

INDC International Nuclear Data Committee

ADS-HE: Evaluated Nuclear Data Library up to 1 GeV

**for ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{235}U , ^{238}U ,
 ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm**

Daniel López Aldama
Instituto de Información Científica y Tecnológica
La Habana, Cuba

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
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Austria

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ABSTRACT

Accelerator Driven Systems (ADS) are being developed for power generation and the transmutation of actinide and fission product waste, and well-defined cross-section libraries suitable for their transport calculations are required. Transport of high energy neutrons and protons near the target assembly requires an extension of the library for incident energies up to 1 GeV. An ADS-HE library for incident neutrons on selected target elements has been developed to meet this request, and assist benchmarking studies linked to ADS experiments and design concepts. New evaluations of high-energy data from 20 MeV up to 1 GeV have been carried out by S.G. Yavshits and O.T. Grudzevich (see [INDC\(NDS\)-0615](#)). The ADS-HE library has been prepared from these high-energy evaluations combined with evaluations below 20 MeV selected from the ENDF/B-VII.1, the JEFF-3.1.2 and the JENDL-4u2 libraries. The ADS-HE library was processed in suitable forms for Monte Carlo transport codes used in the analysis of ADS. ADS-HE is freely available from the IAEA Nuclear Data Section, and is readily accessible on the web site: <http://www-nds.iaea.org/ads/adshe.html>.

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1. Introduction

Advanced nuclear applications increasingly require evaluated nuclear data at higher energies. The general-purpose evaluated data libraries, like ENDF/B-VII.1 [1], JEFF-3.1.2 [2] and JENDL-4u2 [3], include evaluations up to 150 or 200 MeV for several materials, but very few evaluations are available beyond this energy.

Recently, the Nuclear Data Section (NDS) of the International Atomic Energy Agency (IAEA) supported some evaluation work up to 1 GeV for important materials used in Accelerator Driven System (ADS) and nuclear waste transmutation (NWT). Evaluated nuclear data between 20 MeV and 1 GeV were prepared at the V.G. Khlopin Radium Institute, St. Petersburg, Russia for ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm [4, 5].

In order to use these new high-energy evaluated nuclear data in nuclear applications, they must be consistently complemented with low-energy evaluated data. The IAEA/NDS also supported this work to make available a set of evaluated nuclear data files in the energy range between $1 \cdot 10^{-5}$ eV and 1 GeV to end users.

The work carried out to merge low- and high-energy evaluations is described in this technical report. The low-energy nuclear data files were selected from available libraries. Additionally, the prepared data files were processed using NJOY-99.396 [6] into continuous-energy cross section data files in ACE format for use with the MCNP Monte Carlo code [7]. A qualitative verification of processed files was performed; the main findings and recommendations are also reported.

2. Sources of evaluated nuclear data files

Table 1 presents sources of the evaluated nuclear data files. Mercury and major actinides were selected from the ENDF/B-VII.1 library, minor actinides from the JENDL-4.0, and lead and bismuth from the JEFF-3.1.2 library. At high energies, the KRIT2n nuclear data library was used for all nuclides.

Table 1: Sources of evaluated nuclear data files and merging energy

Nuclide	MAT	Low energy file		High energy file		Merging energy E_m [MeV]
		Library	Energy range [MeV]	Library	Energy range [MeV]	
80-Hg-202	8043	ENDF/B-VII.1	10^{-11} to 150	KRIT2n	20 to 1000	20
82-Pb-208	8237	JEFF-3.1.2	10^{-11} to 200	KRIT2n	20 to 1000	20
83-Bi-209	8325	JEFF-3.1.2	10^{-11} to 200	KRIT2n	20 to 1000	20
90-Th-232	9040	ENDF/B-VII.1	10^{-11} to 60	KRIT2n	20 to 1000	60
92-U-235	9228	ENDF/B-VII.1	10^{-11} to 20	KRIT2n	20 to 1000	20
92-U-238	9237	ENDF/B-VII.1	10^{-11} to 30	KRIT2n	20 to 1000	30
93-Np-237	9346	JENDL-4.0u1	10^{-11} to 20	KRIT2n	20 to 1000	20
94-Pu-239	9437	ENDF/B-VII.1	10^{-11} to 20	KRIT2n	20 to 1000	20
95-Am-242	9546	JENDL-4.0	10^{-11} to 20	KRIT2n	20 to 1000	20
96-Cm-246	9640	JENDL-4.0	10^{-11} to 20	KRIT2n	20 to 1000	20

The merging energy E_m is the energy at which low- and high-energy evaluations were merged, therefore data were taken from the low-energy evaluation up to E_m , and from the high-energy evaluation in the energy range between E_m and 1000 MeV.

2.1 Low energy evaluated nuclear data files

2.1.1) ^{202}Hg evaluated nuclear data file

Table 2 shows the evaluation summary for ^{202}Hg . The reaction type number (MT) and the ENDF file number (MF) in ENDF terminology are described in detail in the ENDF Formats Manual [8]. Above the E_{lim} energy limit, the cross sections are equal to zero.

The ^{202}Hg evaluation shows a rather detailed description of neutron and photon data below 20 MeV, but beyond this energy up to 150 MeV, neutron reactions are described by the elastic cross section (n,n) and the (n,x) reaction. Fission reaction is not included.

For reactions with $E_{\text{lim}}=20$ MeV neutron angular-energy distributions are represented using MF files 4 and 5 (MF4, MF5 in short) and photon distributions are given using files MF12, MF14 and MF15. For elastic scattering file MF4 is given and for (n,x) reaction file MF6 is supplied for angular-energy distributions of secondary particles.

2.1.2) ^{208}Pb evaluated nuclear data file

Table 3 shows the evaluation summary for ^{208}Pb . Symbols MT and MF have the same meaning as before. A detailed evaluation is given below 20 MeV, then between 20 and 200 MeV the elastic scattering cross and the (n,x) reaction are used to describe neutron interactions. The angular-energy distributions of secondary particles are given in file MF6. Files MF8 and MF10 contain radioactive product data for (n,np) and (n,d) reactions.

2.1.3) ^{209}Bi evaluated nuclear data file

Table 4 shows the evaluation summary for ^{209}Bi . Symbols MT and MF have the same meaning as before. A detailed evaluation is given below 20 MeV, then between 20 and 200 MeV the elastic scattering cross and the (n,x) reaction are used to describe neutron interactions. The angular-energy distributions of secondary particles are given in file MF6. Files MF8, MF9 and MF10 contain radioactive product data for (n, γ) and (n, ^3He) reactions.

2.1.4) ^{232}Th evaluated nuclear data file

Table 5 shows the evaluation summary for ^{232}Th . Symbols MT and MF have the same meaning as before. It is a complete detailed evaluation up to 60 MeV. Most of the angular-energy distributions of secondary particles are given in file MF6, including fission (MT=18). File MF4 is used for elastic and inelastic scattering and for (n, p_0') and (n, α_0') reactions. Photon multiplicities and angular distributions are given in file MF12 and MF14 respectively for inelastic scattering.

2.1.5) ^{235}U evaluated nuclear data file

Table 6 shows the evaluation summary for ^{235}U . Symbols MT and MF have the same meaning as before. The ^{235}U evaluation contains a detailed description of neutron interactions up to 20 MeV. The reaction (n,x) is not present. Angular distributions for elastic and discrete inelastic scattering are given in file MF4. Fission angular-energy distributions are given in files MF4 and MF5 respectively. The double-differential cross sections for reactions (n,2n), (n,3n), (n,4n) and (n,n γ) are given in file MF6.

Photon multiplicities from inelastic scattering, fission and radiative capture are given in file MF12 between 10^{-5} eV and 1.09 MeV. Photon production cross sections from all non-elastic reactions (MT=3) are given in file MF13 between 1.09 and 20 MeV. Angular-energy distributions for photons are supplied in files MF14 and MF15 respectively.

2.1.6) ^{238}U evaluated nuclear data file

Table 7 shows the evaluation summary for ^{238}U . Symbols MT and MF have the same meaning as before. The ^{238}U evaluation contains a detailed description up to 30 MeV. The reaction (n,x) is not present. Angular distributions for elastic and discrete inelastic scattering are given in file MF4. Fission angular-energy distributions are specified in files MF4 and MF5 respectively. The double-differential cross sections for reactions (n,2n), (n,3n), (n,4n) and (n,n γ) are given in file MF6.

Photon multiplicities from fission and radiative capture are given in file MF12 between 10^{-5} eV and 30 MeV. Photon production cross sections from the rest of the non-elastic reactions are given in file MF13 for MT=3. Angular-energy distributions for photons are supplied in files MF14 and MF15 respectively.

2.1.7) ^{237}Np evaluated nuclear data file

Table 8 shows the evaluation summary for ^{237}Np . Symbols MT and MF have the same meaning as before. The ^{237}Np evaluation contains a detailed description up to 20 MeV. The reaction (n,x) is not present. Files MF4, MF5, MF12, MF14 and MF15 are used to describe the angular-energy distributions of neutrons and photons for fission reaction MT=18. For the rest of particle-producing reactions, file MF6 is supplied. Files MF8 and MF9 contain radioactive product data for the reaction (n,2n).

2.1.8) ^{239}Pu evaluated nuclear data file

Table 9 shows the evaluation summary for ^{239}Pu . Symbols MT and MF have the same meaning as before. The ^{239}Pu evaluation contains a detailed description of neutron interactions up to 20 MeV. The reaction (n,x) is not present. Angular distributions for elastic and discrete inelastic scattering are given in file MF4. Fission angular-energy distributions are given in files MF4 and MF5 respectively. The double-differential cross sections for reactions (n,2n), (n,3n), (n,4n) and (n,n γ) are given in file MF6.

Photon multiplicities from inelastic scattering, fission and radiative capture are given in file MF12 between 10^{-5} eV and 1.09 MeV. Photon production cross sections from all non-elastic

reactions (MT=3) are given in file MF13 between 1.09 and 20 MeV. Angular-energy distributions for photons are supplied in files MF14 and MF15 respectively.

2.1.9) ²⁴²Am evaluated nuclear data file

Table 10 shows the evaluation summary for ²⁴²Am. Symbols MT and MF have the same meaning as before. The ²⁴²Am evaluation contains a detailed description up to 20 MeV. The reaction (n,x) is not present. Files MF4, MF5, MF12, MF14 and MF15 are used to describe the angular-energy distributions of neutrons and photons for fission reaction MT=18. For the rest of particle-producing reactions, file MF6 is supplied.

2.1.10) ²⁴⁵Cm evaluated nuclear data file

Table 11 shows the evaluation summary for ²⁴⁵Cm. Symbols MT and MF have the same meaning as before. The ²⁴⁵Cm evaluation contains a detailed description up to 20 MeV. The reaction (n,x) is not present. Files MF4, MF5, MF12, MF14 and MF15 are used to describe the angular-energy distributions of neutrons and photons for fission reaction MT=18. For the rest of particle-producing reactions, file MF6 is supplied.

Table 2: Summary of ²⁰²Hg low energy evaluation (ENDF/B-VII.1)

MT	Reaction	E _{lim} [*] [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
1	(n,total)	150		X										
2	(n,n)	150		X	X									
4	(n,inelas)	20		X										
5	(n,x)	150		X			X							
16	(n,2n)	20		X	X	X					X		X	X
17	(n,3n)	20		X	X	X					X		X	X
22	(n,nα)	20		X	X	X					X		X	X
28	(n,np)	20		X	X	X					X		X	X
51-69	(n,n _i ')	20		X	X						X		X	
91	(n,n _c ')	20		X	X	X					X		X	X
102	(n,γ)	20		X							X		X	X
103	(n,p)	20		X							X		X	X
104	(n,d)	20		X							X		X	X
107	(n,α)	20		X							X		X	X

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

Table 3: Summary of ^{208}Pb low energy evaluation (JEFF-3.1.2)

MT	Reaction	E_{lim}^* [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
1	(n,total)	200		X										
2	(n,n)	200		X	X									
3	(n,nonelas)	200		X										
4	(n,inelas)	20		X										
5	(n,x)	200		X				X						
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
22	(n,n α)	20		X				X						
24	(n,2n α)	20		X				X						
28	(n,np)	20		X				X	X		X			
32	(n,nd)	20		X				X						
33	(n,nt)	20		X				X						
41	(n,2np)	20		X				X						
51-70	(n,n $_i$ ' γ)	20		X				X						
91	(n,n $_c$ ' γ)	20		X				X						
102	(n, γ)	20		X				X						
103	(n,p)	20		X										
104	(n,d)	20		X					X		X			
105	(n,t)	20		X										
107	(n, α)	20		X										
600-607	(n,p $_i$ ' γ)	20		X				X						
649	(n,p $_c$ ' γ)	20		X				X						
650-655	(n,d $_i$ ' γ)	20		X				X						
699	(n,d $_c$ ' γ)	20		X				X						
700-705	(n,t $_i$ ' γ)	20		X				X						
749	(n,t $_c$ ' γ)	20		X				X						
800-810	(n, α $_i$ ' γ)	20		X				X						
849	(n, α $_c$ ' γ)	20		X				X						

* E_{lim} : Above E_{lim} the cross section is equal zero ($\sigma = 0.0$, if $E > E_{\text{lim}}$)

Table 4: Summary of ²⁰⁹Bi low energy evaluation (JEFF-3.1.2)

MT	Reaction	E _{lim} [*] [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
1	(n,total)	200		X										
2	(n,n)	200		X	X									
3	(n,nonelas)	200		X										
4	(n,inelas)	20		X										
5	(n,x)	200		X				X						
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
22	(n,nα)	20		X				X						
24	(n,2nα)	20		X				X						
28	(n,np)	20		X				X						
32	(n,nd)	20		X				X						
33	(n,nt)	20		X				X						
41	(n,2np)	20		X				X						
51-70	(n,n _i [?])	20		X				X						
91	(n,n _c [?])	20		X				X						
102	(n,γ)	20		X				X	X					
103	(n,p)	20		X										
104	(n,d)	20		X										
105	(n,t)	20		X										
106	(n, ³ He)	20		X					X		X			
107	(n,α)	20		X										
108	(n,2α)	20		X				X						
112	(n,pα)	20		X				X						
600-610	(n,p _i [?])	20		X				X						
649	(n,p _c [?])	20		X				X						
650-655	(n,d _i [?])	20		X				X						
699	(n,d _c [?])	20		X				X						
700-705	(n,t _i [?])	20		X				X						
749	(n,t _c [?])	20		X				X						
750-754	(n, ³ He _i [?])	20		X										
799	(n, ³ He _c [?])	20		X										
800-810	(n,α _i [?])	20		X				X						
849	(n,α _c [?])	20		X				X						

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

Table 5: Summary of ^{232}Th low energy evaluation (ENDF/B-VII.1)

MT	Reaction	E_{lim}^* [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	60	X											
455	ν_d	60	X			X								
456	ν_p	60	X											
458	ε_f	60	X											
1	(n,total)	60		X										
2	(n,n)	60		X	X									
4	(n,inelas)	60		X										
5	(n,x)	60		X			X							
16	(n,2n)	60		X			X							
17	(n,3n)	60		X			X							
18	(n,f)	60		X			X							
22	(n,n α)	60		X			X							
24	(n,2n α)	60		X			X							
28	(n,np)	60		X			X							
41	(n,2np)	60		X			X							
51-89	(n,n $_i'$)	60		X	X						X		X	
91	(n,n $_c'$)	60		X			X							
102	(n, γ)	60		X			X							
112	(n,p)	60		X			X							
600	(n,p $_i'$)	60		X	X									
649	(n,p $_c'$)	60		X			X							
800	(n, α'_i)	60		X	X									
849	(n, α'_c)	60		X			X							

* E_{lim} : Above E_{lim} the cross section is equal zero ($\sigma = 0.0$, if $E > E_{\text{lim}}$)

Table 6: Summary of ^{235}U low energy evaluation (ENDF/B-VII.1)

MT	Reaction	E_{lim}^* [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	20	X											
455	ν_d	20	X			X								
456	ν_p	20	X											
458	ε_f	20	X											
460	$S_\gamma(E, E_\gamma, t)$	20	X								X		X	
1	(n,total)	20		X										
2	(n,n)	20		X	X									
3	(n,nonelas)	20		X								X	X	X
4	(n,inelas)	20		X							X		X	
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
18	(n,fission)	20		X	X	X					X		X	X
19	(n,1f)	20		X										
20	(n,nf)	20		X										
21	(n,2nf)	20		X										
37	(n,4n)	20		X				X						
38	(n,3nf)	20		X										
51-90	(n, n_i')	20		X	X									
91	(n, n_c')	20		X				X						
102	(n, γ)	20		X							X		X	X

* E_{lim} : Above E_{lim} the cross section is equal zero ($\sigma = 0.0$, if $E > E_{\text{lim}}$)

Table 7: Summary of ^{238}U low energy evaluation (ENDF/B-VII.1)

MT	Reaction	E_{lim}^* [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	30	X											
455	ν_d	30	X			X								
456	ν_p	30	X											
458	ε_f	30	X											
1	(n,total)	30		X										
2	(n,n)	30		X	X									
3	(n,nonelas)	30		X								X	X	X
4	(n,inelas)	30		X										
16	(n,2n)	30		X				X						
17	(n,3n)	30		X				X						
18	(n,fission)	30		X	X	X					X		X	X
19	(n,1f)	30		X										
20	(n,nf)	30		X										
21	(n,2nf)	30		X										
37	(n,4n)	30		X				X						
38	(n,3nf)	30		X										
51-90	(n, n_i')	30		X	X									
91	(n, n_c')	30		X				X						
102	(n, γ)	30		X							X		X	X

* E_{lim} : Above E_{lim} the cross section is equal zero ($\sigma = 0.0$, if $E > E_{\text{lim}}$)

Table 8: Summary of ²³⁷Np low energy evaluation (JENDL-4.0u1)

MT	Reaction	E _{lim} * [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	v _t	20	X											
455	v _d	20	X				X							
456	v _p	20	X											
458	ε _f	20	X											
1	(n,total)	20		X										
2	(n,n)	20		X	X									
4	(n,inelas)	20		X										
16	(n,2n)	20		X				X	X	X				
17	(n,3n)	20		X				X						
18	(n,fission)	20		X	X	X					X		X	X
19	(n,1f)	20		X										
20	(n,nf)	20		X										
21	(n,2nf)	20		X										
37	(n,4n)	20		X				X						
38	(n,3nf)	20		X										
51-70	(n,n _i ')	20		X				X						
91	(n,n _c ')	20		X				X						
102	(n,γ)	20		X				X						

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

Table 9: Summary of ²³⁹Pu low energy evaluation (ENDF/B-VII.1)

MT	Reaction	E _{lim} * [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	v _t	20	X											
455	v _d	20	X				X							
456	v _p	20	X											
458	ε _f	20	X											
460	S _γ (E, E _γ , t)	20	X								X		X	
1	(n,total)	20		X										
2	(n,n)	20		X	X									
3	(n,nonelas)	20		X								X	X	X
4	(n,inelas)	20		X							X		X	X
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
18	(n,fission)	20		X	X	X					X		X	X
19	(n,1f)	20		X										
20	(n,nf)	20		X										
21	(n,2nf)	20		X										
37	(n,4n)	20		X				X						
38	(n,3nf)	20		X										
51-90	(n,n _i ')	20		X	X									
91	(n,n _c ')	20		X				X						
102	(n,γ)	20		X							X		X	X

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

Table 10: Summary of ²⁴²Am low energy evaluation (JENDL-4.0)

MT	Reaction	E _{lim} [*] [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	v _t	20	X											
455	v _d	20	X			X								
456	v _p	20	X											
1	(n,total)	20		X										
2	(n,n)	20		X	X									
4	(n,inelas)	20		X										
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
18	(n,fission)	20		X	X	X					X		X	X
19	(n,1f)	20		X										
20	(n,nf)	20		X										
21	(n,2nf)	20		X										
37	(n,4n)	20		X				X						
38	(n,3nf)	20		X										
51-79	(n,n _i ' [?])	20		X				X						
91	(n,n _c ' [?])	20		X				X						
102	(n,γ)	20		X				X						

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

Table 11: Summary of ²⁴⁵Cm low energy evaluation (JENDL-4.0)

MT	Reaction	E _{lim} [*] [MeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	v _t	20	X											
455	v _d	20	X			X								
456	v _p	20	X											
458	ε _f	20	X											
1	(n,total)	20		X										
2	(n,n)	20		X	X									
4	(n,inelas)	20		X										
16	(n,2n)	20		X				X						
17	(n,3n)	20		X				X						
18	(n,fission)	20		X	X	X					X		X	X
19	(n,1f)	20		X										
20	(n,nf)	20		X										
21	(n,2nf)	20		X										
37	(n,4n)	20		X				X						
38	(n,3nf)	20		X										
51-70	(n,n _i ' [?])	20		X				X						
91	(n,n _c ' [?])	20		X				X						
102	(n,γ)	20		X				X						

* E_{lim}: Above E_{lim} the cross section is equal zero (σ = 0.0, if E > E_{lim})

2.2 High energy evaluated nuclear data files

High-energy evaluated nuclear data files from KRIT2n library contain the data types shown in Table 12 for ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm . All evaluations are given between 20 MeV and 1000 MeV.

Table 12: Summary of ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm high-energy evaluations

MT	Reaction	E_{max} [GeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	1	X											
1	(n,total)	1		X										
2	(n,n)	1		X			X							
5	(n,x)	1		X			X							
18	(n,fission)	1		X	X	X								

Neutron interactions are described by the elastic scattering (n,n), the fission reaction (n,fission) and the remaining (n,x) reactions between 20 MeV and 1 GeV. Angular-energy distributions for fission are given in files MF4 and MF5. The neutron angular distributions for elastic scattering are included in file MF6 using LAW=2. The double differential cross sections are also specified in file MF6 using Kalbach-Mann representation for neutrons and protons emerging from the (n,x) reaction. Photon production data are not supplied in the high-energy evaluations.

It is worthwhile to note that secondary energy distributions in file MF5 are given in the centre-of-mass coordinate system (CM), instead of the laboratory system (LAB). It is a deviation from the standard ENDF-6 formats and rules.

3. Preparation of evaluated nuclear data library up to 1 GeV

To prepare evaluated nuclear data files up to 1 GeV a two-step approach was followed for all materials. Firstly, the source files at low- and high-energies were pre-processed for updating and compatibility. Secondly, pre-processed evaluated nuclear data files were merged to prepare the final evaluated nuclear data file for each material.

3.1 Pre-processing and modifications of evaluated nuclear data files for compatibility

3.1.1) Checking original evaluated nuclear data files

Original sources of evaluated nuclear data files at low and high energies were checked using the code CHECKR [9]. No major problems were found and the output warnings were accepted. Nevertheless, for all high-energy evaluations the value of ZAP=0.0 was incorrectly assigned to outgoing neutrons from (n,x) reaction (MF6/MT=5). The correct value of ZAP=1.0 was introduced.

3.1.2) Updating the total number of neutrons per fission (ν_t) for actinides in high energy evaluations

Based on the work presented in reference [10], the values of neutrons emitted per fission were estimated between 20 and 1000 MeV by the expressions:

$$\nu_p(E) = \nu_p(E_0) + [\nu_p^\infty - \nu_p(E_0)] \cdot [1 - e^{-a \cdot (E-E_0)}] \quad (1)$$

$$\nu_t(E) = \nu_p(E) + \nu_d \quad (2)$$

where,

- E incident energy in [MeV]
- $\nu_p(E)$ number of prompt neutrons per fission as a function of incident neutron energy
- $\nu_p(E_0)$ number of prompt neutrons per fission at energy E_0
- ν_p^∞ value of the maximum number of prompt neutrons per fission at very high energies
- a exponential slope [MeV⁻¹]
- $\nu_t(E)$ total number of neutrons per fission as a function of incident neutron energy
- ν_d number of delayed neutron per fission as a function of incident neutron energy

For ²³⁵U and ²³⁸U the values of parameter ν_p^∞ and the exponential slope a , were taken from the reference [10]. It is known, that the value of ν_p^∞ should be directly proportional to the actinide mass and inversely proportional to neutron binding energy. Therefore, parameter ν_p^∞ was estimated by:

$$\nu_{p_i}^\infty = \nu_{p_k}^\infty \cdot \frac{\left(\frac{A}{\varepsilon_n}\right)_i}{\left(\frac{A}{\varepsilon_n}\right)_k} \quad (3)$$

where,

- $\nu_{p_i}^\infty$ value of ν_p^∞ for actinide i (unknown value)
- $\nu_{p_k}^\infty$ value of ν_p^∞ for actinide k (known value)
- $\left(\frac{A}{\varepsilon_n}\right)_i$ ratio of atomic number to neutron binding energy of actinide i
- $\left(\frac{A}{\varepsilon_n}\right)_k$ ratio of atomic number to neutron binding energy of actinide k

The estimation of ν_p^∞ for ²³²Th was based on ²³⁸U data. The ²³⁵U data were applied for the rest of actinides.

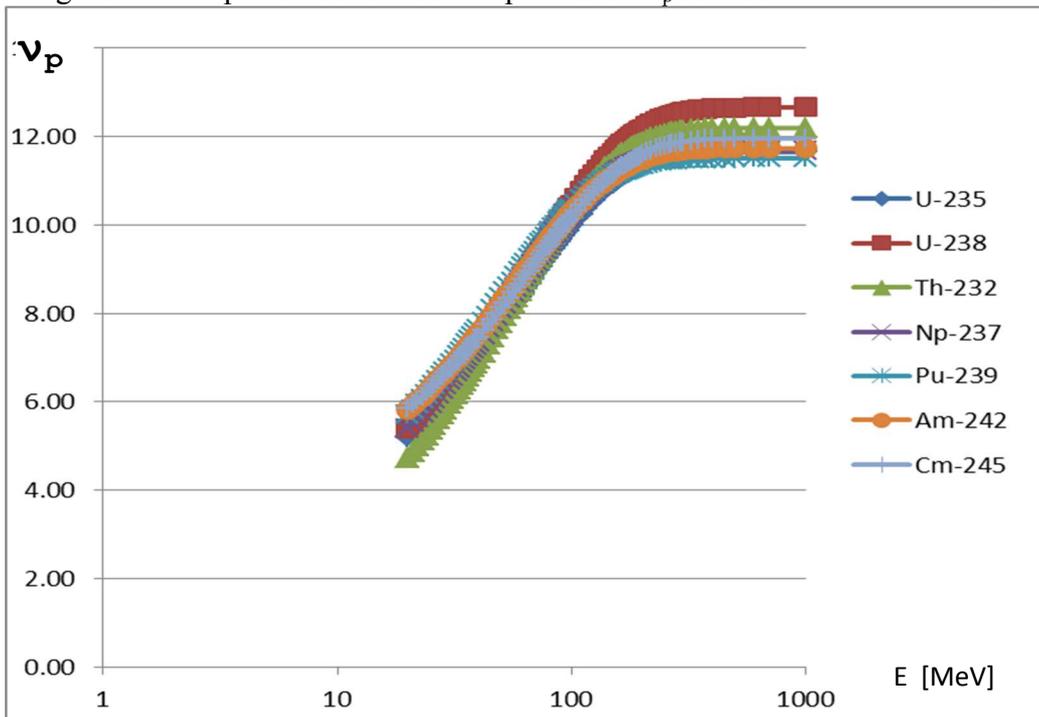
The values of E_0 , $\nu_p(E_0)$, ν_d and a were taken from the corresponding low-energy evaluated nuclear data files. The slope a was estimated using the values of $\nu_p(E)$ in the energy interval between approximately $E_0/4$ and E_0 . This procedure was verified for ²³⁵U and ²³⁸U and results were inside the uncertainty range given for these materials in reference [10].

Table 13 summarizes the parameters used for $\nu_t(E)$ calculation between 20 and 1000 MeV using eqs. (1) and (2); figure 1 shows $\nu_p(E)$ as a function of energy for all actinides.

Table 13: Data used for $\nu_t(E)$ calculation

i	Actinide	E_0 [MeV]	$\nu_p(E_0)$	ν_p^∞	a [MeV ⁻¹]	ν_d
1	²³² Th	60	8.505300	12.18	0.0177	0.014700
2	²³⁵ U	20	5.200845	11.64	0.0170	0.009000
3	²³⁸ U	30	6.388109	12.65	0.0150	0.026000
4	²³⁷ Np	20	5.393000	11.67	0.0187	0.008000
5	²³⁹ Pu	20	5.696949	11.50	0.0205	0.004300
6	²⁴² Am	20	5.808000	11.72	0.0176	0.005627
7	²⁴⁵ Cm	20	5.834000	11.95	0.0156	0.004906

Figure 1: Prompt number of neutron per fission ν_p between 20 and 1000 MeV



3.1.3) Making evaluated nuclear data compatible

The ENDF-6 format [8] allows several models and options to represent the evaluator's intentions, but for merging low- and high-energy evaluations, it is necessary to make compatible the options used at low and high energies. Due to the formalisms used in the original evaluated nuclear data files, the following pre-processing steps were required before merging the data:

1. Linearize the data for the number of neutrons per fission (MF1/MT452, MF1/MT455, MF1/MT456)
2. Linearize the cross section data (MF3)
3. Linearize secondary energy distributions given in file MF5
4. Convert the secondary energy distribution for the elastic scattering from MF6/LAW=2/LANG=12 to MF4/LTT=2 option, for all high-energy evaluated nuclear data files.
5. Convert the secondary angular-energy distribution for the fission reaction given in files MF4/MF5 to Legendre expansion representation (LAW=1/LANG=1) in file MF6 for the ^{232}Th high-energy evaluated nuclear data file.
6. Convert the secondary energy distributions for the fission reaction given in file MF5, from the centre-of-mass coordinate system (CM) to laboratory system (LAB), for all high-energy evaluations but ^{232}Th .
7. Convert the secondary angular-energy distribution for (n,x) reaction given in file MF6/MT5 as Legendre coefficients (LAW=1/LANG=1) to Kalbach-Mann representation (LAW=1/LANG=2) for the ^{232}Th low-energy evaluated nuclear data file.

The code LINEAR from the PREPRO-2012 code system [11] was applied to prepare linearly interpolable data. The code SPECTRA from the same package was used to linearize secondary energy distributions given in file MF5. Two minor corrections were required to run the SPECTRA code. The patches are available on the IAEA/NDS web site: <http://www-nds.iaea.org/ads>.

Furthermore, a set of codes was developed to make the needed format transformations. Conversion of secondary energy distributions from MF6/LAW=2/LANG=12 to MF4/LTT=2 representation requires a rather straightforward algorithm following the ENDF-6 format rules and procedures. The same is applicable to convert secondary angular-energy distribution for the fission reaction given in files MF4/MF5 to the Legendre expansion representation (LAW=1/LANG=1) in file MF6. For the other conversions a brief explanation is given below.

3.1.3.1) Converting from centre-of-mass coordinate system (CM) to laboratory (LAB)

The direct and inverse equations to transform the coordinates (E' , μ) in the laboratory system into the (E'_{cm} , μ_{cm}) coordinates in the centre-of-mass system can be written as:

$$E' = E'_{cm} + c^2 E + 2c\sqrt{E'_{cm}E}\mu_{cm} \quad (4)$$

$$\mu = \sqrt{\frac{E'_{cm}}{E'}} \mu_{cm} + c\sqrt{\frac{E}{E'}} \quad (5)$$

$$E'_{cm} = E' + c^2E - 2c\sqrt{E'E}\mu \quad (6)$$

$$\mu_{cm} = \sqrt{\frac{E'}{E'_{cm}}}\mu - c\sqrt{\frac{E}{E'_{cm}}} \quad (7)$$

where,

$$c = \frac{\sqrt{A'}}{(A+1)} \quad (8)$$

Here, E is the energy of the incident particle, A is the ratio of the atomic mass of target to the mass of incident particle and A' is the ratio of the mass of the emitted particle to the mass of incident particle

Methods to convert angular-energy distributions from the centre-of-mass system (CM) to the laboratory system (LAB) can be found elsewhere [12, 13, 14]. In general, for an isotropic distribution in the centre-of-mass system, it is required to calculate the integral below:

$$a_l^{lab}(E, E') = \frac{1}{2} \int_{\mu_{min}}^1 g\{E, E'_{cm}(E', \mu)\} \cdot J \cdot P_l(\mu) d\mu \quad (9)$$

where ,

J is the Jacobian of the transformation,

E is the incident energy,

E' and μ are respectively the energy and cosine of the secondary particle in the LAB system,

E'_{cm} is the energy of the secondary particle in the CM system,

$g(E, E'_{cm})$ is the isotropic energy distribution given in the CM system,

$P_l(\mu)$ is the l -order Legendre polynomial

$a_l^{lab}(E, E')$ is the l -order Legendre coefficient as a function of E and E' in the LAB system.

The Jacobian is given by,

$$J = \sqrt{\frac{E'}{E'_{cm}}} = \frac{1}{\sqrt{1 + c^2 \frac{E}{E'} - 2c\mu \sqrt{\frac{E}{E'}}}} \quad (10)$$

The value of μ_{min} can be calculated by,

$$\mu_{min} = \frac{1}{2c\sqrt{EE'}} (E' + c^2E - E'_{cm}^{max}) \quad , \quad \mu_{min} \geq -1 \quad (11)$$

$$E'_{cm}^{max} = (\sqrt{E'_{cm}^{max}} + c\sqrt{E})^2 \quad (12)$$

where E'_{cm}^{max} and E'^{max} are the maximum secondary energies in the centre-of-mass and laboratory systems, respectively.

To solve the problem an appropriate grid for the secondary energy E' must be generated. The integral given by equation (9) can then be calculated for each combination of (E, E') using a Gauss quadrature or other integration method.

However, for applications in which the conservation of the number of particles and the average energy are more important than the knowledge of the detailed energy distribution itself, a zero order approximation can be applied for converting the data from the centre-of-mass coordinate system to the laboratory frame of reference.

If the last term in the equation (4) is neglected, then

$$E' = E'_{cm} + c^2 E \quad (13)$$

and the Jacobian can be simplified to

$$J = \sqrt{\frac{E'}{E'_{cm}}} = \sqrt{1 + c^2 \frac{E}{E'_{cm}}} \quad (14)$$

then from expression (9) it follows that

$$f^{lab}(E, E') = a_0^{lab}(E, E') = g(E, E'_{cm}) \cdot \sqrt{1 + c^2 \frac{E}{E'_{cm}}} \quad (15)$$

Equations (13) and (15) were used to convert the secondary energy fission spectra from the centre-of-mass system to the laboratory system for all high-energy evaluated data, but ²³²Th.

3.1.3.2) Converting from Legendre coefficient representation (LAW=1/LANG=1) to Kalbach-Mann formalism (LAW=1/LANG=2) in file MF6.

The Kalbach-Mann systematics representation [8, 14] is very useful for describing the secondary angular-energy distributions (double differential cross sections) at high energies. The high-energy evaluations from the KRIT2n nuclear data library use this formalism to represent data for secondary neutrons and protons for the reaction (n,x). In general, low-energy evaluations selected for merging with KRIT2n data are compatible with the Kalbach-Mann formalism, but not the ²³²Th evaluation, which applied the Legendre-expansion representation.

The angular-energy distribution in the Kalbach-Mann formalism for neutrons and protons is represented by:

$$f(E, E'_{cm}, \mu_{cm}) = \frac{a f_0}{2 \sinh(a)} [\cosh(a \mu_{cm}) + r \sinh(a \mu_{cm})] \quad (16)$$

where

$f_0 = f_0(E, E'_{cm})$ total emission probability
 $r = r(E, E'_{cm})$ is the pre-compound fraction
 $a = a(E, E'_{cm})$ parameterized function that depends also slightly on particle type

A general procedure to convert Legendre expansion representation to Kalbach-Mann formalism is used in the subroutine ACER of the NJOY code [6]. The parameters $r(E, E'_{cm})$

and $a=a(E, E'_{cm})$ are estimated from the average and the difference of the forward ($\mu_{cm}=1$) and backward ($\mu_{cm}=-1$) amplitudes of the Legendre expansion in the centre-of-mass system. This method was also applied in this work.

It is worthwhile to note that in the special case of an isotropic distribution, the conversion from Legendre representation to Kalbach-Mann systematics can be simplified to:

$$f_0(E, E'_{cm}) = g_0(E, E'_{cm}) \quad (17)$$

$$r(E, E'_{cm}) = 0.0 \quad (18)$$

$$a(E, E'_{cm}) = 0.0 \quad (19)$$

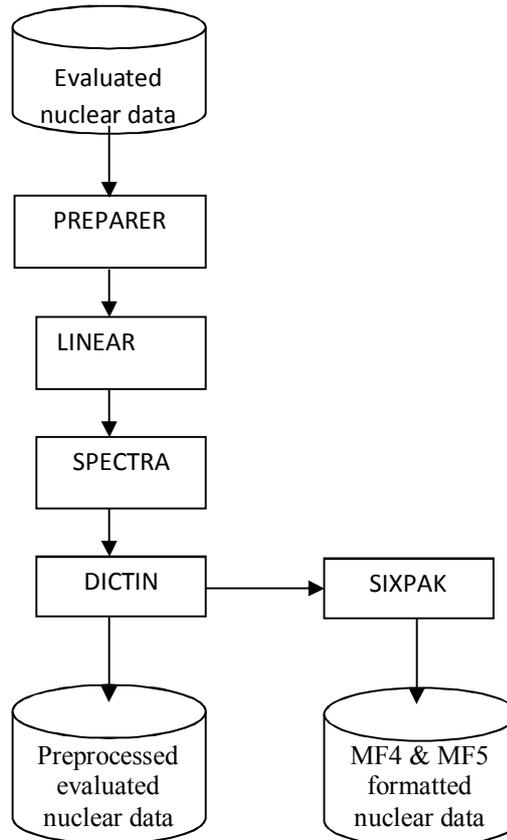
To avoid numerical problems a value of $a(E, E'_{cm})=10^{-8}$ was used inside the code, where $g_0(E, E'_{cm})$ is the isotropic ($l=0$) distribution given in the centre-of-mass system.

The ^{232}Th low-energy evaluation uses isotropic distributions for describing the angular-energy distributions of outgoing neutrons and protons from reaction (n,x).

3.1.3.3) Pre-processing of evaluated nuclear data

Figure 2 shows the pre-processing sequence of low- and high-energy evaluated nuclear data files.

Figure 2: Pre-processing sequence using PREPARER and PREPRO-2012



PREPARER makes compatible the low- and the high-energy evaluations by transforming the corresponding formats and representations. Afterwards, LINEAR and SPECTRA codes are used to linearize cross sections and secondary energy distributions. The reconstruction tolerance was 0.01% and the original data points were kept on the files.

Finally, DICTIN updates the dictionary section and SIXPAK is additionally invoked for checking data in file MF6. After running this sequence of codes successfully, data are prepared for merging.

3.2 Preparing evaluated nuclear data up to 1 GeV

Table 14 and 15 summarize the representation of data after pre-processing high-energy evaluations.

Table 14: Summary of ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm high-energy evaluations after pre-processing

MT	Reaction	E_{\max} [GeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	1	X											
1	(n,total)	1		X										
2	(n,n)	1		X	X									
5	(n,x)	1		X			X							
18	(n,fission)	1		X	X	X								

It can be seen that the angular-energy distribution of fission neutrons is given in file MF6 in the centre-of-mass system for ^{232}Th and it is supplied in files MF4/MF5 in the laboratory coordinate system for the rest of materials.

Table 15: Summary of ^{232}Th high-energy evaluation after pre-processing

MT	Reaction	E_{\max} [GeV]	MF											
			1	3	4	5	6	8	9	10	12	13	14	15
452	ν_t	1	X											
1	(n,total)	1		X										
2	(n,n)	1		X	X									
5	(n,x)	1		X			X							
18	(n,fission)	1		X			X							

A general procedure was applied to merge low- and high-energy evaluated nuclear data files. For each material, an energy value was selected as merging point and denoted by E_m . Below the energy E_m , data are selected from the low-energy evaluated nuclear data file and over E_m , data are taken from the corresponding high-energy evaluation. At E_m , inclusion of a double-energy point and normalization is possible. Table 16 presents the values of E_m for each material. A brief description of the merging procedure is also given below.

Table 16: Selected E_m values

Nuclide	E_m [MeV]
^{202}Hg	20
^{208}Pb	20
^{209}Bi	20
^{232}Th	60
^{235}U	20
^{238}U	30
^{237}Np	20
^{239}Pu	20
^{242}Am	20
^{245}Cm	20

3.2.1 Preparing MF1: General information file

In general in file MF1 the sections MT= 451, 452, 455, 456, 458 and 460 can be found in the selected evaluations.

a) MT=451: Descriptive data and directory

In general, the first four CONT records of section MT=451 were adopted from the low-energy data, except that the fission flag LFI was set to 1 for non-fissionable materials at low energies. Similarly, the NLIB parameter was set equal to 31 to denote the IAEA/NDS evaluated nuclear data library and EMAX was set to 1 GeV in all cases.

The HSUB records were updated and all the descriptive TEXT records from low- and high-energy files were included on the merged MF1 file. Additionally, several new TEXT records were inserted to note that the file was merged at IAEA/NDS.

A new directory was prepared containing all of the sections included in the resulting evaluation.

b) MT=452: Total number of neutrons per fission (ν_t)

For ^{202}Hg , ^{208}Pb , and ^{209}Bi data were taken from the high-energy evaluation between E_m and 1 GeV. For the rest of fissionable materials the total number of neutron per fission was taken from the low-energy evaluation up to E_m and from the high-energy evaluation between E_m and 1 GeV. It is worthwhile to remember that the original values of ν_t in the high-energy evaluations were replaced by the values calculated in paragraph 3.1.2. In this way, normalization at $E = E_m$ is guaranteed.

c) MT=455: Delayed neutron data (ν_d)

Delayed neutron data, if included in the low-energy evaluated nuclear data, were extended from E_m to 1 GeV as constant using the value of ν_d at E_m .

- d) MT=456: Number of prompt neutrons per fission (ν_p)

Number of prompt neutrons per fission is only included in some low-energy evaluated nuclear data files. In this case, the values are calculated by subtracting the number of delayed neutrons per fission from the total number of neutrons per fission:

$$\nu_p(E) = \nu_t(E) - \nu_d(E)$$

The subtraction is performed on the unified energy grid of $\nu_t(E)$ and $\nu_d(E)$. This procedure is backward compatible with the calculation of ν_p and ν_t given above.

- e) MT=458: Components of energy released due to fission

Components of energy released per fission are only included in some low-energy evaluated nuclear data. Taking into account the format used in these cases, the low-energy data were copied to the merged file.

- f) MT=460: Delayed photon data

Delayed photon data are only included in the low-energy evaluated nuclear data files for ^{235}U and ^{239}Pu . The data were copied to the merged file.

3.2.2 Preparing MF2: Resonance parameters

High-energy evaluated nuclear data files do not contain relevant resonance information, therefore low energy resonance data contained on MF2 were copied to the merged file.

3.2.3 Preparing MF3: Reaction cross sections

The following renormalization was applied to cross sections included in the high-energy evaluation ($E \geq E_m$):

$$\sigma_t^{high}(E) = \sigma_{t_0}^{high}(E) \frac{\sigma_t^{low}(E_m)}{\sigma_{t_0}^{high}(E_m)} \quad (20)$$

$$\sigma_s^{high}(E) = \sigma_{s_0}^{high}(E) \frac{\sigma_s^{low}(E_m)}{\sigma_{s_0}^{high}(E_m)} \quad (21)$$

$$\sigma_{R_0}^{high}(E) = \sigma_{t_0}^{high}(E) - \sigma_{s_0}^{high}(E) \quad (22)$$

$$\sigma_R^{high}(E) = \sigma_t^{high}(E) - \sigma_s^{high}(E) \quad (23)$$

$$\sigma_x^{high}(E) = \sigma_{x_0}^{high}(E) \frac{\sigma_R^{high}(E)}{\sigma_{R_0}^{high}(E)} \quad (24)$$

$$\sigma_f^{high}(E) = \sigma_{f_0}^{high}(E) \frac{\sigma_R^{high}(E)}{\sigma_{R_0}^{high}(E)} \quad (25)$$

where the subscripts t, s, R, x, f point to total, scattering, reaction (non-elastic), lumped and fission cross sections, respectively. Subscript 0 denotes values before normalization. The superscripts *low* and *high* mean low- and high-evaluated data. The rest of the symbols have the same meaning as before.

This normalization guarantees that the total, the scattering and the reaction (non-elastic) cross sections are continuous at the merging energy E_m . The fission and the (n,x) cross sections are in the same ratio as they were on the source high-energy evaluation.

In general, the cross sections are taken from the low-energy evaluation up to E_m and from the high-energy evaluation between E_m and 1 GeV. Data are normalized for $E \geq E_m$ according to equations (20) to (25).

If the cross section for the non-elastic reaction (MT=3) is present in the low-energy evaluated nuclear data file, then it is merged with the reaction cross section given by equation (23) at energies higher than E_m . Table 16 summarizes employed normalization factors for total, elastic and reaction (non-elastic) cross sections at energy E_m for each material.

Table 16: Normalization factors for total, elastic and reaction cross sections at E_m .

I	Material	Normalization factors [%] at E_m		
		total MT=1	elastic MT=2	reaction MT=3
1	80-Hg-202	-9.5	-15.6	-0.7
2	82-Pb-208	-1.5	-7.3	7.3
3	83-Bi-209	-1.5	-7.7	8.0
4	90-Th-232	4.5	0.6	8.6
5	92-U -235	1.2	-11.9	20.8
6	92-U -238	-1.6	-19.5	24.8
7	93-Np-237	-0.1	-8.8	12.7
8	94-Pu-239	1.8	-17.0	29.4
9	95-Am-242	-3.0	-14.1	13.1
10	96-Cm-245	3.0	-7.1	17.6

Taking into account the general uncertainties in cross section data at high energies, these normalization factors were considered acceptable.

Redundant partial fission cross sections, MT=19, MT=20, MT=21 and MT=38 describing first to fourth chance fission are removed from the evaluations.

The cross sections not supplied at high energies are extended from E_m to 1 GeV as zero. A double energy point is included at E_m .

3.2.4 Preparing MF4: Angular distributions of secondary particles

Angular distributions $f(\mu, E)$ are represented in file MF4 either as a Legendre expansion coefficient (LTT=1 LI=0), tabulated probability function (LTT=2 LI=0), a combination of Legendre coefficients and tabulated probabilities (LTT=3 LI=0) or as a purely isotropic

distribution (LTT=0 LI=1) for low-evaluated nuclear data files. At high energies, just tabulated probabilities or fully isotropic distributions are usually used.

In general, angular distributions are taken from the low-energy evaluated nuclear data file up to the energy boundary E_m and from the high-energy evaluation between E_m and 1 GeV. A double energy point is included at E_m .

Conversion from purely isotropic representation to tabulated probability function is automatically performed. The angular distributions are given on the same coordinate system after pre-processing.

If the reaction is not included in the low-energy evaluations, then the data are taken from the high-energy evaluation between E_m and 1 GeV.

If the reaction is not included in the high-energy evaluation, then angular distributions are copied from the low-energy evaluated nuclear data file up to the energy boundary E_m and then consistently extended up to 1 GeV using the same distribution specified at E_m .

Table 17 summarizes the possible combinations for merging MF4 file.

Table 17: Format combinations for merging MF4 file

i	Low energy file	High energy file	Merged file
1	LLT=1, LI=0	LLT=2, LI=0	LLT=3, LI=0
2	LLT=2, LI=0	LLT=2, LI=0	LLT=2, LI=0
3	LLT=3, LI=0	LLT=2, LI=0	LLT=3, LI=0
4	LTT=0, LI=1	LLT=2, LI=0	LLT=2, LI=0
5	LLT=1, LI=0	LLT=0, LI=1	LLT=3, LI=0
6	LLT=2, LI=0	LLT=0, LI=1	LLT=2, LI=0
7	LLT=3, LI=0	LLT=0, LI=1	LLT=3, LI=0
8	LTT=0, LI=1	LLT=0, LI=1	LLT=0, LI=1

3.2.5 Preparing MF5: Energy distributions of secondary particles

Energy distributions $f(E,E')$ are represented in file MF5 as a tabulated function (LF=1) after pre-processing the selected evaluations.

In general, energy distributions are taken from the low-energy evaluated nuclear data file up to the energy boundary E_m and from the high-energy evaluation between E_m and 1 GeV. A double energy point is inserted at E_m .

If the reaction is not included in the low-energy evaluations, then data are taken from the high-energy evaluation between E_m and 1 GeV.

If the reaction is not included in the high-energy evaluation, then energy distribution is copied from the low-energy evaluated nuclear data file up to the energy boundary E_m and then consistently extended up to 1 GeV using the same data specified at E_m . Conversion from purely isotropic representation to tabulated probability function is automatically performed. The angular distributions are given on the same coordinate system after pre-processing.

3.2.6 Preparing MF6: Correlated energy-angle distributions

In file MF6, data representations are compatible after pre-processing, but the interpolation law for secondary energies (LEP) could be different in LAW=1. Conversion from LEP=1 to LEP=2 is automatically performed if required.

All high-energy evaluations use the Kalbach-Mann representation (LAW=1/LANG=2) for outgoing protons and neutrons from reaction (n,x). Additionally, the ^{232}Th evaluation describes the secondary angular-energy distribution of fission neutrons using Legendre coefficients (LAW=1/LANG=1).

In general, angular-energy distributions are taken from the low-energy evaluations up to E_m and from high-energy evaluated data files between E_m and 1 GeV. A double energy point is inserted at E_m .

If the reaction is not included in the low-energy evaluations, then data are taken from the high-energy evaluation between E_m and 1 GeV.

If the reaction is not included in the high-energy evaluation, then angular-energy distribution is copied from the low-energy evaluated nuclear data file up to the energy boundary E_m and then consistently extended up to 1 GeV using the same data specified at E_m .

In case of the fission and (n,x) reactions if particles other than neutrons and protons are included in the low-energy evaluation, then angular-energy distributions are taken up to the value of the maximum energy (E_{max}^{low}) found on the corresponding file and extended up to 1 GeV using the data specified at E_{max}^{low} .

3.2.7 Preparing MF8: Radioactive decay data

If file MF8 is specified at low energies, then the radioactive decay information is taken from the low-energy evaluated data file and copied to the merged nuclear data file.

3.2.8 Preparing MF9: Multiplicities for production of radioactive nuclides

If multiplicities are specified in file MF9 at low energies, then they are merged by taking the corresponding data from the low-energy evaluated nuclear data file up to E_m and then extending the data up to 1 GeV using the multiplicity value specified at E_m .

3.2.9 Preparing MF10: Production cross sections for radionuclides

Production cross sections were extended in file MF10 for reactions included on the low-energy evaluation by taking the corresponding data from the low-energy evaluated nuclear data file up to E_m and then extending the data up to 1 GeV as constant equal to zero.

3.2.10 Preparing MF12: Photon production yield data

If file MF12 is specified in the low-energy evaluations, the information is conserved on the merged nuclear data file.

If multiplicities (option LO=1) are specified in file MF12, then data are taken from the low-energy evaluation up to E_m and then extending up to 1 GeV using the multiplicity value specified at E_m . It should be checked that photon data between E_m and 1 GeV are not

represented in file MF6 for each reaction included in file MF12. If it was the case, multiplicities should be extended up to 1 GeV as zero.

On the other hand, if transition probability arrays (option LO=2) are specified in file MF12 in the low-energy evaluation, then data are copied to the merged nuclear data file, because it is implicitly assumed that the transition probability array is independent of incident neutron energy.

3.2.11 Preparing MF13: Photon production cross sections

File MF13 is very often used with the section MT=3 to describe a lumped photon production cross section. If it was the case, data are conserved on the merged file.

In general, photon production cross section data are taken from the low-energy evaluation up to E_m and then extended up to 1 GeV using the value specified at E_m . It should be checked that photon data between E_m and 1 GeV are not represented in file MF6. If it was the case, cross section should be extended up to 1 GeV as zero.

3.2.12 Preparing MF14: Photon angular distributions

Usually, purely isotropic distributions are specified for all reactions found in file MF14, therefore exactly the same distributions were included on the merged evaluations.

3.3.13 Preparing MF15: Continuous photon energy spectra

If MF15 is specified in the low-energy evaluations, then energy distributions are consistently extended for all reactions included in file MF15 by taking the corresponding distributions from the low-energy evaluated nuclear data file up to E_m and then extending the data up to 1 GeV using the same distribution specified at E_m .

4. Preparing evaluated nuclear data files in ACE format for MCNP calculations

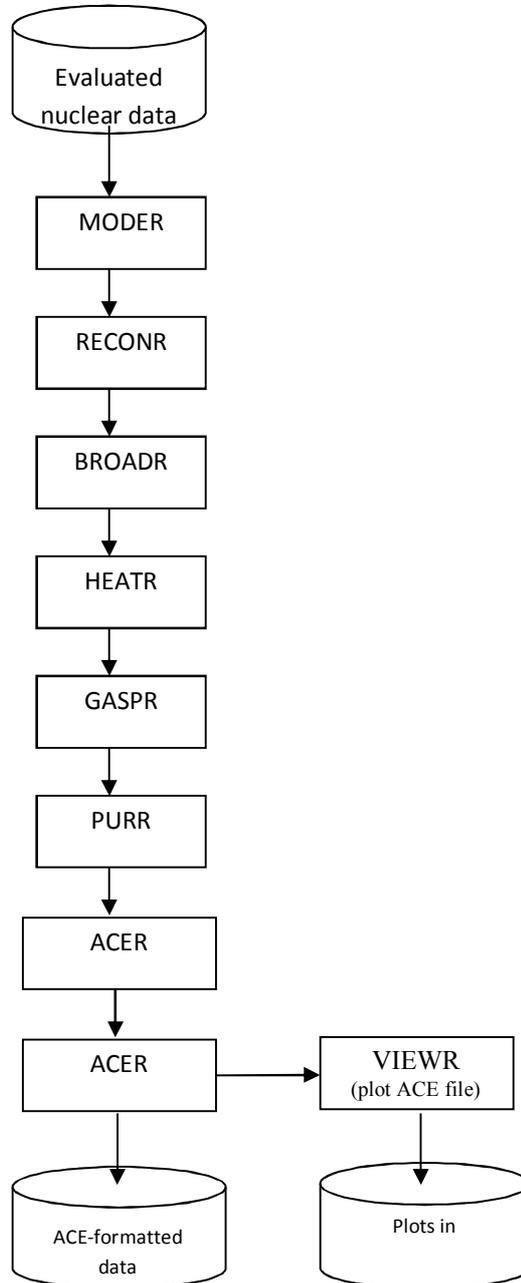
The merged nuclear data files for all materials (Table 18) were processed using the NJOY-99.396 modular code system with additional updates developed at the IAEA-NDS. The new updates are required to process the 1 GeV evaluated nuclear data files and are available from the IAEA/NDS web site: <https://www-nds.iaea.org/ads/>.

Table 18: ENDF-formatted data file

i	Material	E_{max} [MeV]	MAT	ENDF FILE
1	^{202}Hg	1000	8043	hg202.dat
2	^{208}Pb	1000	8237	pb208.dat
3	^{209}Bi	1000	8325	bi209.dat
4	^{232}Th	1000	9040	th232.dat
5	^{235}U	1000	9228	u235.dat
6	^{238}U	1000	9237	u238.dat
7	^{237}Np	1000	9346	np237.dat
8	^{239}Pu	1000	9437	pu239.dat
9	^{242}Am	1000	9546	am242.dat
10	^{245}Cm	1000	9640	cm245.dat

The NJOY processing sequence is shown in Figure 3. The ACE-formatted library is suitable for use by the MCNP family of Monte Carlo codes and other codes that can read the ACE data format.

Figure 3: NJOY processing sequence



A summary of the main processing options is presented below for the sake of completeness:

1. RECONR: Reconstruct cross sections
 - Reconstruction tolerance: 0.1%
 - Resonance-integral-check tolerance: 0.2%
 - Reconstruction temperature: 0.0K

2. BROADR: Doppler broaden cross sections
 - Thinning tolerance: 0.1%
 - Integral criterion tolerance: 0.2%
 - Maximum energy: Doppler broadening was forced to the upper energy limit of the resolved resonance range, but never above 2 MeV
 - Temperature: 300 K
3. HEATR: Add heating kerma and damage
 - MT=302, MT=443, MT = 444 and MT = 445 were requested
 - Kinematic kerma (MT=443) assigned to total kerma (MT=301)
4. GASPR: Add gas production
5. PURR: Process unresolved resonance range if any
 - Number of probability bins: 20
 - Number of resonance ladders: 100
 - Temperature: 300 K
 - Bondarenko σ_0 values (see Table 19)

Table 19: Bondarenko σ_0 values.

Set	Bondarenko σ_0 values	Material
1	10^{10} , 1000, 100, 10, 1	²⁰² Hg, ²⁰⁸ Pb
2	10^{10} , 10000, 1000, 100, 10	²⁰⁹ Bi
3	10^{10} , 10000, 3000, 1000, 300, 100, 30, 10, 3, 1	²³⁵ U
4	10^{10} , 10000, 1000, 100, 30, 10, 3, 1, 0.1, 0.001	Other materials

6. ACER: Prepare ACE formatted files (first run)
 - Type of ACE file: 1
 - ZAID suffix: .30
 - New cumulative angle distribution
 - Detailed photon calculation
 - No thinning
 - Fast data temperature: 300 K
7. ACER: Check ACE formatted files (second run)
 - Type of calculation: Check fast data
8. VIEWR: Plot ACE cross sections
 - Plot ACE formatted file (3D plots)

ACE-formatted files contain point-wise cross-section data for use in the MCNP Monte Carlo code. Two files are supplied for each material: one containing cross-section data with extension “.ace”, and the second containing XSDIR information (extension “.xdr”) to run the MCNP code.

Table 20 summarizes information in the ACE-formatted files. They are also available at the IAEA/NDS web site: <https://www-nds.iaea.org/ads/>.

Table 20: ACE-formatted data for MCNP ($E_{\max} = 1000$ MeV)

Material	ACE Z Aid	Atomic Weight Ratio (AWR)	T [K]	ptable	ACE file	XSDIR File
^{202}Hg	80202.30c	200.2360	300	-	hg202.ace	hg202.xdr
^{208}Pb	82208.30c	206.1900	300	-	pb208.ace	pb208.xdr
^{209}Bi	83209.30c	207.1852	300	-	bi209.ace	bi209.xdr
^{232}Th	90232.30c	230.0450	300	X	th232.ace	th232.xdr
^{235}U	92235.30c	233.0248	300	X	u235.ace	u235.xdr
^{238}U	92238.30c	236.0058	300	X	u238.ace	u238.xdr
^{237}Np	93237.30c	235.0120	300	X	np237.ace	np237.xdr
^{239}Pu	94239.30c	236.9986	300	X	pu239.ace	pu239.xdr
^{242}Am	95242.30c	239.9800	300	X	am242.ace	am242.xdr
^{245}Cm	96245.30c	242.9600	300	X	cm245.ace	cm245.xdr

5. Verification of data

The merged evaluated nuclear data files were analysed using CHECKR and FIZCON codes [8]. No format problems were detected. FIZCON reported some warning messages. They were mainly related to lack of data in the evaluated data source.

A second verification technique was used for evaluated nuclear data files. The evaluations were processed using the PREPRO-2012 package and a set of plots was generated using EVALHARD. All plots were checked by visual inspection and the data were noted as correct.

A third verification was applied on ACE formatted files by checking NJOY output files. All the NJOY messages were understood. The plot files generated by VIEWR were visually inspected and they were taken as an acceptable description of evaluated nuclear data.

After this verification, the evaluated nuclear data up to 1000 MeV were considered acceptable. Annex A presents a selection of plots for each material.

6. Final remarks and recommendations

Evaluated nuclear data files from 10^{-5} eV to 1 GeV were successfully prepared for ten materials: ^{202}Hg , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{242}Am and ^{245}Cm .

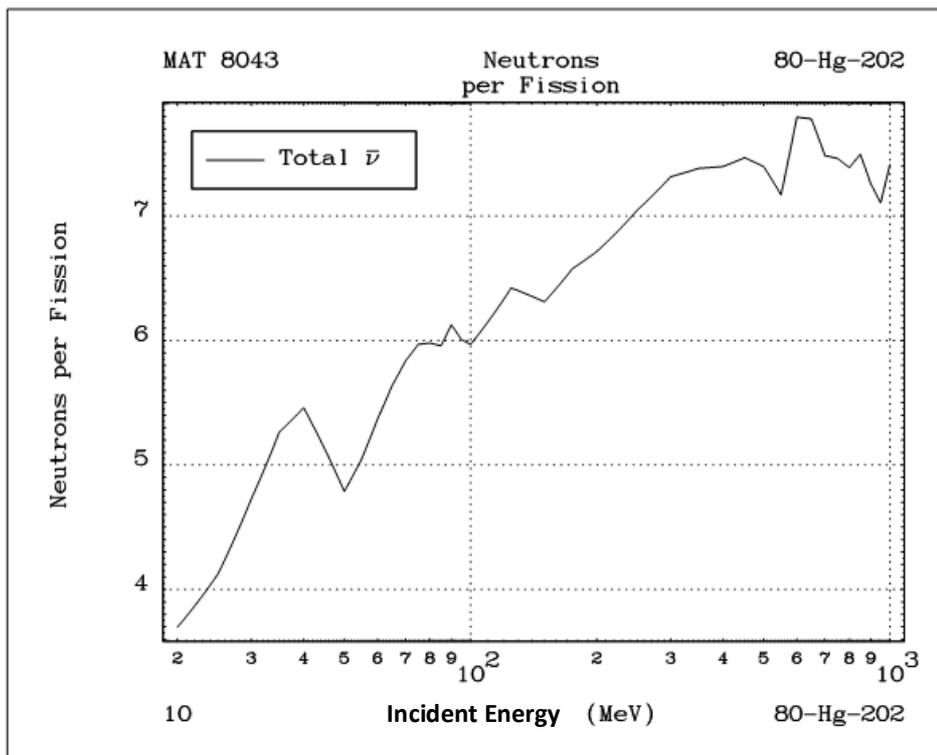
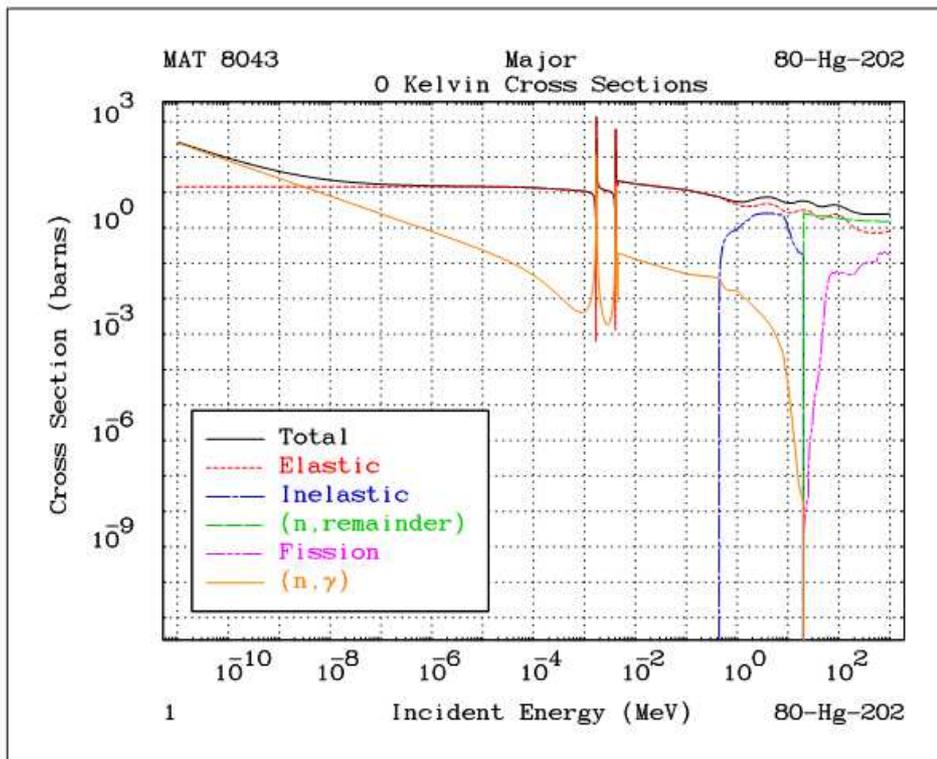
A test library in ACE format was also generated for use in MCNP calculations and made available for end users from the IAEA/NDS web site <https://www-nds.iaea.org/ads/>. These evaluations seem to be reasonable for describing distributions of neutrons and protons at high energies for neutron induced reactions.

It is recommendable to start benchmarking the new ACE-formatted library for ADS applications. At a later stage, the library could be extended to other materials as soon as new evaluations at high energies are released. High-energy evaluations for proton induced reactions on the same material covered in this report are available, and should be used to produce the corresponding high-energy extension; such work is planned.

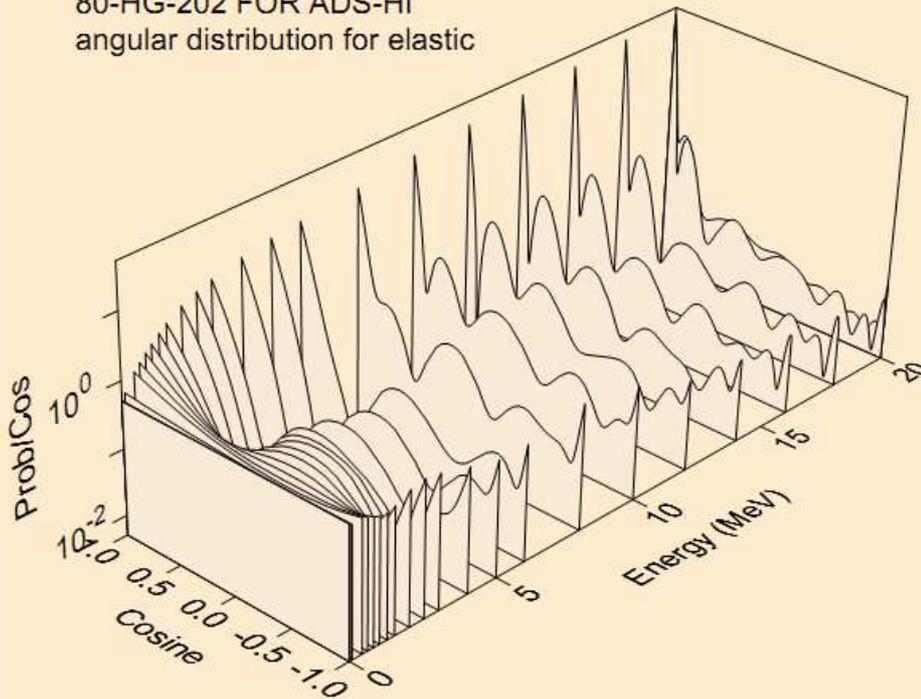
7. References

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- [14] MacFarlane, R. E., et al., “The NJOY Nuclear Data Processing System, Version 2012”, report **LA-UR-12-27079**, Los Alamos National Laboratory, December 20, 2012

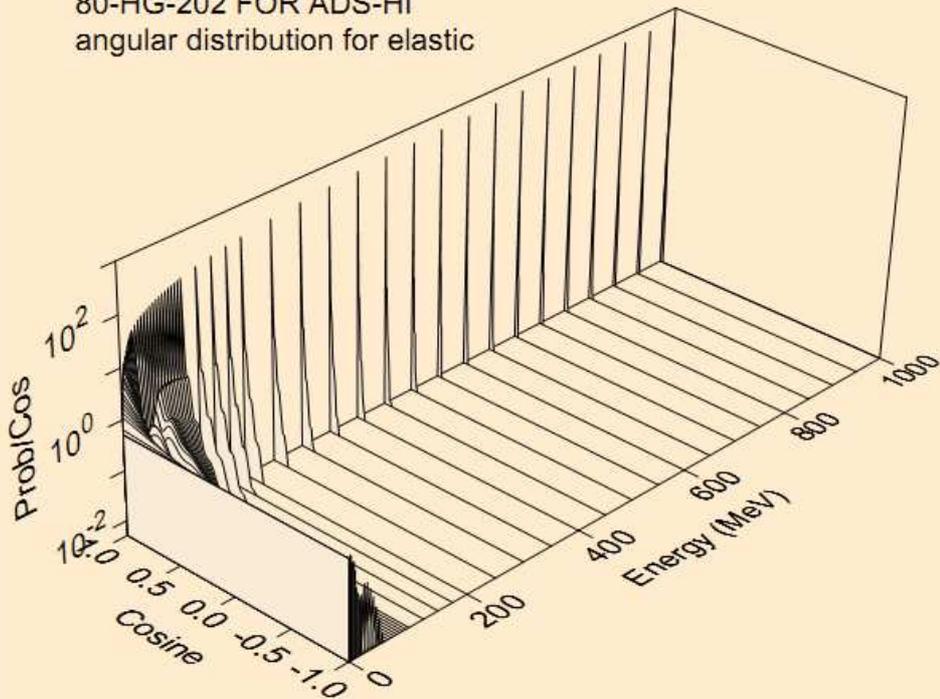
Annex A: Selected plots of evaluated nuclear data files processed by NJOY



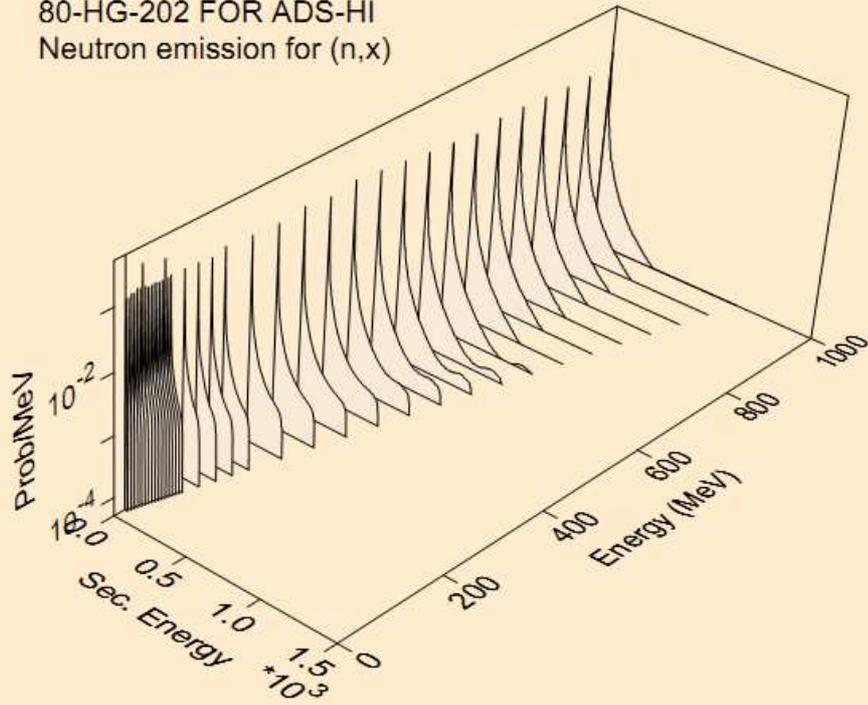
80-HG-202 FOR ADS-HI
angular distribution for elastic



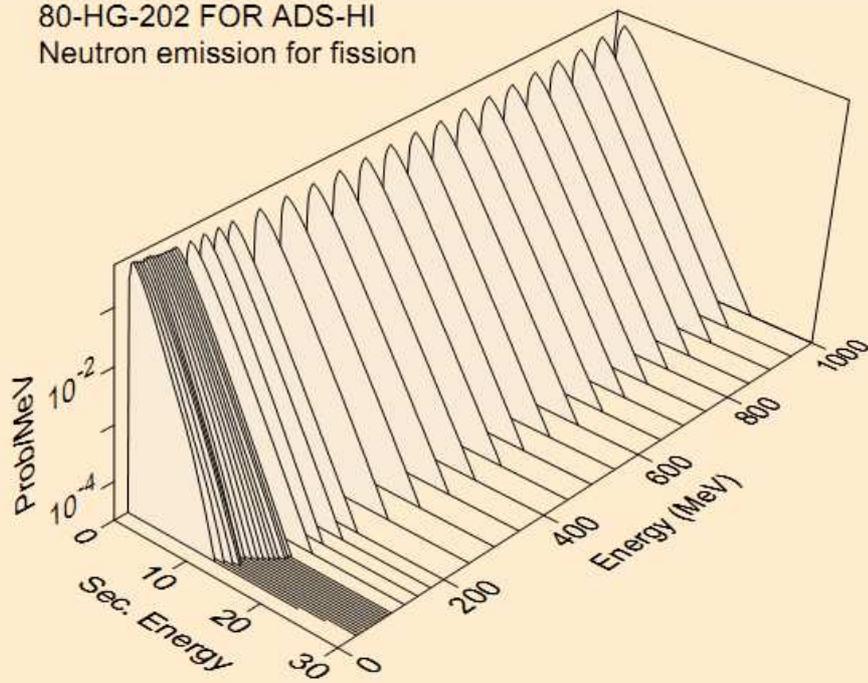
80-HG-202 FOR ADS-HI
angular distribution for elastic

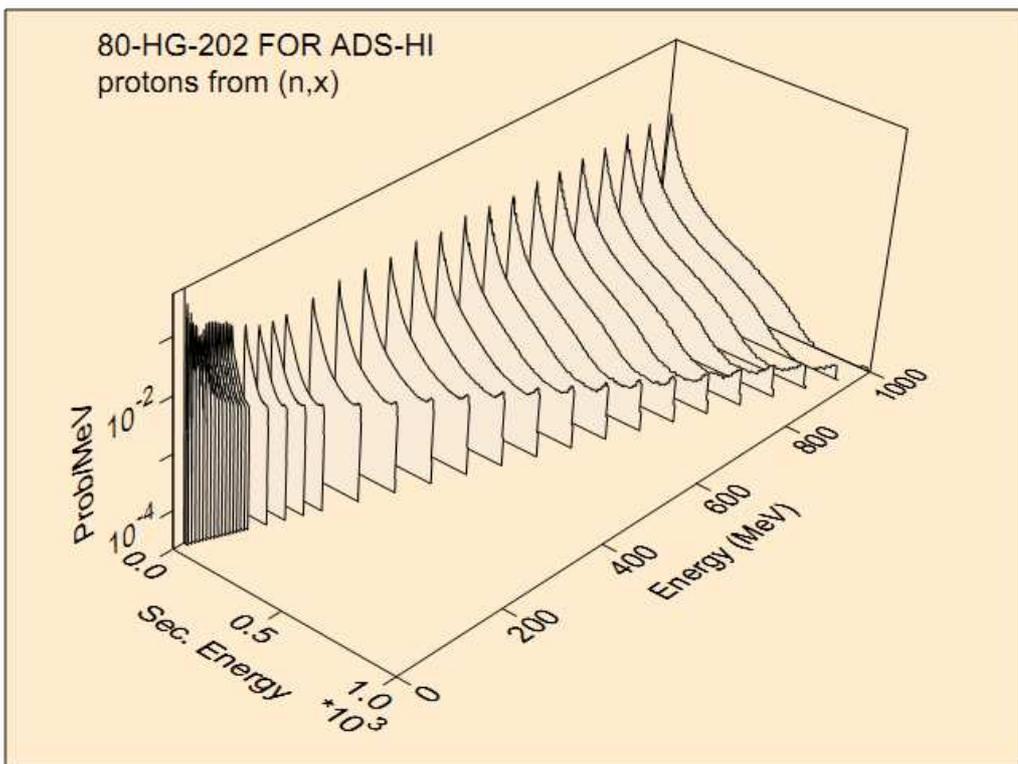
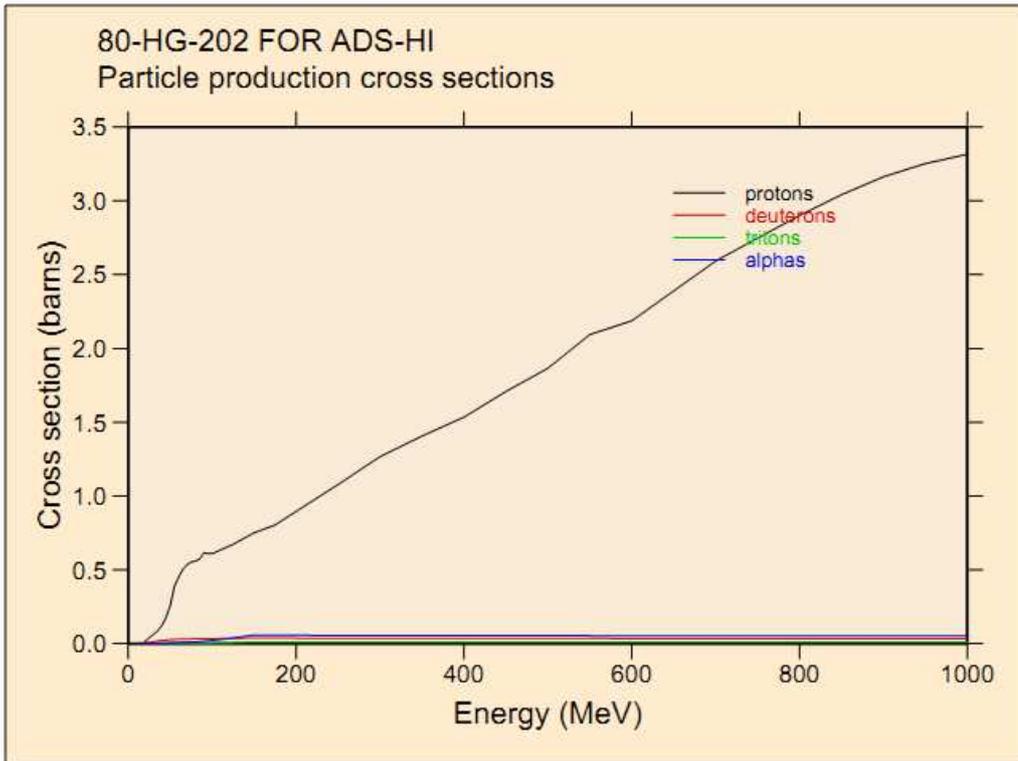


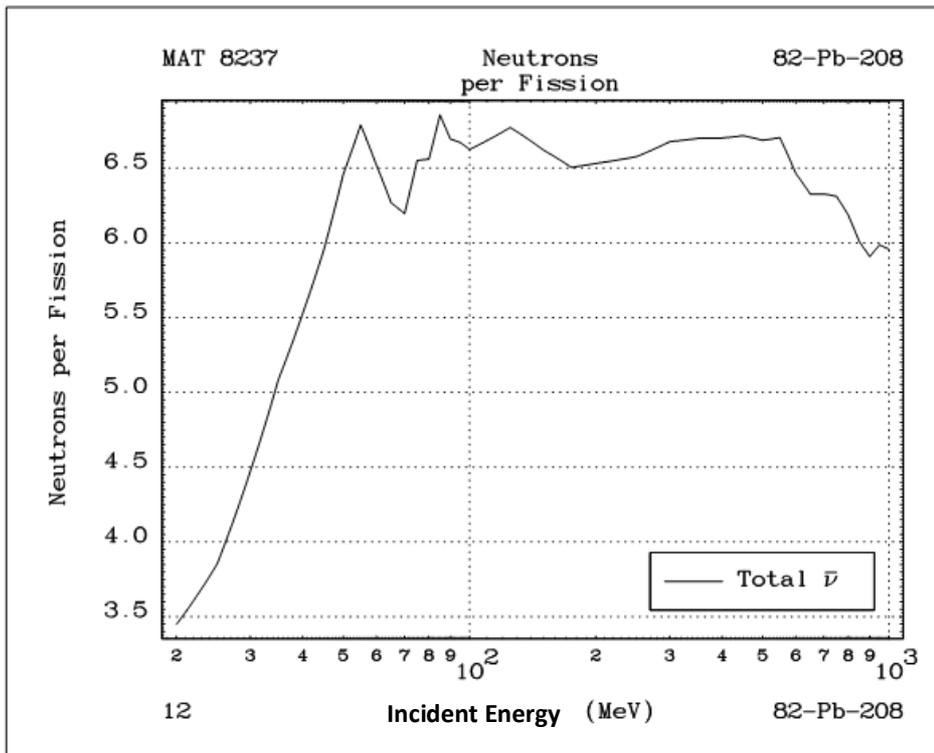
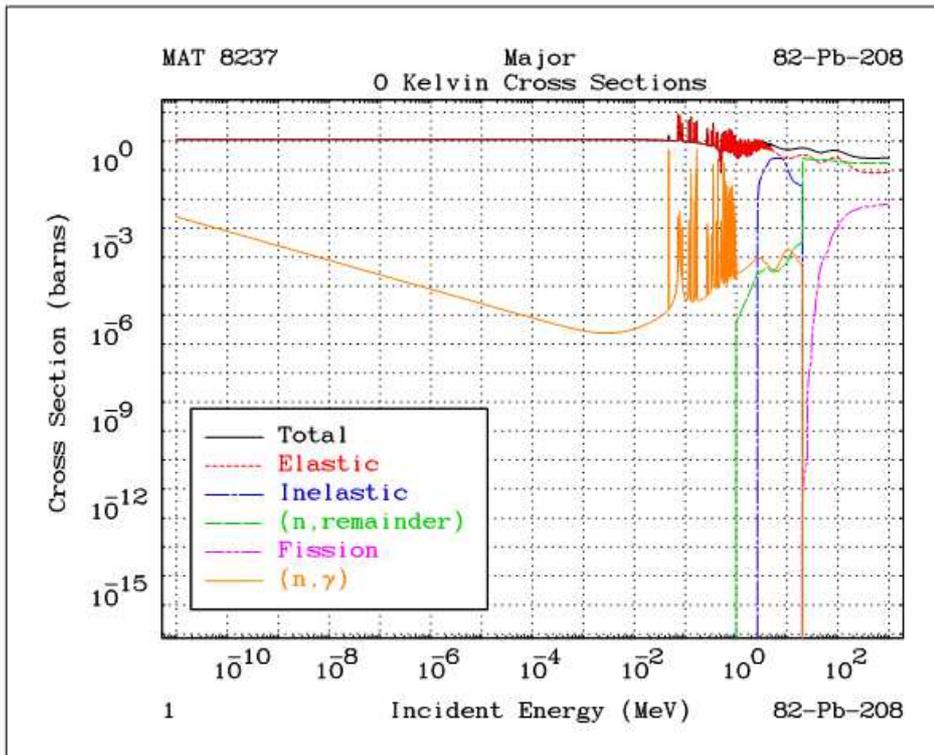
80-HG-202 FOR ADS-HI
Neutron emission for (n,x)



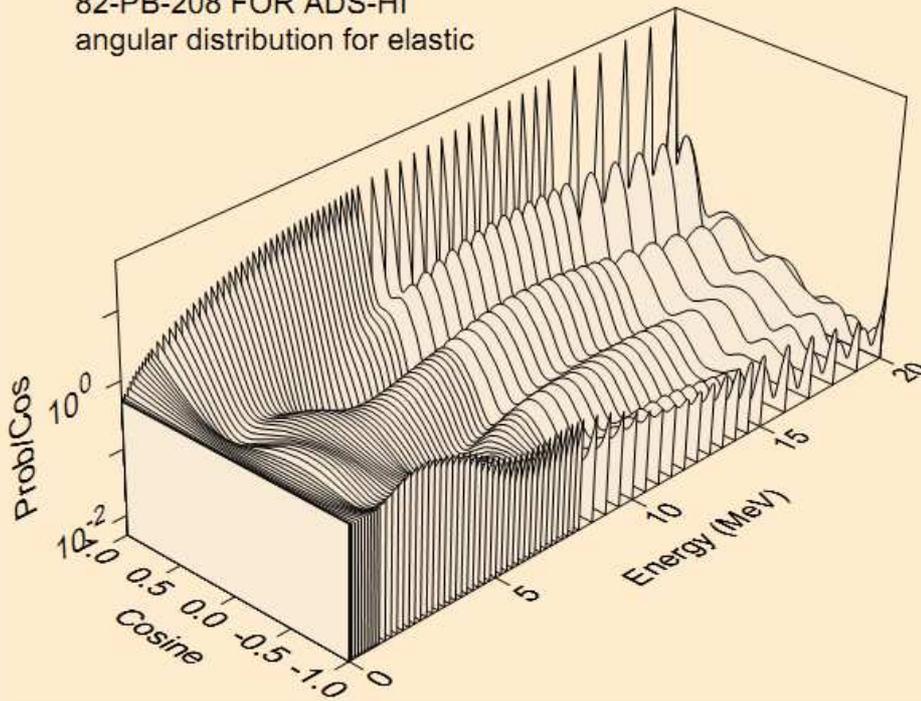
80-HG-202 FOR ADS-HI
Neutron emission for fission



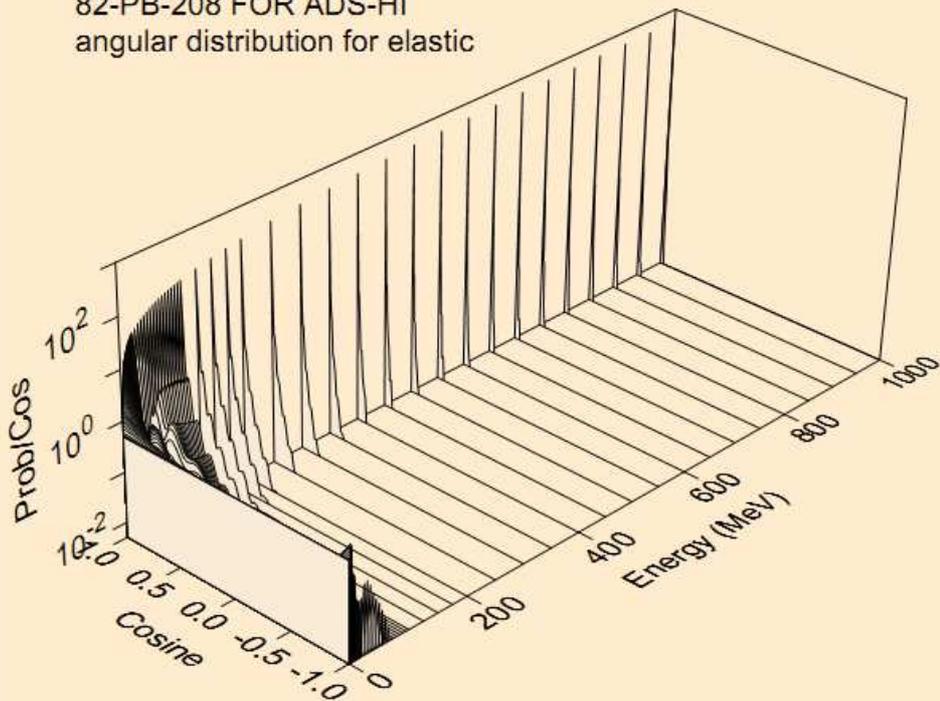




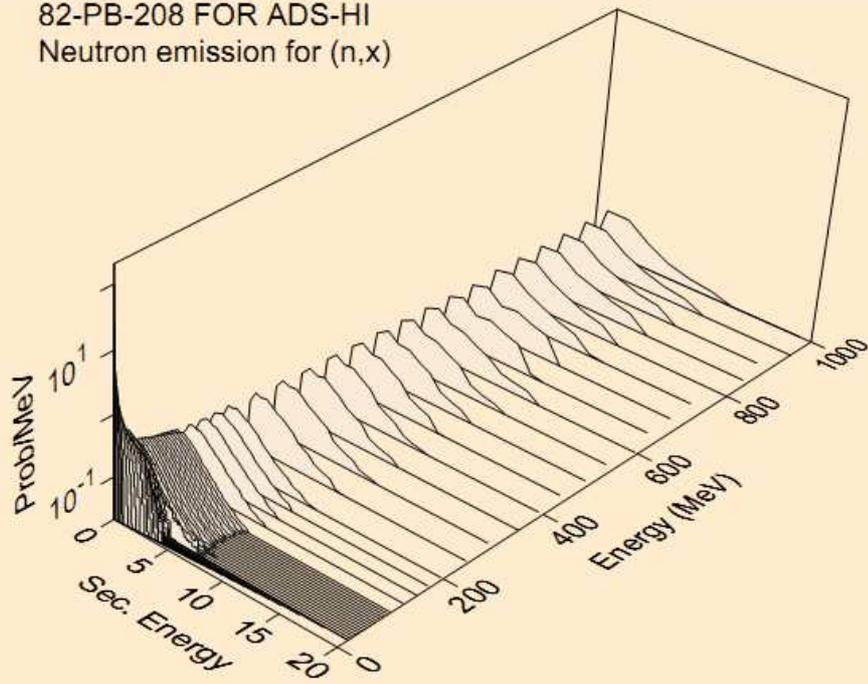
82-PB-208 FOR ADS-HI
angular distribution for elastic



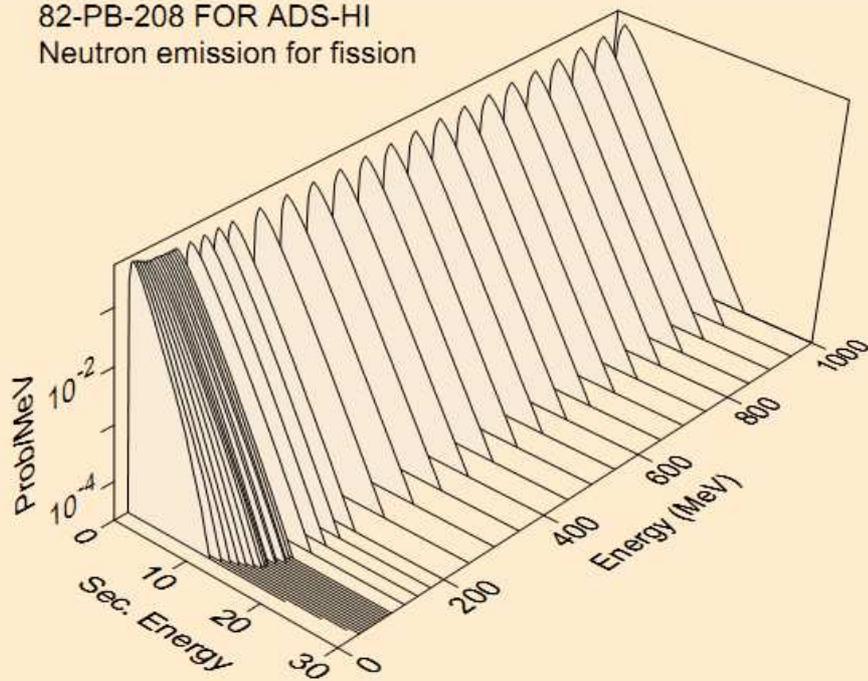
82-PB-208 FOR ADS-HI
angular distribution for elastic

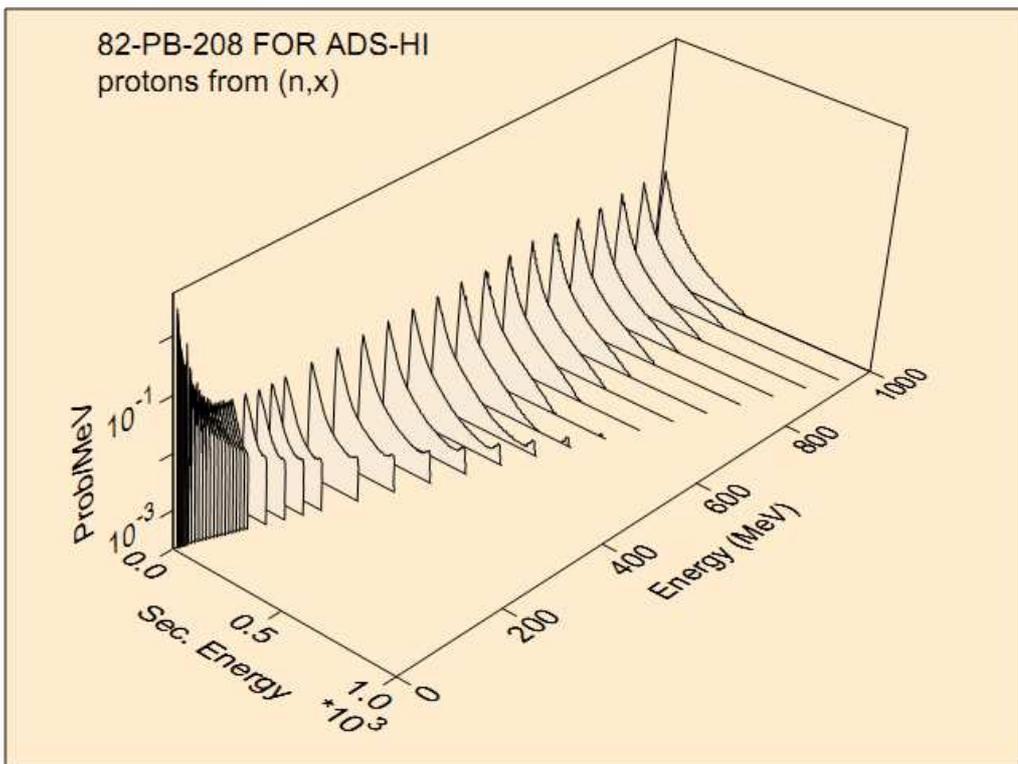
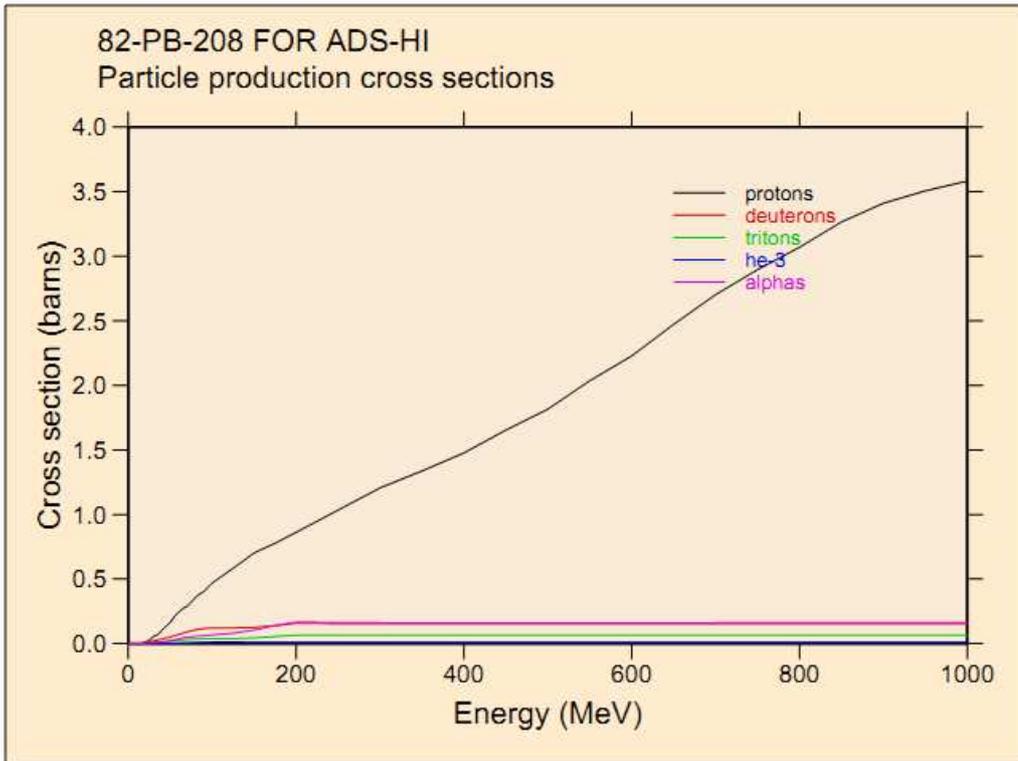


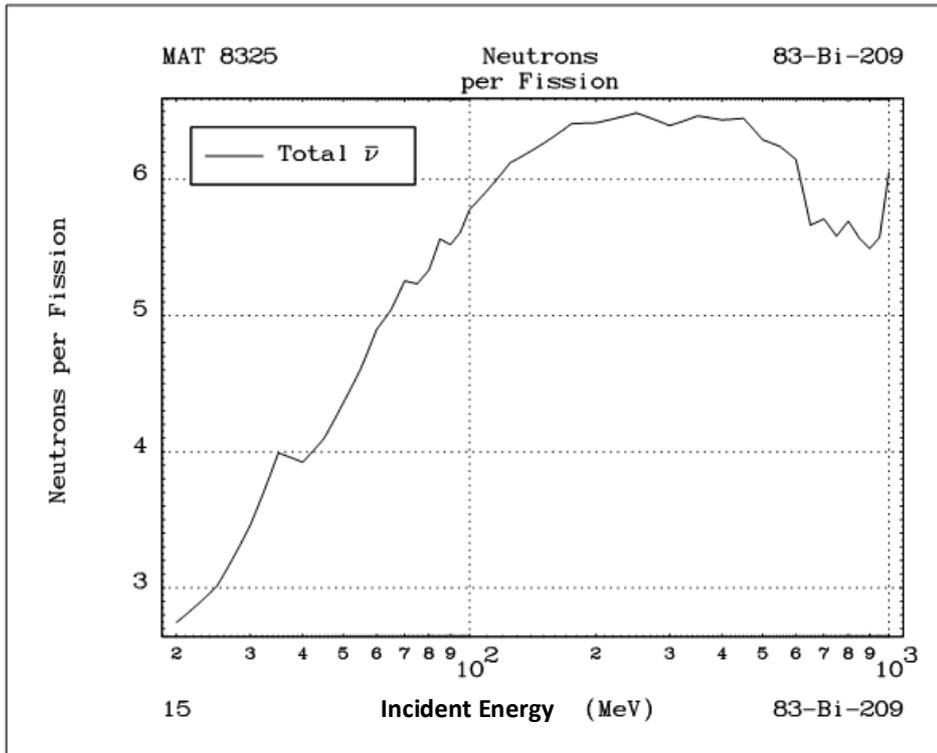
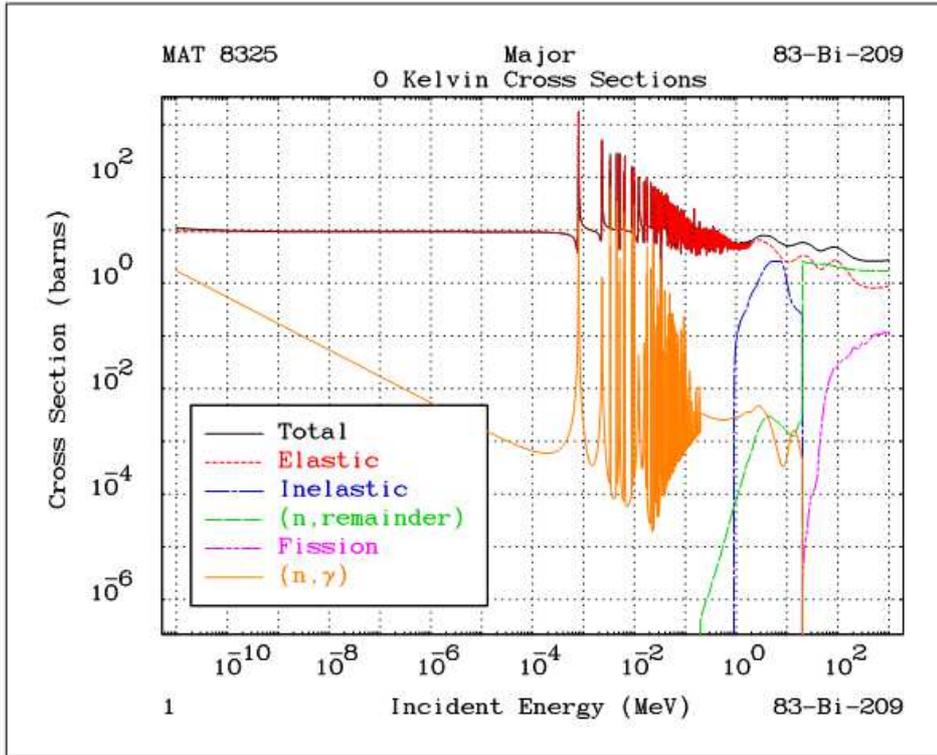
82-PB-208 FOR ADS-HI
Neutron emission for (n,x)



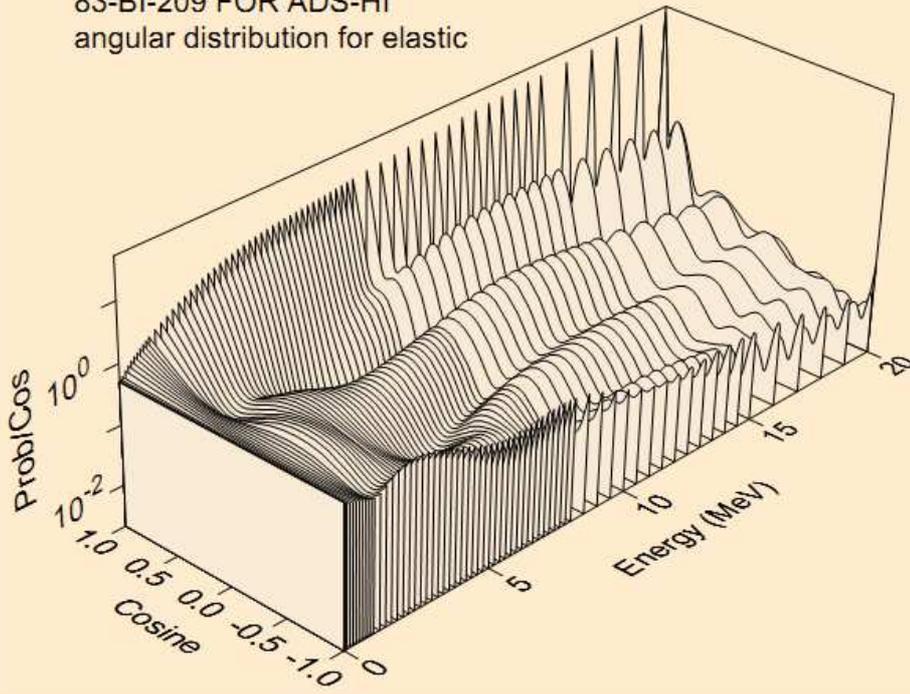
82-PB-208 FOR ADS-HI
Neutron emission for fission



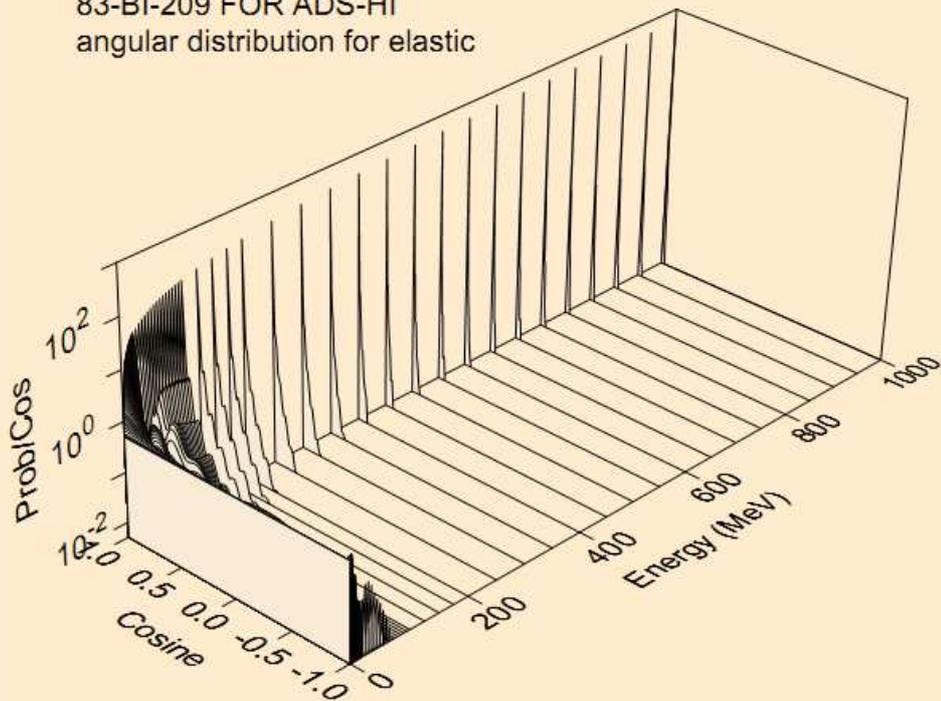




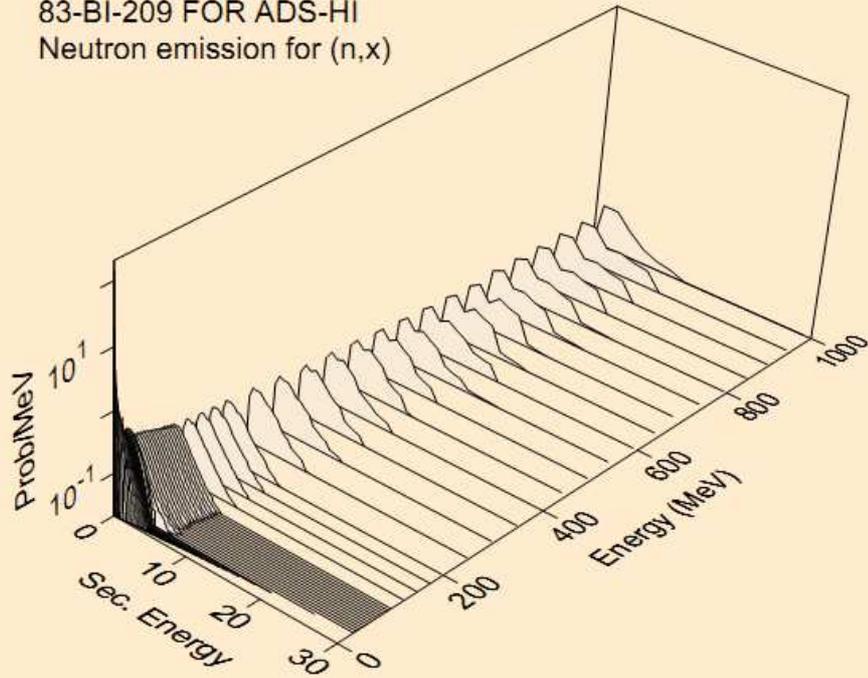
83-BI-209 FOR ADS-HI
angular distribution for elastic



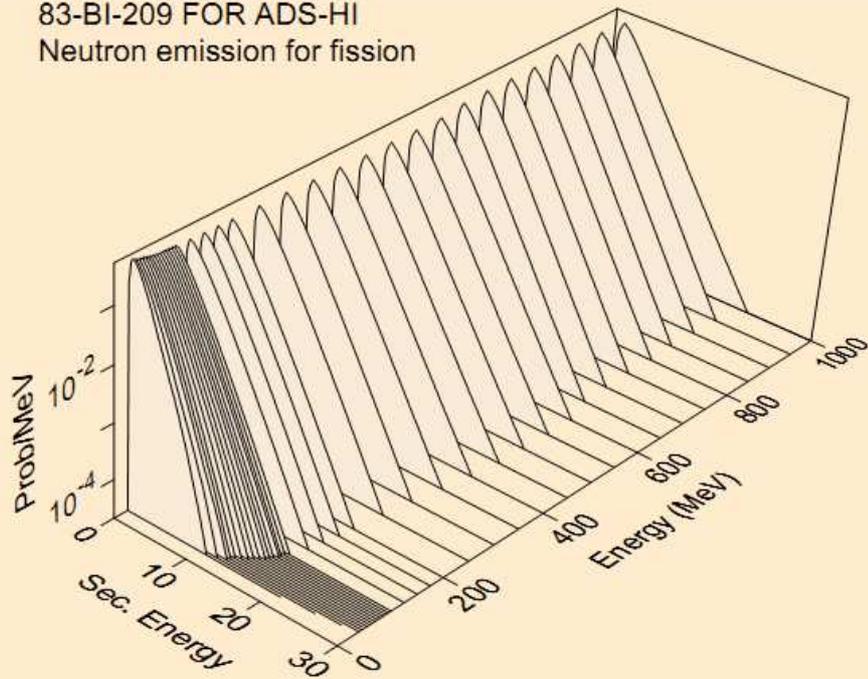
83-BI-209 FOR ADS-HI
angular distribution for elastic

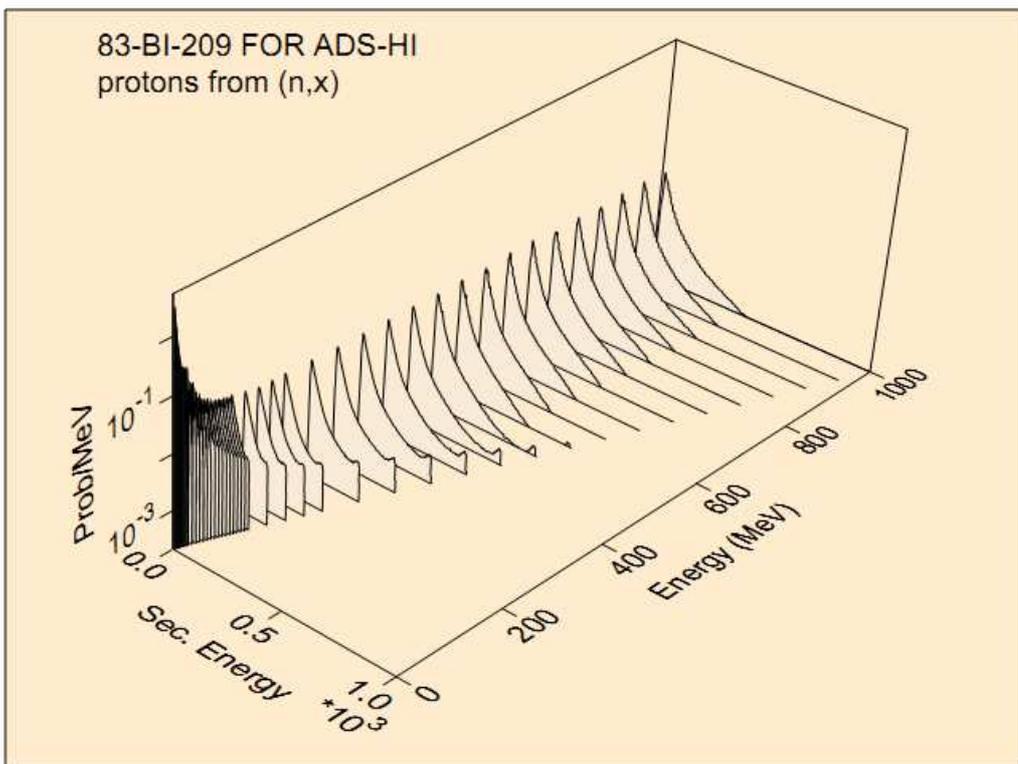
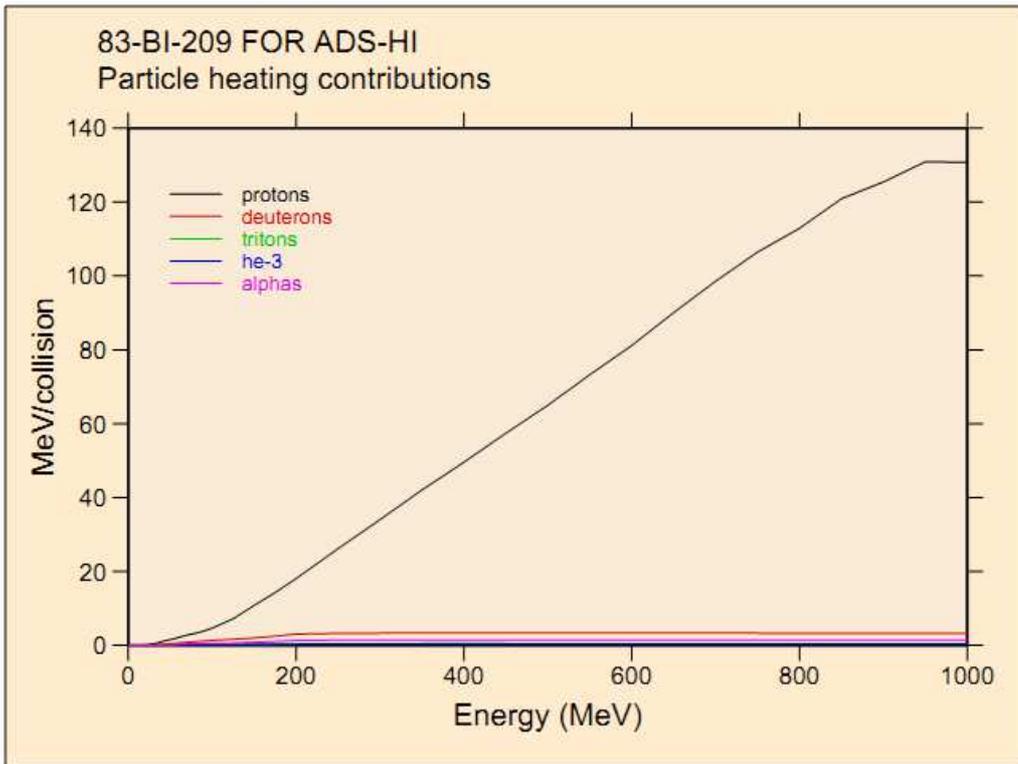


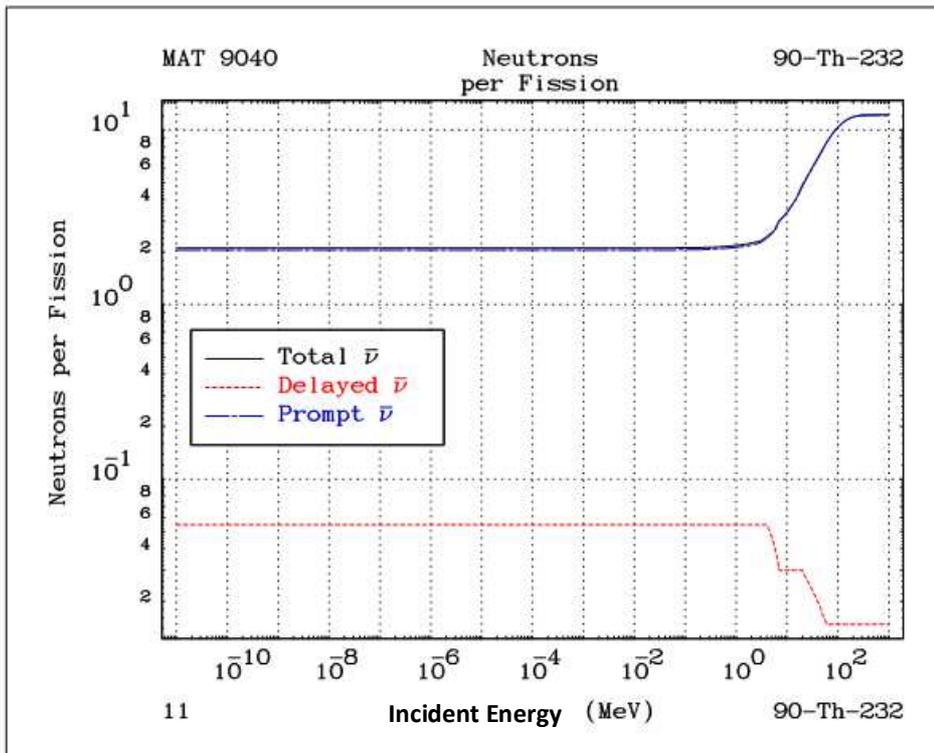
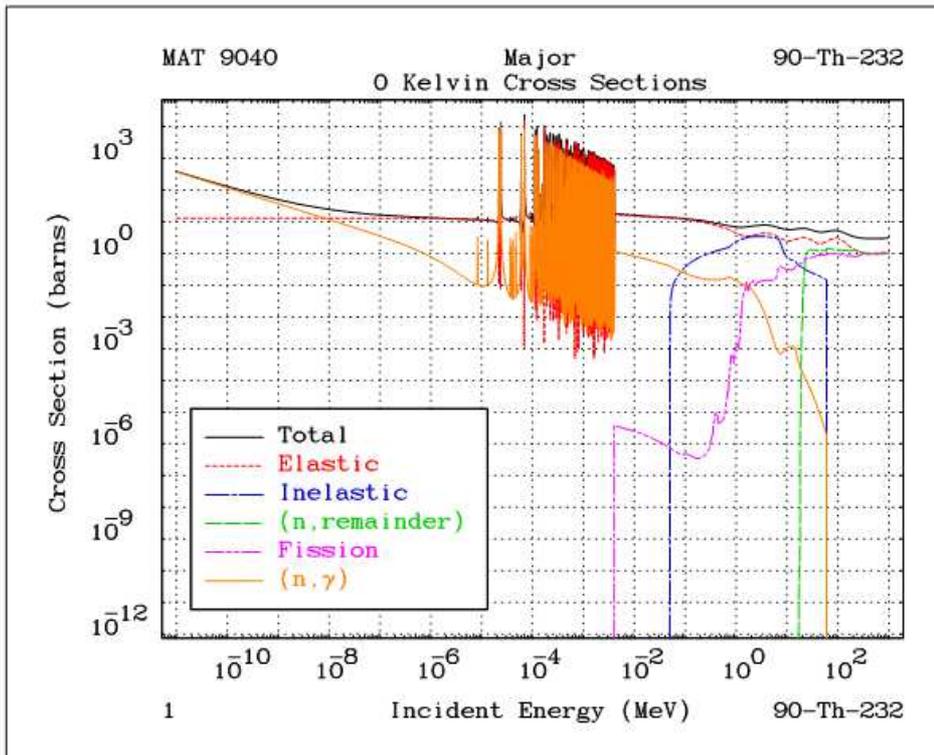
83-BI-209 FOR ADS-HI
Neutron emission for (n,x)



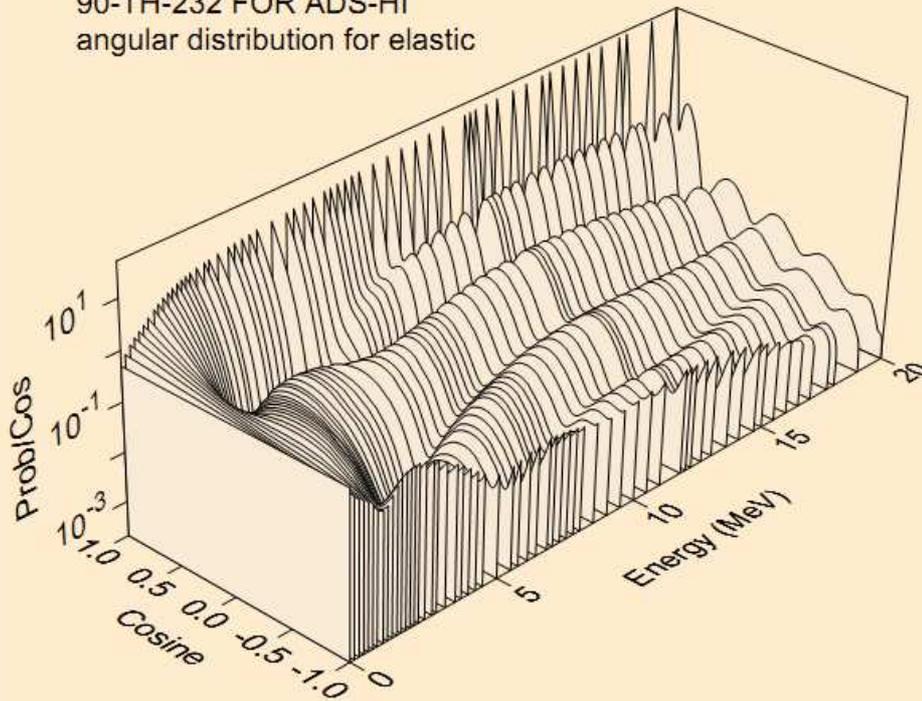
83-BI-209 FOR ADS-HI
Neutron emission for fission



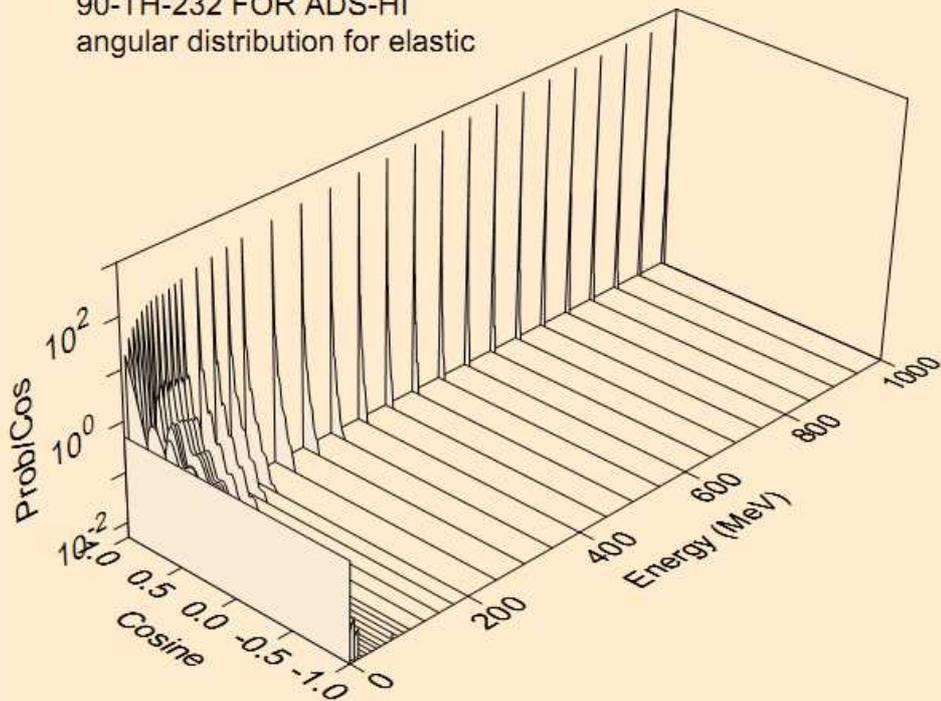




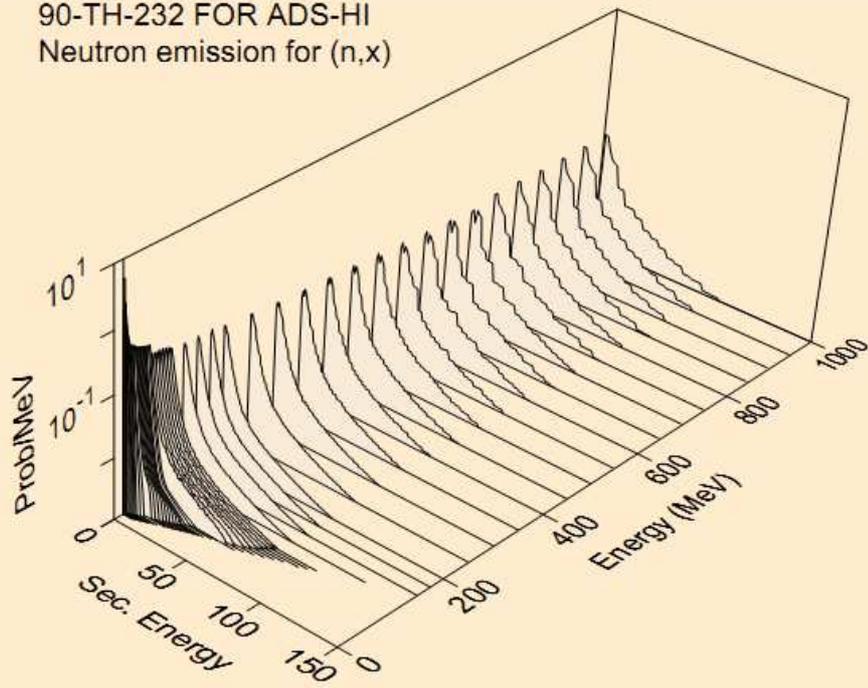
90-TH-232 FOR ADS-HI
angular distribution for elastic



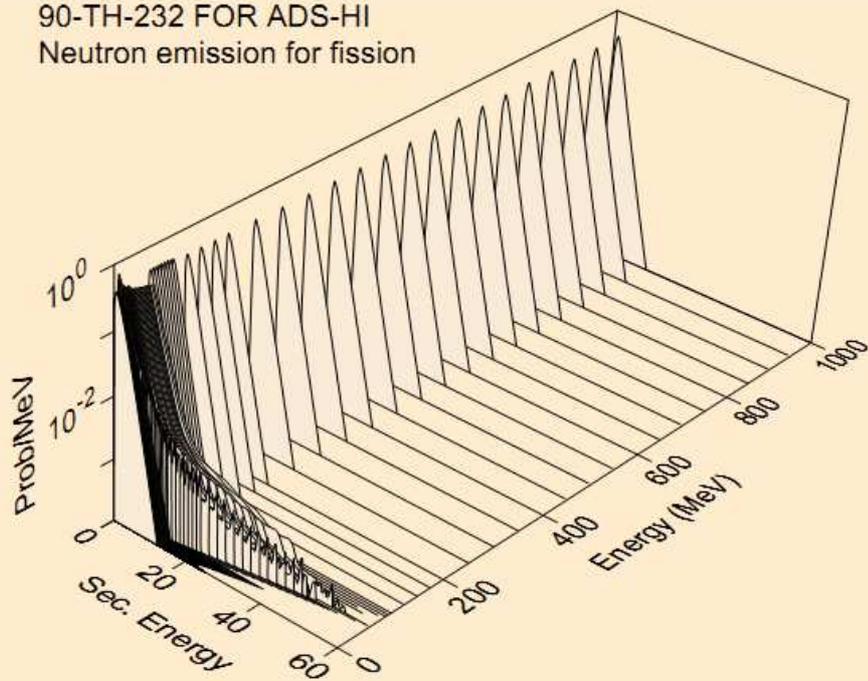
90-TH-232 FOR ADS-HI
angular distribution for elastic

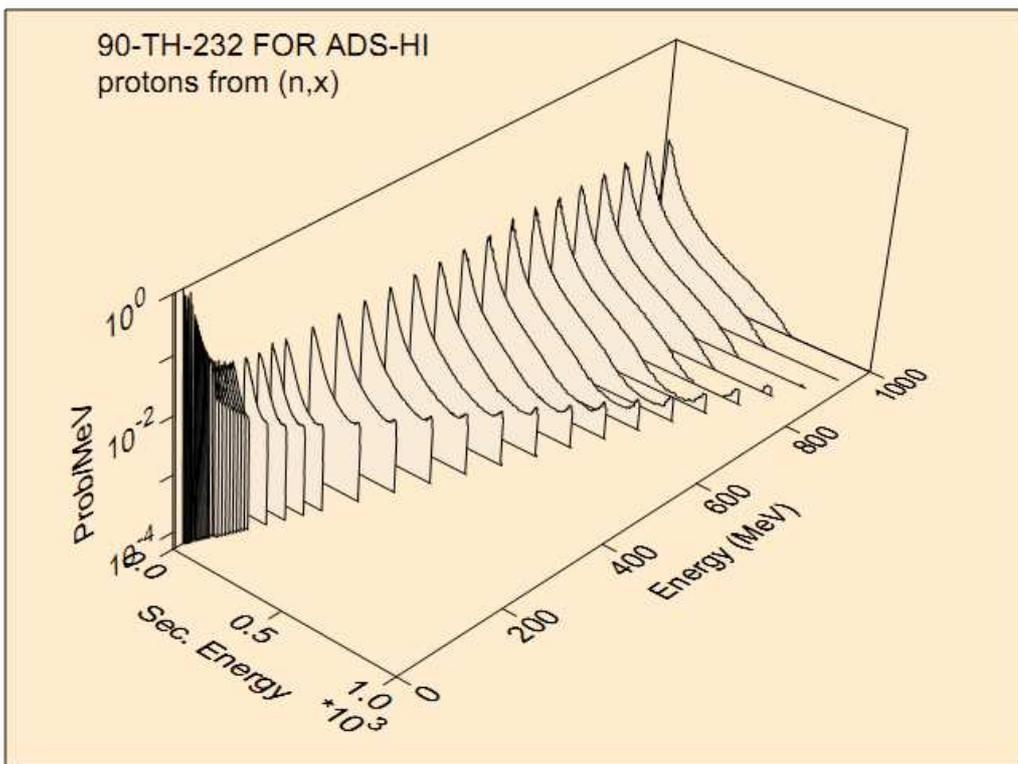
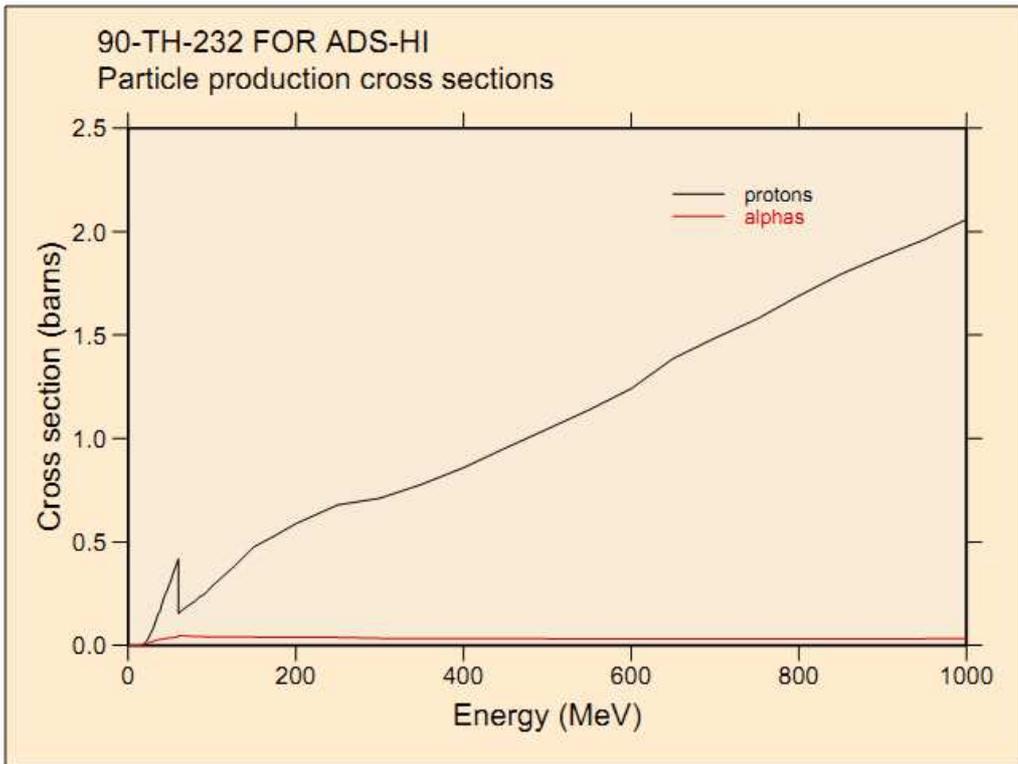


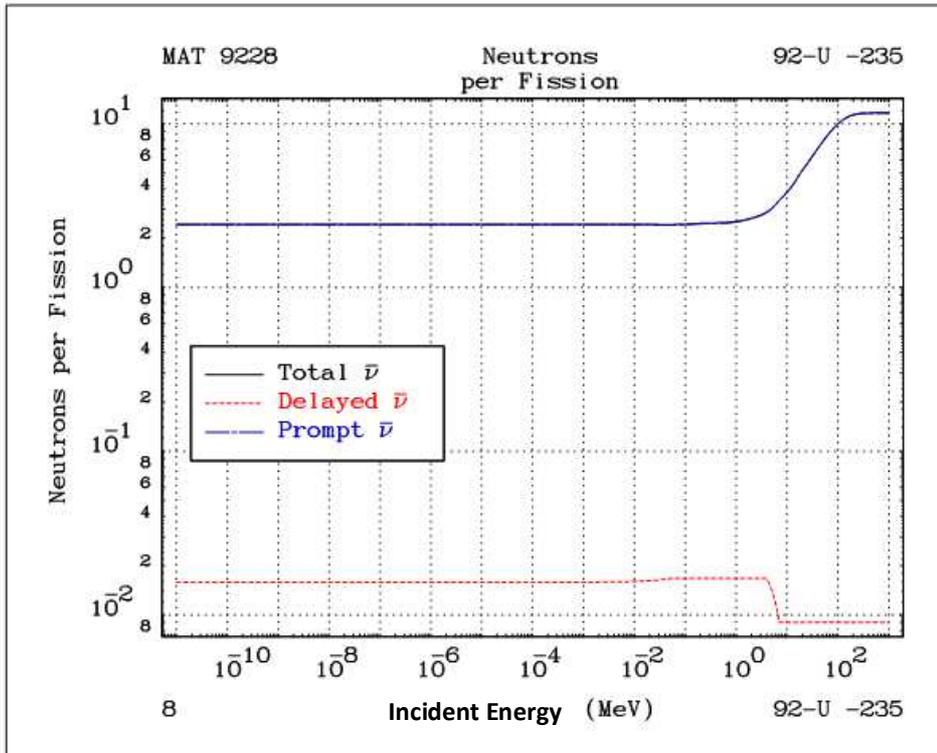
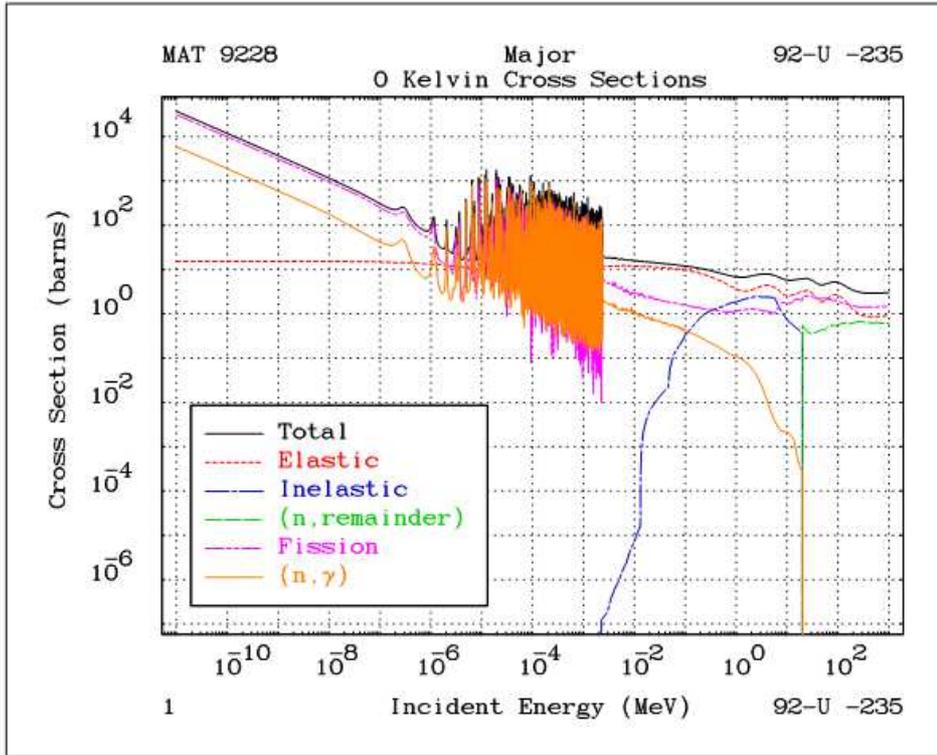
90-TH-232 FOR ADS-HI
Neutron emission for (n,x)



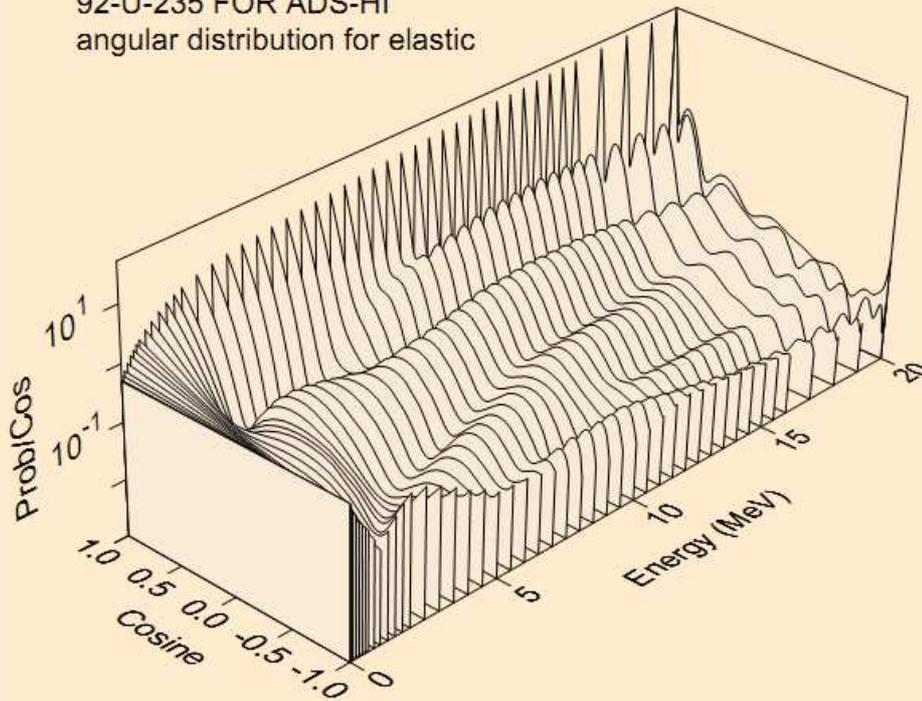
90-TH-232 FOR ADS-HI
Neutron emission for fission



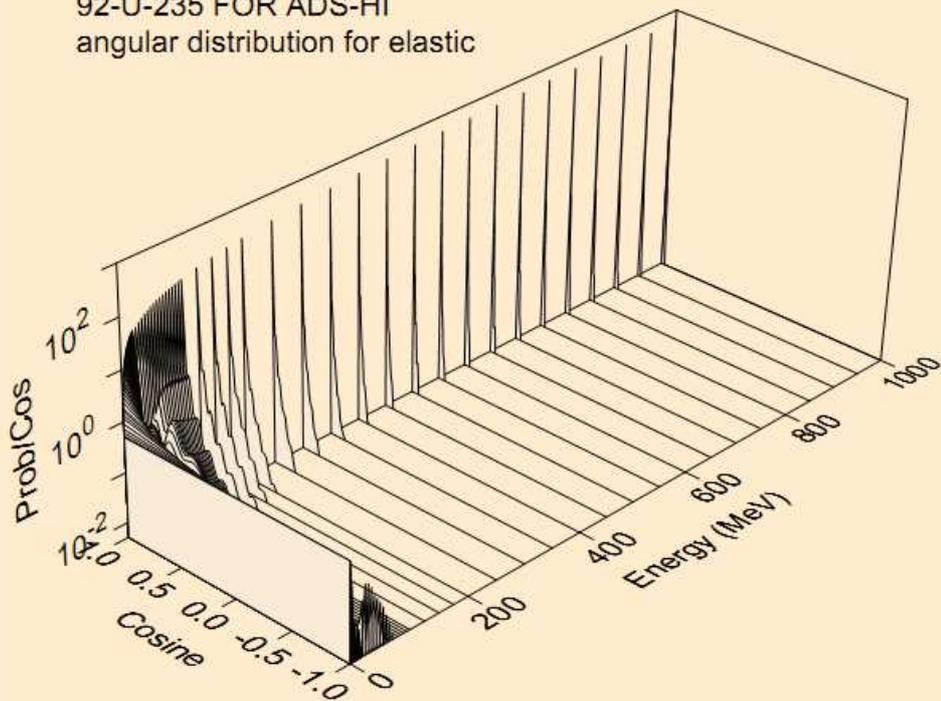




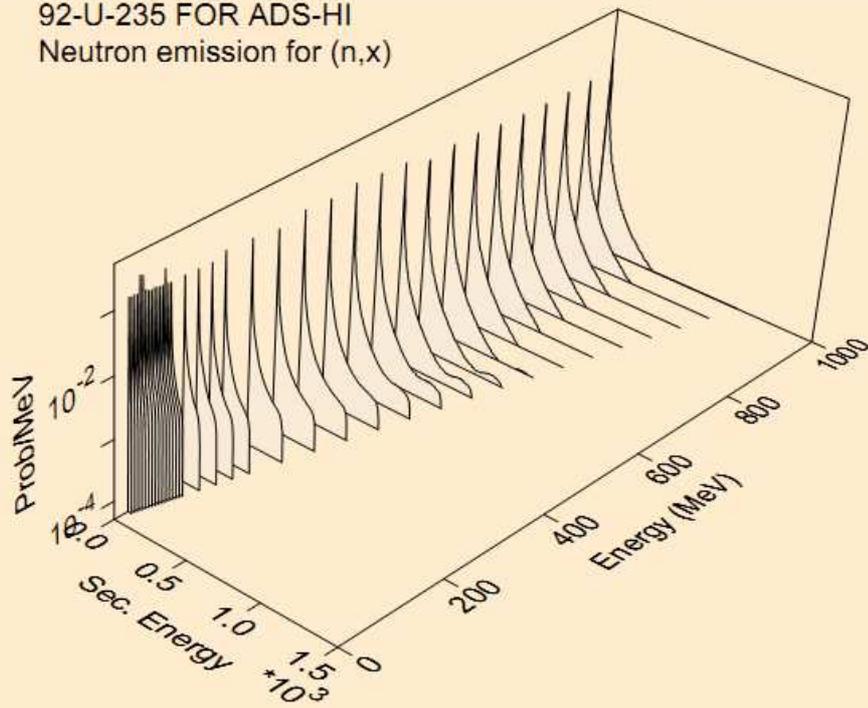
92-U-235 FOR ADS-HI
angular distribution for elastic



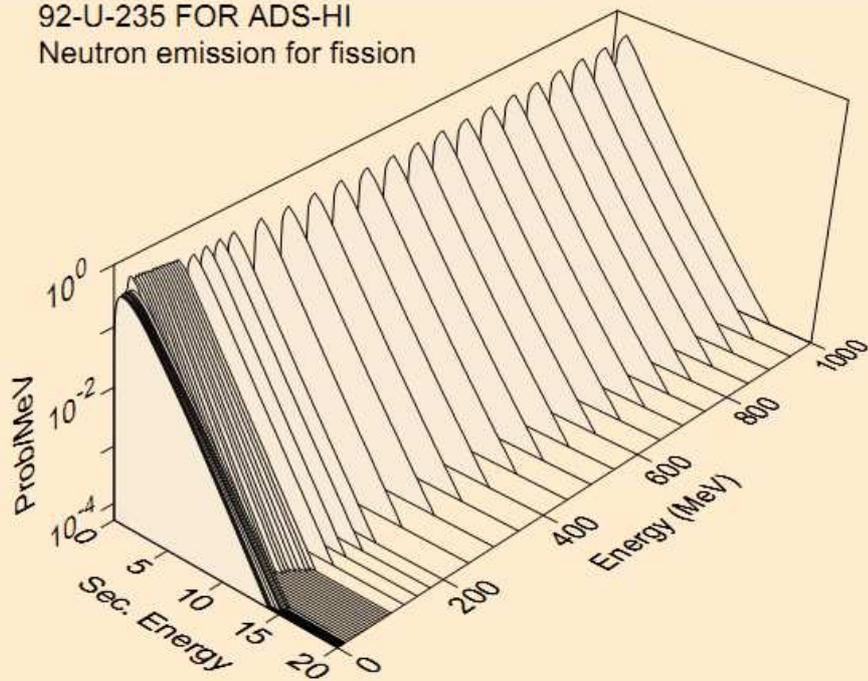
92-U-235 FOR ADS-HI
angular distribution for elastic

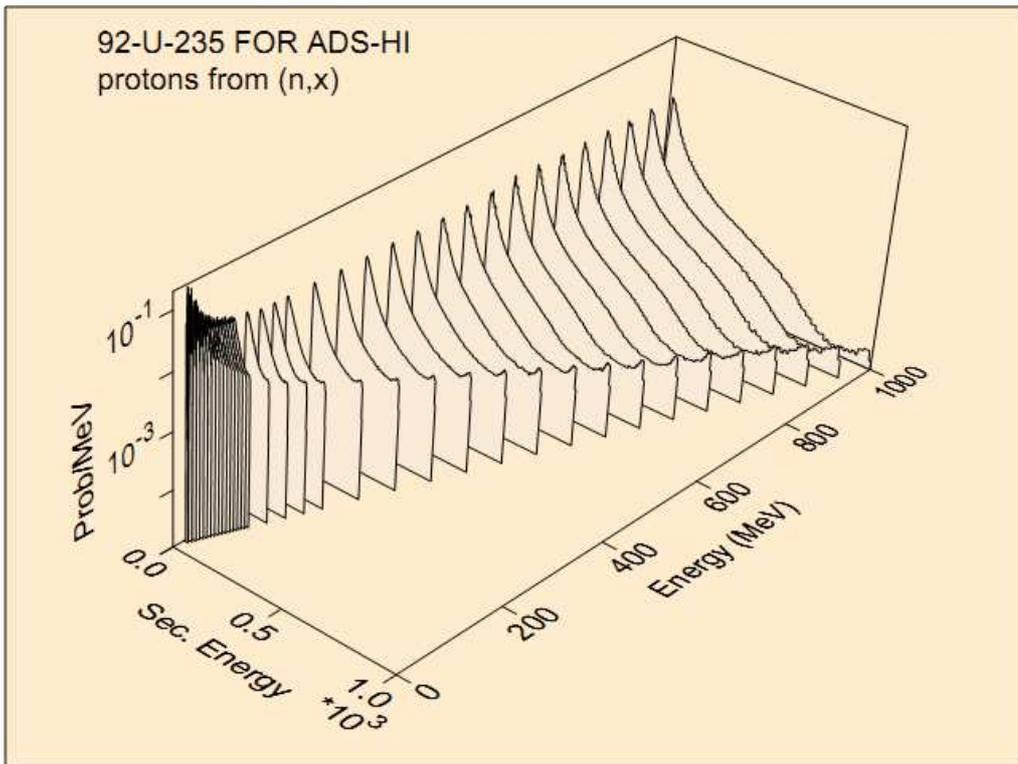
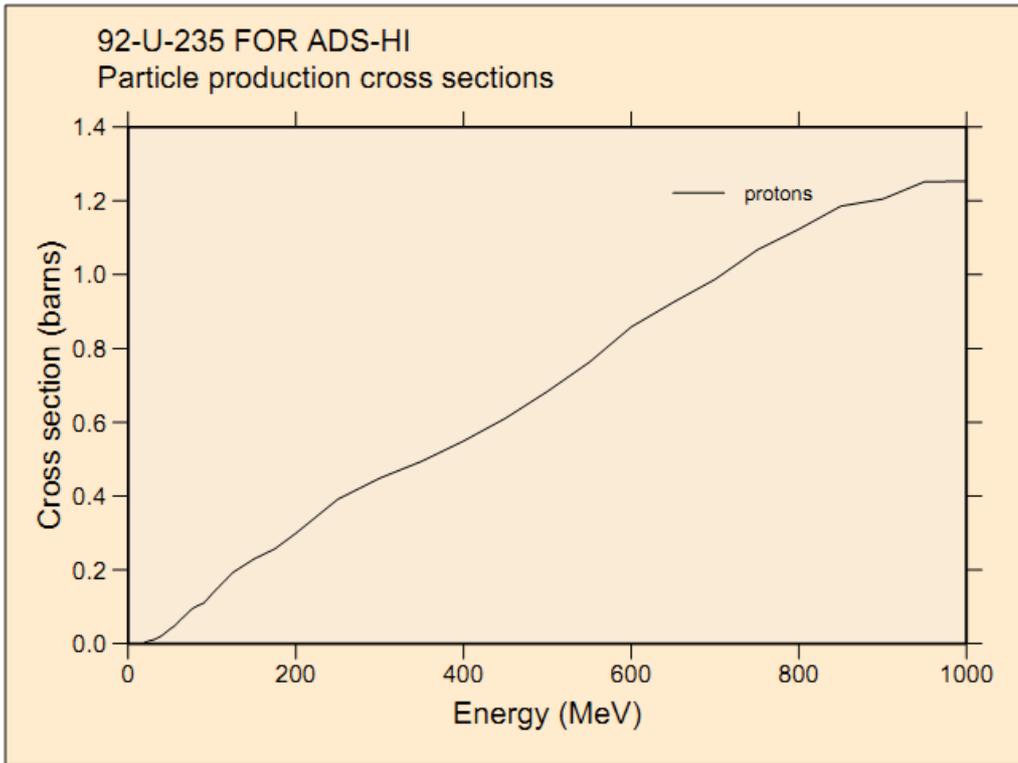


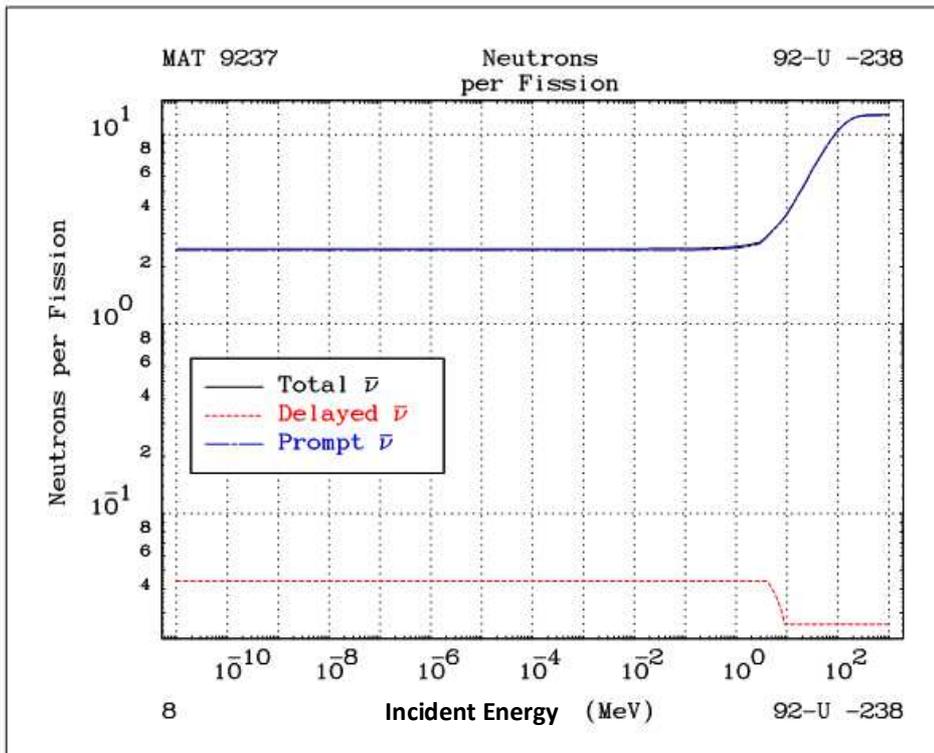
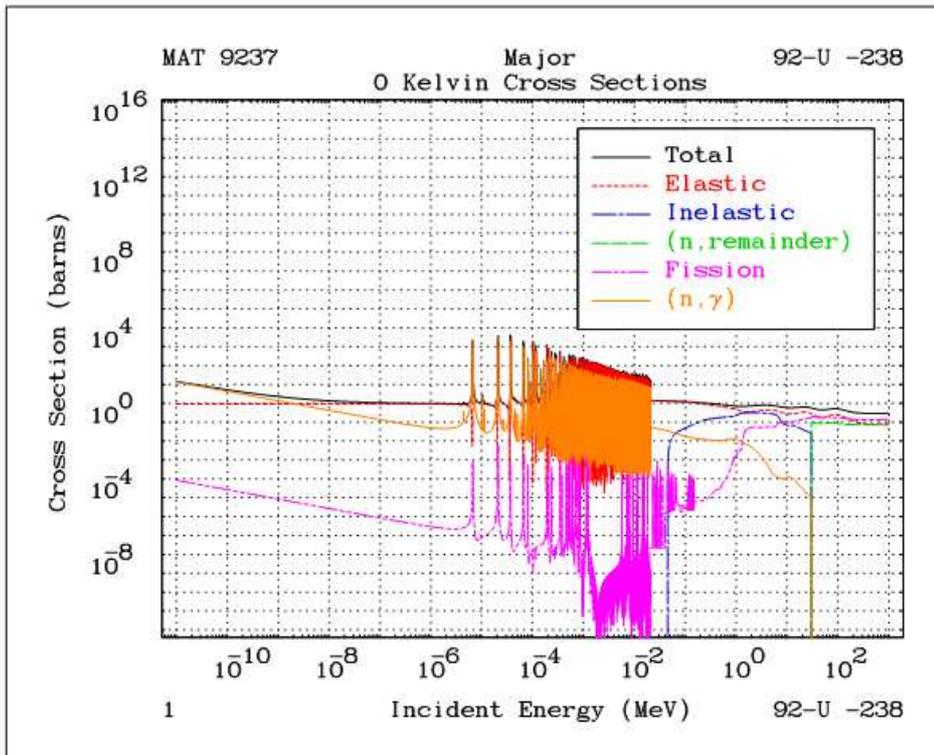
92-U-235 FOR ADS-HI
Neutron emission for (n,x)



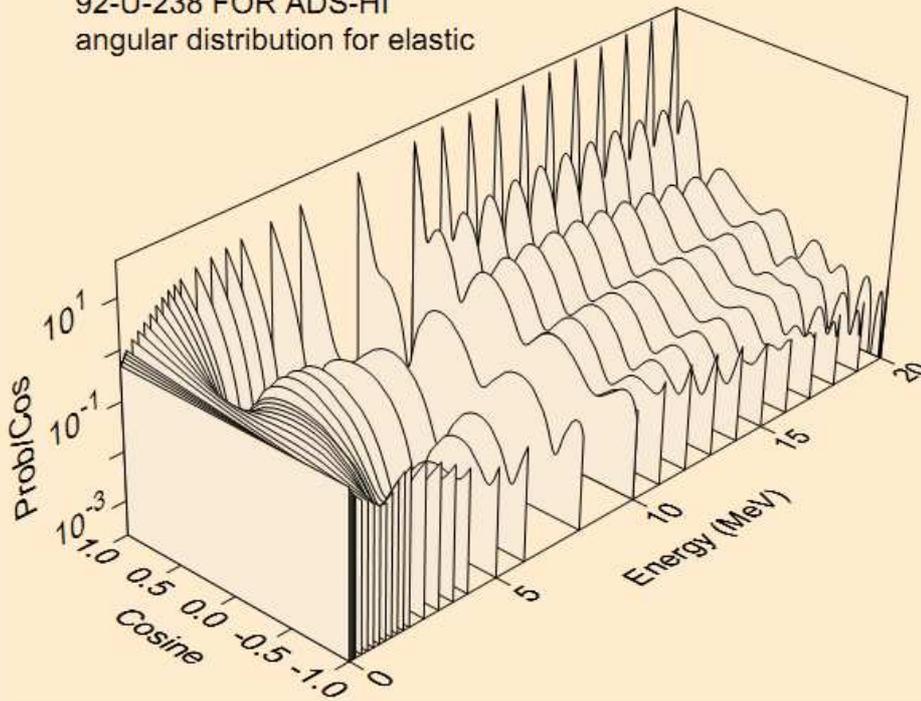
92-U-235 FOR ADS-HI
Neutron emission for fission



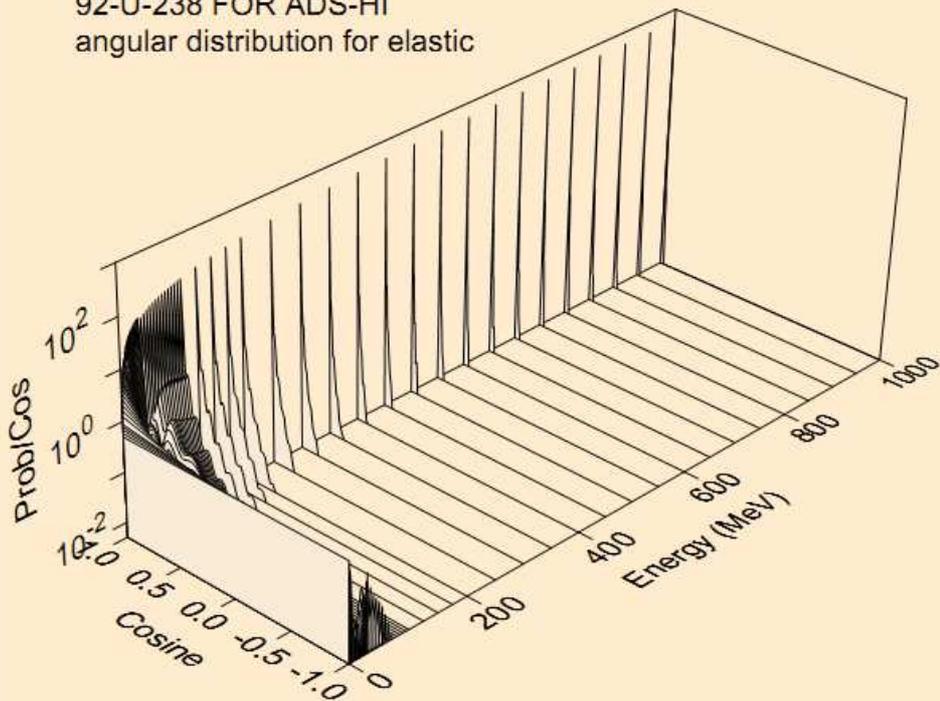




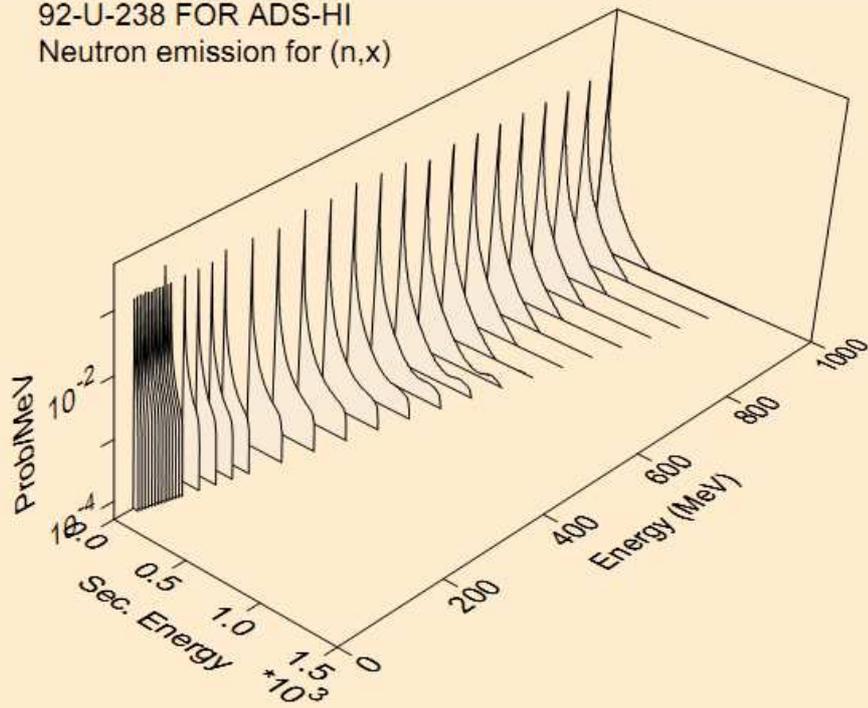
92-U-238 FOR ADS-HI
angular distribution for elastic



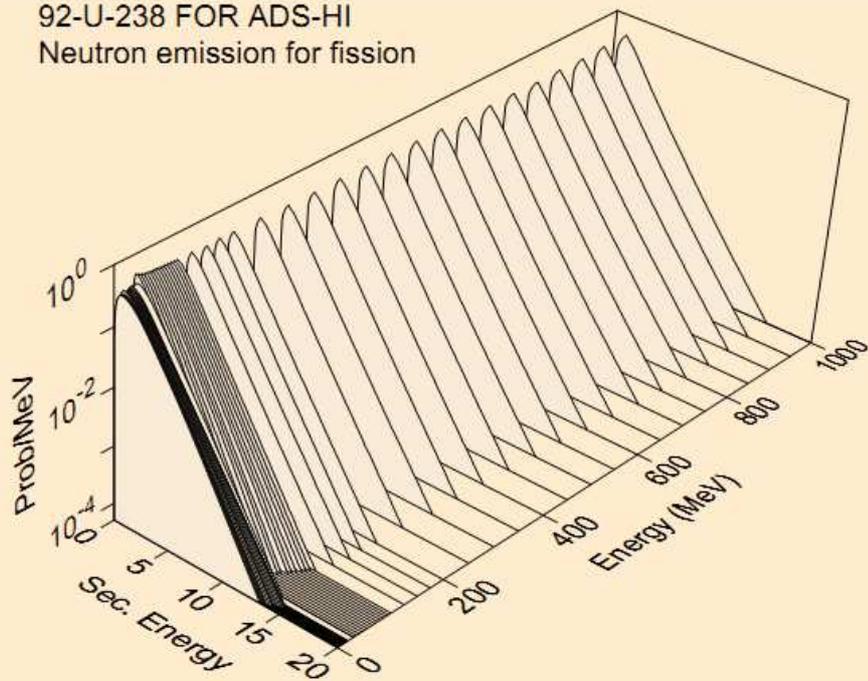
92-U-238 FOR ADS-HI
angular distribution for elastic

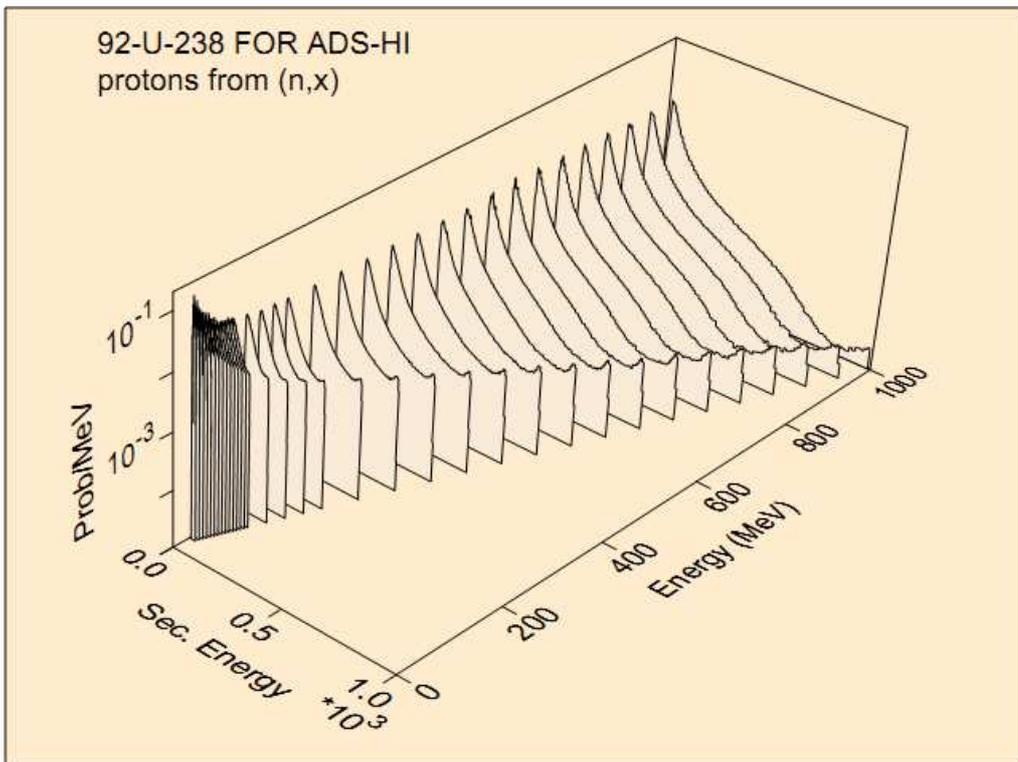
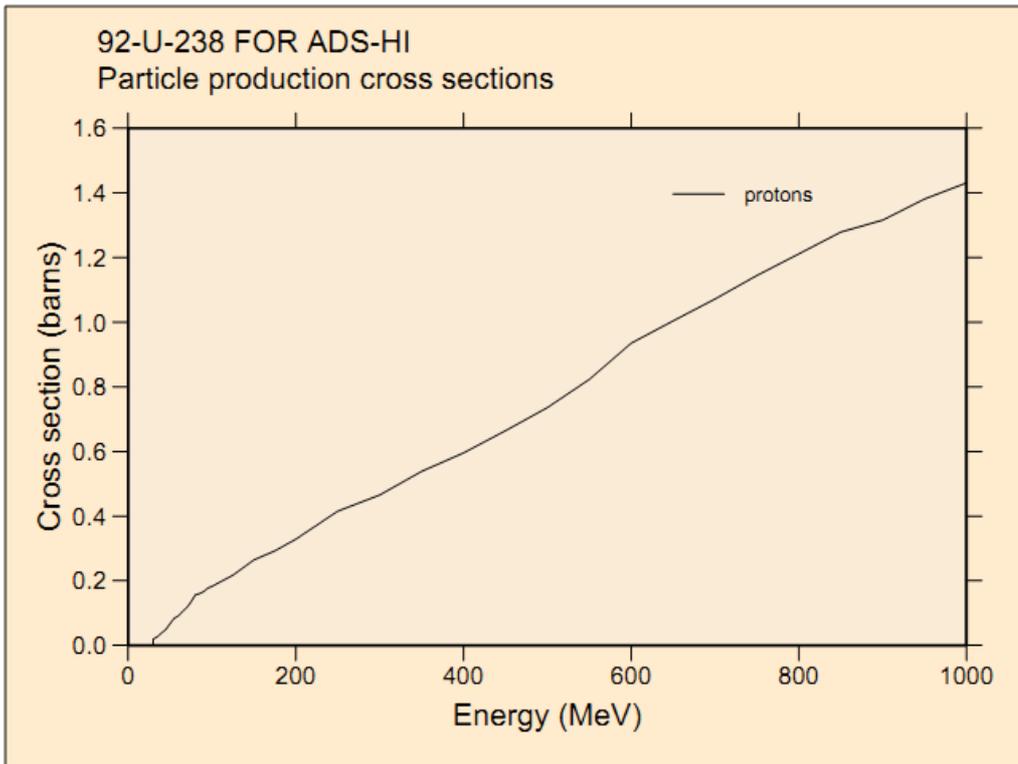


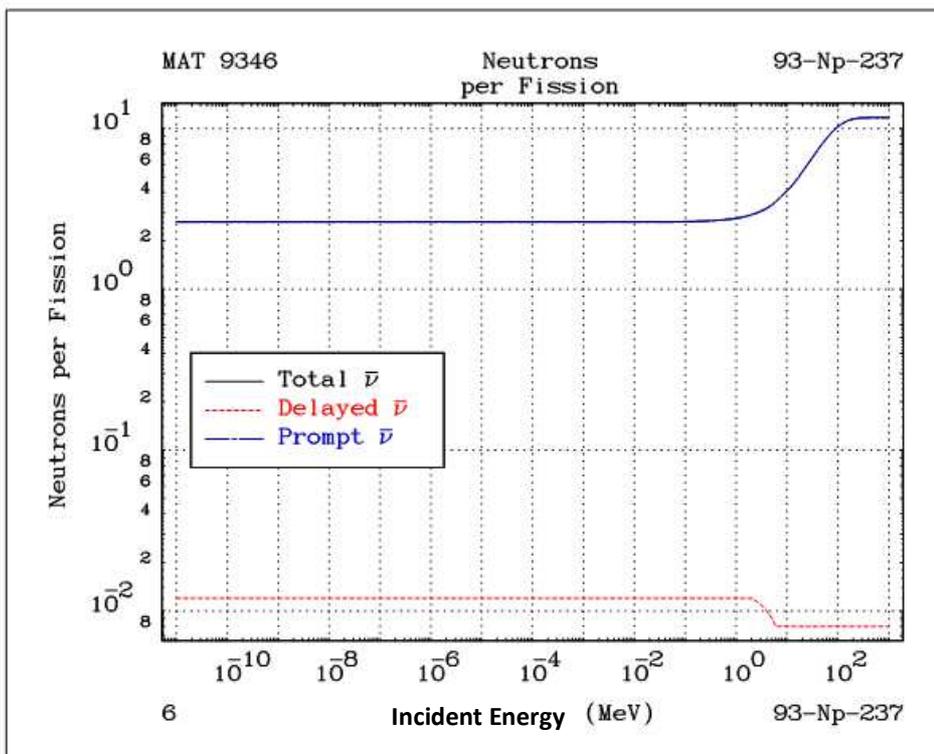
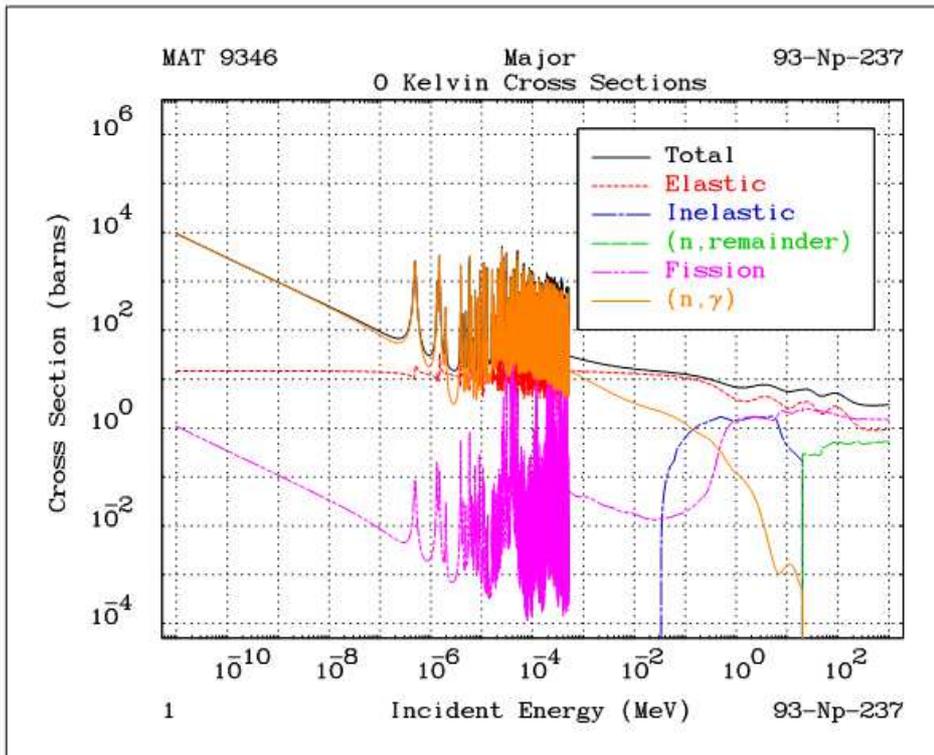
92-U-238 FOR ADS-HI
Neutron emission for (n,x)



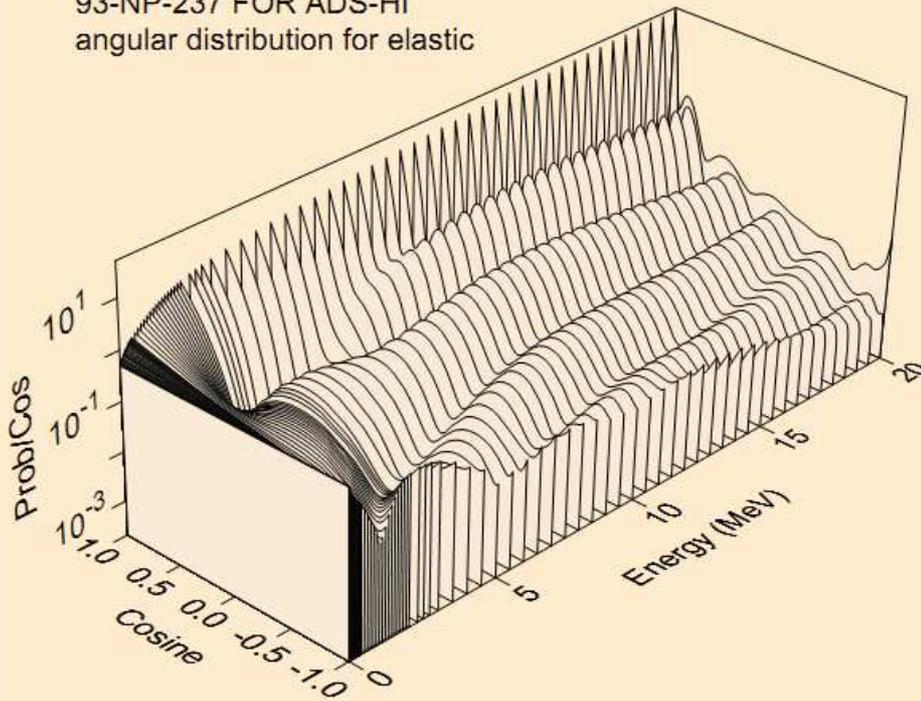
92-U-238 FOR ADS-HI
Neutron emission for fission



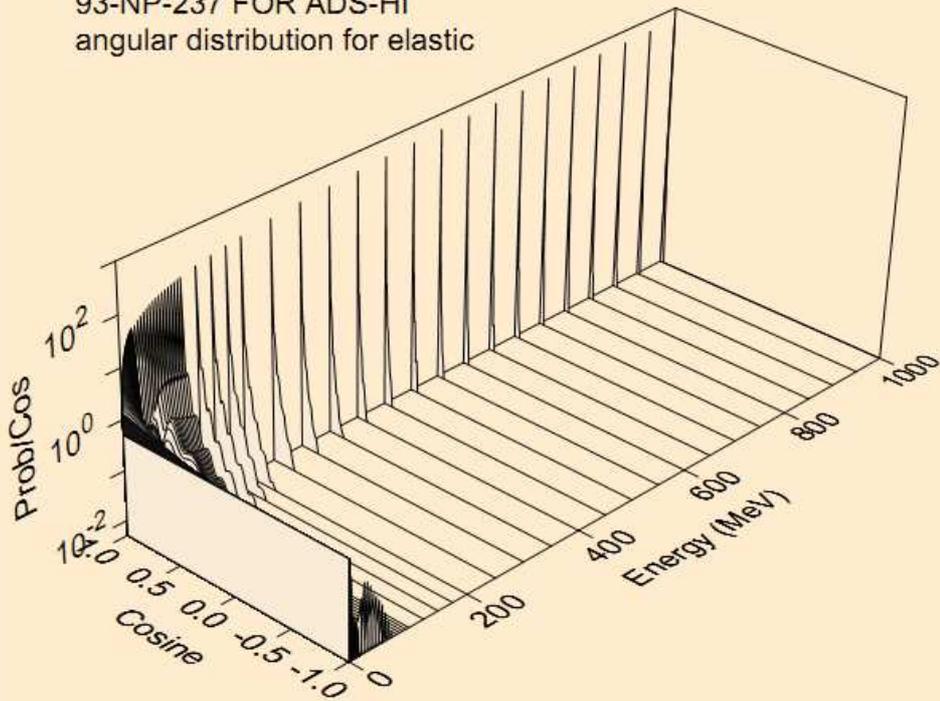




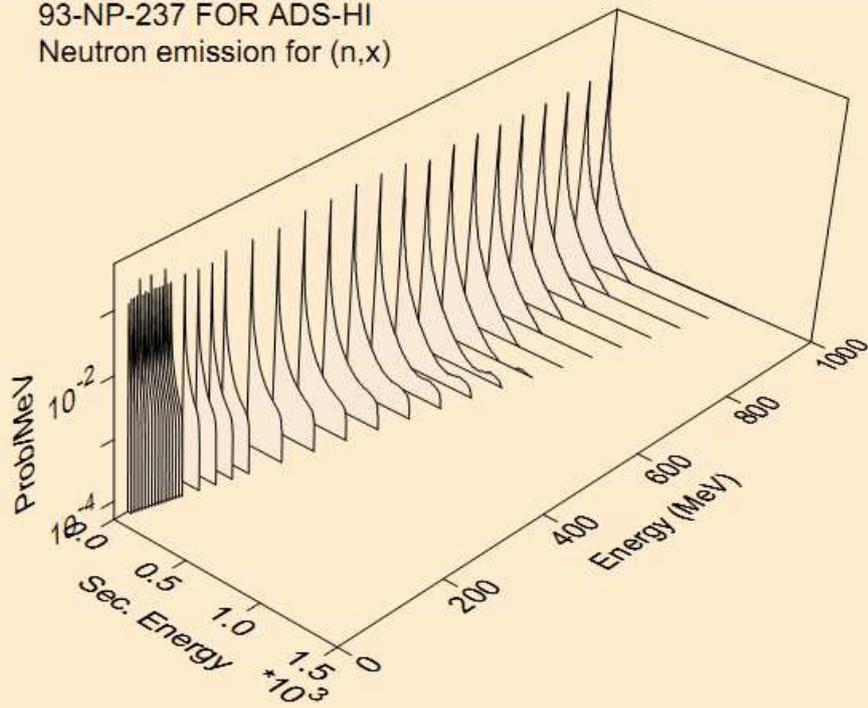
93-NP-237 FOR ADS-HI
angular distribution for elastic



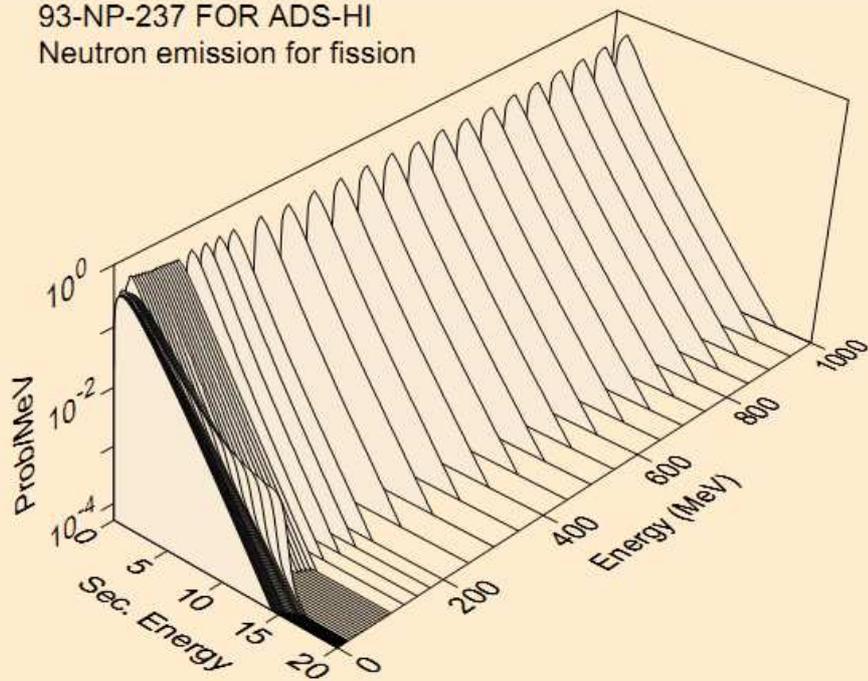
93-NP-237 FOR ADS-HI
angular distribution for elastic

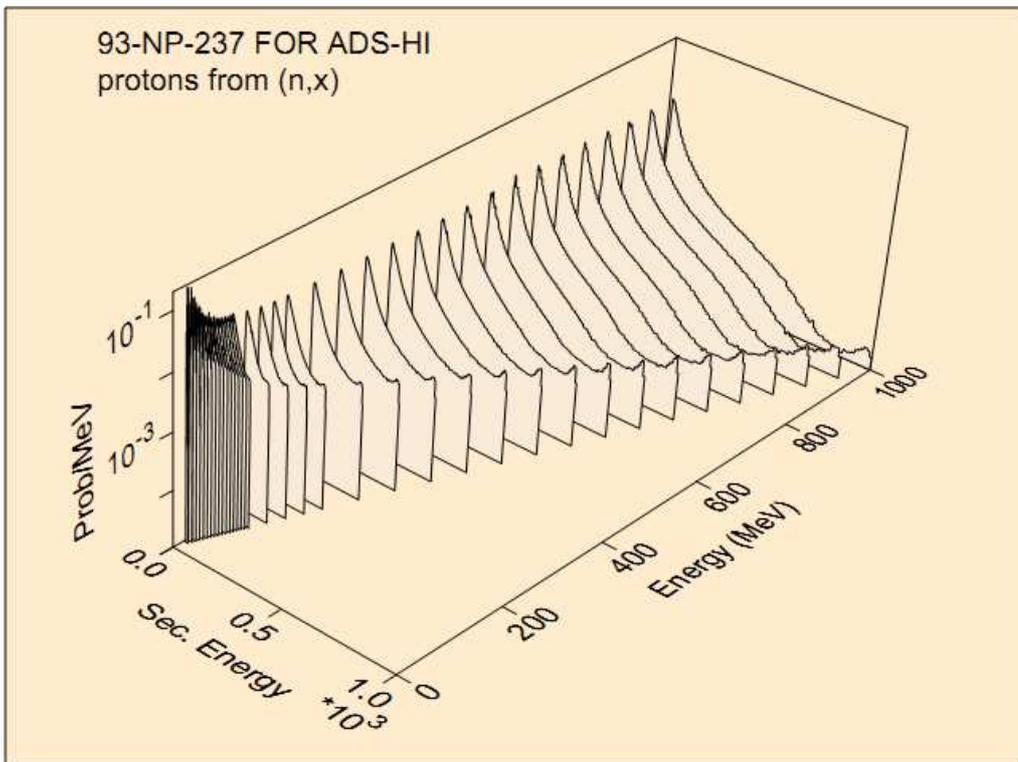
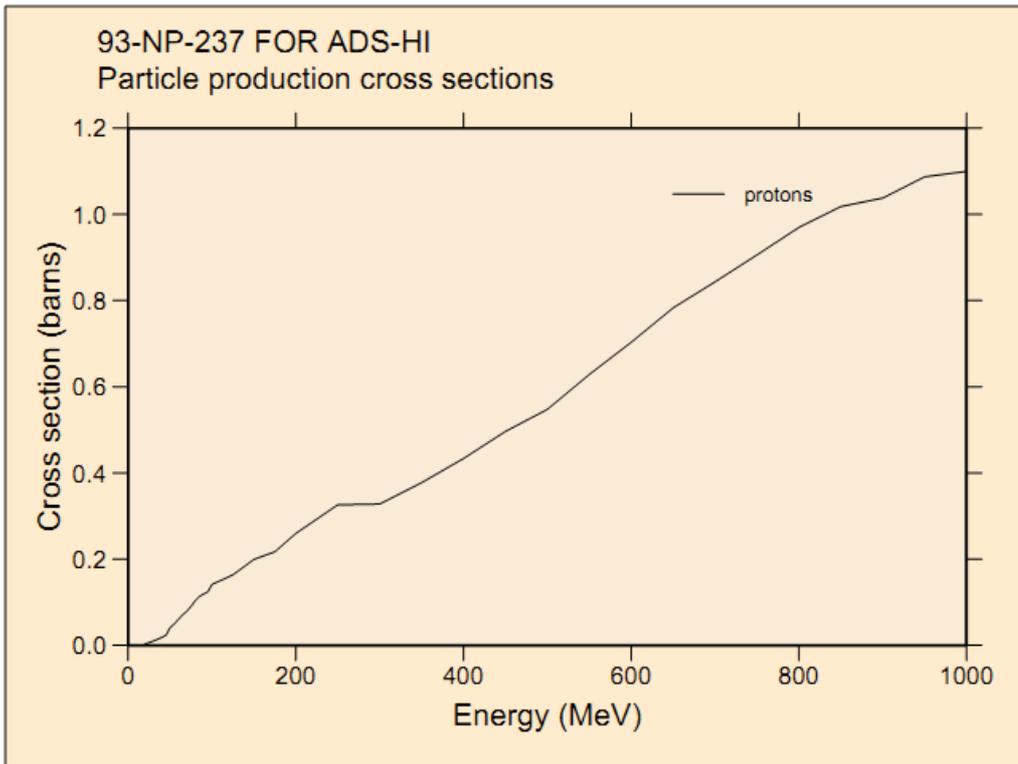


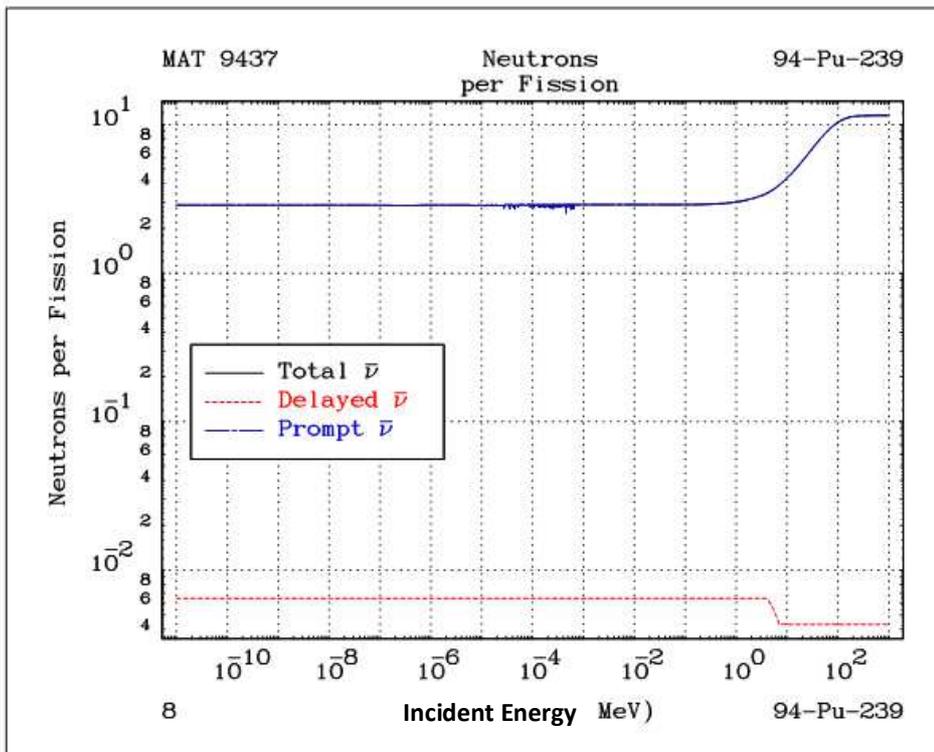
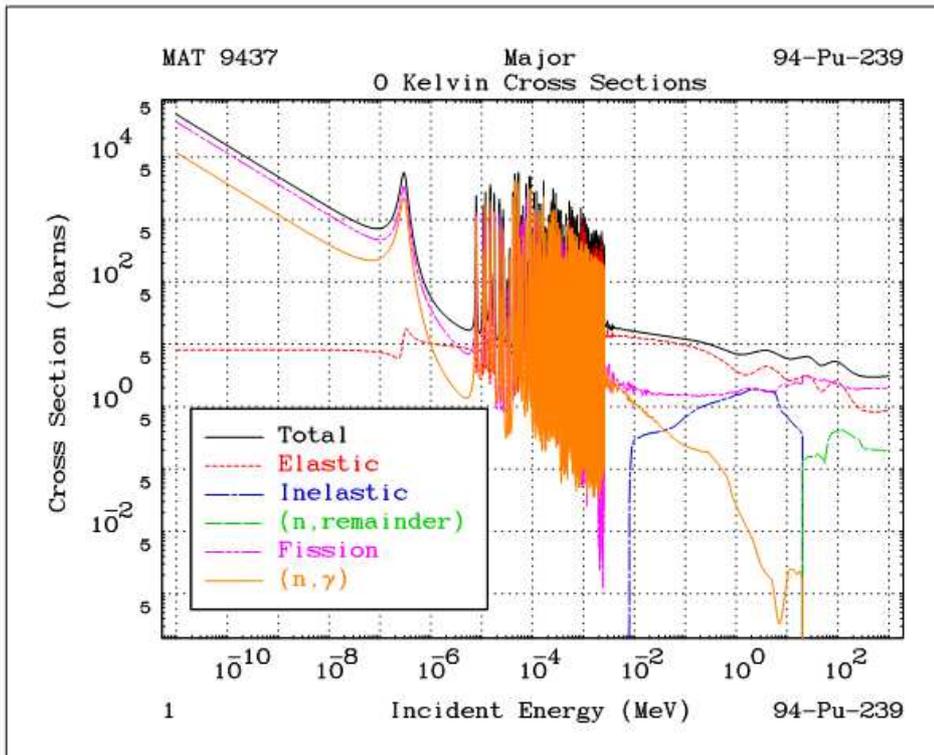
93-NP-237 FOR ADS-HI
Neutron emission for (n,x)



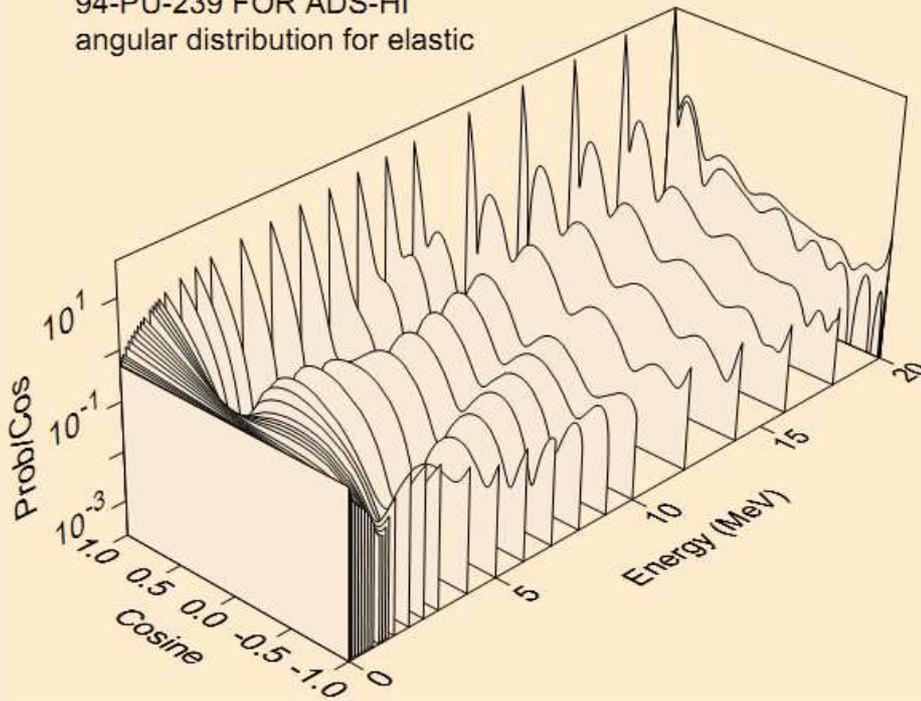
93-NP-237 FOR ADS-HI
Neutron emission for fission



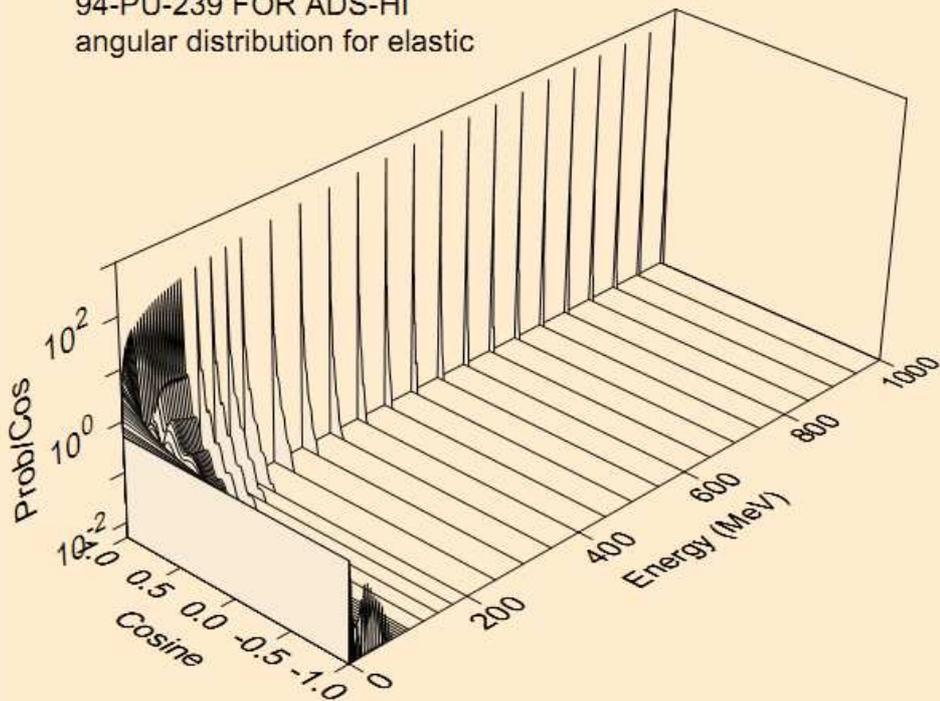




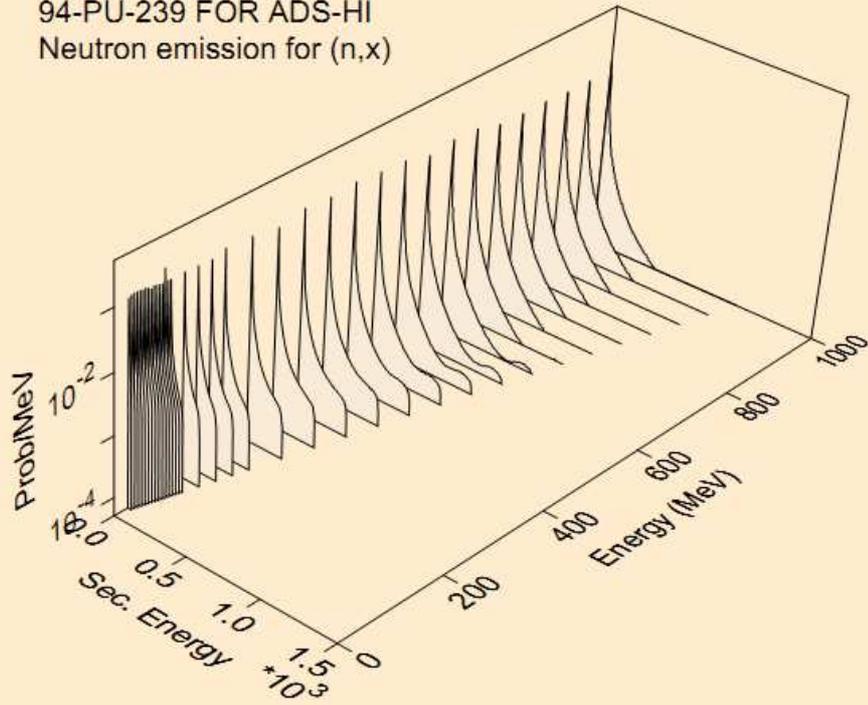
94-PU-239 FOR ADS-HI
angular distribution for elastic



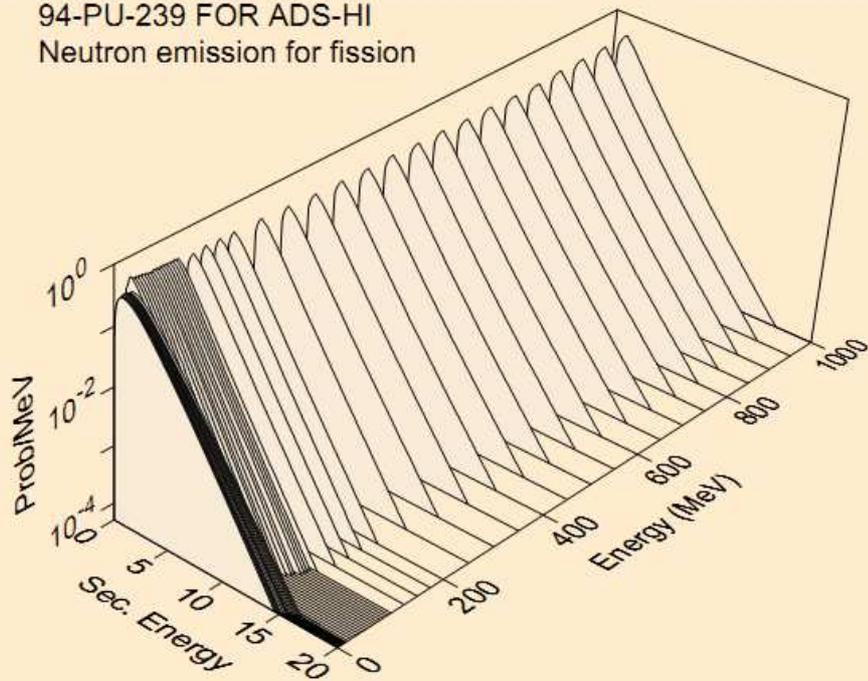
94-PU-239 FOR ADS-HI
angular distribution for elastic

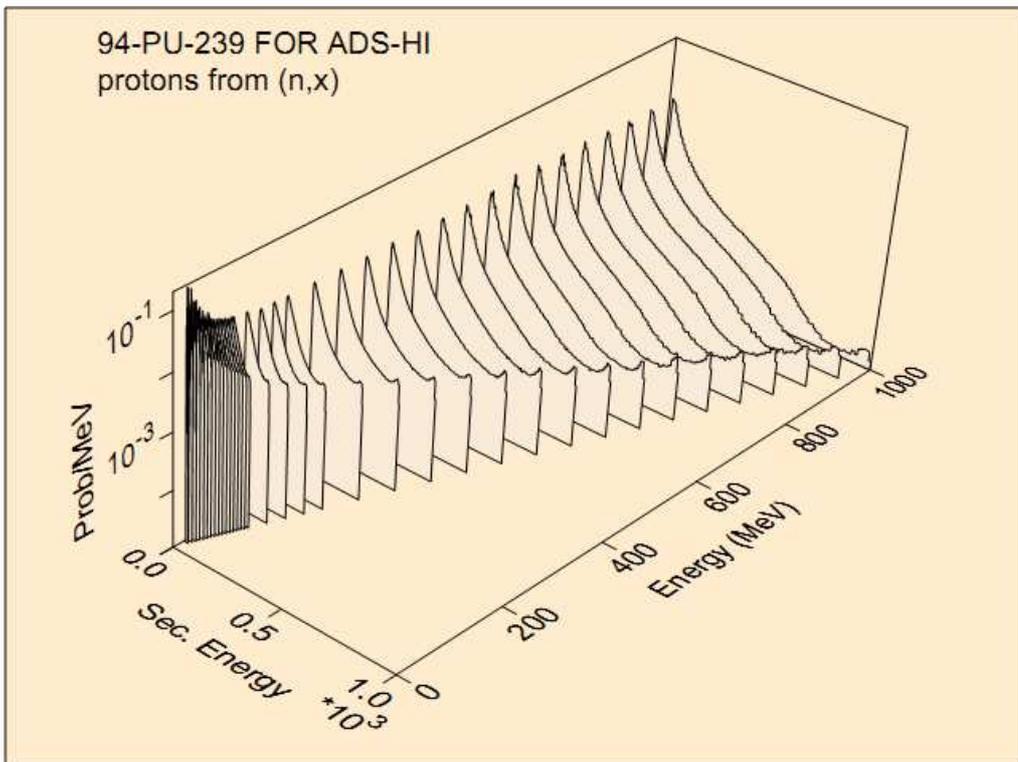
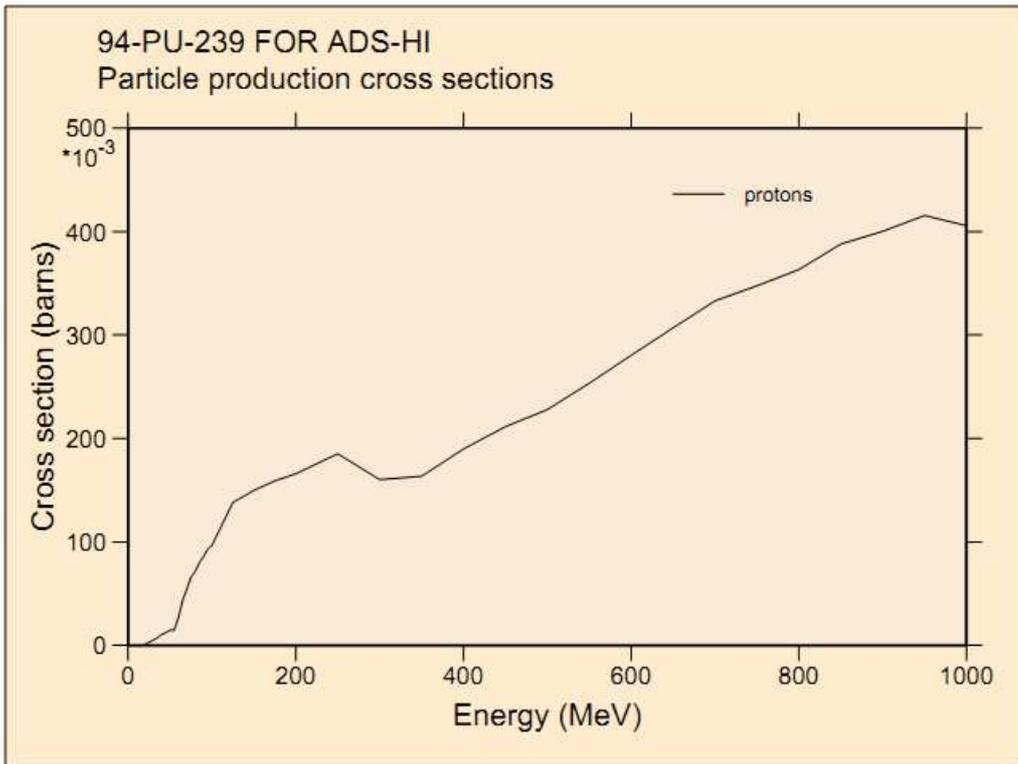


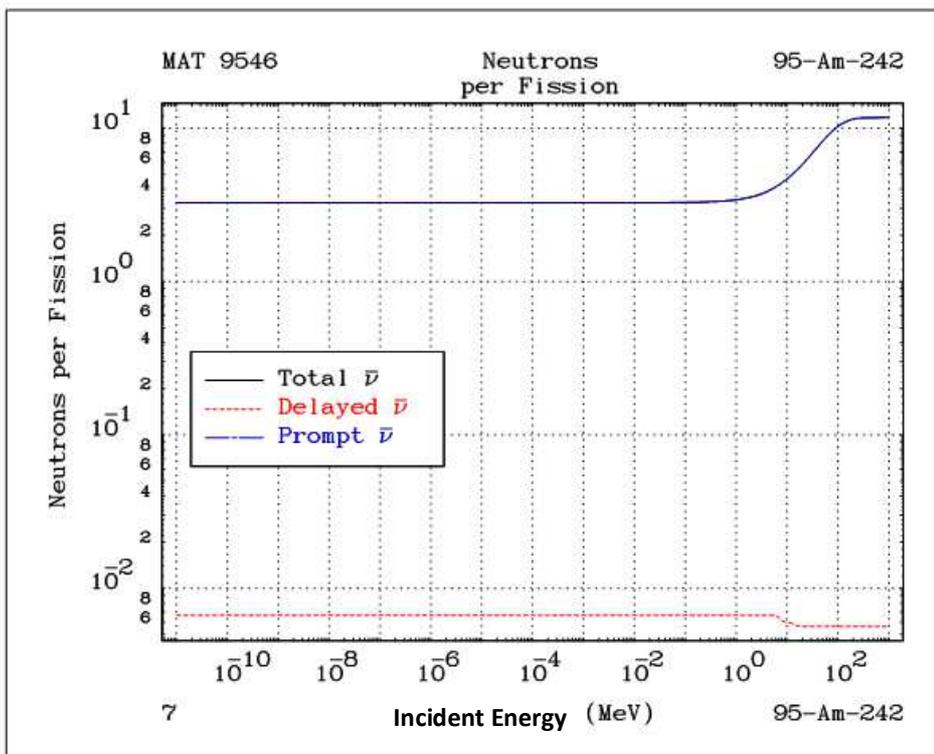
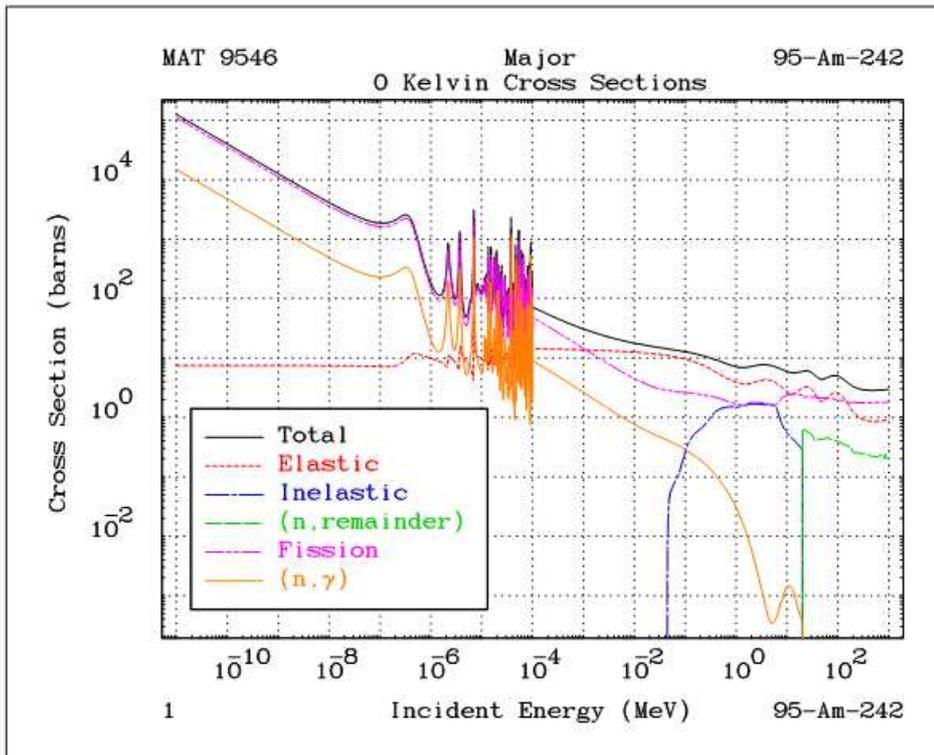
94-PU-239 FOR ADS-HI
Neutron emission for (n,x)



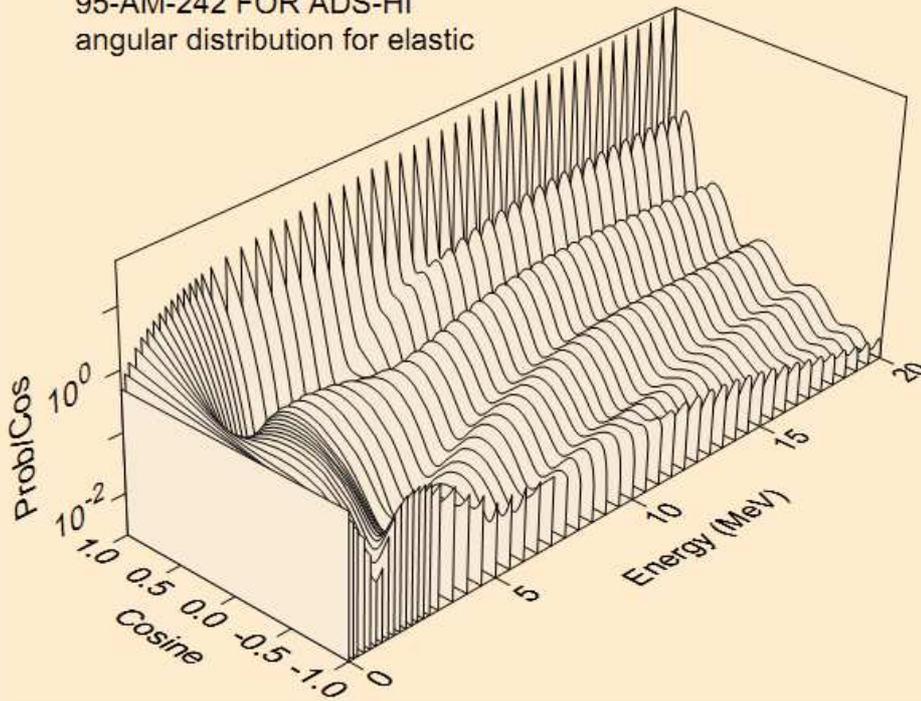
94-PU-239 FOR ADS-HI
Neutron emission for fission



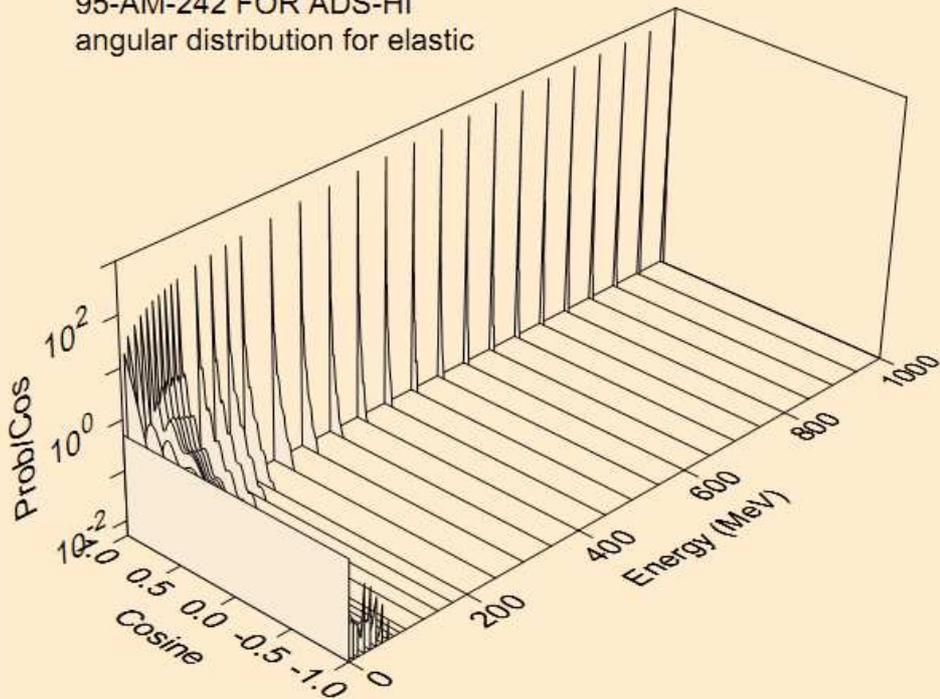




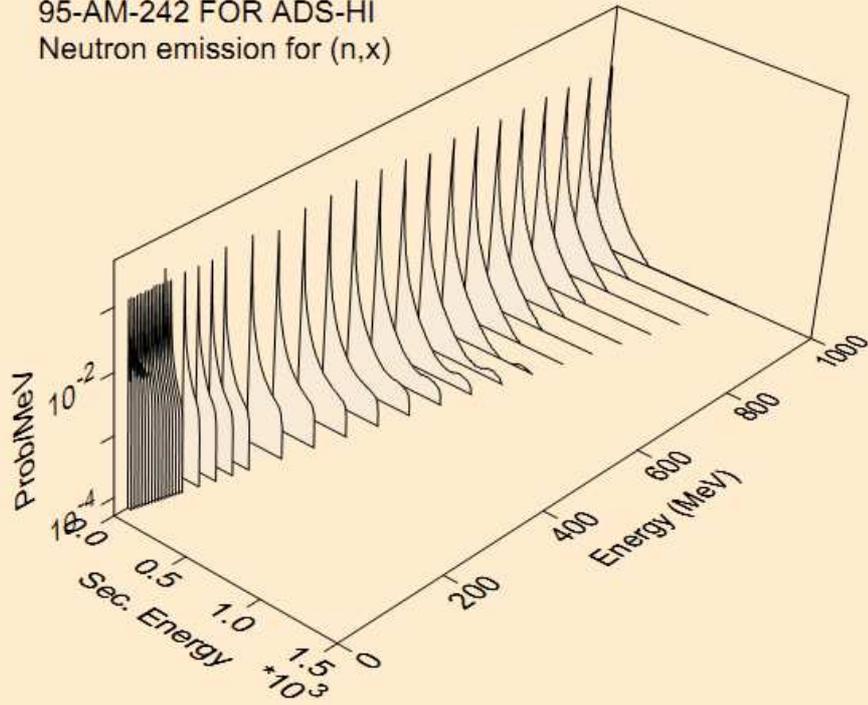
95-AM-242 FOR ADS-HI
angular distribution for elastic



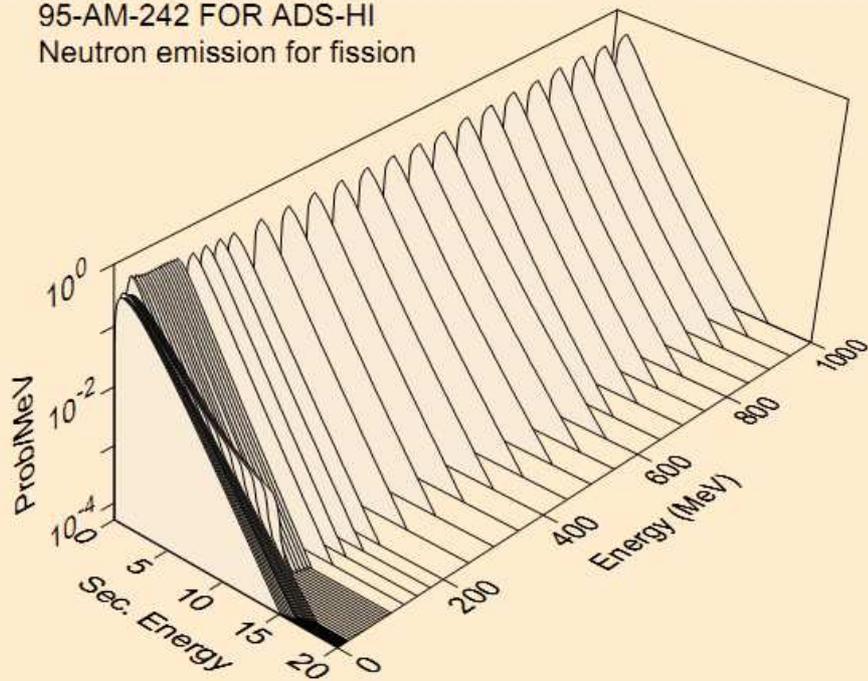
95-AM-242 FOR ADS-HI
angular distribution for elastic

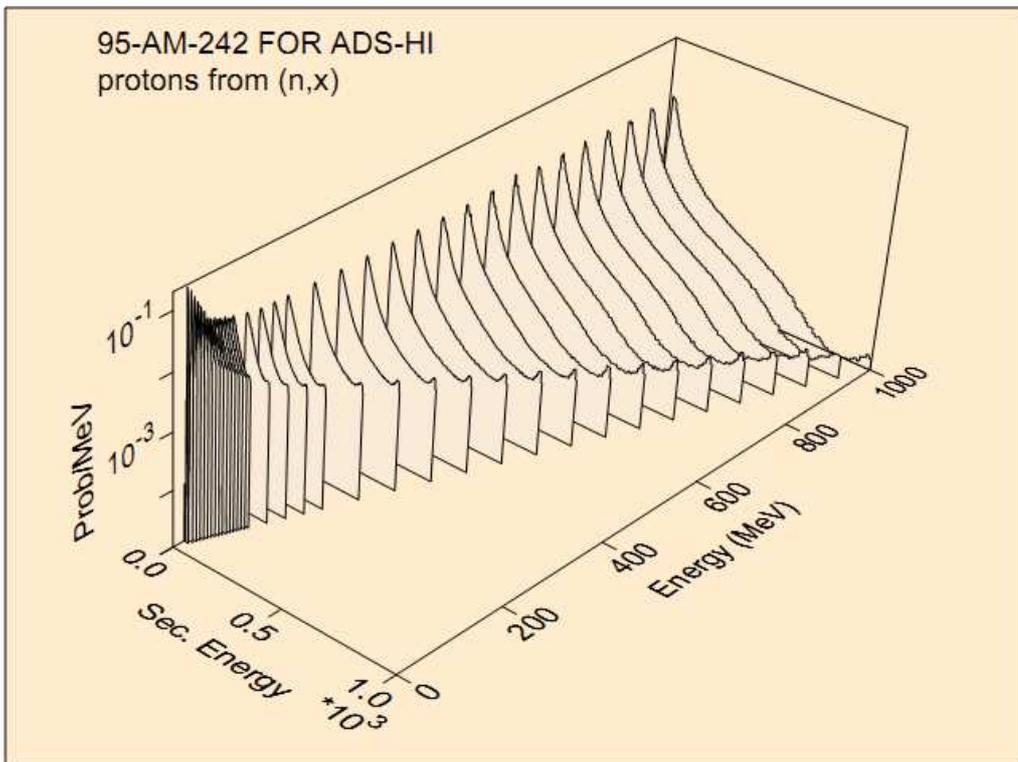
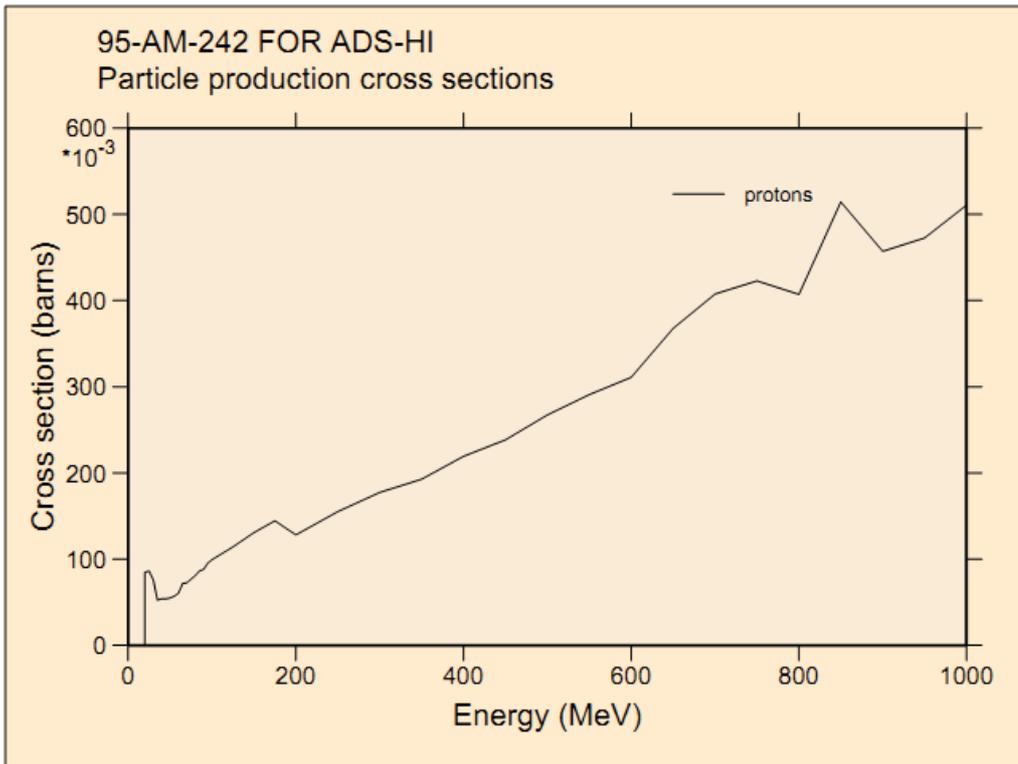


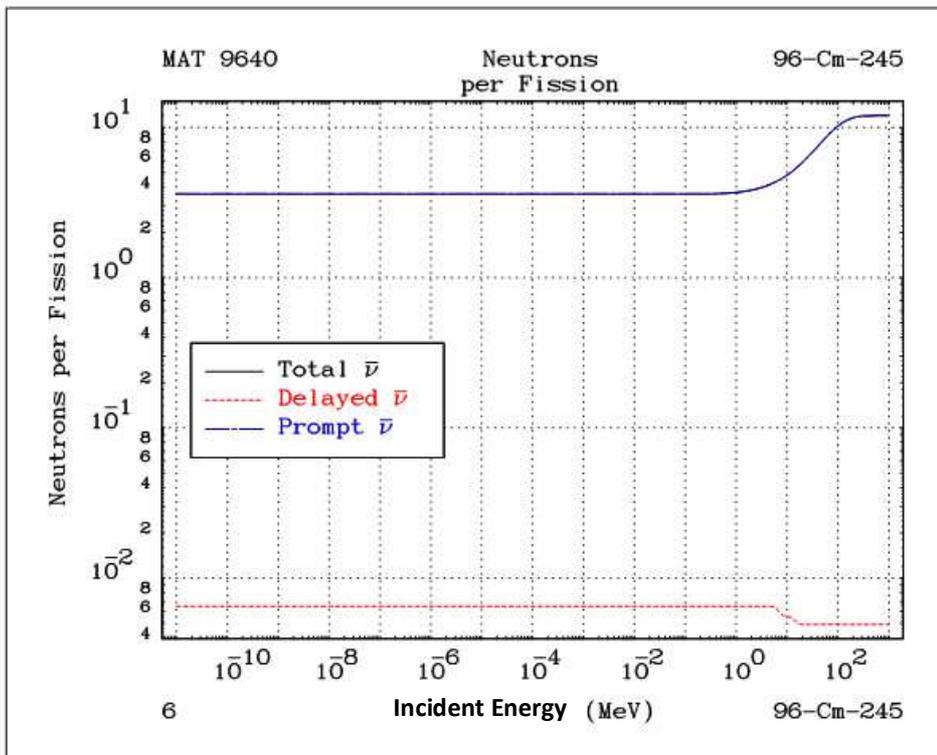
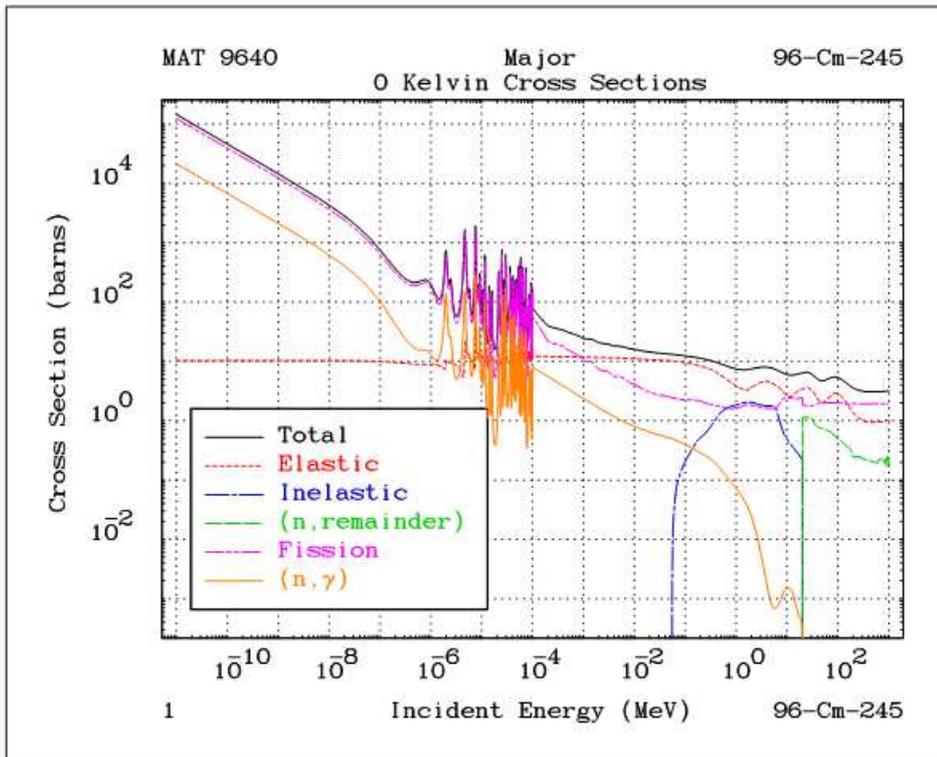
95-AM-242 FOR ADS-HI
Neutron emission for (n,x)



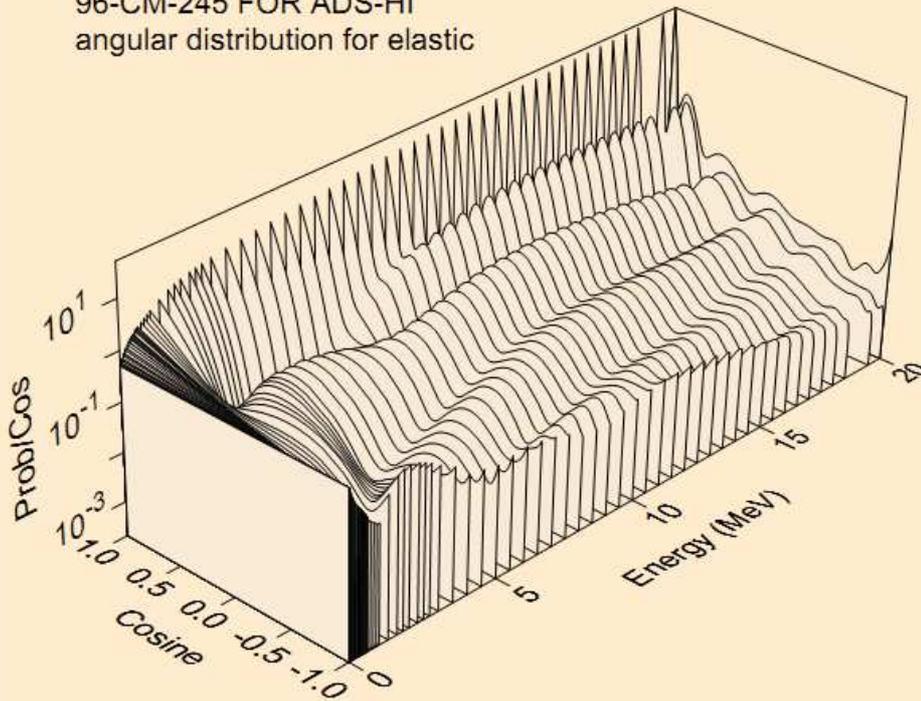
95-AM-242 FOR ADS-HI
Neutron emission for fission



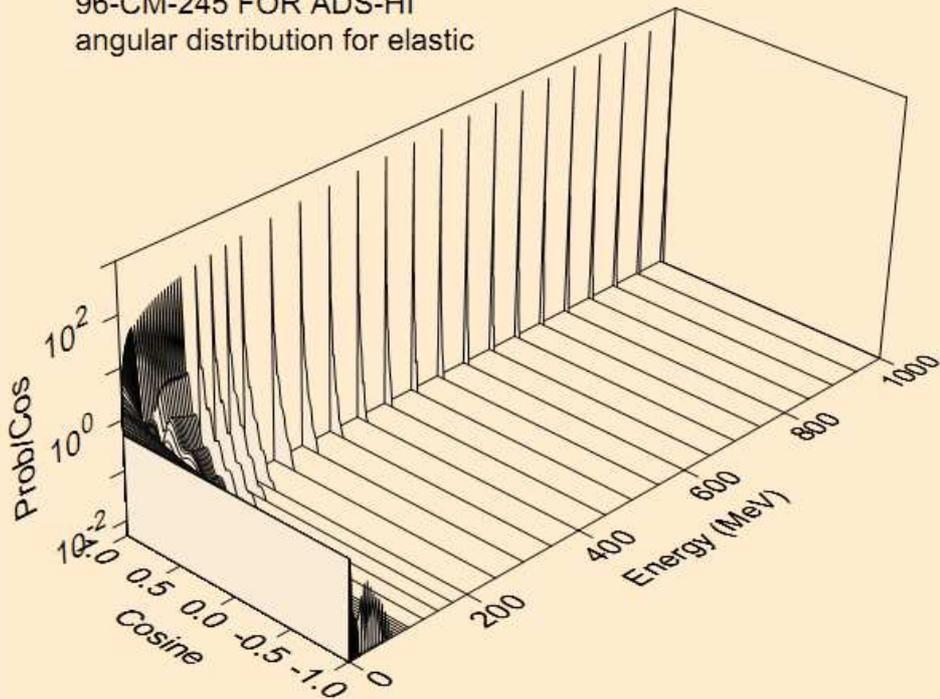




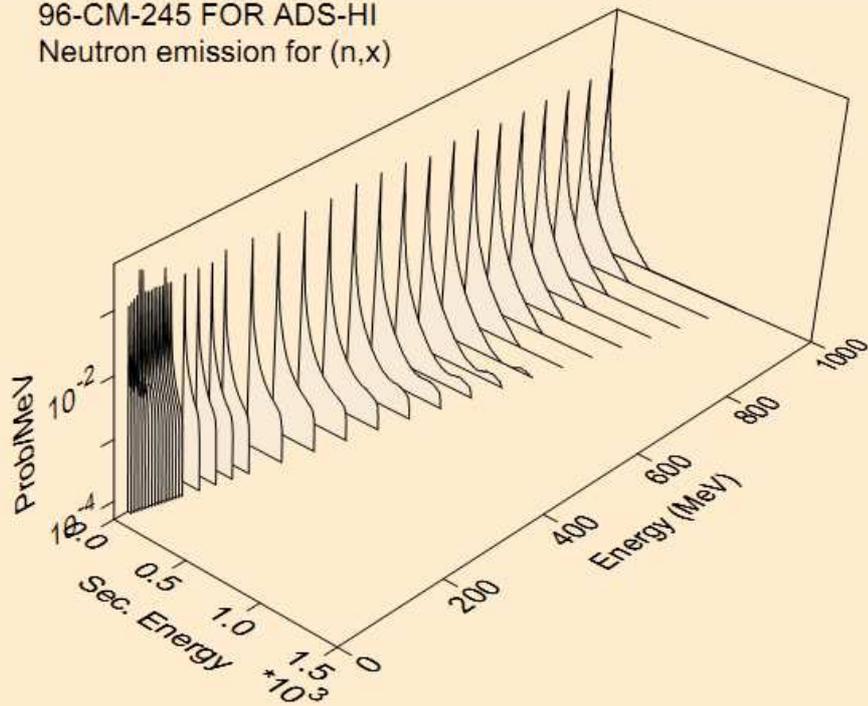
96-CM-245 FOR ADS-HI
angular distribution for elastic



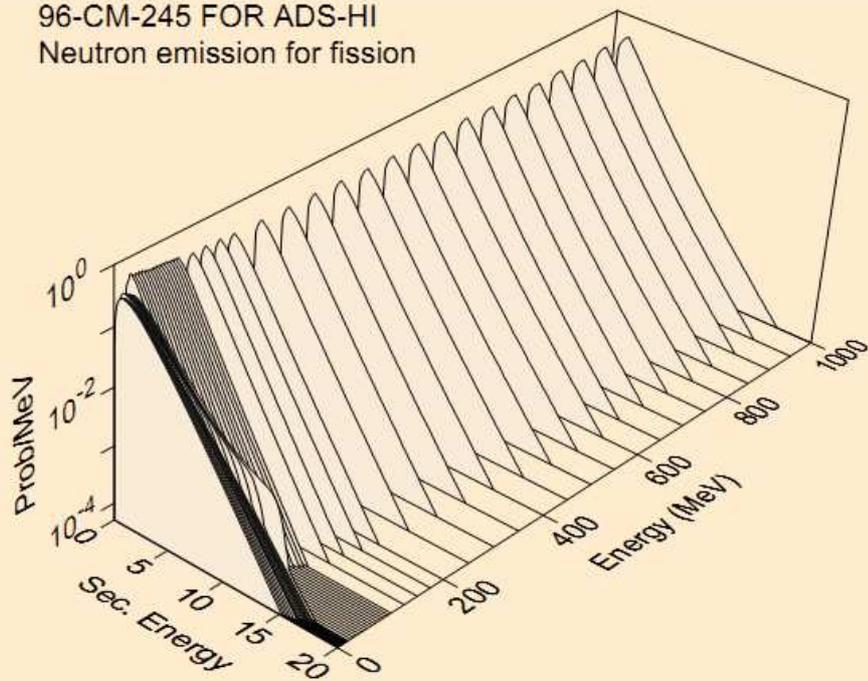
96-CM-245 FOR ADS-HI
angular distribution for elastic

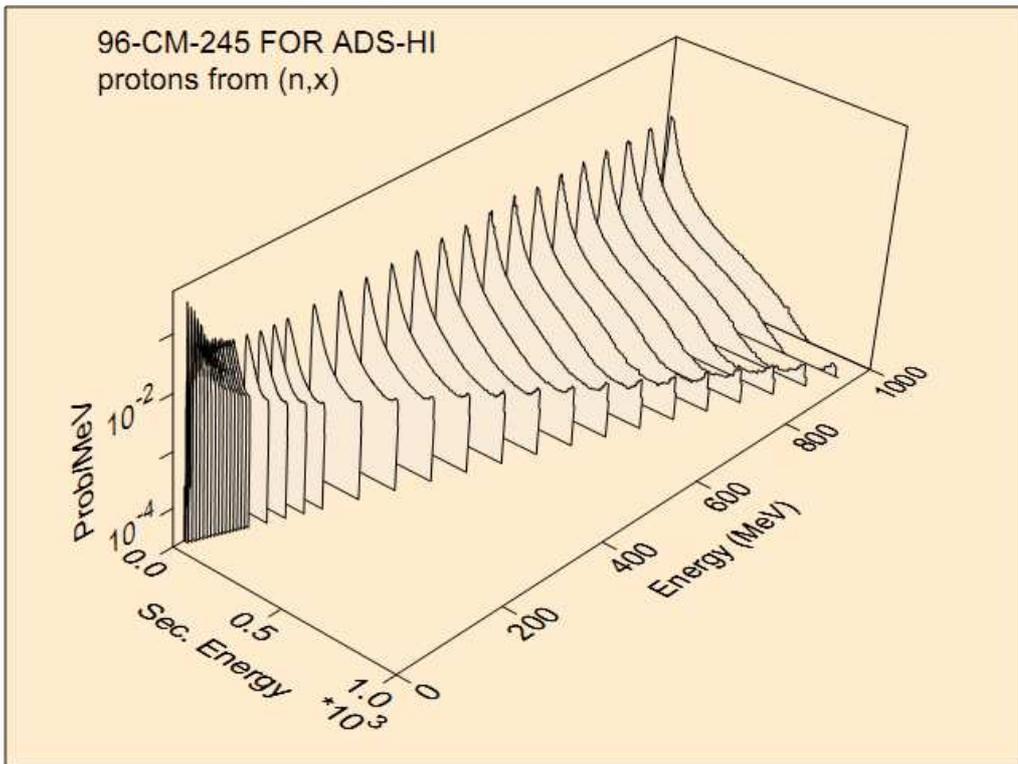
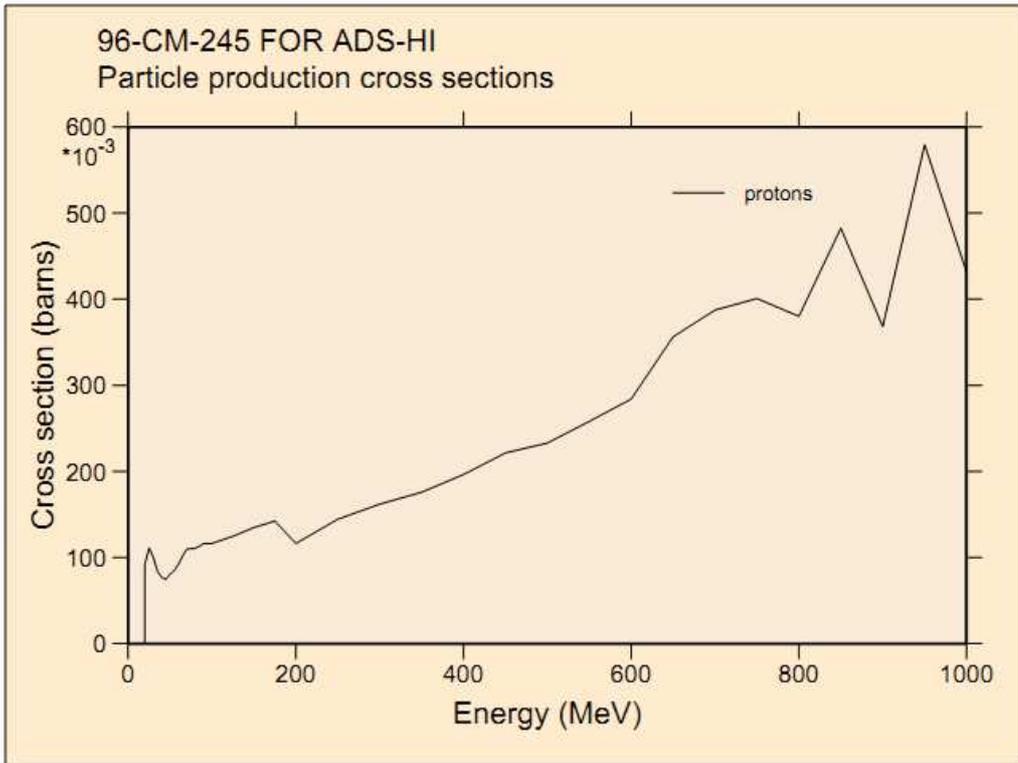


96-CM-245 FOR ADS-HI
Neutron emission for (n,x)



96-CM-245 FOR ADS-HI
Neutron emission for fission





Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: <http://www-nds.iaea.org>
