Integration of the International Standards Evaluation into a Global Data Assessment

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ABSTRACT

We review the methods employed in the GANDR system to perform a global assessment of nuclear data. We then describe the integration the International Evaluation of Neutron Cross Section Standards into a recently initiated global data assessment.

What is GANDR?

***The GANDR system is a suite of* Fortran programs** and associated **data libraries** that can be applied to a variety of tasks in the evaluation of neutron nuclear data. While the underlying statistical engine ZOTTVL is application independent, a number of features have been included in GANDR to support the Global Assessment of Nuclear Data.

What is a Global Assessment?

***This term refers to the simultaneous evaluation, or estimation, of the covariances of nuclear reaction data for many target nuclei (typically over 100), using methods that, while approximate, automatically enforce a* high level of nuclide-to-nuclide consistency**. In this talk, we shall describe an evaluation framework that is suitable for such a global assessment of nuclear data.

Application to Experiment Planning

Probably the most important application of the output covariances from a global data assessment is in the planning of nuclear data experiments. In this field, the two key questions are:

1. **"Are the present data adequate for my application?"**

A covariance library produced via a global data assessment could be used, together with conventional sensitivity analysis, to estimate the uncertainty, due to basic nuclear data, of important calculated quantities such as radiation dose, breeding ratio and critical mass.

2. **"If not, what measurements need to be performed?"**

The very same tools can be used to estimate the impact of a variety of potential future measurements in reducing the uncertainty of the calculations of interest.

The Master PENDF and EXFOR Libraries

A key component of the GANDR system is the Master PENDF Library. It con-tains pointwise data from ENDF/B-VII.0 for the following **130** materials, pre-pared with NJOY99.259. A second important file is the **Master EXFOR Library**, which contains cross sections retrieved from EXFOR for each of the listed materials and for natural elements containing the listed isotopes.

1-H - 1	1-H - 2	2-He- 3	2-He- 4	3-Li- 6	3-Li- 7
4-Be- 9	5-B - 10	5-B - 11	6-C -nat	7-N - 14	7-N - 15
8-O - 16	9-F - 19	11-Na- 23	12-Mg-nat	13-Al- 27	14-Si- 28
14-Si- 29	14-Si- 30	15-P - 31	16-S -nat	17-Cl-nat	18-Ar-nat
19-K -nat	20-Ca-nat	21-Sc- 45	22-Ti-nat	23-V -nat	24-Cr- 50
24-Cr- 52	24-Cr- 53	24-Cr- 54	25-Mn- 55	26-Fe- 54	26-Fe- 56
26-Fe- 57	26-Fe- 58	27-Co- 59	28-Ni- 58	28-Ni- 60	28-Ni- 61
28-Ni- 62	29-Cu- 63	29-Cu- 65	30-Zn-nat	31-Ga-nat	33-As- 75
39-Y - 89	41-Nb- 93	53-I -127	55-Cs-133	73-Ta-nat	74-W -182
74-W -183	74-W -184	74-W -186	75-Re-nat	79-Au-197	80-Hg-nat
81-Tl-nat	82-Pb-206	82-Pb-207	82-Pb-208	83-Bi-209	90-Th-229
90-Th-230	90-Th-232	91-Pa-231	91-Pa-233	92-U -232	92-U -233
92-U -234	92-U -235	92-U -236	92-U -237	92-U -238	93-Np-236
93-Np-237	93-Np-238	93-Np-239	94-Pu-236	94-Pu-238	94-Pu-239
94-Pu-240	94-Pu-241	94-Pu-242	94-Pu-244	95-Am-241	95-Am-42G
95-Am-42M	95-Am-243	96-Cm-242	96-Cm-243	96-Cm-244	96-Cm-245
96-Cm-246	96-Cm-247	96-Cm-248	97-Bk-249	98-Cf-250	98-Cf-251
98-Cf-252					

The 25 GANDR Reactions for Non-Actinides*

(a) ENDF mt=2, elastic scattering

(a1-a3) first three Legendre moments of (a)

(b) ENDF mt=5, high energy reactions

(b1-b6) six tables of secondary particle data (not yet defined) for (b)

(c) all processes other than (b) yielding exactly 2 neutrons

(d) all processes other than (b) yielding exactly 3 neutrons

(e) all processes other than (b) yielding 4 or more neutrons

(f) ENDF mt=51, inelastic scattering to first level

(f1) first Legendre moment of (f)

(g) all other processes yielding exactly one neutron, with a threshold below 1 MeV

(g1) first Legendre moment of (g)

(h) all other processes yielding exactly one neutron, with a threshold of 1 - 6 MeV

(h1) first Legendre moment of (h)

(i) all other processes yielding exactly one neutron, with a threshold above 6 MeV

(j) ENDF mt=102, radiative capture

(k) ENDF mt=103, (n,p)

(l) ENDF mt=107, (n,alpha)

(m) all other neutron absorption

***For actinides, reaction (k) is fission, (l) is nu-bar**, and (m) is all other neutron

GANDR Energy Grid

Index	Δu	u (lethargy)	Energy (eV)
1	---	12.00000	1.00000E-05
2	0.50000	11.50000	3.16228E-05
3	0.50000	11.00000	1.00000E-04
4	0.50000	10.50000	3.16228E-04
5	0.50000	10.00000	1.00000E-03
6	0.25000	9.75000	1.77828E-03
7	0.25000	9.50000	3.16228E-03
8	0.25000	9.25000	5.62341E-03
9	0.25000	9.00000	1.00000E-02
10	0.20000	8.80000	1.58489E-02
11	0.20312	8.59688	2.53000E-02
12	0.14688	8.45000	3.54813E-02
13	0.15000	8.30000	5.01187E-02
14	0.15000	8.15000	7.07946E-02
15	0.15000	8.00000	1.00000E-01
16	0.25000	7.75000	1.77828E-01
17	0.25000	7.50000	3.16228E-01
18	0.25000	7.25000	5.62341E-01
19	0.25000	7.00000	1.00000E+00
20	0.25000	6.75000	1.77828E+00
21	0.25000	6.50000	3.16228E+00
22	0.25000	6.25000	5.62341E+00
23	0.25000	6.00000	1.00000E+01
24	0.25000	5.75000	1.77828E+01
25	0.25000	5.50000	3.16228E+01

GANDR Energy Grid (cont.)

Index	Δu	u (lethargy)	Energy (eV)
26	0.25000	5.25000	5.62341E+01
27	0.25000	5.00000	1.00000E+02
28	0.20000	4.80000	1.58489E+02
29	0.20000	4.60000	2.51189E+02
30	0.20000	4.40000	3.98107E+02
31	0.20000	4.20000	6.30957E+02
32	0.20000	4.00000	1.00000E+03
33	0.20000	3.80000	1.58489E+03
34	0.20000	3.60000	2.51189E+03
35	0.20000	3.40000	3.98107E+03
36	0.20000	3.20000	6.30957E+03
37	0.20000	3.00000	1.00000E+04
38	0.20000	2.80000	1.58489E+04
39	0.20000	2.60000	2.51189E+04
40	0.20000	2.40000	3.98107E+04
41	0.20000	2.20000	6.30957E+04
42	0.20000	2.00000	1.00000E+05
43	0.10000	1.90000	1.25893E+05
44	0.10000	1.80000	1.58489E+05
45	0.10000	1.70000	1.99526E+05
46	0.10000	1.60000	2.51189E+05
47	0.10000	1.50000	3.16228E+05
48	0.10000	1.40000	3.98107E+05
49	0.10000	1.30000	5.01187E+05
50	0.10000	1.20000	6.30957E+05

GANDR Energy Grid (cont.)

Index	Δu	u (lethargy)	Energy (eV)
51	0.10000	1.10000	7.94328E+05
52	0.10000	1.00000	1.00000E+06
53	0.10000	0.90000	1.25893E+06
54	0.10000	0.80000	1.58489E+06
55	0.10000	0.70000	1.99526E+06
56	0.10000	0.60000	2.51189E+06
57	0.10000	0.50000	3.16228E+06
58	0.10000	0.40000	3.98107E+06
59	0.10000	0.30000	5.01187E+06
60	0.10000	0.20000	6.30957E+06
61	0.10000	0.10000	7.94328E+06
62	0.10000	0.00000	1.00000E+07
63	0.10000	-0.10000	1.25893E+07
64	0.10000	-0.20000	1.58489E+07
65	0.10000	-0.30000	1.99526E+07
66	0.10000	-0.40000	2.51189E+07
67	0.10000	-0.50000	3.16228E+07
68	0.10000	-0.60000	3.98107E+07
69	0.10000	-0.70000	5.01187E+07
70	0.10000	-0.80000	6.30957E+07
71	0.10000	-0.90000	7.94328E+07
72	0.10000	-1.00000	1.00000E+08
73	0.10000	-1.10000	1.25893E+08
74	0.07609	-1.17609	1.50000E+08

The GANDR Driver Module: GAPREP

The operation of the GANDR suite of Fortran programs is best illustrated by discussing a simple example. The procedure for performing a GANDR evaluation update normally begins with the user creating a short script, such as that below. For more complex tasks, scripts like this can be "stacked" together.

```
echo yes > permit
grep 74184 /usr/gandr/zott/names > names
gaprep.x << EOF
 0 1 2 0/ inopt,ipick,idef,iprint
 0 0 0/ igrid,ipend,imoc
 1/ retrieve the data for mt=1 from Master EXFOR Library
 1/ select exfor data from knopf (set 1)
 0 0 0/ no exfor covariance modifications
EOF
chmod u+x ganrun
ganrun
```

Line 1 grants execute permission to all modules of the GANDR system. **Line 2** identifies the material of interest as ^{184}W. **Line 3** launches the important **GAPREP** code. In addition to performing a number of parameter and covariance initialization operations, GAPREP also produces a complete set of input data for the **ZOTTVL** code for the experimental data selected from EXFOR (the Knopf measurement of the total cross section), and it produces the GANDR controller script, GANRUN.

The **last line** launches the script GANRUN.

Input to ZOTTVL Code

Below is the ZOTTVL input file generated by GAPREP for this simple example.

```
   4   674     1     0     1    9999   1.0000E+08/
# ZOTTVL input for GANDR system
-5.01187E+00 2.87408E+00 2.69547E+00 -4.95456E-01
74184
         3*0.0000000E+00           3.0304156E+00           1.7884542E+00
       572*0.0000000E+00           7.3533129E+00           4.3396899E+00
        95*0.0000000E+00
*****
74184
        18*0.0000000E+00           2.8371318E+00           1.4232752E+00
       572*0.0000000E+00           1.5017328E-01           7.5335913E-02
        80*0.0000000E+00
*****
74184
        20*0.0000000E+00           7.3831820E-01           3.4542191E+00
       572*0.0000000E+00           1.6199324E-02           7.5788479E-02
        78*0.0000000E+00
*****
74184
        42*0.0000000E+00           4.0021895E+00           4.4202905E+00
       350*0.0000000E+00           8.6624958E-02           9.5674502E-02
       220*0.0000000E+00           4.3087634E-02           4.7588916E-02
        56*0.0000000E+00
*****
# Covariance matrix for GANDR evaluation update
 1     4 /
 6.40000E-01 /
 9.00000E-02 /
 4.00000E-02 /
 2.50000E-01 /
```

The GANRUN Controller Script

At the heart of the operation of the GANDR system is the GANRUN controller script generated automatically by GAPREP. GANRUN first invokes the least squares solver **ZOTTVL**, then invokes the **GAPOST** module to read the ZOTTVL output and prepare listings and plotting instructions, and then invokes the NJOY **PLOTR** module to prepare high quality PostScript plots. In each case the module reads "user input" and data files prepared by earlier modules. The script finally organizes the output files into standard directories.

```
zottvl.x2 < zottvl.in
mv zottvl.out.* zottvl.out
gapost.x
xnjoy < plotr.in
mv tape32 gapost.ps
mkdir -p      0120.000
mv ganrun      0120.000
mv gaprep.out      0120.000
mv zottvl.in      0120.000
mv zottvl.out      0120.000
mv gapost.out      0120.000
cp /usr/gandr/zott/list/74184      0120.000/list
mv tape50      0120.000
mv tape51      0120.000
mv plotr.in      0120.000
mv output      0120.000
cp gapost.ps      0120.000
```

GANDR Documentation

To provide a detailed description of the GANDR project and the associated software and hardware, we have produced a six-volume set of reports in Word format. These cover a wide range of topics ranging from theoretical and programming aspects to user input instructions and sample problems. We list below the topics that are covered in the reports.

Volume 1. Project Overview

Volume 2. The ZOTTVL Program

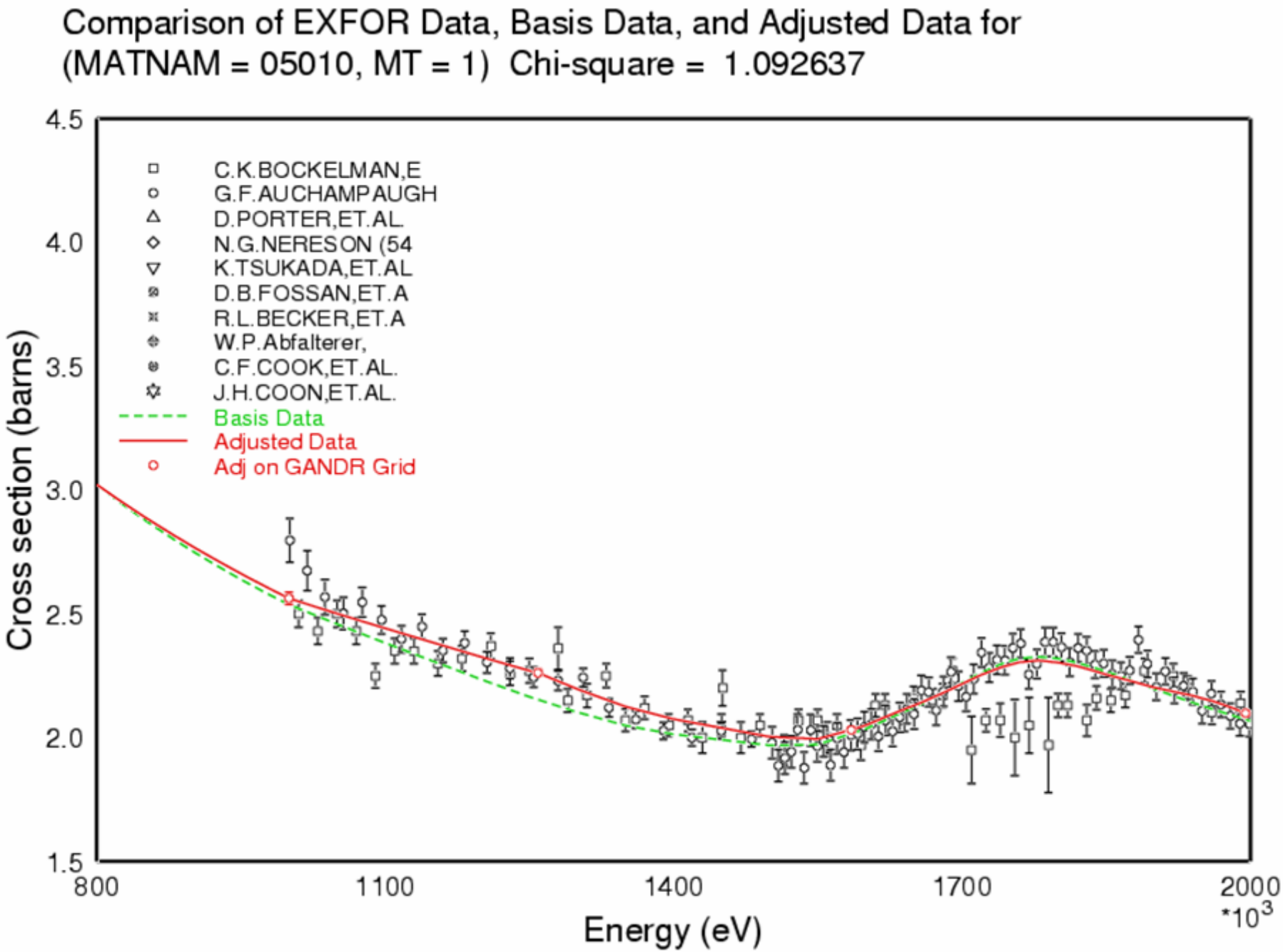
Volume 3. Auxiliary Programs GAPREP, GAPOST and GABROW

Volume 4. User Input Instructions and Five Sample Problems Based on EXFOR Data

Volume 5. Preparation of the EXFOR Master Library for the GANDR Project

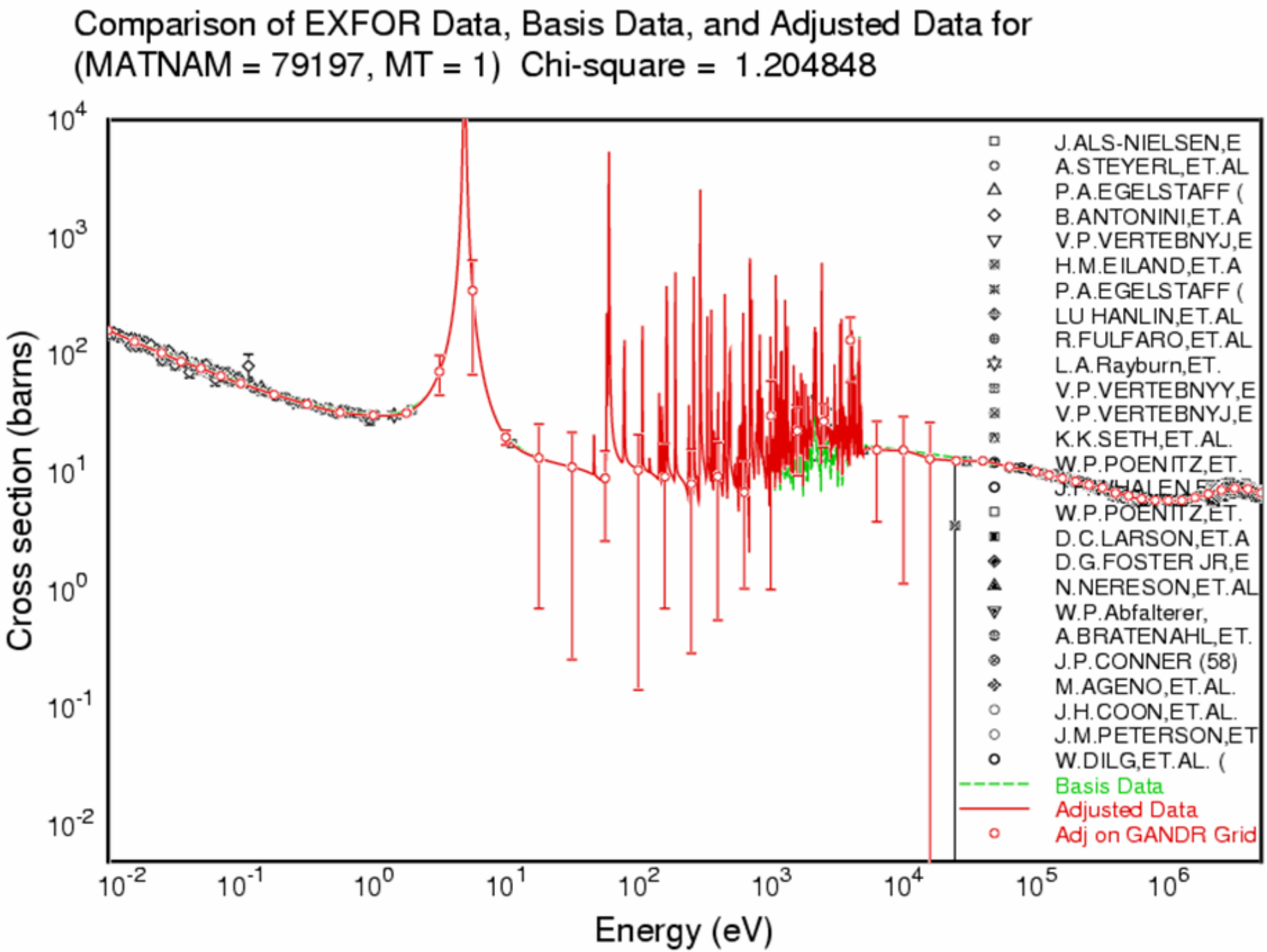
Volume 6. Multigroup Sensitivities

These six reports are available, along with much additional information, online at **www-nds.iaea.org/gandr**.


Comparison of EXFOR Data, Basis Data, and Adjusted Data for
(MATNAM = 05010, MT = 1) Chi-square = 1.092637
C.K.BOCKELMAN,E
G.F.AUCHAMPAUGH
D.PORTER,ET.AL.
N.G.NERESON (54
K.TSUKADA,ET.AL
D.B.FOSSAN,ET.A
R.L.BECKER,ET.A
W.P.Abfalterer,
C.F.COOK,ET.AL.
J.H.COON,ET.AL.
Basis Data
Adjusted Data
Adj on GANDR Grid
Cross section (barns)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
800
1100
1400
1700
2000
*10^3
Energy (eV)

Response of All ^{10}B Partials at 1.995 MeV to Measured Total Cross Sections from EXFOR

Reaction type	Parameter index/value	Orig. σ (b)	Final σ (b)	Change (b)
elastic	**46 1.16051**	**1.46135**	**1.69591**	**0.23456**
1st level	266 2.63499	0.07305	0.19249	**0.11944**
(n,p)	**478 1.12524**	**0.01390**	**0.01564**	**0.00174**
(n,α0)	543 0.19540	0.34804	0.06801	**-0.28003**
(n,α1)	608 0.63674	0.11408	0.07264	**-0.04144**
(n,t2α)	673 0.86273	0.06273	0.05411	-0.00861
Total		**2.07315**	**2.09880**	**0.02566**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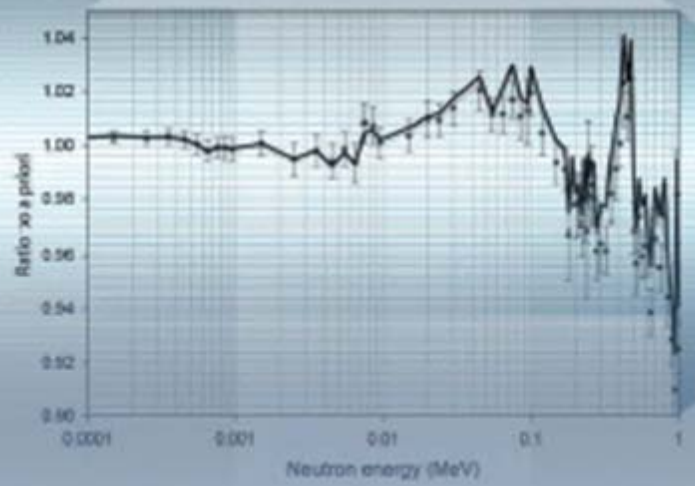
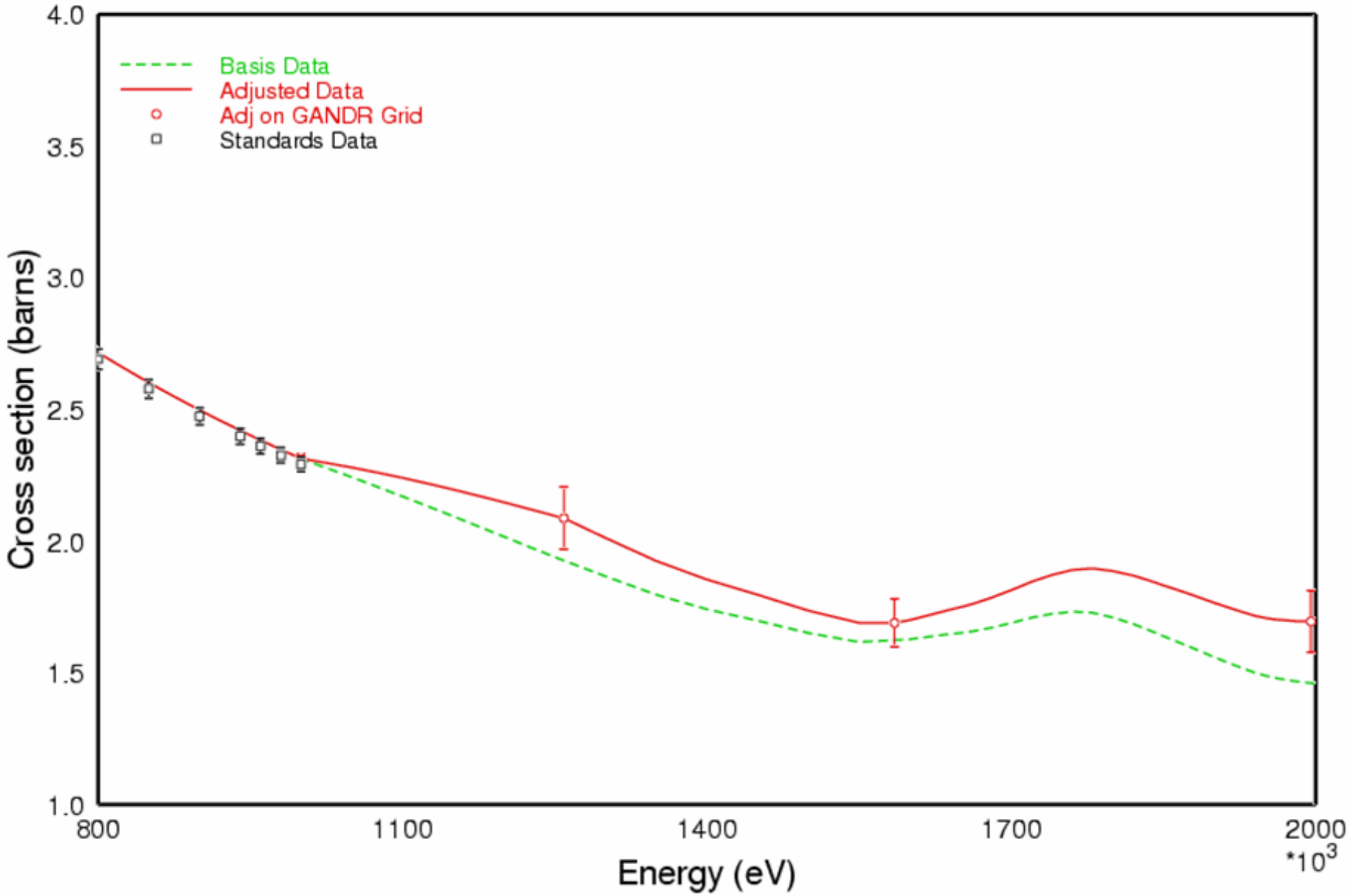
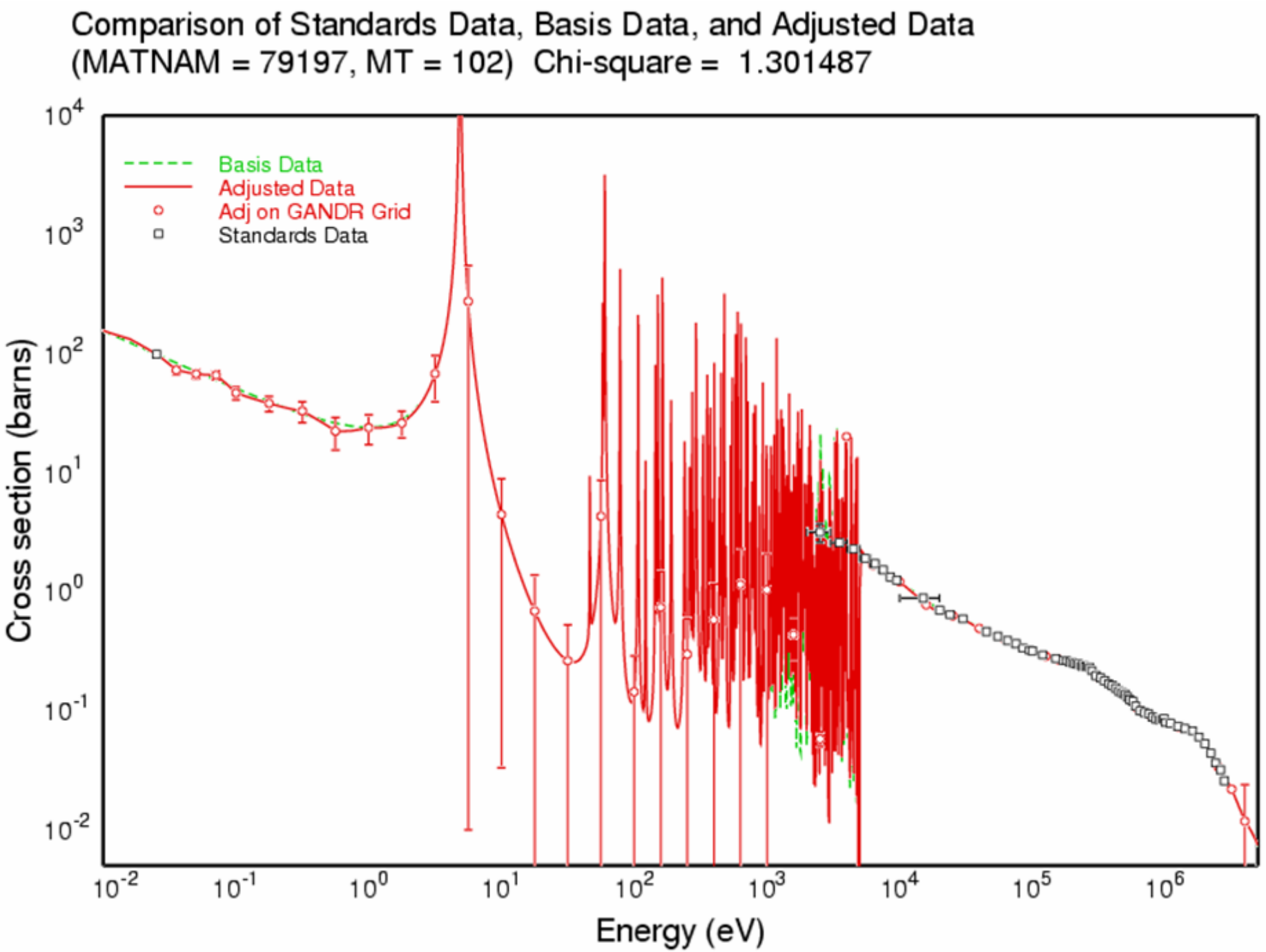
(MATNAM = 79197, MT = 1) Chi-square = 1.204848
Cross section (barns)
Energy (eV)
J.ALS-NIELSEN,E
A.STEYERL,ET.AL
P.A.EGELSTAFF (
B.ANTONINI,ET.A
V.P.VERTEBNYJ,E
H.M.EILAND,ET.A
P.A.EGELSTAFF (
LU HANLIN,ET.AL
R.FULFARO,ET.AL
L.A.Rayburn,ET.
V.P.VERTEBNYY,E
V.P.VERTEBNYJ,E
K.K.SETH,ET.AL.
W.P.POENITZ,ET.
W.P.POENITZ,ET.
D.C.LARSON,ET.A
D.G.FOSTER JR,E
N.NERESON,ET.AL
W.P.Abfalterer,
A.BRATENAHL,ET.
J.P.CONNER (58)
M.AGENO,ET.AL.
J.H.COON,ET.AL.
J.M.PETERSON,ET
W.DILG,ET.AL. (
Basis Data
Adjusted Data
Adj on GANDR Grid

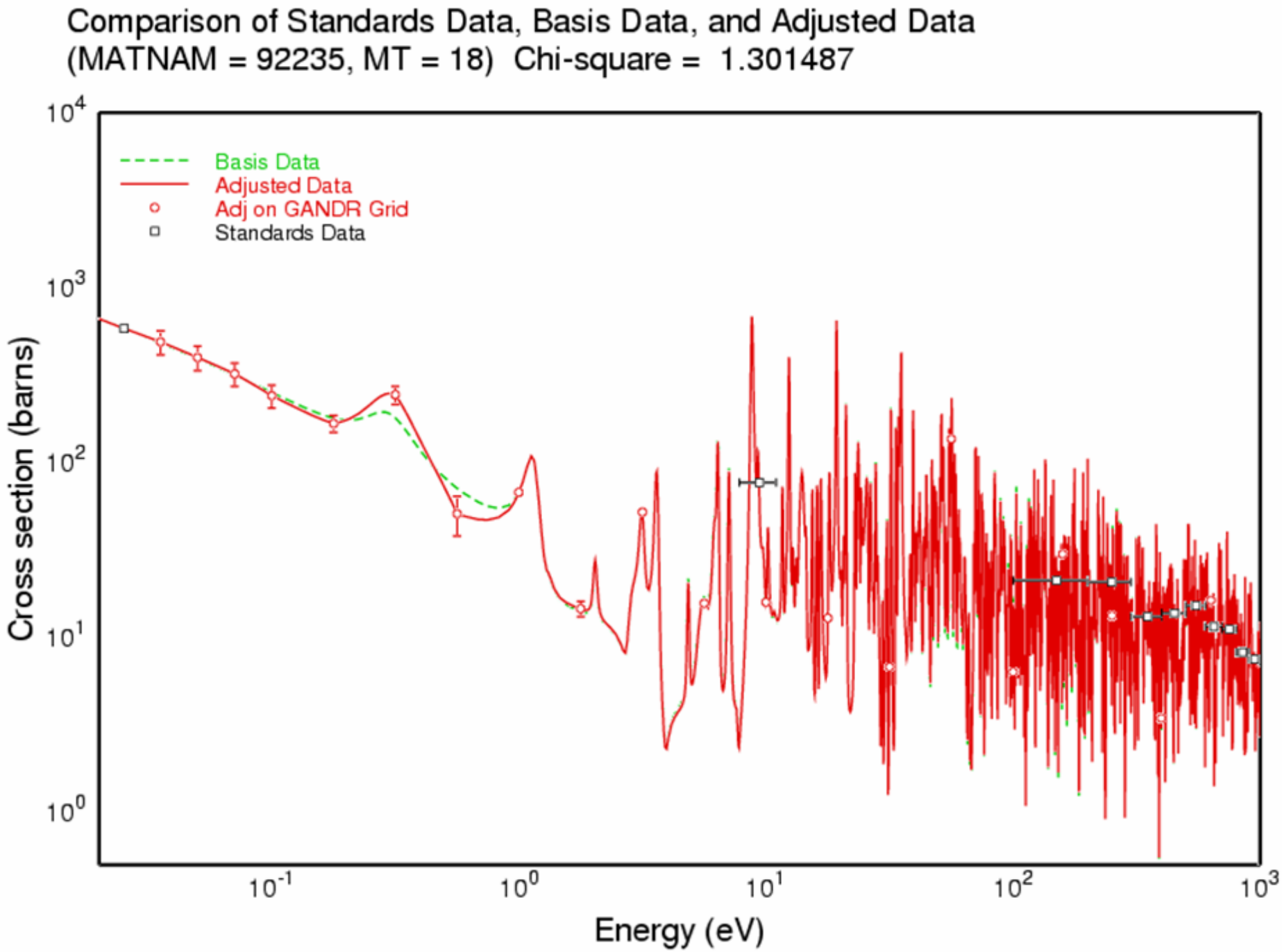
International Evaluation of Neutron Cross-Section Standards



IAEA
International Atomic Energy Agency


Comparison of Standards Data, Basis Data, and Adjusted Data
(MATNAM = 05010, MT = 2) Chi-square = 1.301487
Basis Data
Adjusted Data
Adj on GANDR Grid
Standards Data
Cross section (barns)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
800
1100
1400
1700
2000
Energy (eV)
*10^3


Comparison of Standards Data, Basis Data, and Adjusted Data
(MATNAM = 79197, MT = 102) Chi-square = 1.301487
Basis Data
Adjusted Data
Adj on GANDR Grid
Standards Data
Cross section (barns)
Energy (eV)
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-2
10^-1
10^0
10^1
10^2
10^3
10^4
10^5
10^6


Comparison of Standards Data, Basis Data, and Adjusted Data
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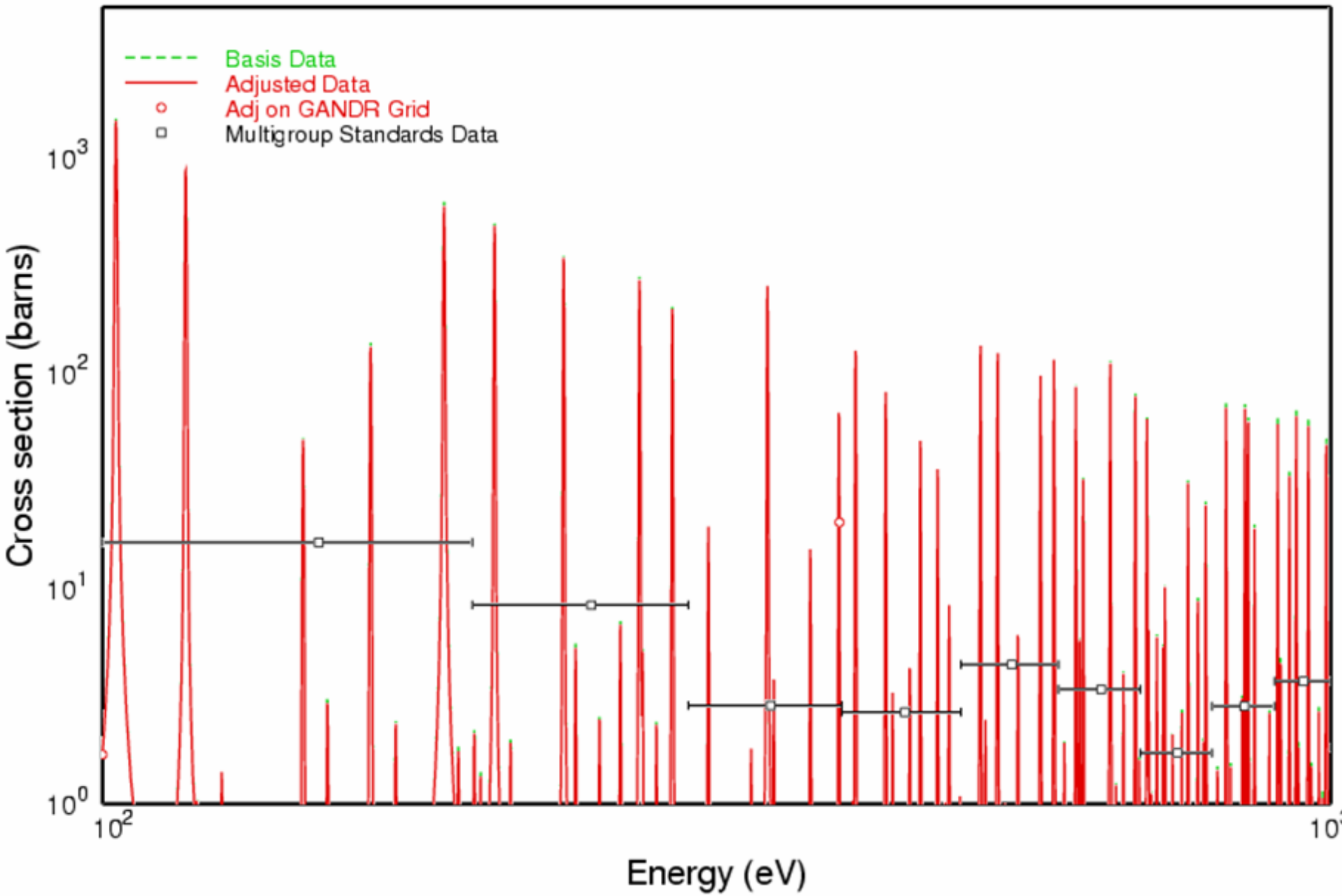
Basis Data
Adjusted Data
Adj on GANDR Grid
Standards Data
Cross section (barns)
Energy (eV)
10^4
10^3
10^2
10^1
10^0
10^-1
10^0
10^1
10^2
10^3


Comparison of Standards Data, Basis Data, and Adjusted Data
(MATNAM = 92238, MT = 102) Chi-square = 1.301487
Basis Data
Adjusted Data
Adj on GANDR Grid
Multigroup Standards Data
Cross section (barns)
10^3
10^2
10^1
10^0
10^2
10^3
Energy (eV)

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Global Assessment of Nuclear Data Requirements
The GANDR Project

An IAEA Nuclear Data Section Data Development Project

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Available files

- g3readme.txt 20 kB, 2008-04-28 21:21
- g3files.tar.gz 260 MB, 2008-04-20 00:42
- g3install.tar.gz 451 kB, 2008-04-28 21:22
- upn3.1 1 kB, 2008-06-13 13:16

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Response of ^{10}B Partials at 1.995 MeV to Measured Total Cross Sections from EXFOR

Reaction type	Parameter index	Parameter value	Original σ (b)	Final σ (b)	Change (b)
elastic	46	1.16051	1.46135	1.69591	0.23456
1st level	266	2.63499	0.07305	0.19249	0.11944
(n,p)	478	1.12524	0.01390	0.01564	0.00174
(n,α_0)	543	0.19540	0.34804	0.06801	−0.28003
(n,α_1)	608	0.63674	0.11408	0.07264	−0.04144
(n,t2α)	673	0.86273	0.06273	0.05411	−0.00861
Sums	---	---	2.07315	2.09880	0.02566