.0	1993	500	20	80	coh
grph.13t	grph.23t	endf70sab	ENDF/B-VII.0	1993	600	20	80	coh
grph.14t	grph.24t	endf70sab	ENDF/B-VII.0	1993	700	20	80	coh
grph.15t	grph.25t	endf70sab	ENDF/B-VII.0	1993	800	20	80	coh
grph.16t	grph.26t	endf70sab	ENDF/B-VII.0	1993	1000	20	80	coh
grph.17t	grph.27t	endf70sab	ENDF/B-VII.0	1993	1200	20	80	coh
grph.18t	grph.28t	endf70sab	ENDF/B-VII.0	1993	1600	20	80	coh
grph.19t	grph.29t	endf70sab	ENDF/B-VII.0	1993	2000	20	80	coh
			Hydrogen in Zirconium Hydride (1001)					
h-zr.10t	h-zr.20t	endf70sab	ENDF/B-VII.0	1993	293.6	20	80	inco
h-zr.11t	h-zr.21t	endf70sab	ENDF/B-VII.0	1993	400	20	80	inco
h-zr.12t	h-zr.22t	endf70sab	ENDF/B-VII.0	1993	500	20	80	inco
h-zr.13t	h-zr.23t	endf70sab	ENDF/B-VII.0	1993	600	20	80	inco
h-zr.14t	h-zr.24t	endf70sab	ENDF/B-VII.0	1993	700	20	80	inco
h-zr.15t	h-zr.25t	endf70sab	ENDF/B-VII.0	1993	800	20	80	inco
h-zr.16t	h-zr.26t	endf70sab	ENDF/B-VII.0	1993	1000	20	80	inco

[a] All of the S(α, β) data is taken from the ENDF/B-VII.0 [1] release. The lone exception is `sio2` which comes from ENDF/B-VII.1 [2].

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Table 1: S(α, β) cross section libraries available in MCNP (continued).

Discrete ZAID	Continuous ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Data
h-zr.17t	h-zr.27t	endf70sab	ENDF/B-VII.0	1993	1200	20	80	inco
			Ortho Hydrogen (1001)					
hortho.10t	hortho.20t	endf70sab	ENDF/B-VII.0	1993	20	20	80	none
			Para Hydrogen (1001)					
hpara.10t	hpara.20t	endf70sab	ENDF/B-VII.0	1993	20	20	80	none
			Deuterium in Heavy Water (1002)					
hwtr.10t	hwtr.20t	endf70sab	ENDF/B-VII.0	2004	293.6	20	80	none
hwtr.11t	hwtr.21t	endf70sab	ENDF/B-VII.0	2004	350	20	80	none
hwtr.12t	hwtr.22t	endf70sab	ENDF/B-VII.0	2004	400	20	80	none
hwtr.13t	hwtr.23t	endf70sab	ENDF/B-VII.0	2004	450	20	80	none
hwtr.14t	hwtr.24t	endf70sab	ENDF/B-VII.0	2004	500	20	80	none
hwtr.15t	hwtr.25t	endf70sab	ENDF/B-VII.0	2004	550	20	80	none
hwtr.16t	hwtr.26t	endf70sab	ENDF/B-VII.0	2004	600	20	80	none
hwtr.17t	hwtr.27t	endf70sab	ENDF/B-VII.0	2004	650	20	80	none
			Hydrogen in Liquid Methane (1001)					
lmeth.10t	lmeth.20t	endf70sab	ENDF/B-VII.0	1993	100	20	80	none
			Hydrogen in Light Water (1001)					
lwtr.10t	lwtr.20t	endf70sab	ENDF/B-VII.0	2006	293.6	20	80	none
lwtr.11t	lwtr.21t	endf70sab	ENDF/B-VII.0	2006	350	20	80	none
lwtr.12t	lwtr.22t	endf70sab	ENDF/B-VII.0	2006	400	20	80	none
lwtr.13t	lwtr.23t	endf70sab	ENDF/B-VII.0	2006	450	20	80	none
lwtr.14t	lwtr.24t	endf70sab	ENDF/B-VII.0	2006	500	20	80	none
lwtr.15t	lwtr.25t	endf70sab	ENDF/B-VII.0	2006	550	20	80	none
lwtr.16t	lwtr.26t	endf70sab	ENDF/B-VII.0	2006	600	20	80	none
lwtr.17t	lwtr.27t	endf70sab	ENDF/B-VII.0	2006	650	20	80	none
lwtr.18t	lwtr.28t	endf70sab	ENDF/B-VII.0	2006	800	20	80	none
			Oxygen in Beryllium Oxide (8016, 8017, 8018)					
o-be.10t	o-be.20t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
o-be.11t	o-be.21t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
o-be.12t	o-be.22t	endf70sab	ENDF/B-VII.0	2005	500	20	80	coh
o-be.13t	o-be.23t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh
o-be.14t	o-be.24t	endf70sab	ENDF/B-VII.0	2005	700	20	80	coh
o-be.15t	o-be.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh
o-be.16t	o-be.26t	endf70sab	ENDF/B-VII.0	2005	1000	20	80	coh
o-be.17t	o-be.27t	endf70sab	ENDF/B-VII.0	2005	1200	20	80	coh
			Oxygen in UO2 (8016, 8017, 8018)					
o2-u.10t	o2-u.20t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
o2-u.11t	o2-u.21t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
o2-u.12t	o2-u.22t	endf70sab	ENDF/B-VII.0	2005	500	20	80	coh
o2-u.13t	o2-u.23t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh

[a] All of the S(α, β) data is taken from the ENDF/B-VII.0 [1] release. The lone exception is `sio2` which comes from ENDF/B-VII.1 [2].

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Table 1: S(α, β) cross section libraries available in MCNP (continued).

Discrete ZAID	Continuous ZAID	Library Name	Source	Eval Date	Temp (K)	Num of Angles	Num of Energies	Elastic Data
o2-u.14t	o2-u.24t	endf70sab	ENDF/B-VII.0	2005	700	20	80	coh
o2-u.15t	o2-u.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh
o2-u.16t	o2-u.26t	endf70sab	ENDF/B-VII.0	2005	1000	20	80	coh
o2-u.17t	o2-u.27t	endf70sab	ENDF/B-VII.0	2005	1200	20	80	coh
Hydrogen in Polyethylene (1001)								
poly.10t	poly.20t	endf70sab	ENDF/B-VII.0	1969	293.6	20	80	inco
poly.11t	poly.21t	endf70sab	ENDF/B-VII.0	1969	350	20	80	inco
Silicon and Oxygen in Silicon Dioxide (8016, 14028, 14029)								
—	sio2.20t[a]	endf71sab	ENDF/B-VII.1	2010	293.6	20	80	coh
—	sio2.21t[a]	endf71sab	ENDF/B-VII.1	2010	350	20	80	coh
—	sio2.22t[a]	endf71sab	ENDF/B-VII.1	2010	400	20	80	coh
—	sio2.23t[a]	endf71sab	ENDF/B-VII.1	2010	500	20	80	coh
—	sio2.24t[a]	endf71sab	ENDF/B-VII.1	2010	800	20	80	coh
—	sio2.25t[a]	endf71sab	ENDF/B-VII.1	2010	1000	20	80	coh
—	sio2.26t[a]	endf71sab	ENDF/B-VII.1	2010	1200	20	80	coh
Hydrogen in Solid Methane (1001)								
smeth.10t	smeth.20t	endf70sab	ENDF/B-VII.0	1993	22	20	80	inco
Uranium-238 in Uranium Oxide (92238)								
u-o2.10t	u-o2.20t	endf70sab	ENDF/B-VII.0	2005	293.6	20	80	coh
u-o2.11t	u-o2.21t	endf70sab	ENDF/B-VII.0	2005	400	20	80	coh
u-o2.12t	u-o2.22t	endf70sab	ENDF/B-VII.0	2005	500	20	80	coh
u-o2.13t	u-o2.23t	endf70sab	ENDF/B-VII.0	2005	600	20	80	coh
u-o2.14t	u-o2.24t	endf70sab	ENDF/B-VII.0	2005	700	20	80	coh
u-o2.15t	u-o2.25t	endf70sab	ENDF/B-VII.0	2005	800	20	80	coh
u-o2.16t	u-o2.26t	endf70sab	ENDF/B-VII.0	2005	1000	20	80	coh
u-o2.17t	u-o2.27t	endf70sab	ENDF/B-VII.0	2005	1200	20	80	coh
Zirconium in Zirconium Hydride (40000, 40090, 40091, 40092, 40094, 40096)								
zr-h.10t	zr-h.20t	endf70sab	ENDF/B-VII.0	1993	293.6	20	80	inco
zr-h.11t	zr-h.21t	endf70sab	ENDF/B-VII.0	1993	400	20	80	inco
zr-h.12t	zr-h.22t	endf70sab	ENDF/B-VII.0	1993	500	20	80	inco
zr-h.13t	zr-h.23t	endf70sab	ENDF/B-VII.0	1993	600	20	80	inco
zr-h.14t	zr-h.24t	endf70sab	ENDF/B-VII.0	1993	700	20	80	inco
zr-h.15t	zr-h.25t	endf70sab	ENDF/B-VII.0	1993	800	20	80	inco
zr-h.16t	zr-h.26t	endf70sab	ENDF/B-VII.0	1993	1000	20	80	inco
zr-h.17t	zr-h.27t	endf70sab	ENDF/B-VII.0	1993	1200	20	80	inco

[a] All of the S(α, β) data is taken from the ENDF/B-VII.0 [1] release. The lone exception is `sio2` which comes from ENDF/B-VII.1 [2].

References

[1] M. B. Chadwick, P. Obložinskỳ, M. Herman, N. M. Greene, R. D. McKnight, D. L. Smith, P. G. Young, R. E. MacFarlane, G. M. Hale, S. C. Frankle, A. C. Kahler, T. Kawano, R. C. Little, D. G. Madland, P. Moller, R. D. Mosteller, P. R. Page, P. Talou, H. Trellue, M. C. White, W. B. Wilson, R. Arcilla, C. L. Dunford, S. F. Mughabghab, B. Pritychenko, D. Rochman, A. A. Sonzogni, C. R. Lubitz, T. H. Trumbull, J. P. Weinman, D. A. Brown, D. E. Cullen, D. P. Heinrichs, D. P. McNabb, H. Derrien, M. E. Dunn, N. M. Larson, L. C. Leal, A. D. Carlson, R. C. Block, J. B. Briggs, E. T. Cheng, H. C. Huria, M. L. Zerkle, K. S. Kozier, A. Courcelle, V. Pronyaev, and S. C. van der Marck. ENDF/B-VII.0: Next generation evaluated nuclear data library for nuclear science and technology. *Nuclear Data Sheets*, 107(12):2931–3059, December 2006.

[2] M.B. Chadwick, M. Herman, P. Obložinskỳ, M.E. Dunn, Y. Danon, A.C. Kahler, D.L. Smith, B. Pritychenko, G. Arbanas, R. Arcilla, R. Brewer, D.A. Brown, R. Capote, A.D. Carlson, Y.S. Cho, H. Derrien, K. Guber, G.M. Hale, S. Hoblit, S. Holloway, T.D. Johnson, T. Kawano, B.C. Kiedrowski, H. Kim, S. Kunieda, N.M. Larson, L. Leal, J.P. Lestone, R.C. Little, E.A. McCutchan, R.E. MacFarlane, M. MacInnes, C.M. Mattoon, R.D. McKnight, S.F. Mughabghab, G.P.A. Nobre, G. Palmiotti, A. Palumbo, M.T. Pigni, V.G. Pronyaev, R.O. Sayer, A.A. Sonzogni, N.C. Summers, P. Talou, I.J. Thompson, A. Trkov, R.L. Vogt, S.C. van der Marck, A. Wallner, M.C. White, D. Wiarda, and P.G. Young. ENDF/B-VII.1 nuclear data for science and technology: Cross sections, covariances, fission product yields and decay data. *Nuclear Data Sheets*, 112(12):2887 – 2996, 2011.

[3] D. E. Cullen, L. F. Hansen, E. M. Lent, and E. F. Plechaty. Thermal scattering law data: Implementation and testing using the monte carlo neutron transport codes cog, mcnp and tart. Technical Report UCRL-ID-153656, Lawrence Livermore National Laboratory, May 17 2003.

[4] Holly R. Trellue and Robert C. Little. Release of new mcnp s(alpha,beta) library ENDF70SAB based on ENDF/B-VII.0. Technical Report LA-UR-08-3628, Los Alamos National Laboratory, 2008.

A Sample MCNP Input File

```
test of ENDF/B-VII data
1  1 -1.0 -1 2 -3  imp:n=1
2  0       -2:3    imp:n=0
3  0    1 -4 2 -3  imp:n=1

1   cx 1.0e-8
2   px 0
3   px 1.0e5
4   cx 1.0e99

print
nps 1E10
sdef pos=5.0e4 0 0 erg=0.0253e-6 vec=1 0 0 nrm=1  dir=1
tmp 2.53e-08 2.53e-08 2.53e-08
ctme 15.0
m1  1001.70c    2.0   8016.70c 1.0
mt1    lwtr.20t
f1:n 1
f11:n 2
c11   -1.0 199I 1.0
e11   1.0e-6
f21:n 3
c21   -1.0 199I 1.0
e21   1.0e-6
e0  1.0e-10 300ilog 1.0e-6
f31:n 2
c31   -1.0 499I 0.90 249I 0.99 100I 1.0
e31   1.0e-6
f41:n 3
c41   -1.0 499I 0.90 249I 0.99 100I 1.0
e41   1.0e-6
```

B Sample NJOY Input Files

B.1 Temperature Independent NJOY Input

```
moder
20 -21
reconr
-21 -22
'pendf tape for ENDF/B-VII 1-H-1'/
125 14 0/
.001/
'1-H-1 from ENDF/B-VII'/
'processed with njoy at 0.1%'/
'the following reaction types are added'/
'     mt20x   gas production'/
'     mt221   free thermal scattering'/
'     mt222   h in h2o thermal scattering'/
'     mt223   h in poly inelastic thermal scattering'/
'     mt224   h in poly elastic thermal scattering'/
'     mt225   h in zrh inelastic thermal scattering'/
'     mt226   h in zrh elastic thermal scattering'/
'     mt227   h in benzine thermal scattering'/
'     mt301   total heating kerma factor'/
'     mt443   kinematic kerma'/
'     mt444   total damage energy production'/
0/
broadr
-21 -22 -23
125 9/
.001/
293.6  350  400  450  500  550  600  650  800 /
0/
heatr
-21 -23 -24/
125 4/
302 402 443 444 /
thermr
30 -24 -25
1 125 20 9 4 0 2 222 1/
293.6  350  400  450  500  550  600  650  800
.001 10./
gaspr
-21 -25 -27
moder
-27 28
stop
```

B.2 Temperature Dependent Input for ACER Module

```
acer
30 28 0 31 32
2 0 1 .28/
'H in h2o at 800K from ENDF/B-VII'/
125 800 'lwtr'/
1001/
222 80 0 0 1 10.1 2/
acer
0 31 35 33 34/
7 1/
'H in h2o at 800K from ENDF/B-VII'/
stop
```

C Secondary Distributions Plots

C.1 Continuous

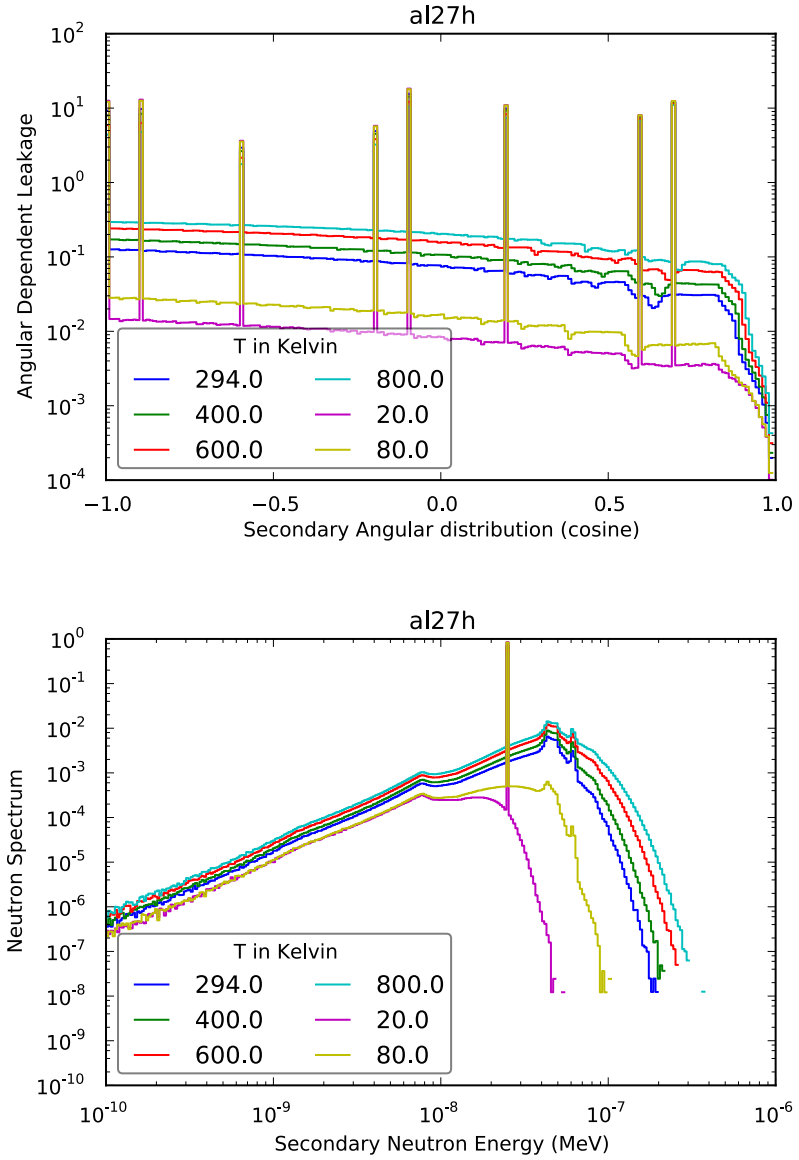


Figure 1: Continuous al27h

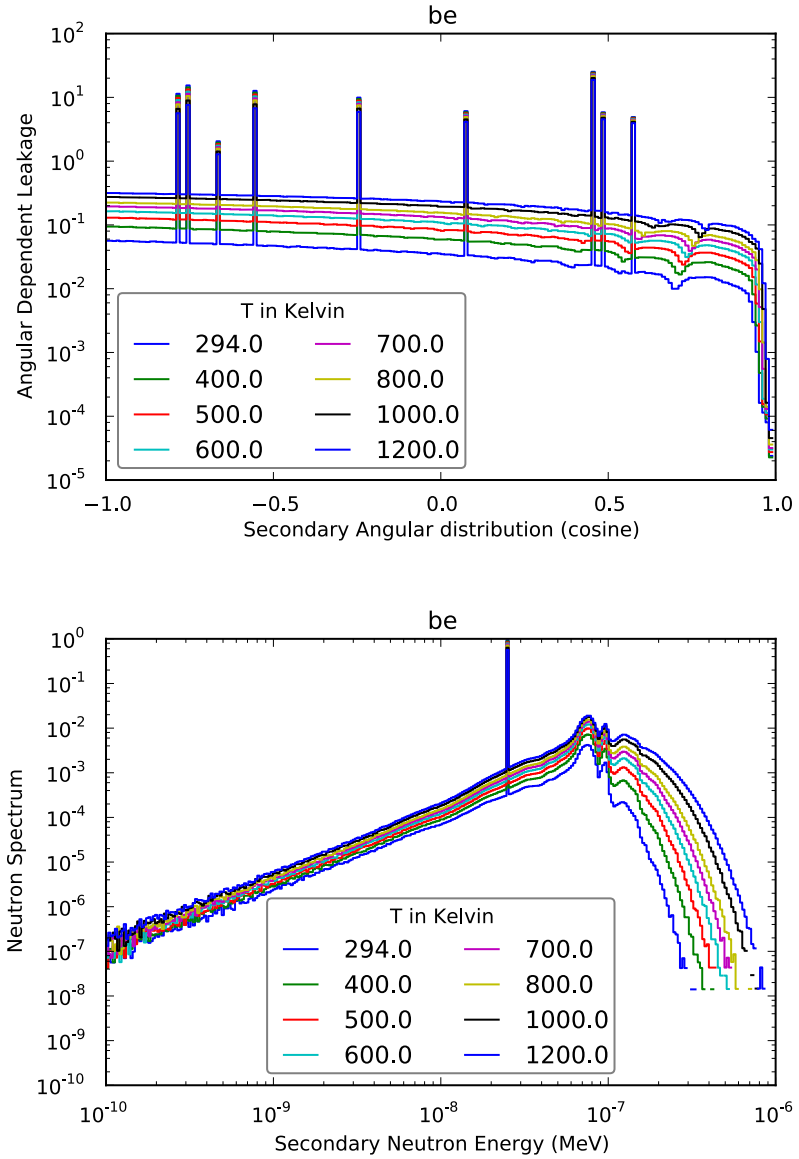


Figure 2: Continuous be

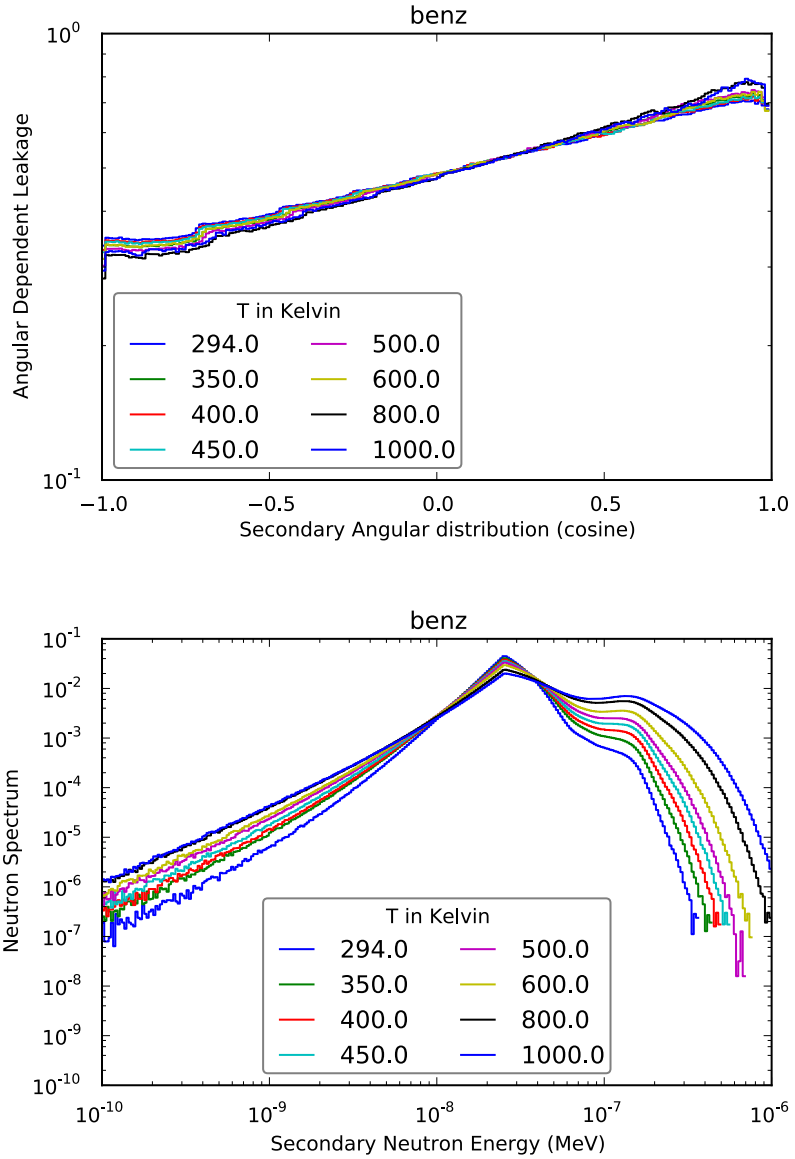


Figure 3: Continuous benz

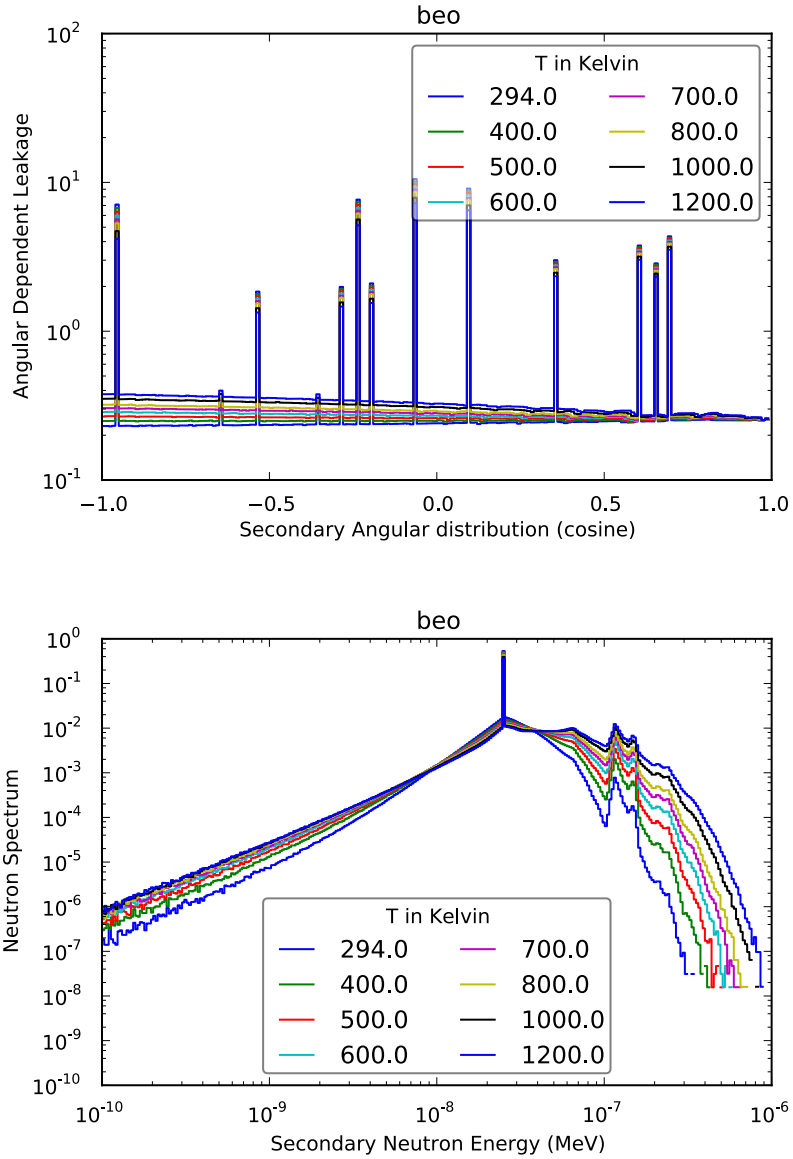


Figure 4: Continuous beo

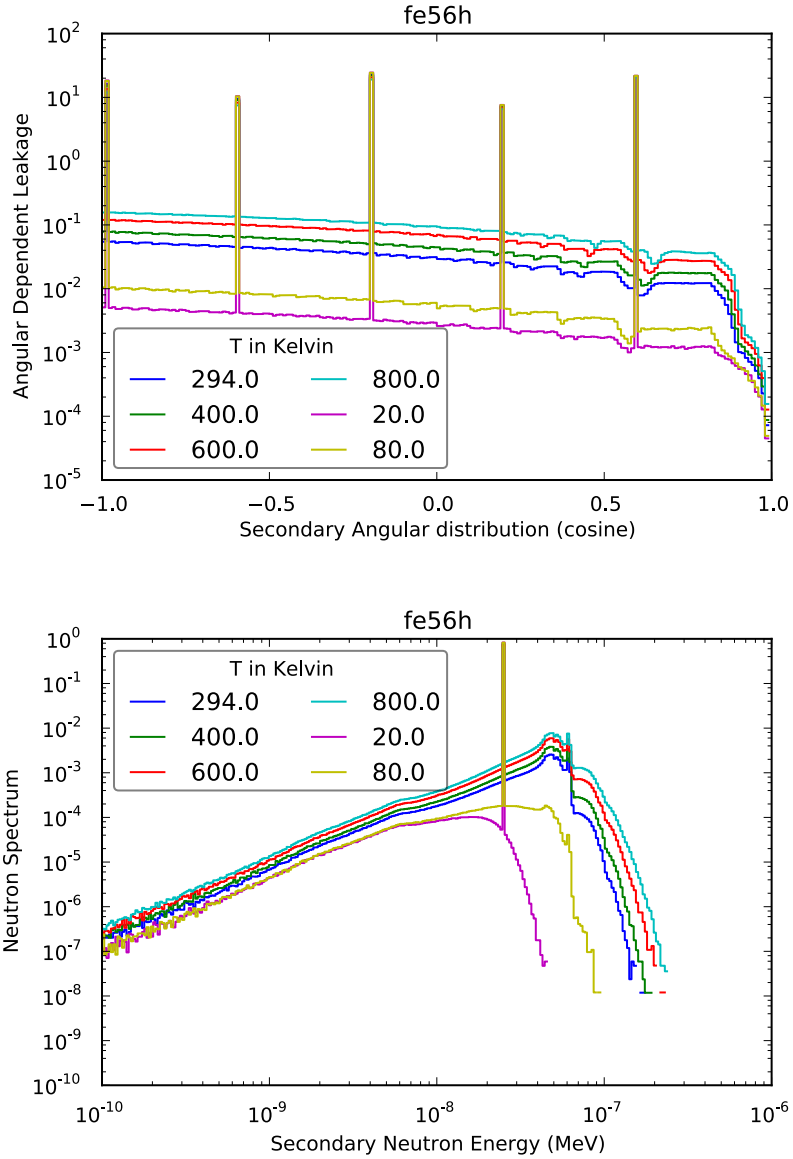


Figure 5: Continuous fe56h

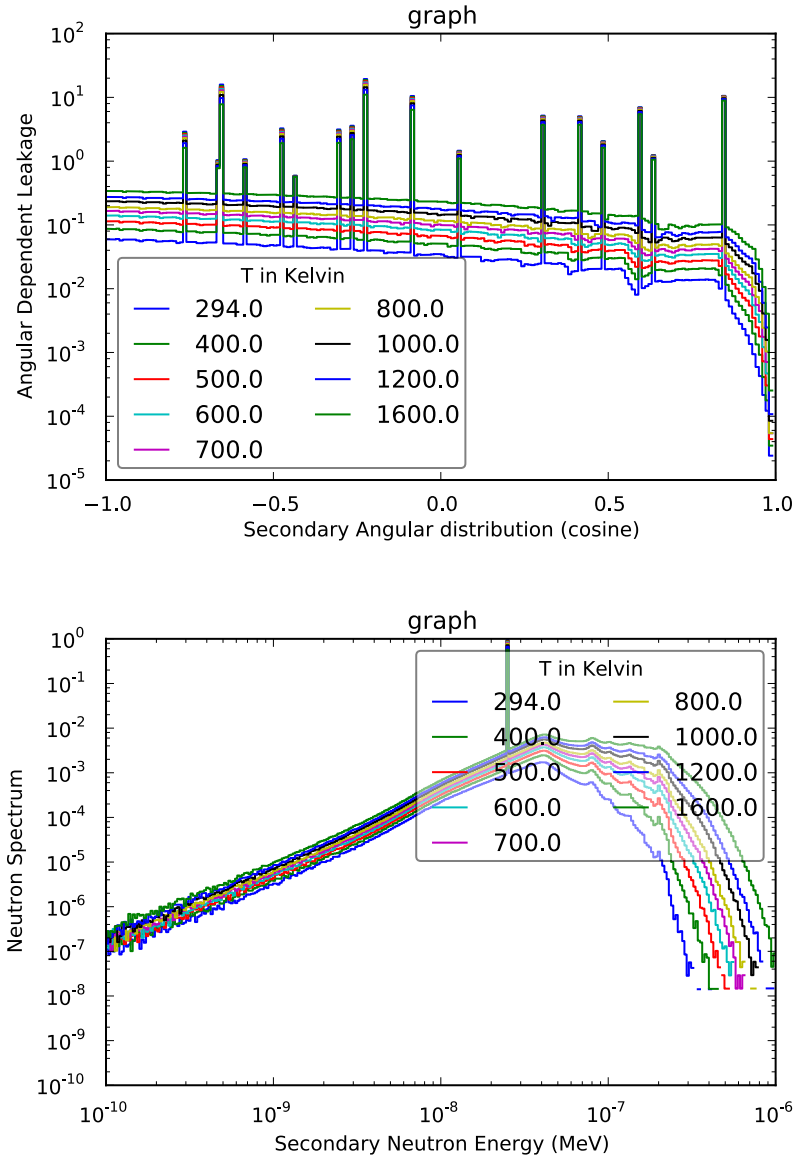


Figure 6: Continuous graph

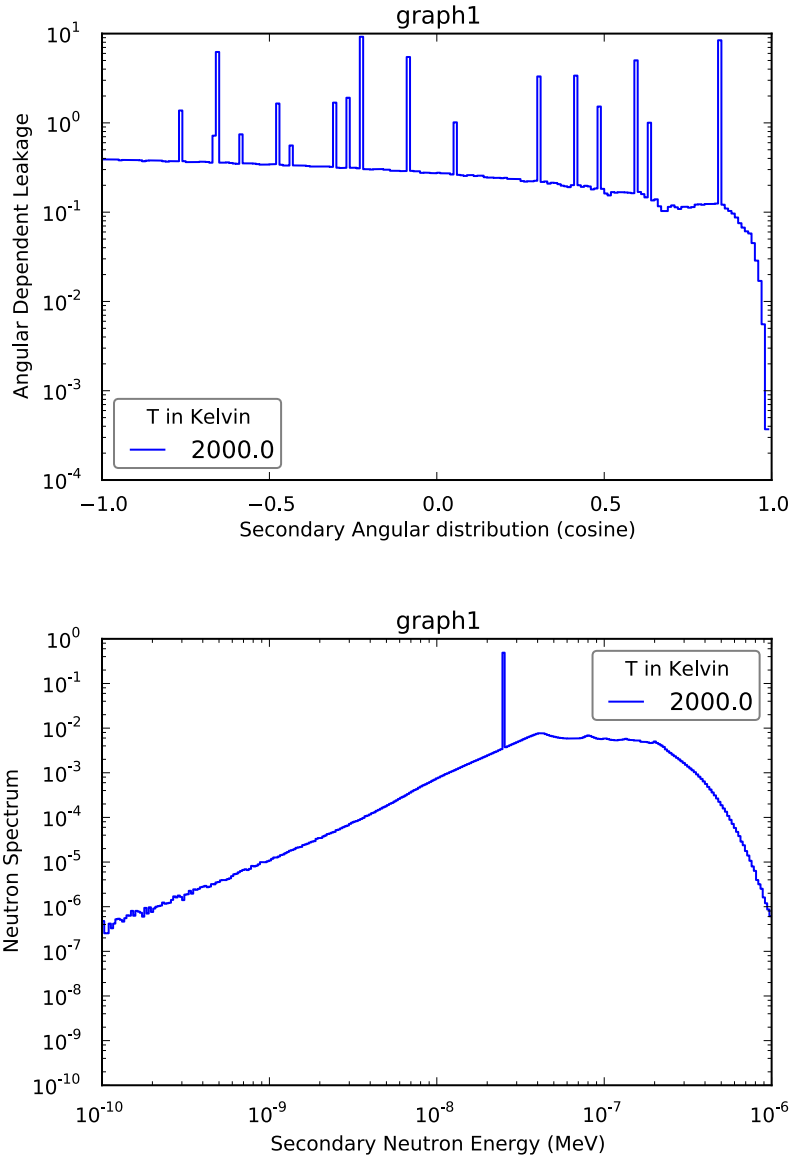


Figure 7: Continuous graph1

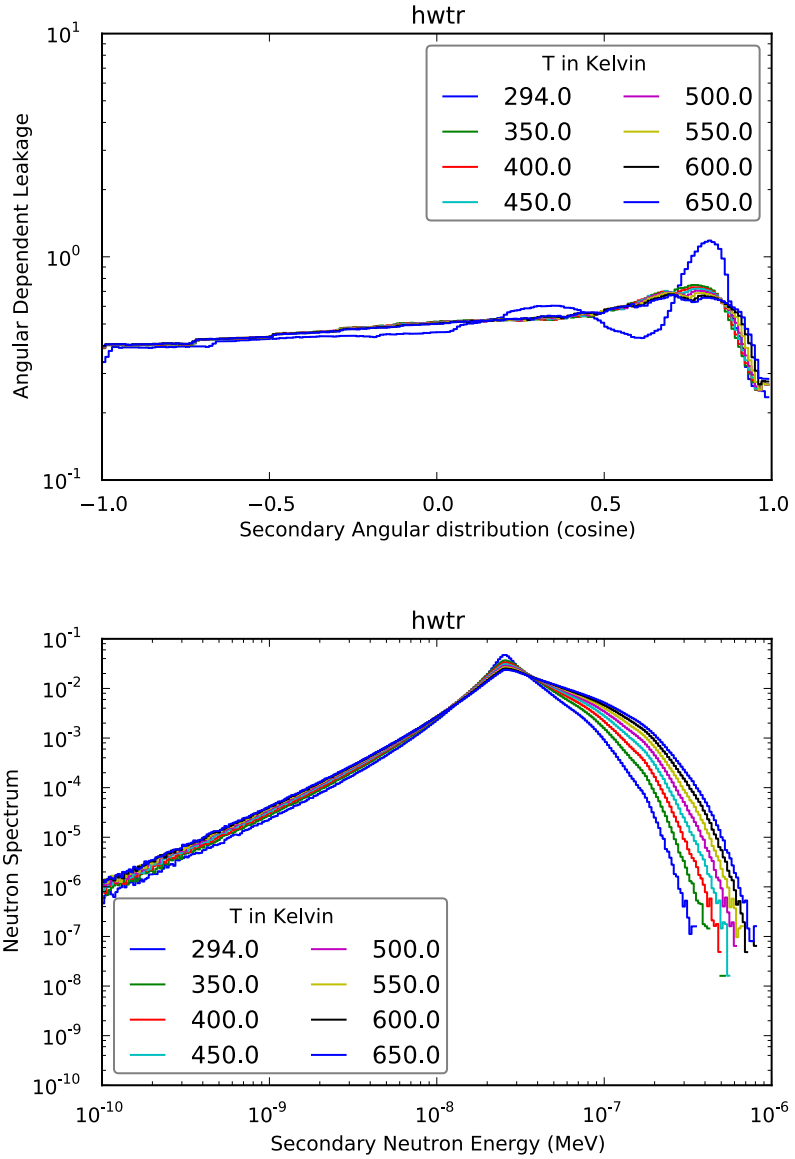


Figure 8: Continuous hwtr

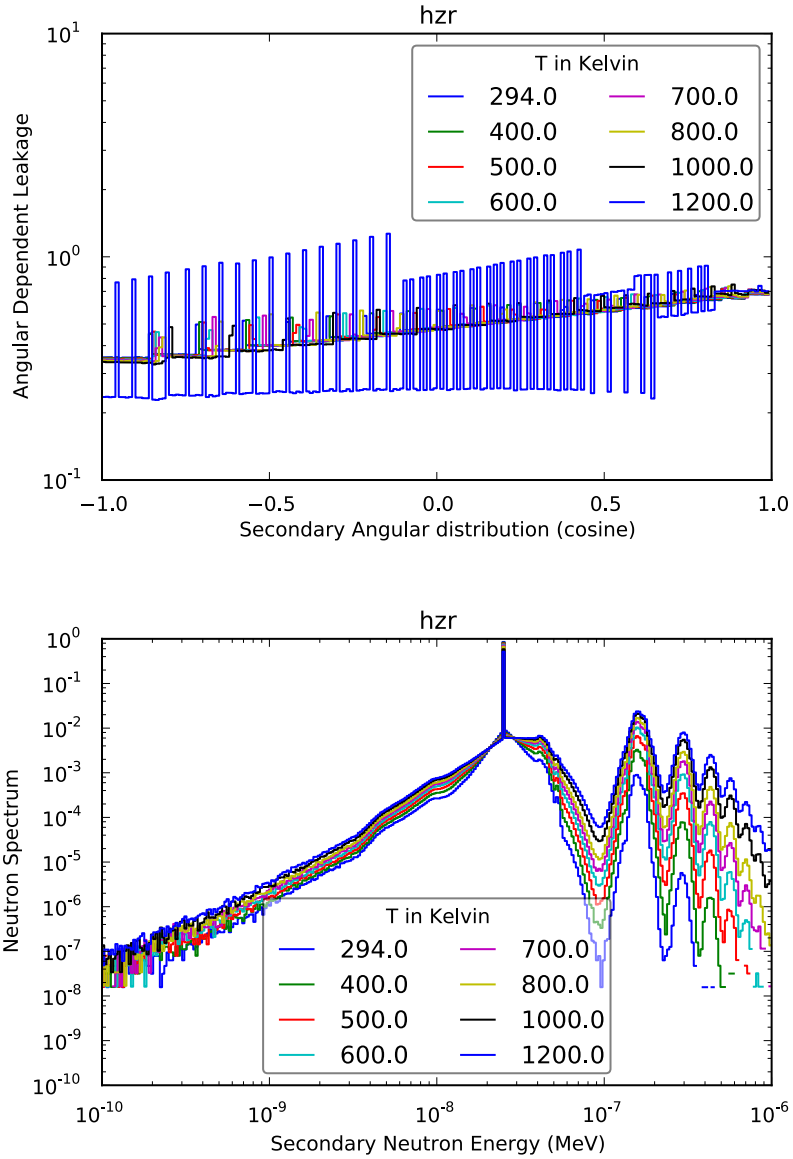


Figure 9: Continuous hzr

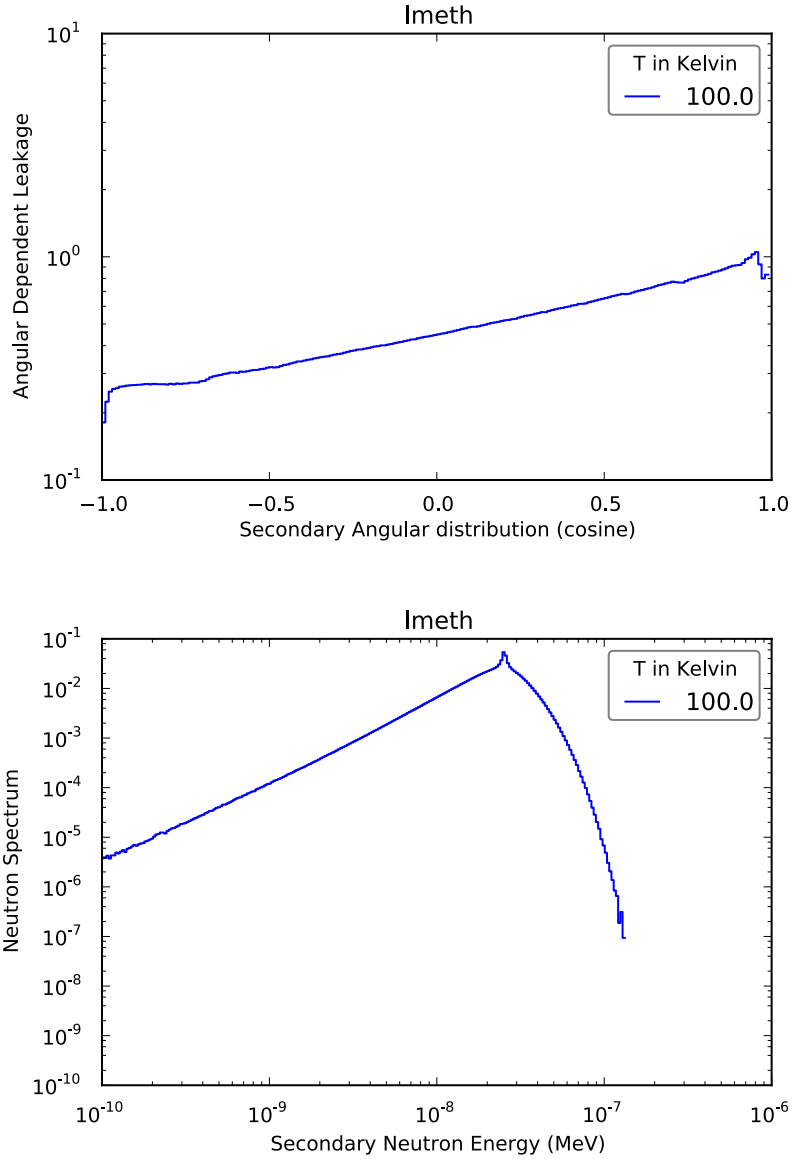


Figure 10: Continuous lmeth

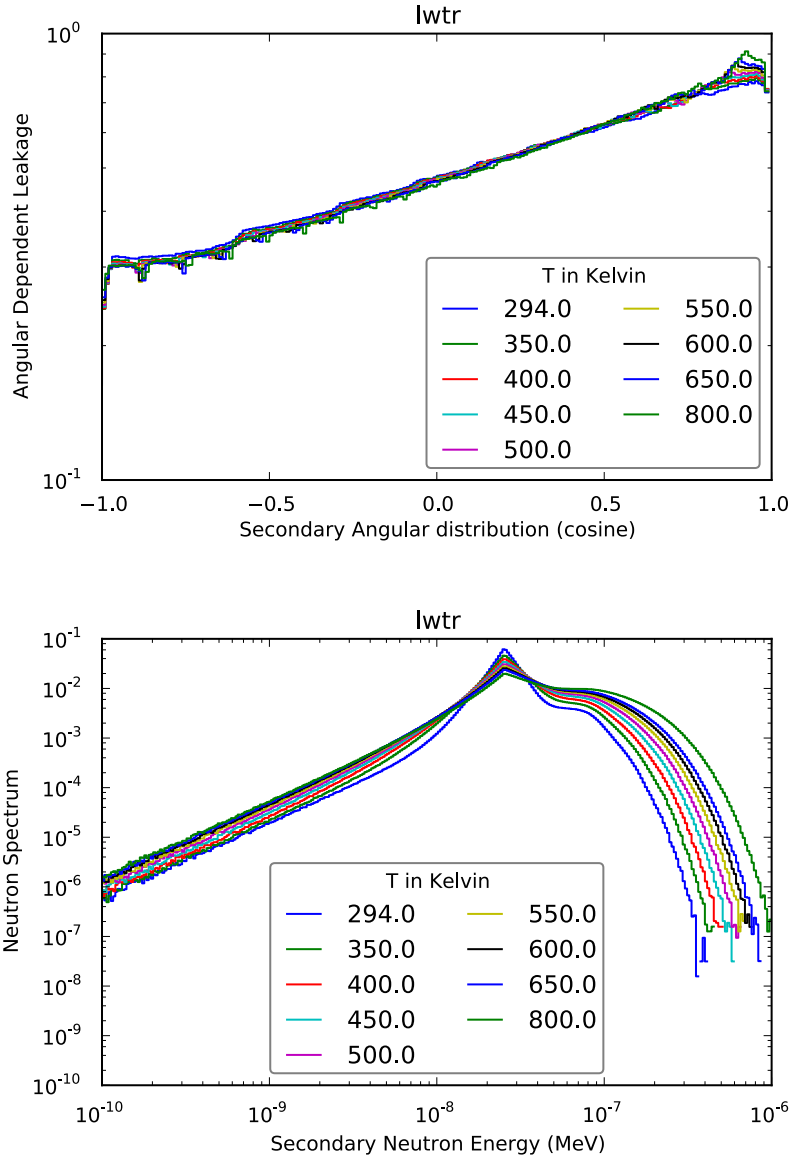


Figure 11: Continuous lwtr

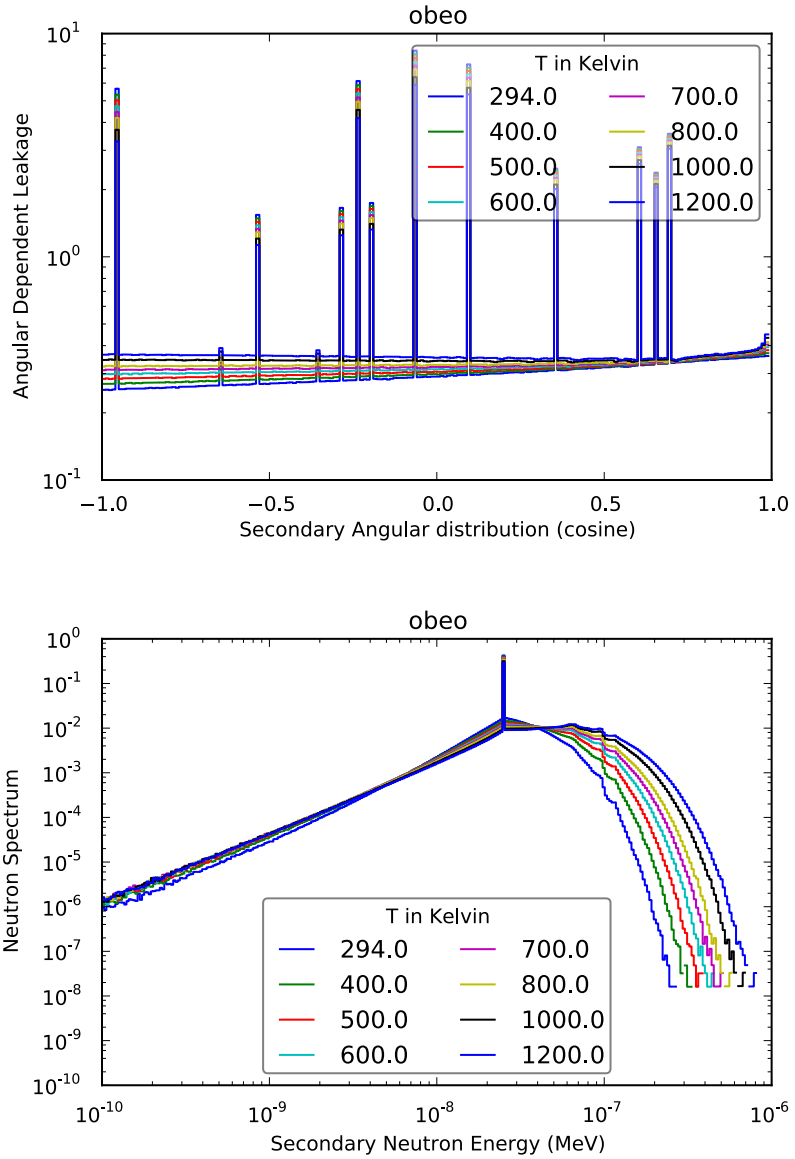


Figure 12: Continuous obeo

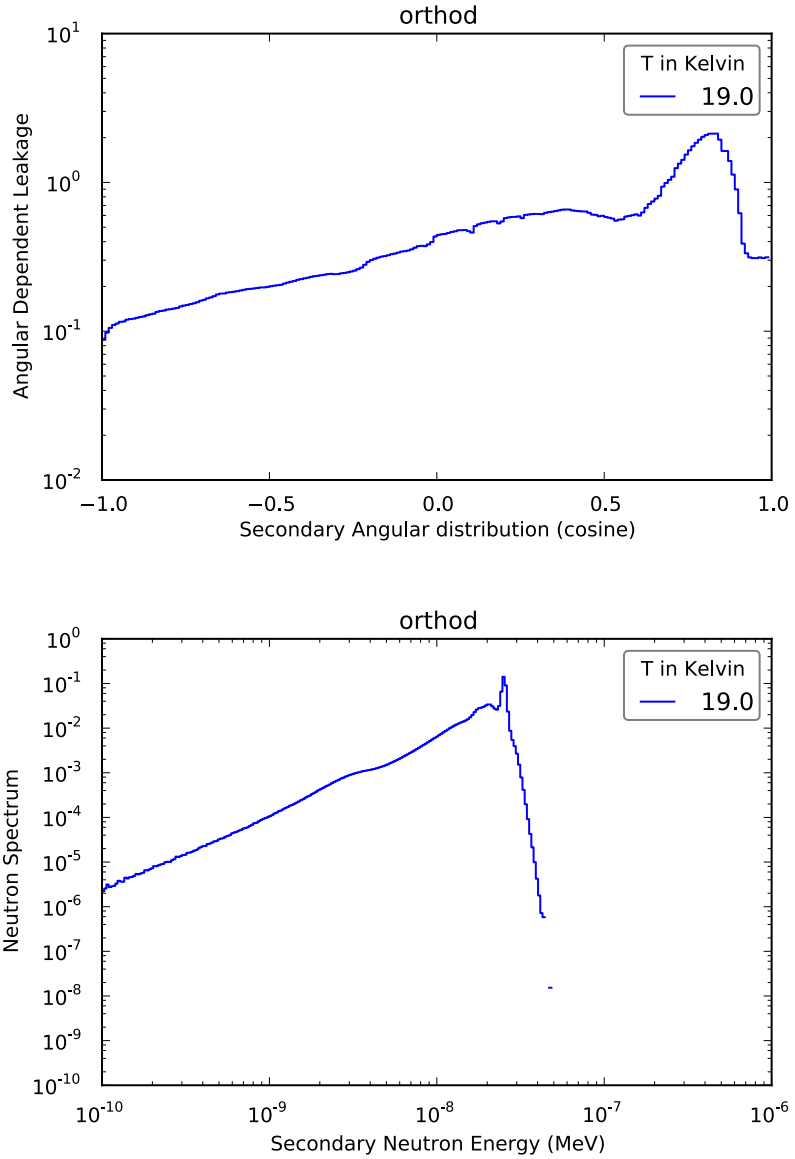


Figure 13: Continuous orthod

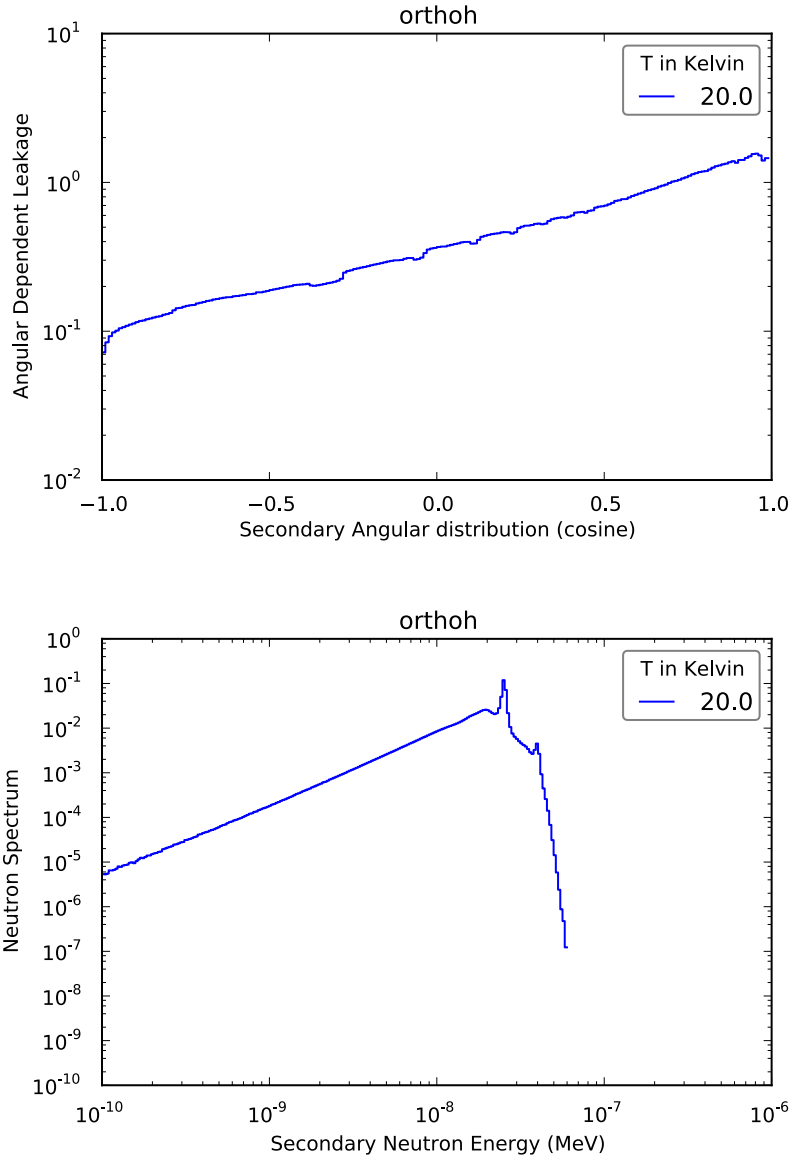


Figure 14: Continuous orthoh

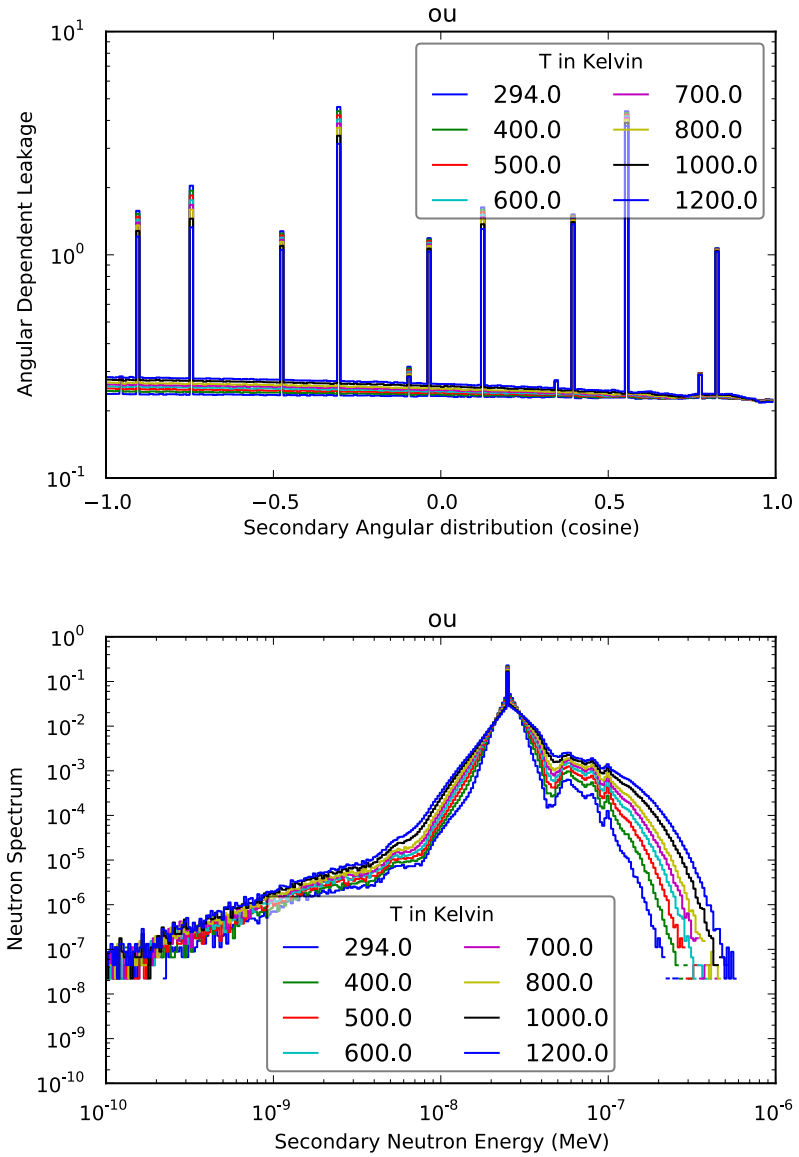


Figure 15: Continuous ou

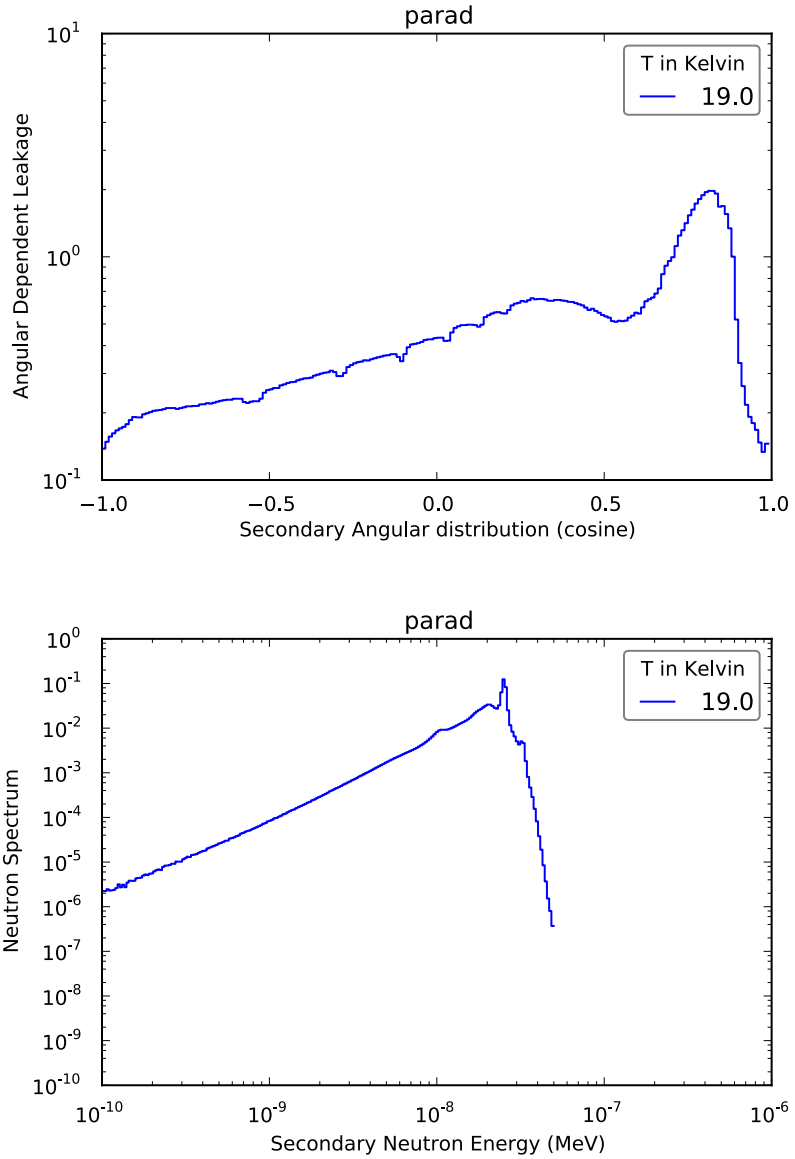


Figure 16: Continuous parad

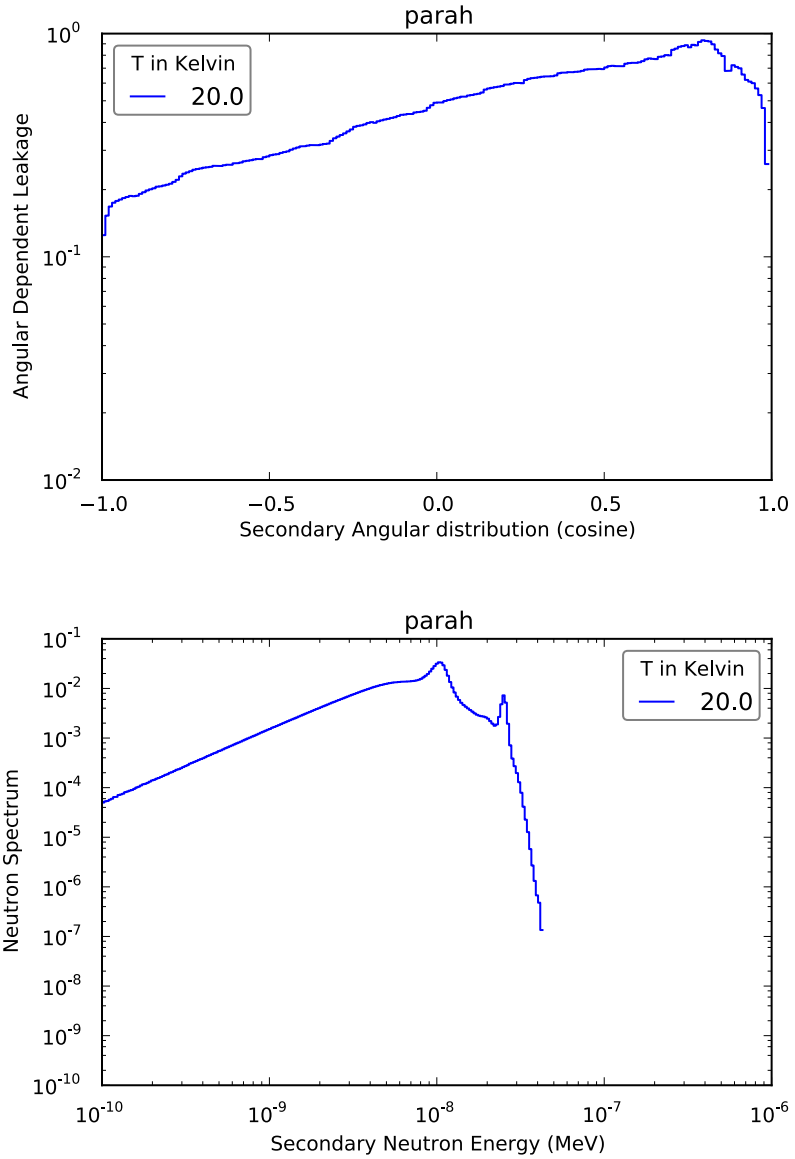
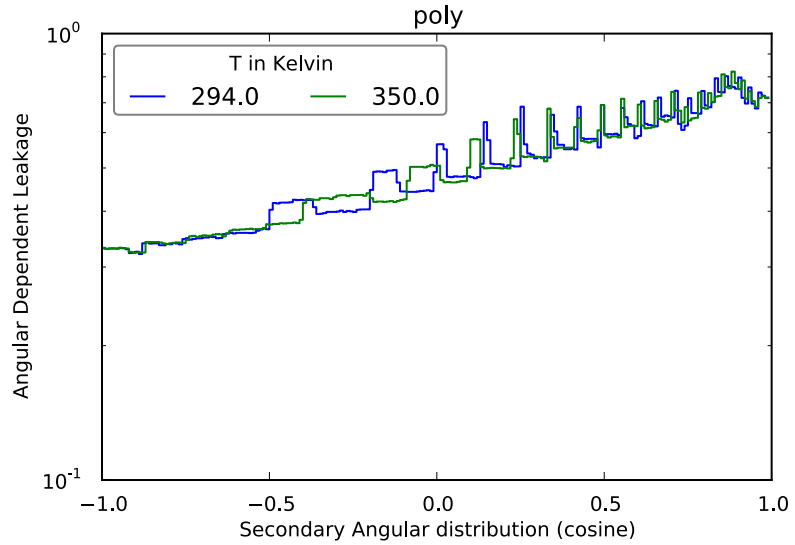


Figure 17: Continuous parah



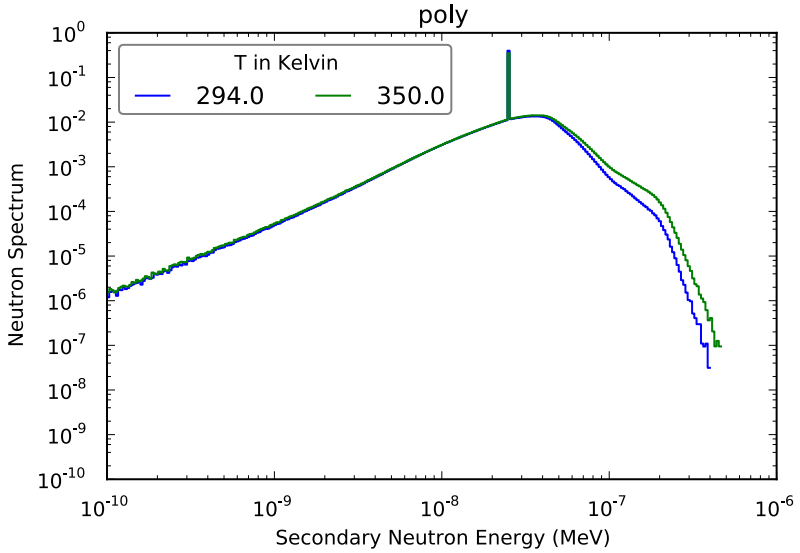


Figure 18: Continuous poly

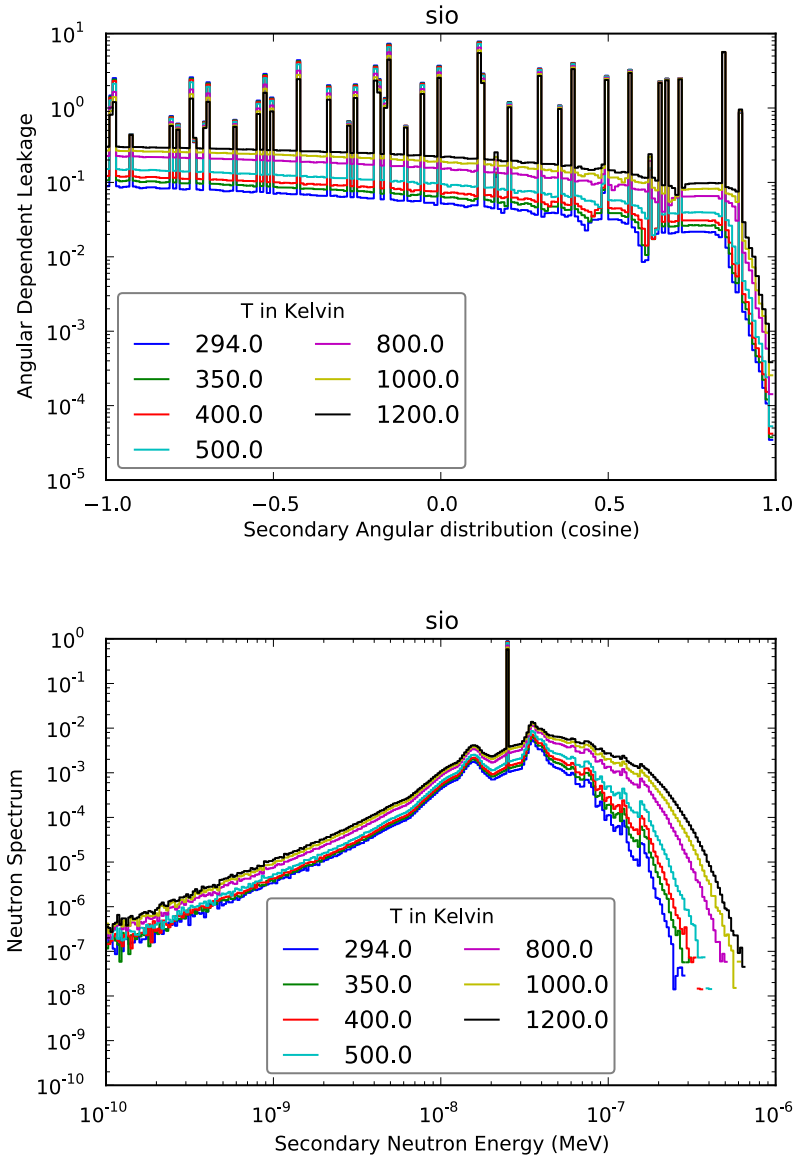


Figure 19: Continuous sio

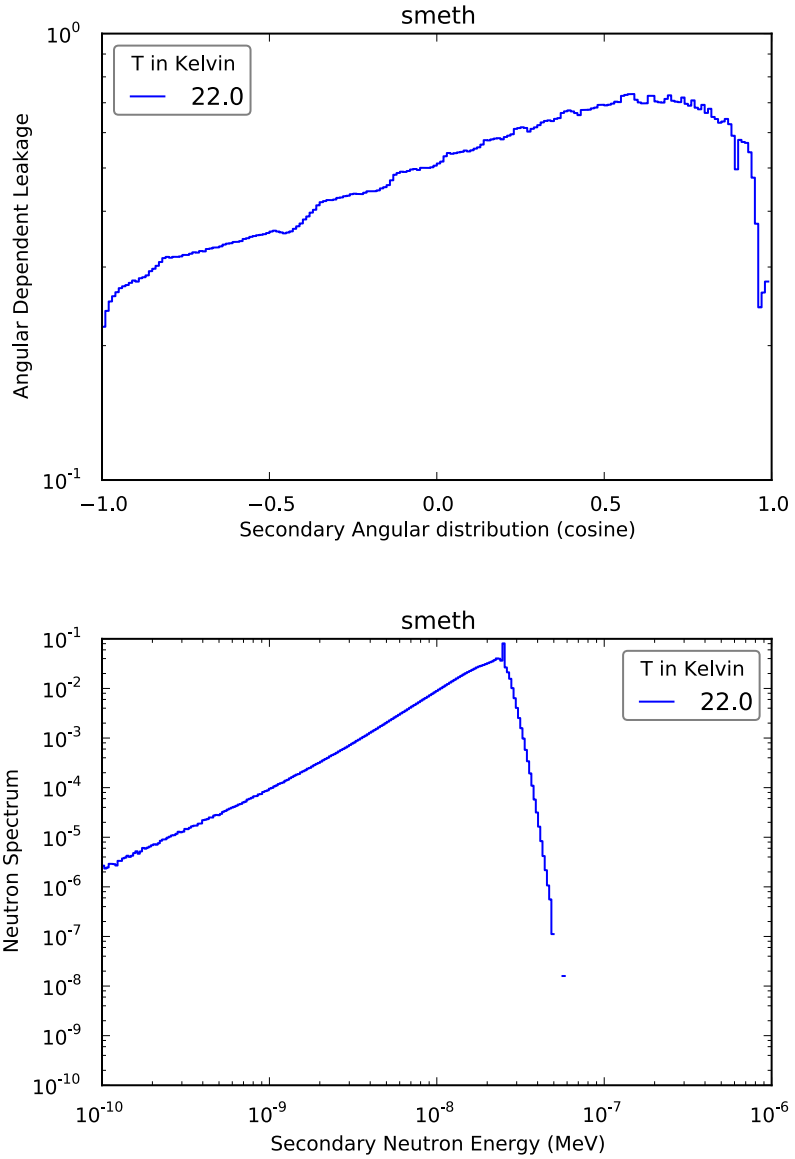


Figure 20: Continuous smeth

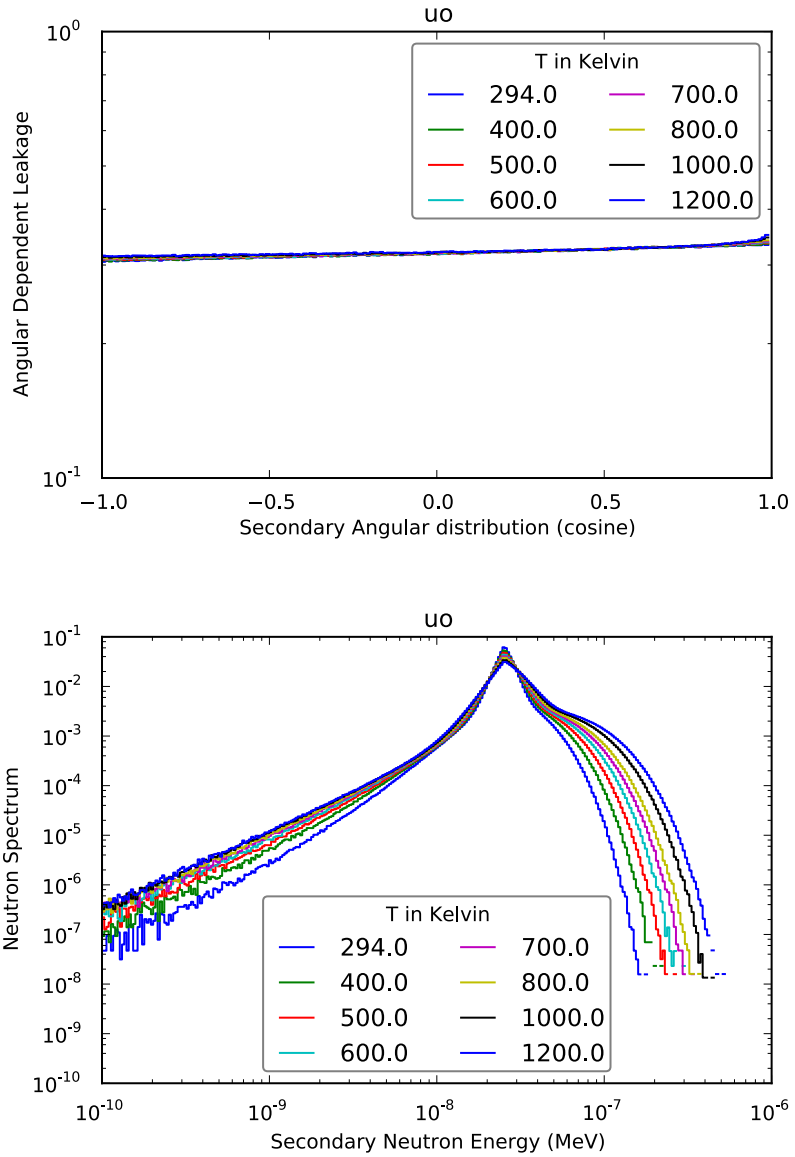


Figure 21: Continuous uo

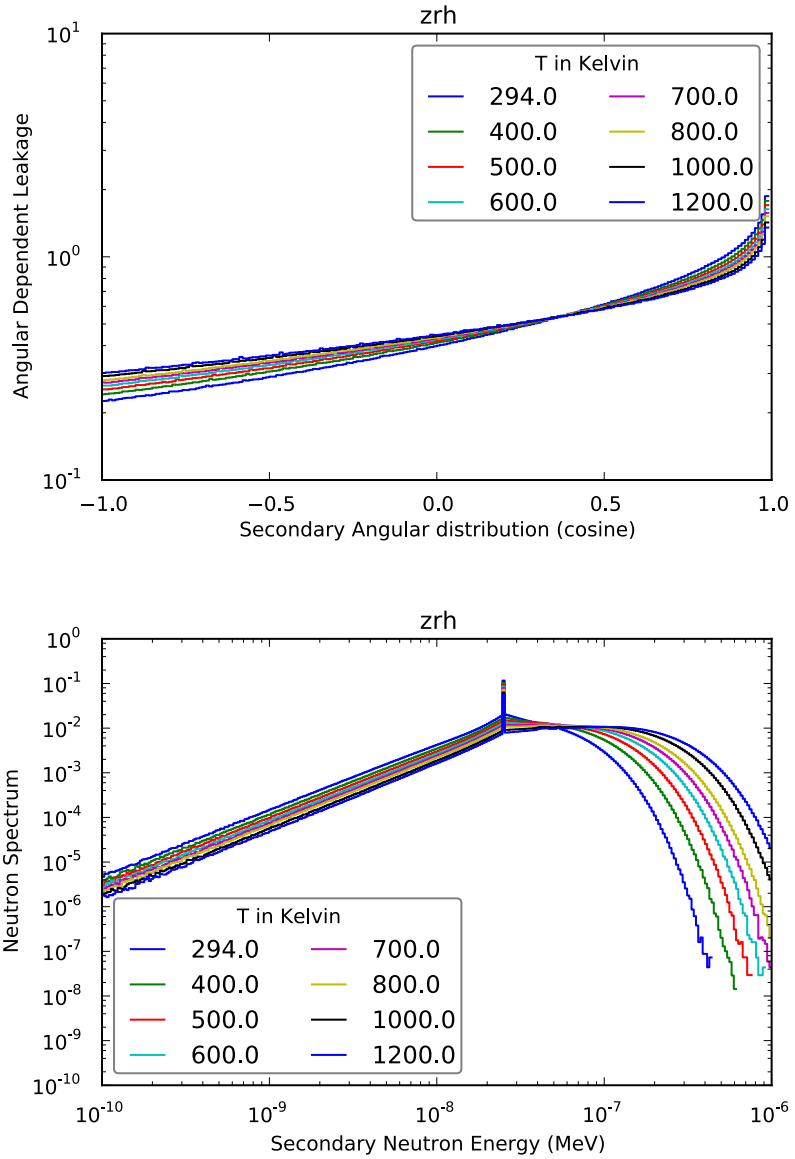


Figure 22: Continuous zrh

C.2 Discrete

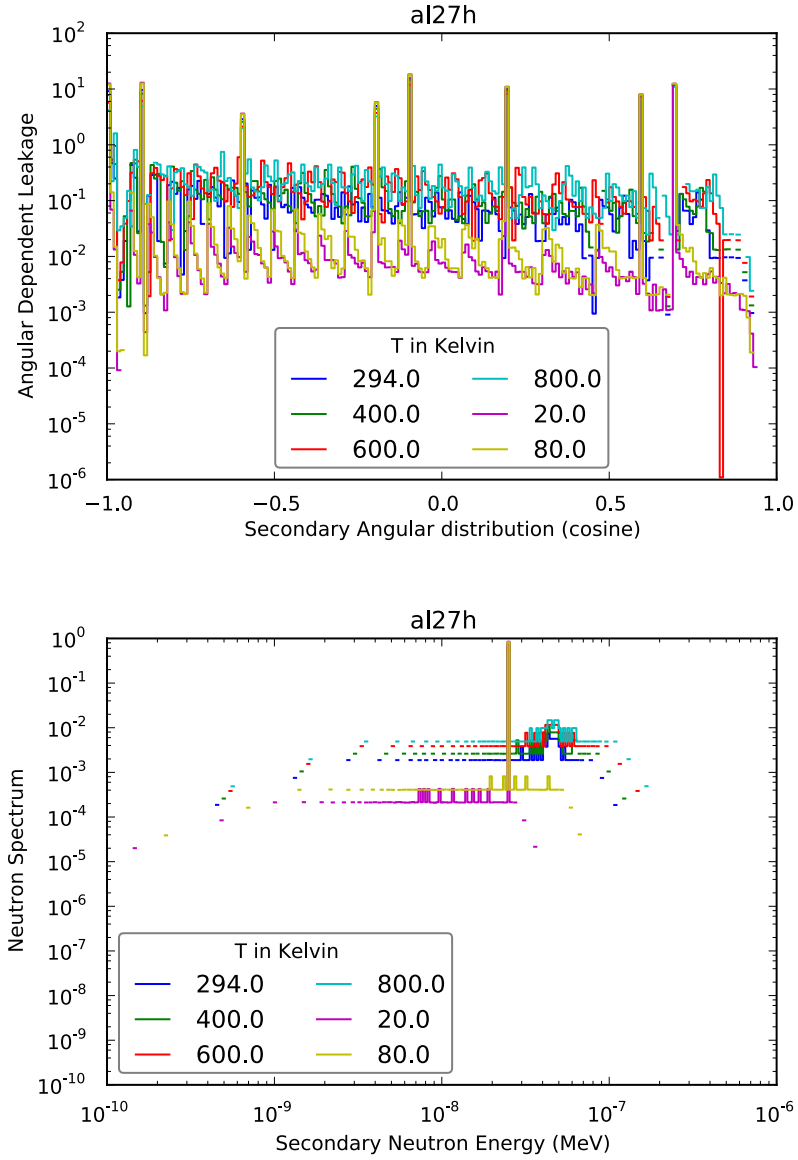


Figure 23: Discrete al27h

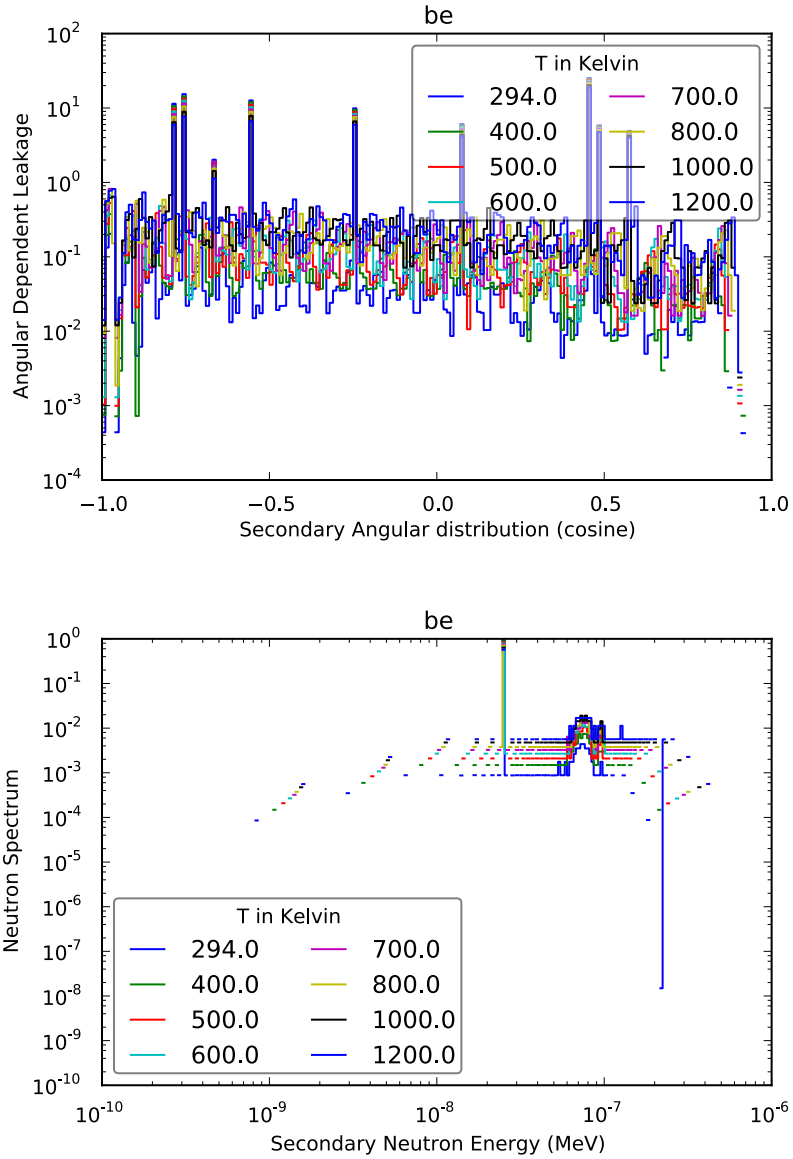


Figure 24: Discrete be

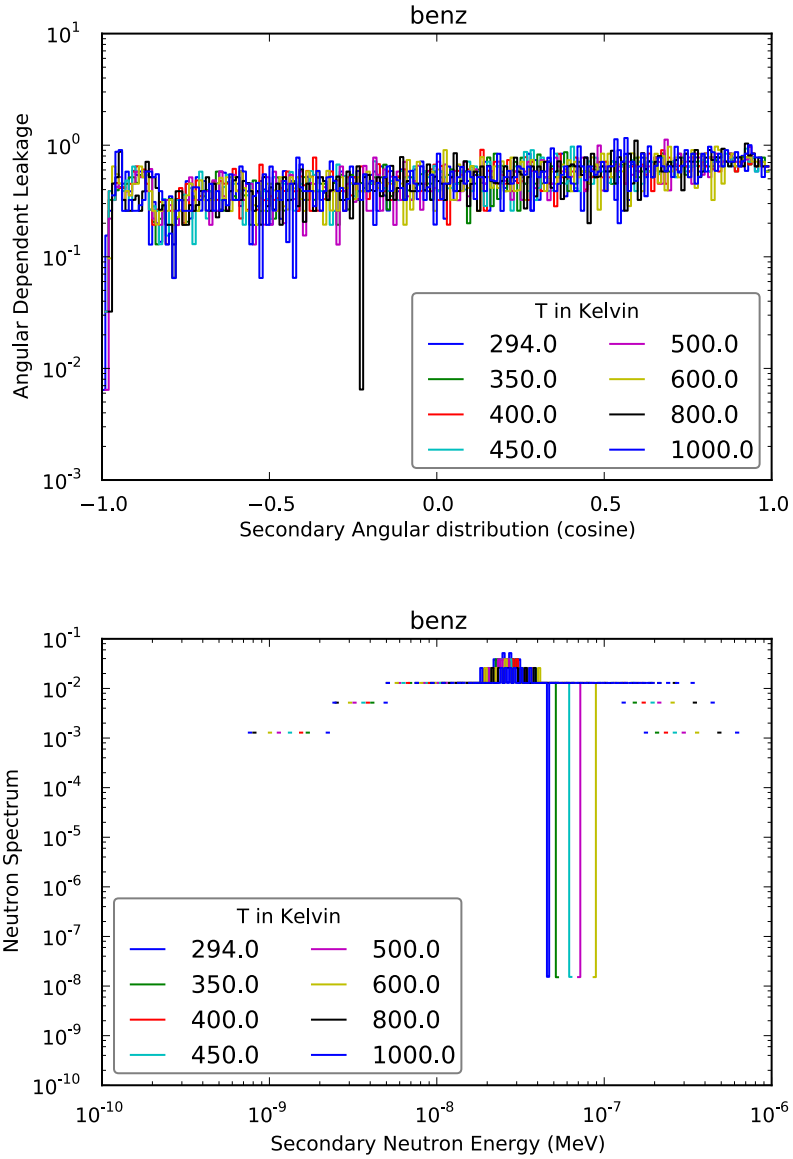


Figure 25: Discrete benz

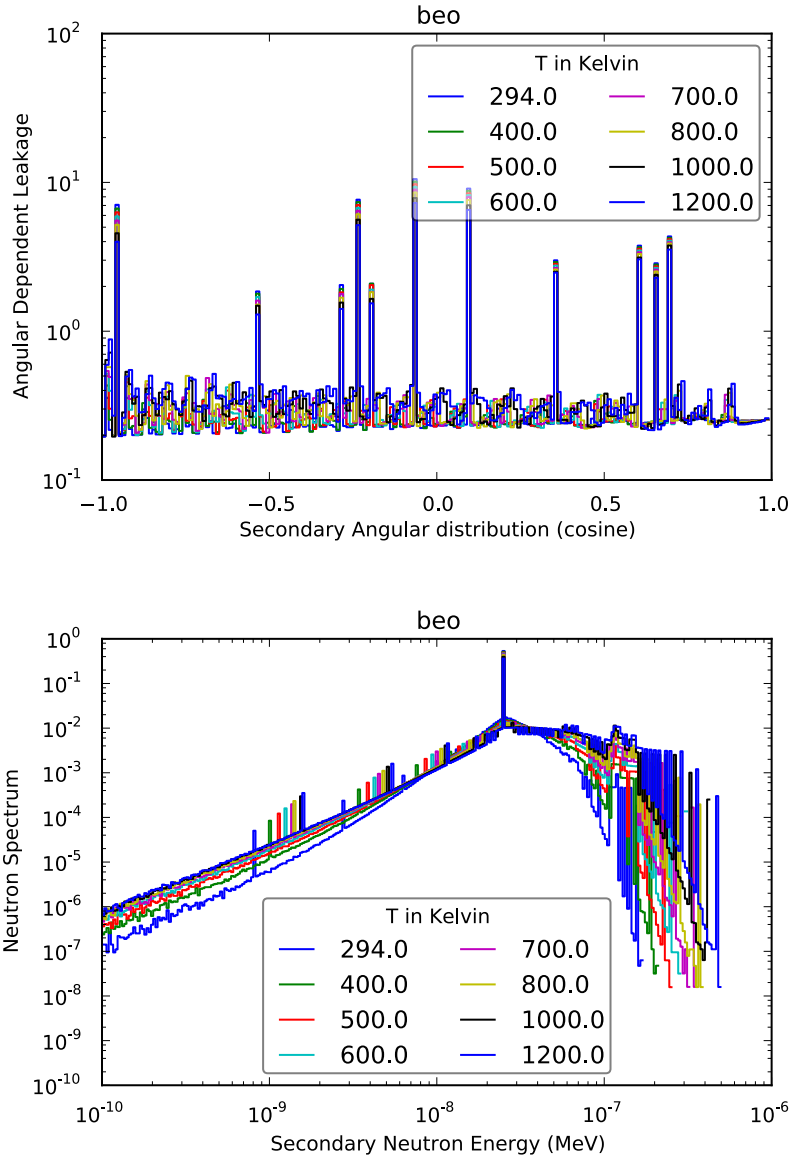


Figure 26: Discrete beo

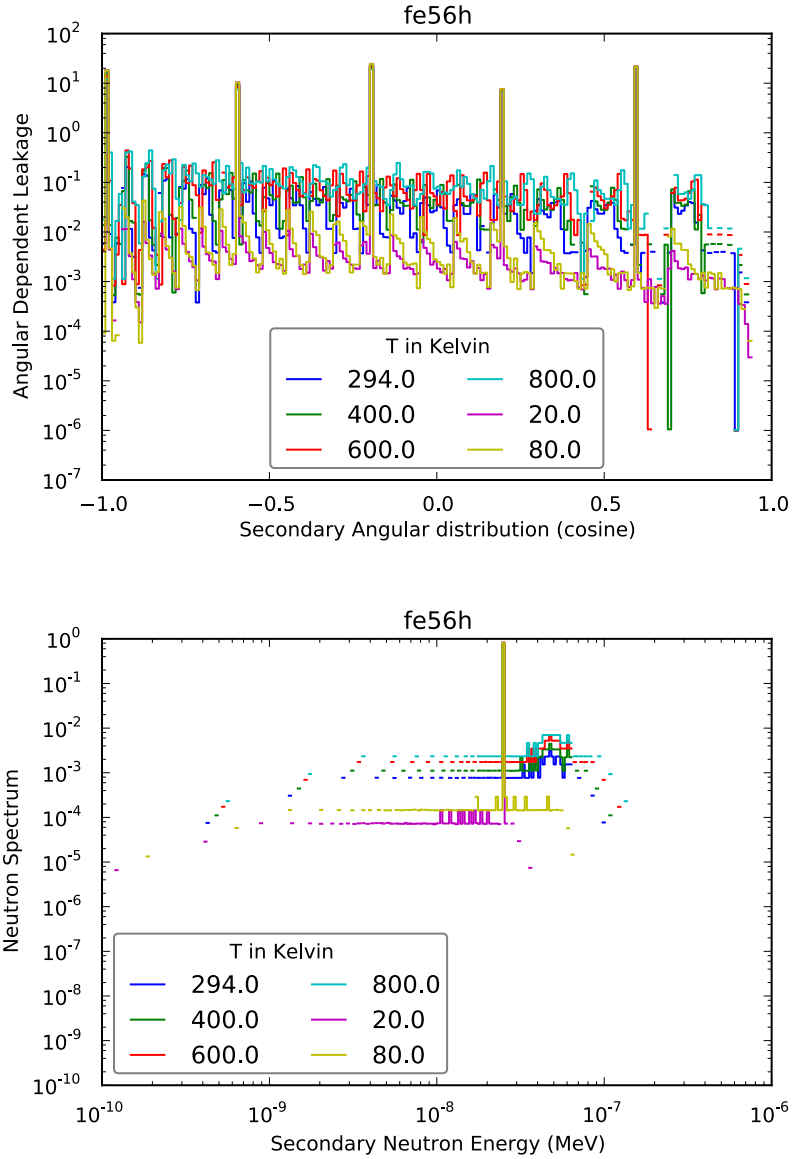


Figure 27: Discrete fe56h

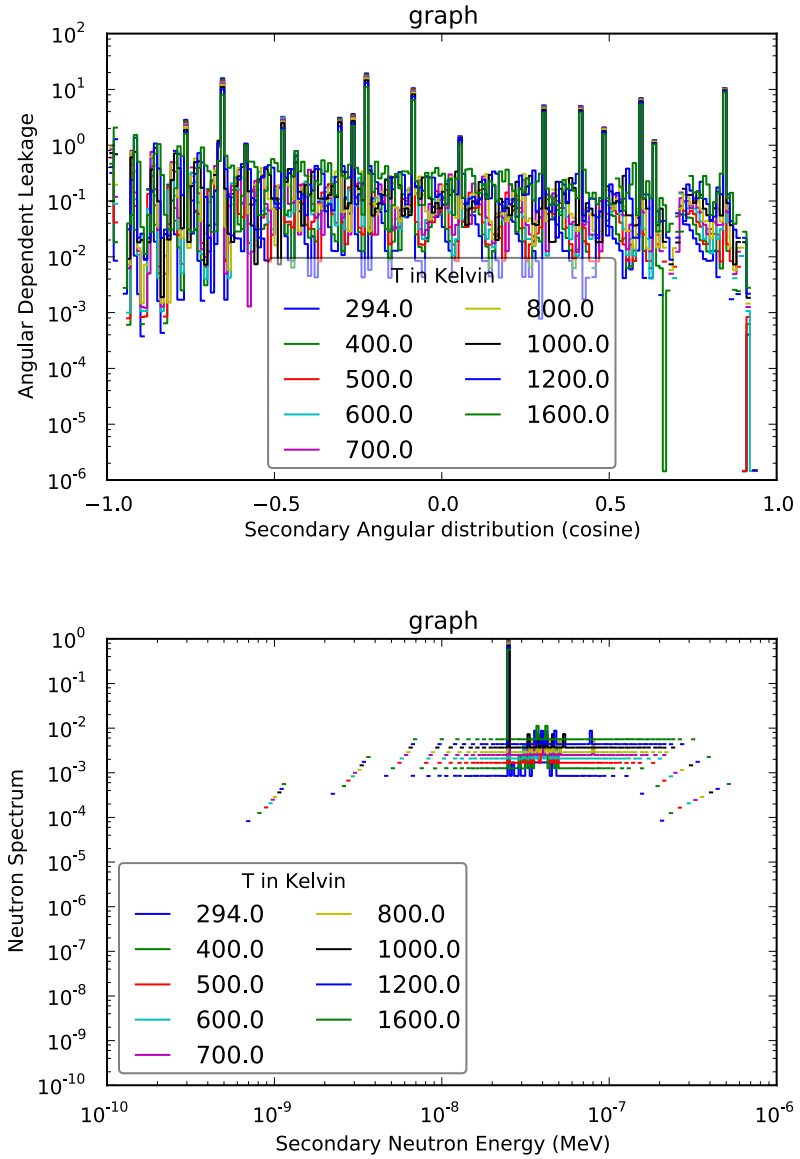


Figure 28: Discrete graph

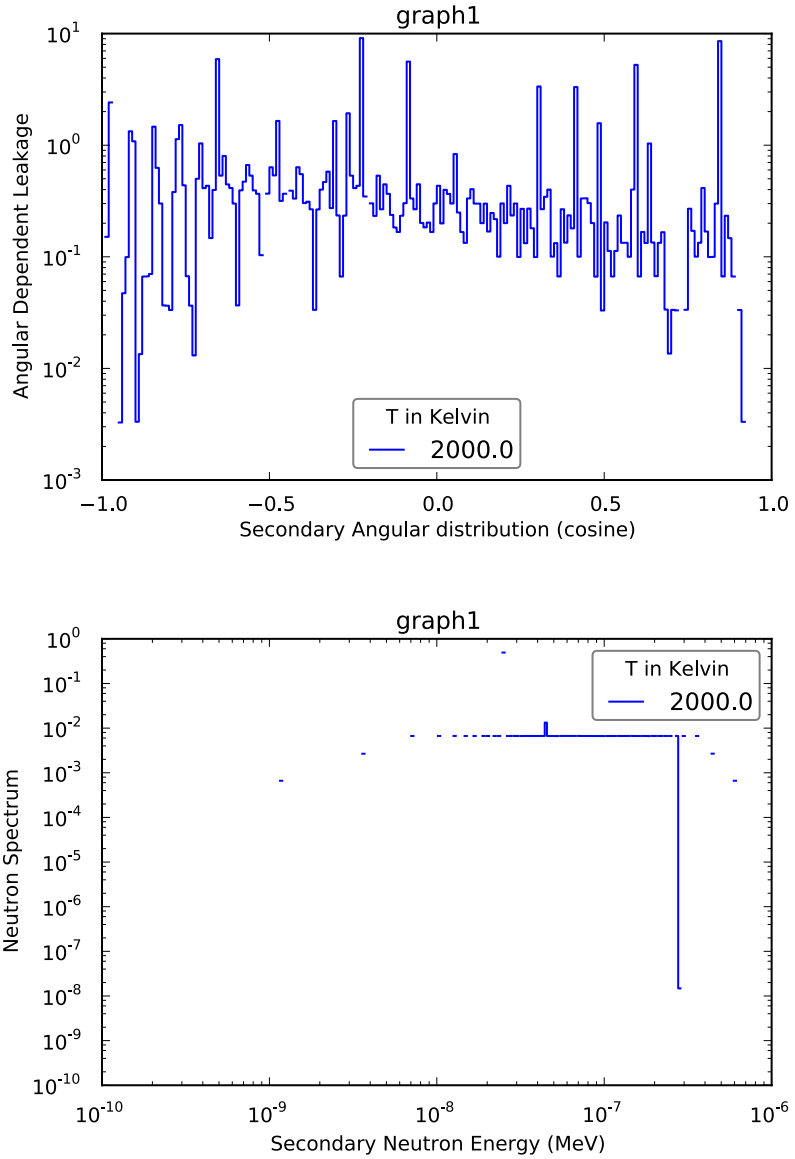


Figure 29: Discrete graph1

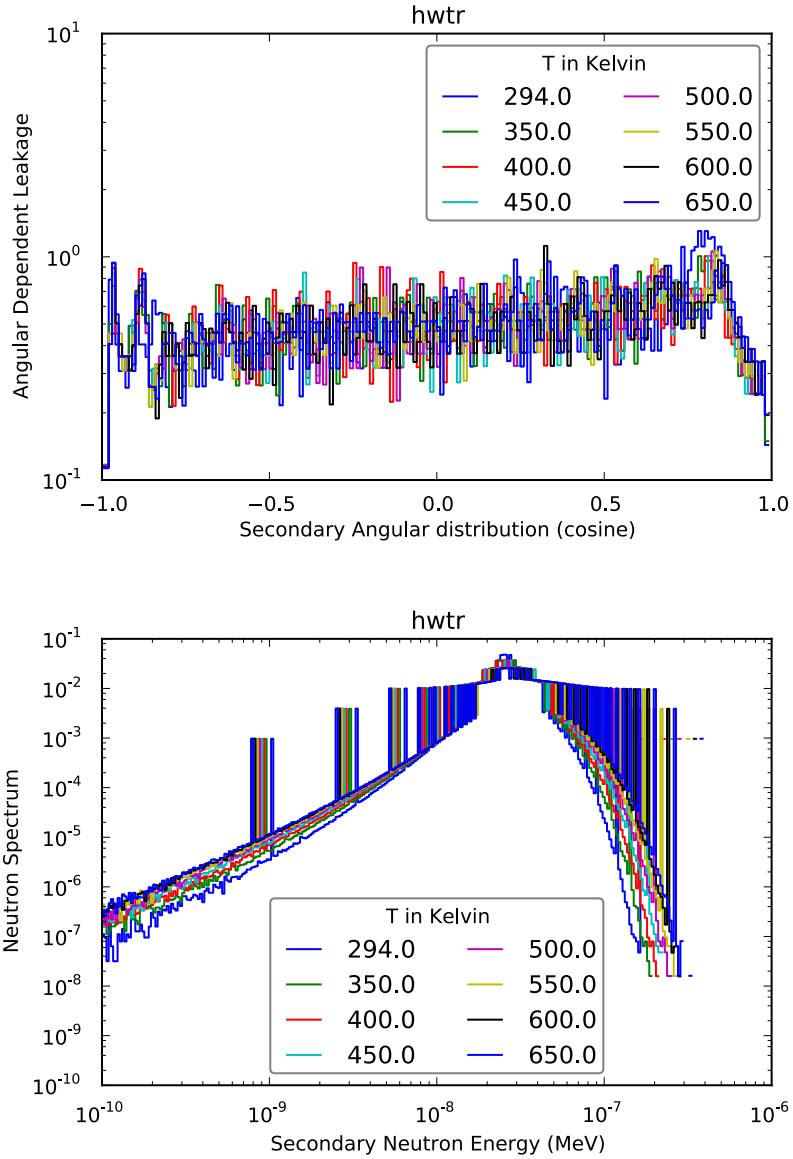


Figure 30: Discrete hwtr

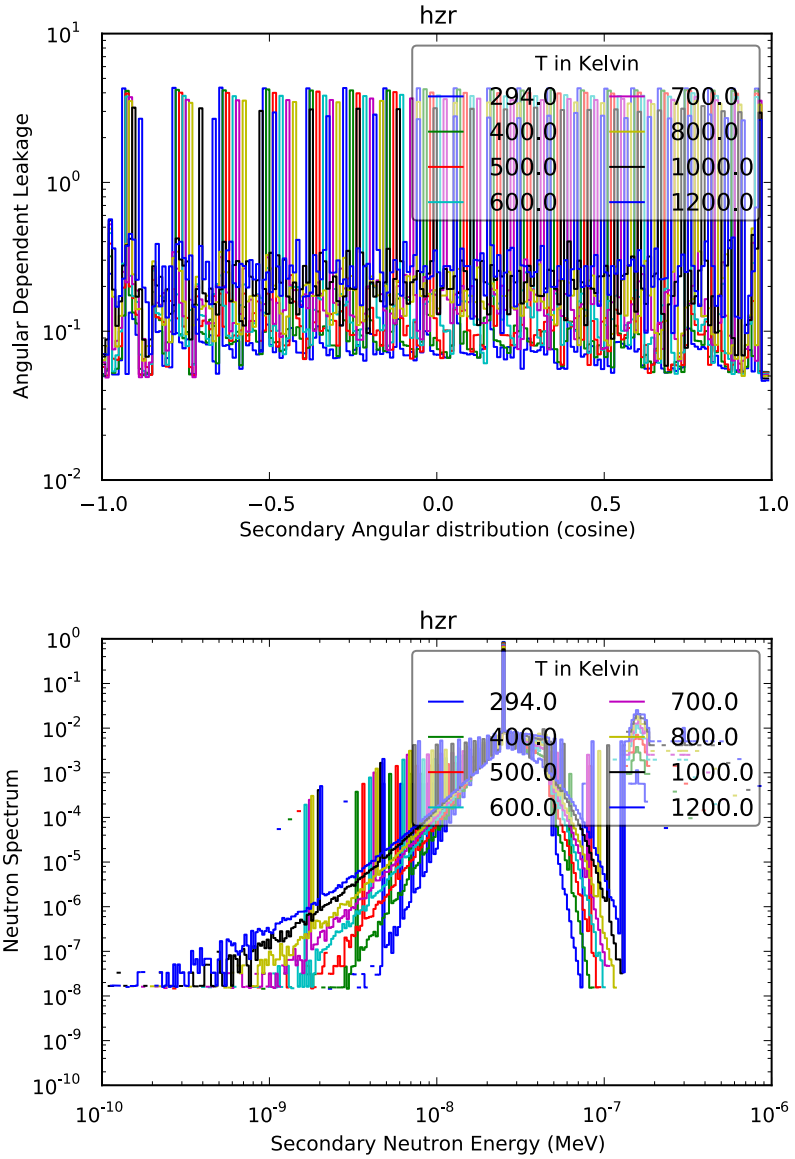


Figure 31: Discrete hzr

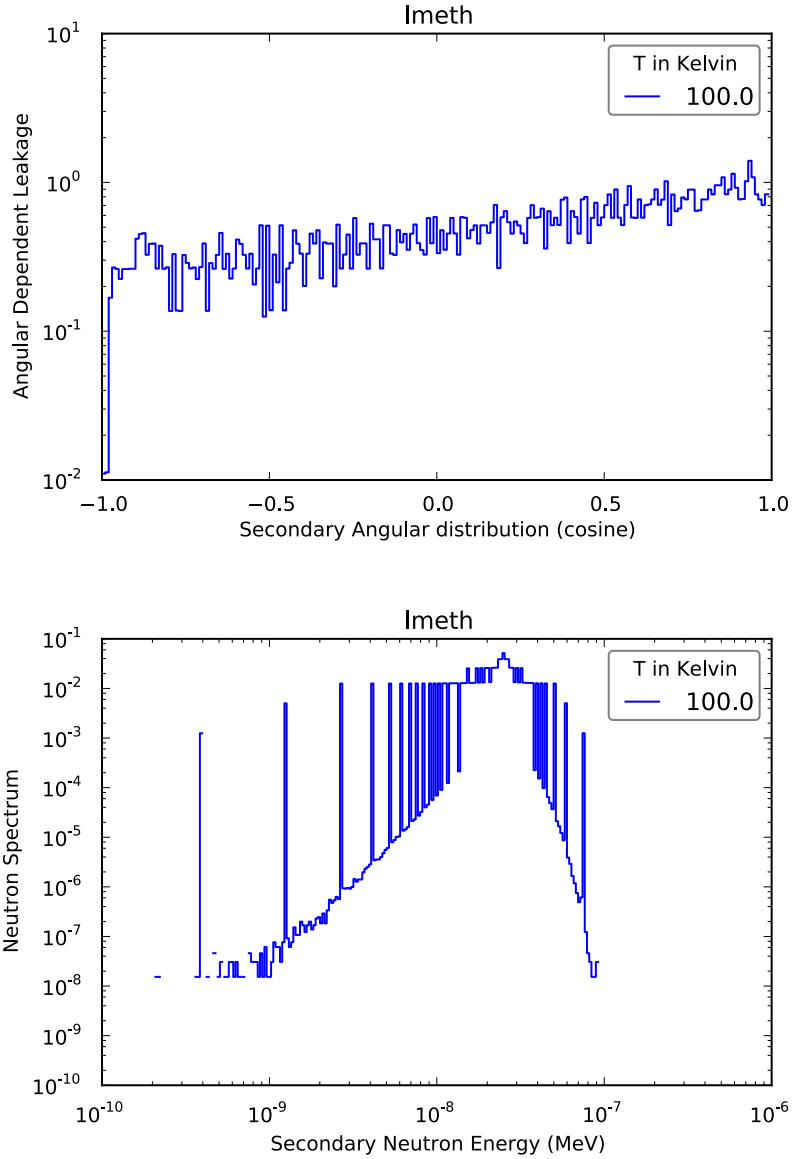


Figure 32: Discrete lmeth

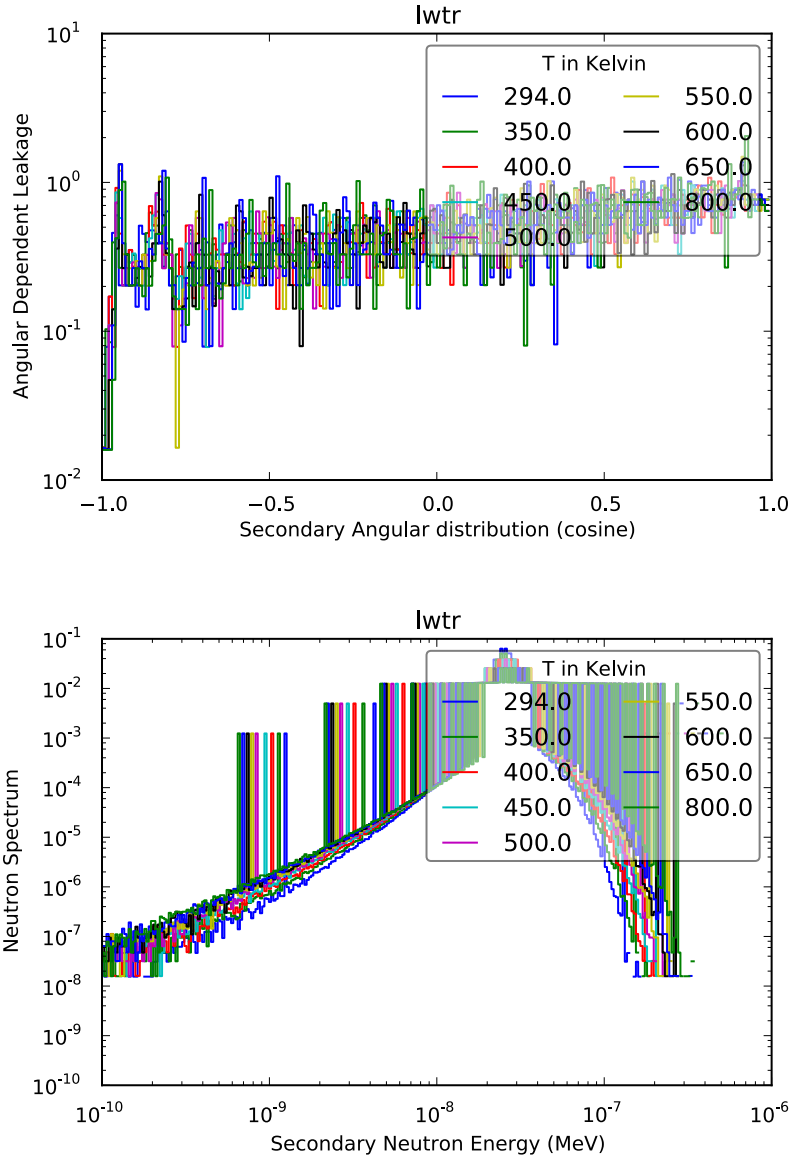


Figure 33: Discrete lwtr

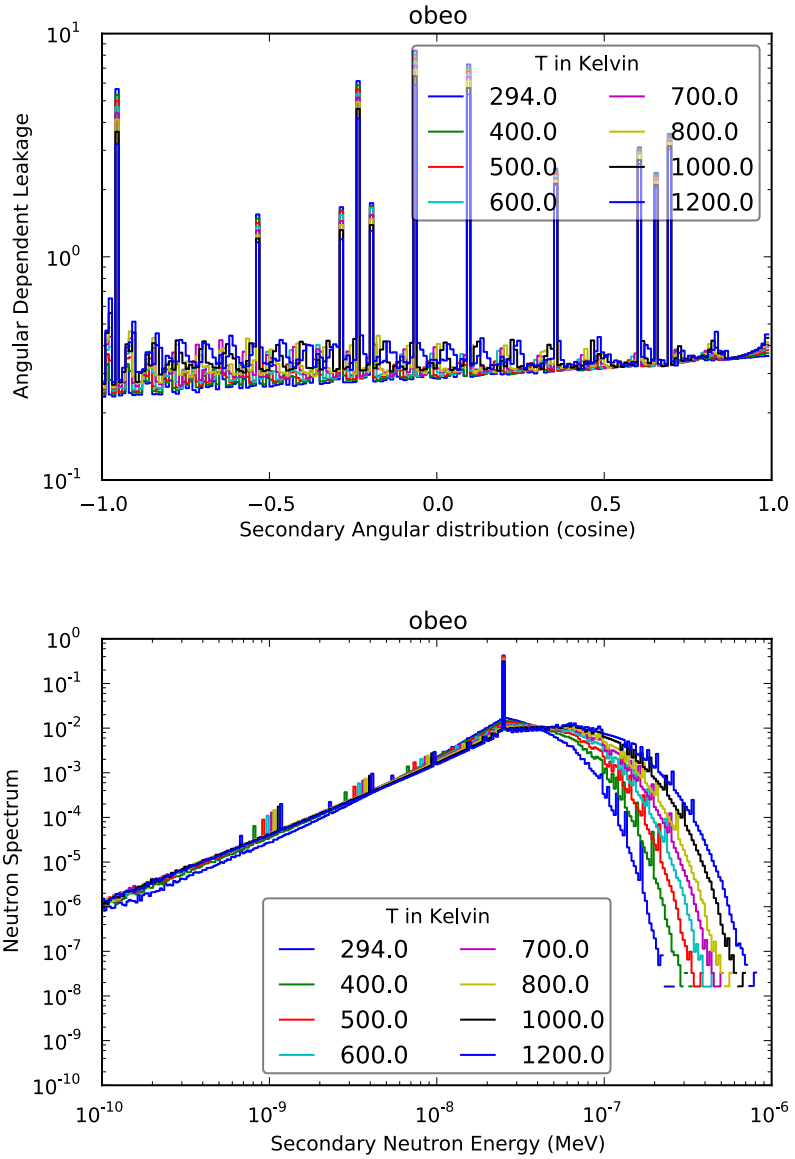


Figure 34: Discrete obeo

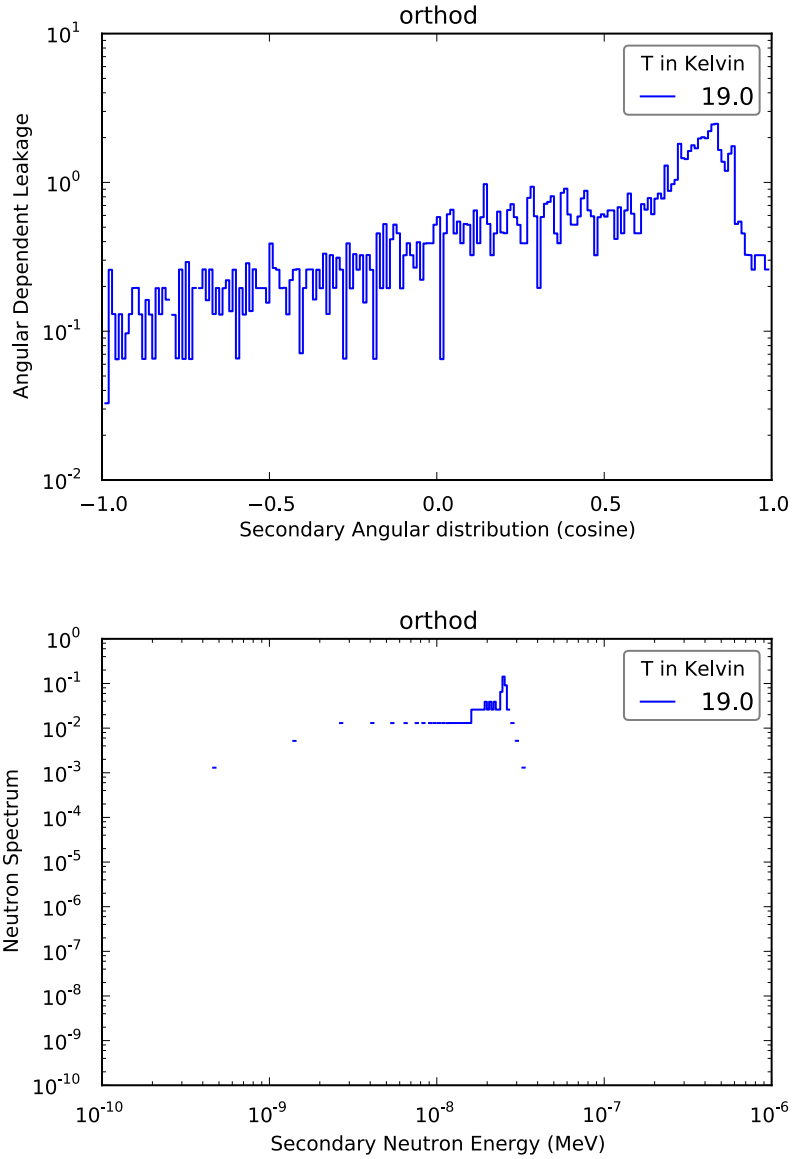
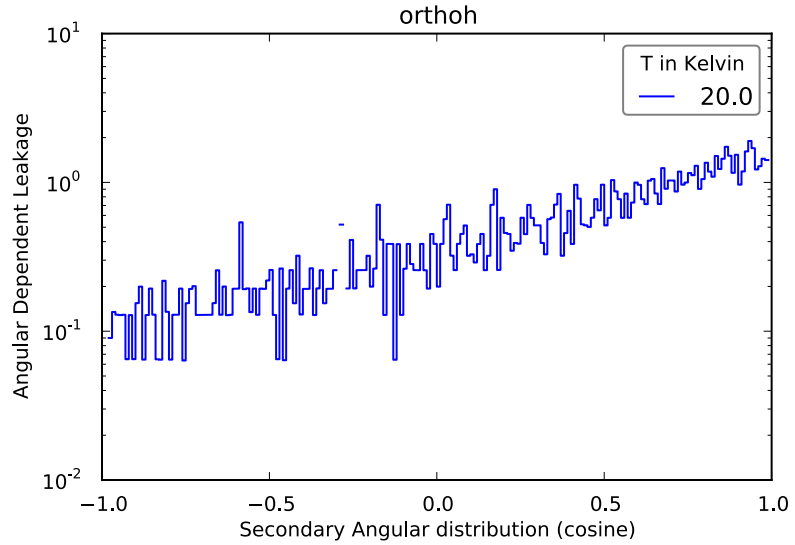


Figure 35: Discrete orthod



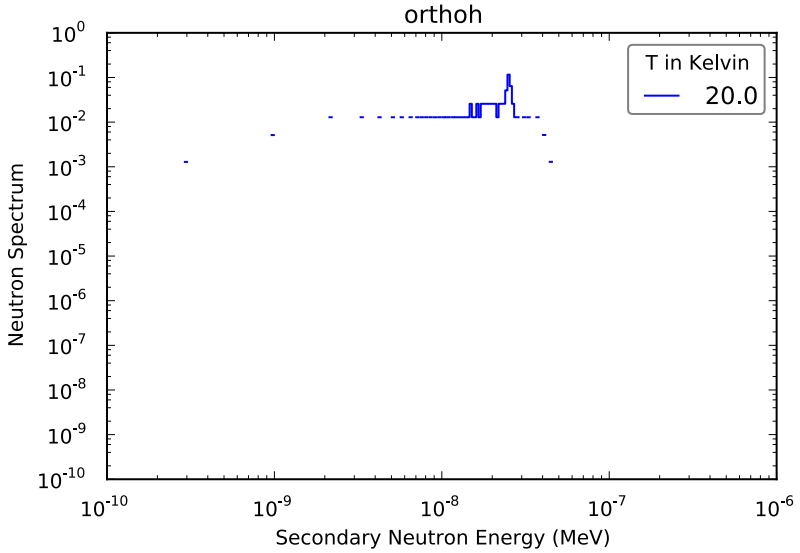


Figure 36: Discrete orthoh

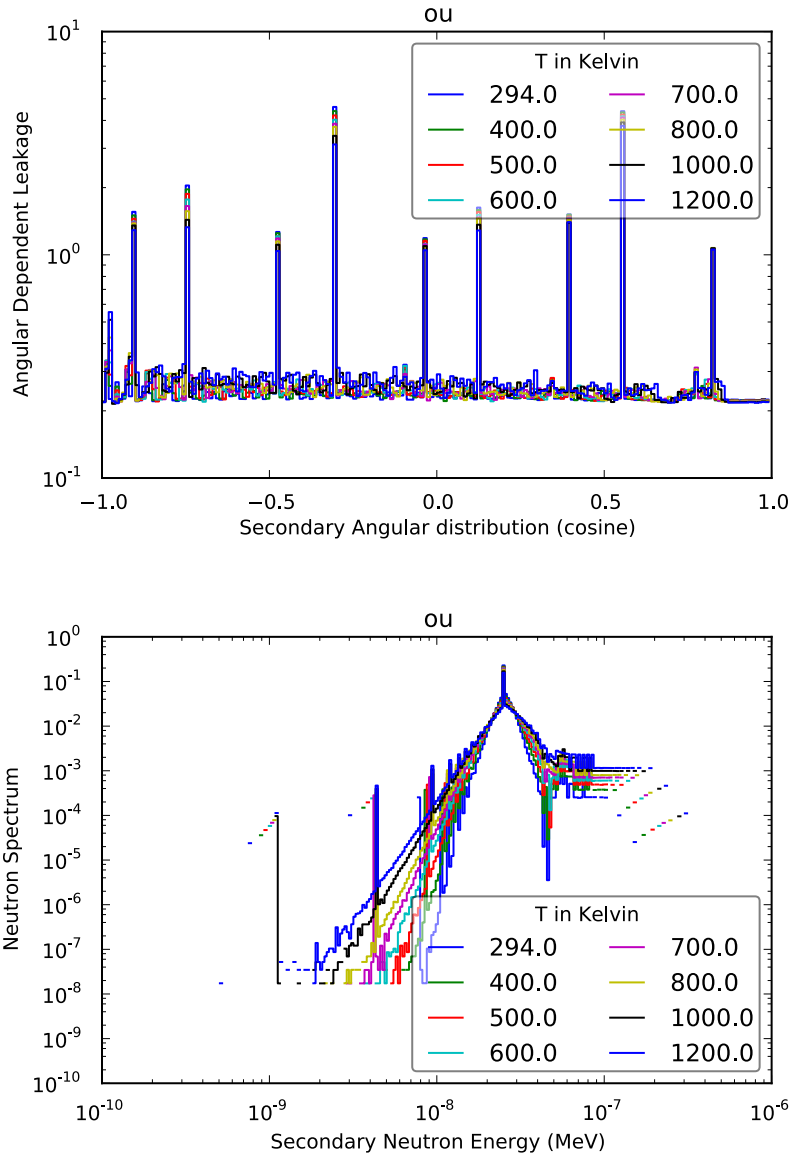


Figure 37: Discrete ou

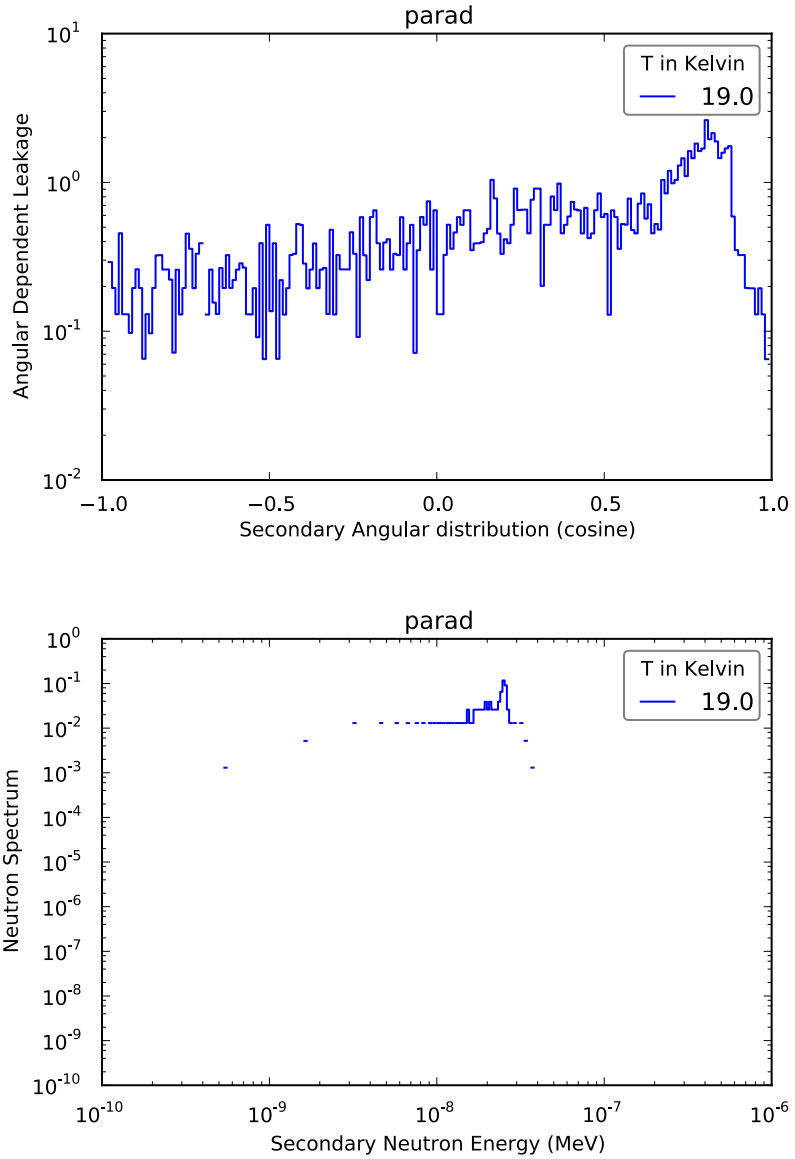


Figure 38: Discrete parad

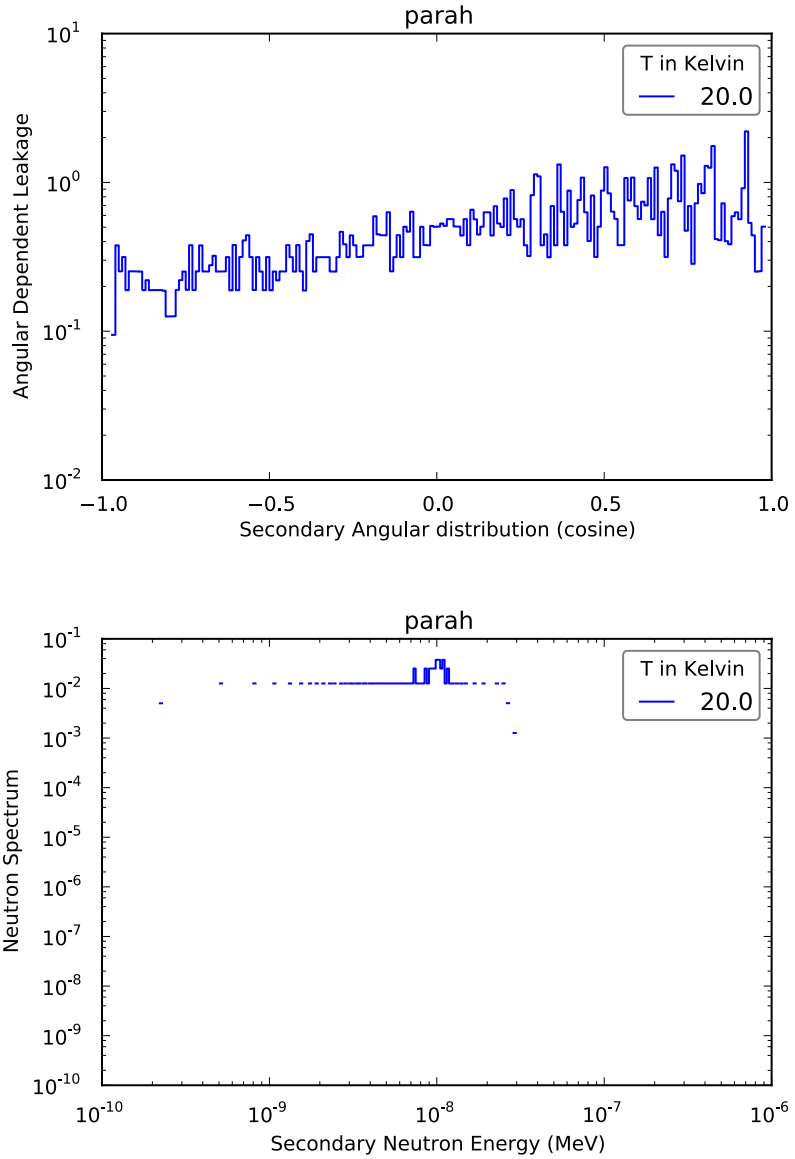


Figure 39: Discrete parah

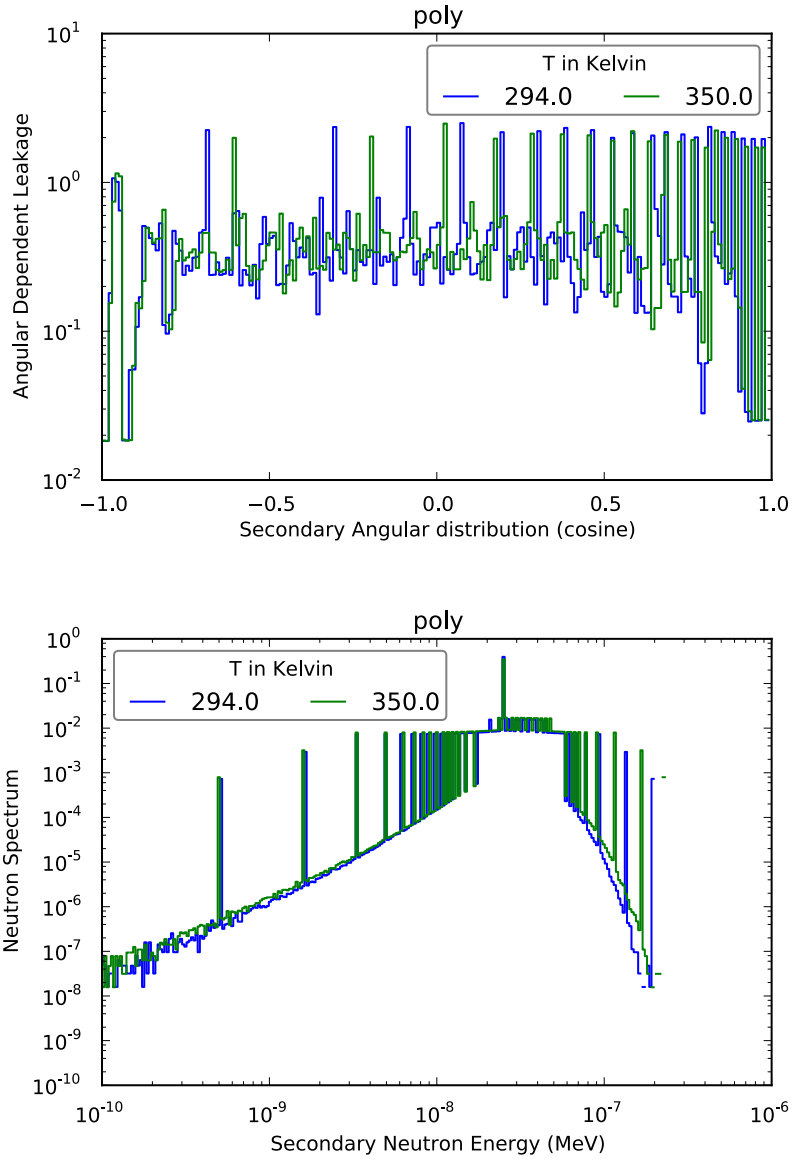


Figure 40: Discrete poly

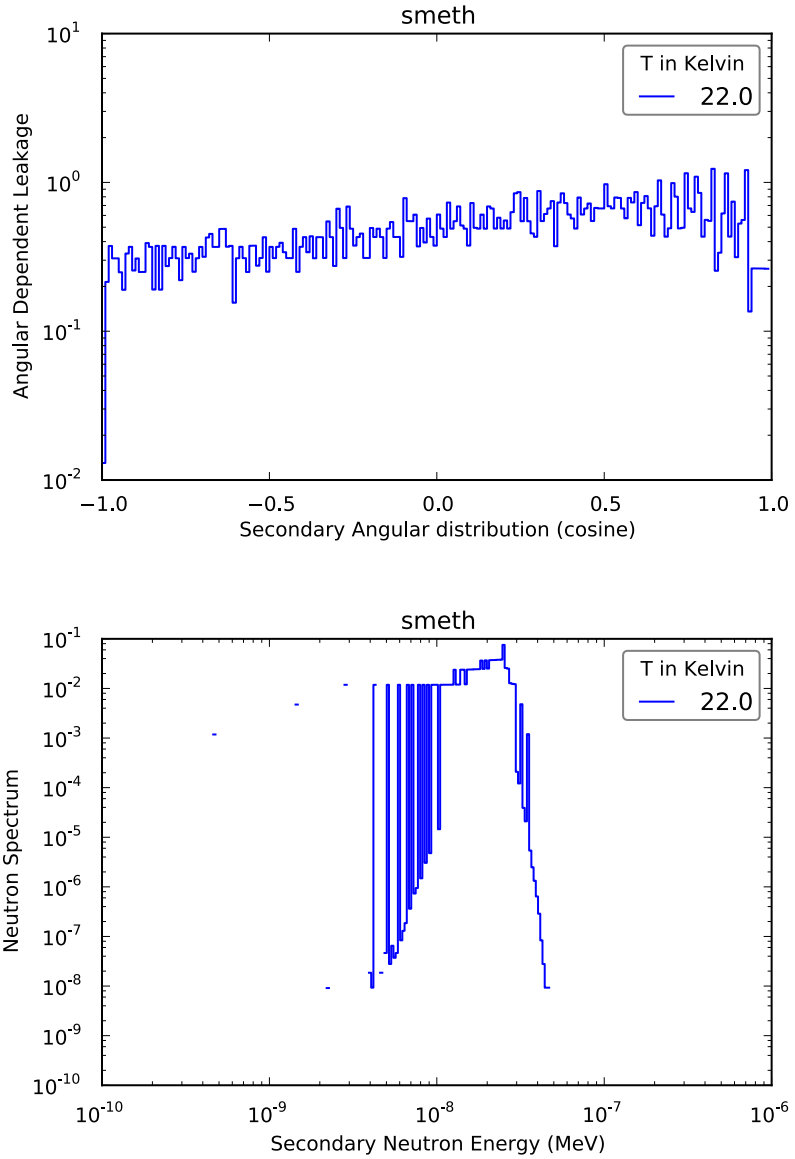


Figure 41: Discrete smeth

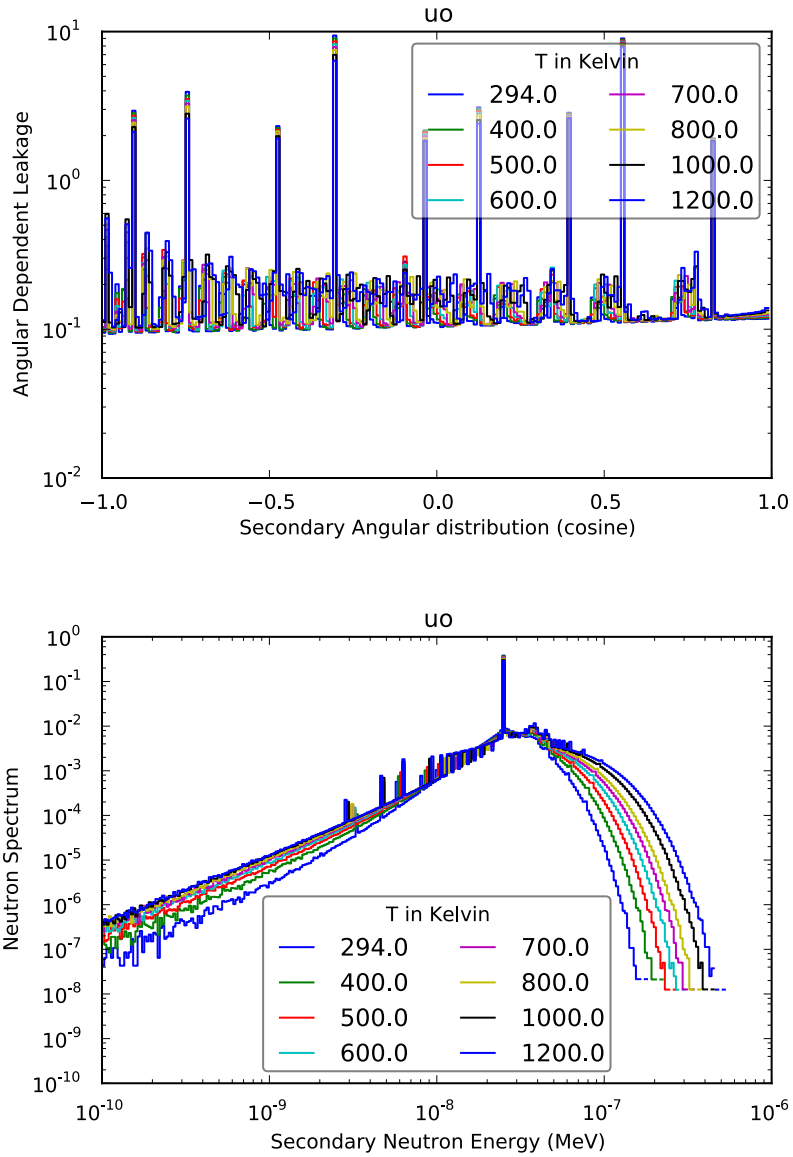


Figure 42: Discrete uo

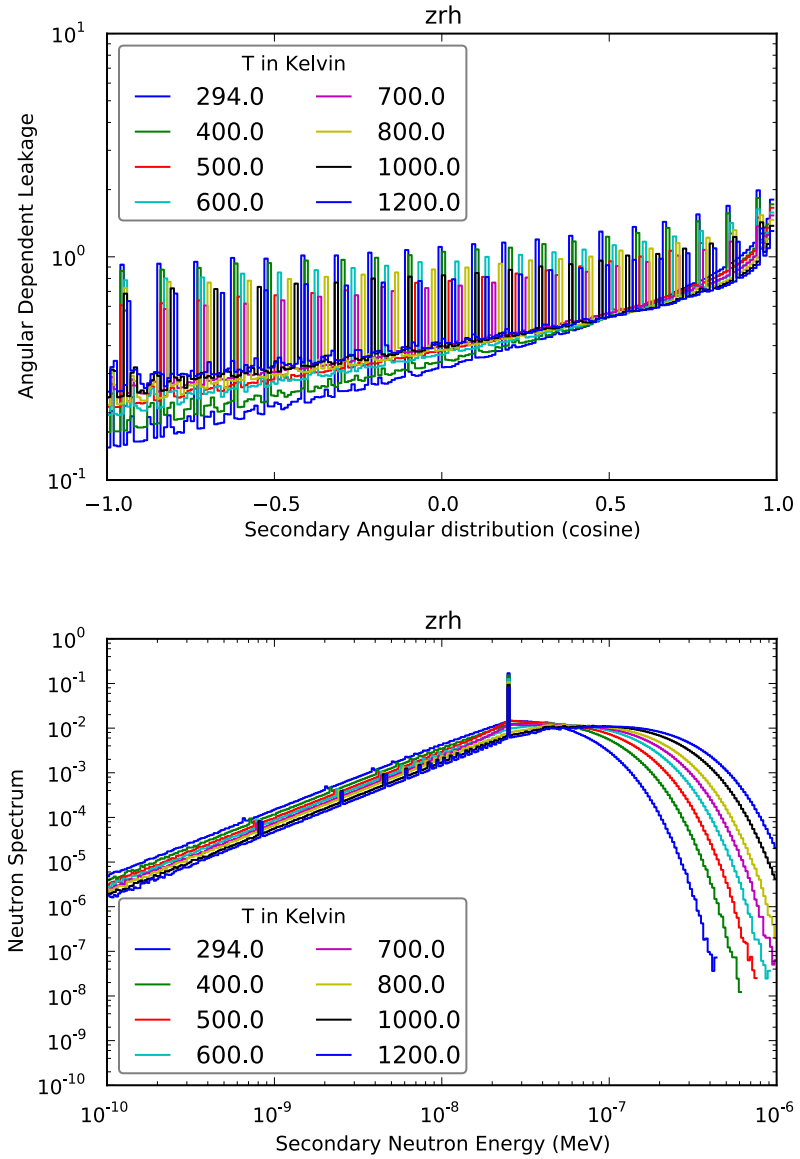


Figure 43: Discrete zrh

C.3 FreeGas

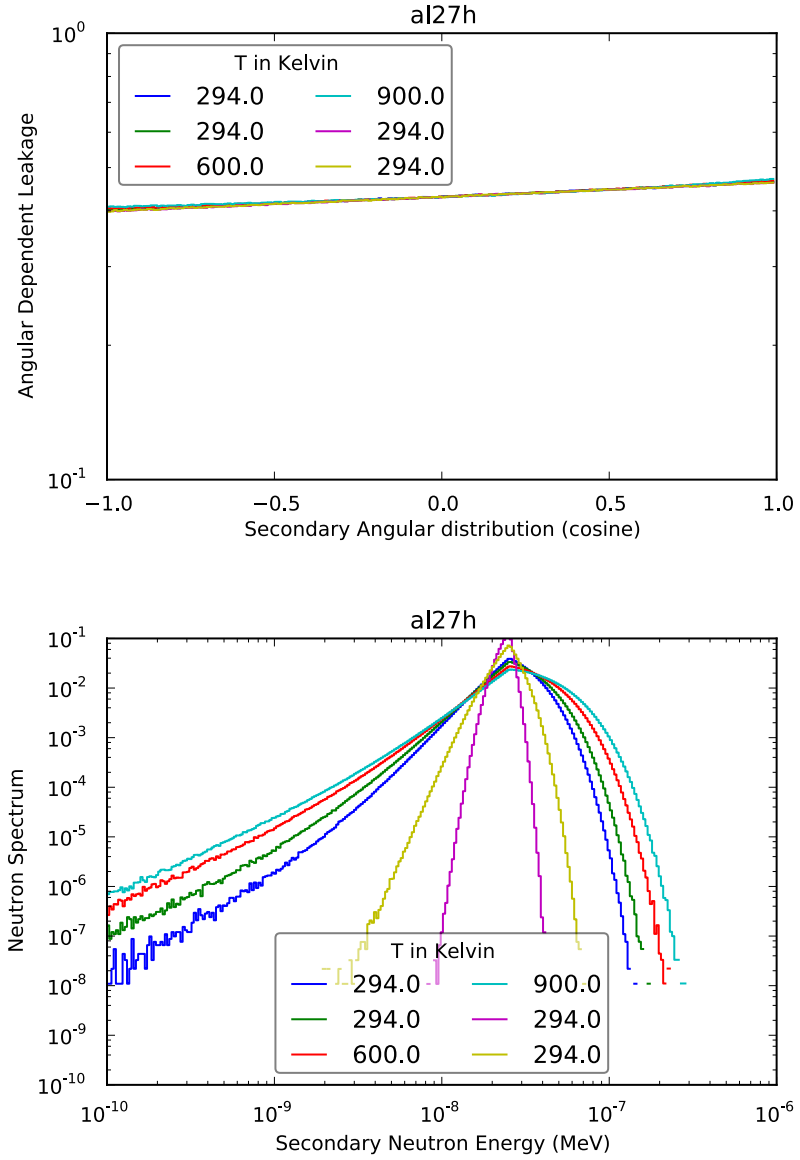


Figure 44: FreeGas al27h

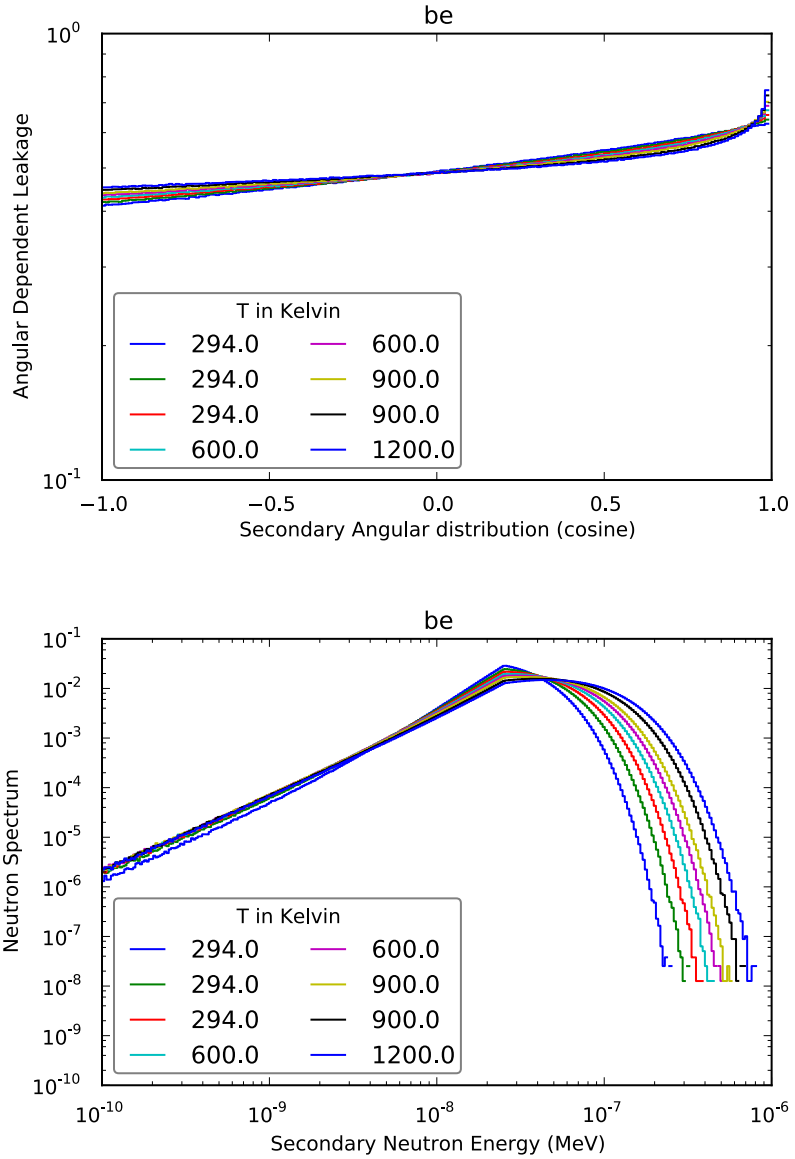


Figure 45: FreeGas be

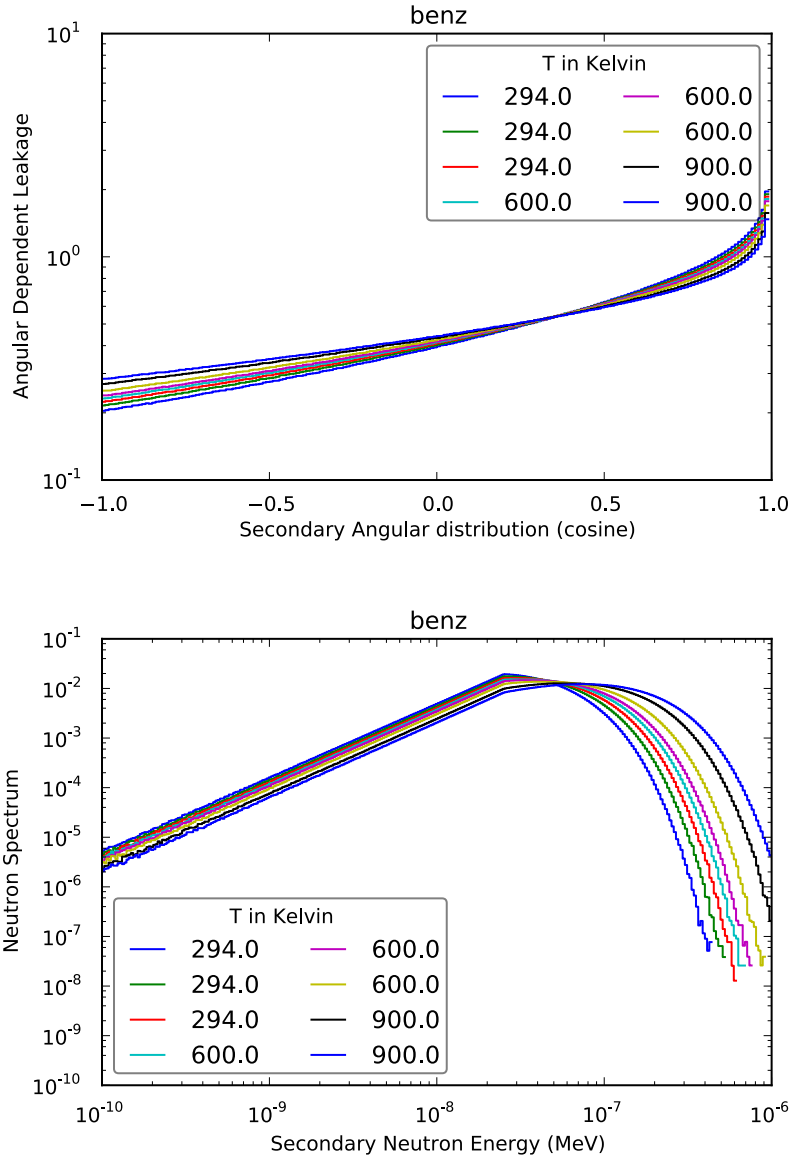


Figure 46: FreeGas benz

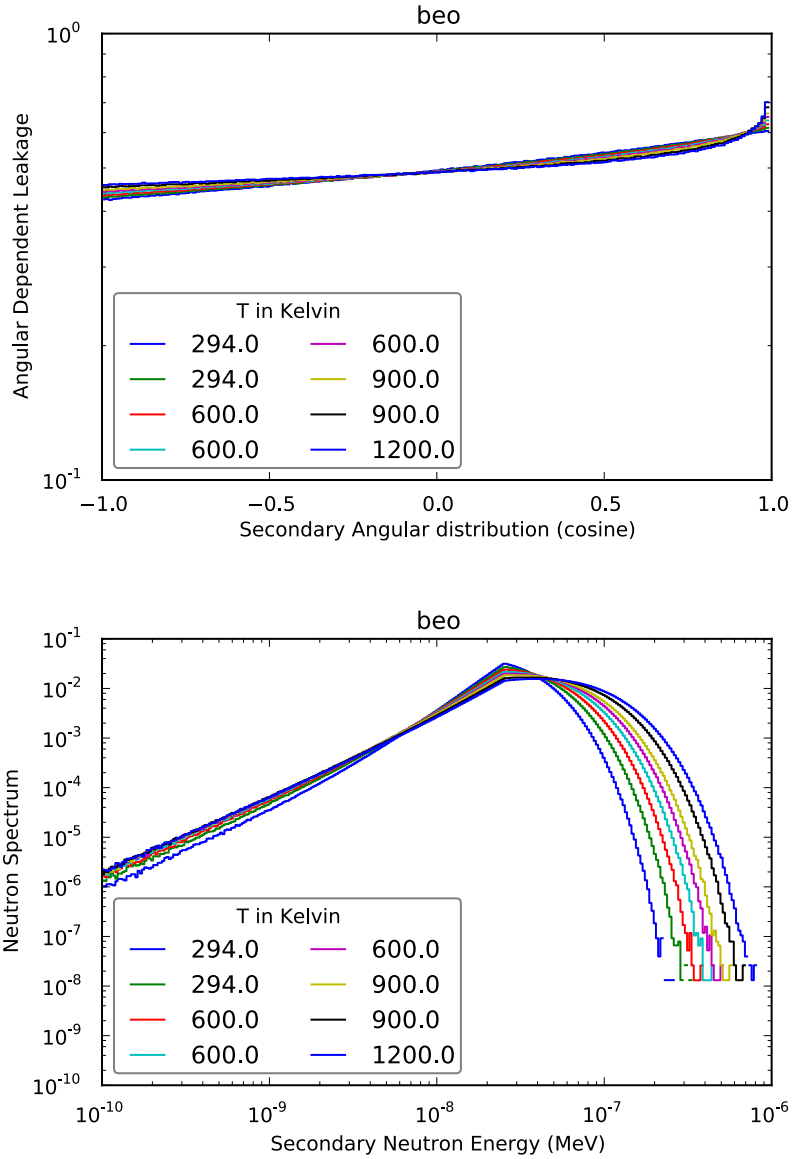


Figure 47: FreeGas beo

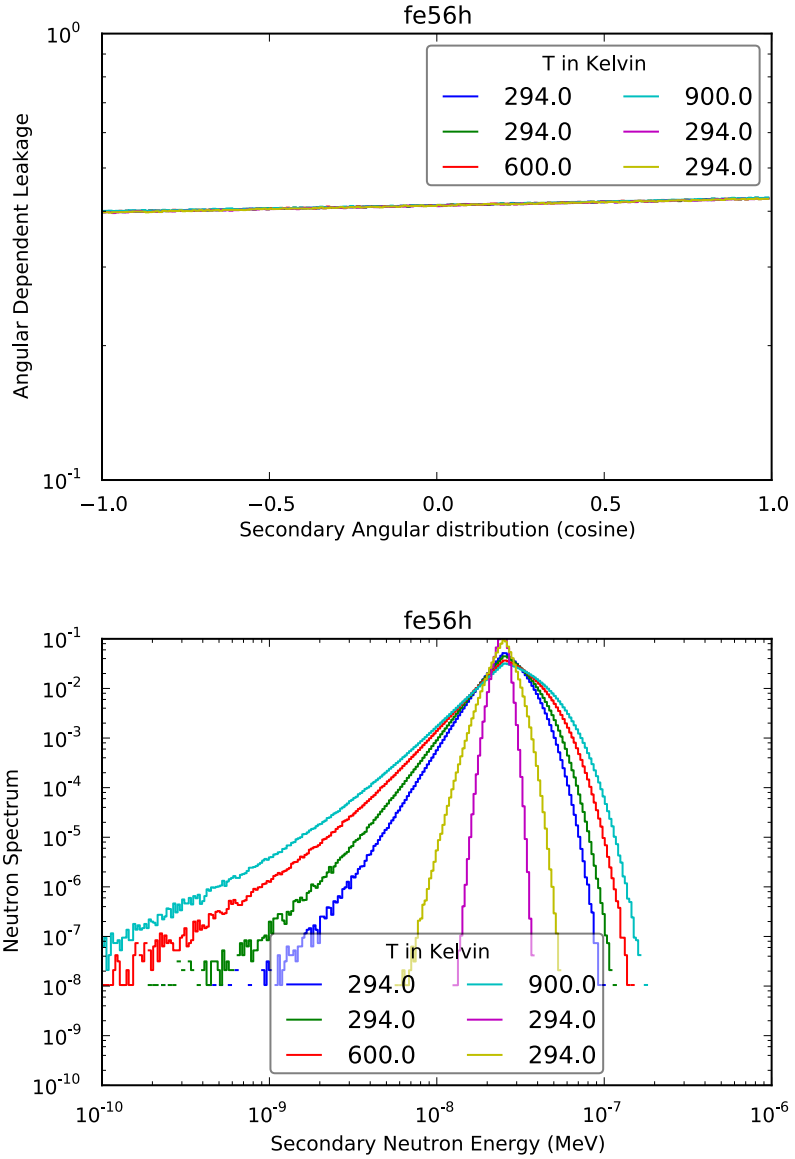


Figure 48: FreeGas fe56h

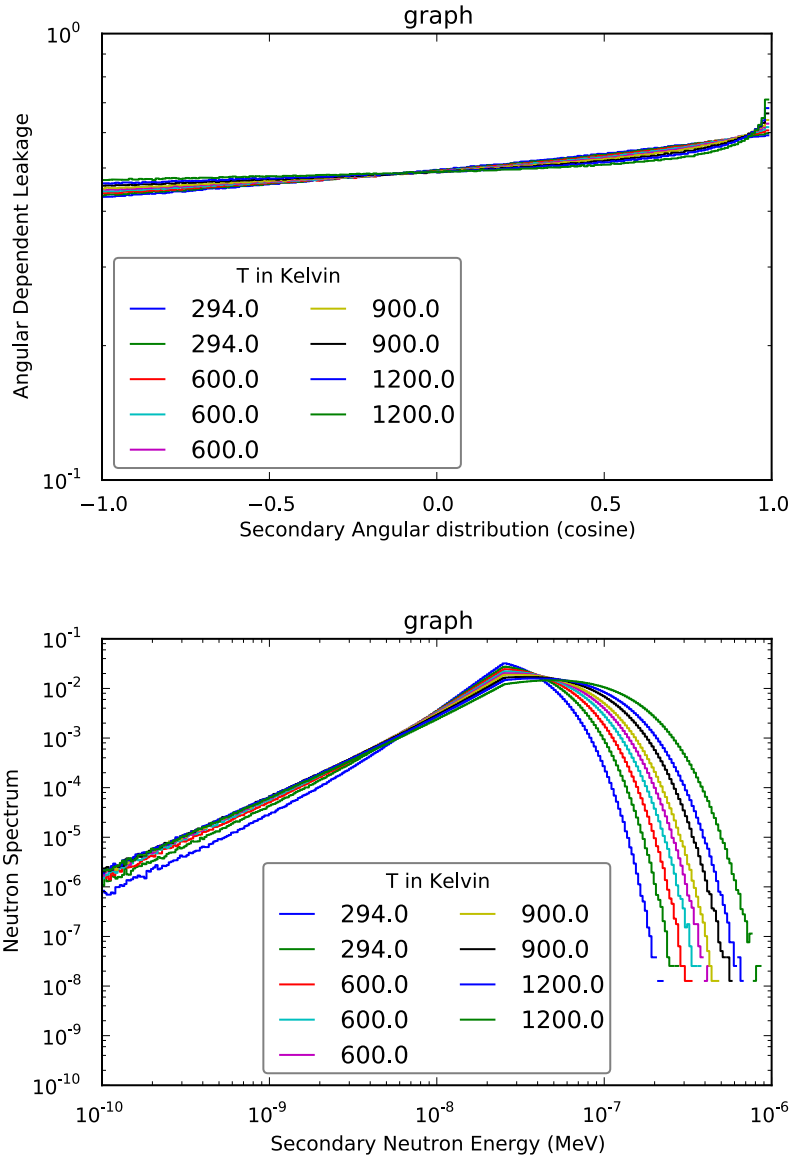


Figure 49: FreeGas graph

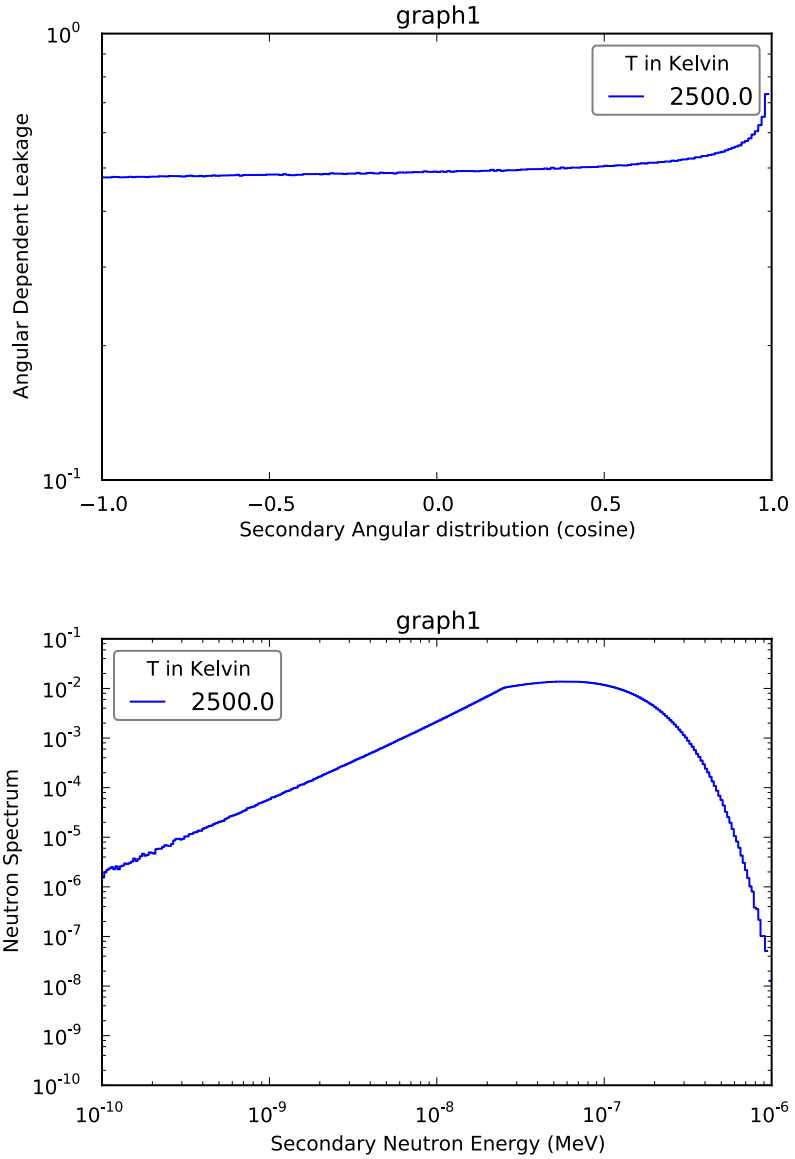


Figure 50: FreeGas graph1

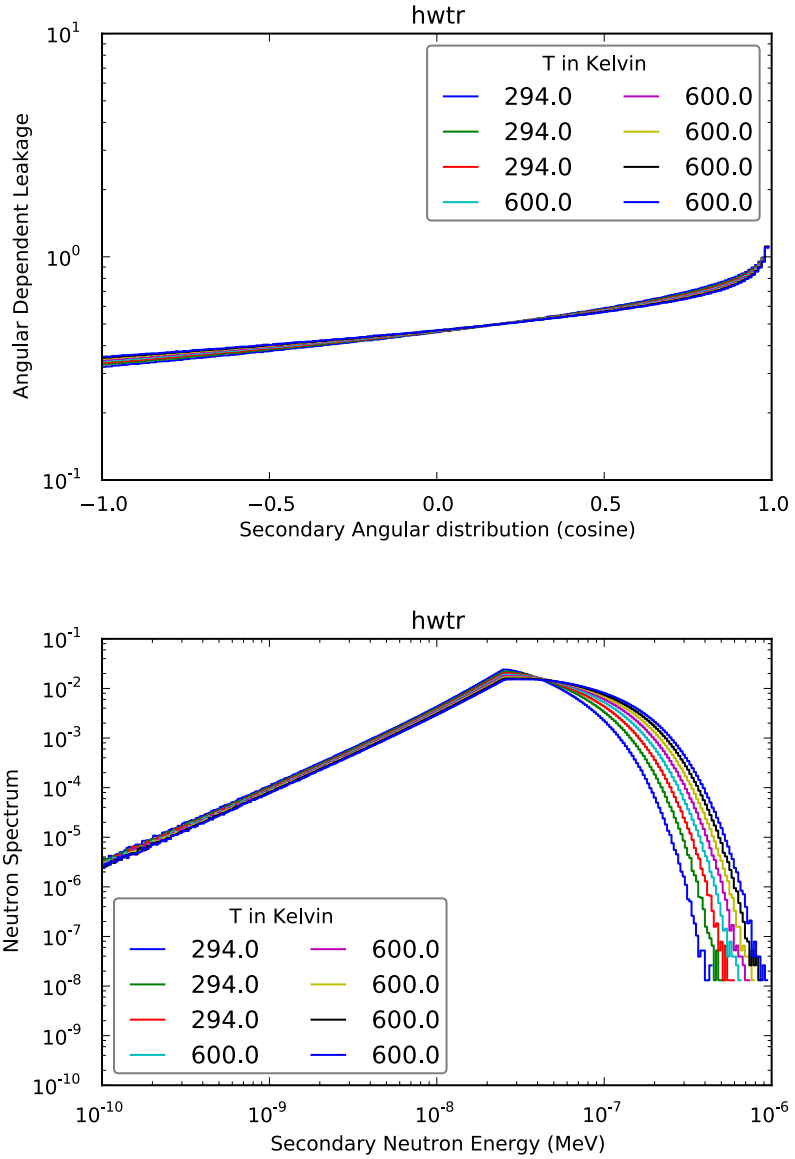


Figure 51: FreeGas hwtr

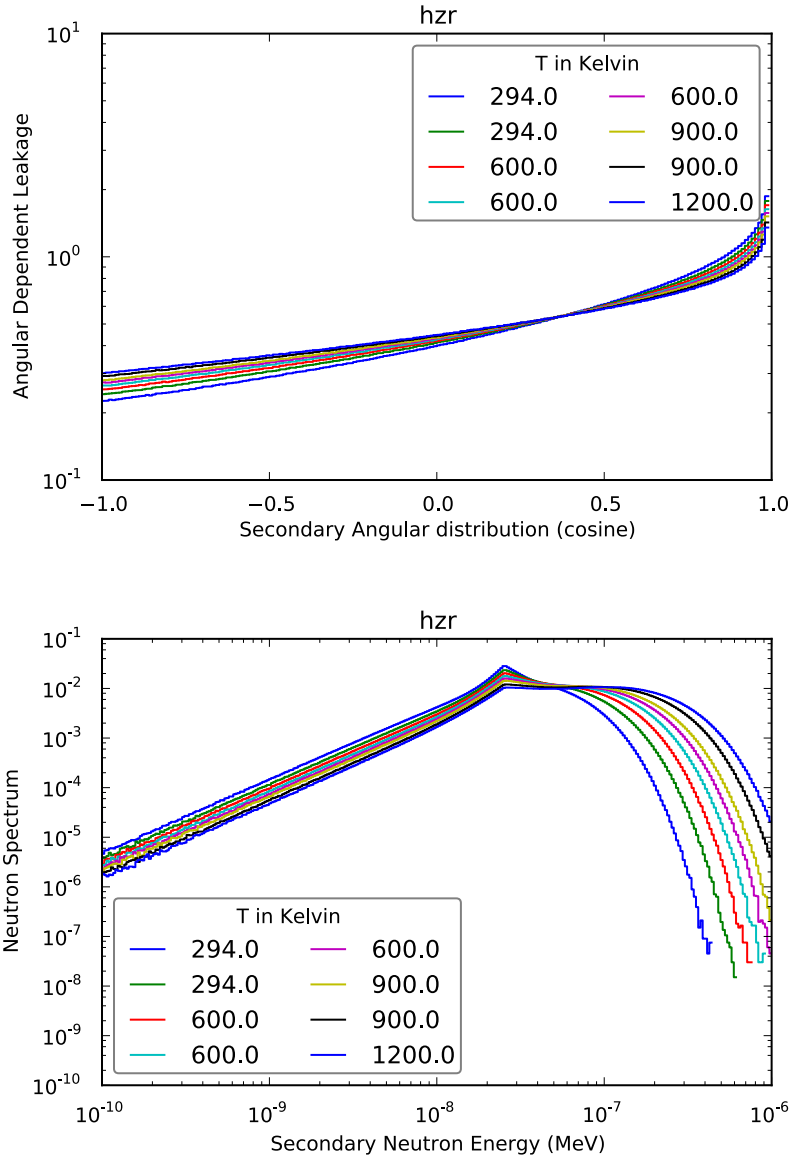


Figure 52: FreeGas hzr

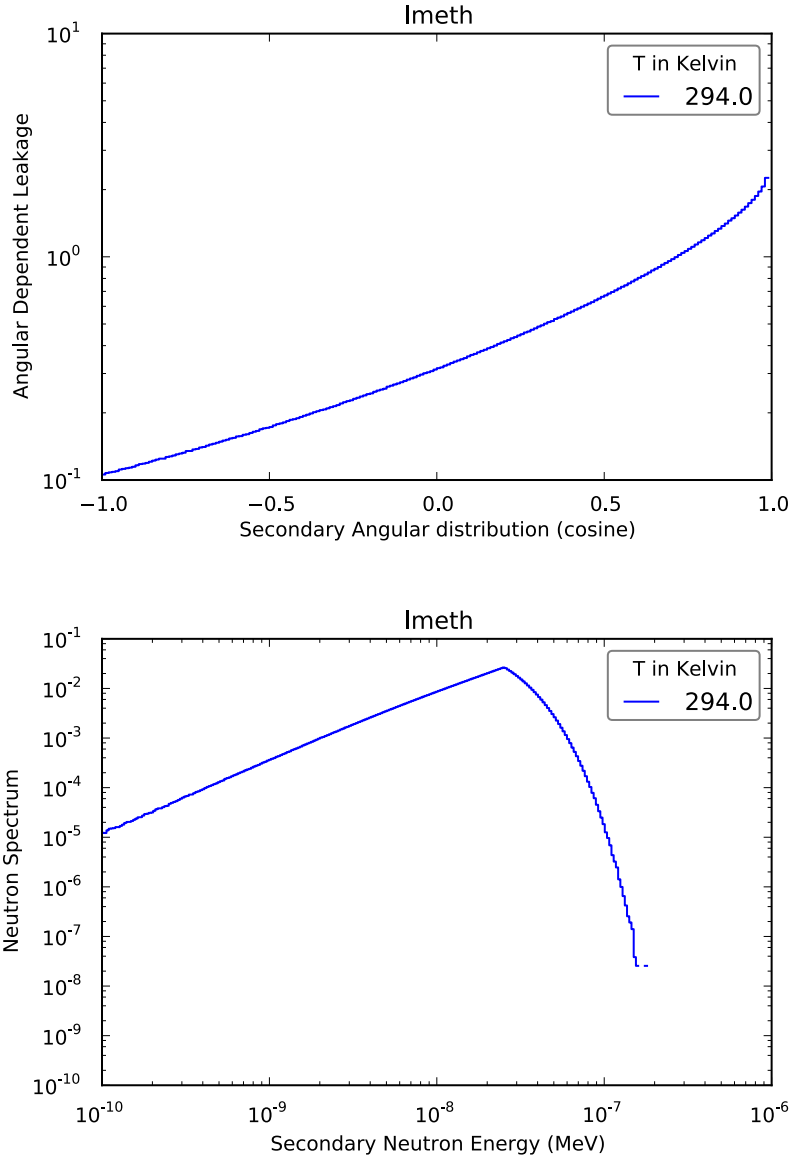


Figure 53: FreeGas lmeth

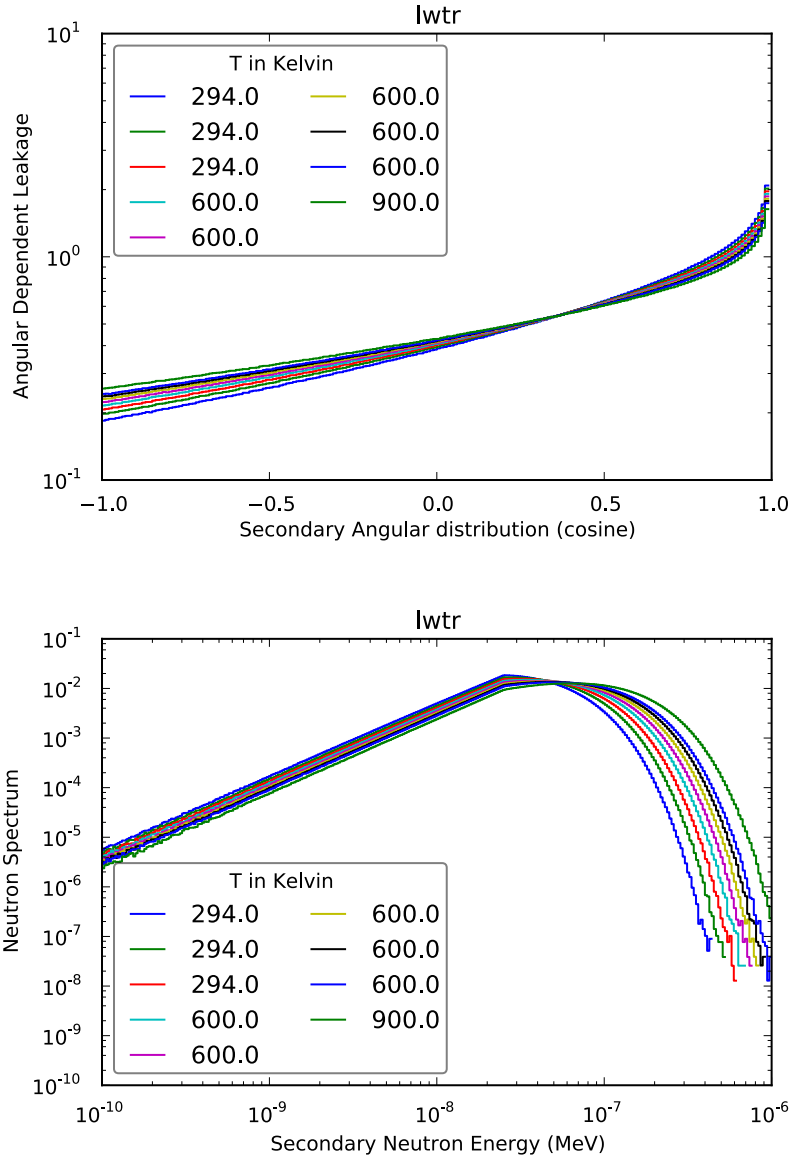


Figure 54: FreeGas lwtr

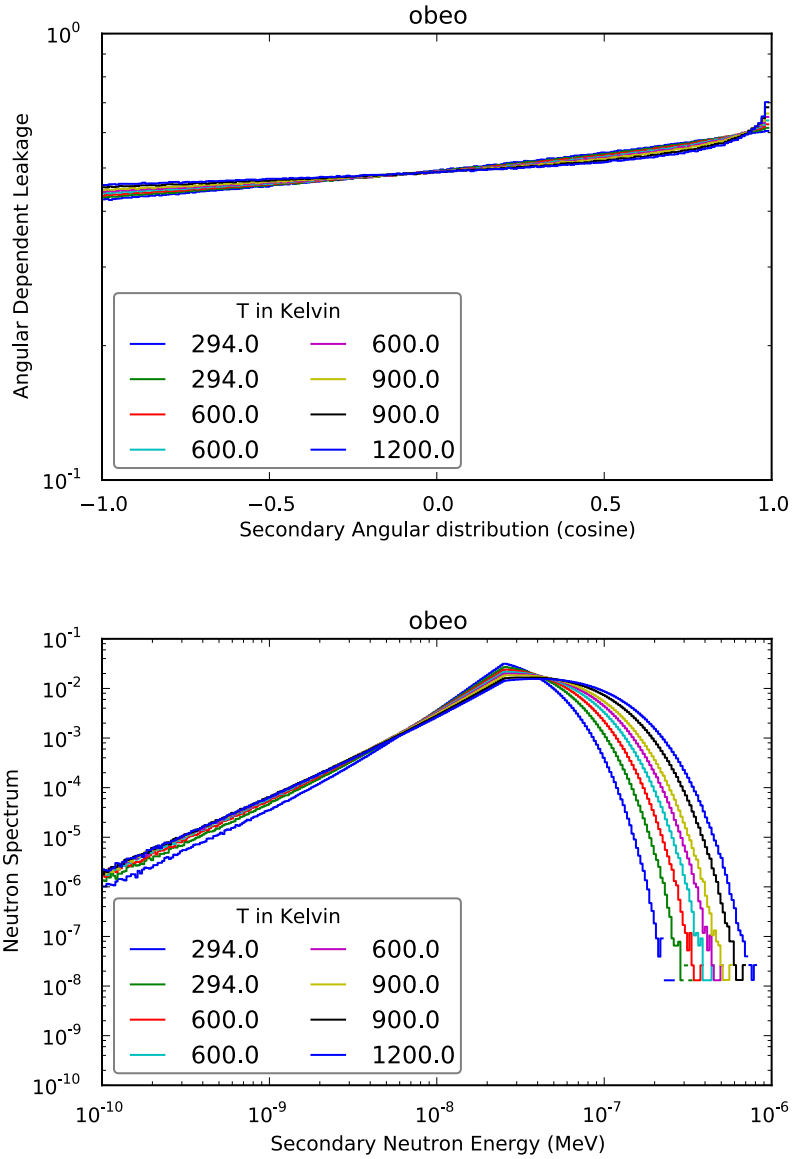


Figure 55: FreeGas obeo

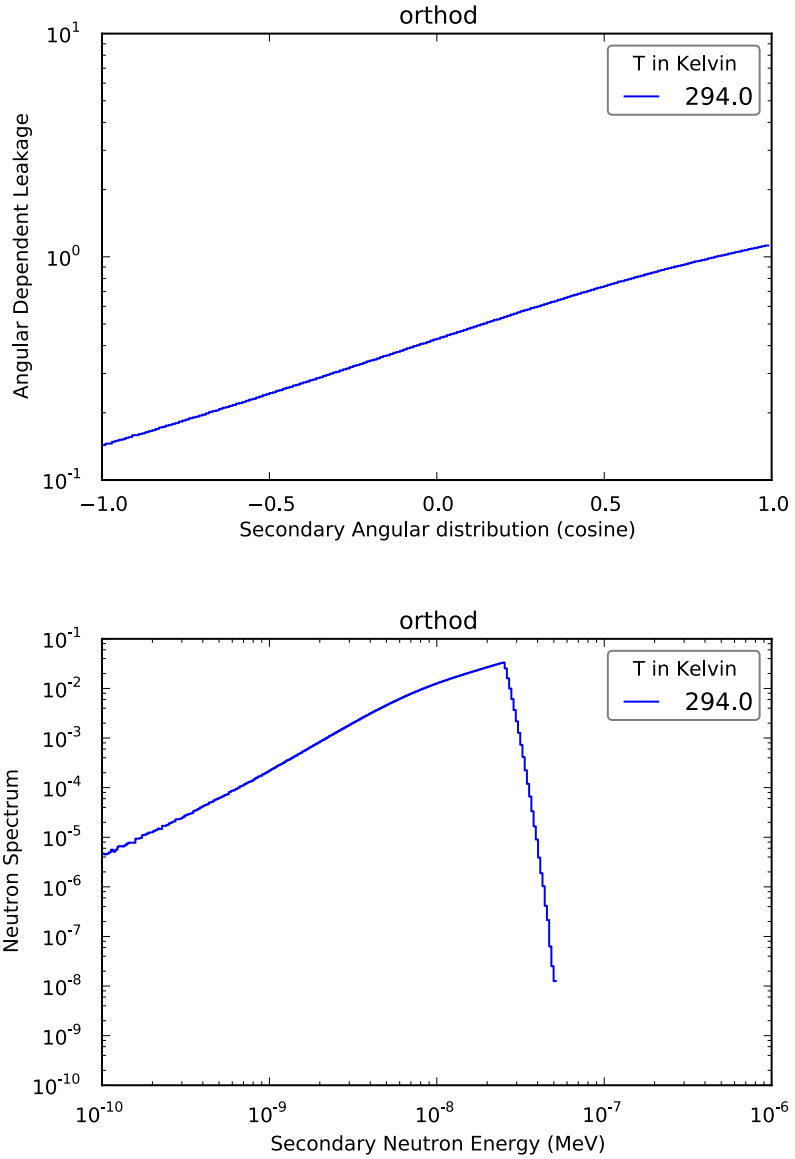


Figure 56: FreeGas orthod

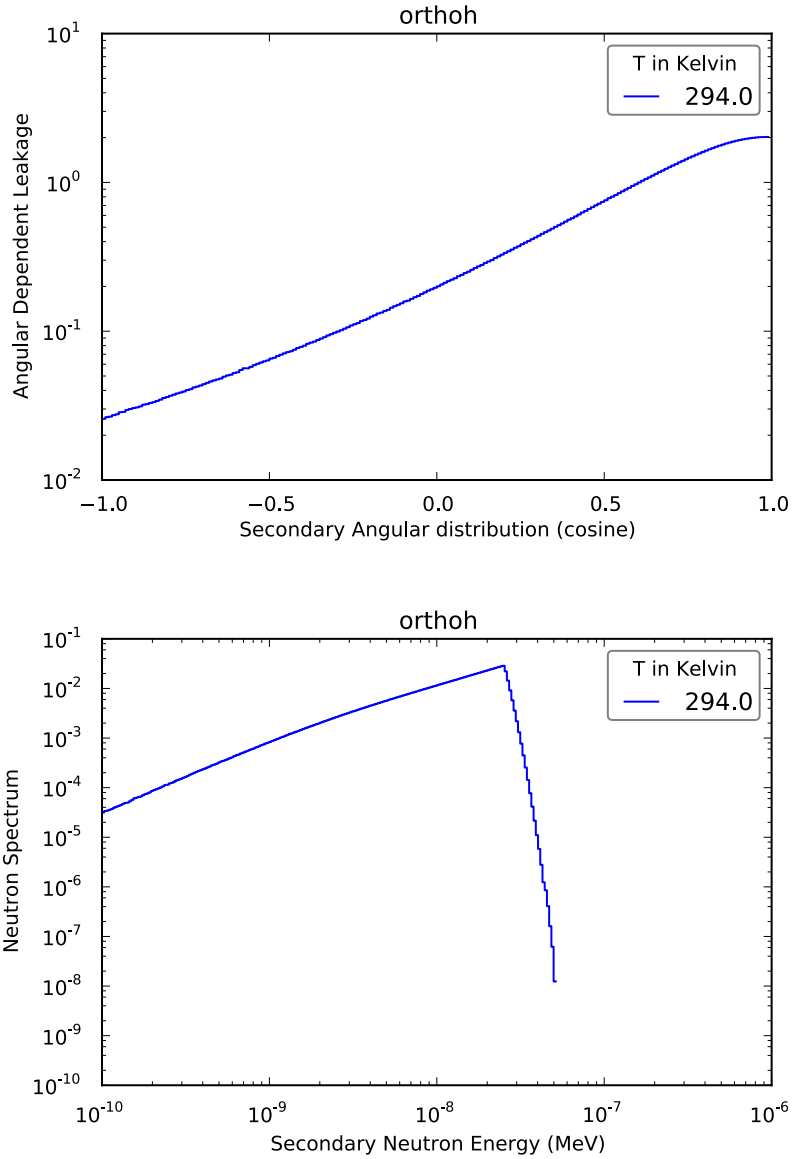


Figure 57: FreeGas orthoh

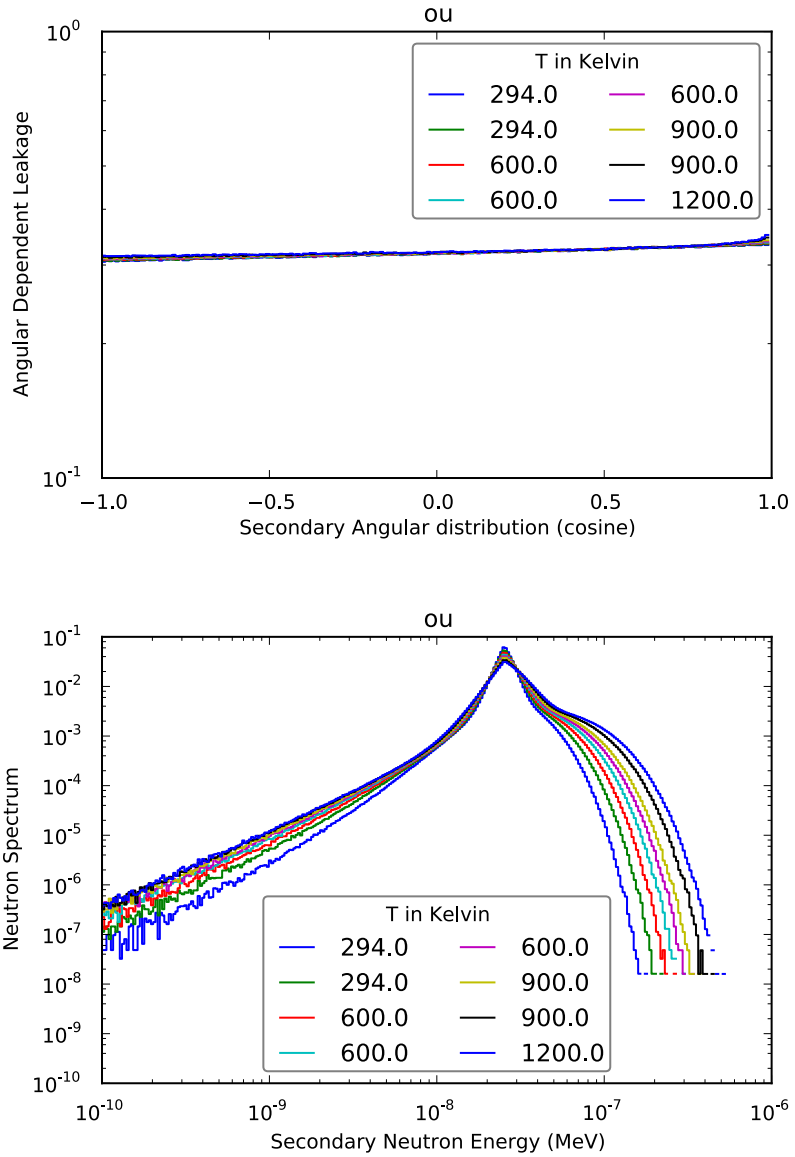


Figure 58: FreeGas ou

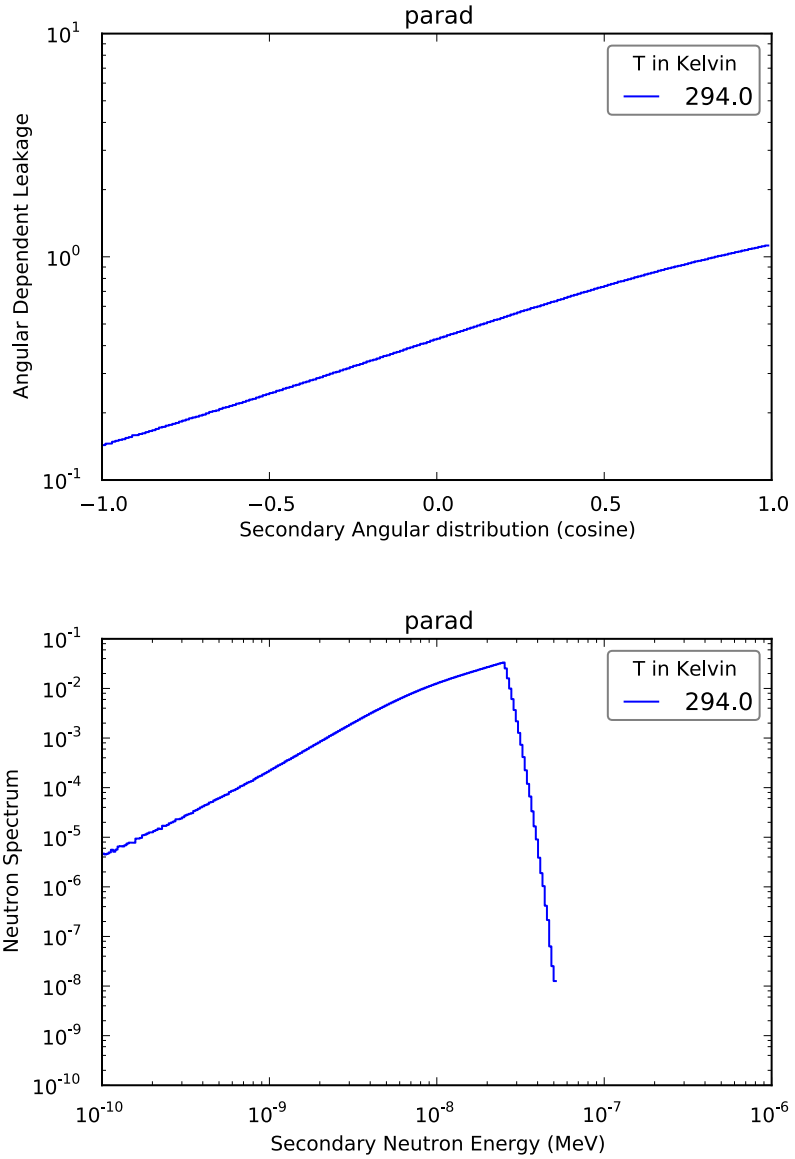


Figure 59: FreeGas parad

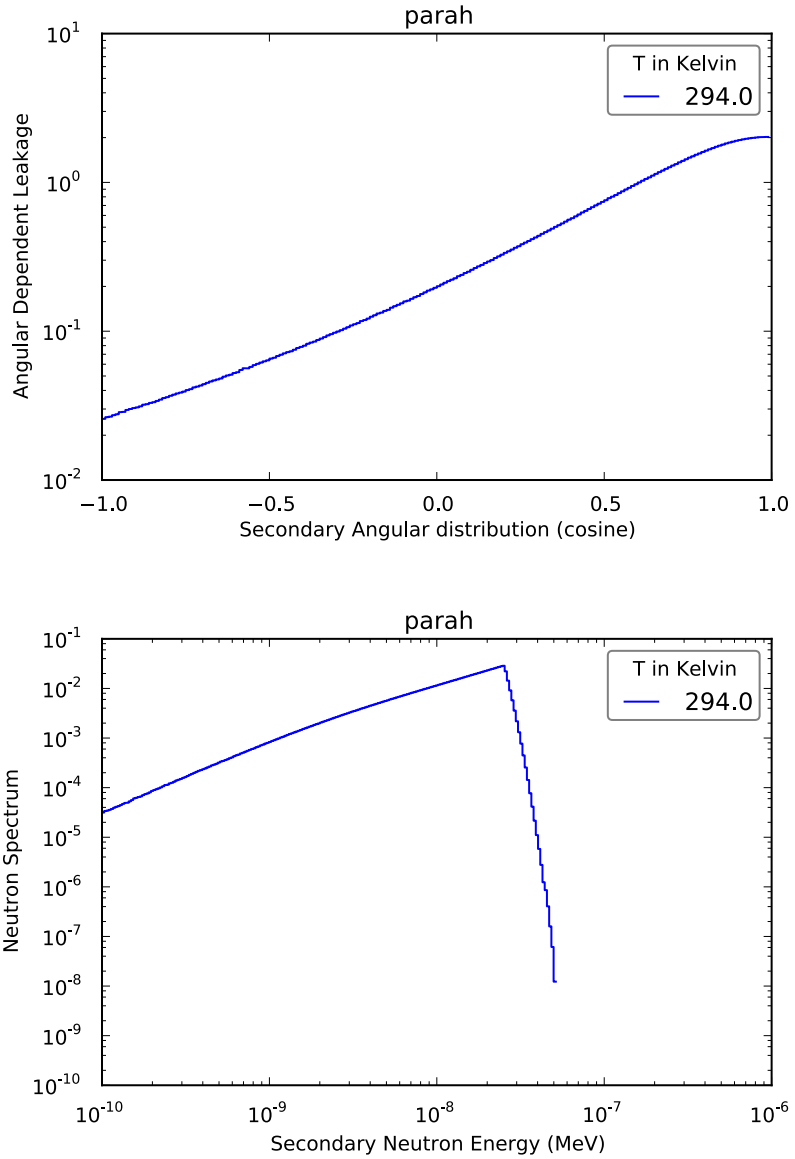


Figure 60: FreeGas parah

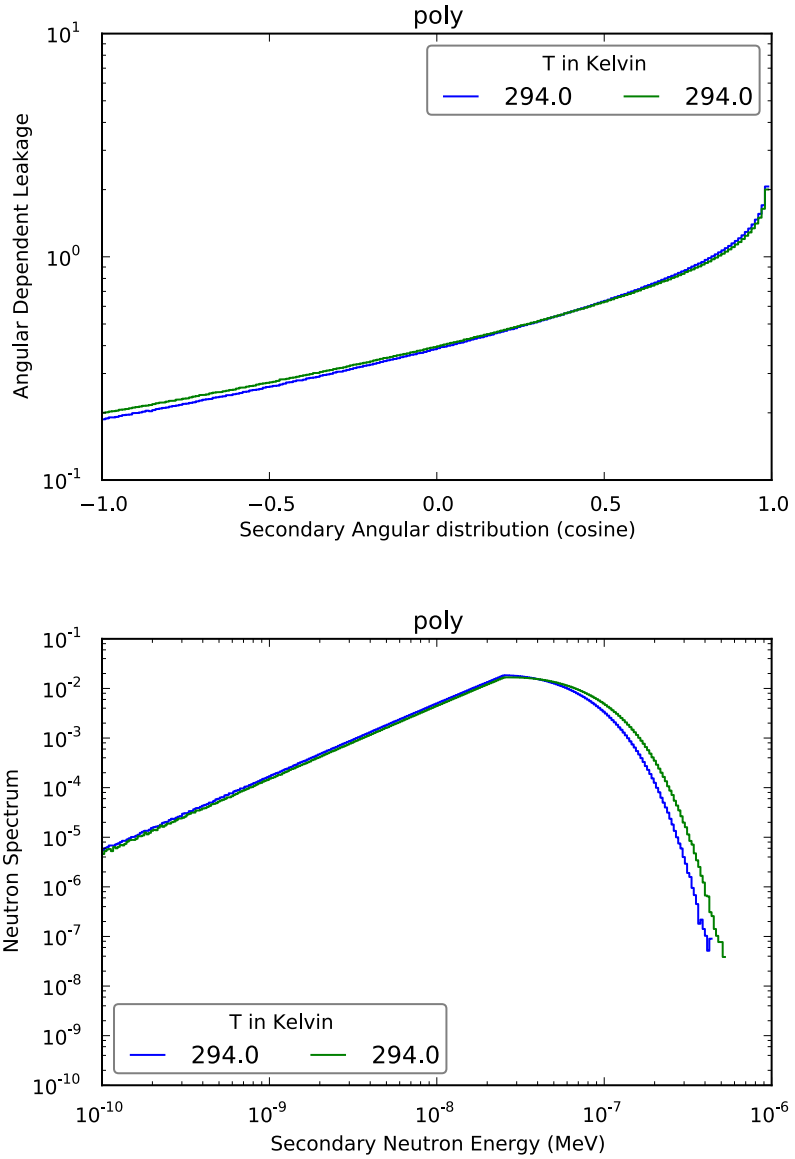


Figure 61: FreeGas poly

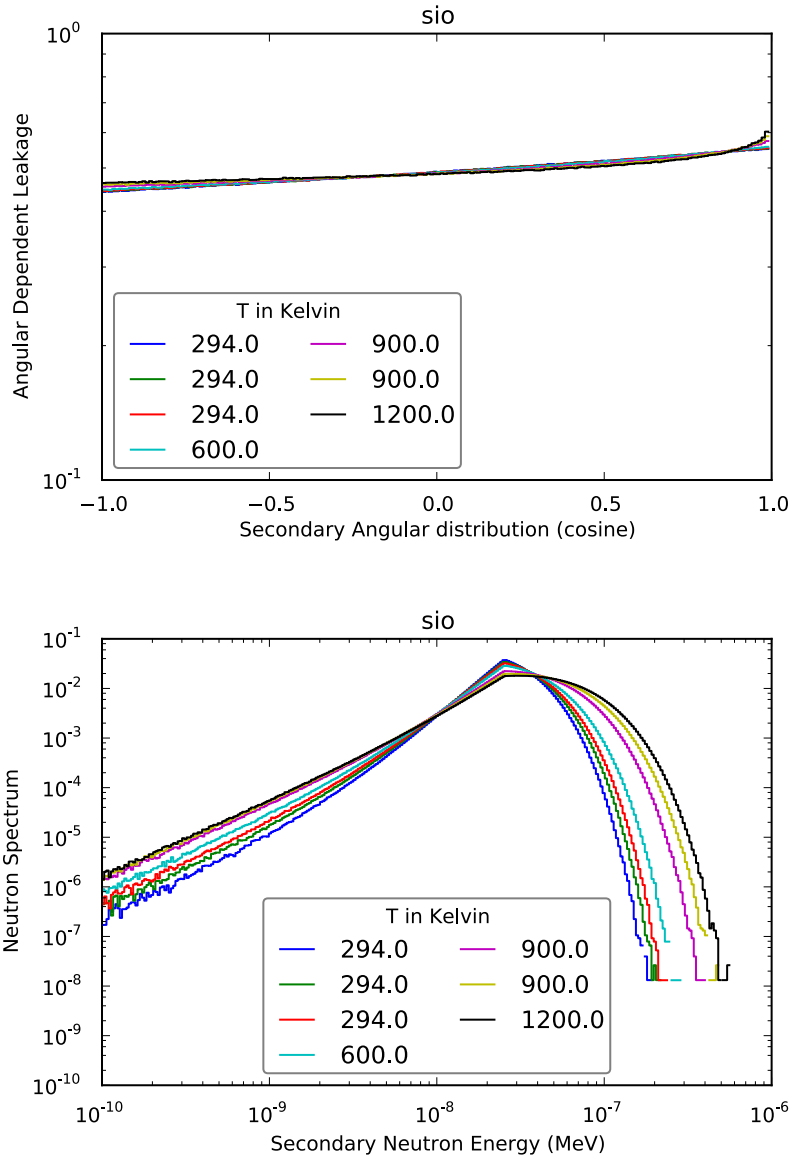


Figure 62: FreeGas sio

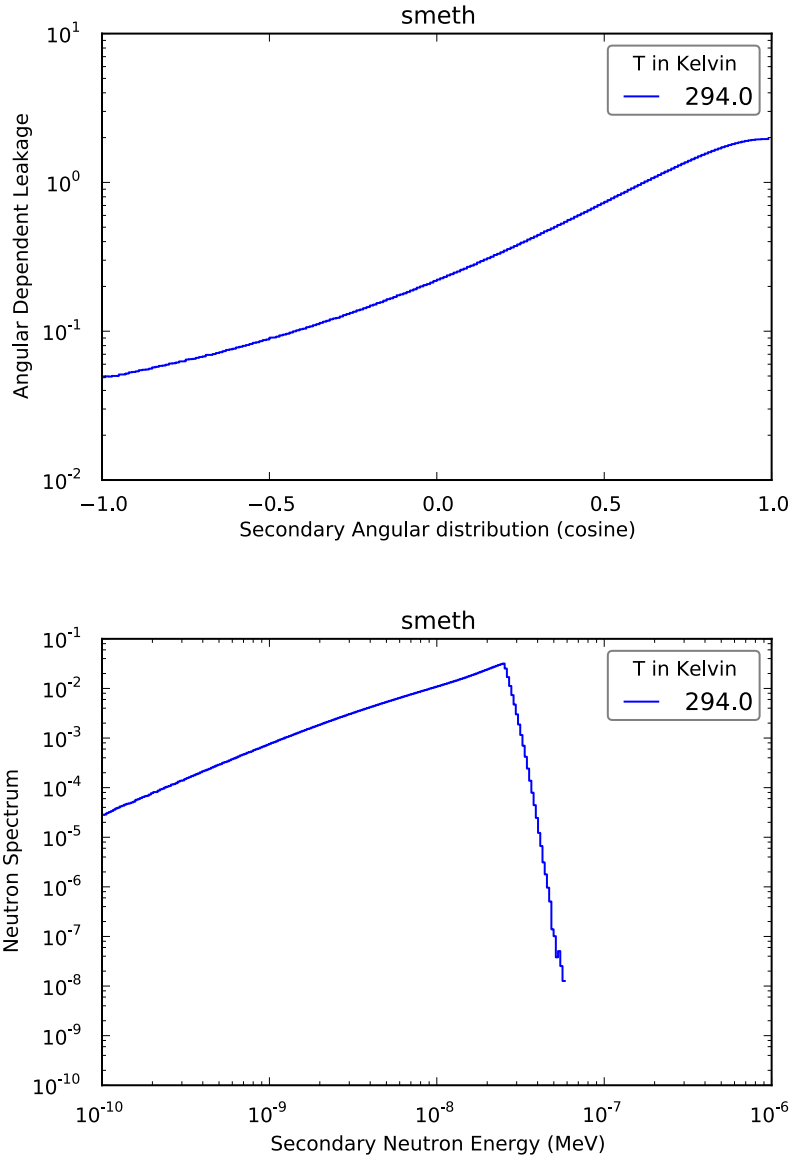


Figure 63: FreeGas smeth

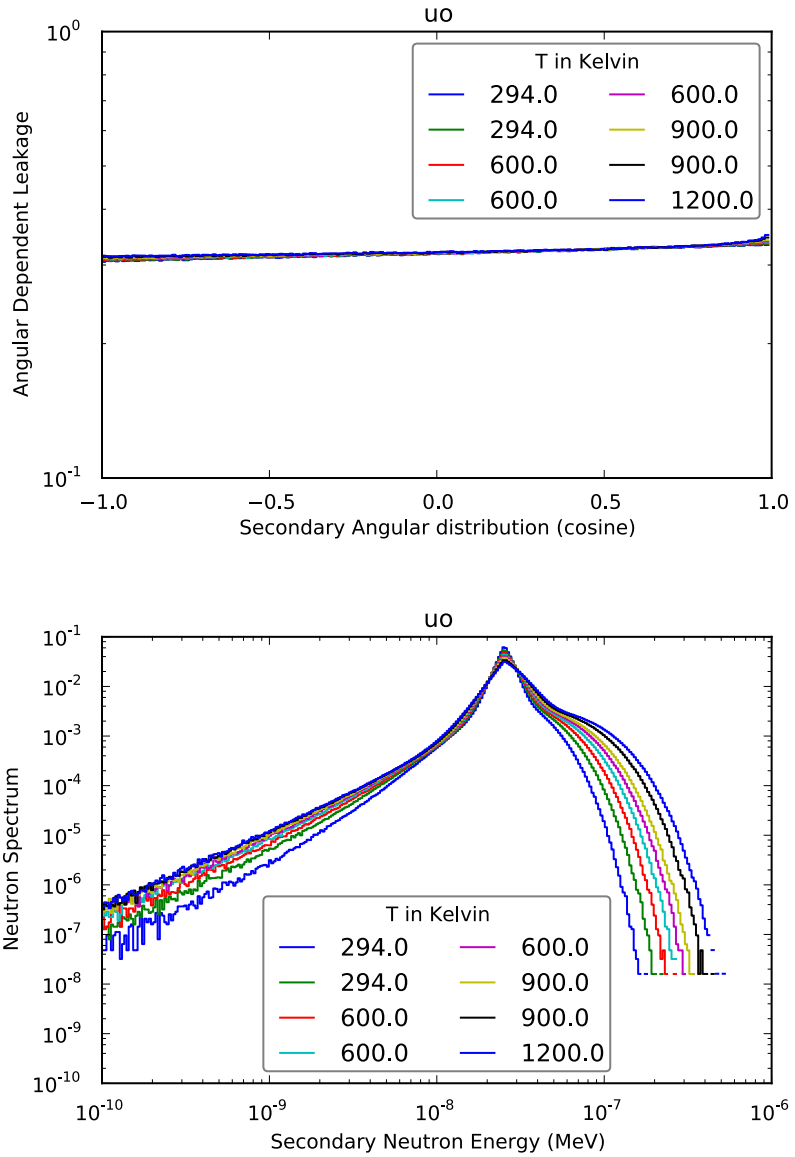


Figure 64: FreeGas uo

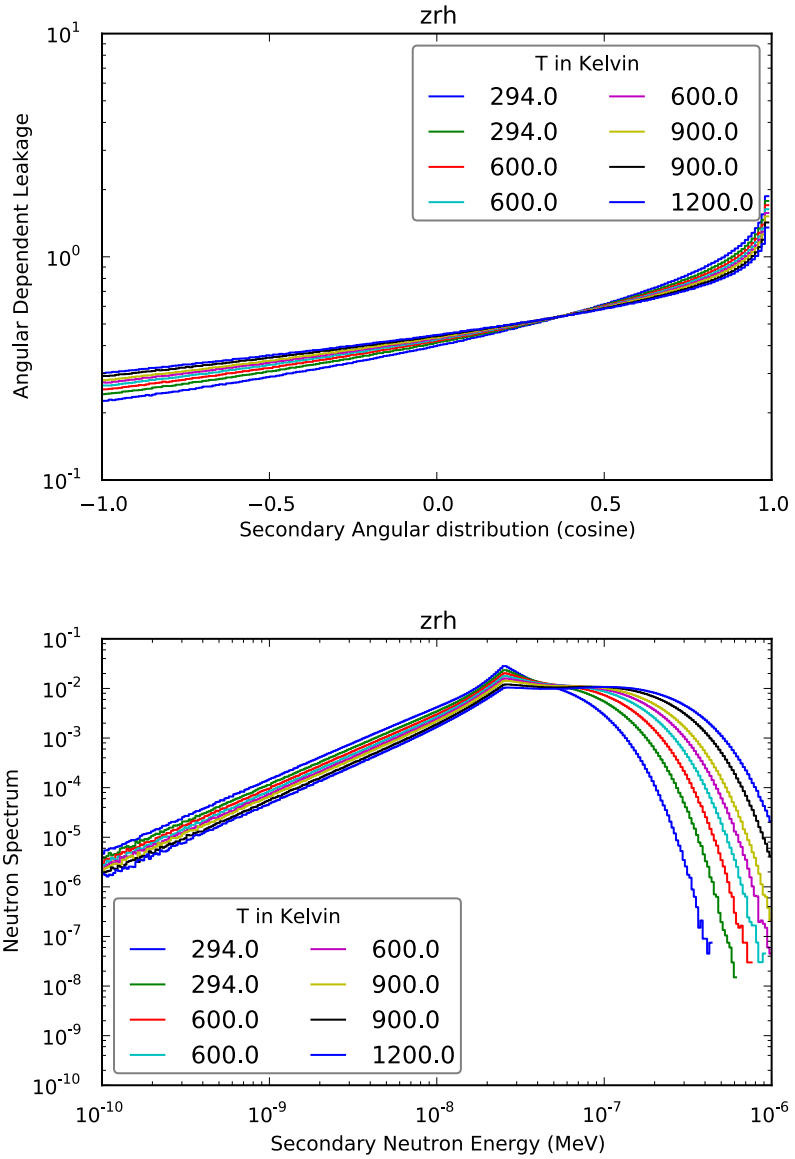


Figure 65: FreeGas zrh

D Plots of the S(α, β) Cross Sections

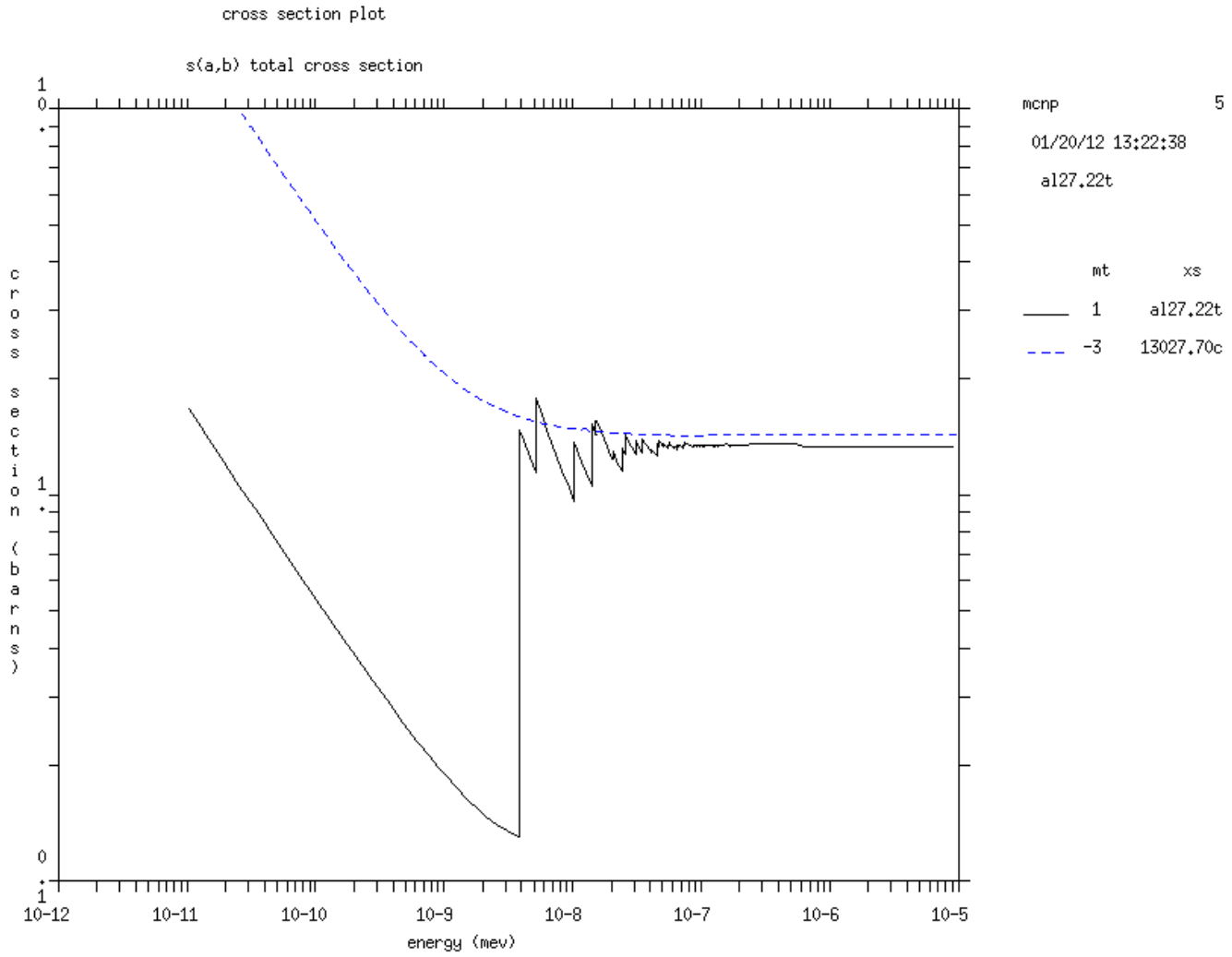


Figure 66: Plot of cross section for S(α, β) material: `al27`

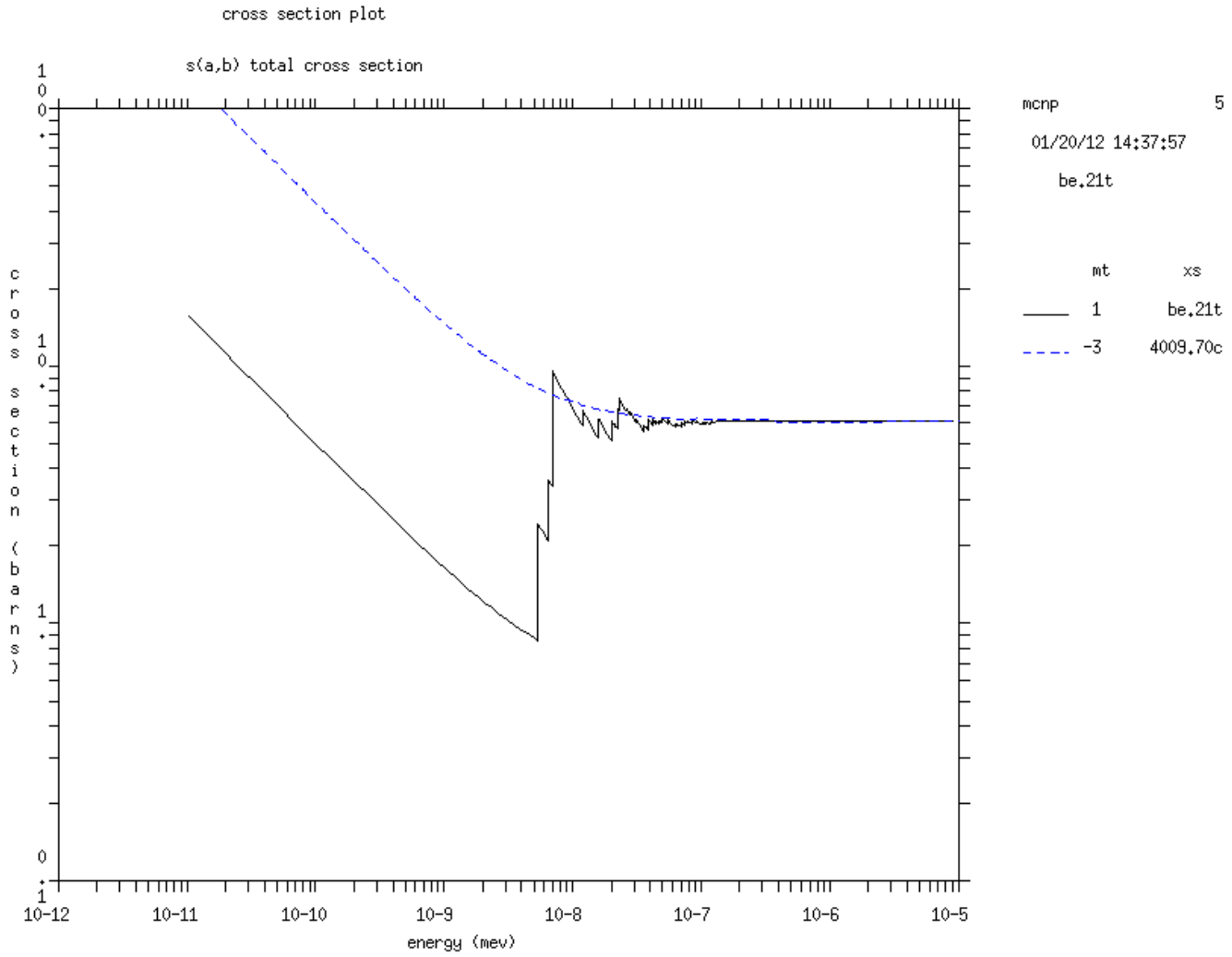


Figure 67: Plot of cross section for S(α, β) material: `be`

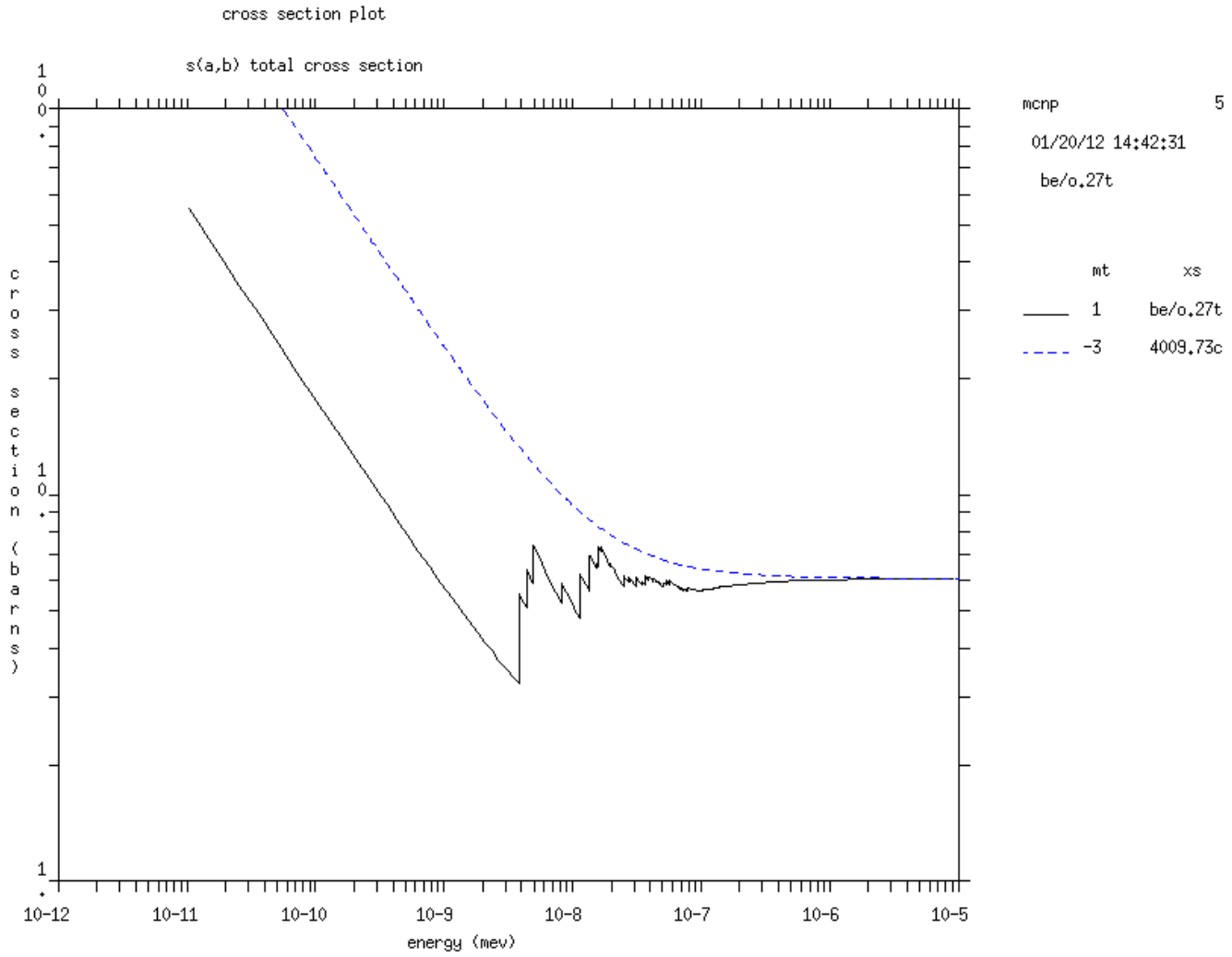


Figure 68: Plot of cross section for S(α, β) material: `beo`

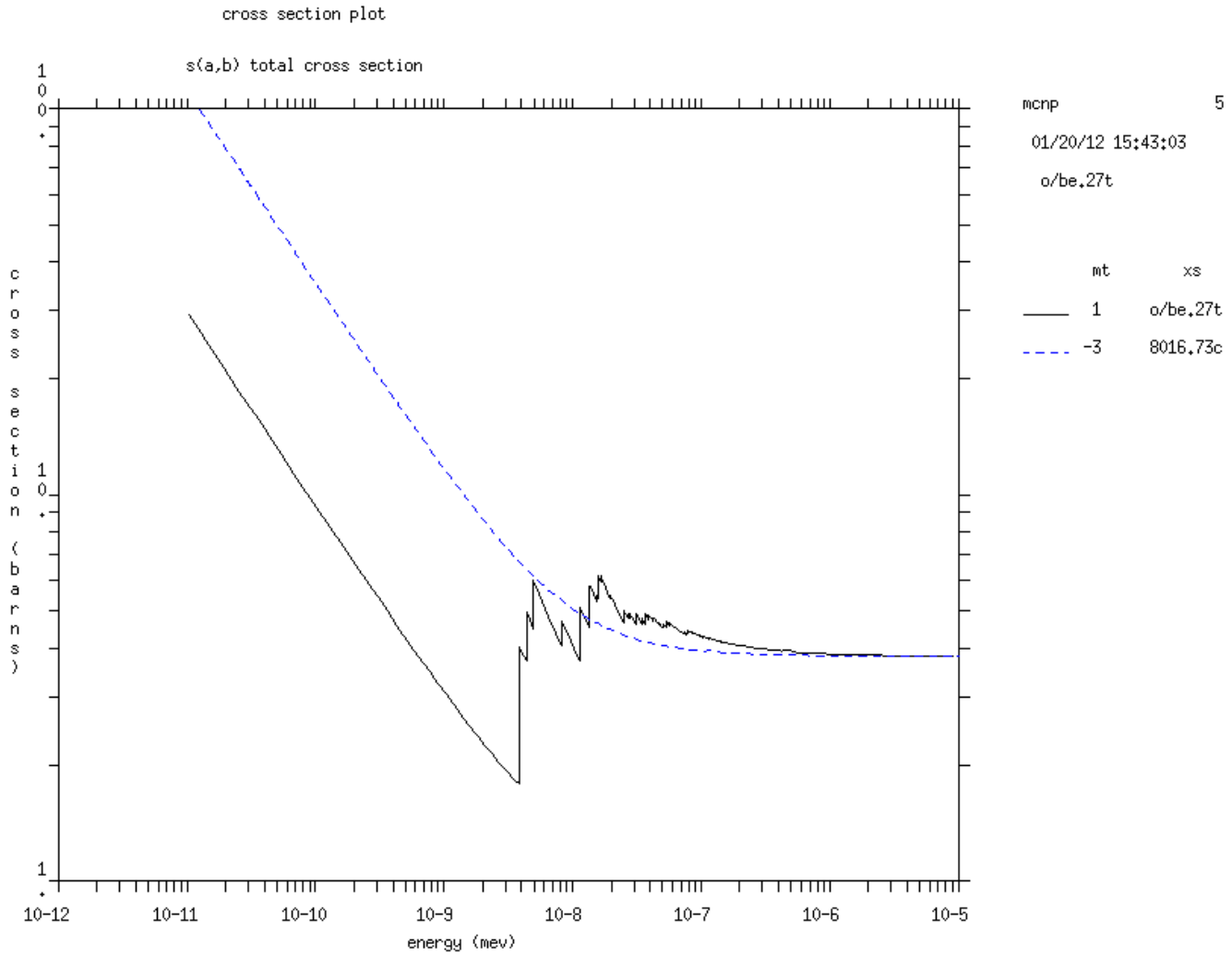


Figure 69: Plot of cross section for S(α, β) material: `obe`

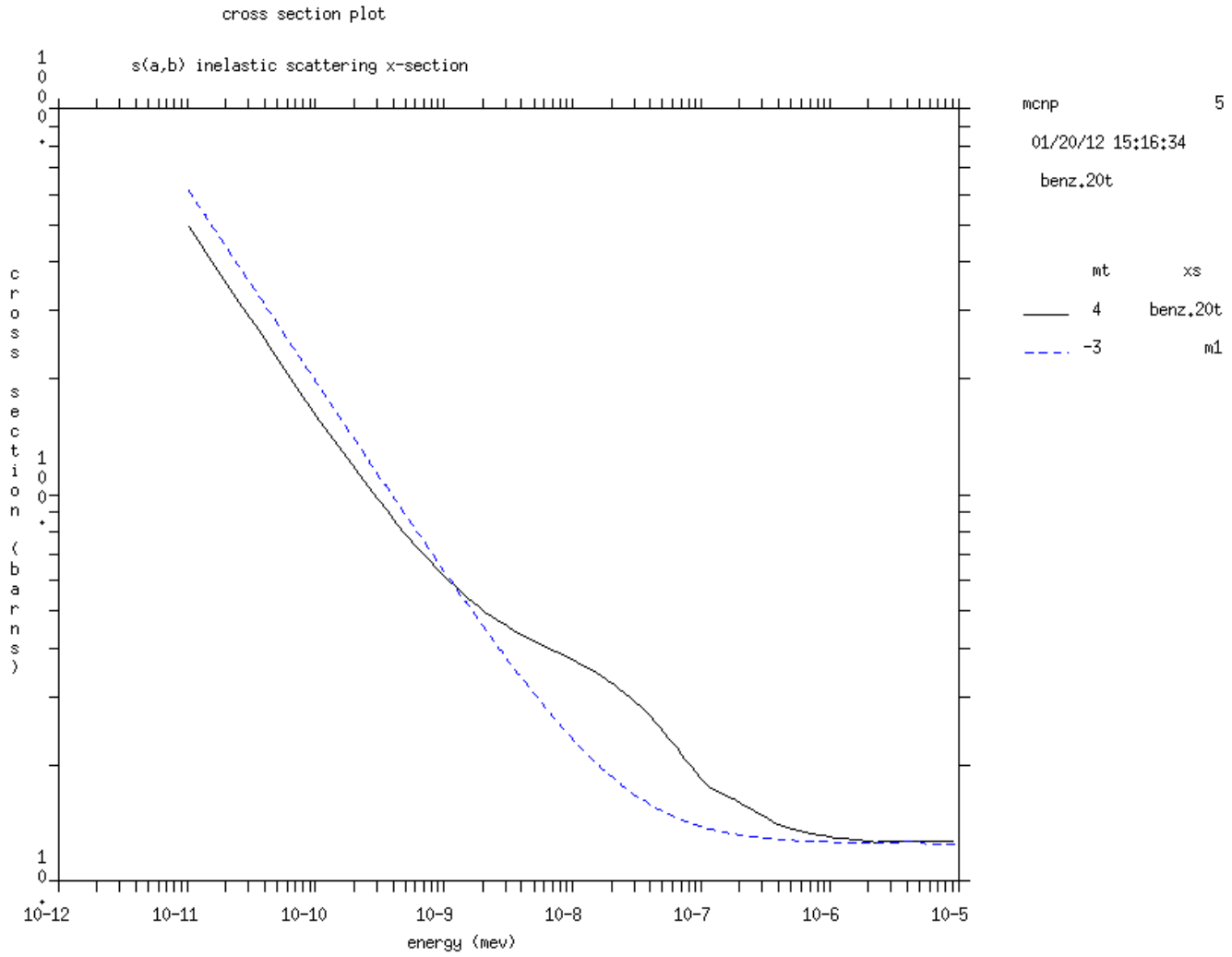


Figure 70: Plot of cross section for S(α, β) material: `benz`

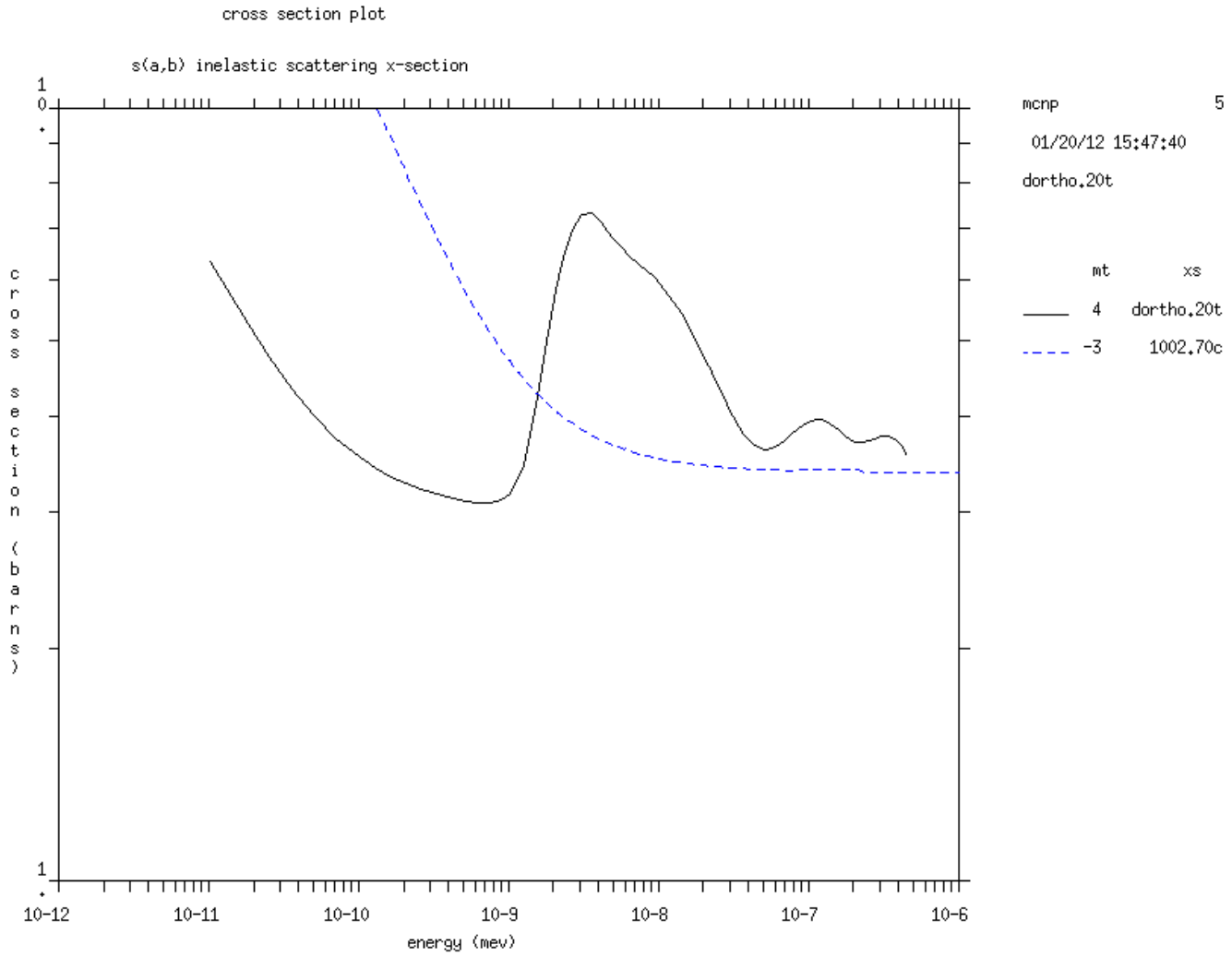


Figure 71: Plot of cross section for S(α, β) material: `dortho`

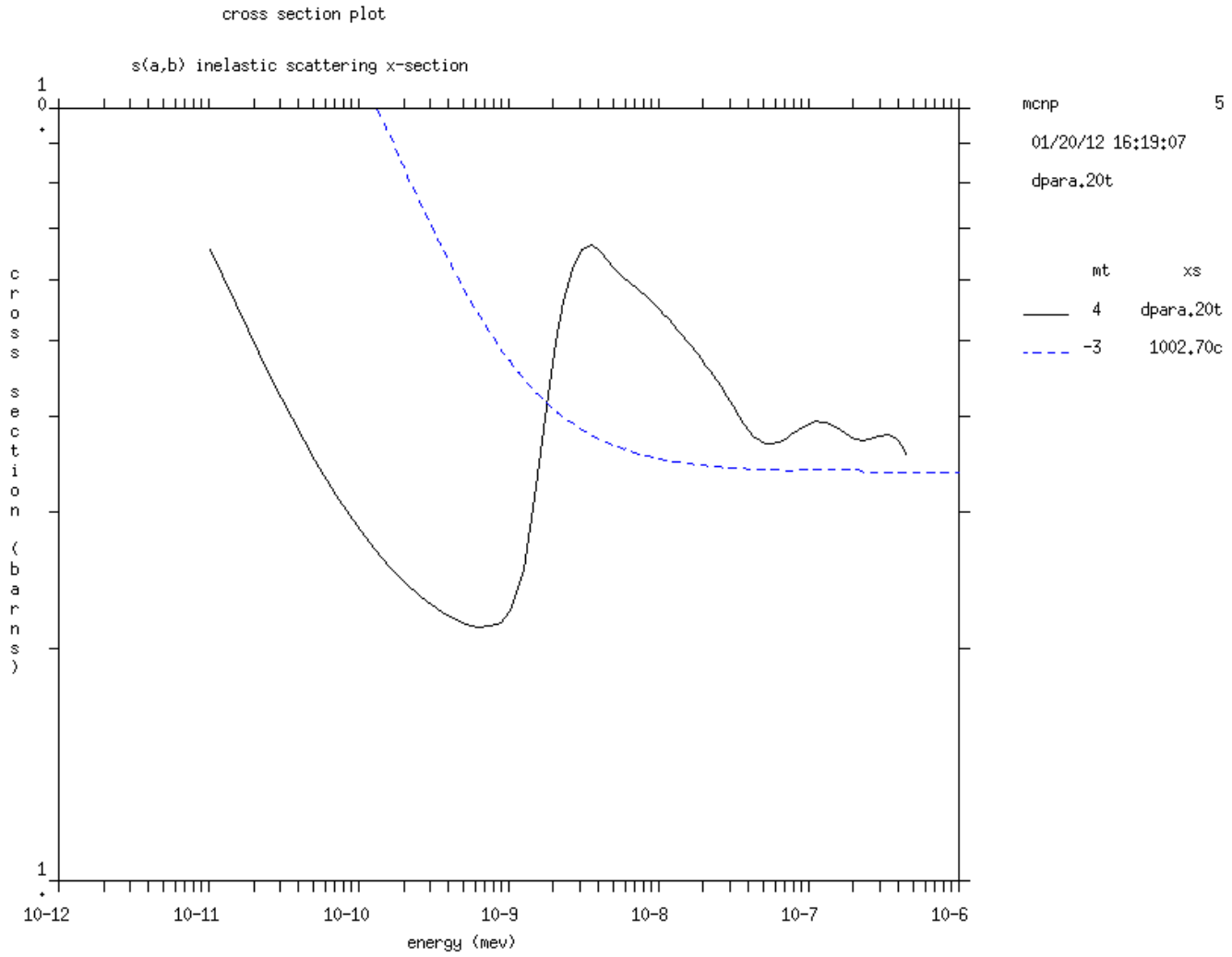


Figure 72: Plot of cross section for S(α, β) material: `dpara`

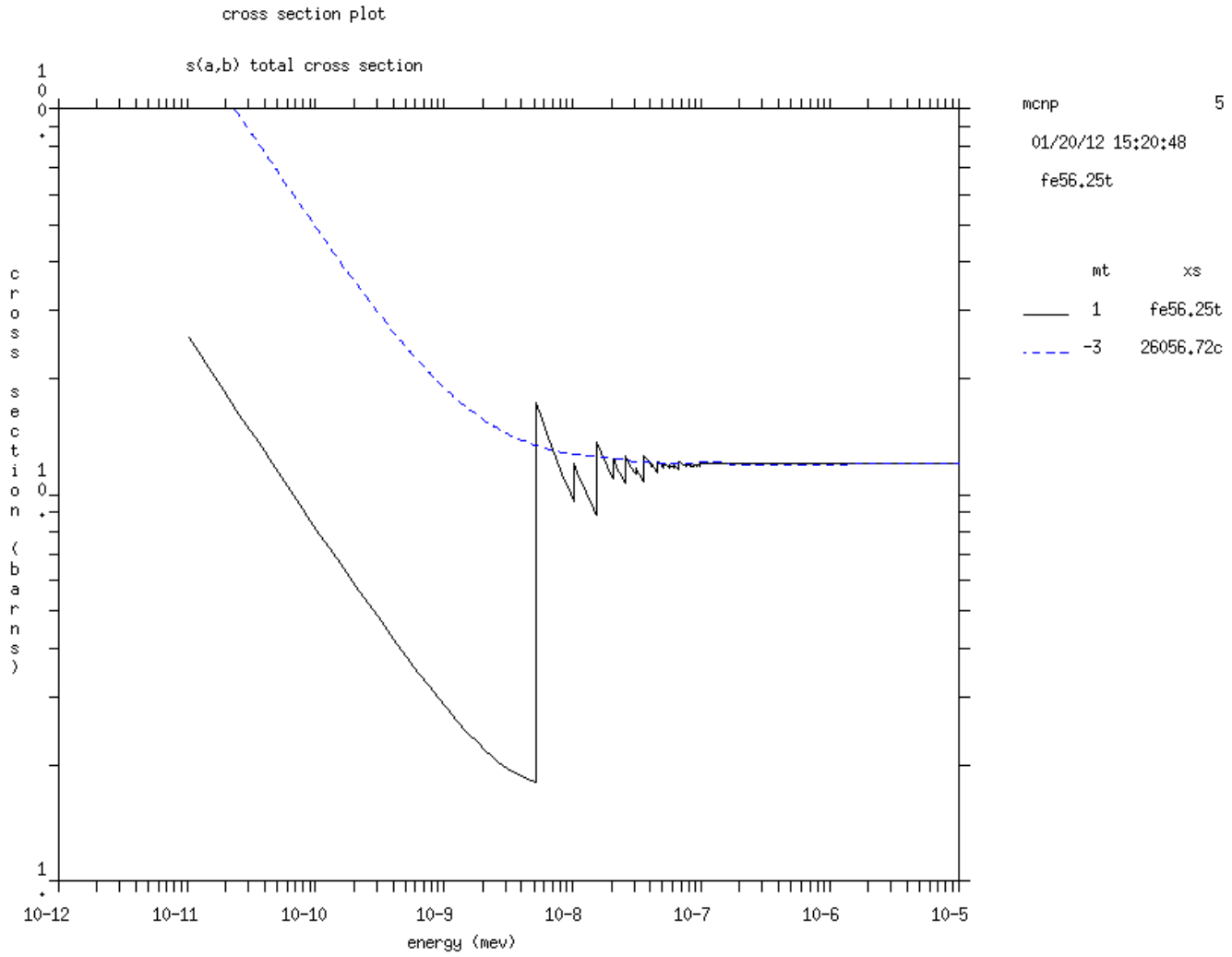


Figure 73: Plot of cross section for S(α, β) material: `fe56`

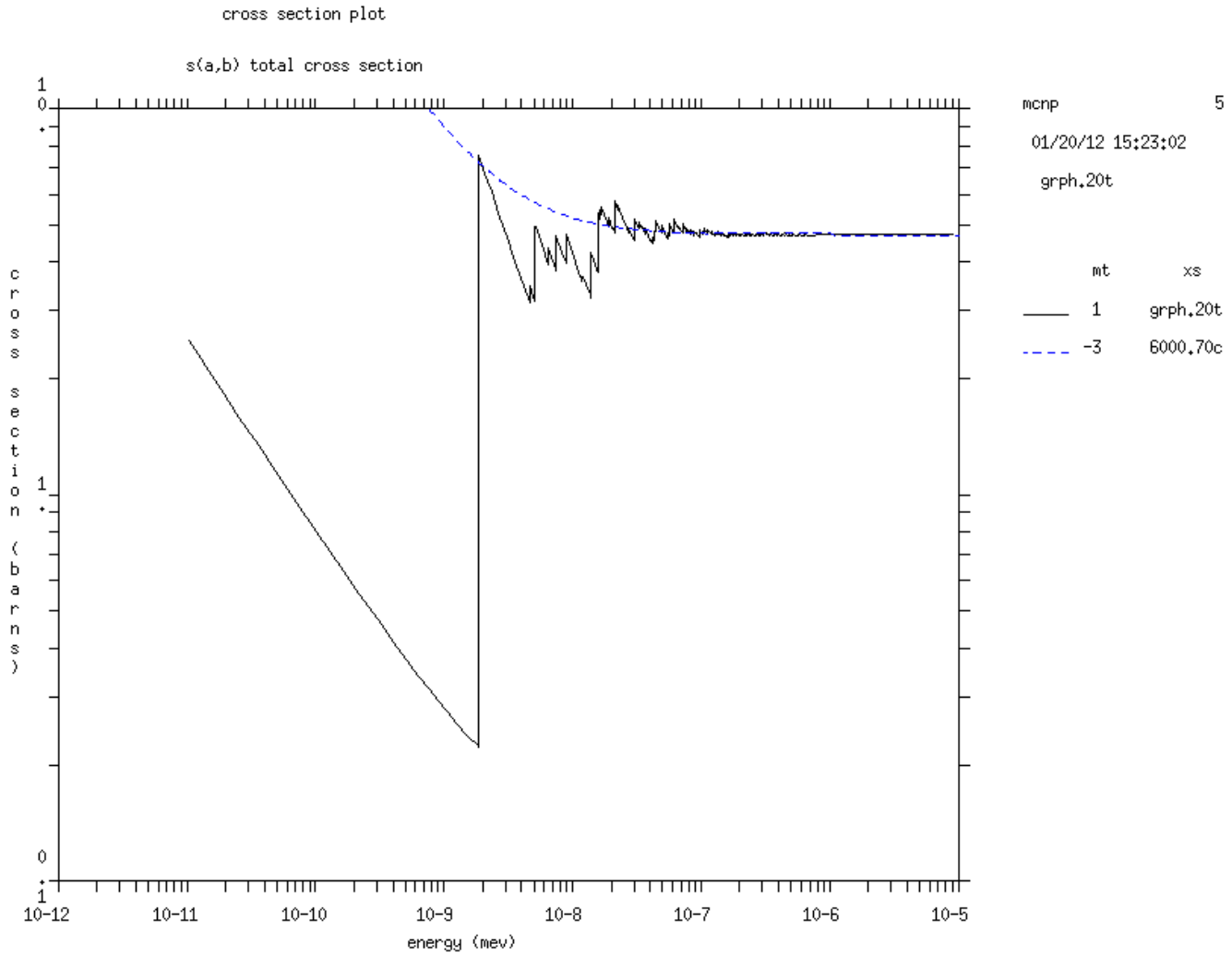


Figure 74: Plot of cross section for S(α, β) material: `graph`

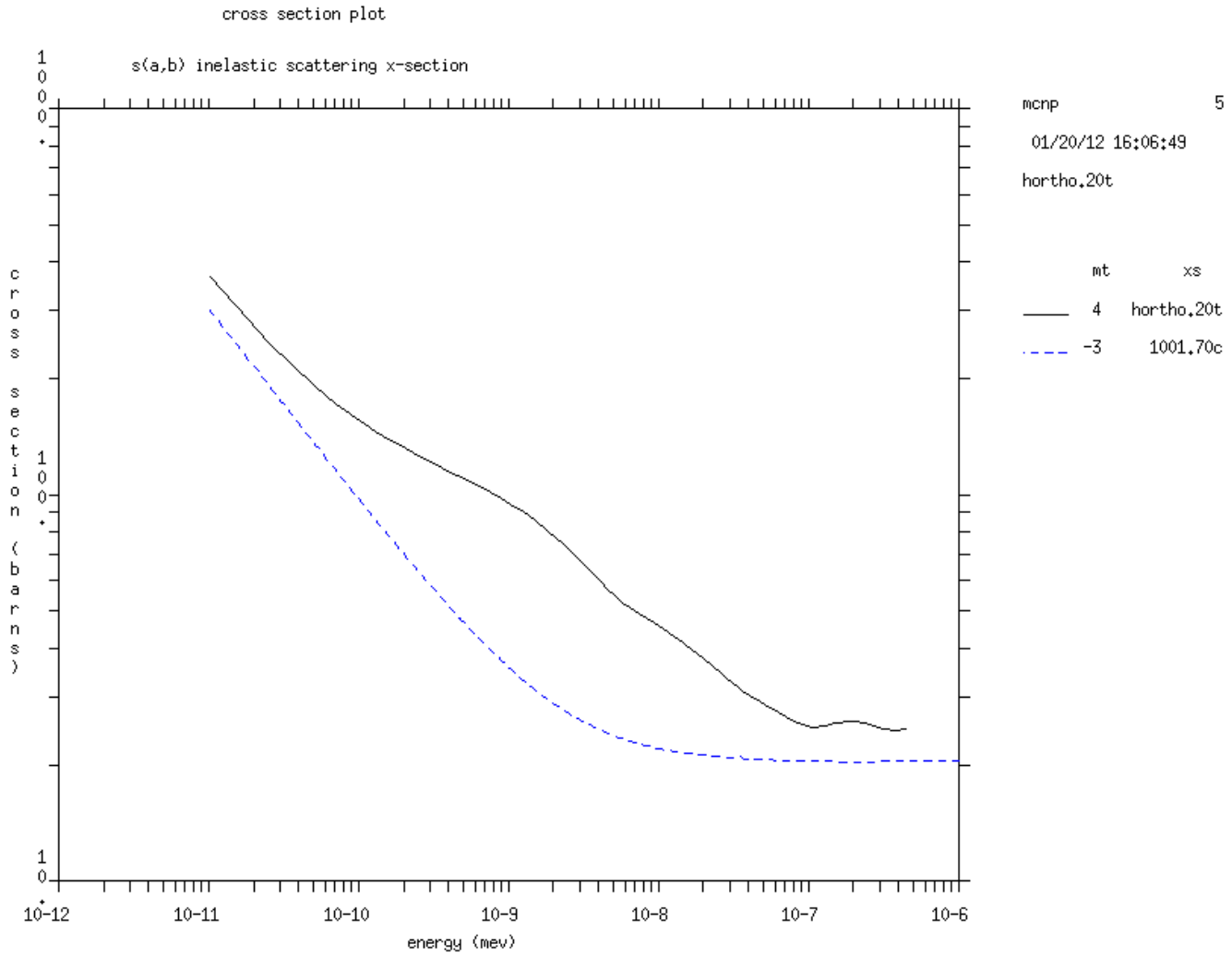


Figure 75: Plot of cross section for S(α, β) material: `hortho`

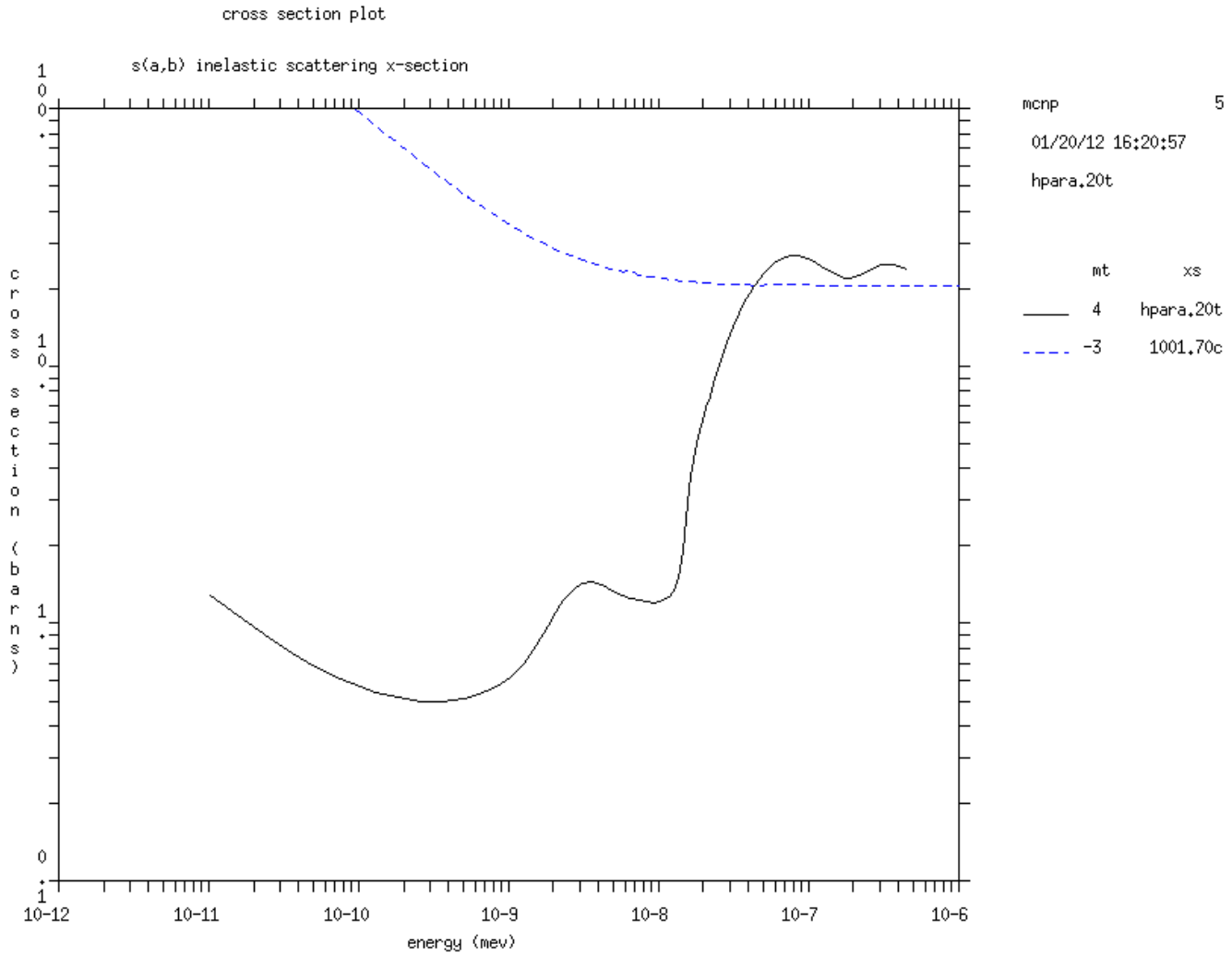


Figure 76: Plot of cross section for S(α, β) material: `hpara`

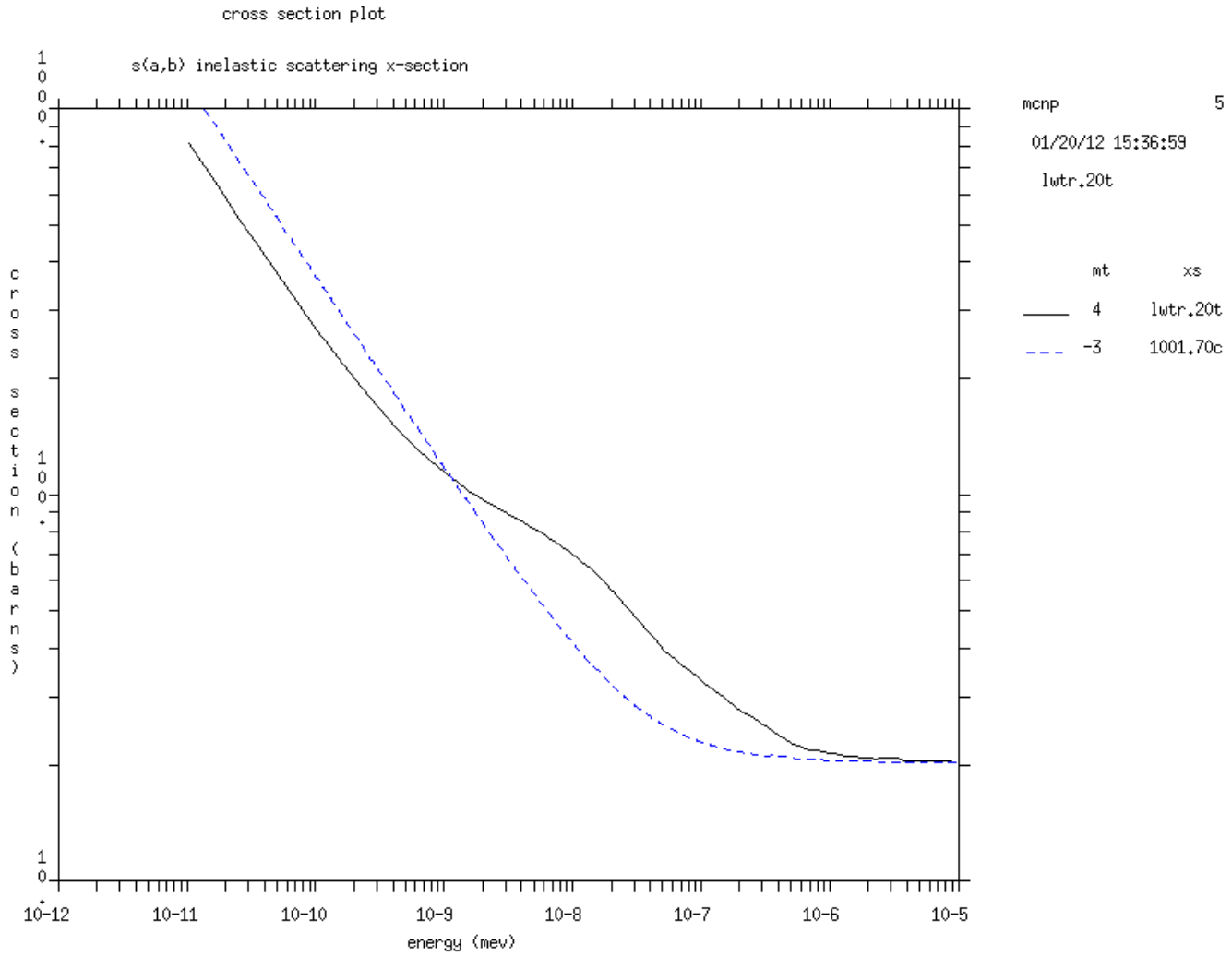


Figure 77: Plot of cross section for S(α, β) material: `lwtr`

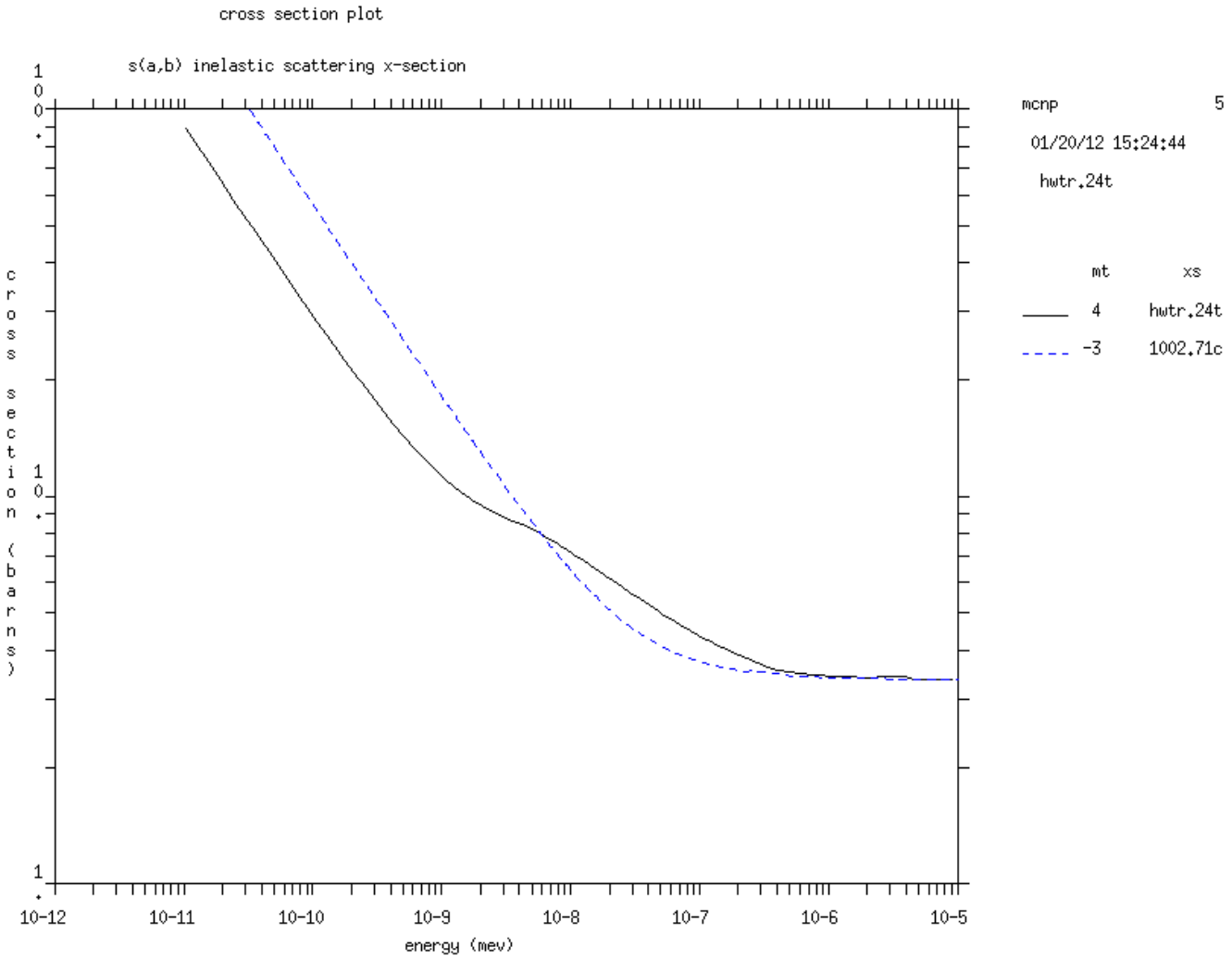


Figure 78: Plot of cross section for S(α, β) material: `hwtr`

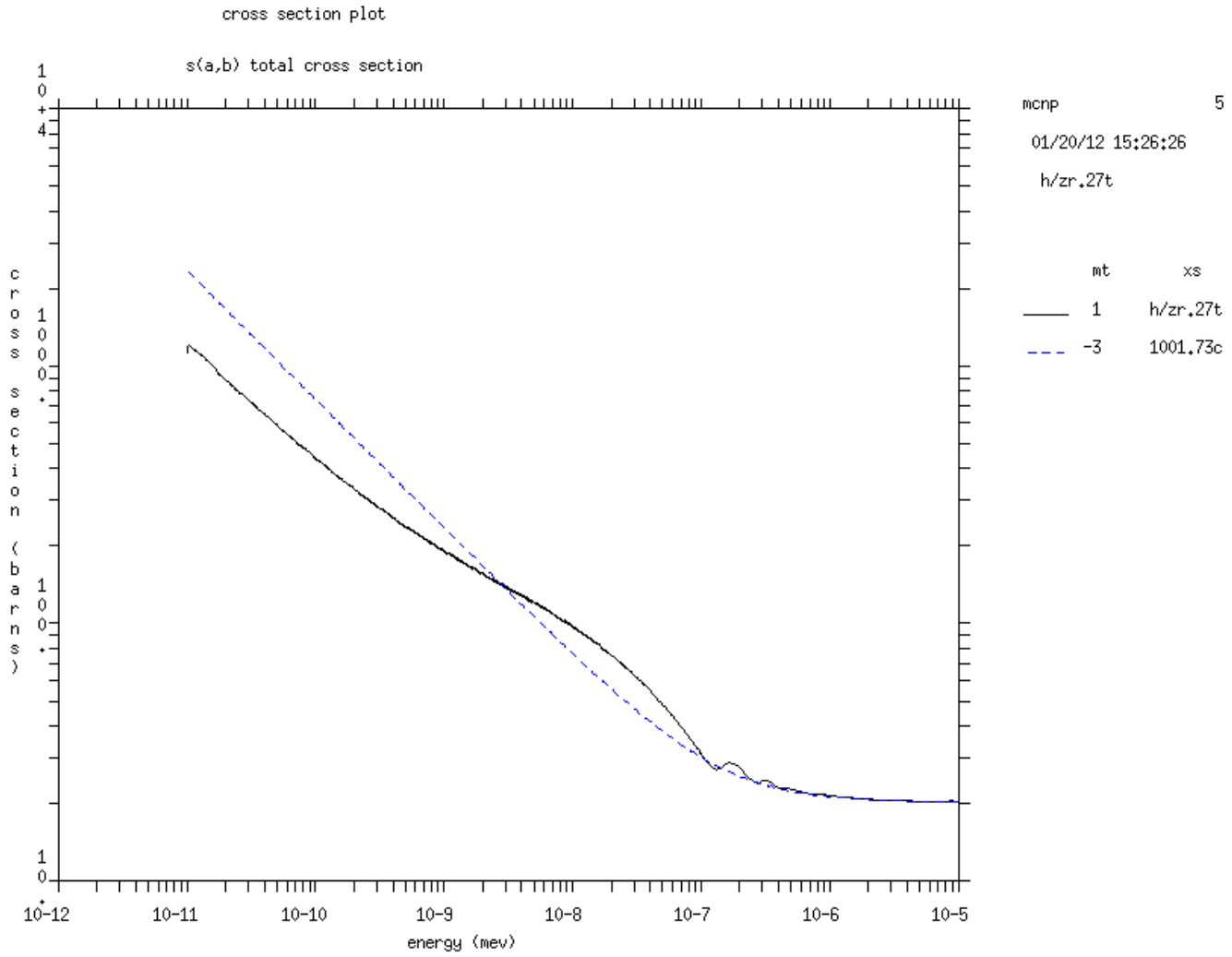


Figure 79: Plot of cross section for S(α, β) material: `hzr`

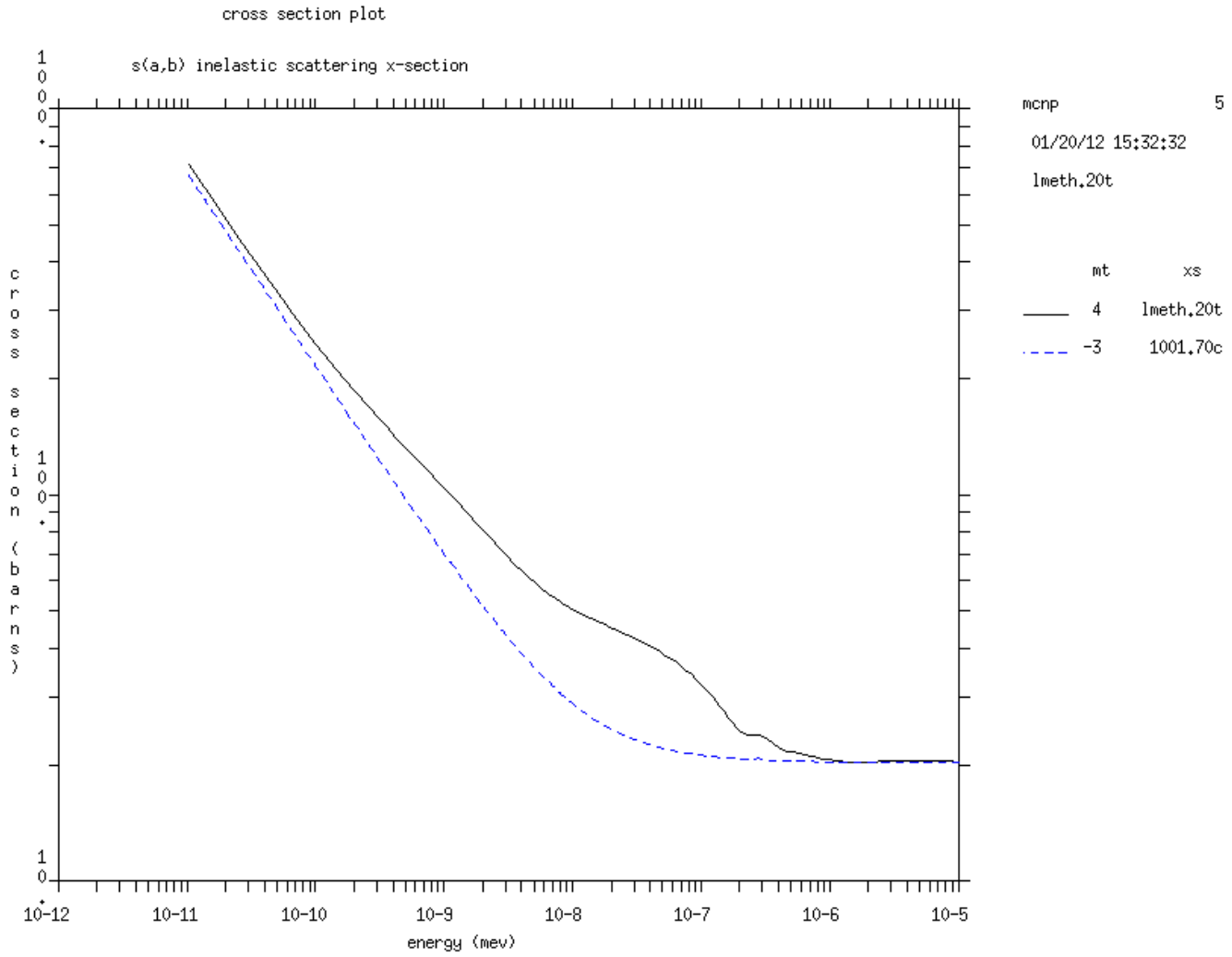


Figure 80: Plot of cross section for S(α, β) material: `lmeth`

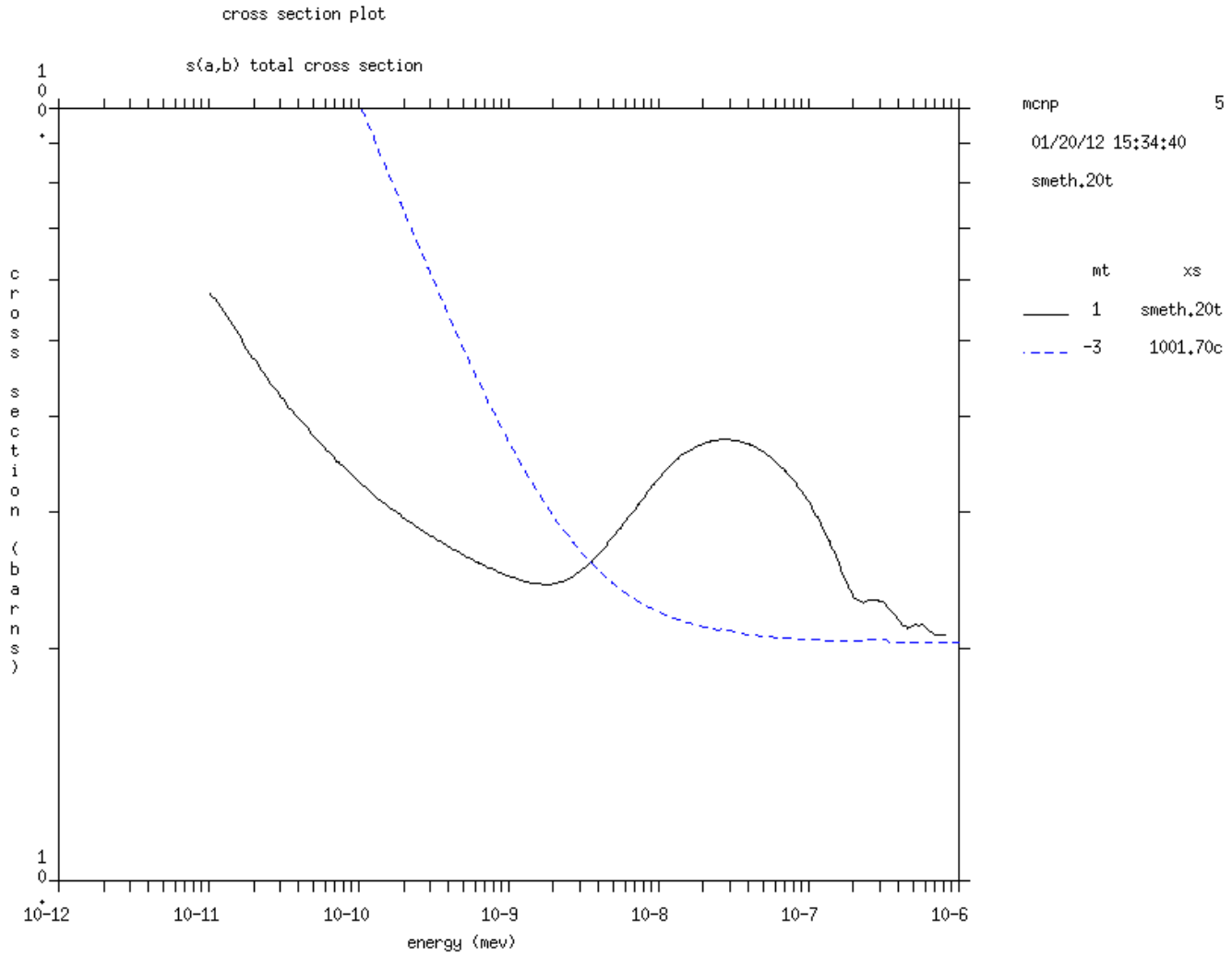


Figure 81: Plot of cross section for S(α, β) material: `smeth`

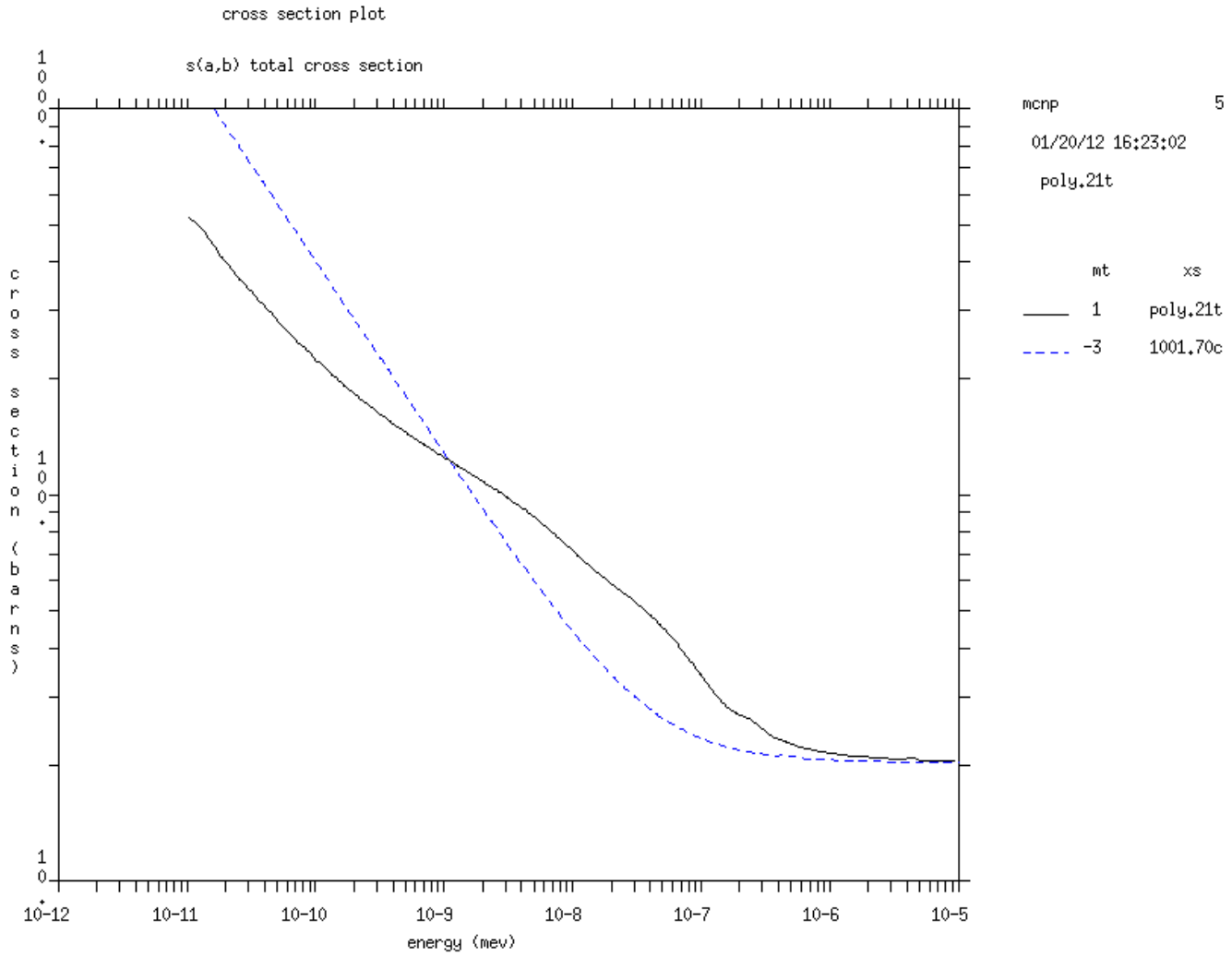


Figure 82: Plot of cross section for S(α, β) material: `poly`

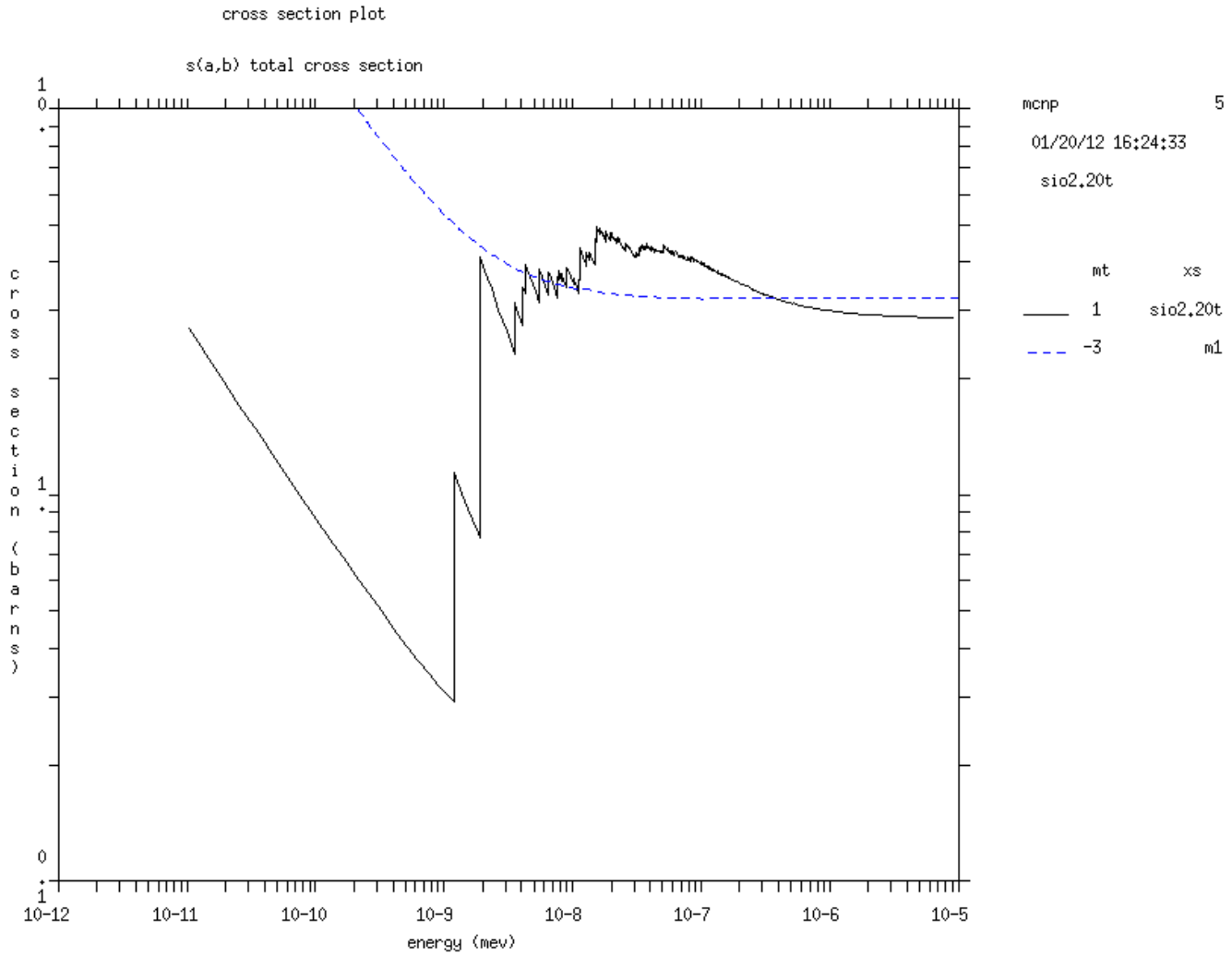


Figure 83: Plot of cross section for S(α, β) material: `si02`

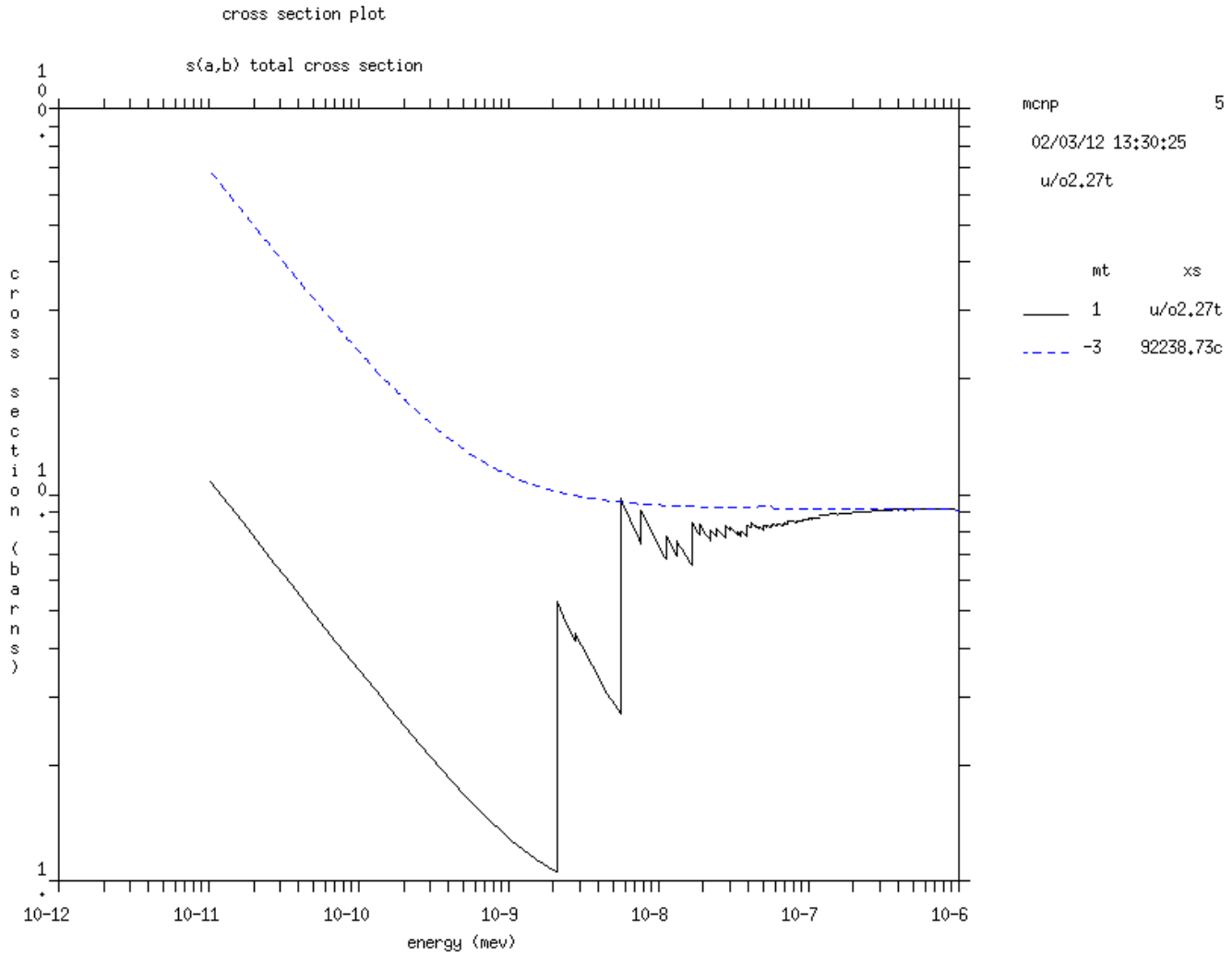


Figure 84: Plot of cross section for S(α, β) material: `uo2`

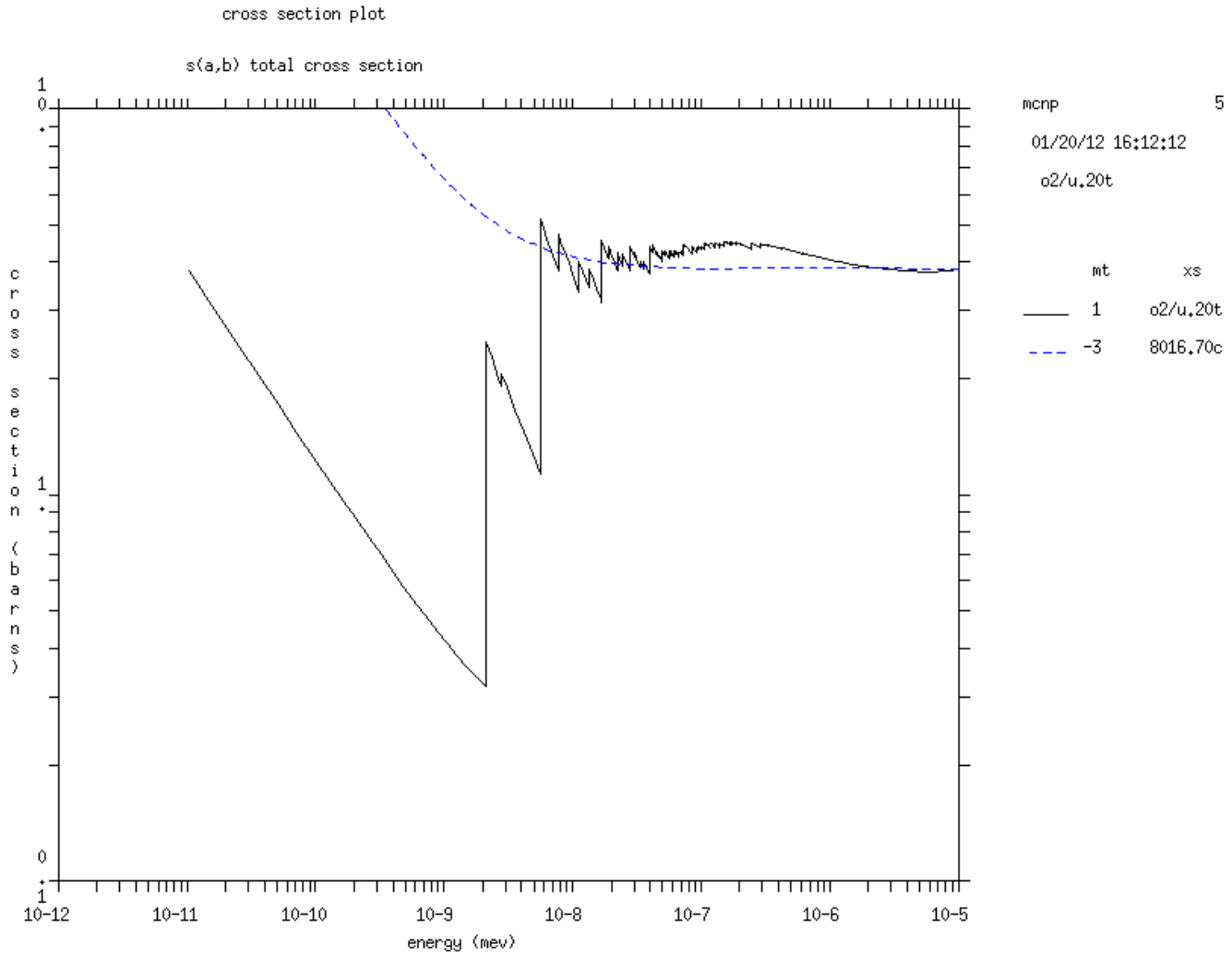


Figure 85: Plot of cross section for S(α, β) material: `o2u`