
Iron
in fast neutron range
β_0 evaluation for ^{56}Fe
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WPEC 2015 , SG40 meeting
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β_0 CIELO evaluation of ^{56}Fe

- New RR evaluation by ORNL merged with the new fast-neutron evaluation produced at BNL
- Fast-neutron file based on:
  - experimental data included in the previous evaluations (with some renormalization when needed)
  - new data not included in the previous evaluations (e.g. Geel data, LANCE data, RPI semi-differential data…)
  - fully represented by EMPIRE calculations informed by differential data

NO adjustment to integral data at this stage!

β_0 evaluation identification tag (49)

- Released: Apr 23, 2015 on NNDC GForge server
- Identifier: Subversion rev.49
- Content:
  - Resolved Resonance range
    - Produced at: ORNL
    - Posted at GForge: March 23, 2015
    - Identifier: Subversion rev. 41 (unofficially referred as ‘ORNL4’)
    - Energy ange: 1.0E-5 eV - 2 MeV
    - Data source: RPI transmission exp. and Geel inelastic scattering + ORNL Perrey data
  - Unresolved Resonance range: none
  - Fast neutron range
    - Produced at: BNL using EMPIRE code
    - Posted at GForge: Apr 20, 2015
    - Identifier: Subversion rev. 48
    - Energy range: 2 MeV - 20 MeV
  - Covariances: none

Experimental database

- Excellent compilation and analysis by CNDC (too many experiments to be listed!)
- Tagessen,Vonach, Pronayev => EFF-3.1 around 1995 (JEFF-3.0 'contaminated' by adjustment to integral experiments). Caveat: model based parts of EFF-3.1 can't be used!
- recent inelastic data from Geel
- less recent inelastic data from LANCE



Modeling fast region

- Incident channel & inelastic to collective levels
  - coupled-channels with soft-rotor dispersive OMP (RIPL #614)
  - OPTMAN module used
- DWBA to selected 13 discrete levels
- Non-collective outgoing channels - spherical OM

Coupled levels		
N	E (MeV)	Jπ
1	0	0
2	0.84678	2
3	2.08510	4
4	2.65759	2
5	2.94150	0
11	3.44535	3
16	3.74413	2
33	4.50956	-3

Modeling fast region

- Preequilibrium
  - MSD with ORION+TRISTAN for (n,n')
  - Heidelberg MSC for (n,n')
  - Exciton model (PCROSS) for (n,p) and (n,γ)
  - Iwamoto-Harada model for cluster emission
  - Kalbach systematics angular distributions for PCROSS

Use of direct and preequilibrium models

Exit channel	ECIS	MSD	MSC	HMS	PCROSS
neut. disc.	1	0	0	0	0
neut. cont.	0	1	1	0	0
prot. disc.	0	0	0	0	0
prot. cont.	0	0	0	0	1
gammas	0	0	0	0	1
alpha cont.	0	0	0	0	1
deut. cont.	0	0	0	0	1
trit. cont.	0	0	0	0	1
He-3 cont.	0	0	0	0	1
LI cont.	0	0	0	0	0
alpha disc.	0	0	0	0	0
deut. disc.	0	0	0	0	0
trit. disc.	0	0	0	0	0
He-3 disc.	0	0	0	0	0

Modeling fast region

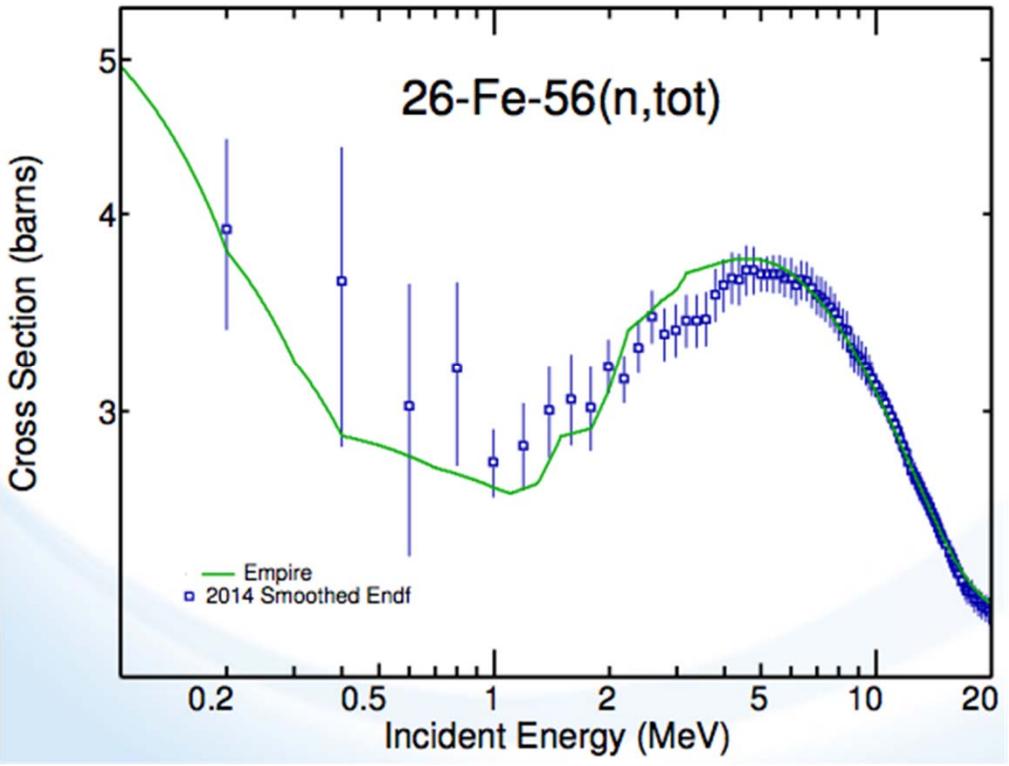
- Compound nucleus
  - HRTW width fluctuations up to 8.00 MeV
  - T_{lj} coupling for the top CN bin up to incident 8.00 MeV
  - CN anisotropy calculated using Blatt-Biedenharn
  - CN decay and Direct cross sections added incoherently
  - Hauser-Feshbach with full γ-cascade
  - Microscopic, parity dependent, HFB level dens. (RIPL-3)
  - Discrete levels from the updated RIPL-3 (ENSDF 2014)
  - E1 strength function set to RIPL MLO1
  - GDR parameters from RIPL/Exp.data+Plujko systematics

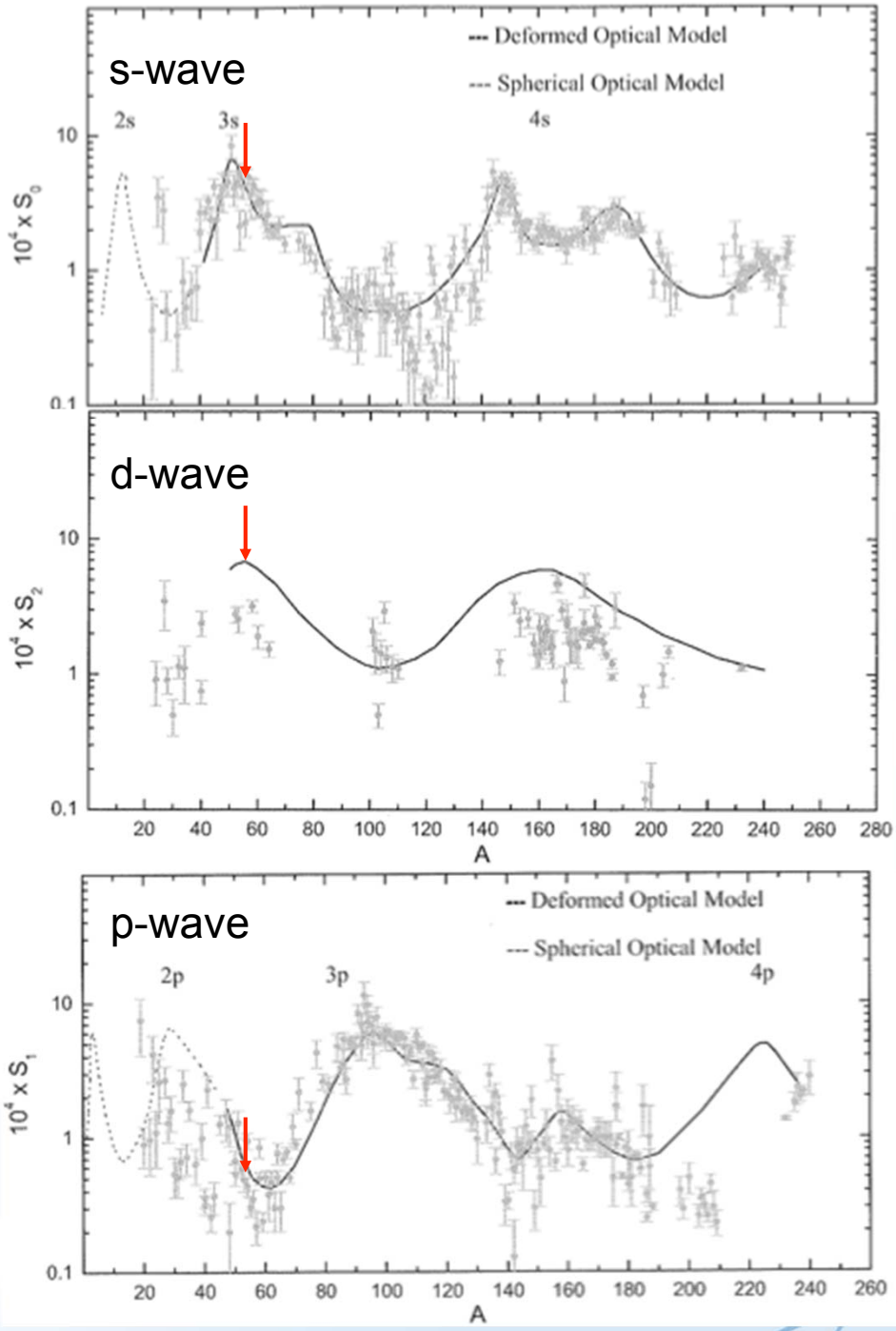
β_o evaluation strategy

- Apply selected models with default parameters
- Adjust only when it's evidently needed and supported by good experimental data
  - total and reaction cross sections below 3 MeV
  - (n,p) reaction cross sections (dosimetry reaction)
  - neutron spectra - DWBA to discrete levels
  - (n,g) at ~14 MeV (magic 1 mb)
- No explicit adjustment for other reactions
- No fine tuning at this stage*)

*) Except for (n,p) because of very well known cross sections

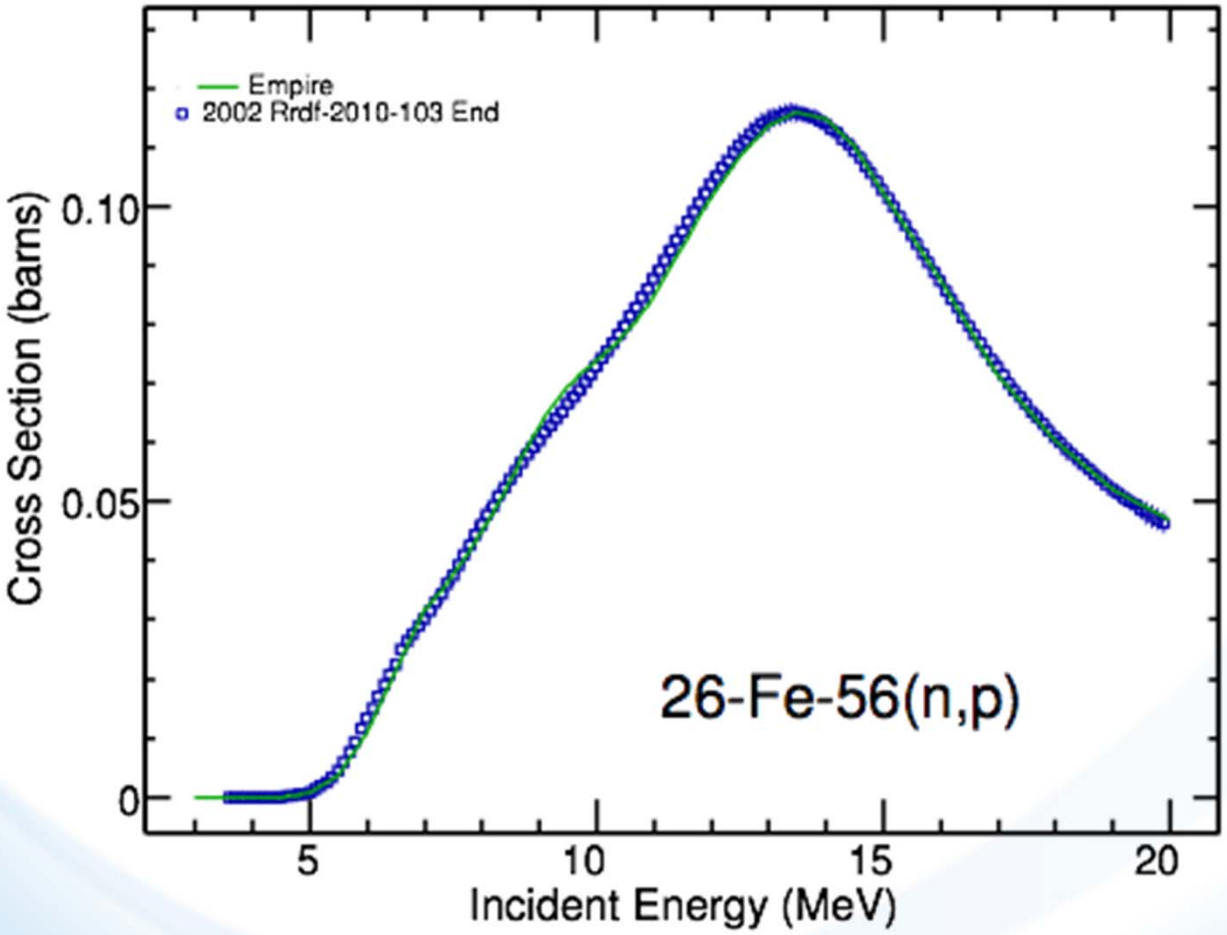
OM problem < 3 MeV





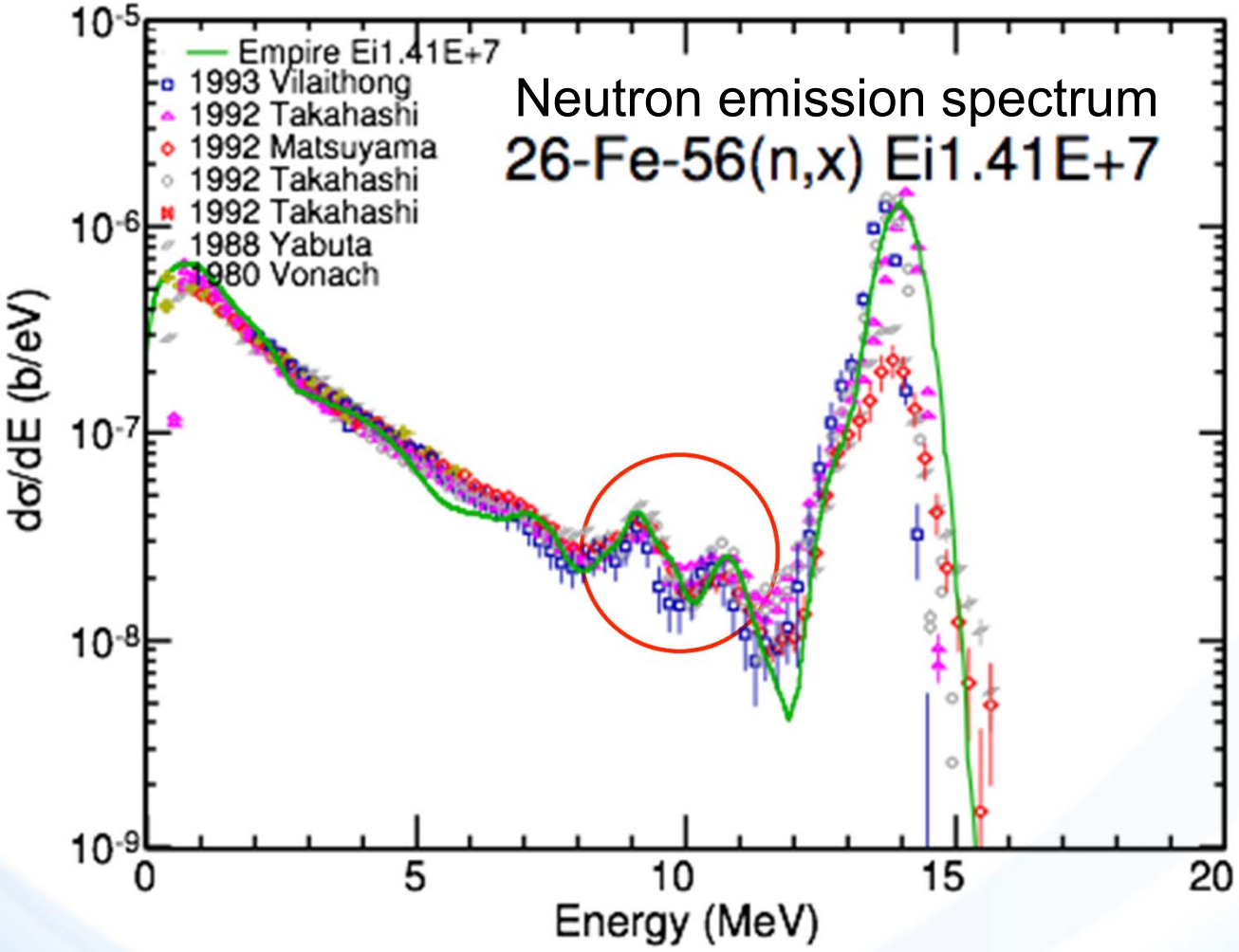
- OM total scaled down to reproduce exp. data (factor 0.65 at 1 keV increasing to 1 at 3 MeV)

(n,p) cross sections



- Adjusted through
  - 56Fe & 55Mn level densities
  - Preequilibrium strength

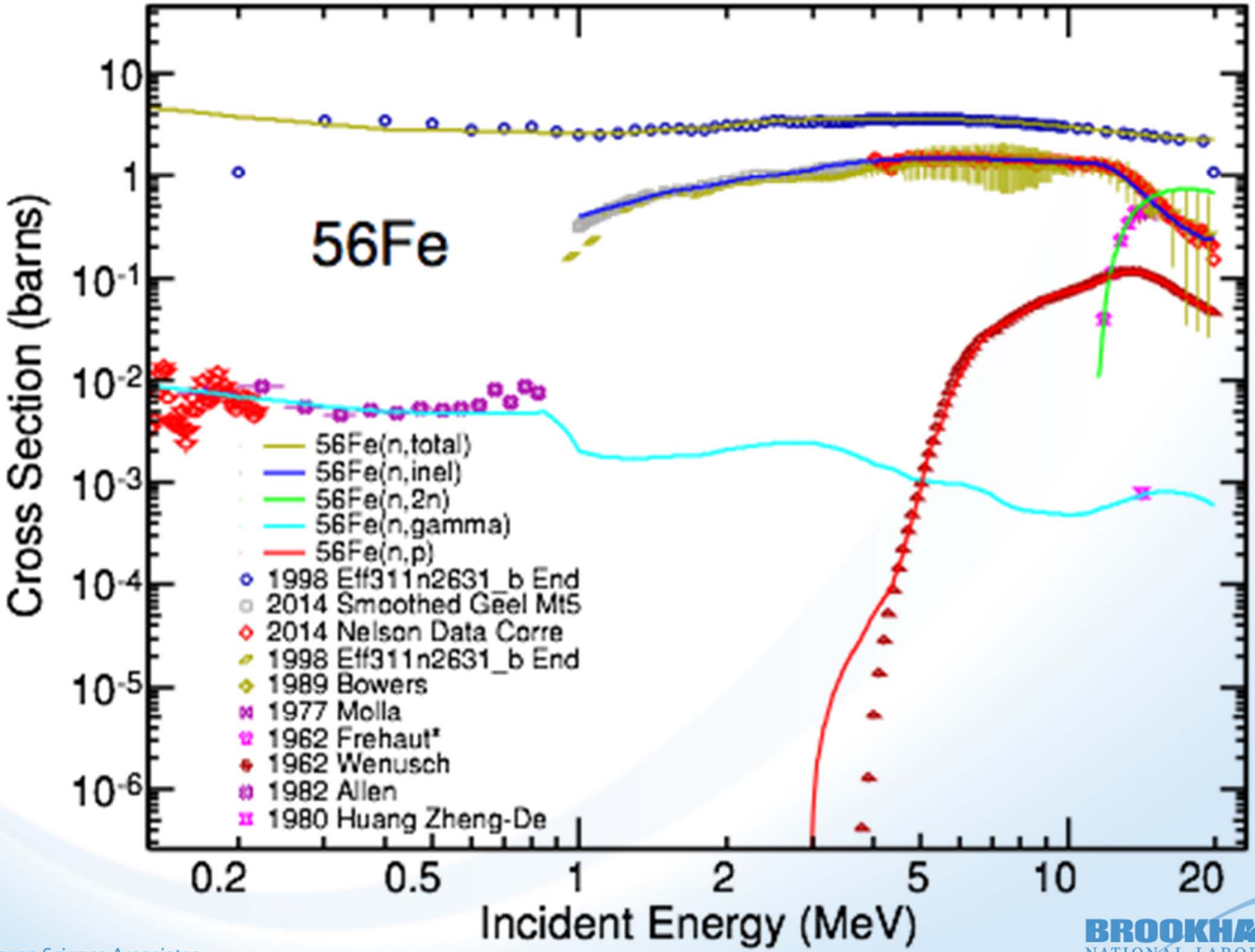
DWBA to discrete levels

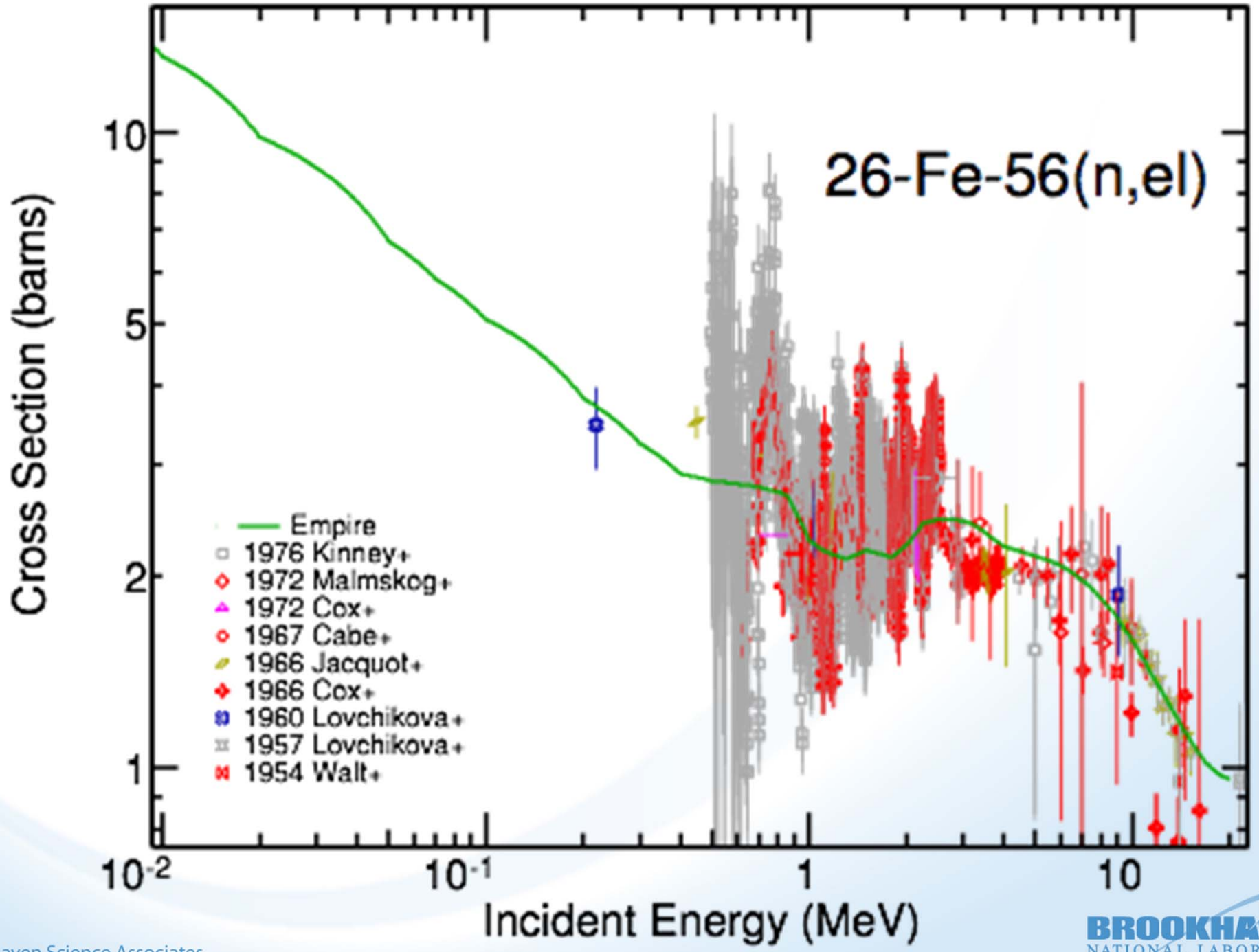


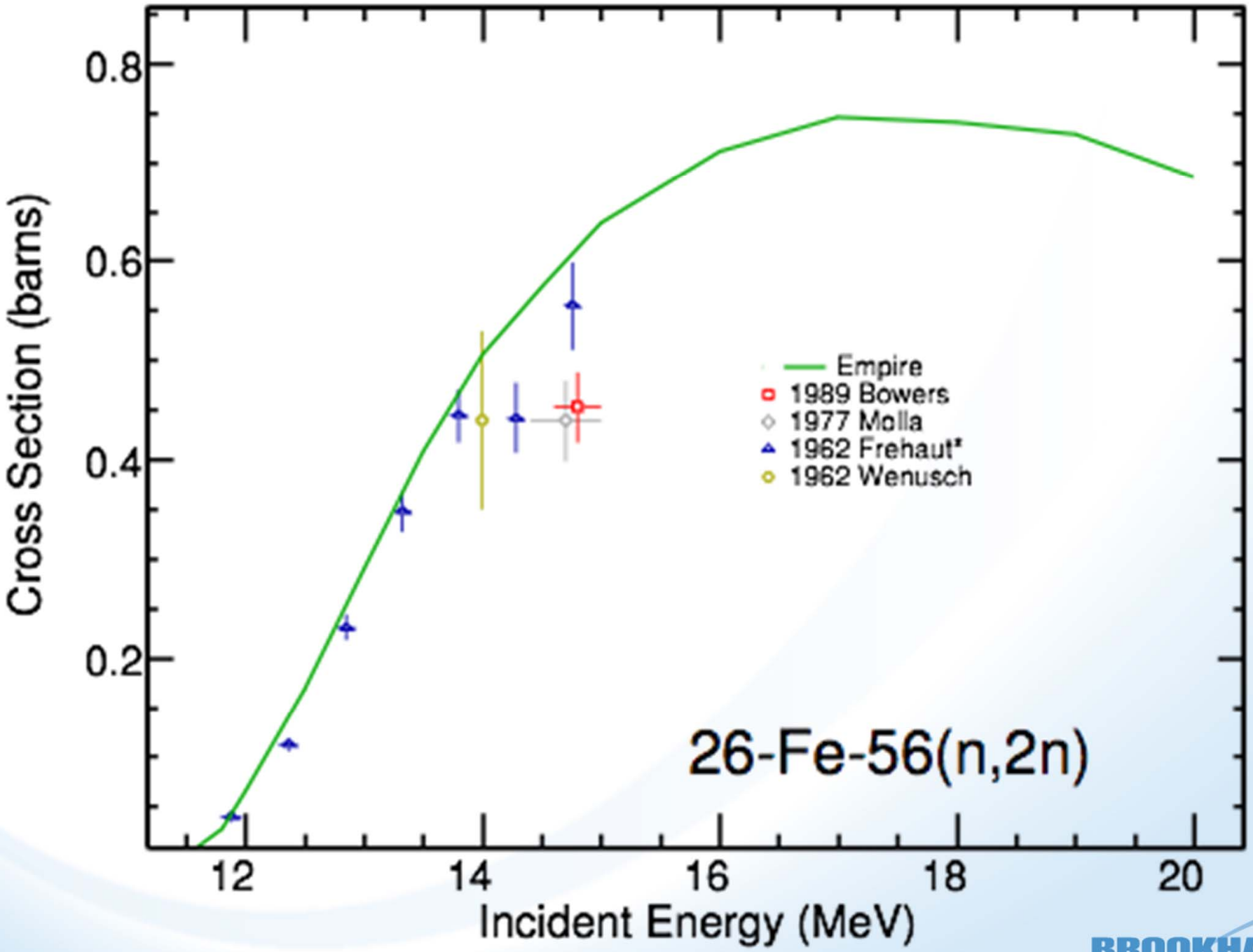
- 13 uncoupled levels treated within DWBA in addition to 8 CC

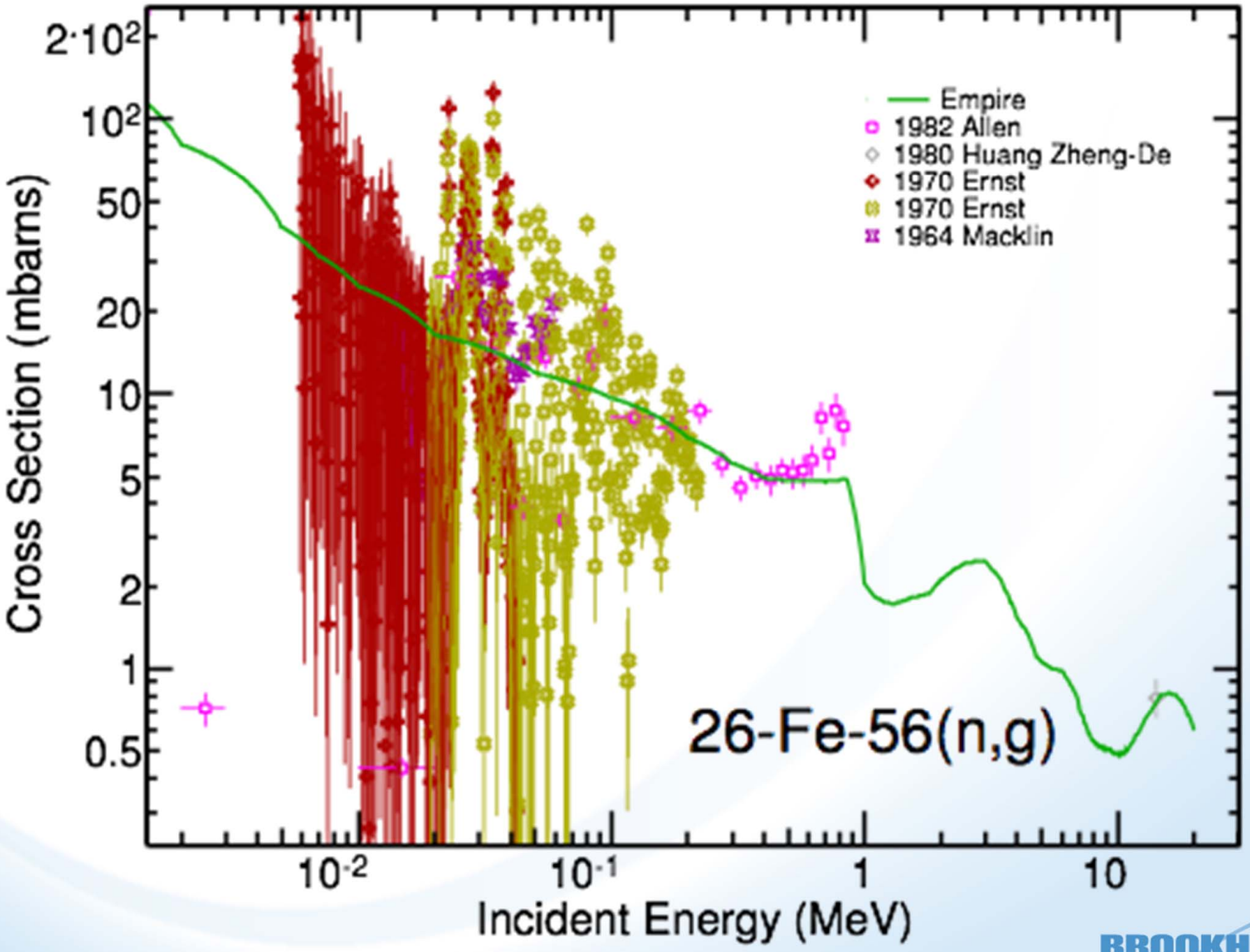
E_{level}	J	Def.
2.95997	2.	0.08115
3.12011	1.	0.00500
3.12297	4.	0.04115
3.36995	2.	0.06000
3.60021	2.	0.00500
3.60569	2.	0.00500
3.61021	0.	0.00500
3.82977	2.	0.07000
3.85649	3.	0.04000
4.04889	3.	0.04000
4.08593	2.	0.04000
4.10036	4.	0.03000
4.11994	3.	0.03000

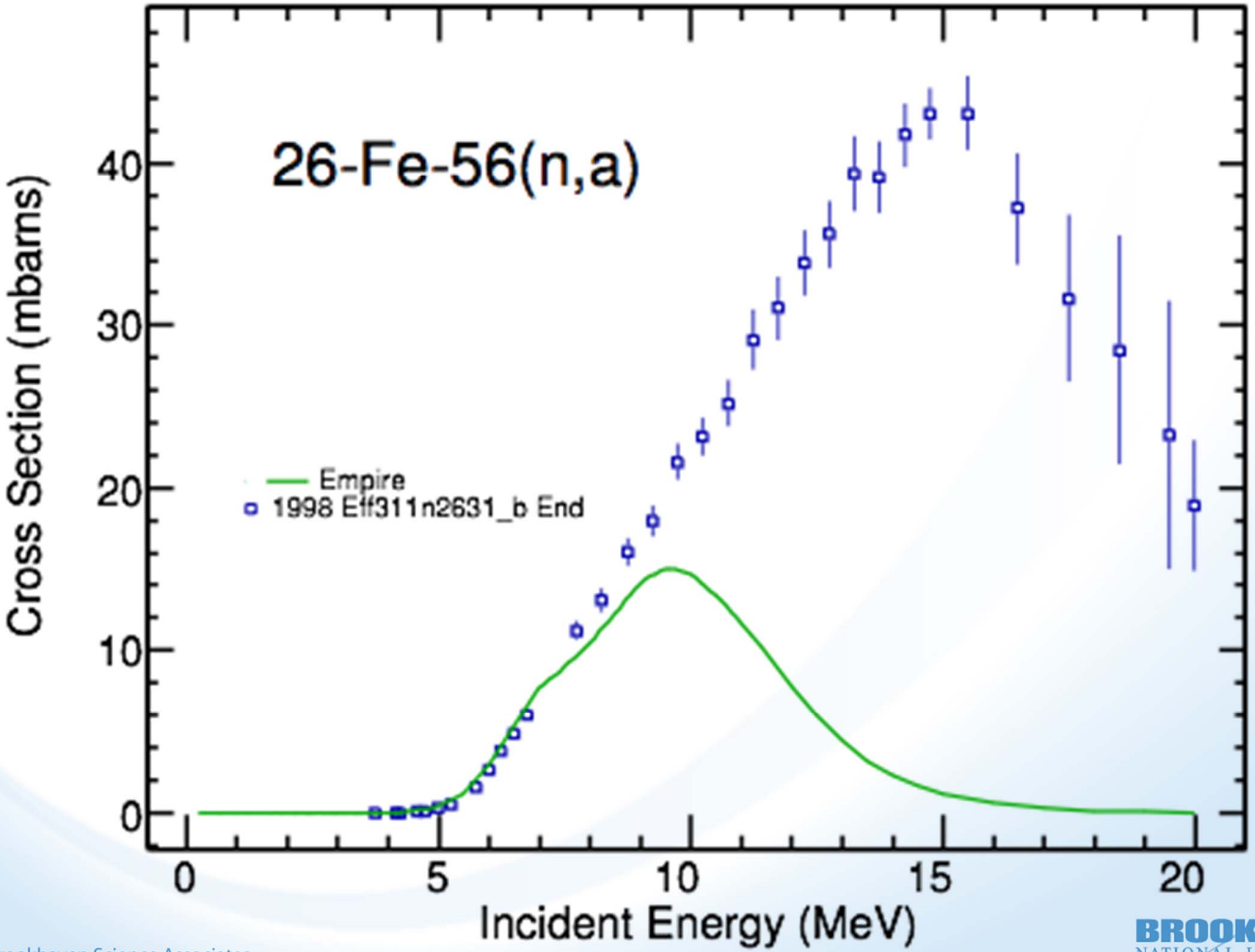
Applying these adjustments produces cross sections shown on the slides that follow

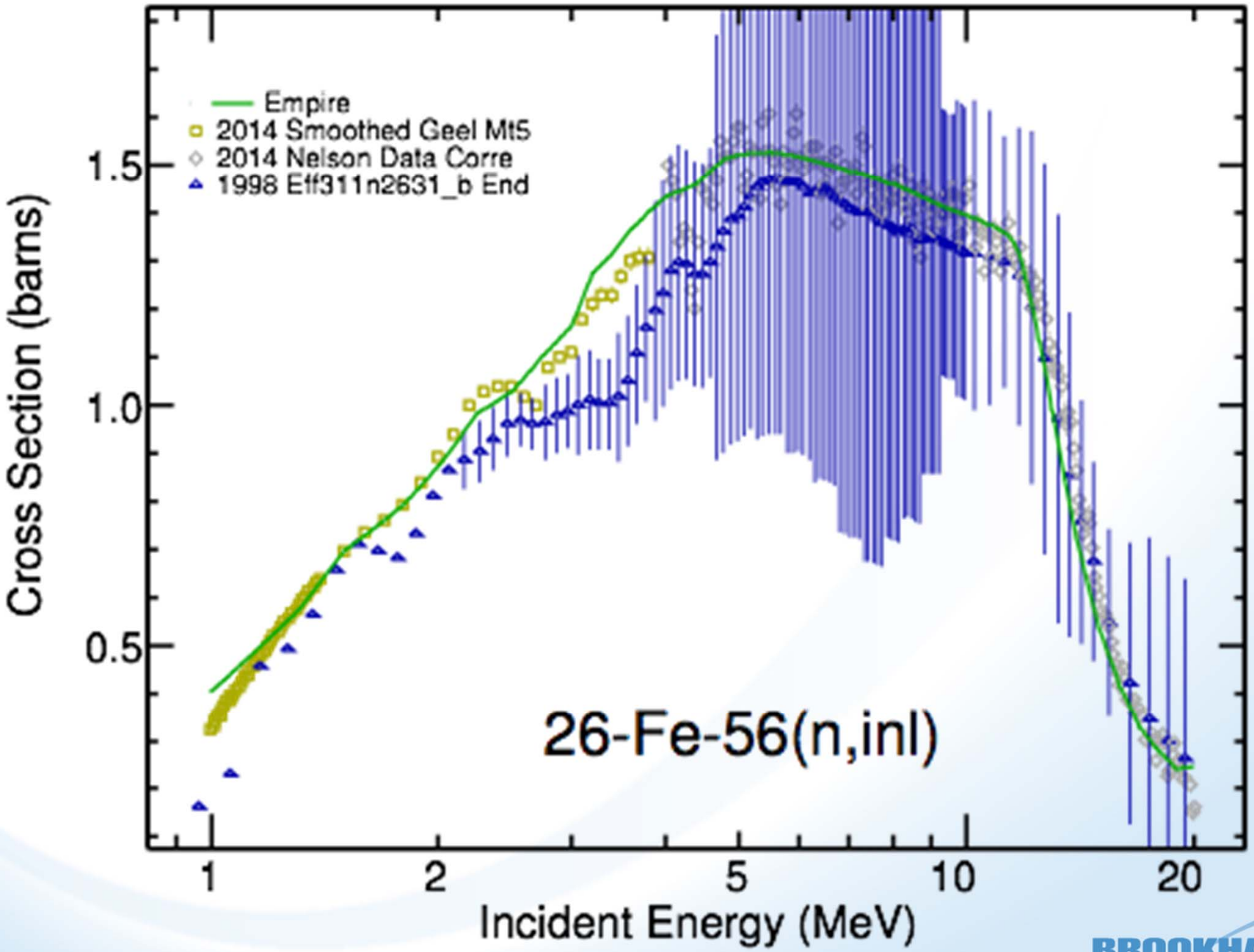

56Fe
Cross Section (barns)
Incident Energy (MeV)
10
1
10-1
10-2
10-3
10-4
10-5
10-6
0.2
0.5
1
2
5
10
20
56Fe(n,total)
56Fe(n,inel)
56Fe(n,2n)
56Fe(n,gamma)
56Fe(n,p)
1998 Eff311n2631_b End
2014 Smoothed Geel Mt5
2014 Nelson Data Corre
1998 Eff311n2631_b End
1989 Bowers
1977 Molla
1962 Frehaut*
1962 Wenusch
1982 Allen
1980 Huang Zheng-De

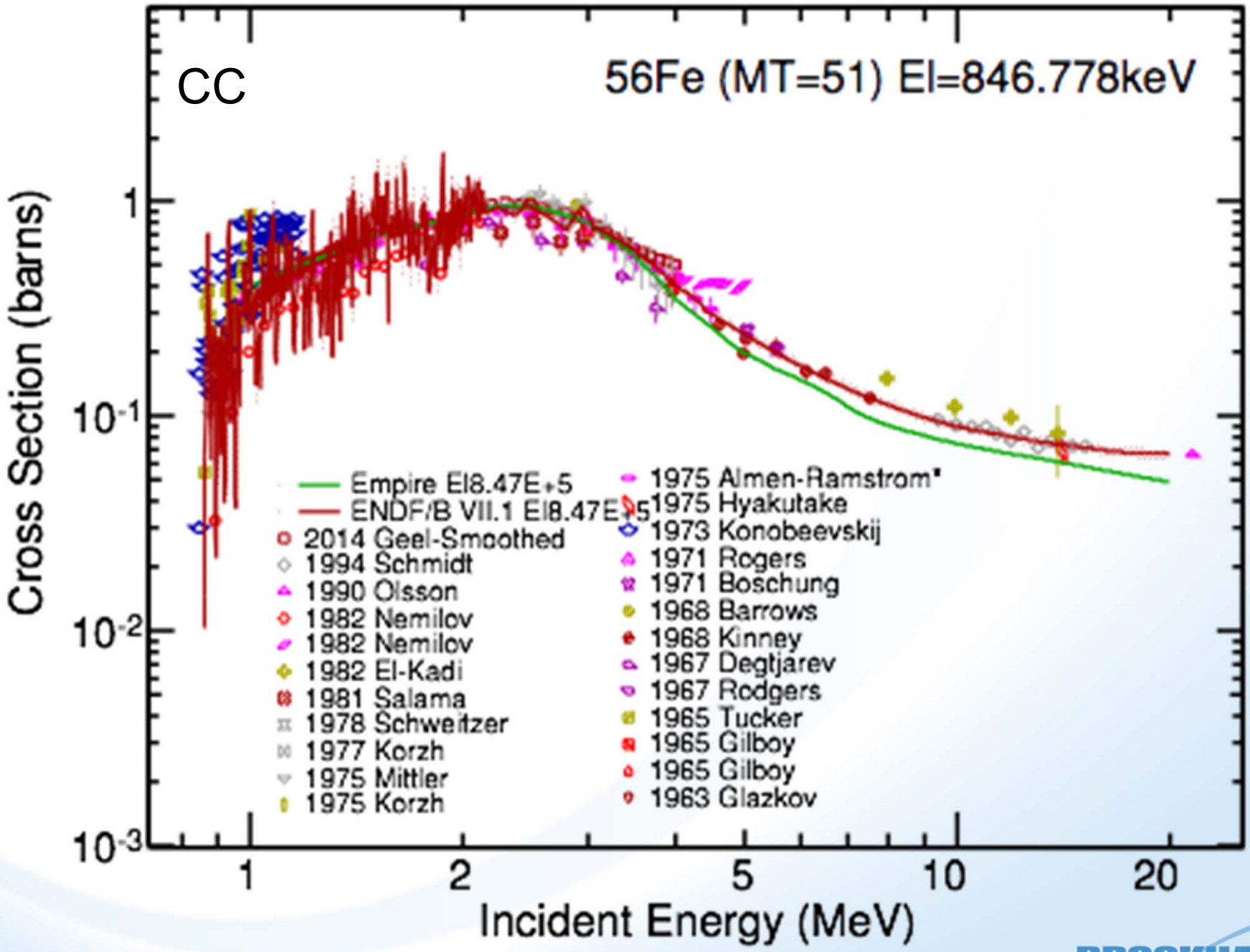

26-Fe-56(n,el)
Cross Section (barns)
Incident Energy (MeV)
10
5
2
1
10^{-2}
10^{-1}
1
10
Empire
1976 Kinney
1972 Malmskog
1972 Cox
1967 Cabe
1966 Jacquot
1966 Cox
1960 Lovchikova
1957 Lovchikova
1954 Walt

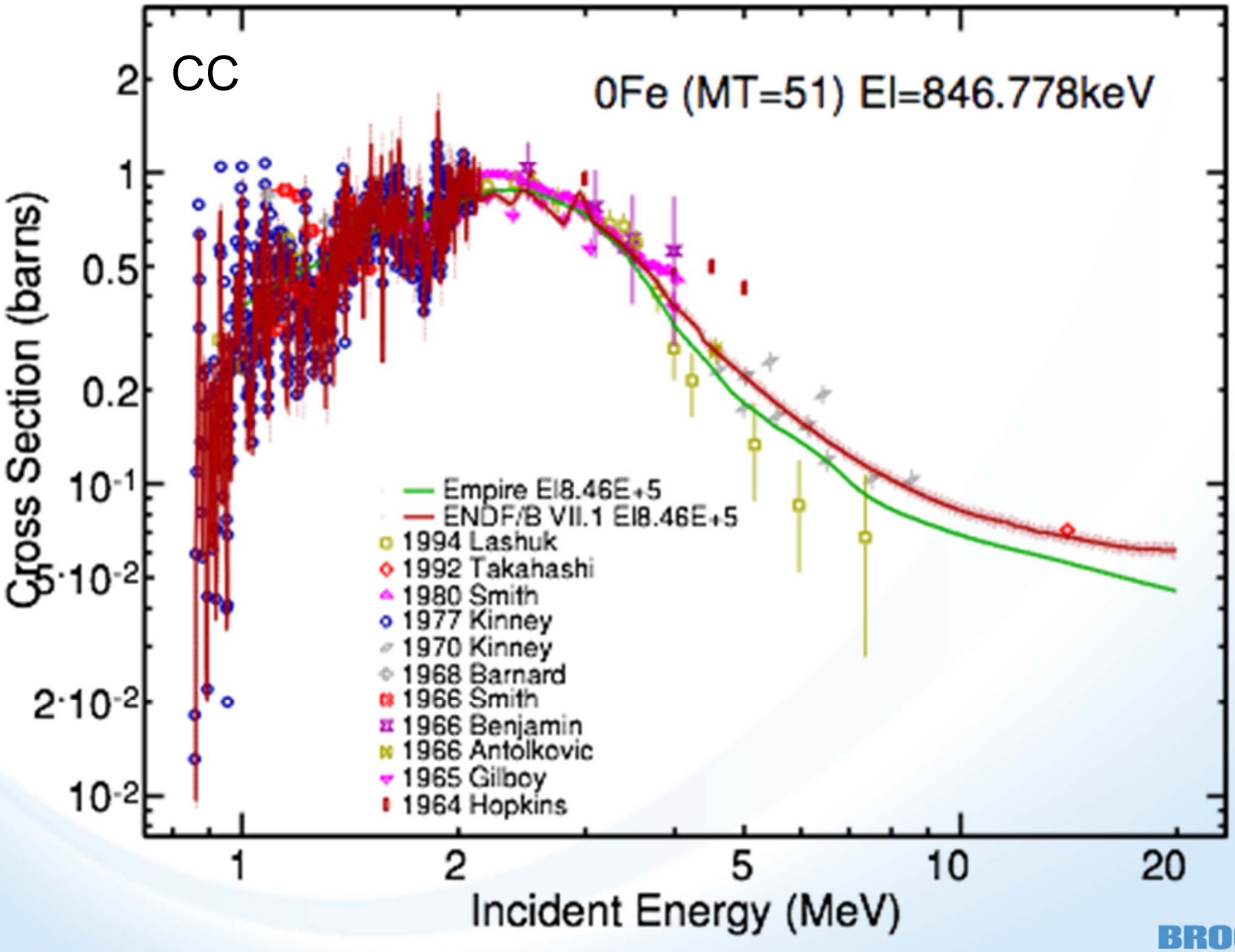

Cross Section (barns)
0.8
0.6
0.4
0.2
12
14
16
18
20
Incident Energy (MeV)
Empire
1989 Bowers
1977 Molla
1962 Frehaut*
1962 Wenusch
26-Fe-56(n,2n)

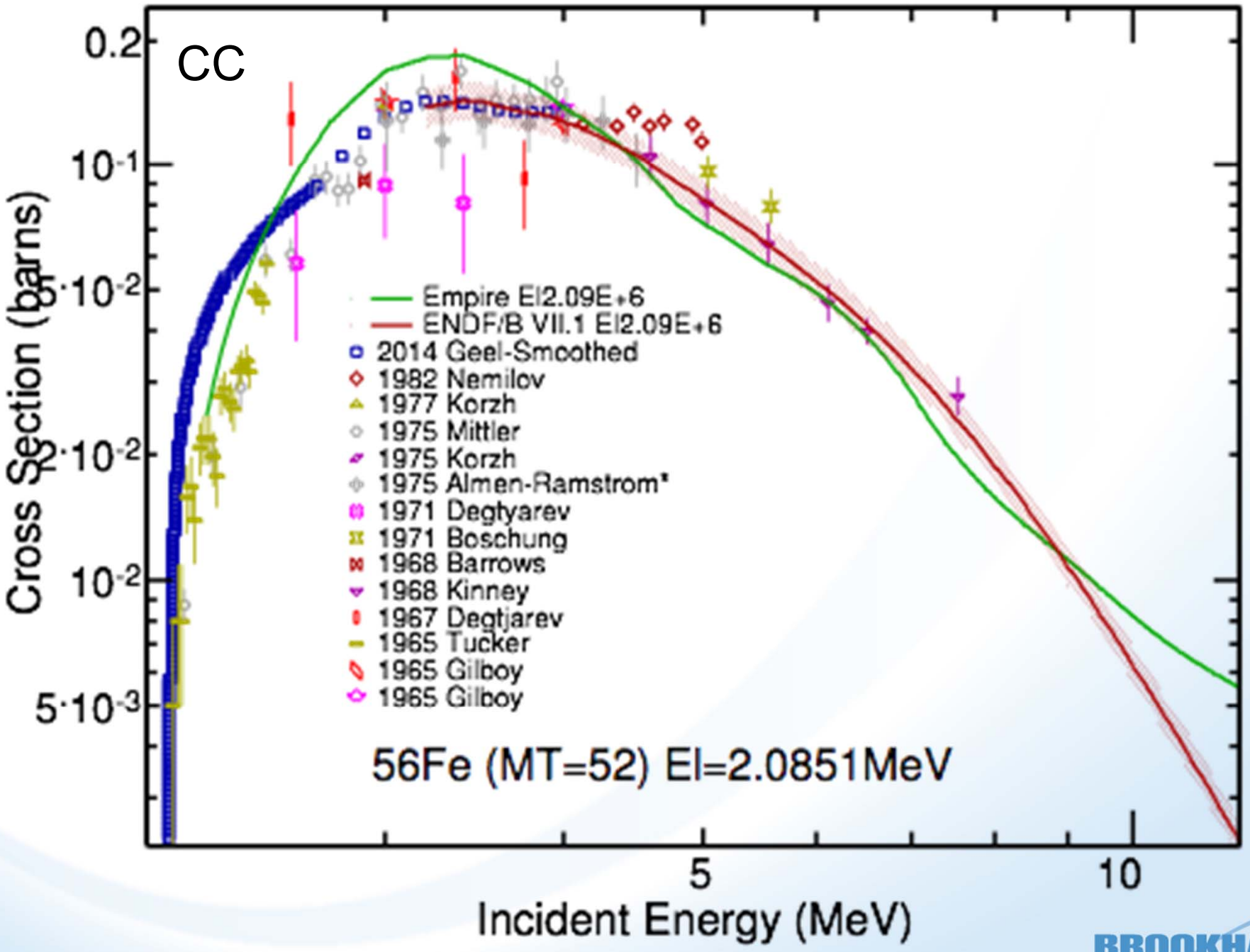

Empire
1982 Allen
1980 Huang Zheng-De
1970 Ernst
1970 Ernst
1964 Macklin
26-Fe-56(n,g)
Cross Section (mbarms)
Incident Energy (MeV)
2·10²
10²
50
20
10
5
2
1
0.5
10⁻²
10⁻¹
1
10

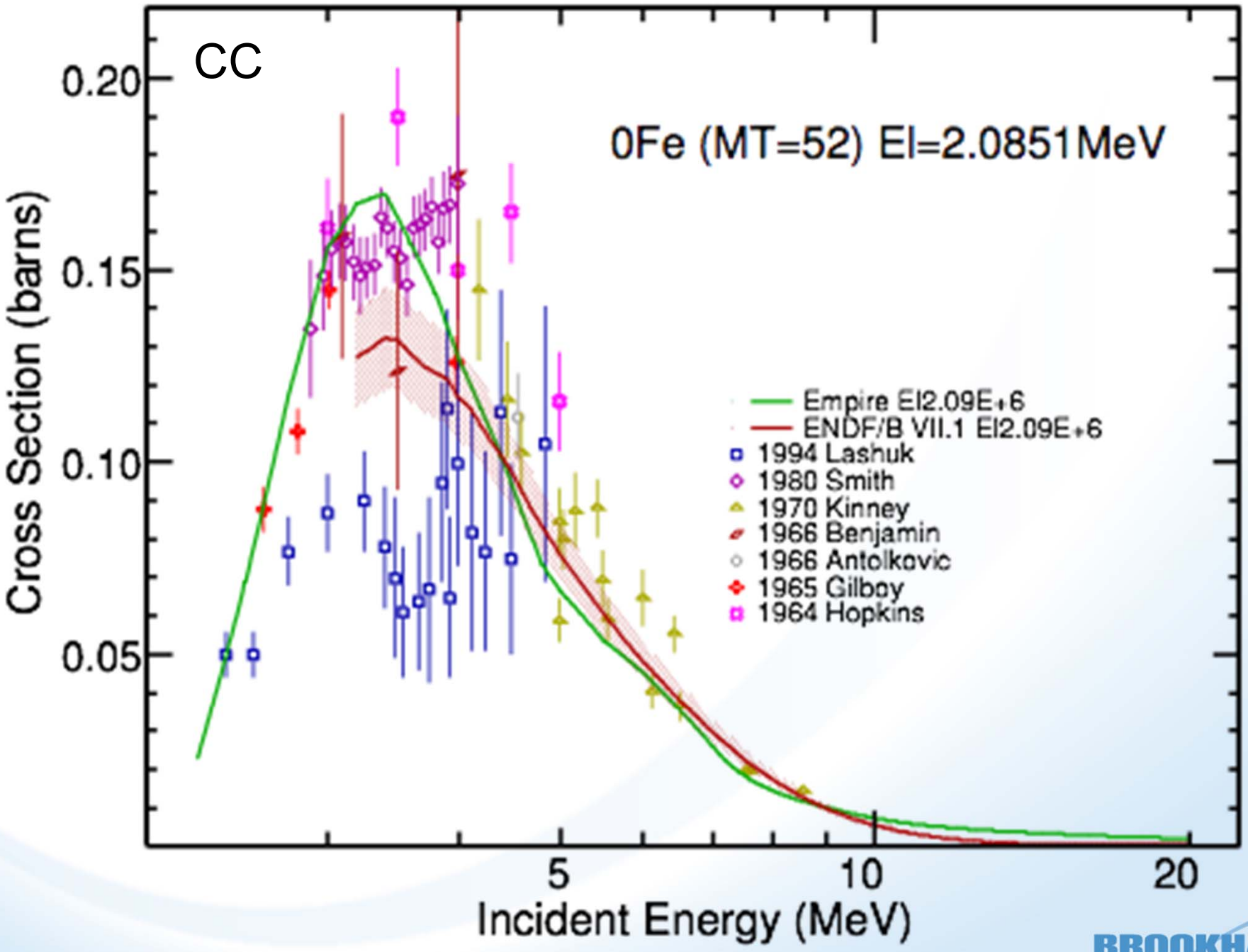

26-Fe-56(n,a)
Empire
1998 Eff311n2631_b End
Cross Section (mbarns)
Incident Energy (MeV)
0
10
20
30
40
0
5
10
15
20

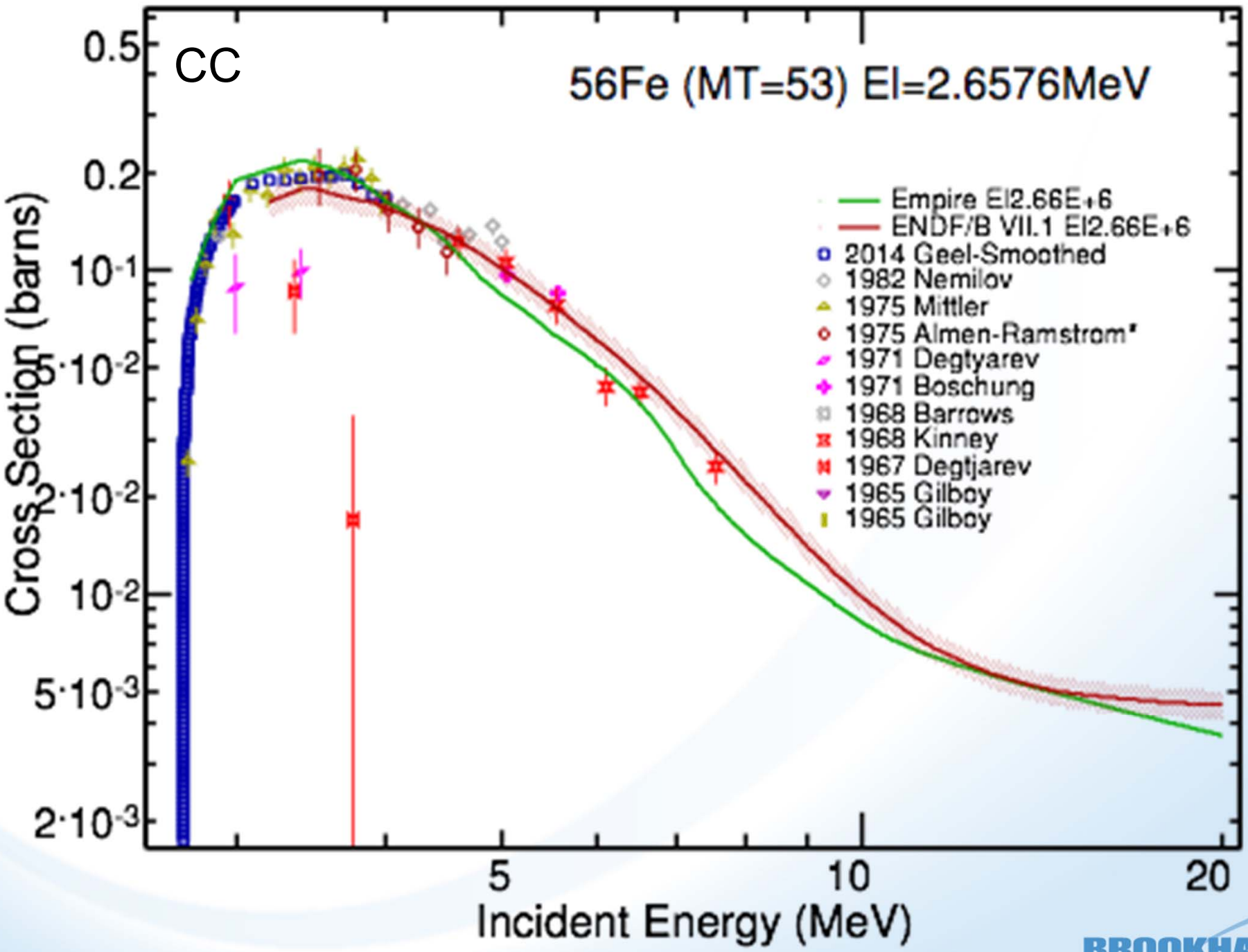

Empire
2014 Smoothed Geel Mt5
2014 Nelson Data Corre
1998 Eff311n2631_b End
Cross Section (barns)
1.5
1.0
0.5
26-Fe-56(n,inl)
1
2
5
10
20
Incident Energy (MeV)

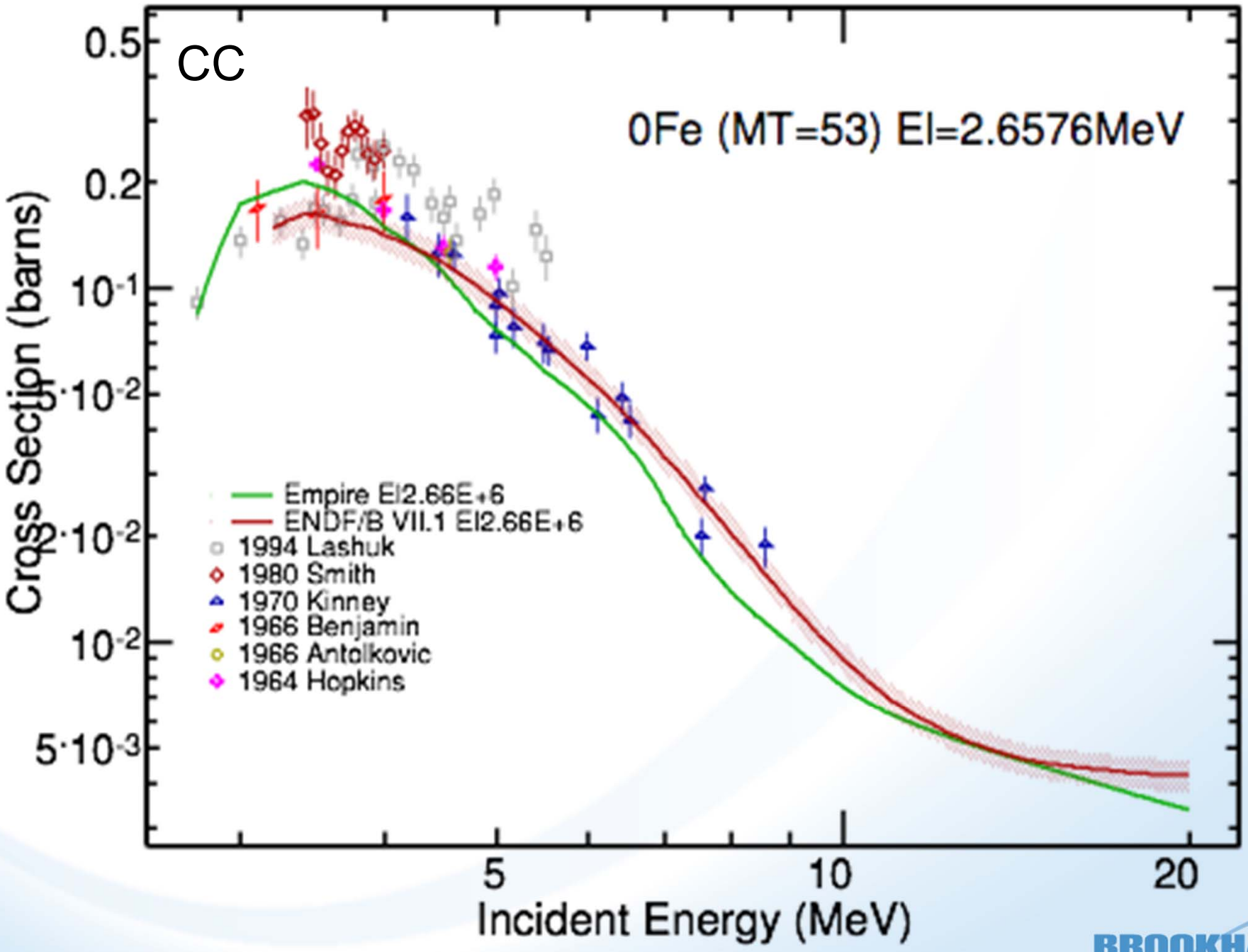

CC
56Fe (MT=51) El=846.778keV
Cross Section (barns)
1
10-1
10-2
10-3
1
2
5
10
20
Incident Energy (MeV)
Empire El8.47E+5
ENDF/B VII.1 El8.47E+5
2014 Geel-Smoothed
1994 Schmidt
1990 Olsson
1982 Nemilov
1982 Nemilov
1982 El-Kadi
1981 Salama
1978 Schweitzer
1977 Korzh
1975 Mittler
1975 Korzh
1975 Almen-Ramstrom*
1975 Hyakutake
1973 Konobeevskij
1971 Rogers
1971 Boschung
1968 Barrows
1968 Kinney
1967 Degtjarev
1967 Rodgers
1965 Tucker
1965 Gilboy
1965 Gilboy
1963 Glazkov

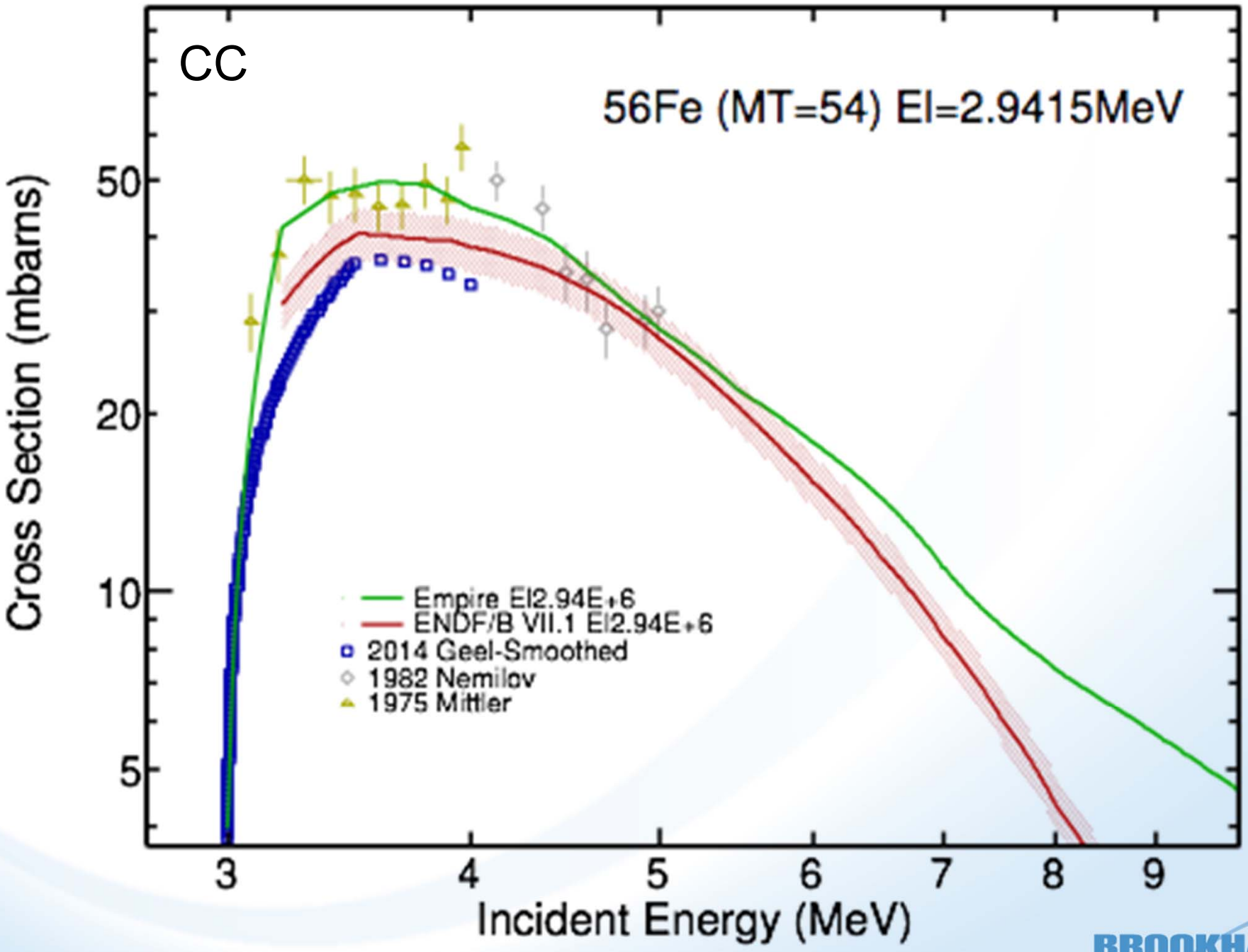

CC
0Fe (MT=51) El=846.778keV
Cross Section (barns)
2
1
0.5
0.2
10-1
5·10-2
2·10-2
10-2
Empire El8.46E+5
ENDF/B VII.1 El8.46E+5
1994 Lashuk
1992 Takahashi
1980 Smith
1977 Kinney
1970 Kinney
1968 Barnard
1966 Smith
1966 Benjamin
1966 Antolkovic
1965 Gilboy
1964 Hopkins
1
2
5
10
20
Incident Energy (MeV)

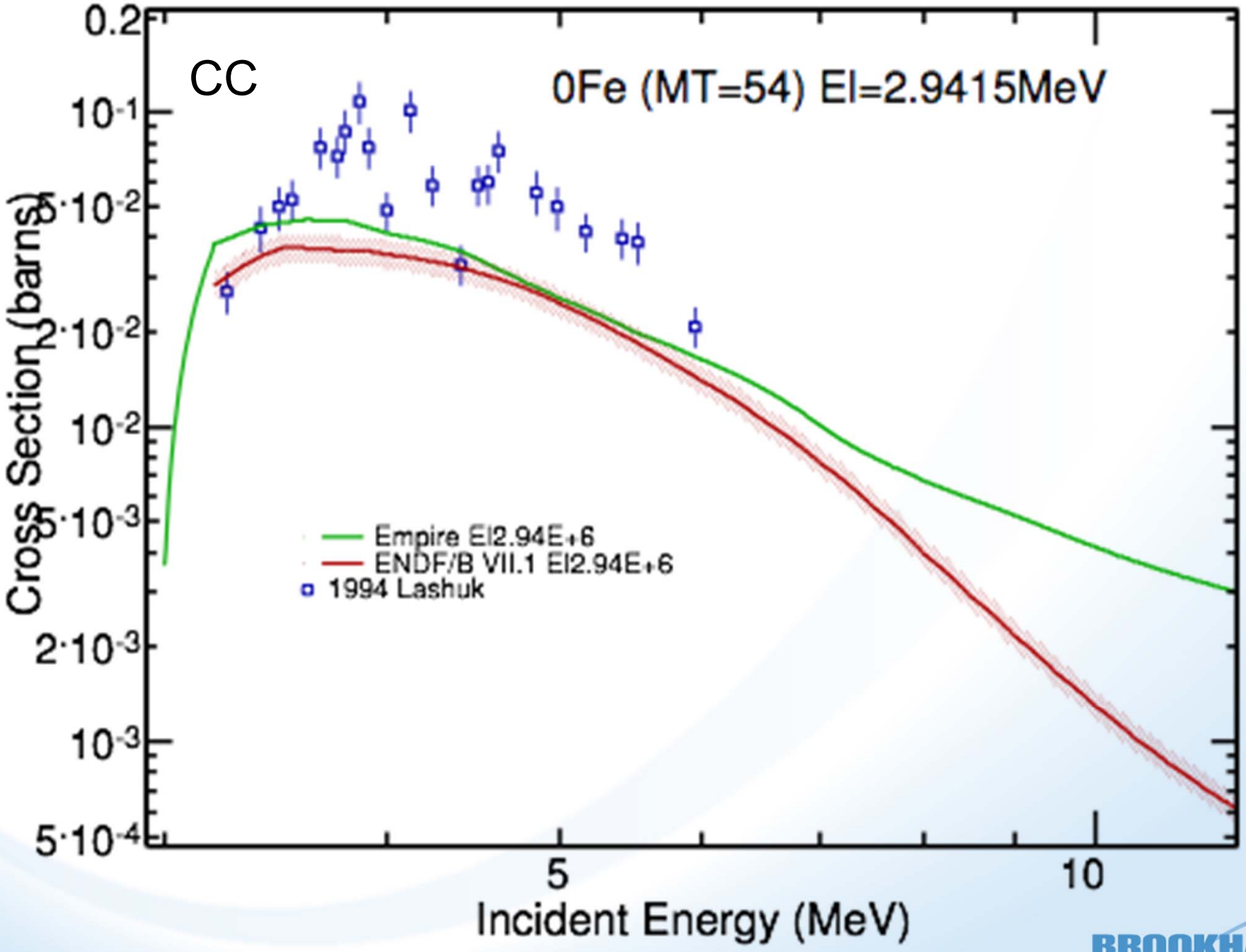

CC
0.2
10-1
5·10-2
2·10-2
10-2
5·10-3
Cross Section (barns)
Empire EI2.09E+6
ENDF/B VII.1 EI2.09E+6
2014 Geel-Smoothed
1982 Nemilov
1977 Korzh
1975 Mittler
1975 Korzh
1975 Almen-Ramstrom*
1971 Degtyarev
1971 Boschung
1968 Barrows
1968 Kinney
1967 Degtjarev
1965 Tucker
1965 Gilboy
1965 Gilboy
56Fe (MT=52) EI=2.0851MeV
5
10
Incident Energy (MeV)

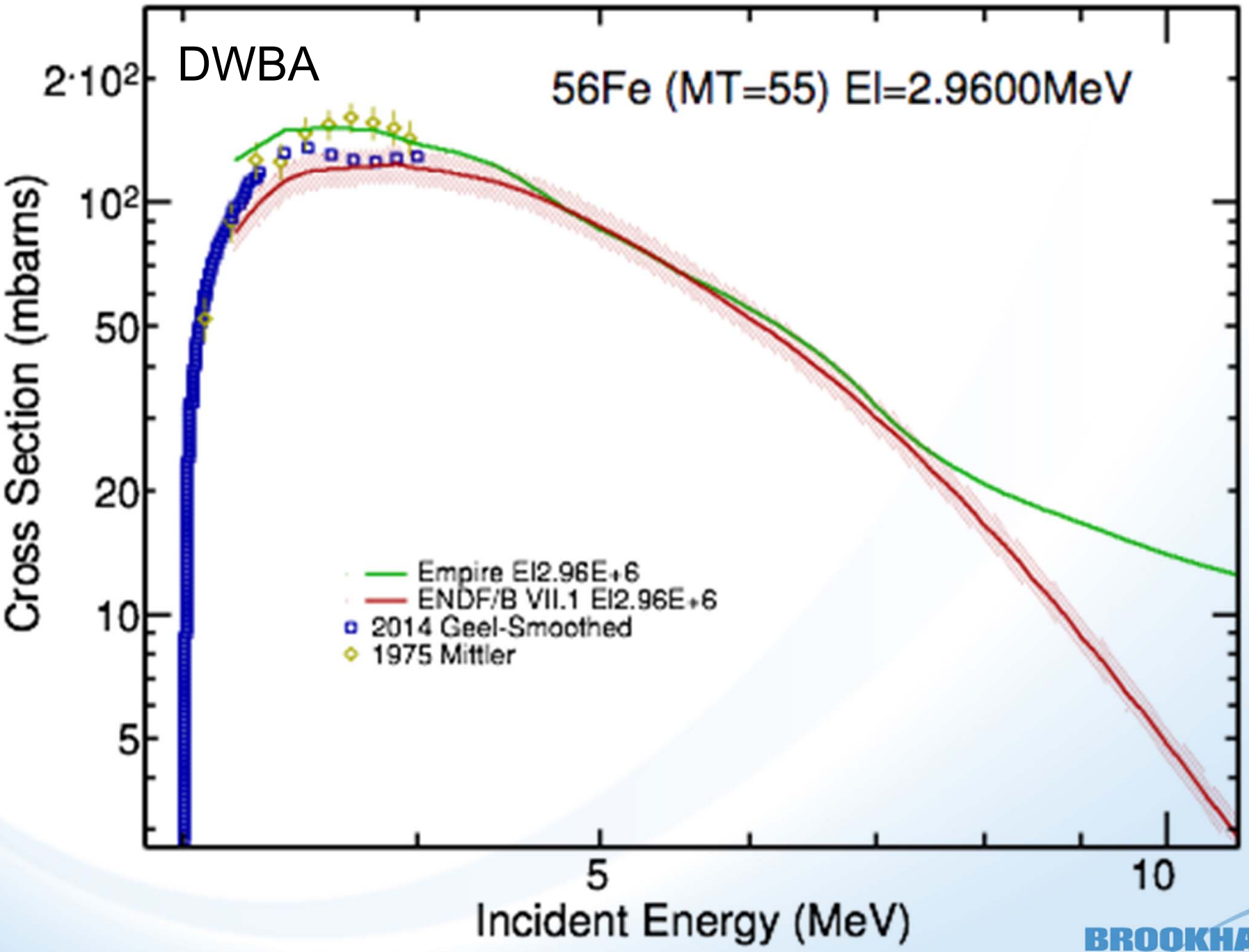

CC
0Fe (MT=52) EI=2.0851MeV
Cross Section (barns)
0.20
0.15
0.10
0.05
5
10
20
Incident Energy (MeV)
Empire EI2.09E+6
ENDF/B VII.1 EI2.09E+6
1994 Lashuk
1980 Smith
1970 Kinney
1966 Benjamin
1966 Antolkovic
1965 Gilboy
1964 Hopkins

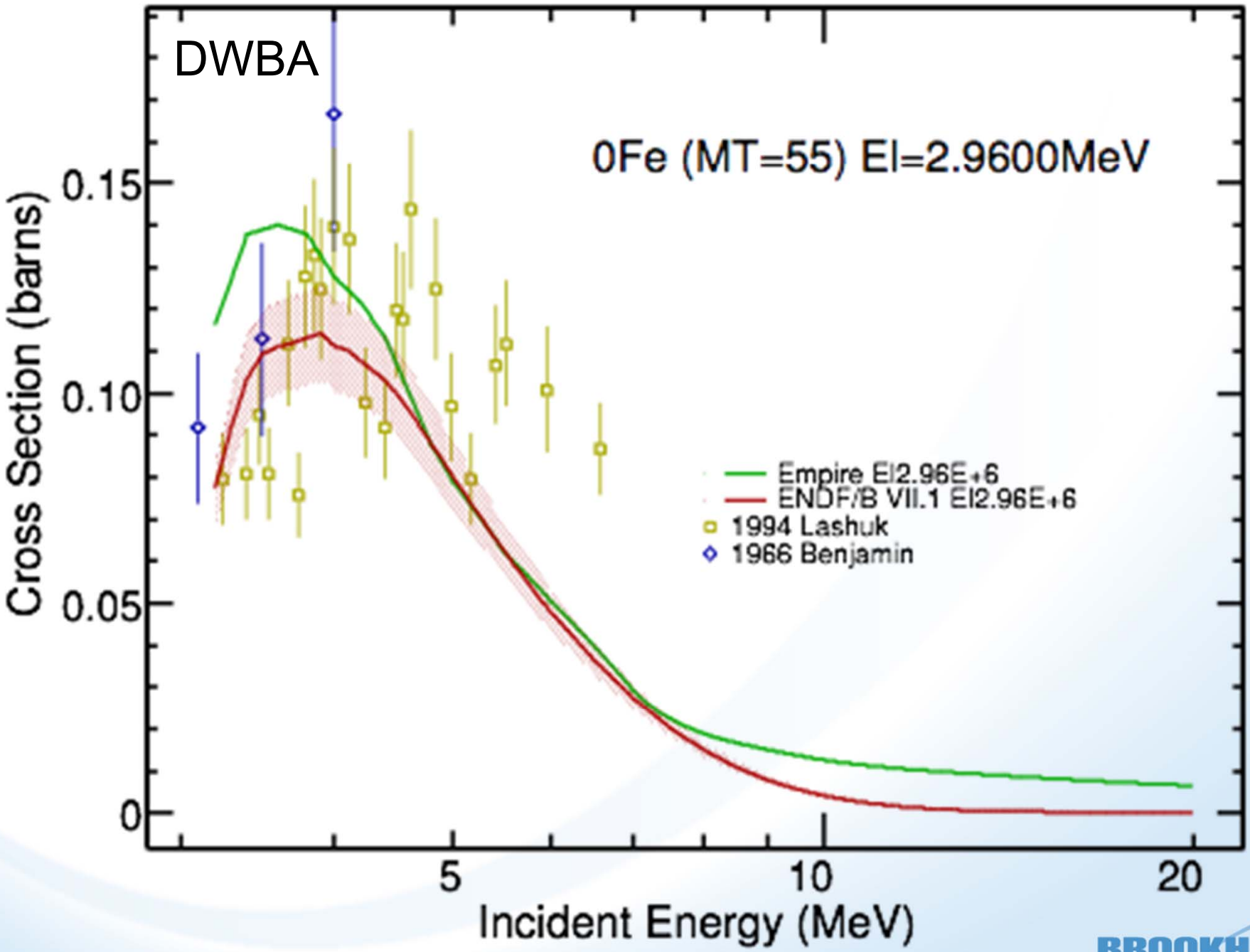

CC
56Fe (MT=53) EI=2.6576MeV
Cross Section (barns)
Incident Energy (MeV)
0.5
0.2
10-1
5·10-2
2·10-2
10-2
5·10-3
2·10-3
5
10
20
Empire EI2.66E+6
ENDF/B VII.1 EI2.66E+6
2014 Geel-Smoothed
1982 Nemilov
1975 Mittler
1975 Almen-Ramstrom*
1971 Degtyarev
1971 Boschung
1968 Barrows
1968 Kinney
1967 Degtjarev
1965 Gilboy
1965 Gilboy

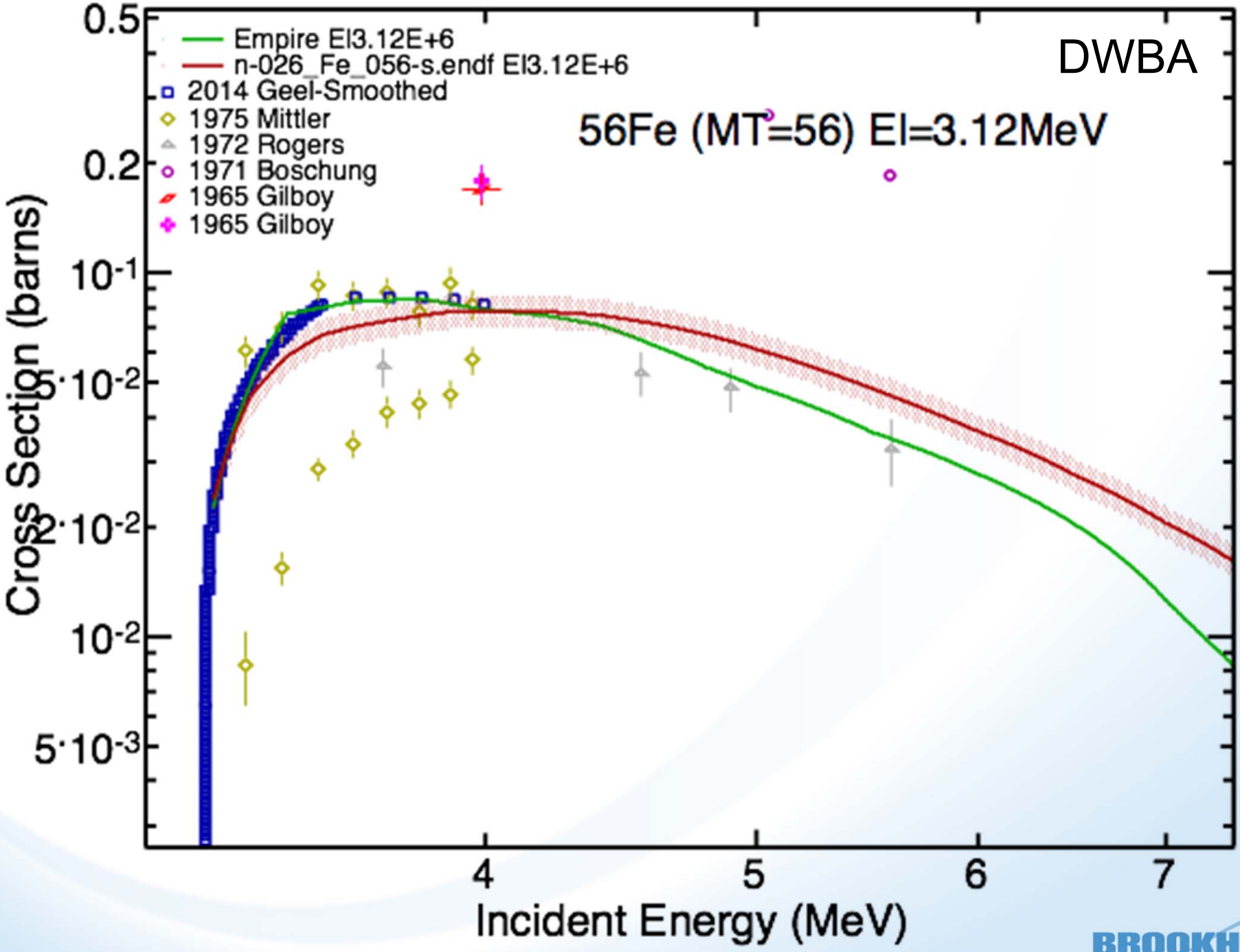

CC
0Fe (MT=53) El=2.6576MeV
Cross Section (barns)
0.5
0.2
10-1
5·10-2
2·10-2
10-2
5·10-3
5
10
20
Incident Energy (MeV)
Empire El2.66E+6
ENDF/B VII.1 El2.66E+6
1994 Lashuk
1980 Smith
1970 Kinney
1966 Benjamin
1966 Antolkovic
1964 Hopkins

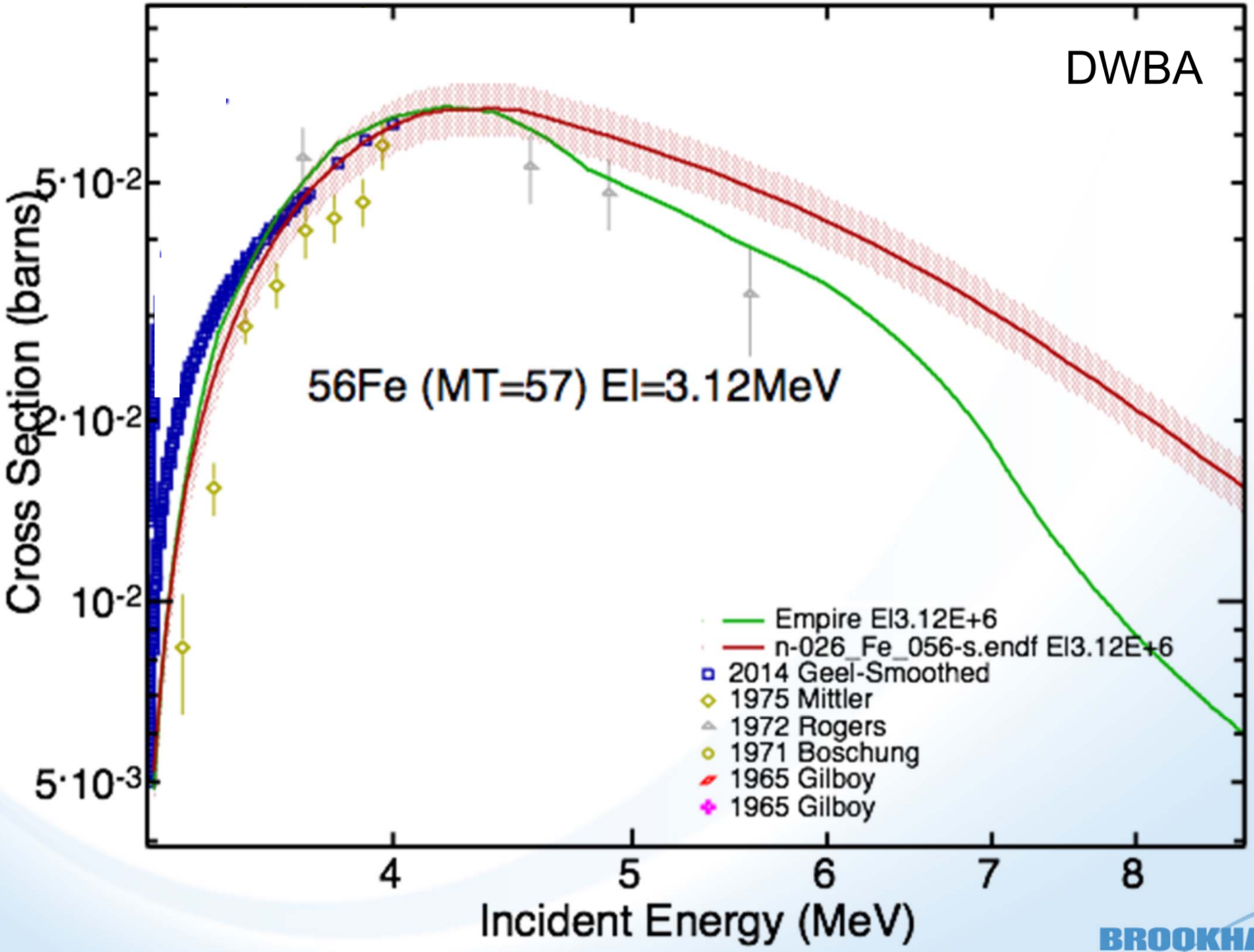

CC
56Fe (MT=54) EI=2.9415MeV
Cross Section (mbarms)
50
20
10
5
3
4
5
6
7
8
9
Incident Energy (MeV)
Empire EI2.94E+6
ENDF/B VII.1 EI2.94E+6
2014 Geel-Smoothed
1982 Nemilov
1975 Mittler

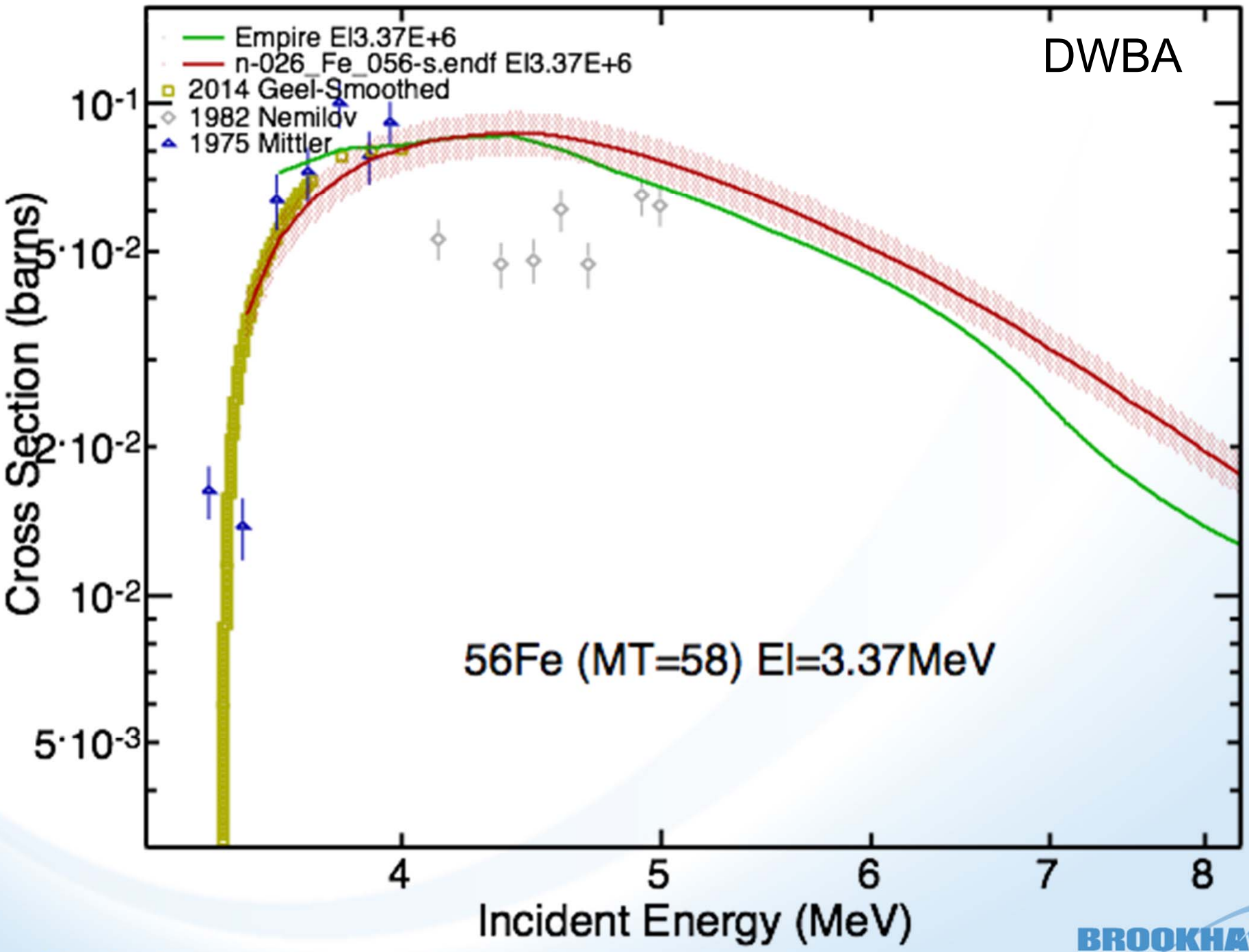

CC
0Fe (MT=54) El=2.9415MeV
Cross Section (barns)
0.2
10-1
8·10-2
2·10-2
10-2
5·10-3
2·10-3
10-3
5·10-4
5
10
Incident Energy (MeV)
Empire El2.94E+6
ENDF/B VII.1 El2.94E+6
1994 Lashuk

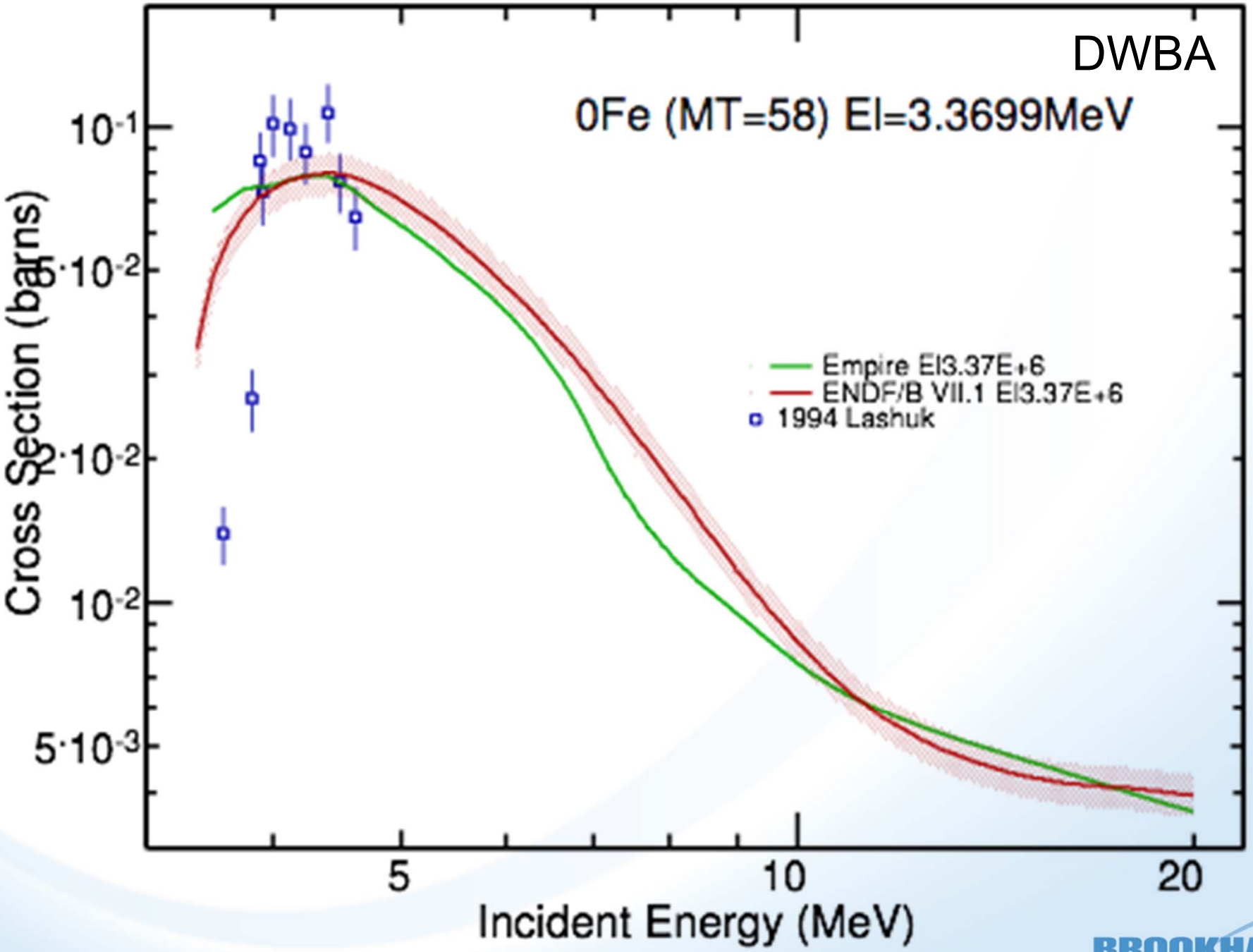

DWBA
56Fe (MT=55) El=2.9600MeV
Cross Section (mbarms)
2·10²
10²
50
20
10
5
5
10
Incident Energy (MeV)
Empire El2.96E+6
ENDF/B VII.1 El2.96E+6
2014 Geel-Smoothed
1975 Mittler

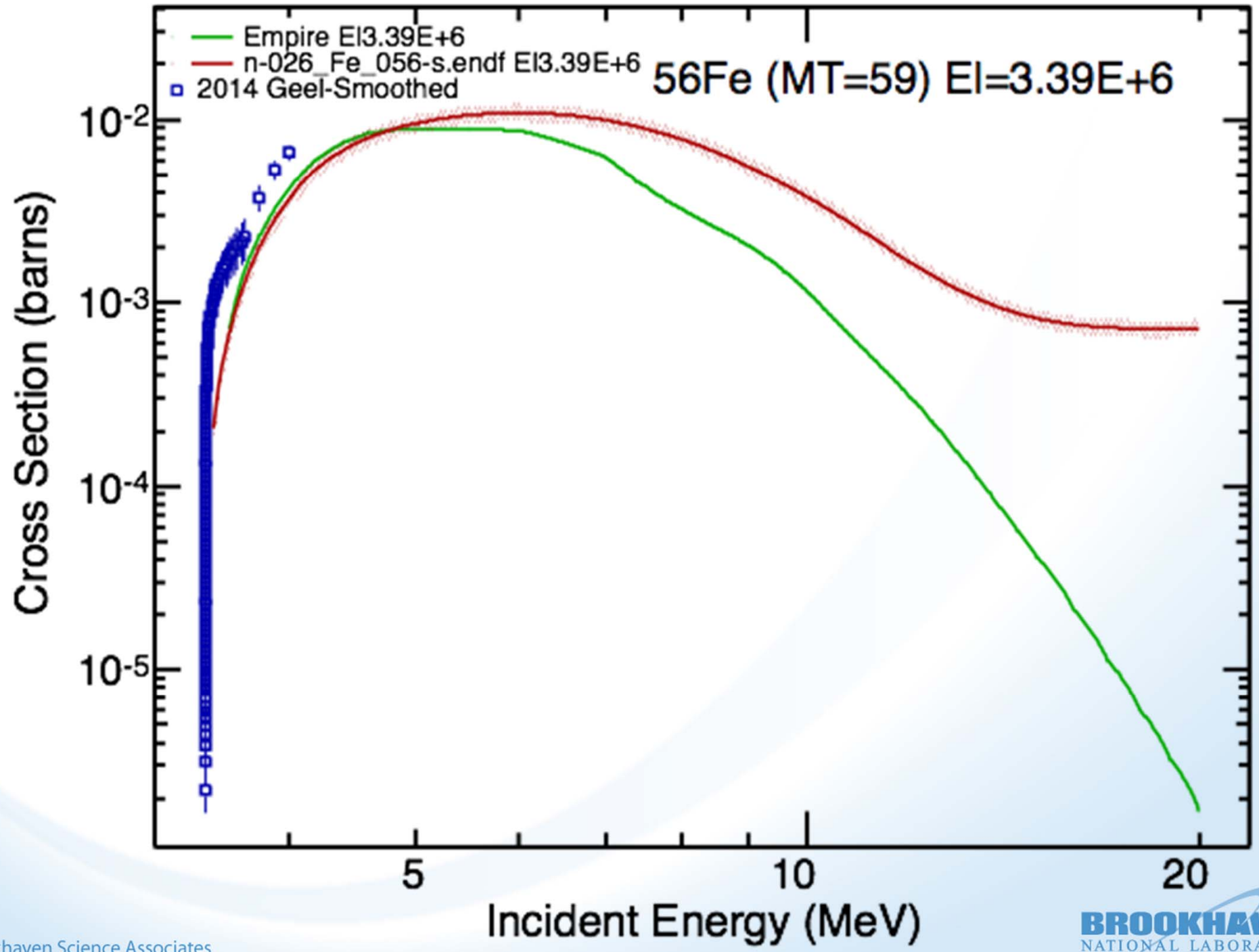

DWBA
0Fe (MT=55) El=2.9600MeV
Cross Section (barns)
0.15
0.10
0.05
0
5
10
20
Incident Energy (MeV)
Empire El2.96E+6
ENDF/B VII.1 El2.96E+6
1994 Lashuk
1966 Benjamin

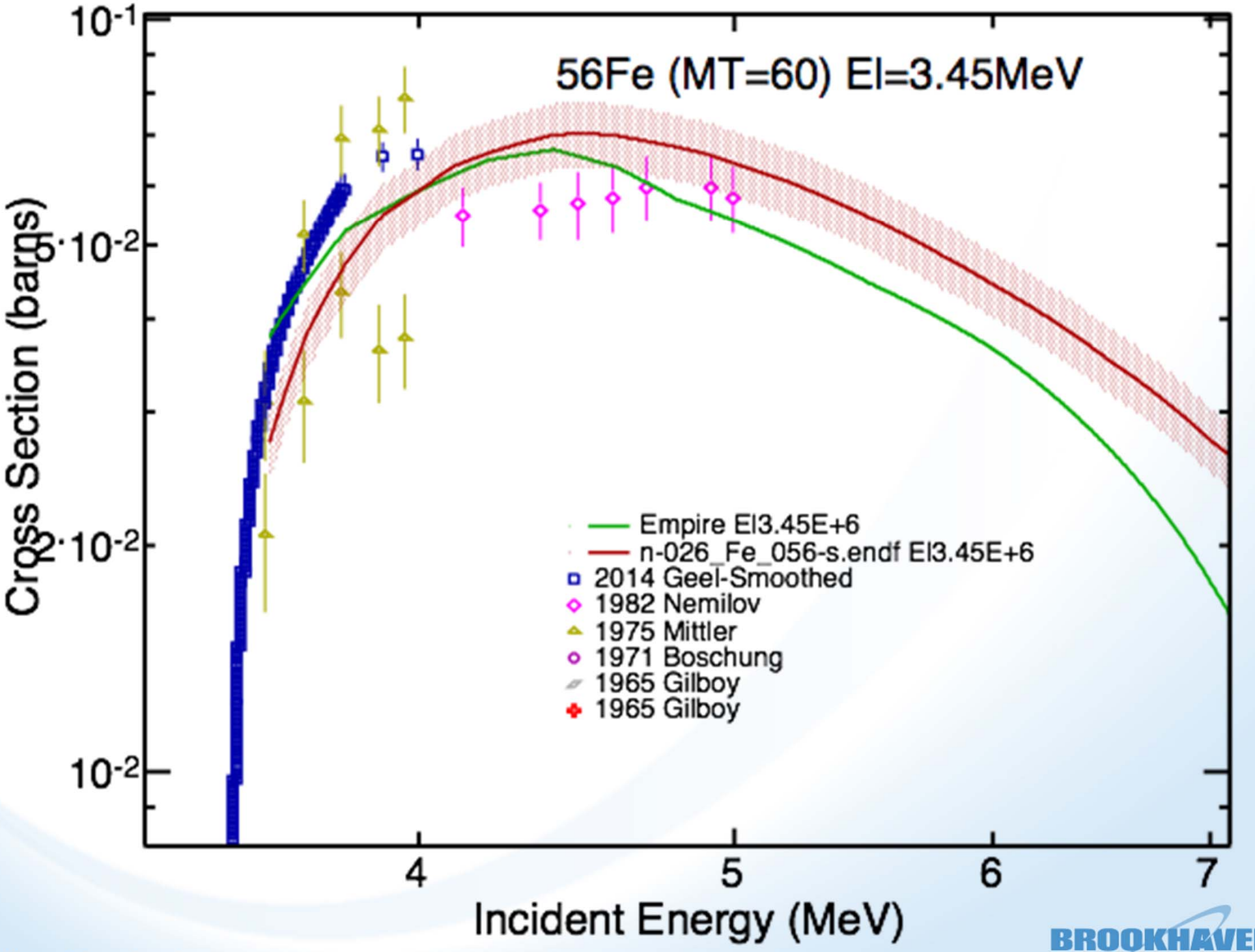

DWBA
56Fe (MT=56) EI=3.12MeV
Empire EI3.12E+6
n-026_Fe_056-s.endf EI3.12E+6
2014 Geel-Smoothed
1975 Mittler
1972 Rogers
1971 Boschung
1965 Gilboy
1965 Gilboy
Cross Section (barns)
0.5
0.2
10-1
5·10-2
2·10-2
10-2
5·10-3
4
5
6
7
Incident Energy (MeV)

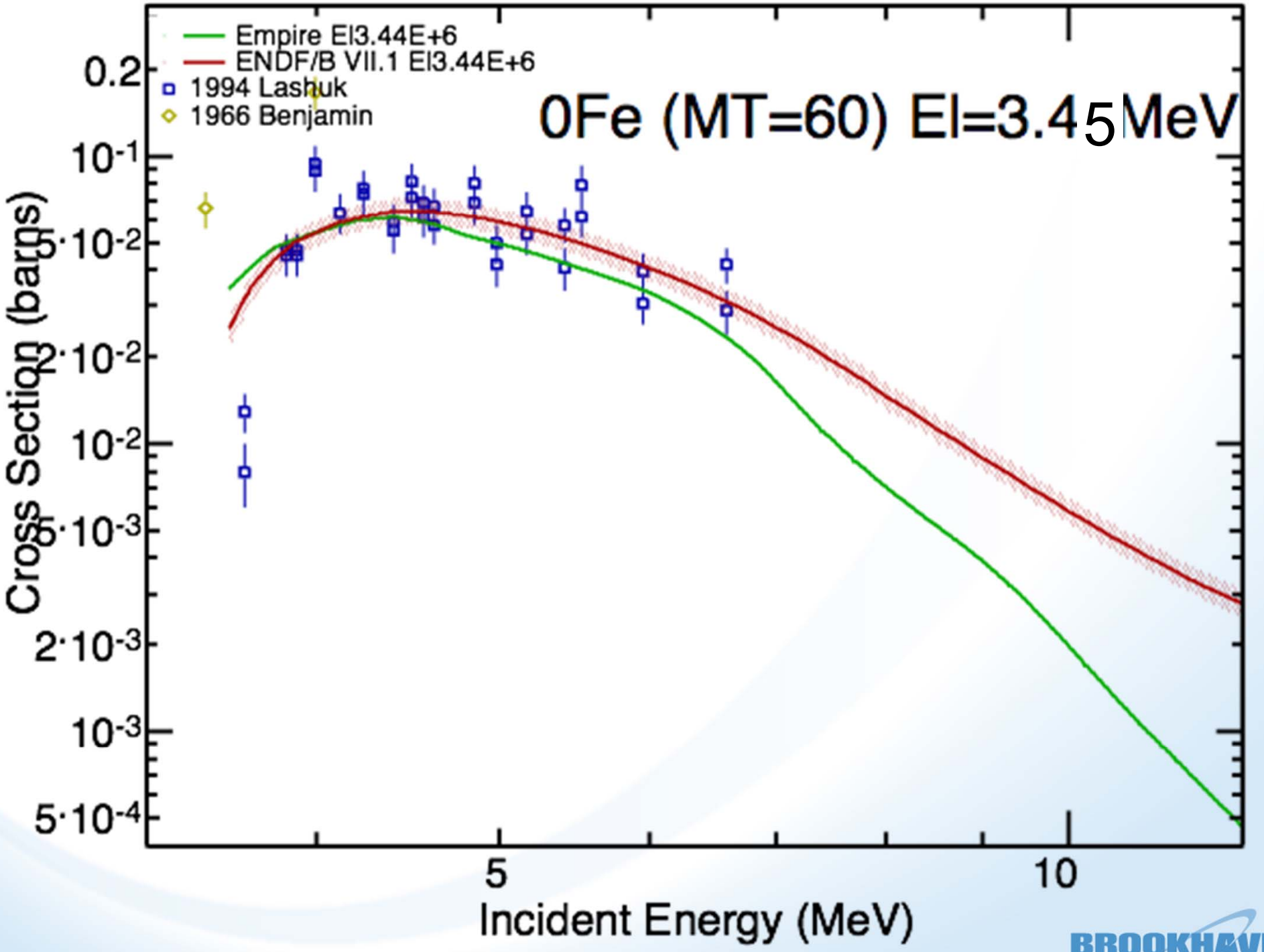

DWBA
56Fe (MT=57) El=3.12MeV
Cross Section (barns)
5·10-2
2·10-2
10-2
5·10-3
4
5
6
7
8
Incident Energy (MeV)
Empire El3.12E+6
n-026_Fe_056-s.endf El3.12E+6
2014 Geel-Smoothed
1975 Mittler
1972 Rogers
1971 Boschung
1965 Gilboy
1965 Gilboy


Empire El3.37E+6
n-026_Fe_056-s.endf El3.37E+6
2014 Geel-Smoothed
1982 Nemilov
1975 Mittler
DWBA
Cross Section (barns)
10-1
5·10-2
2·10-2
10-2
5·10-3
4
5
6
7
8
Incident Energy (MeV)
56Fe (MT=58) El=3.37MeV

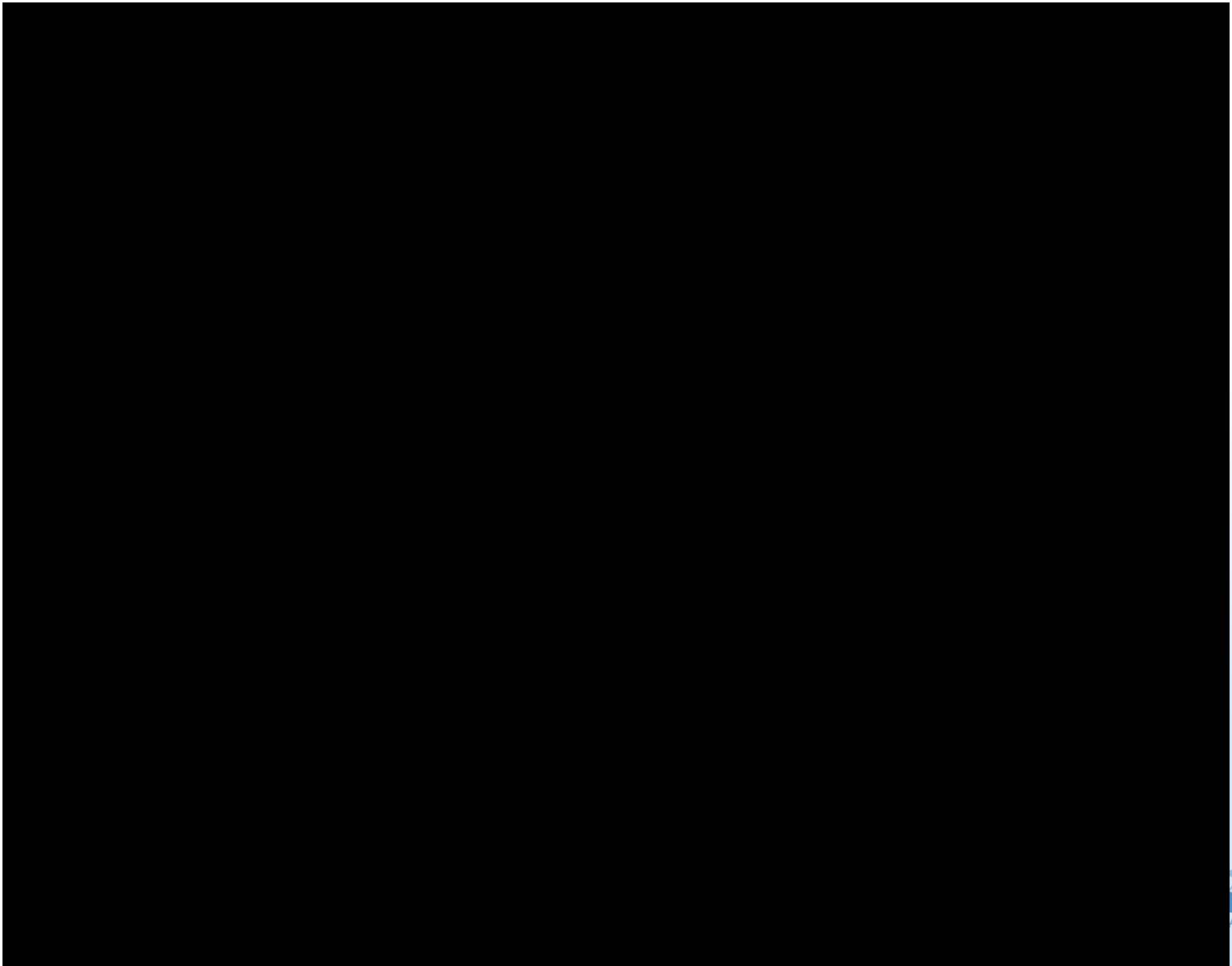

DWBA
0Fe (MT=58) EI=3.3699MeV
Empire EI3.37E+6
ENDF/B VII.1 EI3.37E+6
1994 Lashuk
Cross Section (barns)
10-1
8·10-2
2·10-2
10-2
5·10-3
5
10
20
Incident Energy (MeV)


Empire EI3.39E+6
n-026_Fe_056-s.endf EI3.39E+6
2014 Geel-Smoothed
56Fe (MT=59) EI=3.39E+6
Cross Section (barns)
10-2
10-3
10-4
10-5
5
10
20
Incident Energy (MeV)

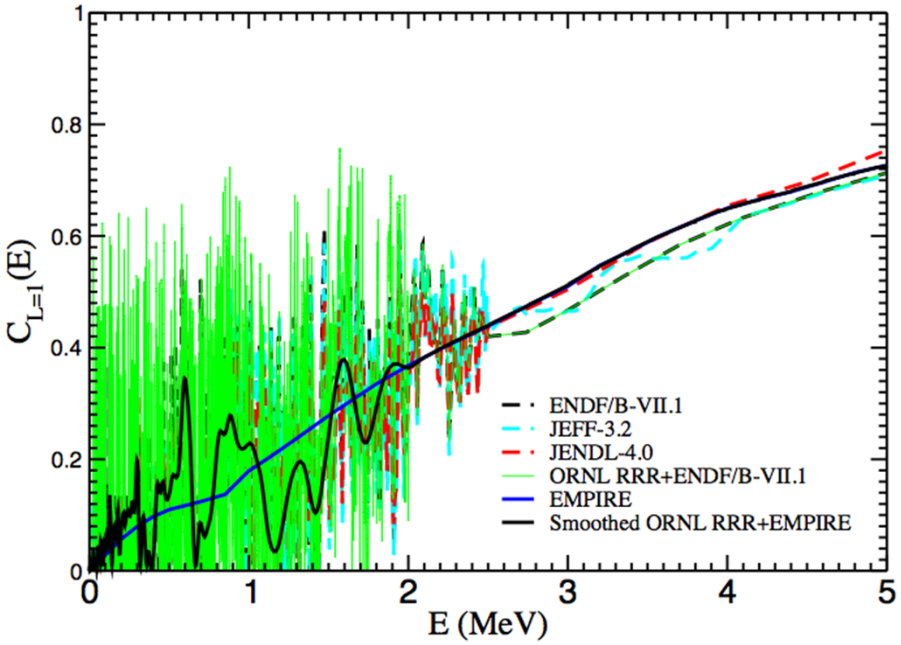

56Fe (MT=60) El=3.45MeV
Cross Section (barns)
Incident Energy (MeV)
Empire El3.45E+6
n-026_Fe_056-s.endf El3.45E+6
2014 Geel-Smoothed
1982 Nemilov
1975 Mittler
1971 Boschung
1965 Gilboy
1965 Gilboy

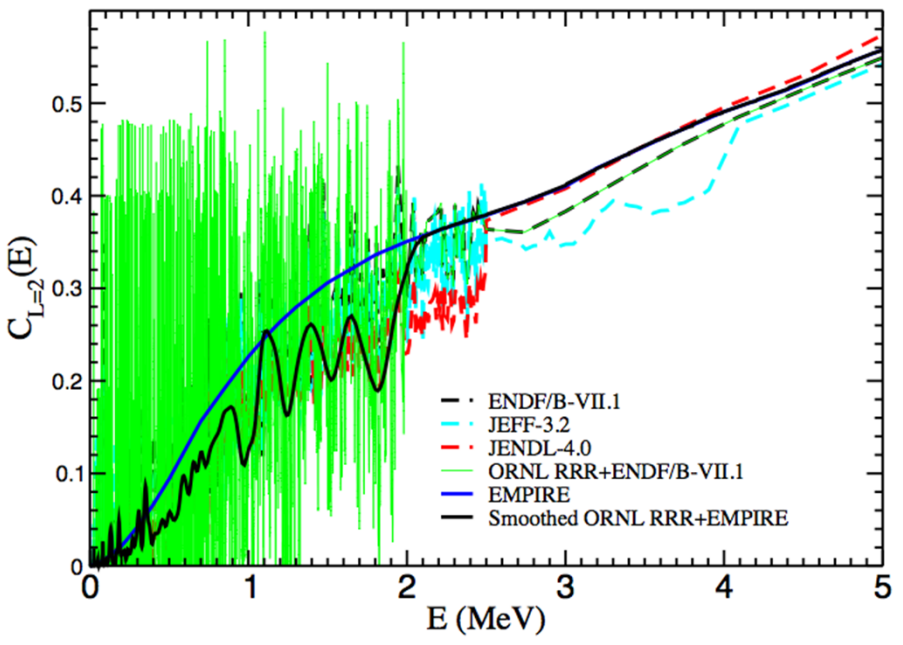

Empire El3.44E+6
ENDF/B VII.1 El3.44E+6
1994 Lashuk
1966 Benjamin
0Fe (MT=60) El=3.45MeV
Cross Section (barns)
0.2
10-1
2·10-2
10-2
8·10-3
2·10-3
10-3
5·10-4
5
10
Incident Energy (MeV)

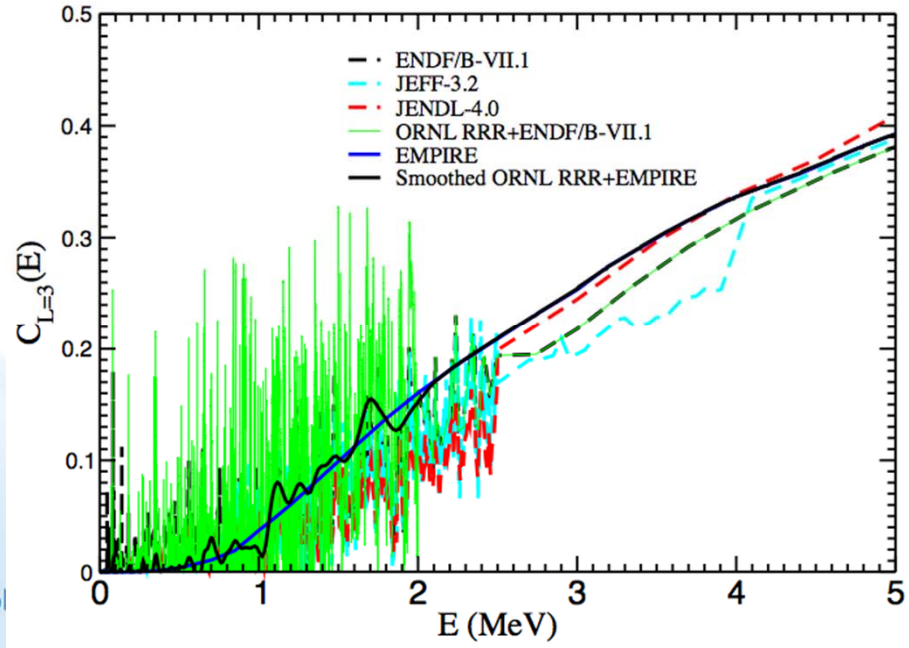
Elastic angular distributions

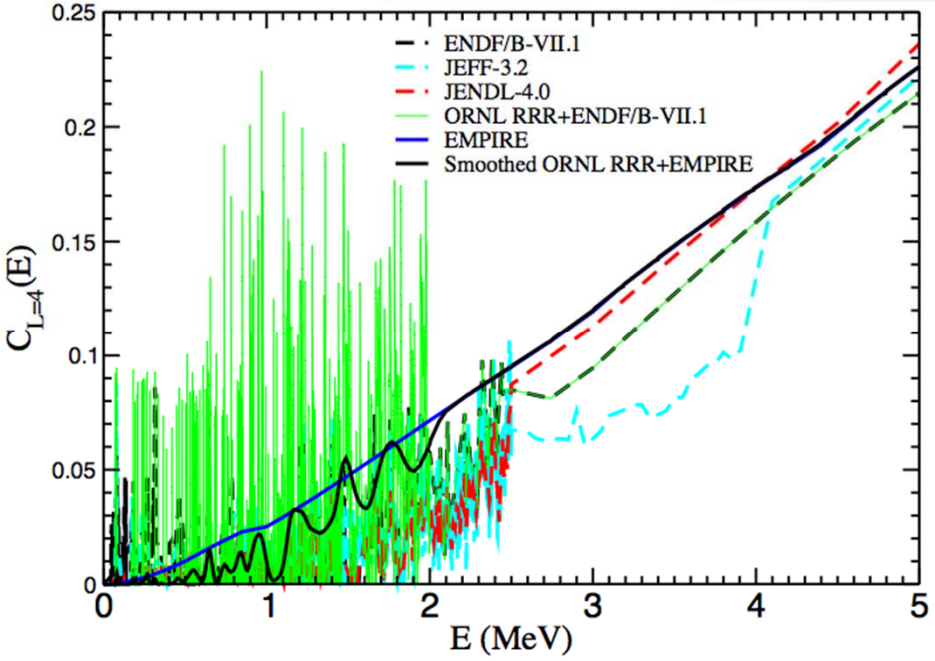


Smoothed Legendre coefficients in various libraries (case of elastic)

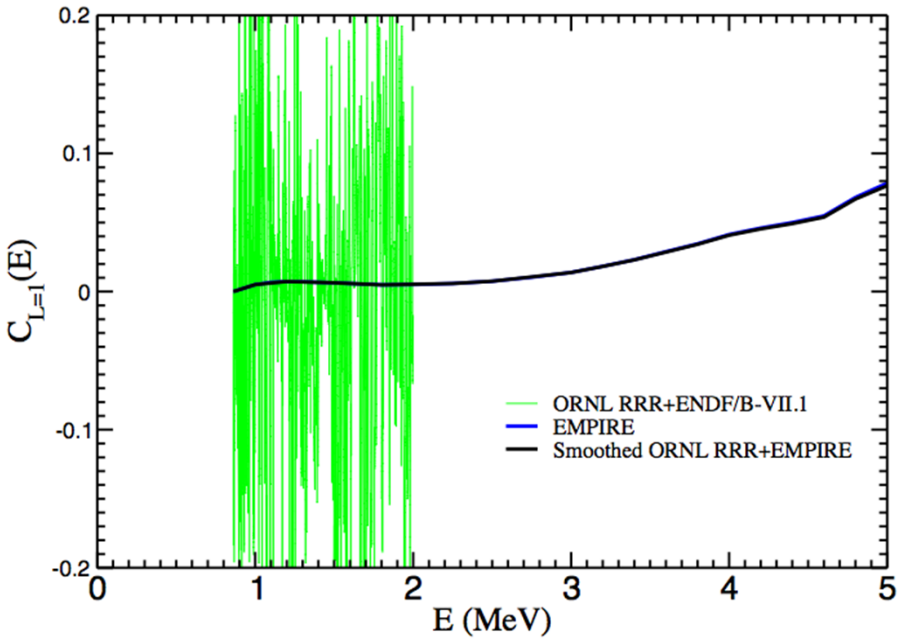


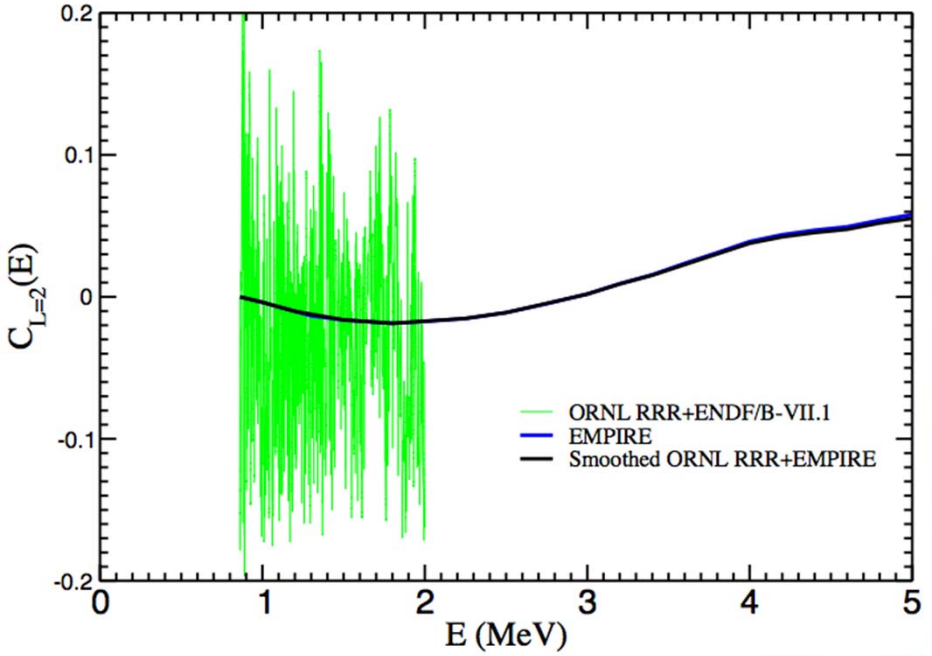


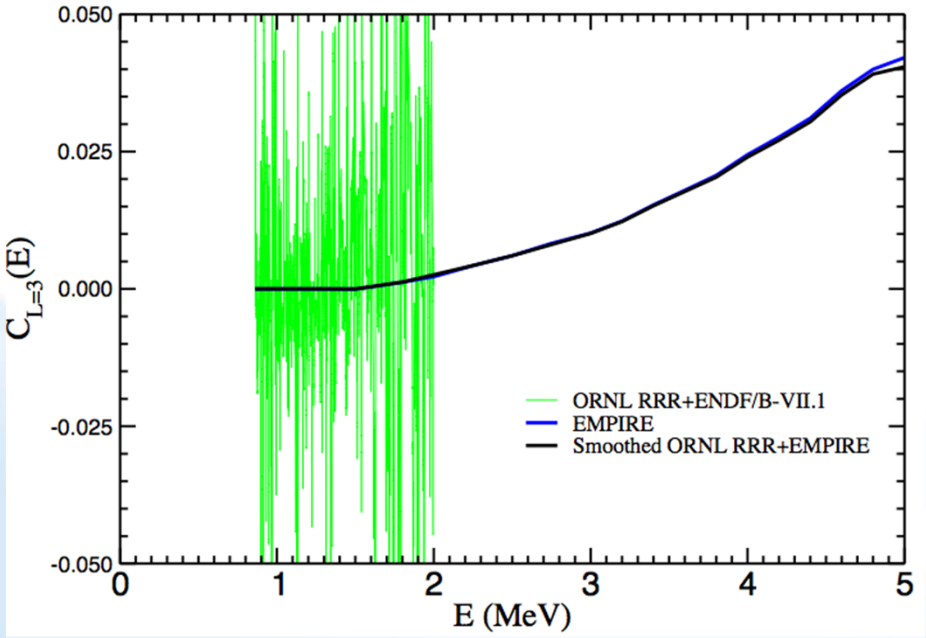


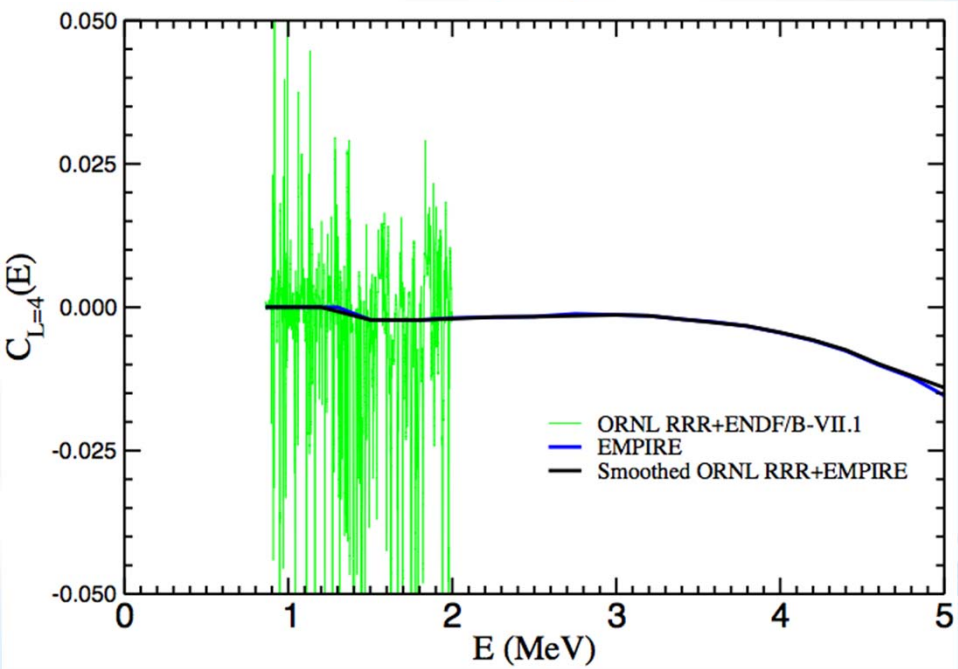


Smoothed Legendre coefficients in various libraries (case of 1st inelastic)









Angular distributions - conclusions

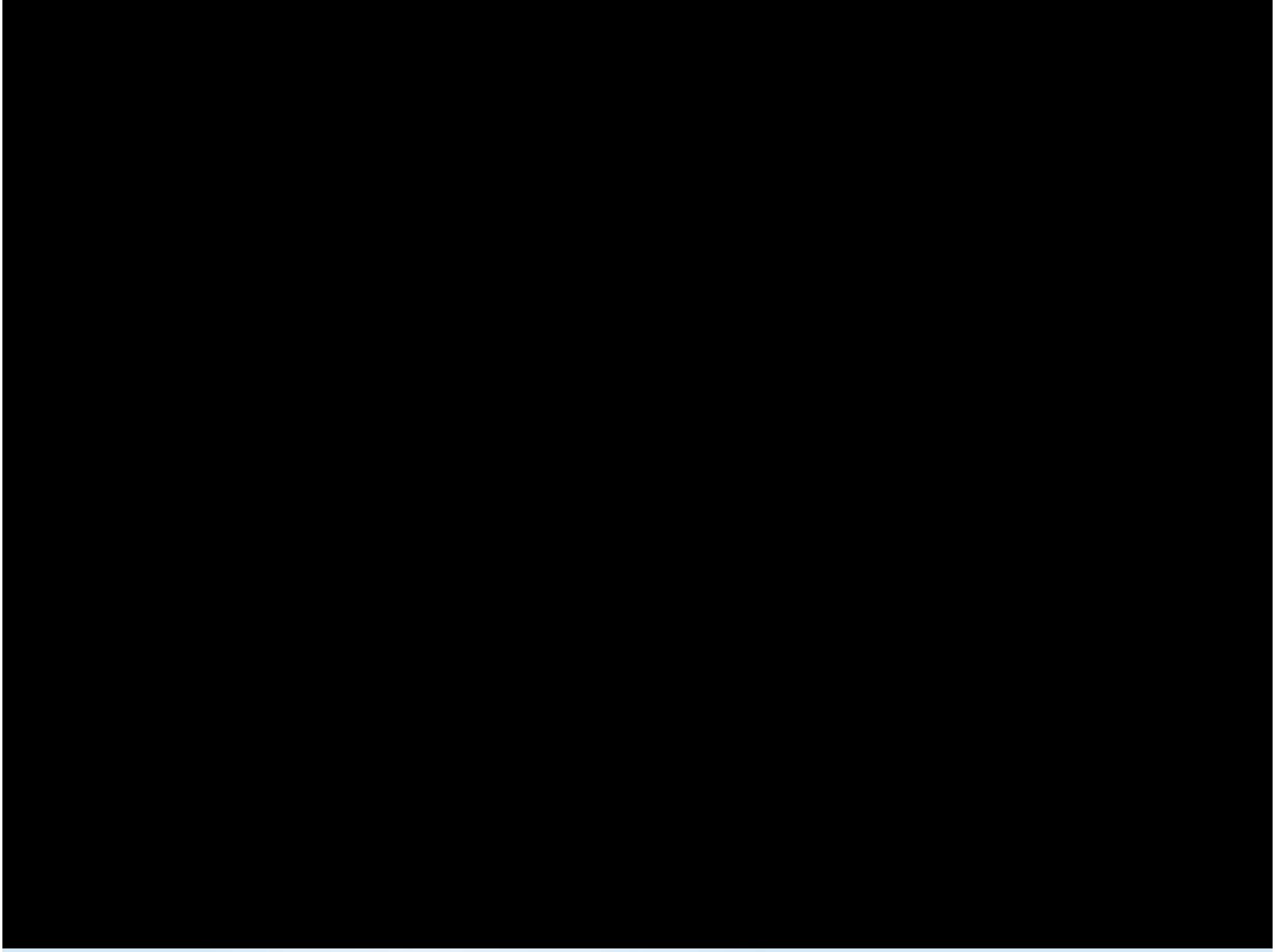
Fast neutron range

- Calculations provide very good overall description of averaged elastic angular distributions
- JEFF-3.2 has a strange behavior - probably due to fitting fluctuating data
- ENDF/B-VII.1 Leg. coeffs. are lower than CIELO
- JENDL-4.0 Leg. coeffs. agree very well with CIELO

Resonance Range

- Reasonable agreement of averaged Leg. coeffs. between RR and OM for odd L (on average)
- For even Leg. coffees. OM tends to be higher than RR
- We may need to resort to integral testing to make a choice

Double differential spectra



D. diff. spectra - conclusions

- Agreement with exp. data is reasonable but there is room for improvement
  - fine tuning of DWBA to discrete levels
  - exaggerated structure at low emission energies for neutrons
  - too low PE component for protons (however there is (n,p) constrain!)
- Several experimental set are not very reliable and should be probably taken out of consideration

To do list

- Fix (n,α) and check other complex particle channels
- Accounting for cross section fluctuations (to do or not to do?)
- Decide on angular distribution representation
- Adding other isotopes
- Final fine tuning (including semi-differential RPI data)
- Extending to higher incident energies
- Produce covariances
- Final validation
- Adjust to integral data if needed (CIELO/B ?)


We are getting it into shape