Iron

in fast neutron range
Forging CIELO evaluation plan

M. Herman , D. Brown, A. Trkov, ...

Tentative Evaluation Team

- **Leal** (ORNL) - resonances
- **Danon** (RPI), **Plompen** (IRM) - experiment guidance
- **Ahlassid** (Yale) - microscopic level densities
- **Capote** (IAEA) - soft-rotor CC potential
- N. **Iwamoto**, O. **Iwamoto** (JAEA) - ?
- **Brown**, **Hoblit**, **Herman** (BNL) - fast neutron calculations, covariances, consistent adjustment
- HI **Kim**, Young-Sik **Cho** (KAERI) - fast neutron calculations
- **Trkov** (IAEA) - file assembly, verification, validation
- **MacFarlane** (LANL), **Sublet** (UKAEA), **Palmiotti** (INL), **Salvatores** (CEA), **Aliberti** (ANL) - validation, adjustment
- **Koning** (NRG), **Goadage** - ?
- **Ruirui Xu** (CNDC) - ?
- **Pronyaev** (IPPE) - legacy consultation

TO BE COMPLETED!

Summary/comparison of evaluations

ENDF/B-VII.1

- 1991-1996-2000-2004-2011
- 1996: Chadwick, Young, Koning - 20<E<150 MeV extension
  - GNASH (OM+CC+HF +PE)
- 1991: Fu, Perey, Hetrick, Perey - basic file <20MeV
  - TNG code
  - isotopic with recoils
  - covariances MF=33,34

JEFF-3.1

- 2009-2001-2000-1998-1990
- 2009: Koning, Duijvestijn - 20<E<200 MeV extension
  - TALYS (OM+DWBA+HF +PE)
- 1998: major update below 20 MeV
  - High resolution Geel data for total and inelastic
  - MF=6 using EMPIRE's MSD/MSC
- Basic EFF-3.0
  - covariances MF=33,34
  - Elastic ang. distr. in URR

JENDL-4.0

- 1987...2010
- Iijma, Yamakoshi, Shibata, Igarasi <20 MeV
  - POD, OPTMAN, GNASH, CASTHY - CC +HF+PE
  - Geel high resolution data
  - covariances MF=33,34 obtained using Kalman

Summary/comparison of evaluations

ENDF/B-VII.1

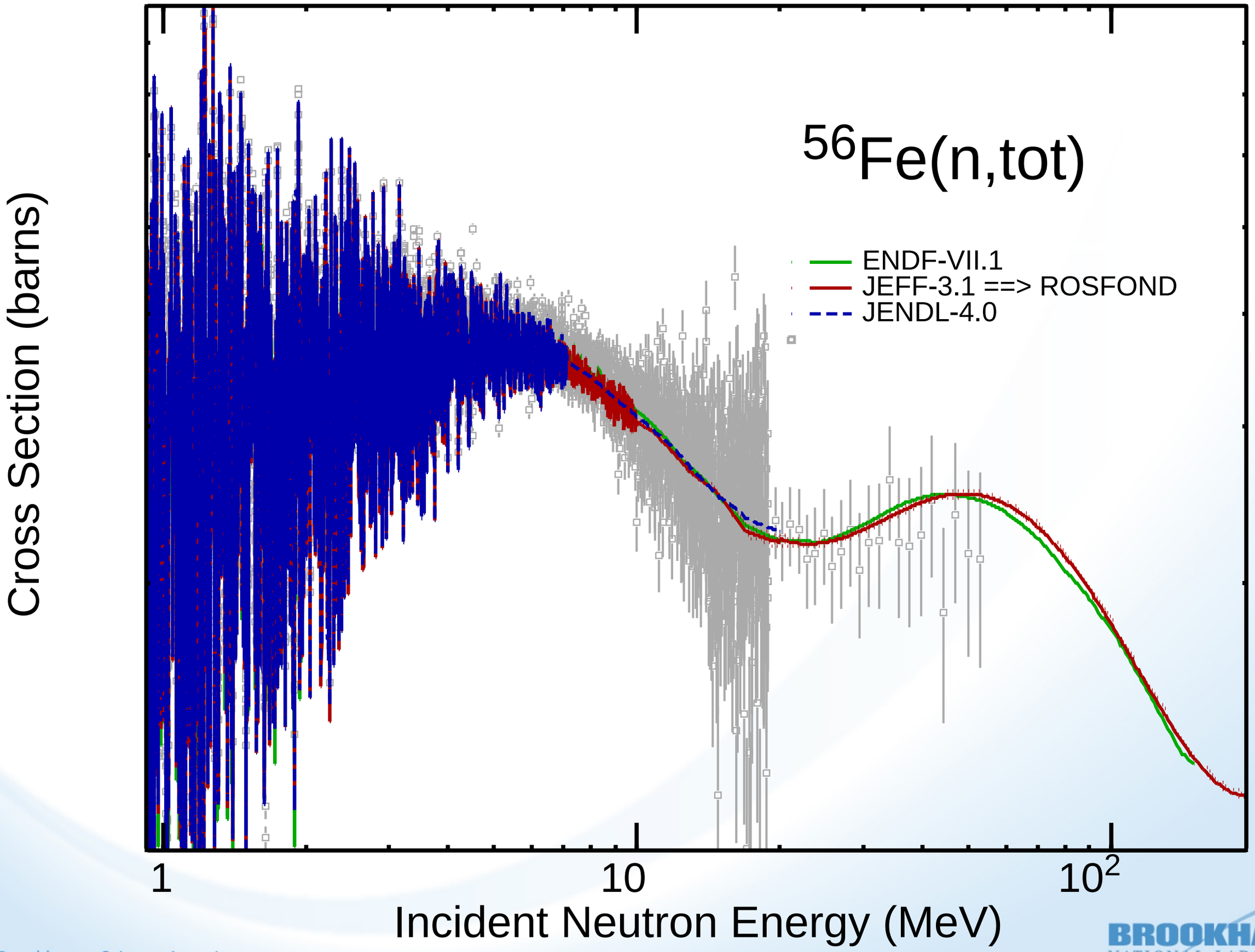
```
   MF=   1  2  3  4  6 12 14 15 33 34
 MT1  : __.__.__X__.__.__.__.__.__X__. (N,TOT)
 MT2  : __.__.__X__X__.__.__.__.__X__X (N,EL)-L0
 MT3  : __.__.__X__.__.__.__.__.__X__. (N,NON)
 MT4  : __.__.__X__.__.__.__.__.__X__. (N,INL)
 MT5  : __.__.__X__.__X__.__.__.__.__. (N,X)
 MT16 : __.__.__X__.__X__.__.__.__X__. (N,2N)
 MT22 : __.__.__X__.__X__.__.__.__X__. (N,N+A)
 MT28 : __.__.__X__.__X__.__.__.__X__. (N,N+P)
 MT51 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L1
 MT52 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L2
...
 MT75 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L25
 MT91 : __.__.__X__.__X__.__.__.__X__. (N,N`)-C
 MT102: __.__.__X__.__.__X__X__X__X__. (N,G)
 MT103: __.__.__X__.__X__.__.__.__X__. (N,P)
 MT104: __.__.__X__.__.__.__.__.__X__. (N,D)
 MT105: __.__.__X__.__.__.__.__.__X__. (N,T)
 MT106: __.__.__X__.__.__.__.__.__X__. (N,HE3)
 MT107: __.__.__X__.__X__.__.__.__X__. (N,A)
 MT151: __.__X__.__.__.__.__.__.__.__. (N,RES)
 MT451: __X__.__.__.__.__.__.__.__.__. INFO
```

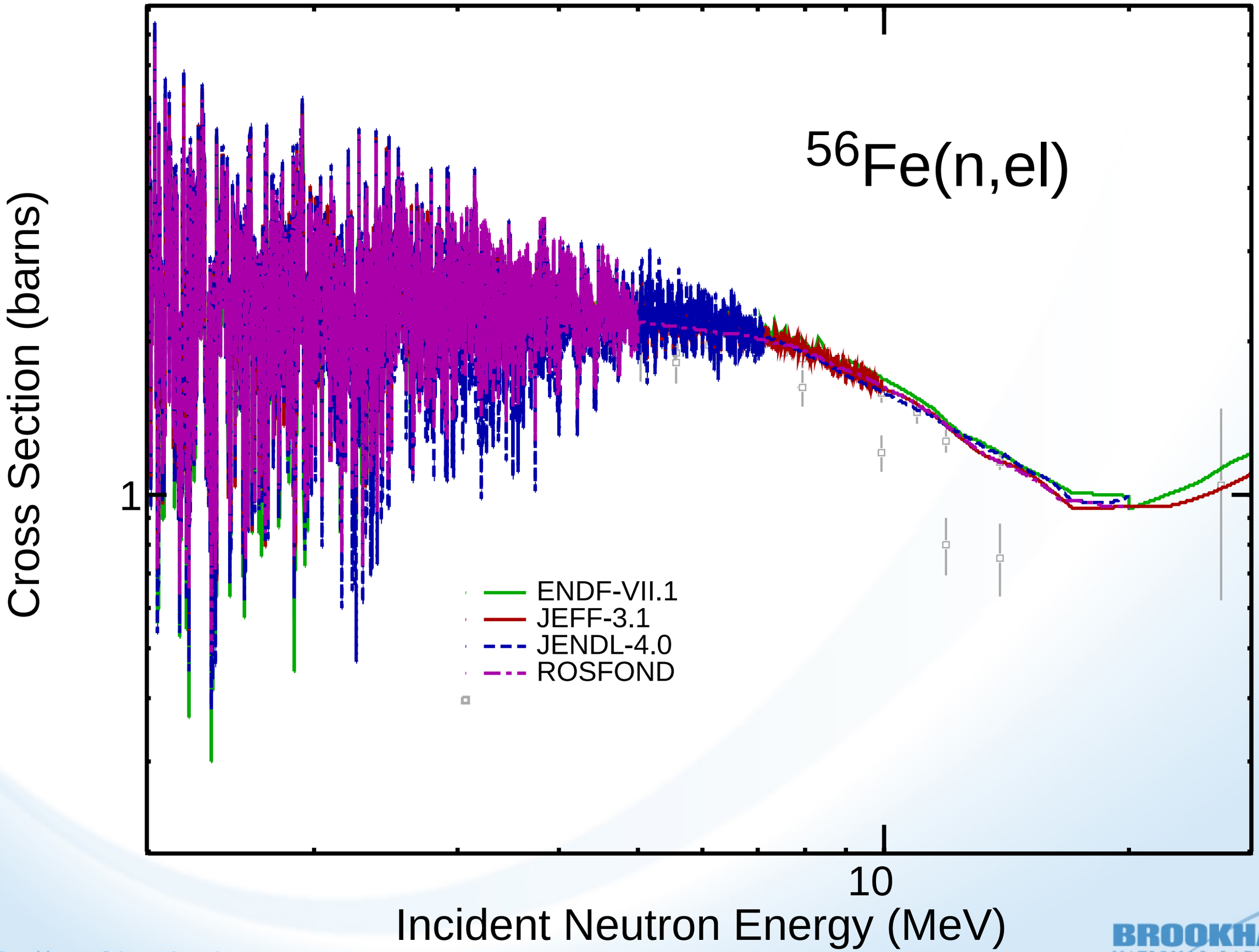
JEFF-3.1

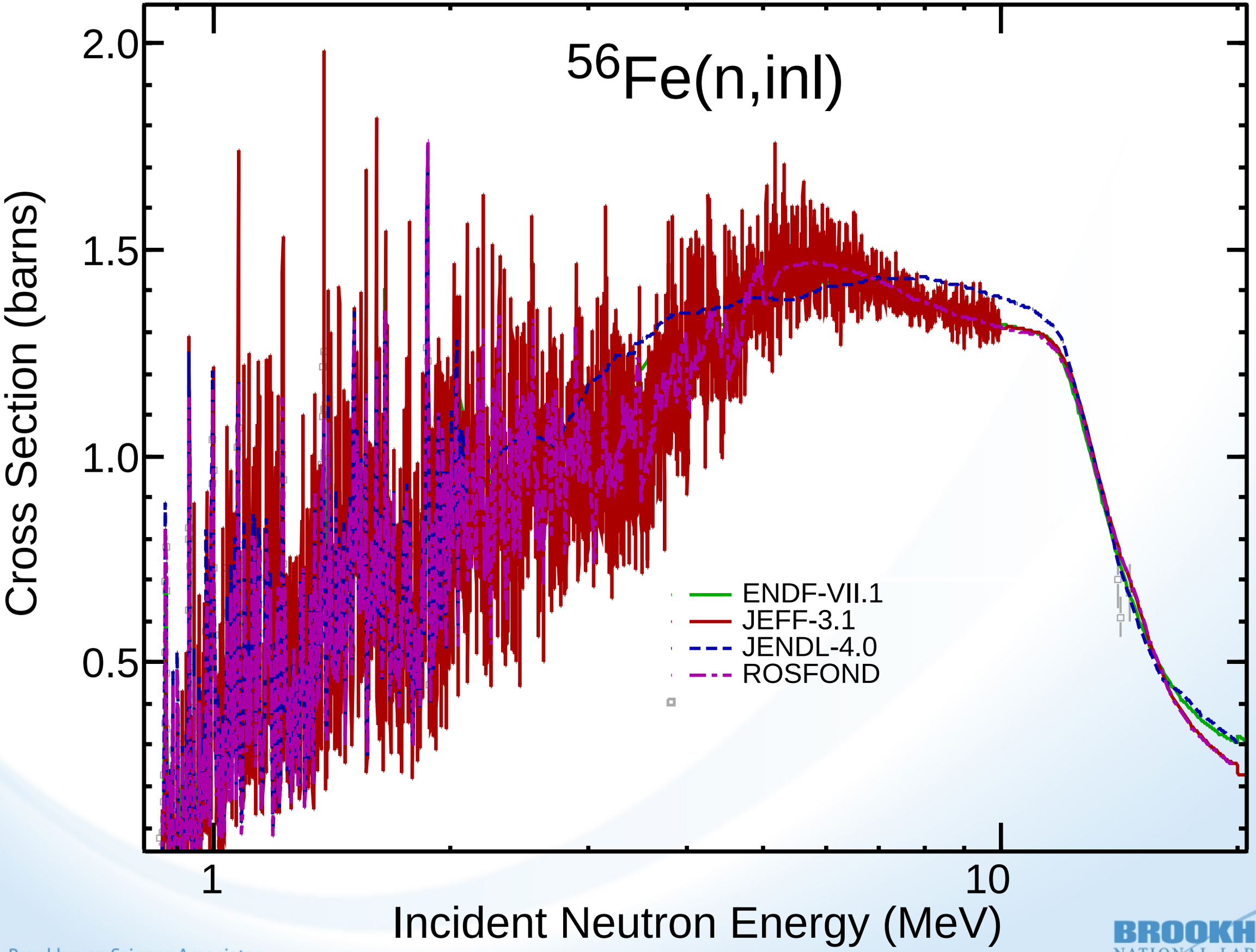
```
   MF=   1  2  3  4  6 12 14 15 33 34
MT1  : __.__.__X__.__.__.__.__.__X__. (N,TOT)
MT2  : __.__.__X__X__.__.__.__.__X__X (N,EL)-L0
MT3  : __.__.__X__.__.__.__.__.__X__. (N,NON)
MT4  : __.__.__X__.__.__.__.__.__X__. (N,INL)
MT5  : __.__.__X__.__X__.__.__.__.__. (N,X)
MT16 : __.__.__X__.__X__.__.__.__X__. (N,2N)
MT22 : __.__.__X__.__X__.__.__.__X__. (N,N+A)
MT28 : __.__.__X__.__X__.__.__.__X__. (N,N+P)
MT51 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L1
...
MT82 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L32
MT91 : __.__.__X__.__X__.__.__.__X__. (N,N`)-C
MT102: __.__.__X__.__.__X__X__X__X__. (N,G)
MT103: __.__.__X__.__.__.__.__.__X__. (N,P)
MT104: __.__.__X__.__.__.__.__.__X__. (N,D)
MT105: __.__.__X__.__.__.__.__.__X__. (N,T)
MT106: __.__.__X__.__.__.__.__.__X__. (N,HE3)
MT107: __.__.__X__.__.__.__.__.__X__. (N,A)
MT151: __.__X__.__.__.__.__.__.__.__. (N,RES)
MT451: __X__.__.__.__.__.__.__.__.__. INFO
MT600: __.__.__X__X__.__.__.__.__X__. (N,P`)-L0
MT601: __.__.__X__X__.__X__X__.__X__. (N,P`)-L1
MT602: __.__.__X__X__.__X__X__.__X__. (N,P`)-L2
...
MT649: __.__.__X__.__X__.__.__.__X__. (N,P`)-C
MT800: __.__.__X__X__.__.__.__.__X__. (N,A`)-L0
MT801: __.__.__X__X__.__X__X__.__X__. (N,A`)-L1
...
MT810: __.__.__X__X__.__X__X__.__X__. (N,A`)-L10
MT849: __.__.__X__.__X__.__.__.__X__. (N,A`)-C
MT851: __.__.__.__.__.__.__.__.__X__.
MT852: __.__.__.__.__.__.__.__.__X__.
MT853: __.__.__.__.__.__.__.__.__X__.
```

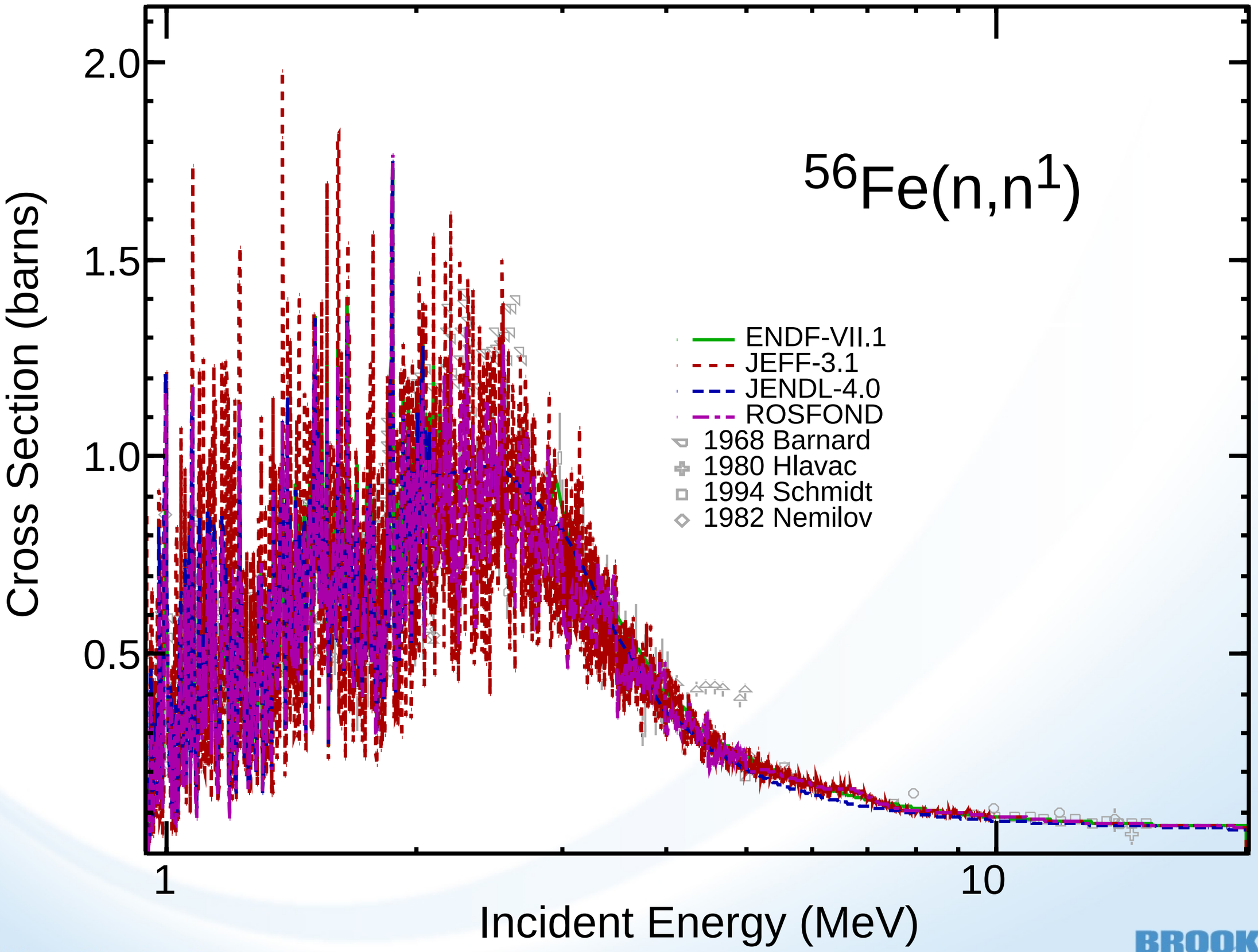
JENDL-4.0

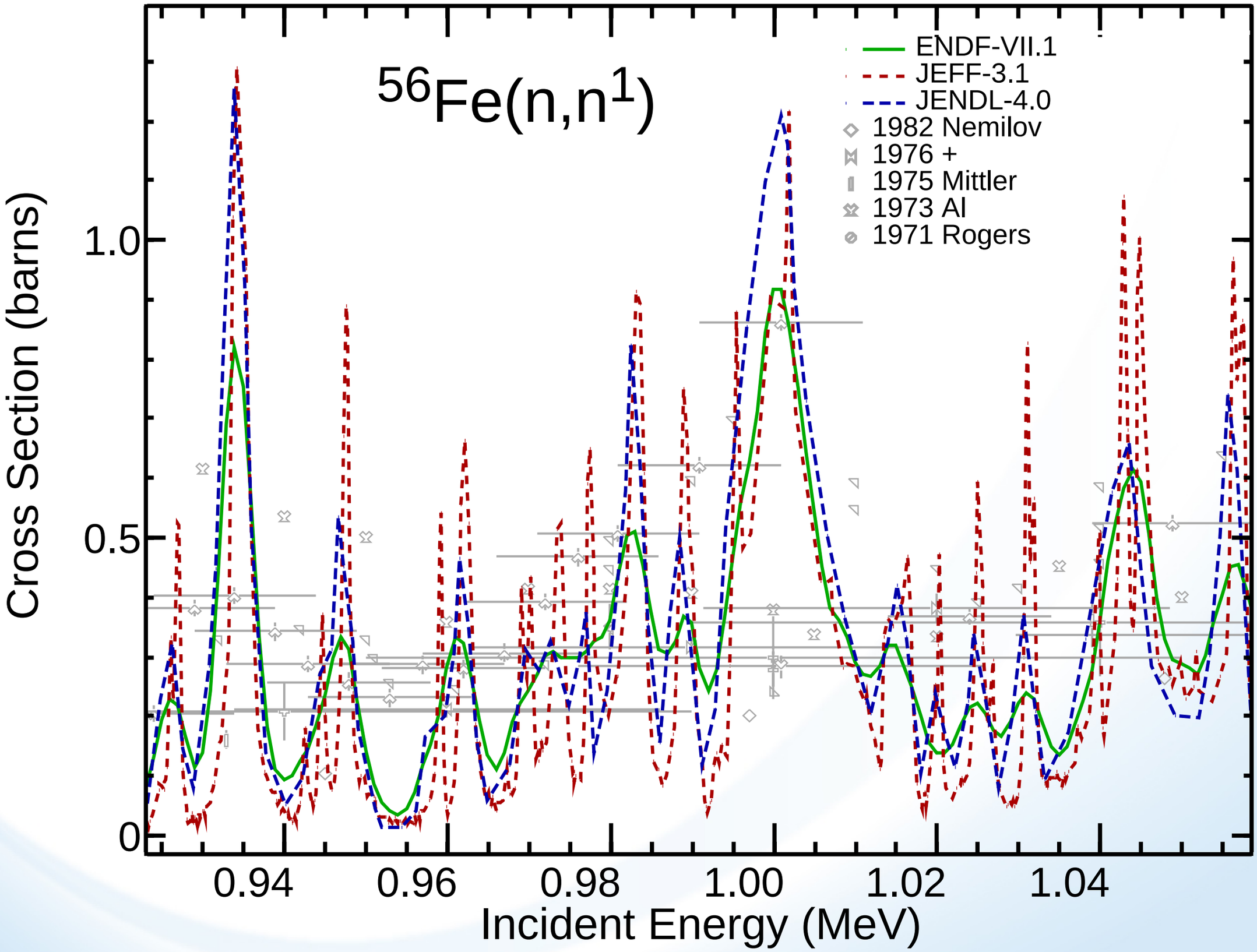
```
   MF=   1  2  3  4  6 12 14 15 33 34
MT1  : __.__.__X__.__.__.__.__.__X__. (N,TOT)
MT2  : __.__.__X__X__.__.__.__.__X__X (N,EL)-L0
MT4  : __.__.__X__.__.__.__.__.__X__. (N,INL)
MT16 : __.__.__X__.__X__X__X__X__X__. (N,2N)
MT22 : __.__.__X__.__X__X__X__X__X__. (N,N+A)
MT28 : __.__.__X__.__X__X__X__X__X__. (N,N+P)
MT51 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L1
MT52 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L2
...
MT77 : __.__.__X__X__.__X__X__.__X__. (N,N`)-L27
MT91 : __.__.__X__.__X__X__X__X__X__. (N,N`)-C
MT102: __.__.__X__.__.__X__X__X__X__. (N,G)
MT103: __.__.__X__.__.__X__X__X__X__. (N,P)
MT107: __.__.__X__.__.__X__X__X__X__. (N,A)
MT151: __.__X__.__.__.__.__.__.__.__. (N,RES)
MT203: __.__.__X__.__X__.__.__.__.__. (N,XP)
MT207: __.__.__X__.__X__.__.__.__.__. (N,XA)
MT451: __X__.__.__.__.__.__.__.__.__. INFO
```

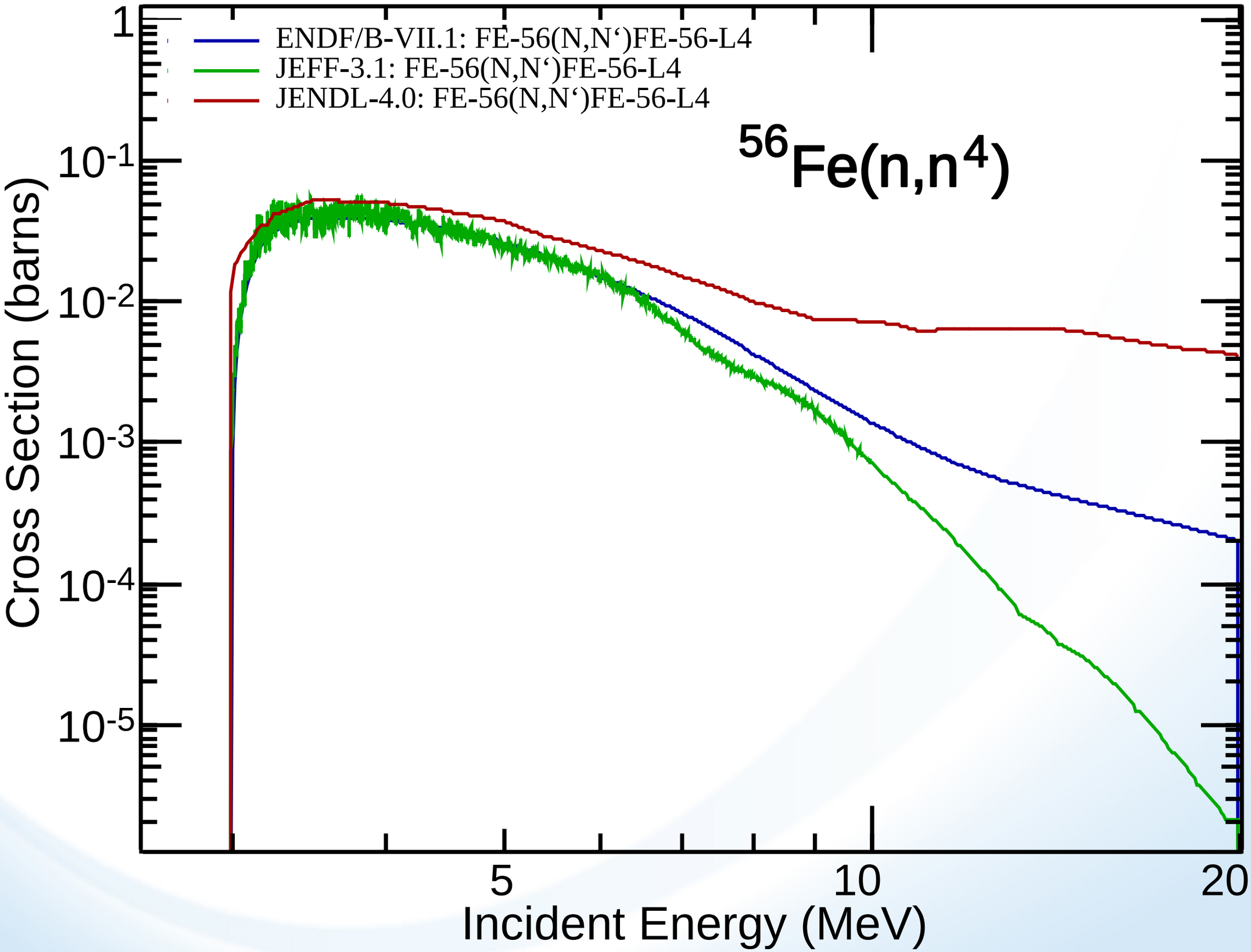

^{56}Fe(n,tot)
ENDF-VII.1
JEFF-3.1 ==> ROSFOND
JENDL-4.0
Cross Section (barns)
1
10
10^2
Incident Neutron Energy (MeV)

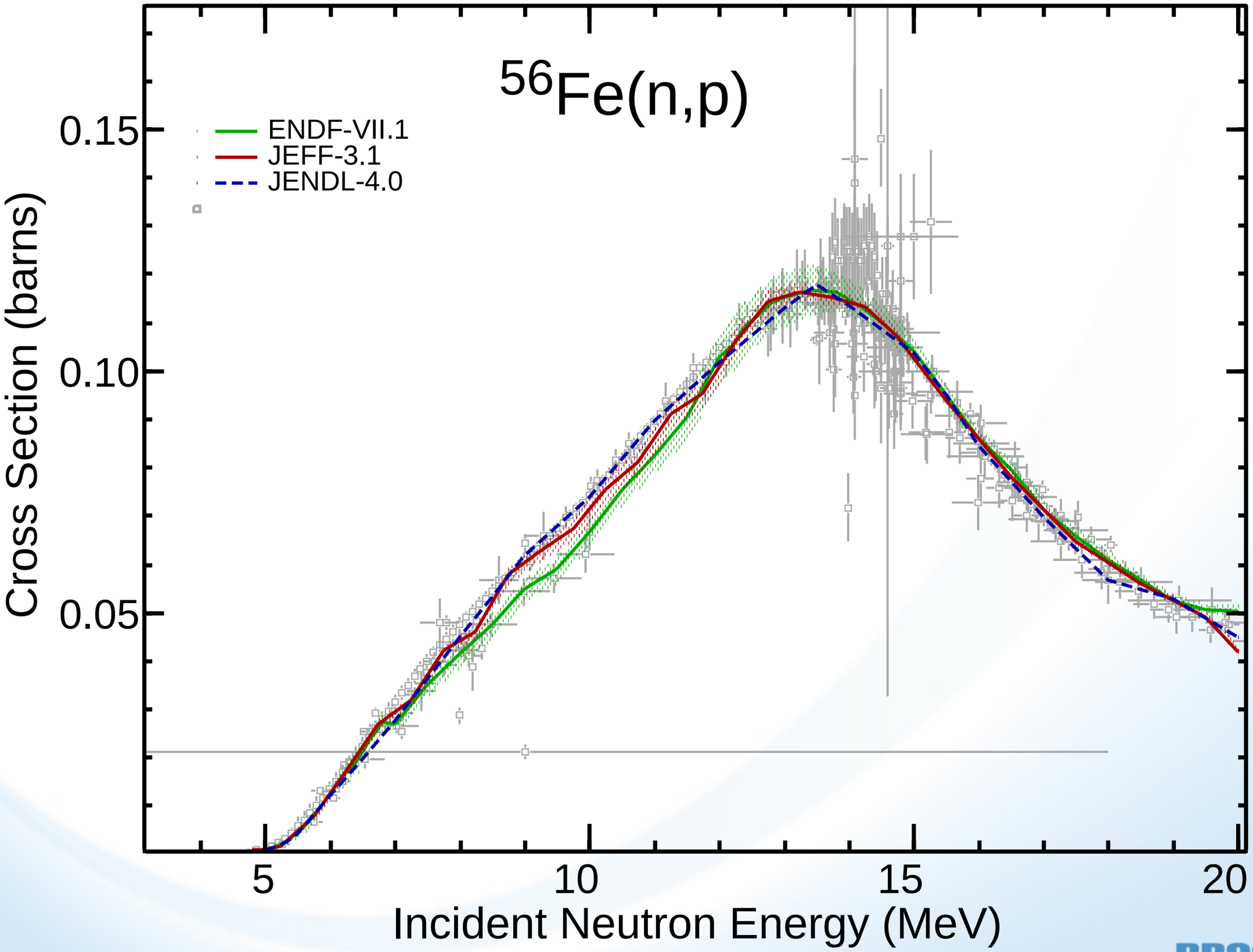

^{56}Fe(n,el)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
ROSFOND
Cross Section (barns)
1
10
Incident Neutron Energy (MeV)

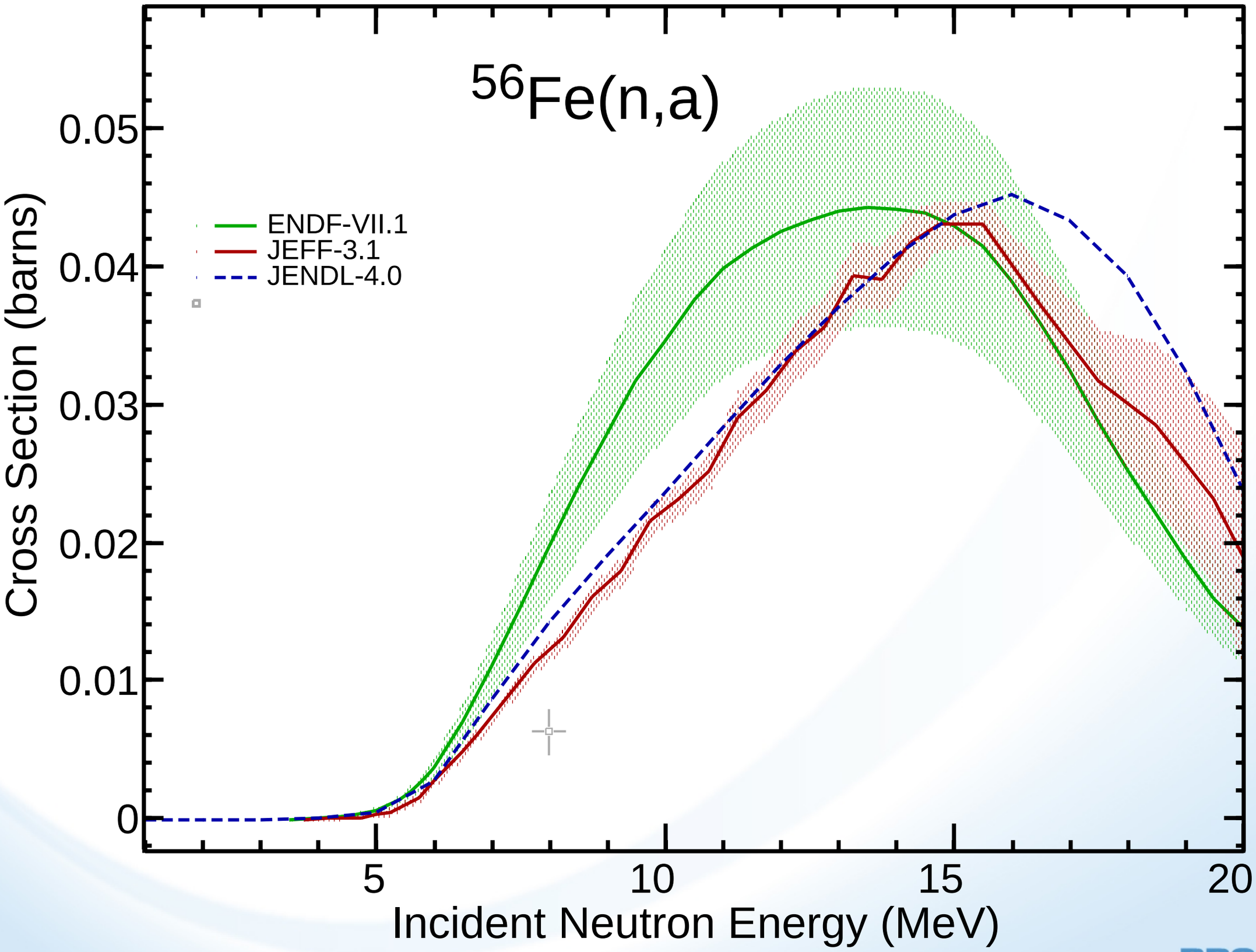

^{56}Fe(n,inl)
Cross Section (barns)
2.0
1.5
1.0
0.5
1
10
Incident Neutron Energy (MeV)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
ROSFOND

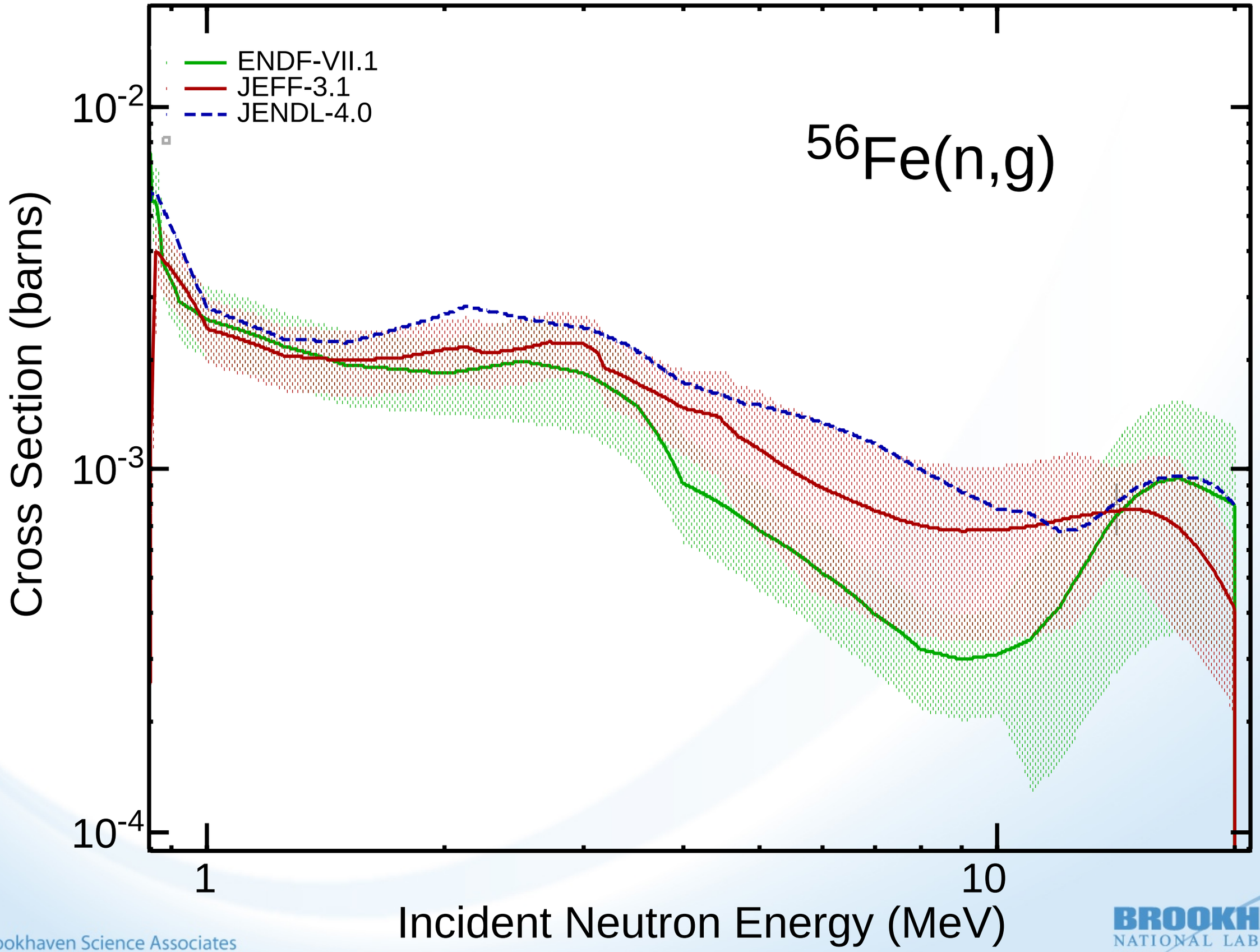

^{56}Fe(n,n^{1})
ENDF-VII.1
JEFF-3.1
JENDL-4.0
ROSFOND
1968 Barnard
1980 Hlavac
1994 Schmidt
1982 Nemilov
Cross Section (barns)
2.0
1.5
1.0
0.5
1
10
Incident Energy (MeV)

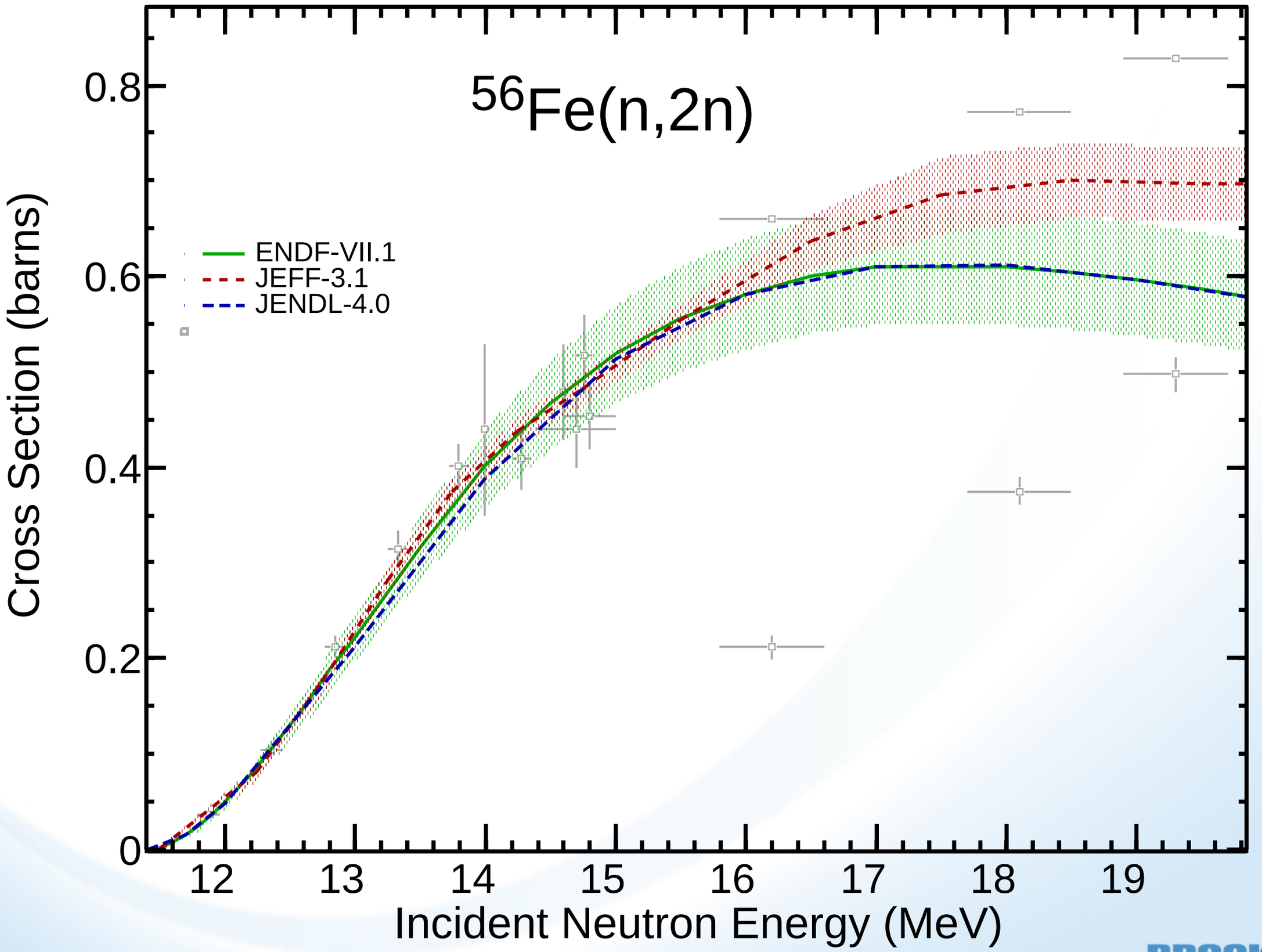

^{56}Fe(n,n^1)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
1982 Nemilov
1976 +
1975 Mittler
1973 Al
1971 Rogers
Cross Section (barns)
1.0
0.5
0
0.94
0.96
0.98
1.00
1.02
1.04
Incident Energy (MeV)

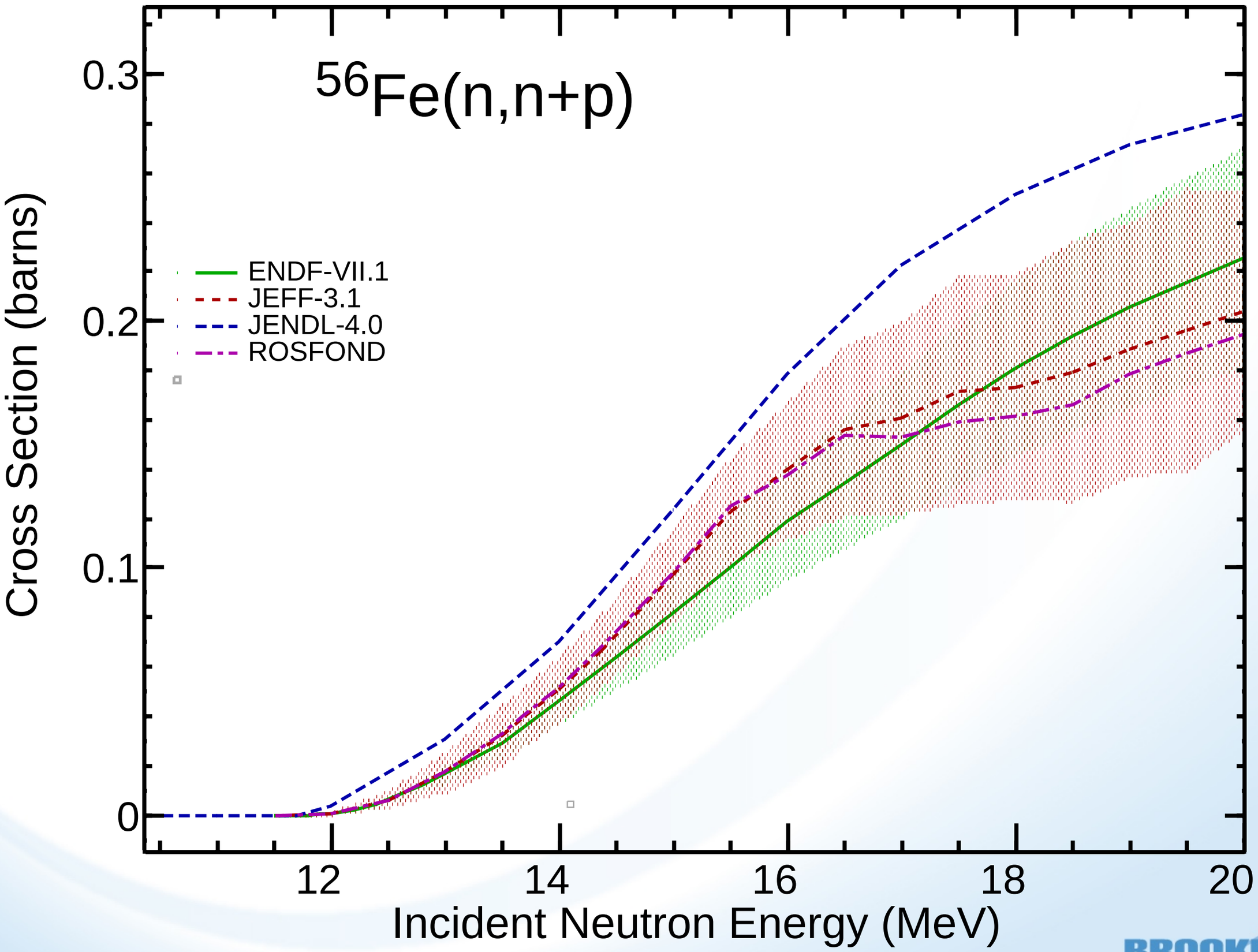

ENDF/B-VII.1: FE-56(N,N')FE-56-L4
JEFF-3.1: FE-56(N,N')FE-56-L4
JENDL-4.0: FE-56(N,N')FE-56-L4
56Fe(n,n4)
Cross Section (barns)
1
10-1
10-2
10-3
10-4
10-5
5
10
20
Incident Energy (MeV)

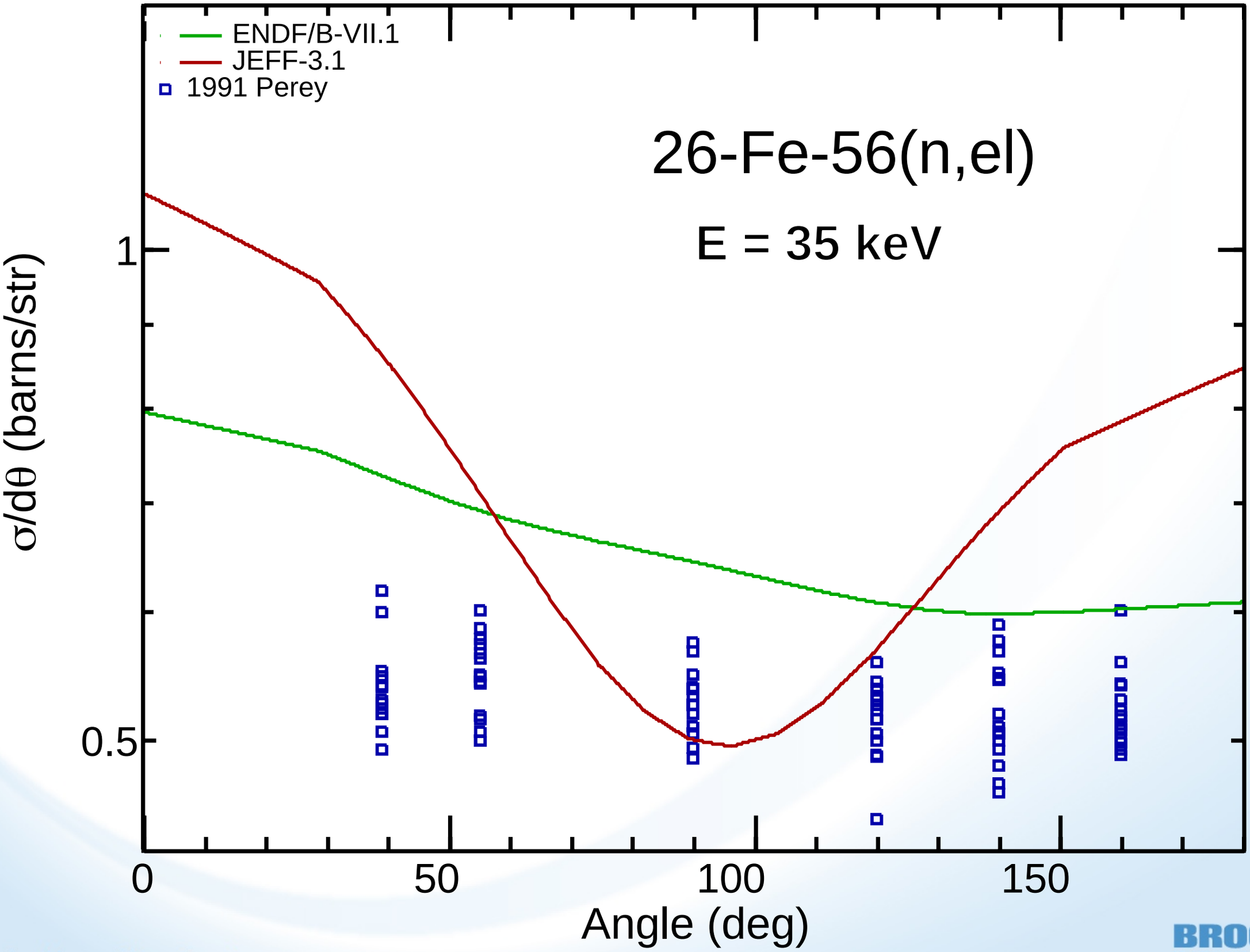

^{56}Fe(n,p)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
Cross Section (barns)
0.15
0.10
0.05
5
10
15
20
Incident Neutron Energy (MeV)

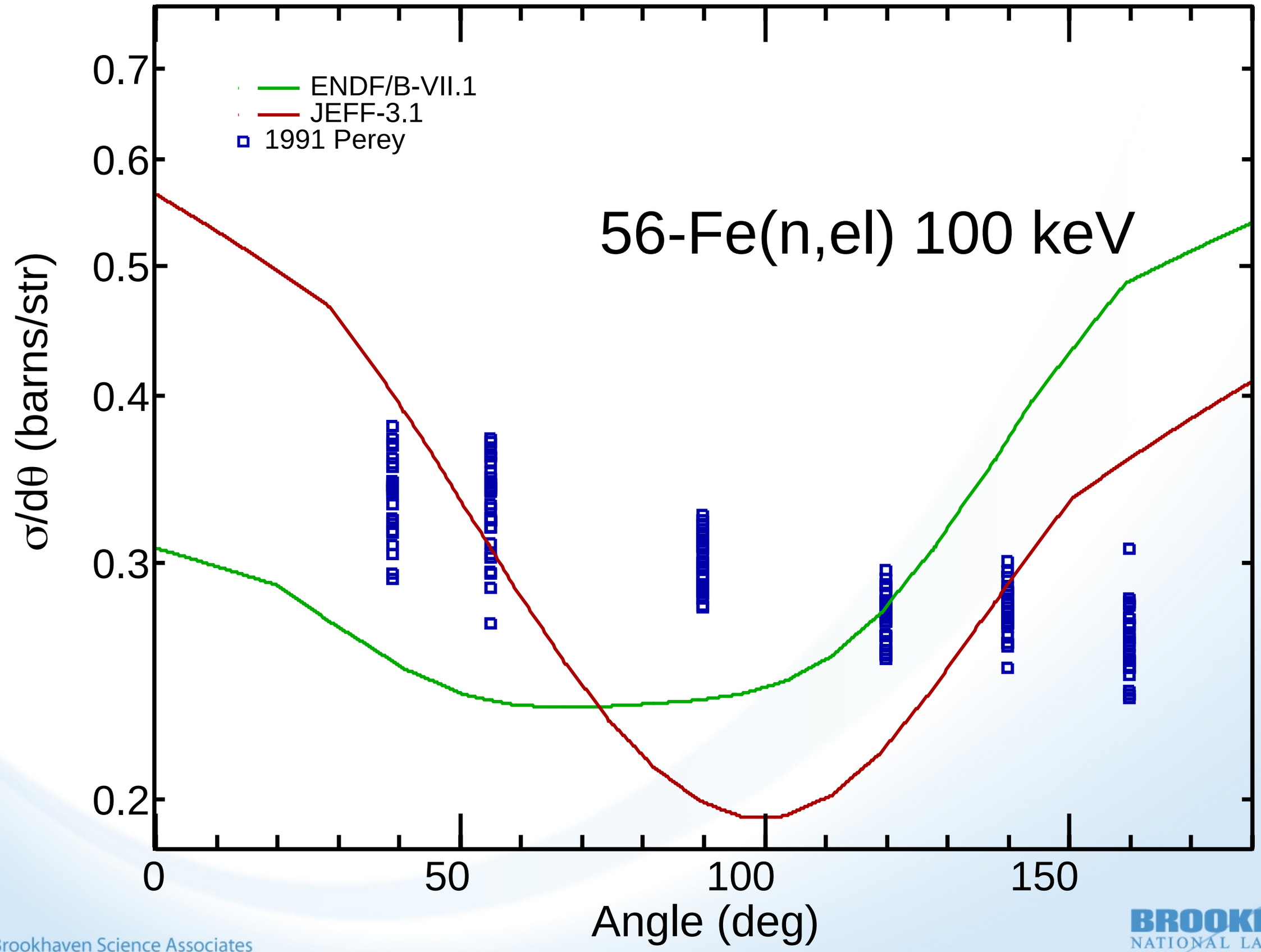

^{56}Fe(n,a)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
Cross Section (barns)
0.05
0.04
0.03
0.02
0.01
0
5
10
15
20
Incident Neutron Energy (MeV)

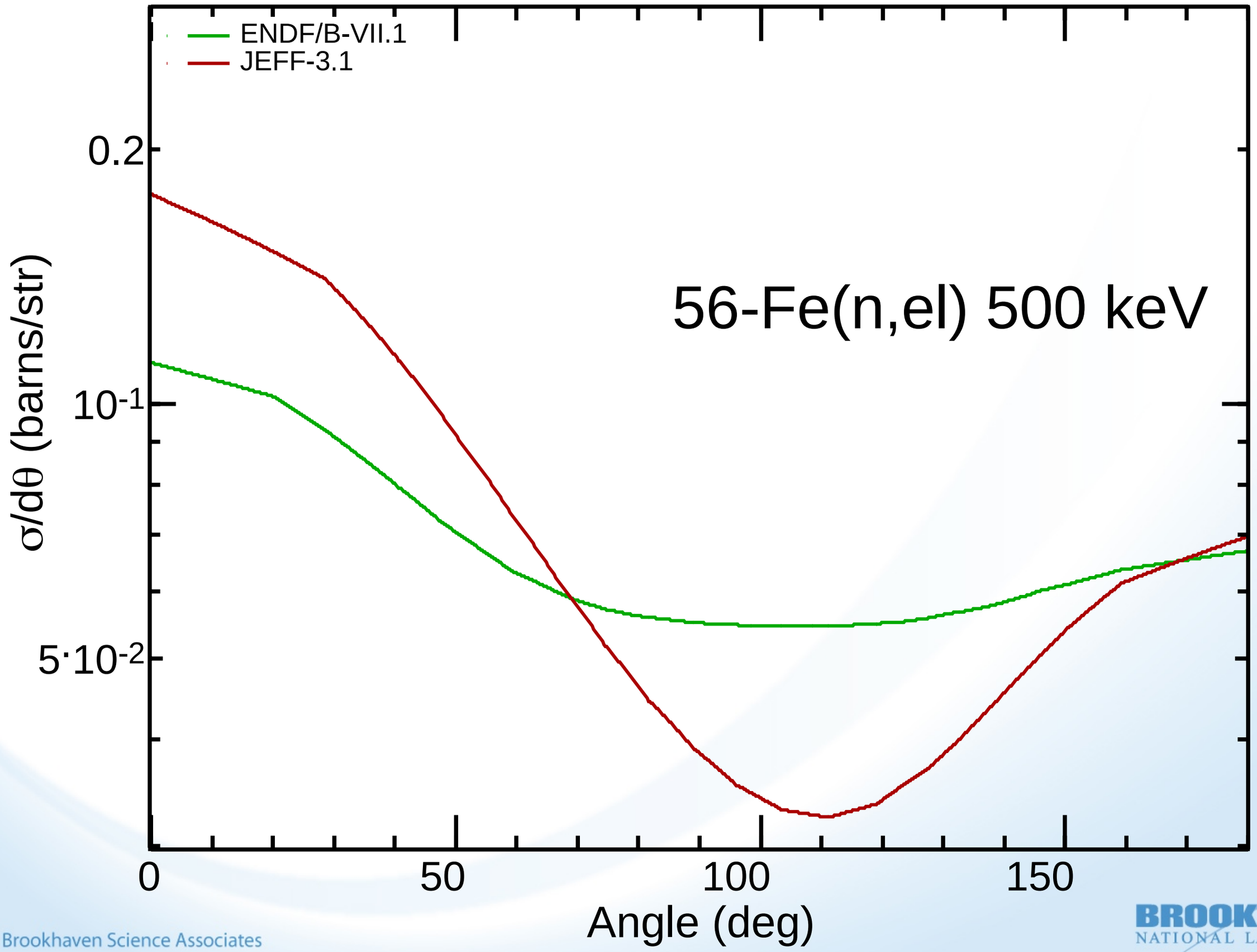

ENDF-VII.1
JEFF-3.1
JENDL-4.0
^{56}Fe(n,g)
Cross Section (barns)
10^{-2}
10^{-3}
10^{-4}
1
10
Incident Neutron Energy (MeV)

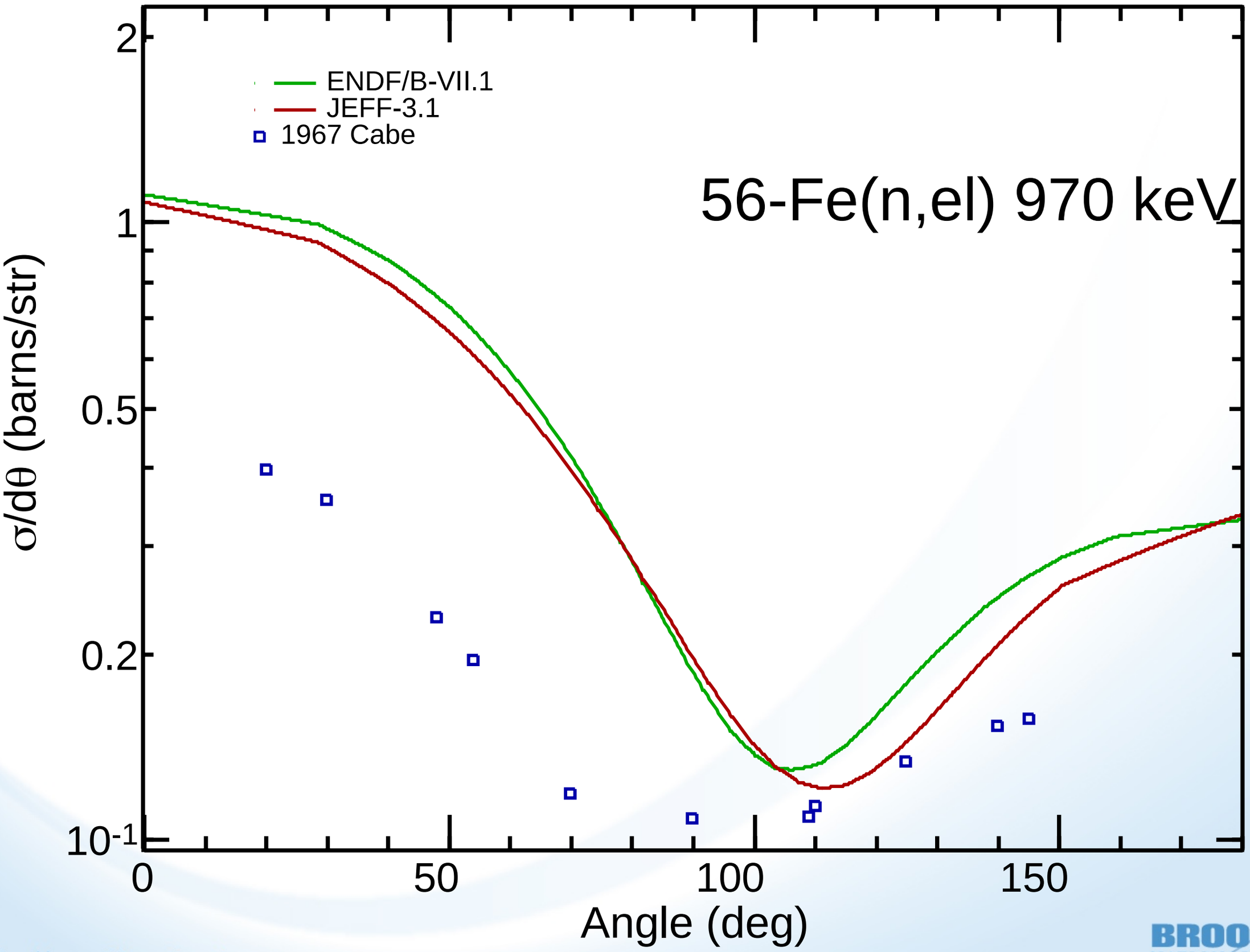

^{56}Fe(n,2n)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
Cross Section (barns)
0
0.2
0.4
0.6
0.8
12
13
14
15
16
17
18
19
Incident Neutron Energy (MeV)

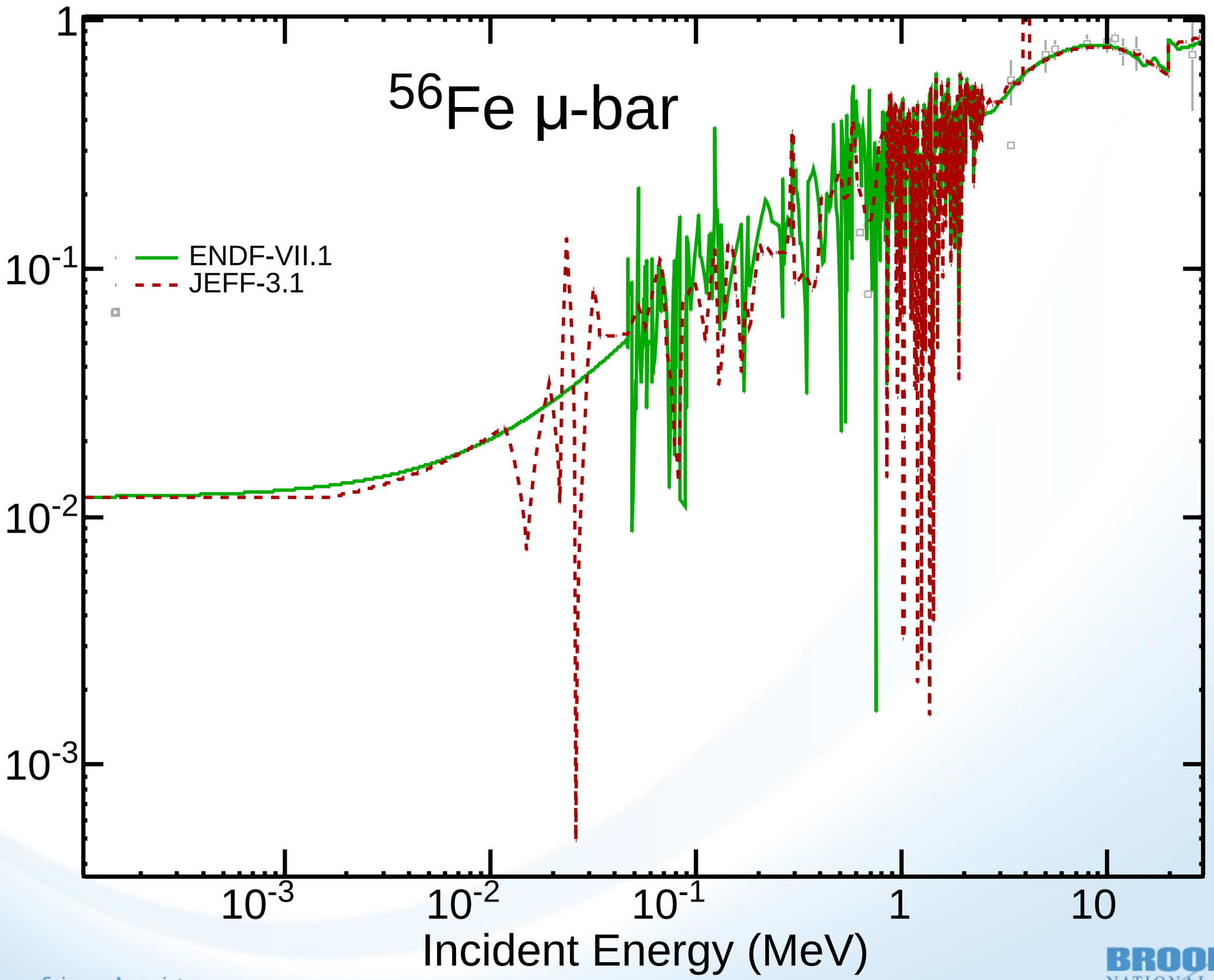

^{56}Fe(n,n+p)
ENDF-VII.1
JEFF-3.1
JENDL-4.0
ROSFOND
Cross Section (barns)
0
0.1
0.2
0.3
12
14
16
18
20
Incident Neutron Energy (MeV)


ENDF/B-VII.1
JEFF-3.1
1991 Perey
26-Fe-56(n,el)
E = 35 keV
1
0.5
σ/dθ (barns/str)
0
50
100
150
Angle (deg)


ENDF/B-VII.1
JEFF-3.1
1991 Perey
56-Fe(n,el) 100 keV
σ/dθ (barns/str)
0.7
0.6
0.5
0.4
0.3
0.2
0
50
100
150
Angle (deg)


ENDF/B-VII.1
JEFF-3.1
56-Fe(n,el) 500 keV
0.2
10-1
5·10-2
σ/dθ (barns/str)
0
50
100
150
Angle (deg)

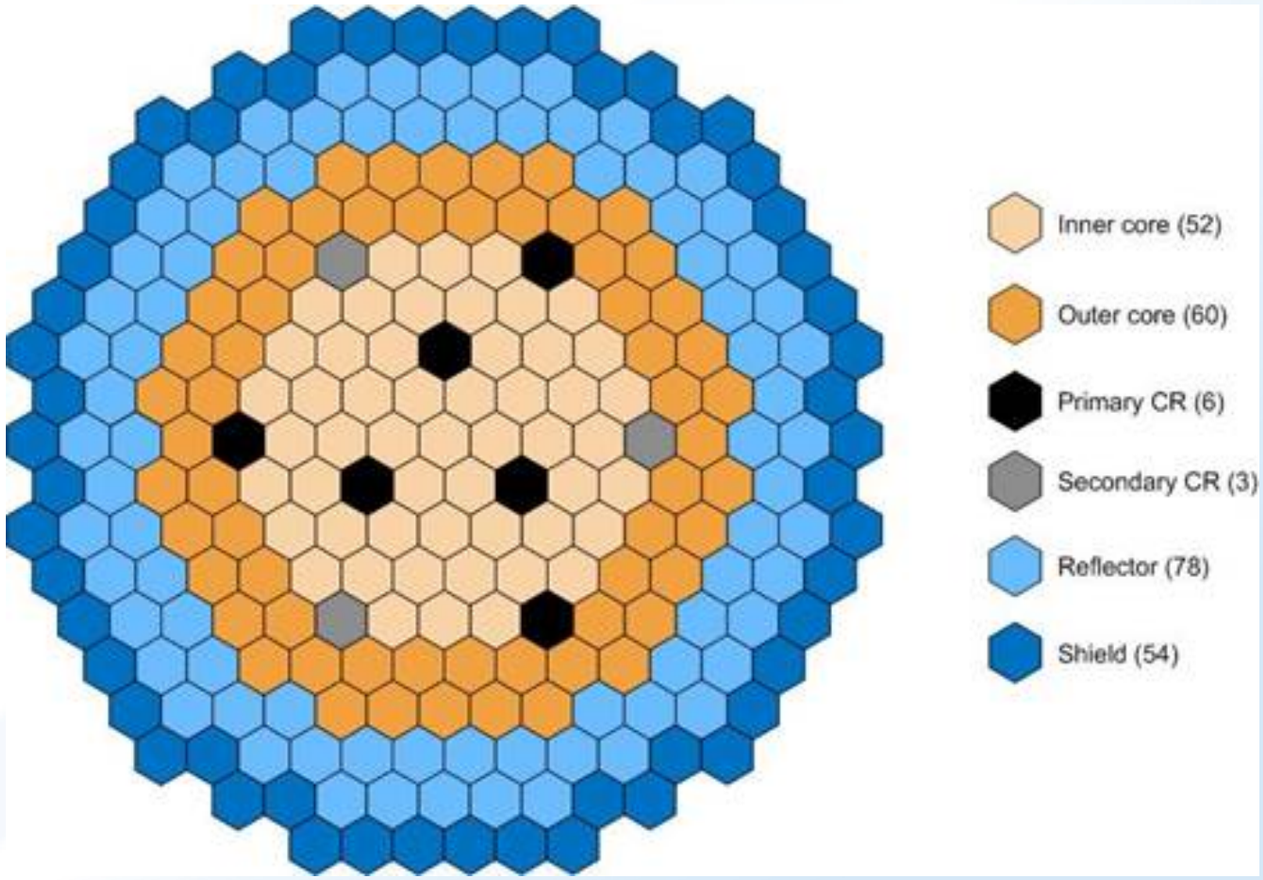

ENDF/B-VII.1
JEFF-3.1
1967 Cabe
56-Fe(n,el) 970 keV
dσ/dθ (barns/str)
Angle (deg)
2
1
0.5
0.2
10-1
0
50
100
150


^{56}Fe μ-bar
ENDF-VII.1
JEFF-3.1
1
10^{-1}
10^{-2}
10^{-3}
10^{-3}
10^{-2}
10^{-1}
1
10
Incident Energy (MeV)

Sensitivities for Sodium Fast Reactor (SFR)

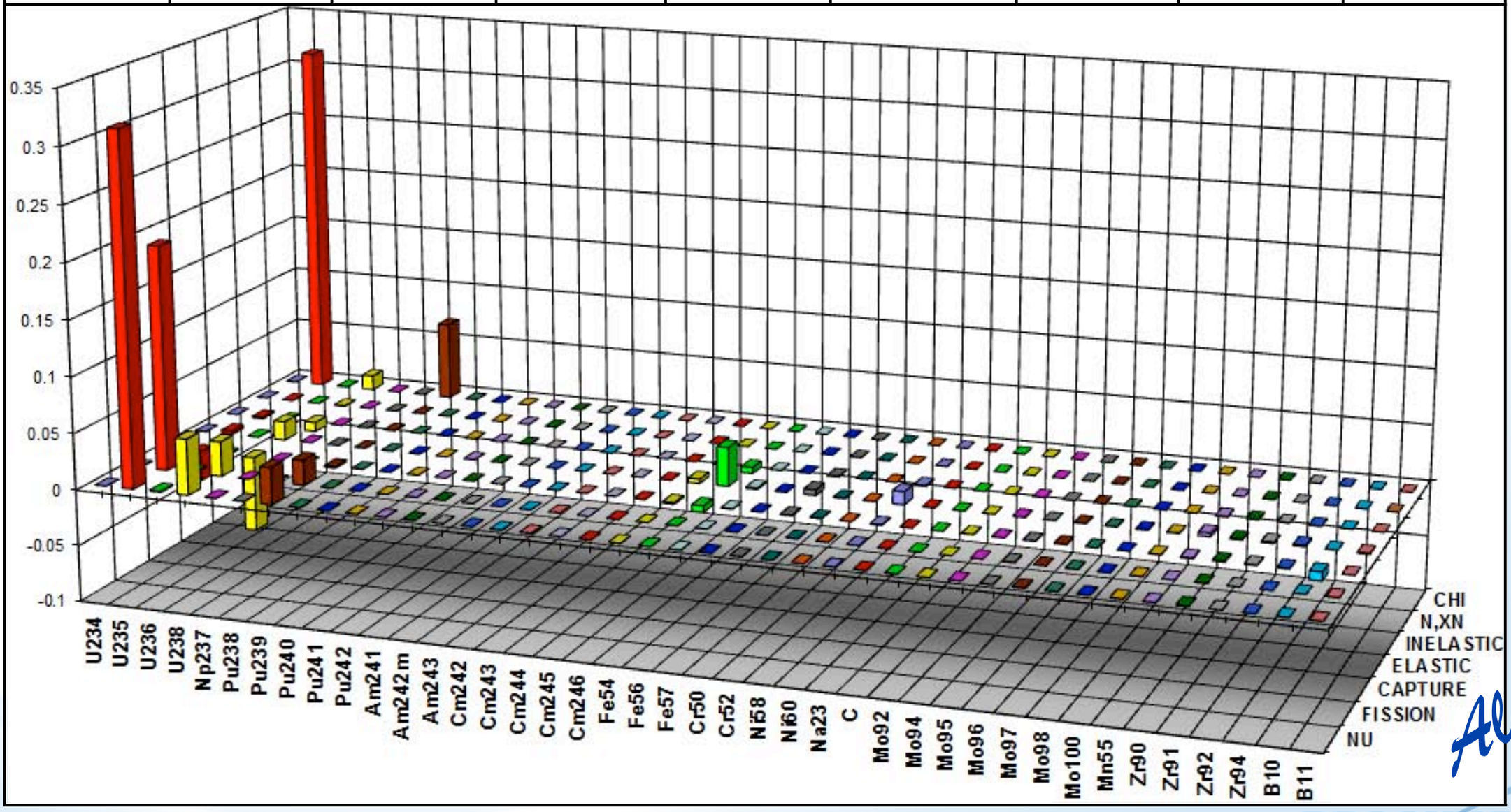
Aliberti

- Pitch: 13.7 cm
- Fuel assemblies contain pins of U-10Zr fuel with HT9M clad.
- Aliberti performed sensitivity analysis of the following parameters:
  - k-effective
  - Reactivity worth (coolant void, Doppler, control rod, etc.);
  - and others..



keff sensitivities

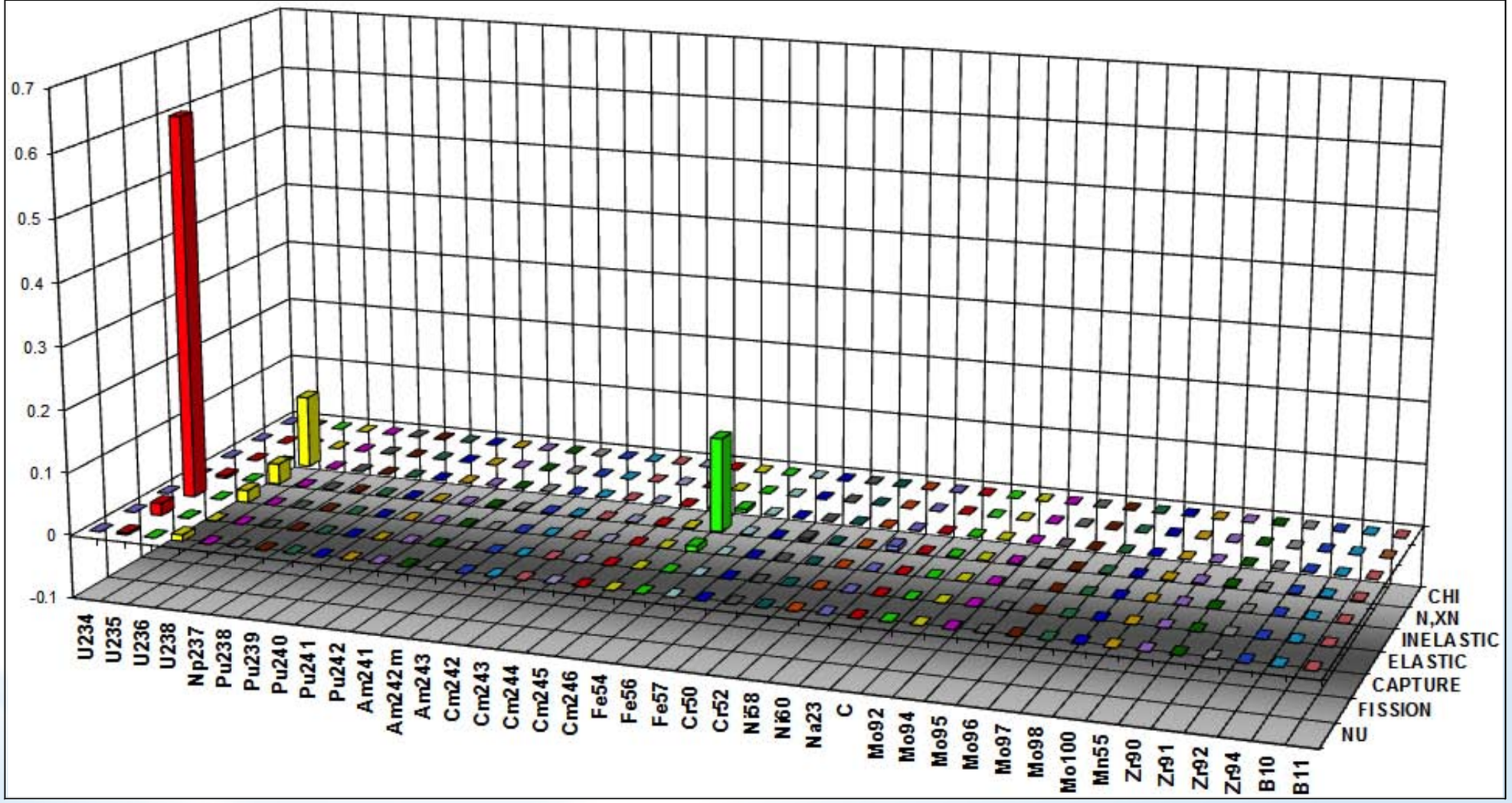
ISOTOPE	NU	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	CHI	SUM
U235	0.791	0.504	-0.066	0.008	-0.003		0.792	2.025
U238	0.125	0.078	-0.167	0.042	-0.021	-0.001	0.033	0.088
Pu239	0.081	0.056	-0.004	0.001			0.174	0.308
Fe56			-0.014	0.087	-0.014			0.059
Cr52			-0.001	0.012	-0.001			0.010
Na23			-0.001	0.029	-0.002			0.025
B10			-0.020					-0.020
SUM	1.000	0.640	-0.287	0.207	-0.047	-0.002	1.000	2.511



Aliberti

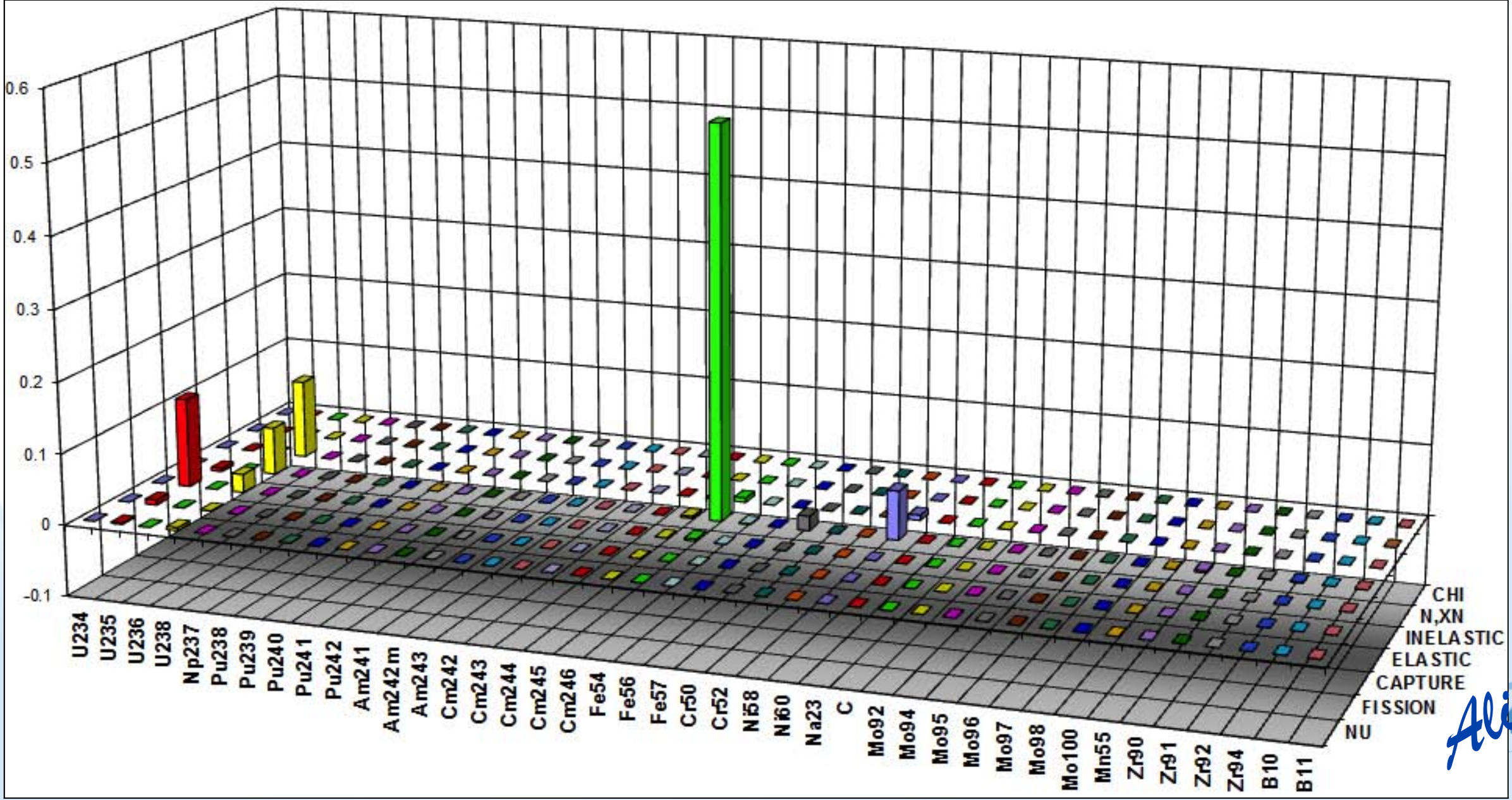
k_{eff} uncertainties with COMMARA-2.0

ISOTOPE	NU	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	CHI	SUM
U235	0.08	0.21	1.17	0.10	0.03			1.20
U236	0.01	0.04	0.01					0.04
U238	0.15	0.04	0.21	0.27	0.51	0.01		0.63
Pu239	0.01	0.02	0.03				0.04	0.05
Fe54			0.03	0.04				0.06
Fe56			0.14	0.58	0.11			0.60
Fe57			0.01	0.02				0.02
Cr52			0.01	0.10	0.01			0.10
Na23				0.12	0.01			0.12
Zr90			0.02	0.03	0.01			0.04
Zr92			0.02	0.02	0.01			0.03
Total	0.17	0.22	1.20	0.67	0.52	0.01	0.04	1.49



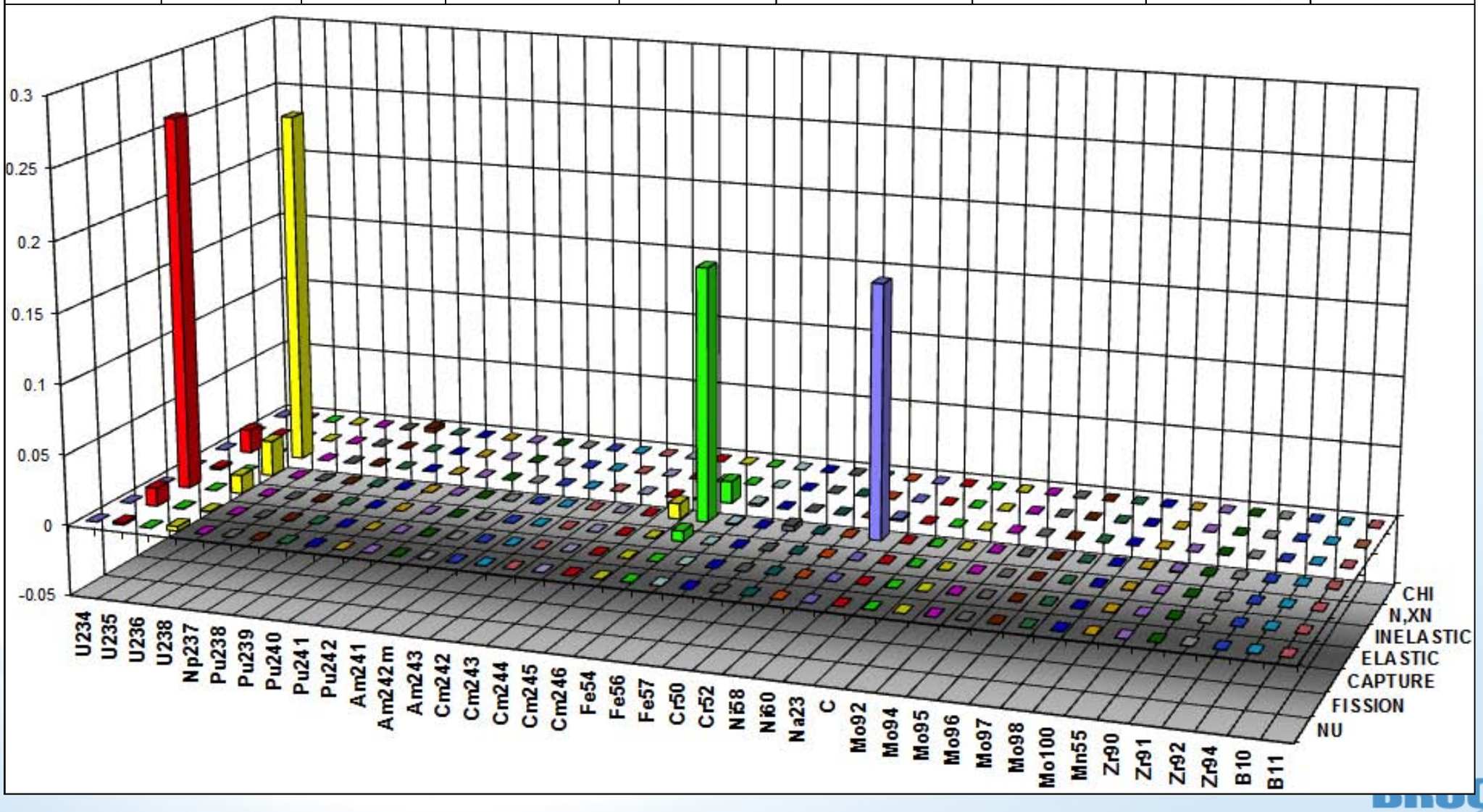
Void uncertainties with COMMARA-2.0

ISOTOPE	NU	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	CHI	SUM
U235	0.63	1.31	5.46	1.07i	0.23	0.02		5.55
U238	0.97	0.30	2.47	3.99	5.10	0.23		7.01
Fe54			0.24	0.81	0.03			0.85
Fe56			0.86	11.42	1.19			11.52
Cr52			0.07	2.20	0.12			2.20
Na23			0.11	4.02	1.31			4.23
Zr90			0.14	0.80	0.13			0.83
Total	1.16	1.38	6.07	12.97	5.41	0.23	0.29	15.42



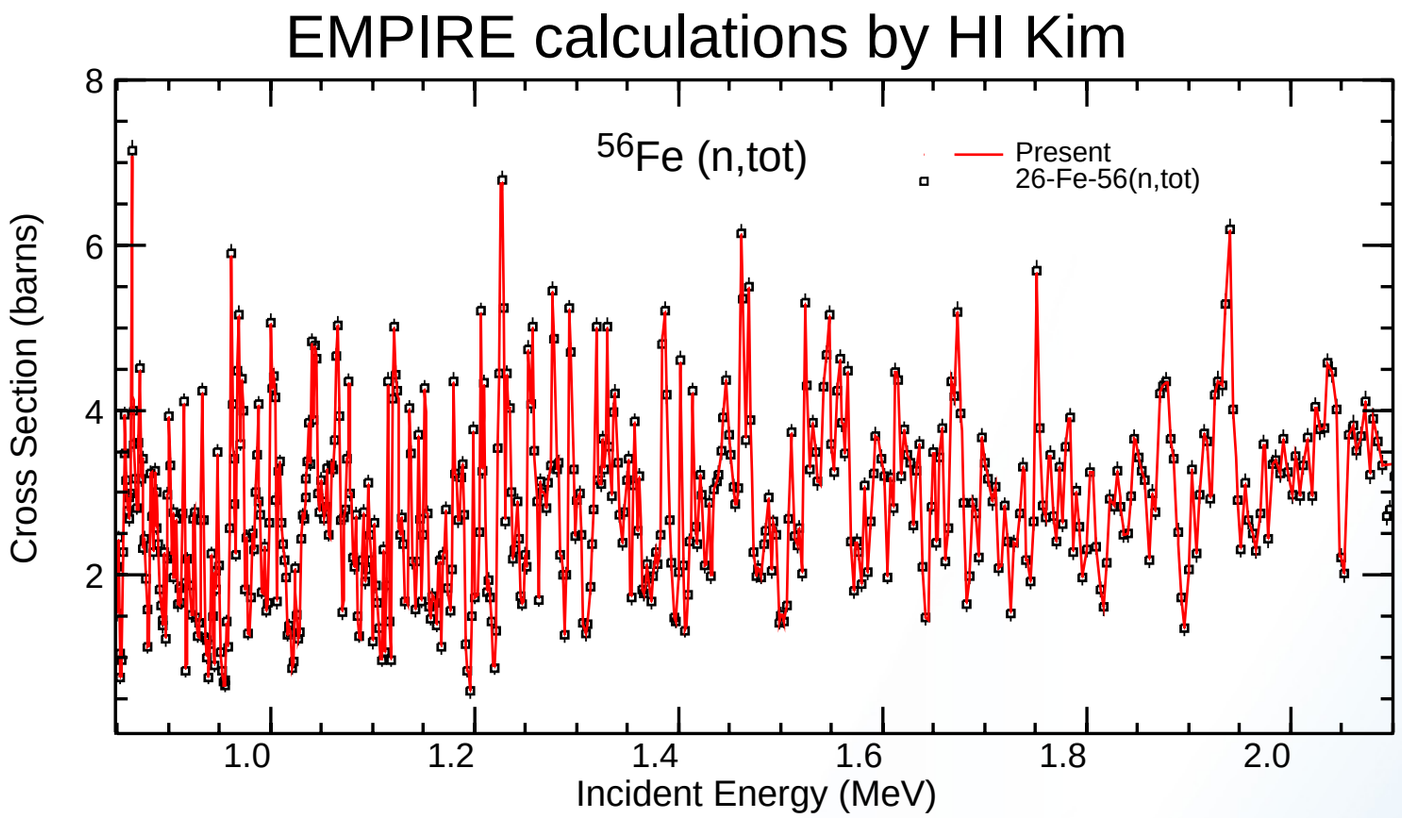
Doppler uncertainties with COMMARA-2.0

ISOTOPE	NU	FISSION	CAPTURE	ELASTIC	INELASTIC	N,XN	CHI	SUM
U235	0.21	0.61	2.80	0.20	0.70			2.97
U236	0.01	0.10	0.03		0.04			0.11
U238	0.31	0.11	0.62	0.86	2.72	0.04		2.94
Pu239	0.02	0.07	0.12	0.02	0.13		0.30	0.36
Fe54			0.08	0.57	0.01			0.57
Fe56			0.46	2.30	0.68			2.44
Fe57			0.07	0.16	0.21			0.27
Cr52			0.04	0.33	0.04			0.33
Na23				2.29	0.19			2.30
Zr90			0.04	0.14	0.03			0.14
Total	0.37	0.64	2.91	3.44	2.91	0.04	0.30	5.42

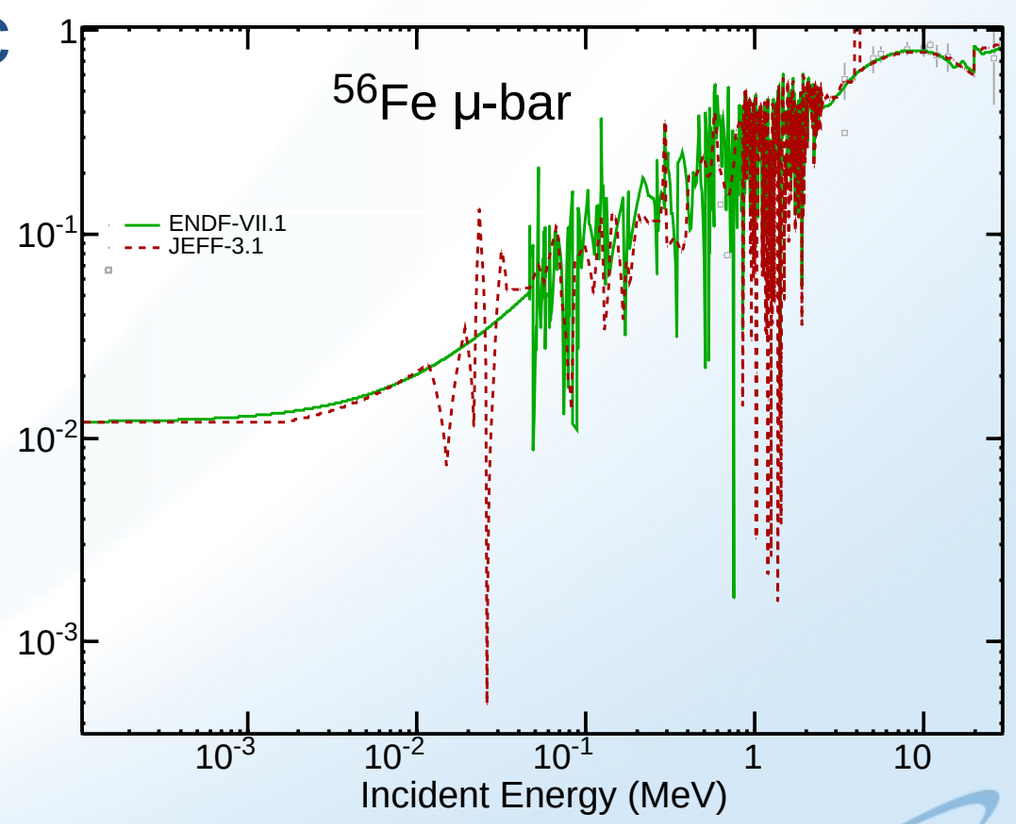


Challenges

- Fluctuations and their distribution among reaction channels



- If RRR is extended to the inelastic region how do we merge it with the CC inelastic scattering?



- Elastic angular distributions

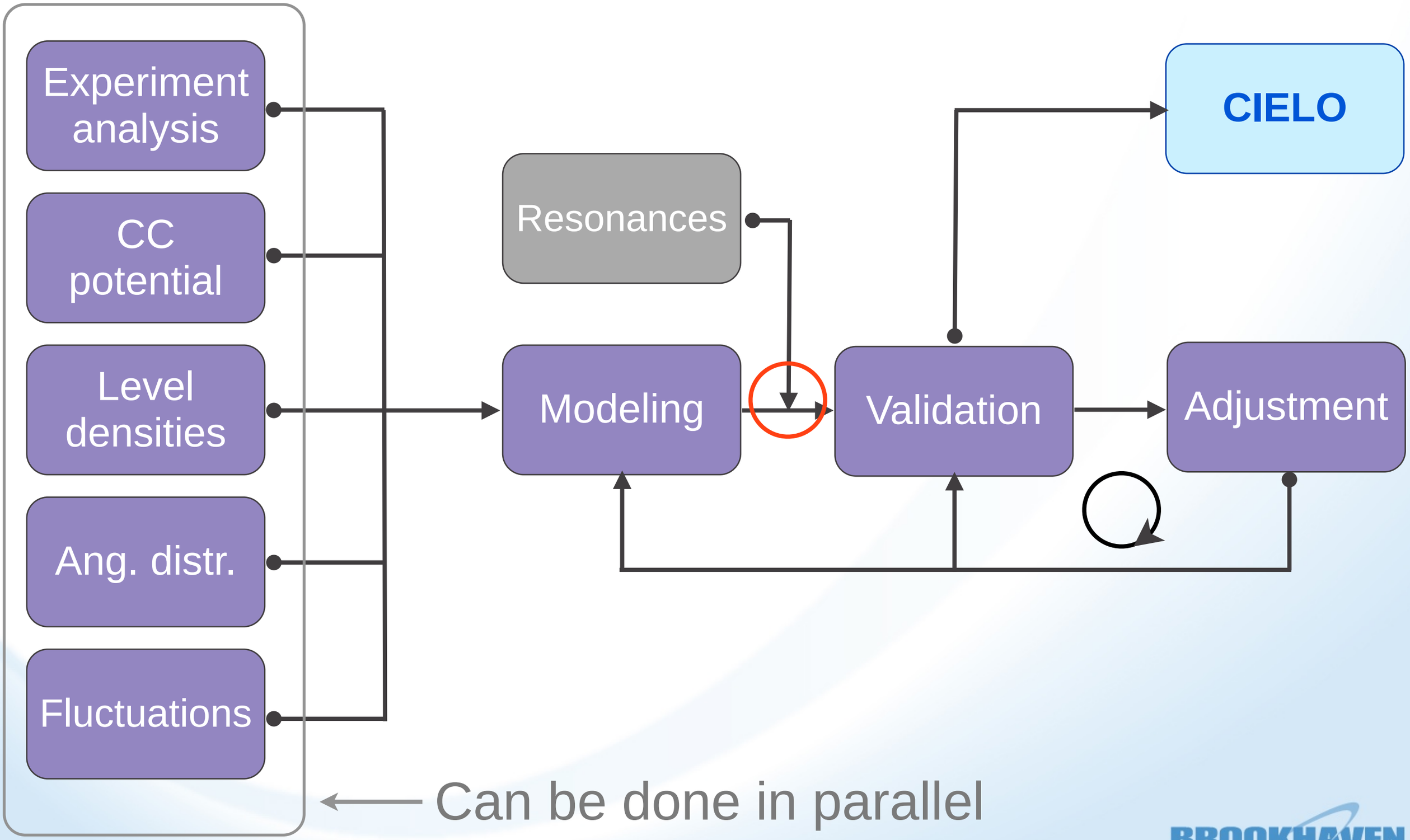
Tasks

- Experiment selection, renormalization & covariances
- Elastic angular distributions in resonance region
- Optical Model Potential
- Level densities
- Calculations in fast neutron region (x-sec, ang. distr., energy spectra)
- Accounting for cross section fluctuations
- File assembly, merging resonance & fast regions
- Covariances
- Validation
- Adjustment (consistent)

New opportunities

- New differential/semi-differential experimental data
- Renormalization of old experimental data
- Extended resonance range (L.Leal)
- Soft-rotor CC potential (Capote et al.)
- Microscopic level densities with parity dependence (Alhassid)
- Elastic angular distributions (resonances, omp, HF)
- MSC/MSD preequilibrium
- Complete covariance matrix with cross-reaction terms
- Consistent adjustment

Fast neutron evaluation flow-chart



← Can be done in parallel

Modus operandi: split into sub^3-groups

- analysis of experimental data
  - total
  - inelastic
  - spectra…
  - experimental covariances
- level densities
- soft-rotor CC potential
- fluctuations
- angular distributions

- fast neutron modeling
- file assembly
- verification & validation
- (consistent) adjustment
- covariances

Means of cooperation

- Mailing list
- GForge
  - storing and updating results
  - storing/sharing documentation
  - filing trackers
  - posting announcements
  - Wiki, Blog, Forum
- Video conferencing
- Meetings (at least once a year!)

56Fe EXFOR Data Triage

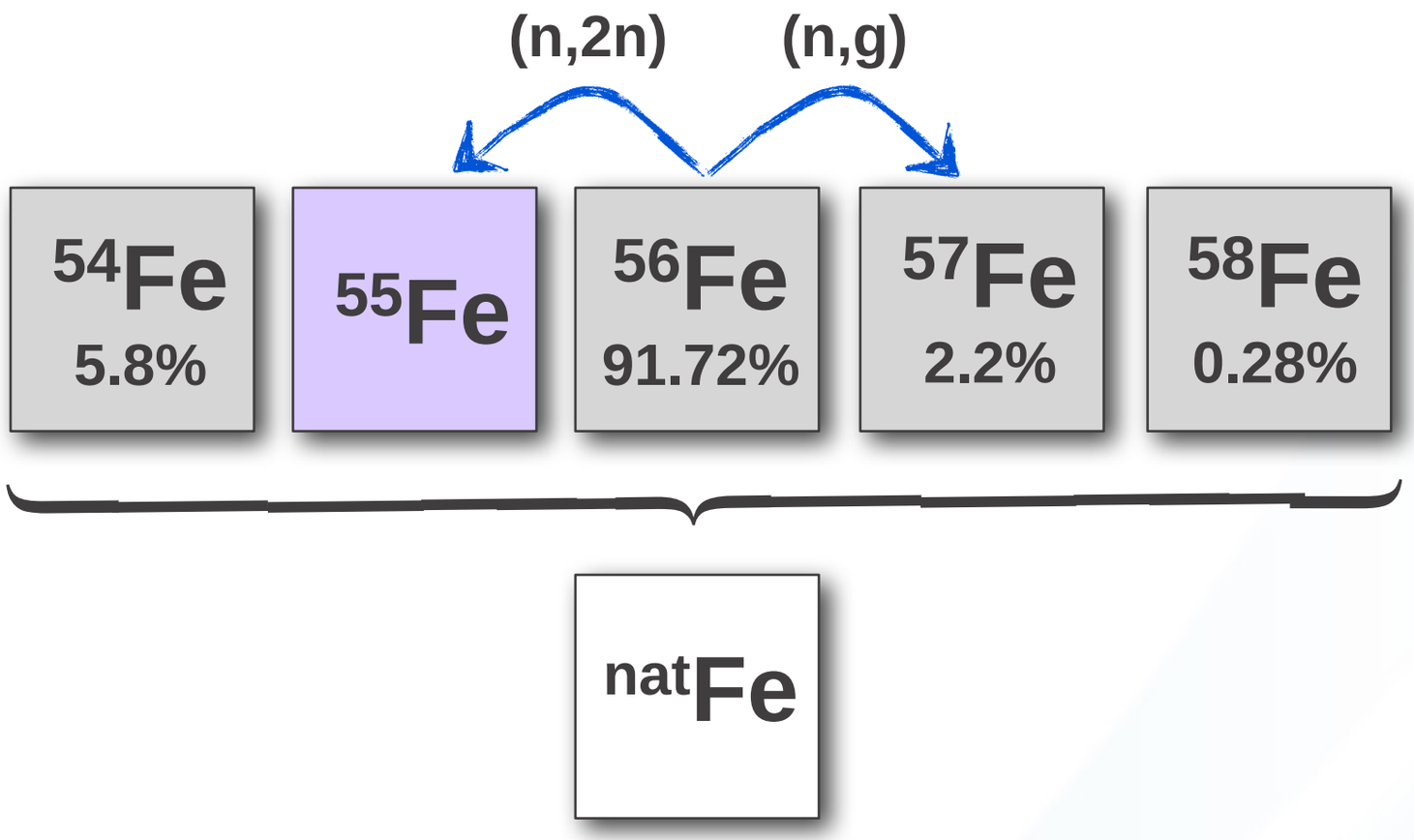
D. Brown

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

We need to consider more than 56Fe



- **56Fe** (obviously), but...
- **natFe** since 56Fe is dominant isotope
- **55Fe** and **57Fe** to nail down level densities
- **54Fe** as dominant “contaminant” to natFe

Iron is a very popular material for (n,*)

Isotope	# EXFOR SUBENTs
^{54}Fe 5.8%	419 (5 evals)
^{55}Fe	2 (1 eval)
^{56}Fe 91.72%	636 (7 evals)

Isotope	# EXFOR SUBENTs
^{57}Fe 2.2%	85 (3 evals)
^{58}Fe 0.28%	72 (2 evals)
^{nat}Fe	918 (1 eval)

Not all of this is useful, must down-select to what is useful for CIELO

- No polarization data
- No (FIS, SPA) since not well defined;
  Limited integral data (RI, MXW) are OK
- No evaluated data (RECOM,EVAL,DERIV, SUBENT begins with ‘V’)
- No quasi-evaluated data (CN,SEQ)
- No atomic data (BA,FA)
- No thermal scattering (THS,COH,INC)
- No kerma (KER)
- No high-energy (DI)

A lot of the remaining data is really only good for validation

- Partial data: PAR
- Poorly defined reactions: INL, NON, SCT, ABS
- Coupled data (ratio data, etc) or ALF
- Isotope/particle production

This is what's left

	Resonance*	Fast*	Validation*	Total*
^{54}Fe	101 sets	161 sets	137 sets	399 sets
^{55}Fe	0 sets	0 sets	0 sets	0 sets
^{56}Fe	223 sets	134 sets	313 sets	670 sets
^{57}Fe	89 sets	23 sets	13 sets	125 sets
^{58}Fe	50 sets	23 sets	17 sets	90 sets
^{nat}Fe	38 sets	327 sets	511 sets	876 sets

*This is number of data sets, not SUBENTs

This is what's left

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I volunteer for this

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I volunteer for this

Sorry Luiz

I have produced text files breaking down the data

- **resonancesFe.txt**: *resonance data*
- **fastFe.txt**: *fast data that we can fit to*
- **validationFe.txt**: *the data usable for validation only*
- **allFe.txt**: *everything*

```
FE-54 :
    26-FE-54(N,TOT) :
        Cross sections :
            SIG :
                ('40556003', ' '),('11180005', ' '),('11368013', ' '),...
    26-FE-54(N,P)25-MN-54 :
        Cross sections :
            SIG :
                ('20841002', ' '),('30221006', ' '),('30457003', ' '),...
        Angular dists :
            DA :
                ('40699007', ' ')
        Energy/Angle dists :
            DA/DE :
                ('12948002', ' ')
   ...
```

SUBENT

pointer