Iron Isotope Advances

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National Nuclear Data Center
Brookhaven National Laboratory

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CIELO-Iron collaboration

BNL, CNDC, IAEA, IRM, JSI, LANL, ORNL, RPI, IRSN

- Exp. data analysis: CNDC
- Resonance range: ORNL & IRSN & BNL & IAEA
- Fast neutron range: EMPIRE (BNL, IAEA)
- File assembly: IAEA, BNL
- Testing: IAEA, RPI, BNL, LANL, JSI

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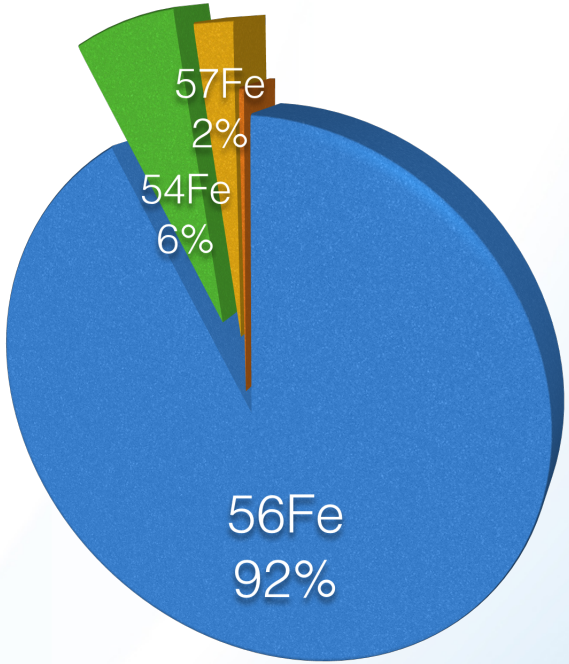
1. BNL, Upton, NY, USA
2. IAEA, Vienna, Austria
3. ORNL, Oak Ridge, TN, USA
4. EC-JRC-IRMM, Geel, Belgium
5. RPI, Troy, NY, USA
6. CNDC, Beijing, P.R.China
7. CIAE, Beijing, P.R.China
8. IRSN, Paris, France
9. ITA, Sao José dos Campos, Brazil
10. Bucharest University, Bucharest-Magurele, Romania

Features of CIELO Iron evaluation

- Strong reliance on experimental data including recent Geel, LANL and RPI
- IRDFF data adopted whenever available
- Model calculations adjusted to reproduce IRDFF and exp. data
- Special attention devoted to angular distributions (AD)
  - AD derived from resonance parameters
  - anisotropic AD compound nucleus inelastic scattering
  - influence of AD on benchmark results



- All reaction channels up to (n,a), (n,xn) and (n,xp) treated as exclusive and continued smoothly to 150 MeV
- Exclusive spectra for exclusive reactions also above 20 MeV
- Simultaneous evaluation of minor isotopes ^{54}Fe, ^{57}Fe and ^{58}Fe

Summary of releases

^{56}Fe	RRR	Fast
β-1	• JENDL-4.0 up to 850 keV • Artificial "background" added to capture around 20 keV • Background near 800 keV was reduced by 50% • Elas. ang. dist. from JENDL-4.0 • Tweak of P2 and P4 Legendre coefficients of elastic above 0.3 MeV • Res. @ 766.7 keV was corrected	• Gilbert-Cameron level-densities • Total taken from JEFF-3.2 • Ang. dist. up to 4MeV taken from JEFF-3.2 • Tweak of P2 and P4 Legendre coefficients of elastic below 1.5 MeV
β-2	• Revised resonance region from IRSN up to 850 keV in the LRF=7 format • No P2, P4 tweaks • Elastic angular distributions reconstructed from resonance parameters - IRSN < 850 keV	• Elastic and inelastic cross sections and angular distributions taken from beta 1 • Remainder of Fast Region: EMPIRE • Switch from pure GDR strength function to Weisskopf improving agreement of inelastic with experiment.
β-3	• Back to Beta-1 • P2, P4 tweaks were brought back • Elas. ang. dist. taken from resonance parameters of JENDL-4.0 < 850 keV	• Capture above 860keV adjusted to RPI data • Higher energies: EMPIRE as in β-2 • Corrected inclusive/exclusive spectra @ high E • Improved alpha production • HMS

Minor Isotopes

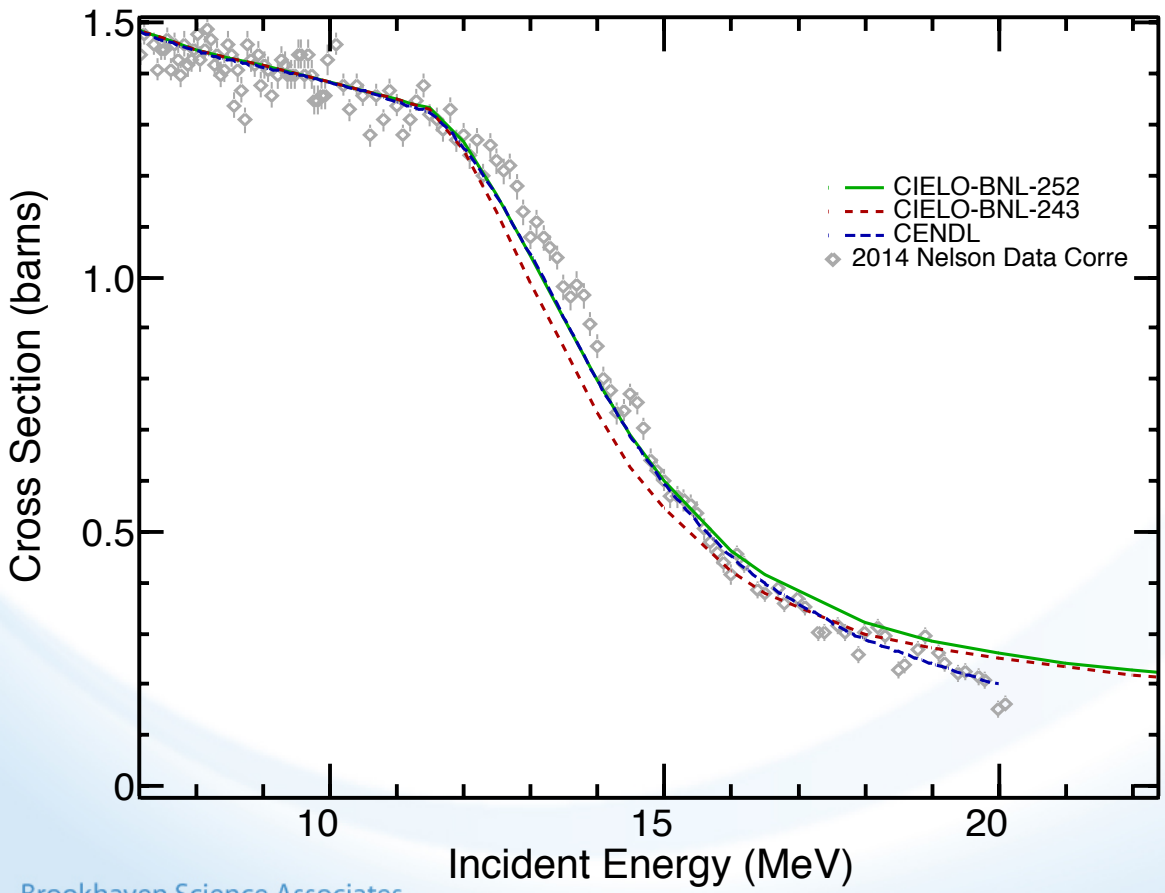
^{54}Fe	RRR	Fast
β-2	• Evaluation based on Atlas up to 1.2 MeV • Improved several resonances	• Capture artificially scaled down across the board in an attempt to improve matching with resonance region
β-3	• IRSN resonances up to 1.036 MeV	• Better fit of (n,p), (n,a), (n,2n) to IRDFF evaluation • Energy-dependent scaling of total in order to reproduce Guenther elastic data below 2 MeV and improve agreement with ave. VII.1 between 700 keV and 1.2 MeV

^{57}Fe	RRR	Fast
β-2	• New LRF=7 evaluation from Atlas • Converted from MLBW to Reich-Moore LRF=7 to include first inelastic	• Gilbert-Cameron level densities
β-3	• Same as β-2	• Corrected coupled and DWBA levels • HMS

^{58}Fe	RRR	Fast
β-3=β-2	• Moxon evaluation	• EMPIRE

Rose inelastic shoulder - ^{56}Fe

Compared to CENDL and VII.1 our CIELO rev.243 inelastic was too low between 12 and 16 MeV. How to bring it up without destroying perfect agreement for (n,p)?



Solution:
Increase competition of gammas against neutron emission from ^{56}Fe by increasing gamma-ray strength function in ^{56}Fe.

Inelastic goes up, (n,2n) goes down (we like it), (n,p) remains untouched and gamma spectra calculate closer to the experiment.

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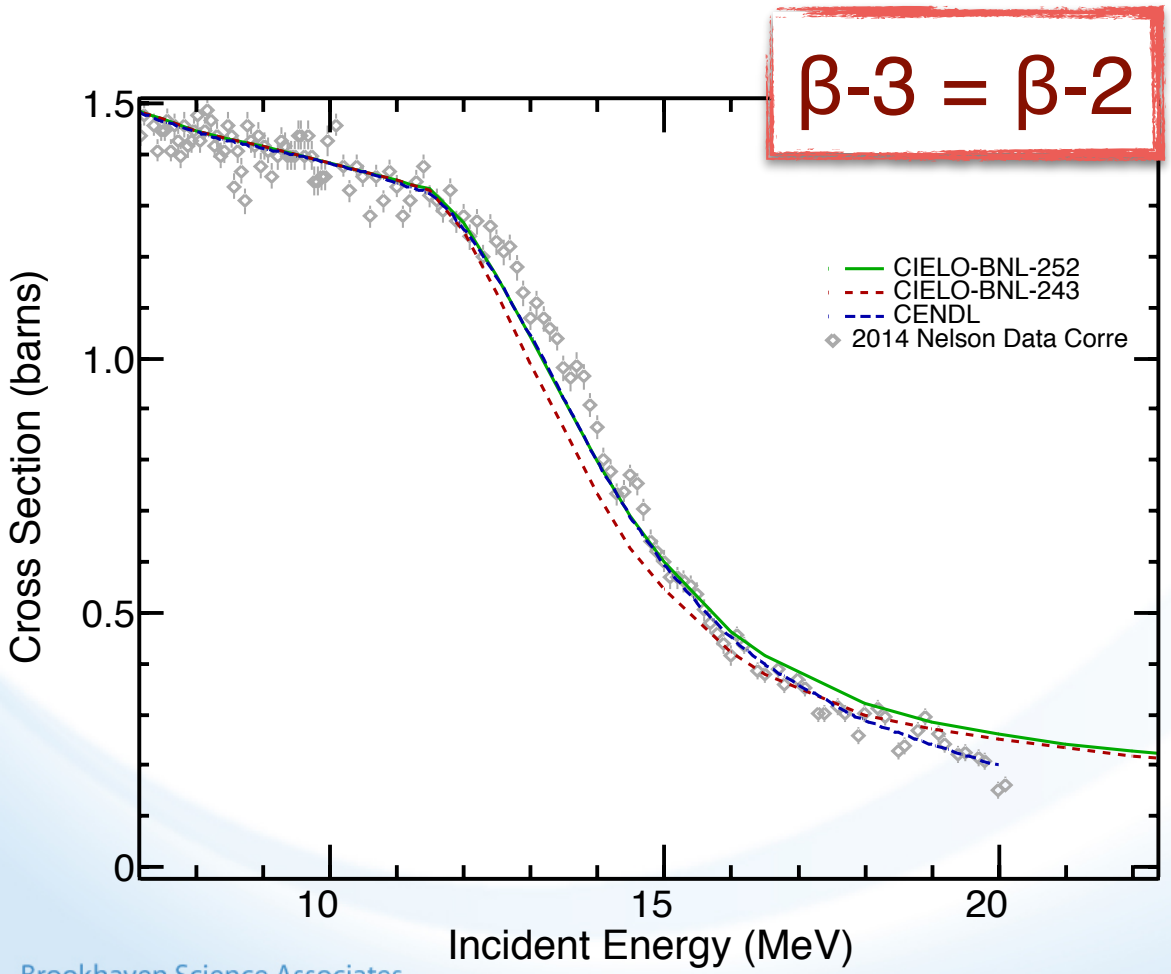

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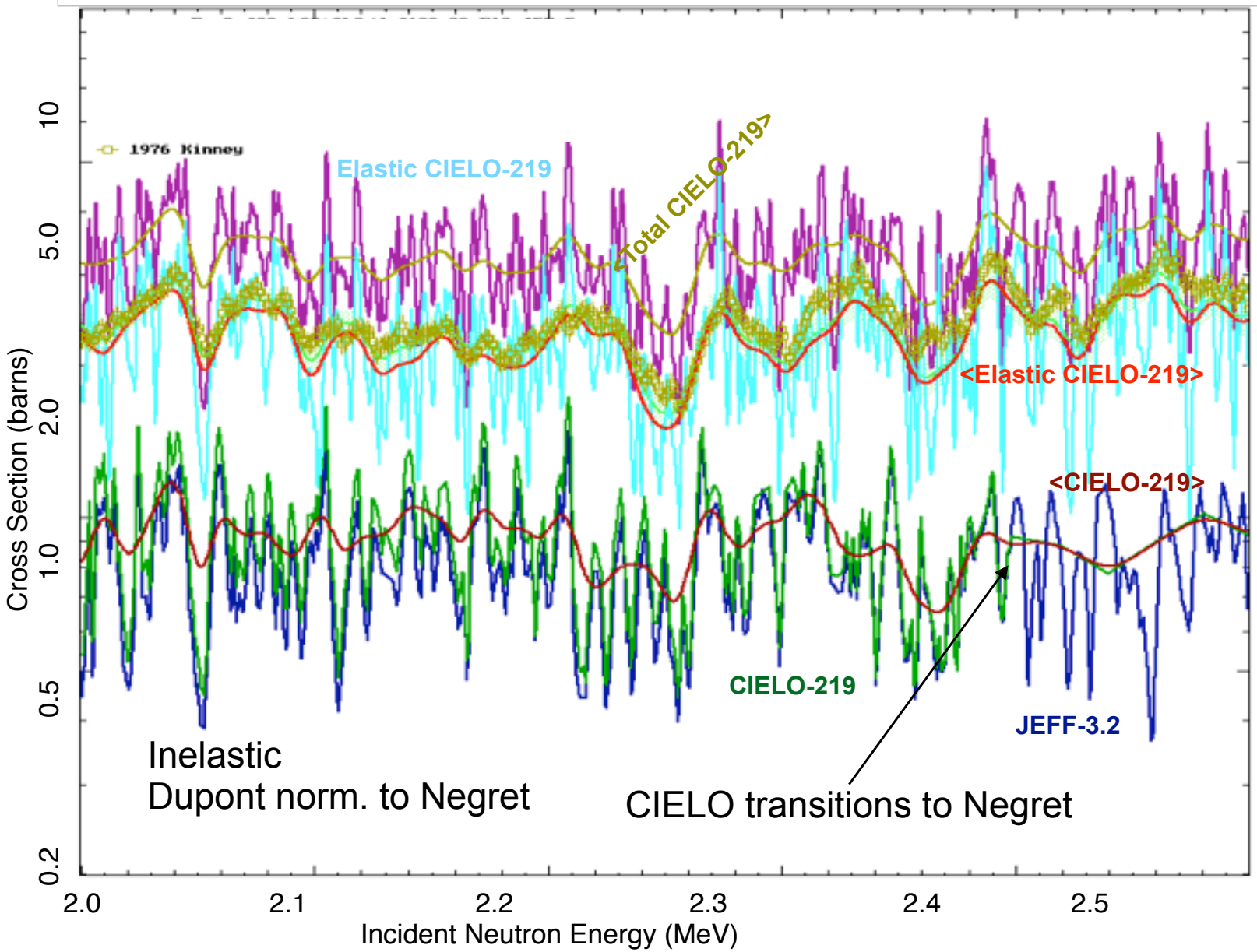
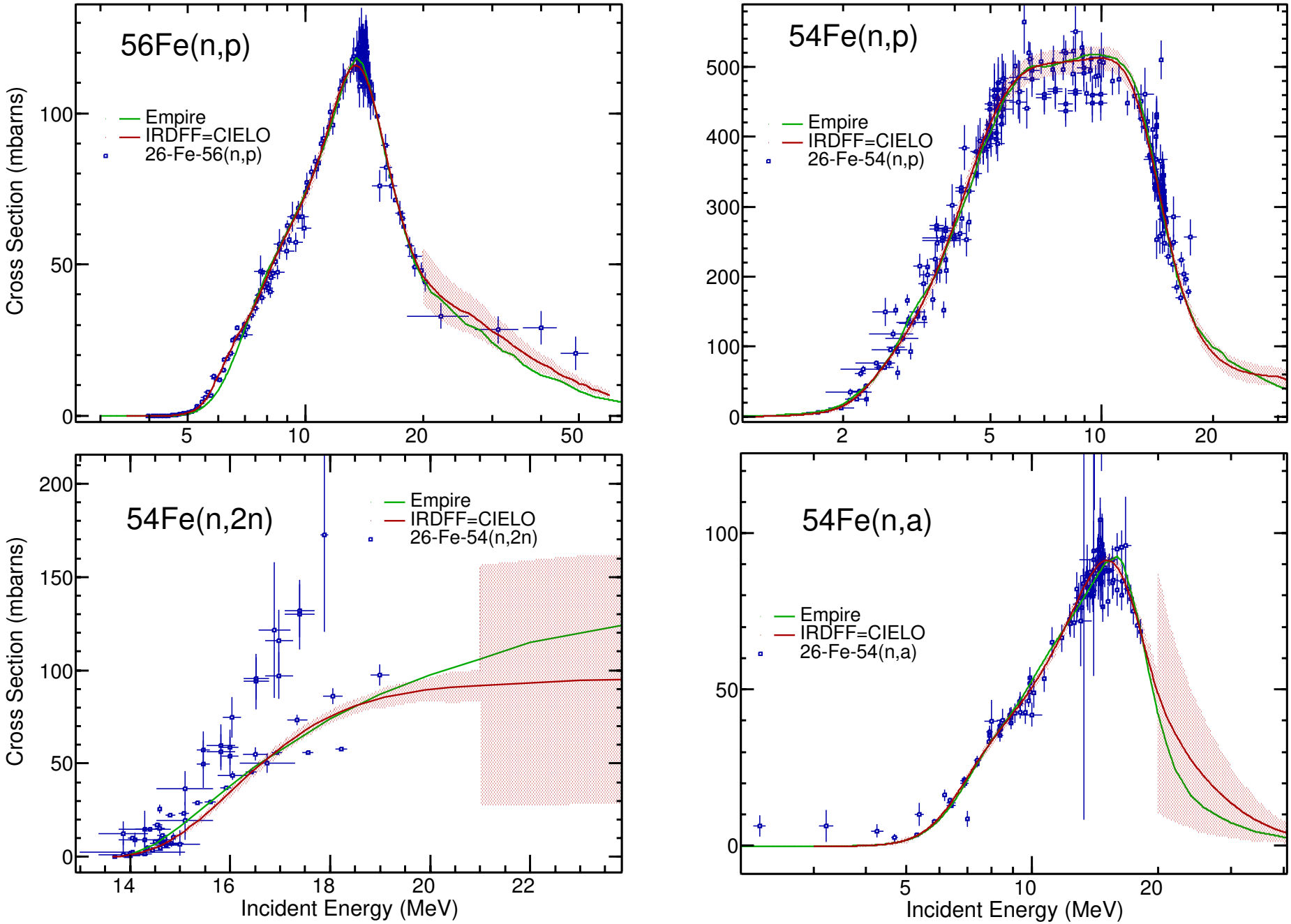
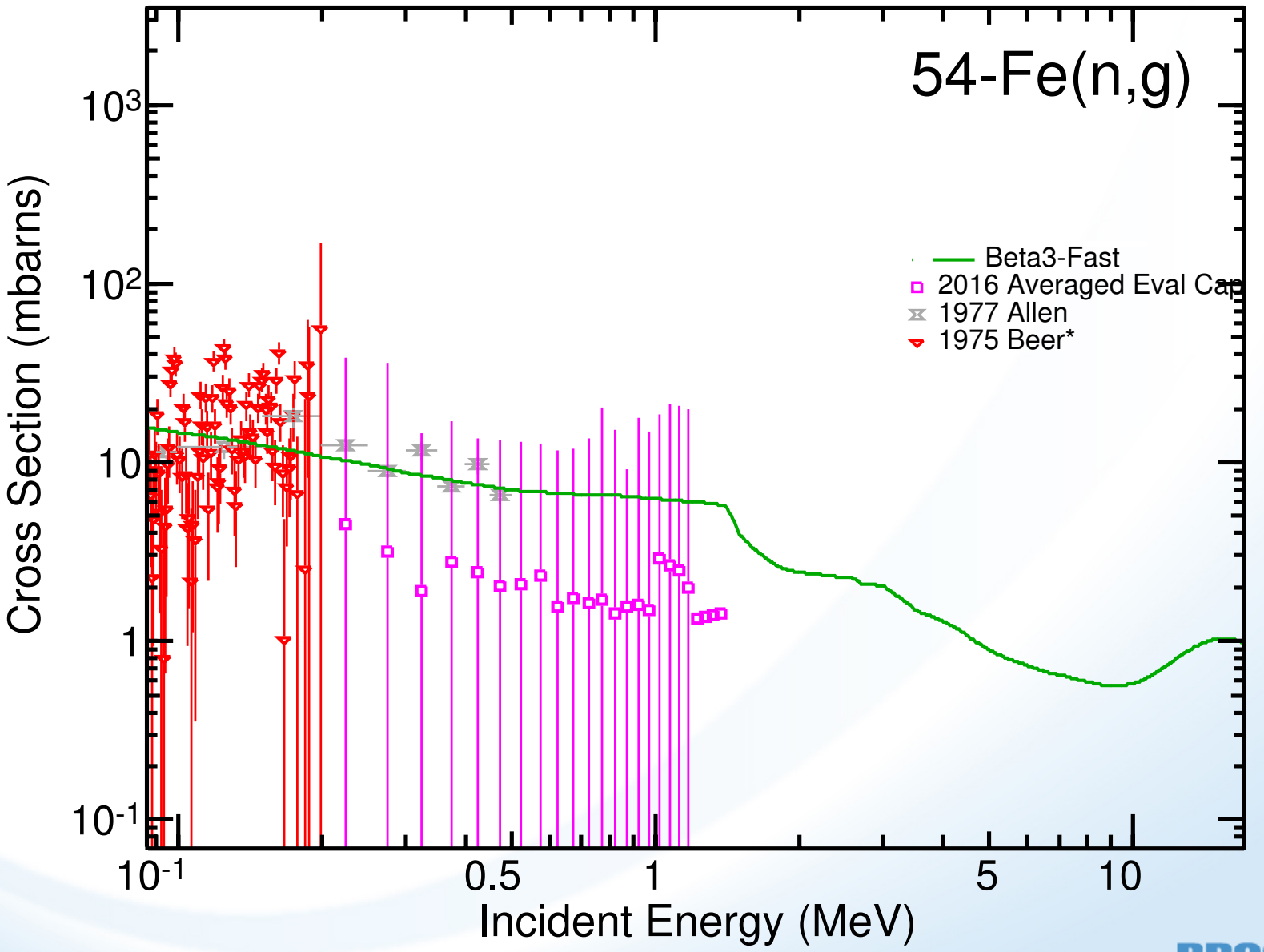
Consistent usage of exp. data:
(i) total from Berthold (corrected for minor isotopes)
(ii) inelastic - Dupont normalized to Negret up to 2.4 MeV, Negret above,
(iii) elastic = total - inelastic. Resolution broadened elastic agrees with Kinney data.



Dosimetry file (IRDFF)



^{54}Fe capture issue



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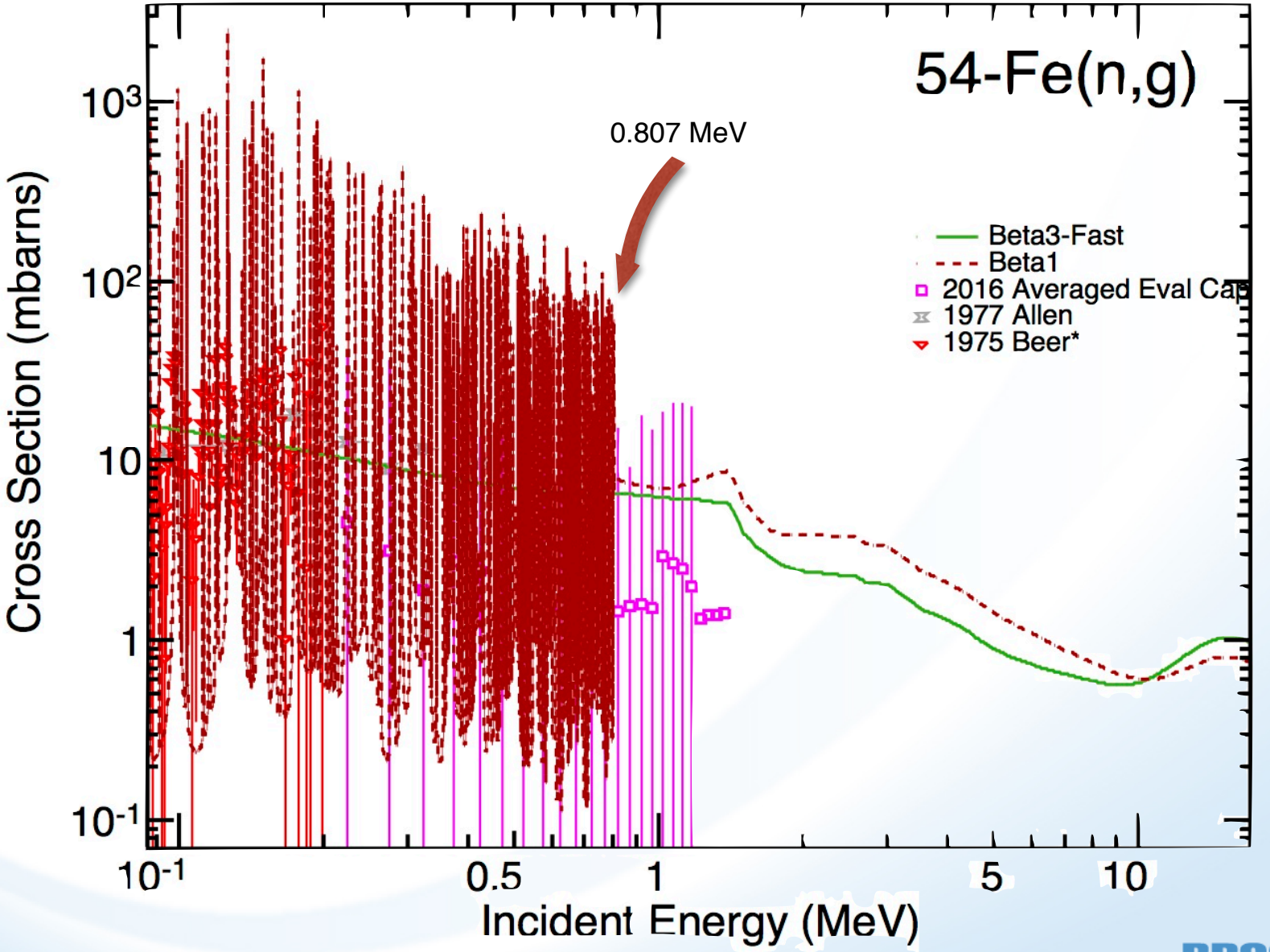

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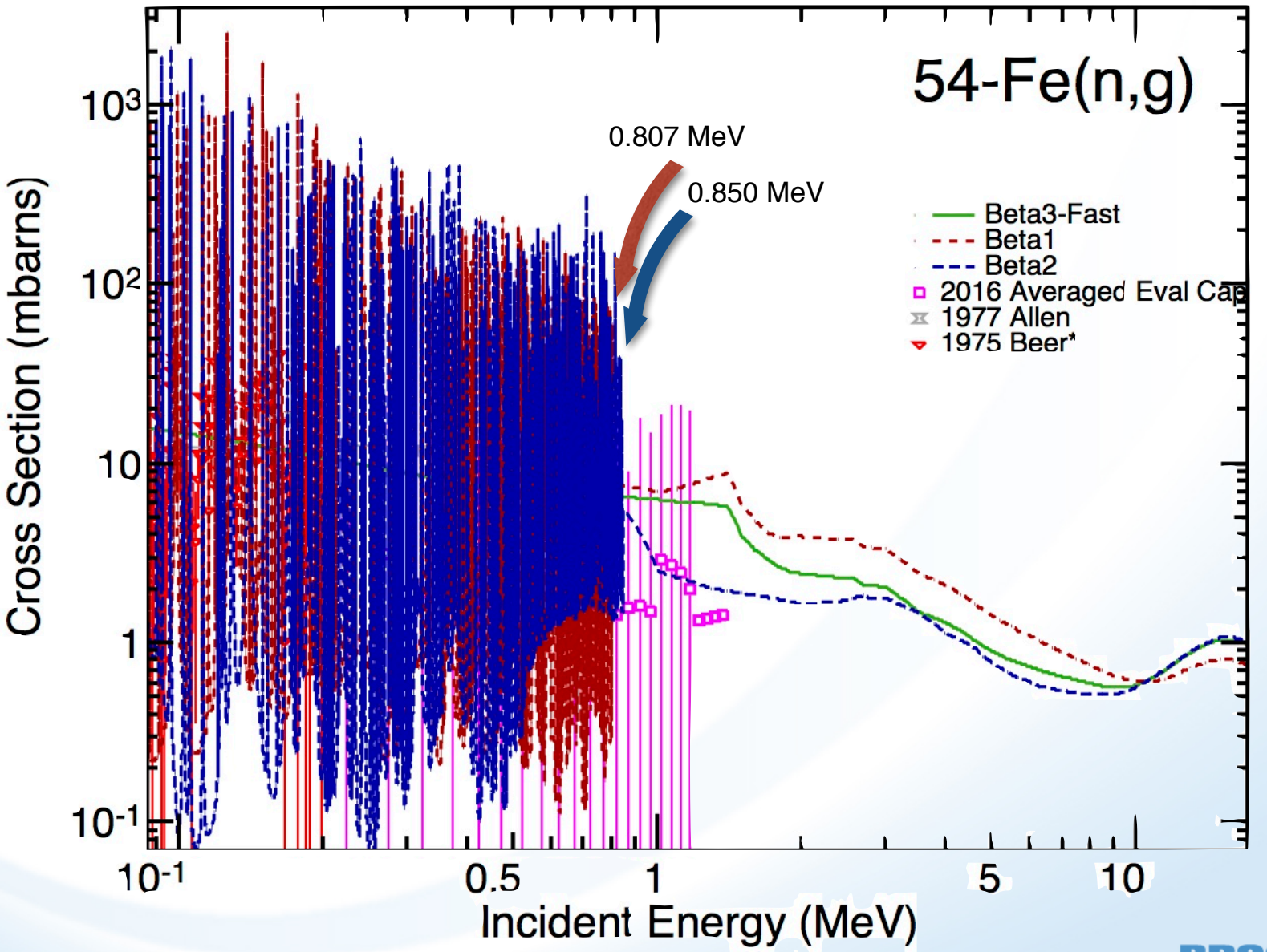
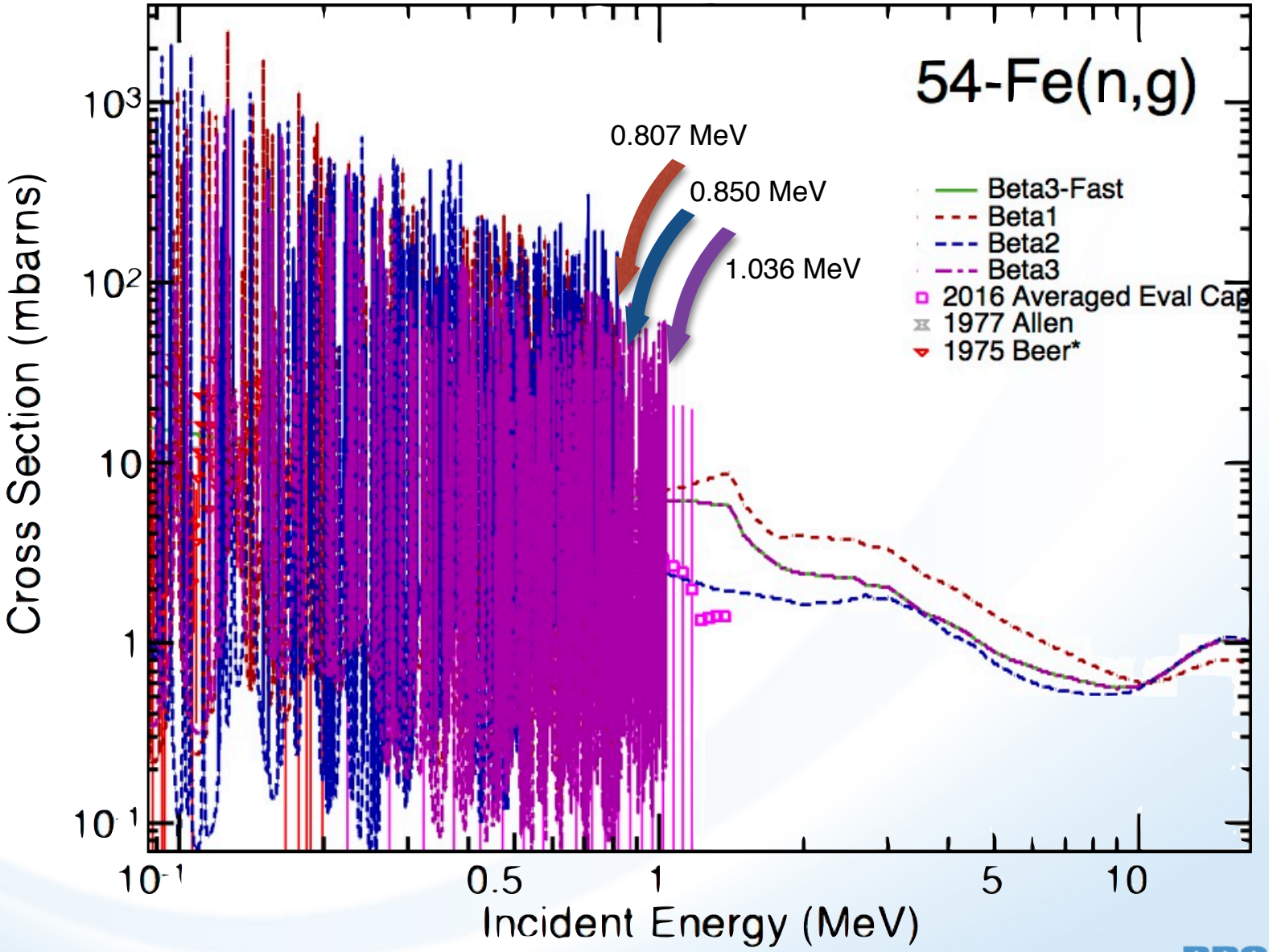
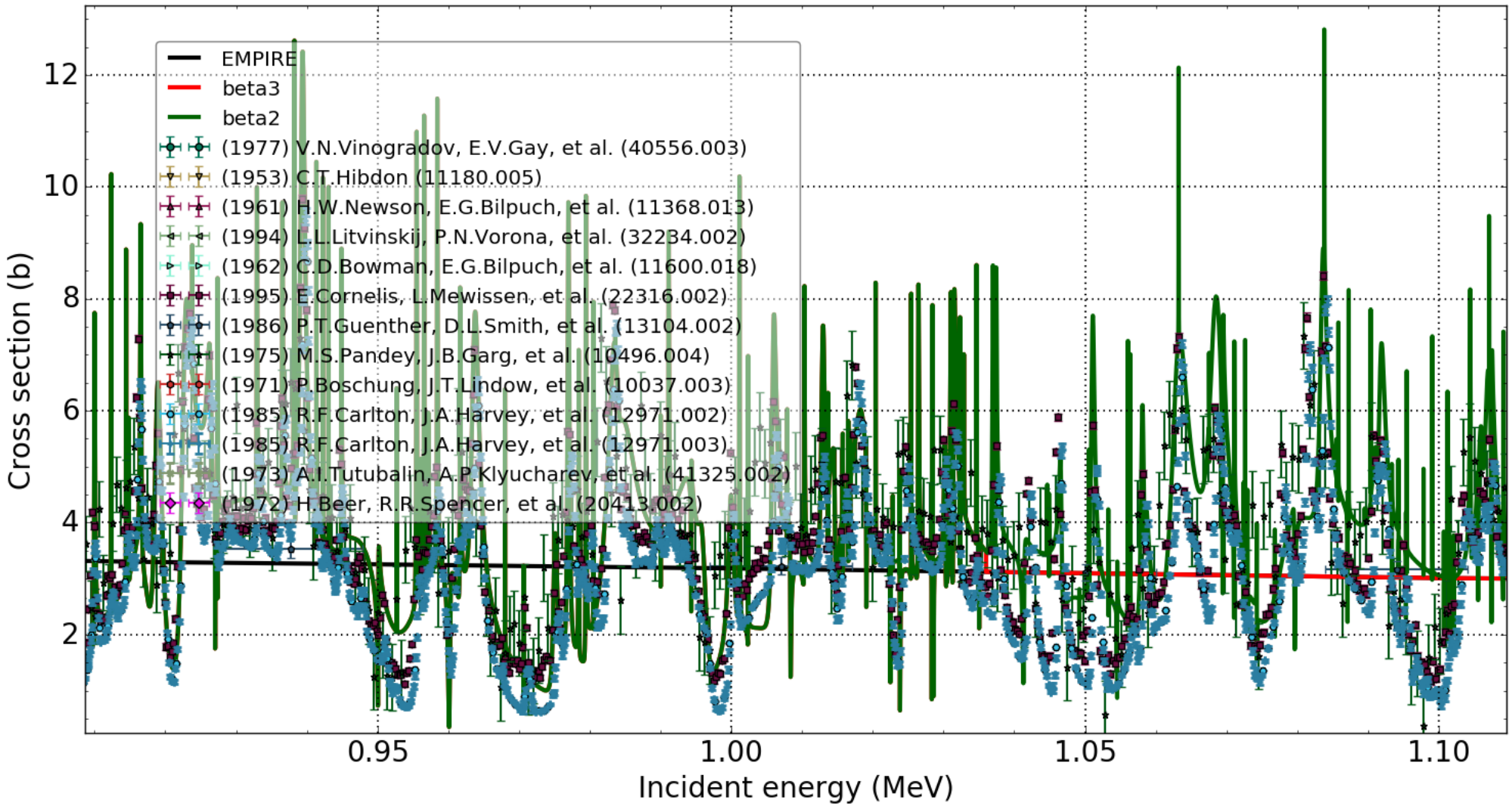


^{54}Fe capture issue

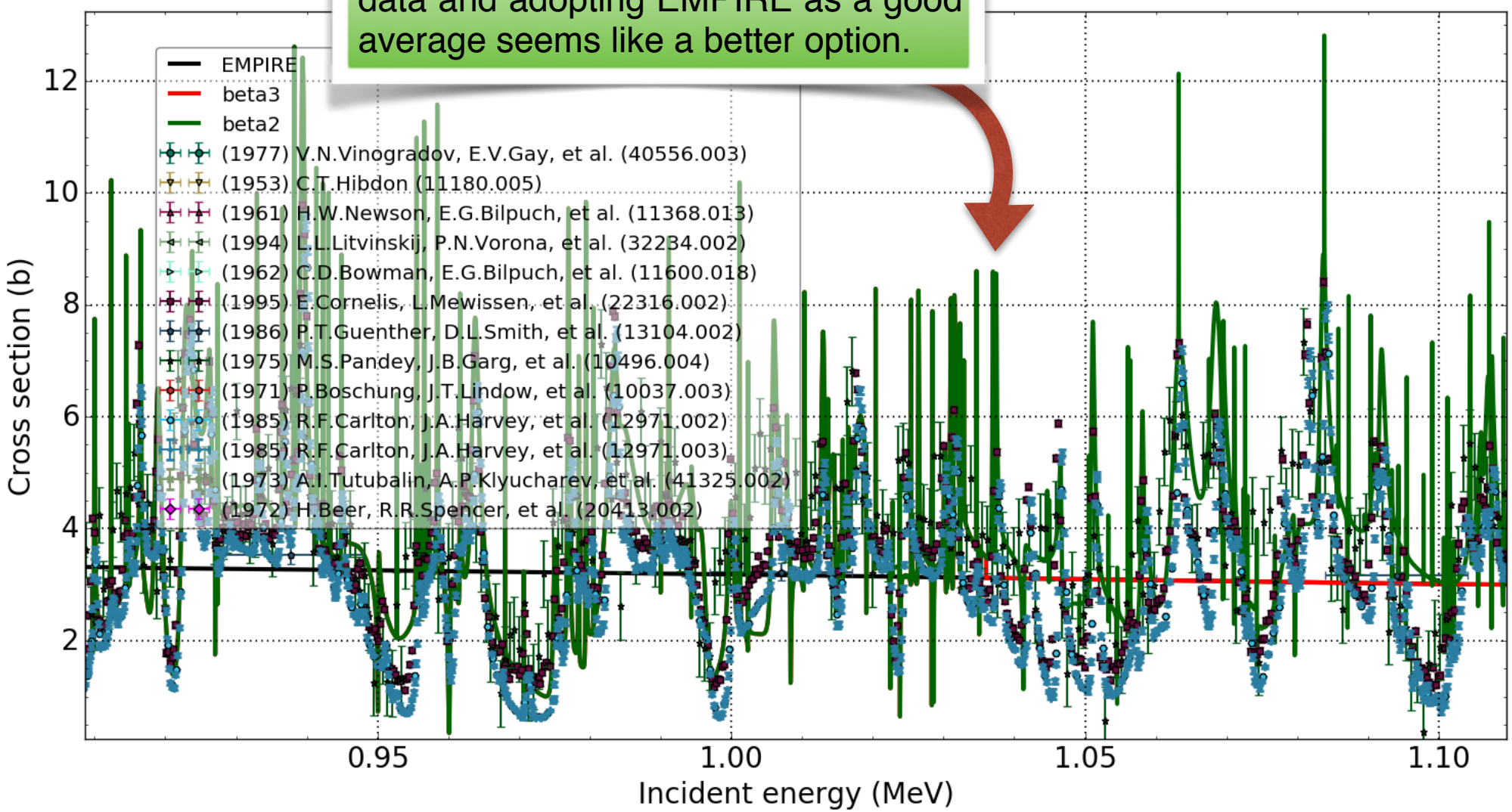


Resonance cut-off in ^{54}Fe(n,tot)

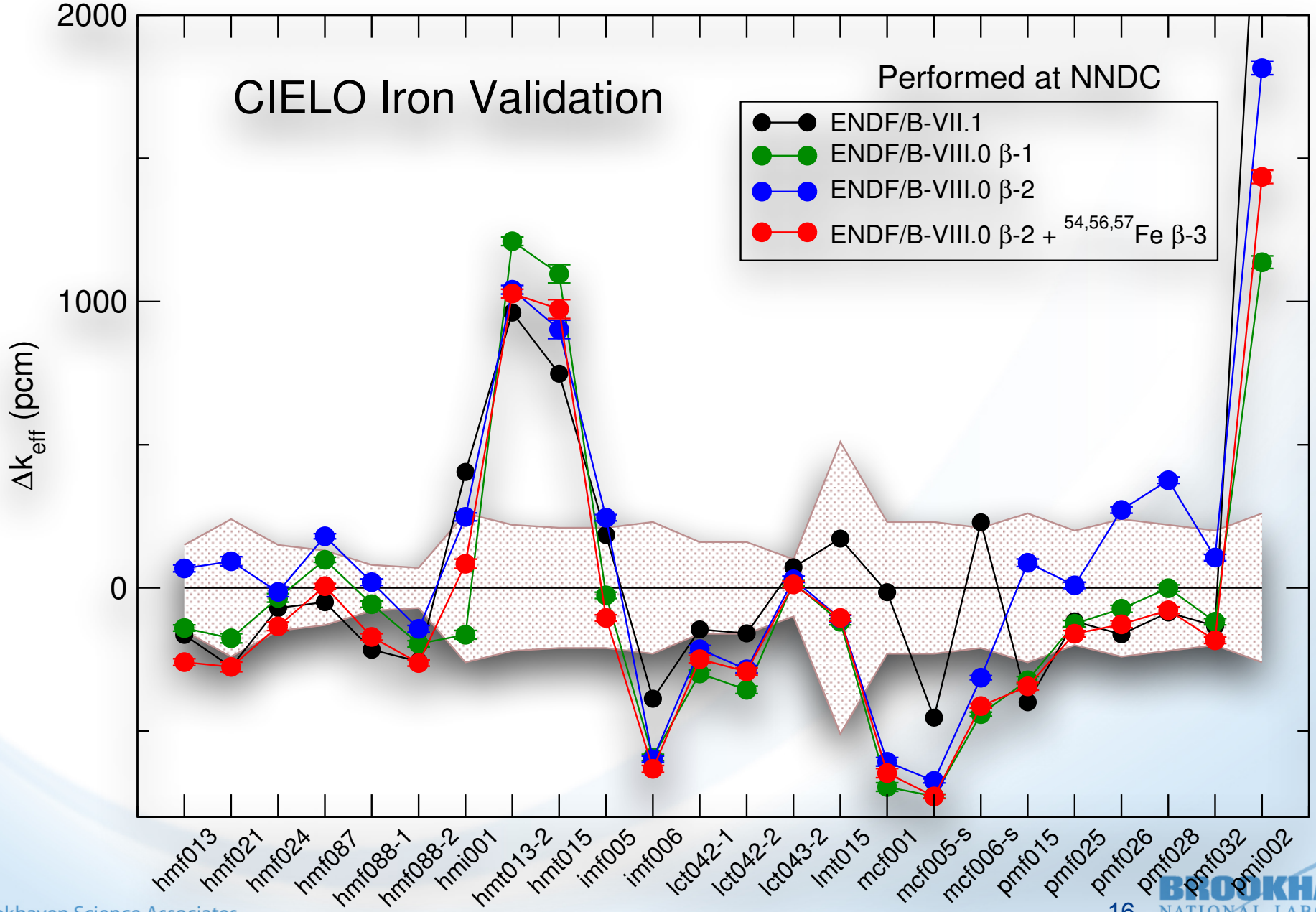


Resonance cut-off in ^{54}Fe(n,tot)

1.036 MeV: Where IRSN from β-2 becomes consistently higher than exp. data and adopting EMPIRE as a good average seems like a better option.



Validation


CIELO Iron Validation
Performed at NNDC
ENDF/B-VII.1
ENDF/B-VIII.0 β-1
ENDF/B-VIII.0 β-2
ENDF/B-VIII.0 β-2 + 54,56,57Fe β-3
Δk_eff (pcm)
2000
1000
0
hmf013
hmf021
hmf024
hmf087
hmf088-1
hmf088-2
hmi001
hmt013-2
hmt015
imf005
imf006
lct042-1
lct042-2
lct043-2
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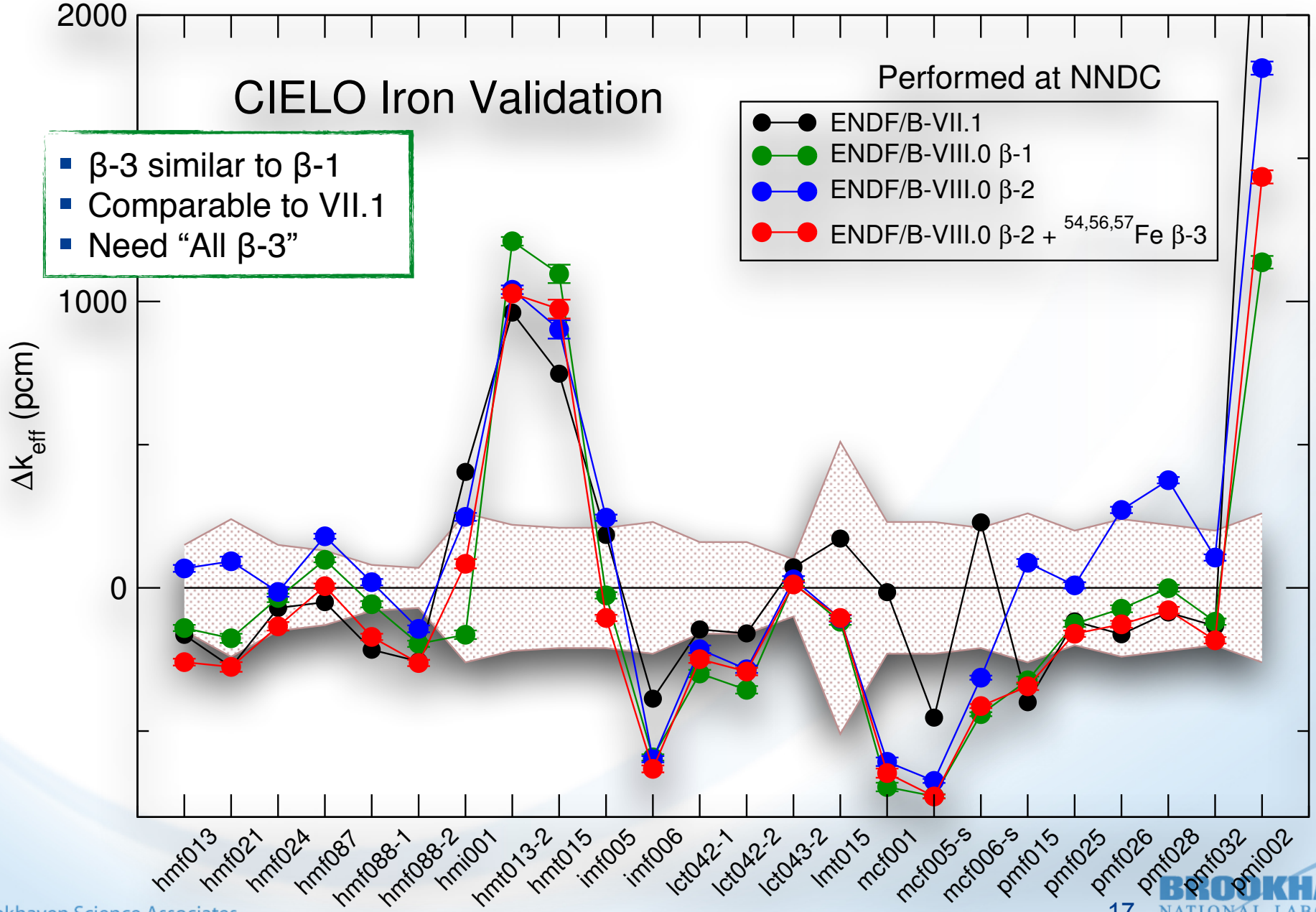
pmf025
pmf026
pmf028
pmf032
pmi002

Validation



- β-3 similar to β-1
- Comparable to VII.1
- Need "All β-3"

Current State of Iron - CIELO

- β-3: incorporates the best of β-1 and β-2 while addressing problems of both (with moderate success…)
- Minor isotopes have small effect on benchmarks (except hmi001)
- ^{56}Fe: β-2 performed well but RPI feedback pointed to β-1 performing significantly better. **Why?**
- Issues in resonance: Luiz's resonances don't have tweaks but are shifted (among other issues…)
- We've had several improvements (soft-rotor OMP, anisotropic compound, etc.); need more (RRR, HMS, inelastic γ's…)
- Decision - β-4?
- Comments?