^{56}Fe Evaluation for the CIELO Project

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mini-CSEWG 2016, April 11-12

^{56}Fe CIELO collaboration

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

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

- **Recent developments**
  - Update of 56Fe
    - Modifications of RR
    - Elastic angular distributions
    - New fast neutron evaluation using PE exciton model for all channels
    - Capture above 1.3 MeV lowered (following RPI data)
    - (n,2n) slightly changed, inelastic consistent with v.88
  - New evaluations for 54,57,58Fe
    - RR for 54,57 (LRF=7),
  - Covariances for 54,56,57Fe

Status of ^{56}Fe CIELO evaluation

- **Rev.49**
  - RR - ORNL rev.43 up to 2 MeV
  - Fast - EMPIRE calculations with HFB level dens. rev.48
  - X-sec fluctuations ignored
  - Elastic ang. distributions
    - RR: JENDL-4.0 (aver. fluct.)
    - rest: EMPIRE (no fluctuations)

- **Rev.88 (CSEWG-2015)**
  - RR - ORNL rev.43 up to **846** keV
  - **Total 846 keV - 4 MeV: JEFF-3.2 (smoothed Berthold data)**
  - **MT51,52 up to 4 MeV: Negret (Geel) data**
  - All the rest except elastic: EMPIRE calculations with **GC** level densities
  - X-sec fluctuations **included**
  - Elastic ang. distributions
    - RR: JENDL-4.0 (aver. fluct.)
    - rest: EMPIRE (no fluctuations)

Status of ^{56}Fe CIELO evaluation

- Rev.49
  - Rev.88 (CSEWG-2015)
    - RR - ORNL rev.43 up to 846 keV
    - Total 846 keV - 4 MeV: JEFF-3.2 (smoothed Berthold data)
    - MT51,52 up to 4 MeV: Negret (Geel) data
    - All the rest except elastic: EMPIRE calculations with GC level densities
    - X-sec fluctuations included
    - Elastic ang. distributions
      - RR: JENDL-4.0 (aver. fluct.)
      - rest: EMPIRE (no fluctuations)

- Rev.219 (mini-CSEWG-16) 'fe56ib15k'
  - RR - JENDL-4.0 up to 850 keV
    - resonance energy at 766.7 keV was corrected
    - background added to capture around 24.5 keV
    - background below 400 keV reduced by 40% (capture, elastic)
  - Total 850 keV - 6 MeV: JEFF-3.2 (smoothed Berthold data)
  - MT51,52 up to 3.5 MeV: **consistent combination of Dupont and Negret data**
  - All the rest except elastic: EMPIRE calculations with GC level densities
  - X-sec fluctuations included
  - Elastic ang. distributions
    - RR: JENDL-4.0 (aver. fluct.)
    - **above RR up to 4 MeV fluct. taken from JEFF-3.2 (JEF-2.2) following Kinney data**
    - rest: EMPIRE (no fluctuations)

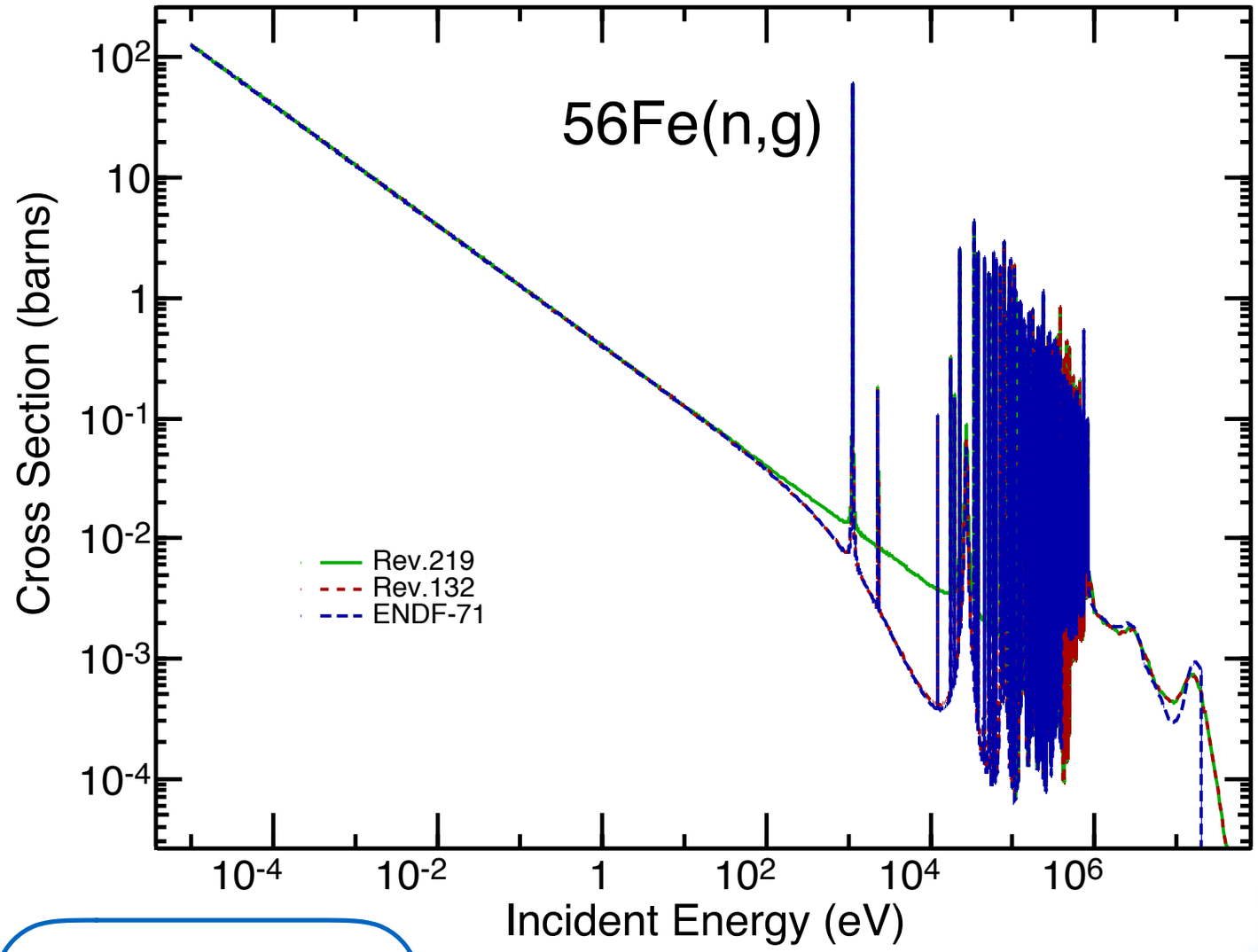
Summary of EMPIRE calculations (56Fe)

- CC for incident/outgoing channels + DWBA to uncoupled levels
- Lane-consistent soft-rotator dispersive OMP by Soukhovitski et al (PRC 2015)
- Rev. 88 replaces microscopic HFB level densities with Gilbert-Cameron (open issue of parity distribution!)
- Width fluctuation correction (HRTW) up to 8 MeV (difference HRTW v. Moldauer <1%)
- Default gamma-ray strength function (Plujko MLO1)
- Exciton model (PCROSS) for PE emission including Iwamoto-Harada model for PE cluster emission
- Rev. 88 fitted LD parameters to IRDFF for (n,p) and to experimental data for α production
- Rev. 219 energy range extended to 150 MeV
- Rev. 219 adds Kalman generated covariances in the fast region

Elastic angular distributions

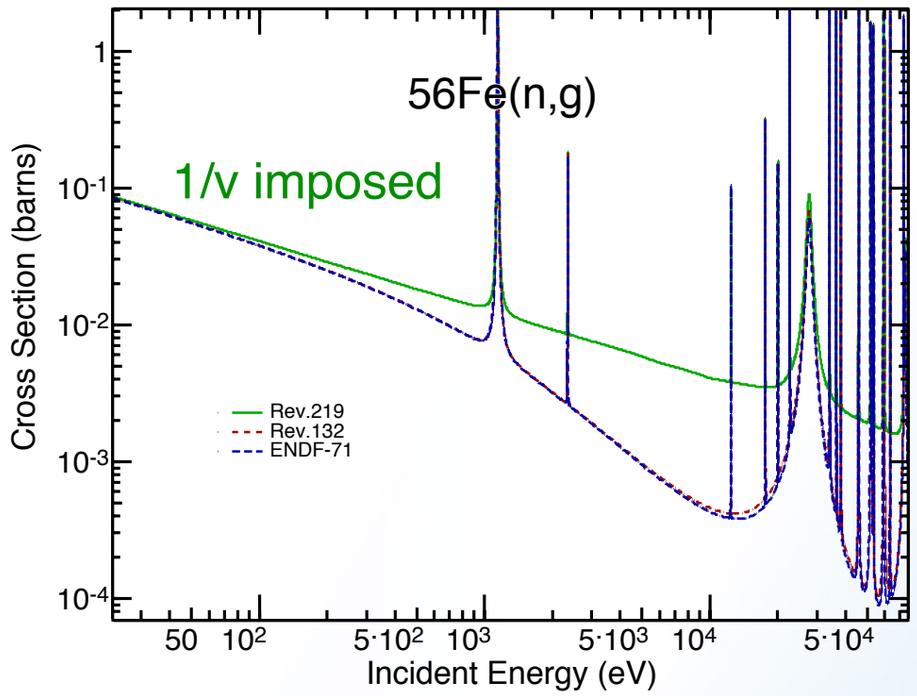
- Kinney data are the most extensive and detailed above the inelastic threshold
- JEF-2.2=>JEFF-3.2 ang. distr. are fitted to the Kinney data
- Whenever low energy-resolution experimental data are available they are closer to EMPIRE than to Kinney
- However, RPI semi-integral experiment favors JEF(F)s so we adopted it between 846 keV and 4 MeV
- RPI broad-average data to be compared with EMPIRE and broad-averaged evaluations

Changes to the RR region



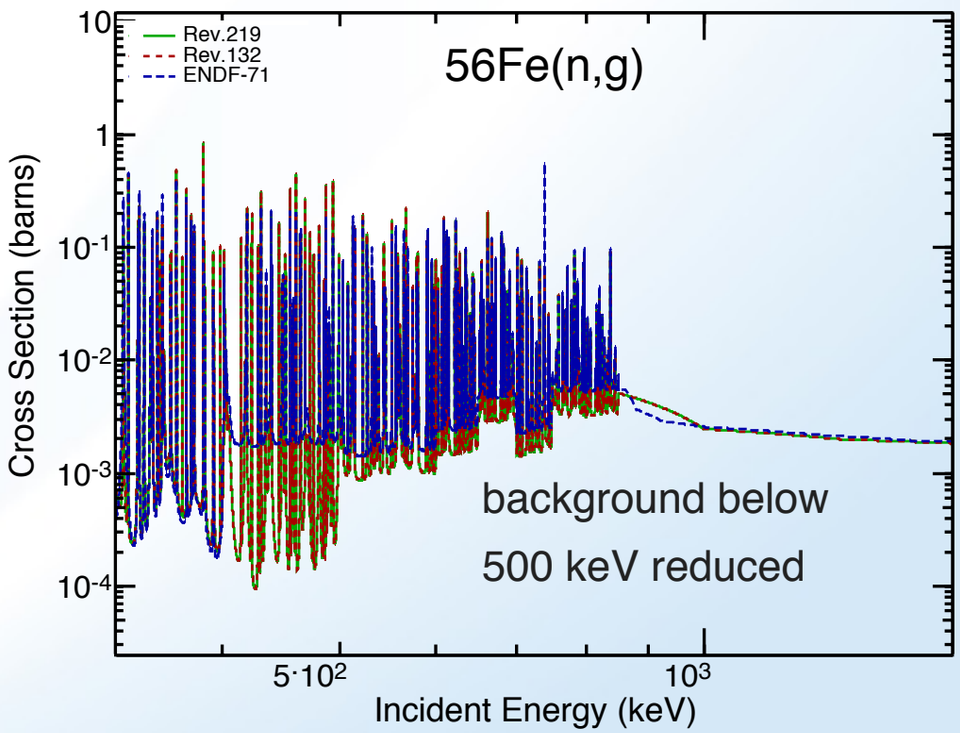
Thermal capture x-sec

Atlas:	2.59(14)
EGAF:	2.71(4)
CIELO r.291:	2.6051
ENDF/B-VII.1:	2.58936
ENDF/B-VII.0:	2.58933

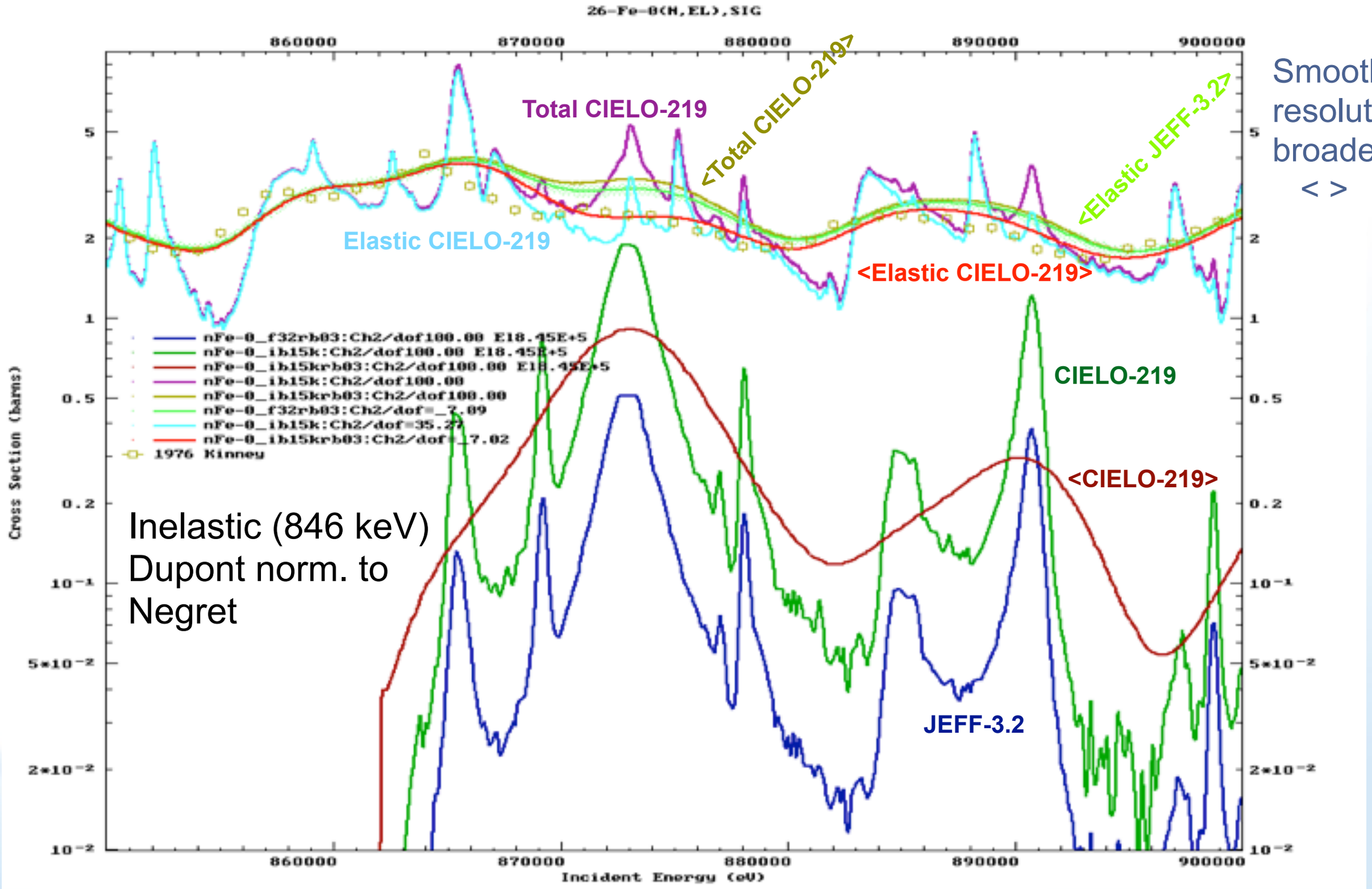


Changes driven by integral testing…

We don't like backgrounds…but there might be physics reasons behind them: (i) direct capture or (ii) forcing negative resonances to maintain 1/v trend up to 25 keV, (iii)



nat-Fe: Total, Elastic, Inelastic 850-900 keV



Smooth lines resolution-broadened
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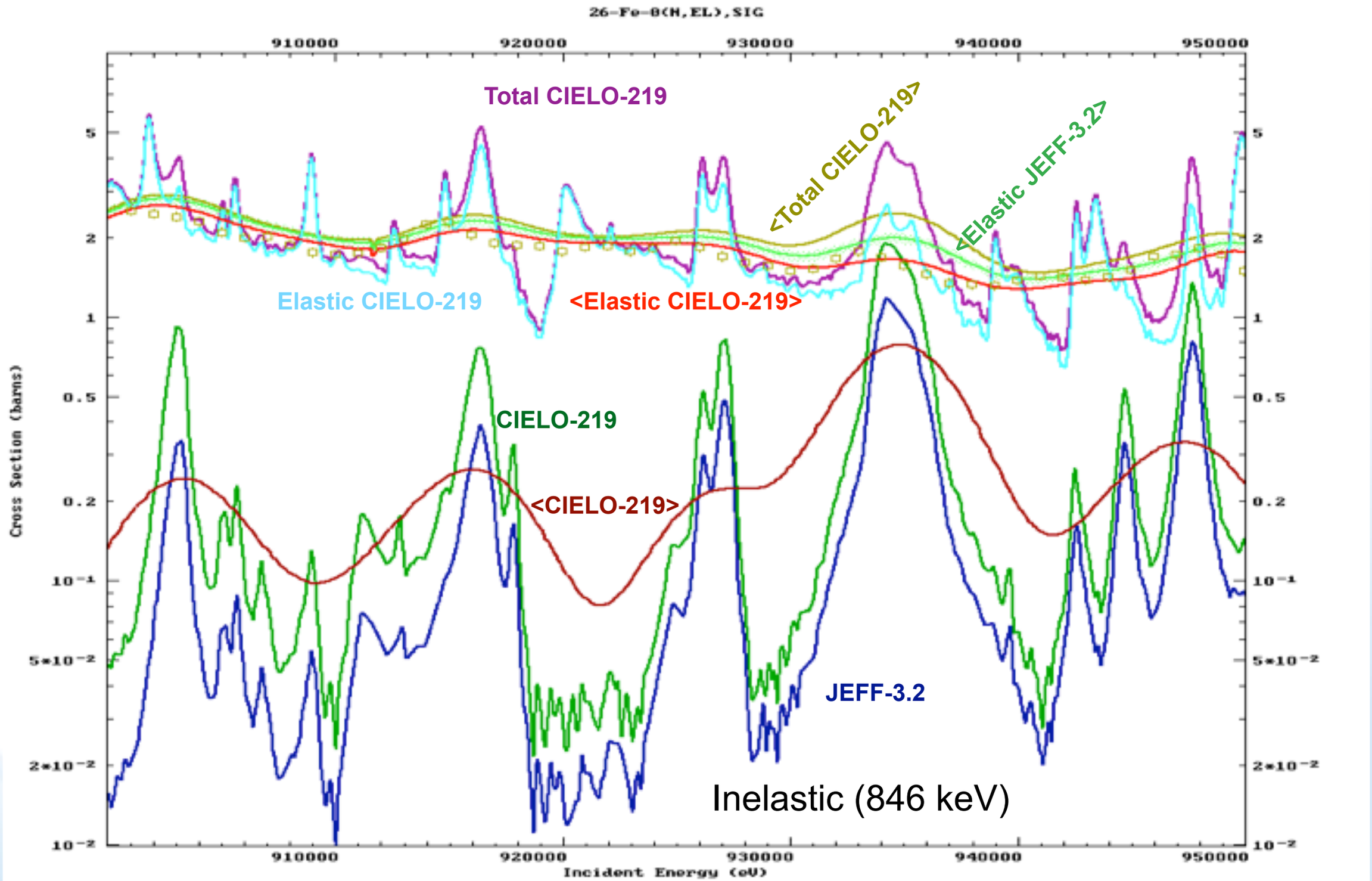
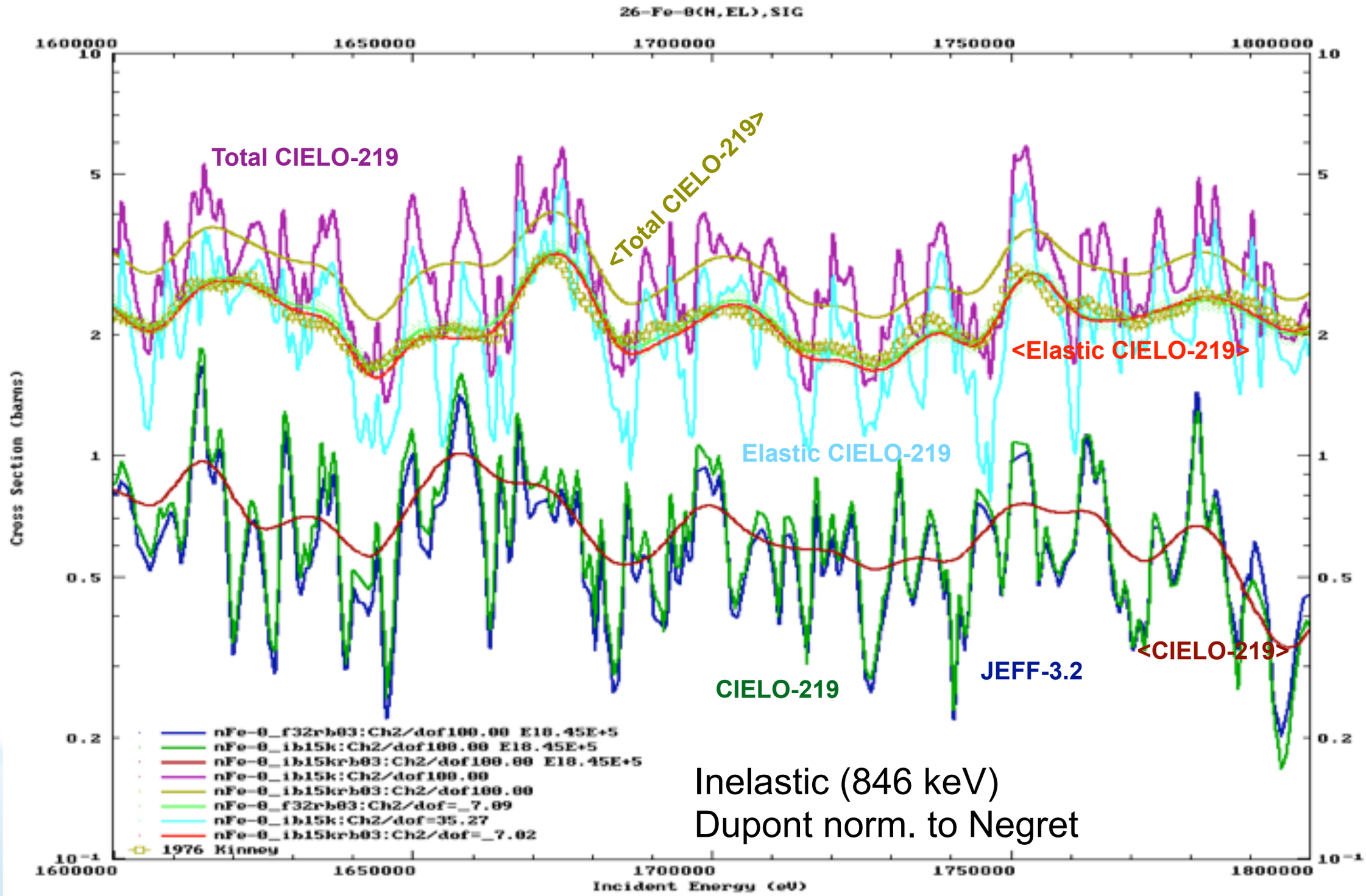
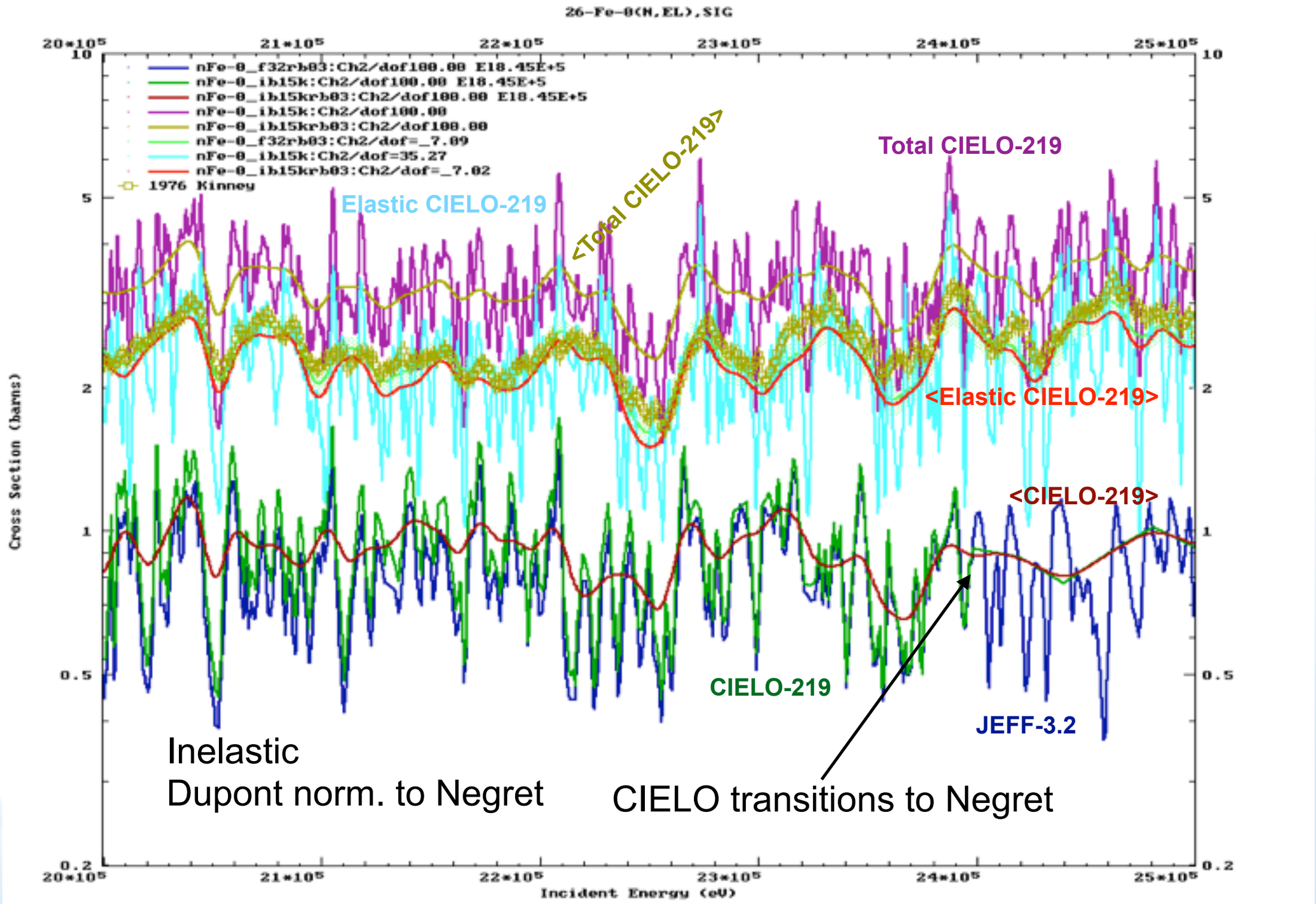
nat-Fe: Total, Elastic, Inelastic 900-950 keV



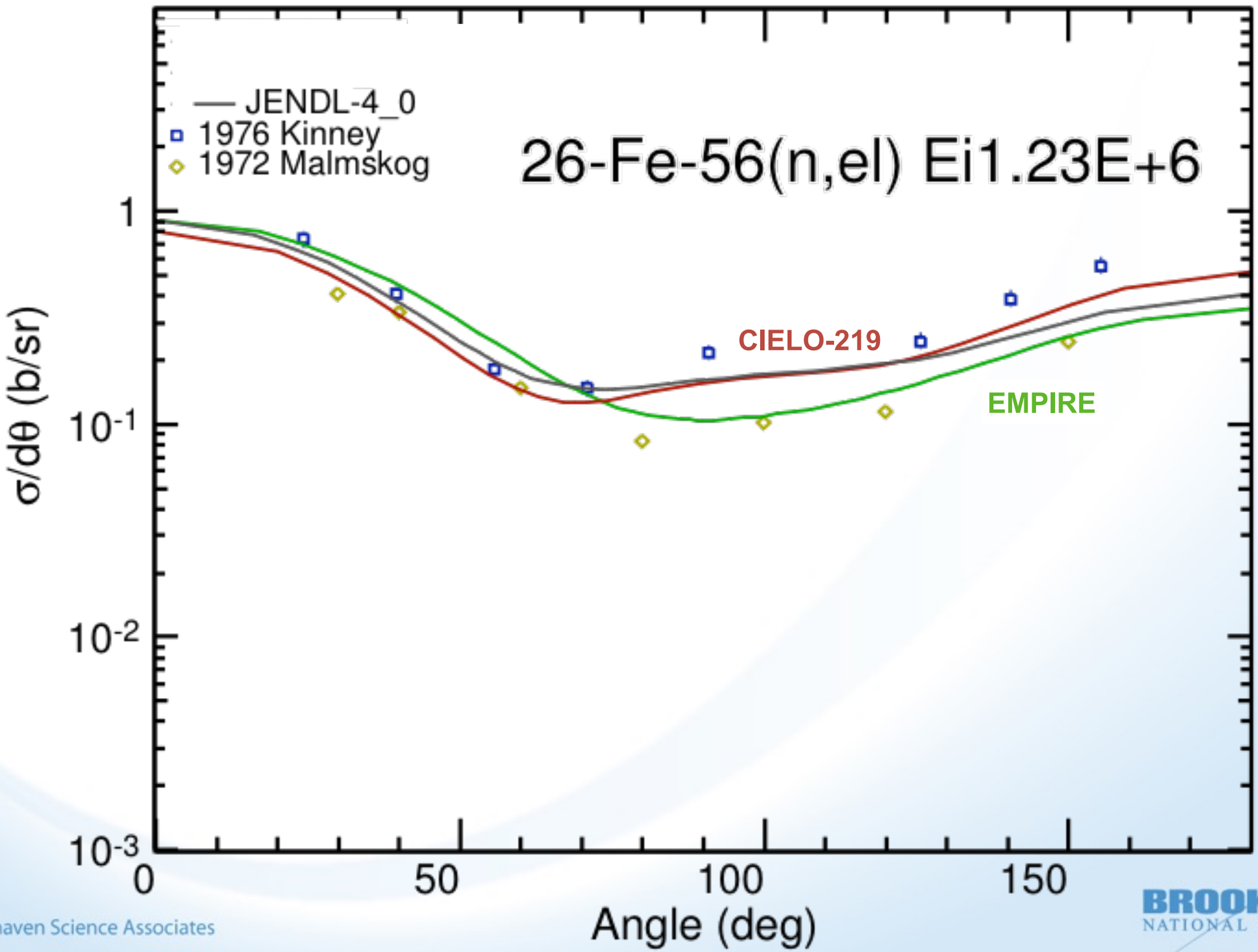
nat-Fe: Total, Elastic, Inelastic 1.60-1.80 MeV



nat-Fe: Total, Elastic, Inelastic 2.00-2.50 MeV



Elastic angular distributions – Kinney data



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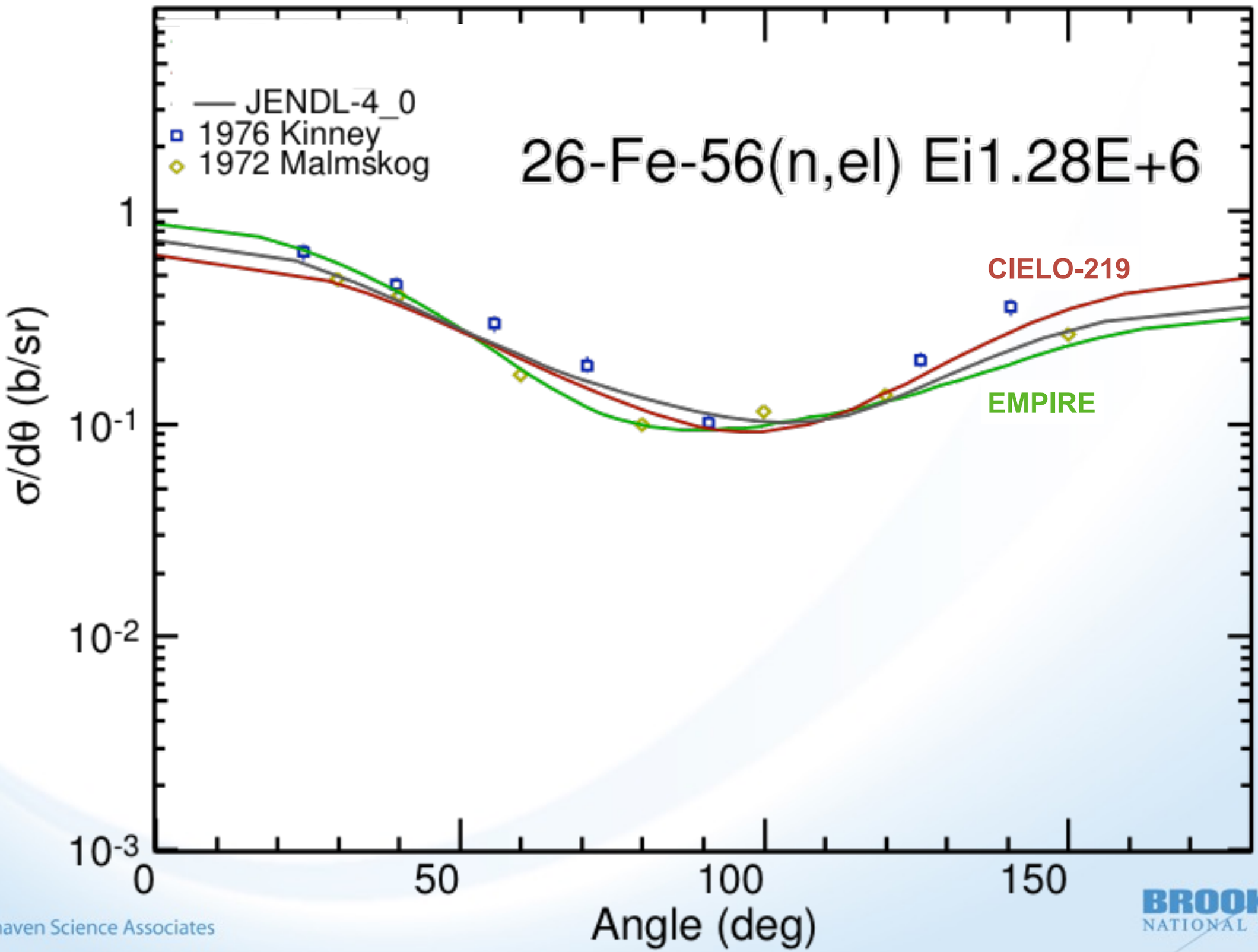

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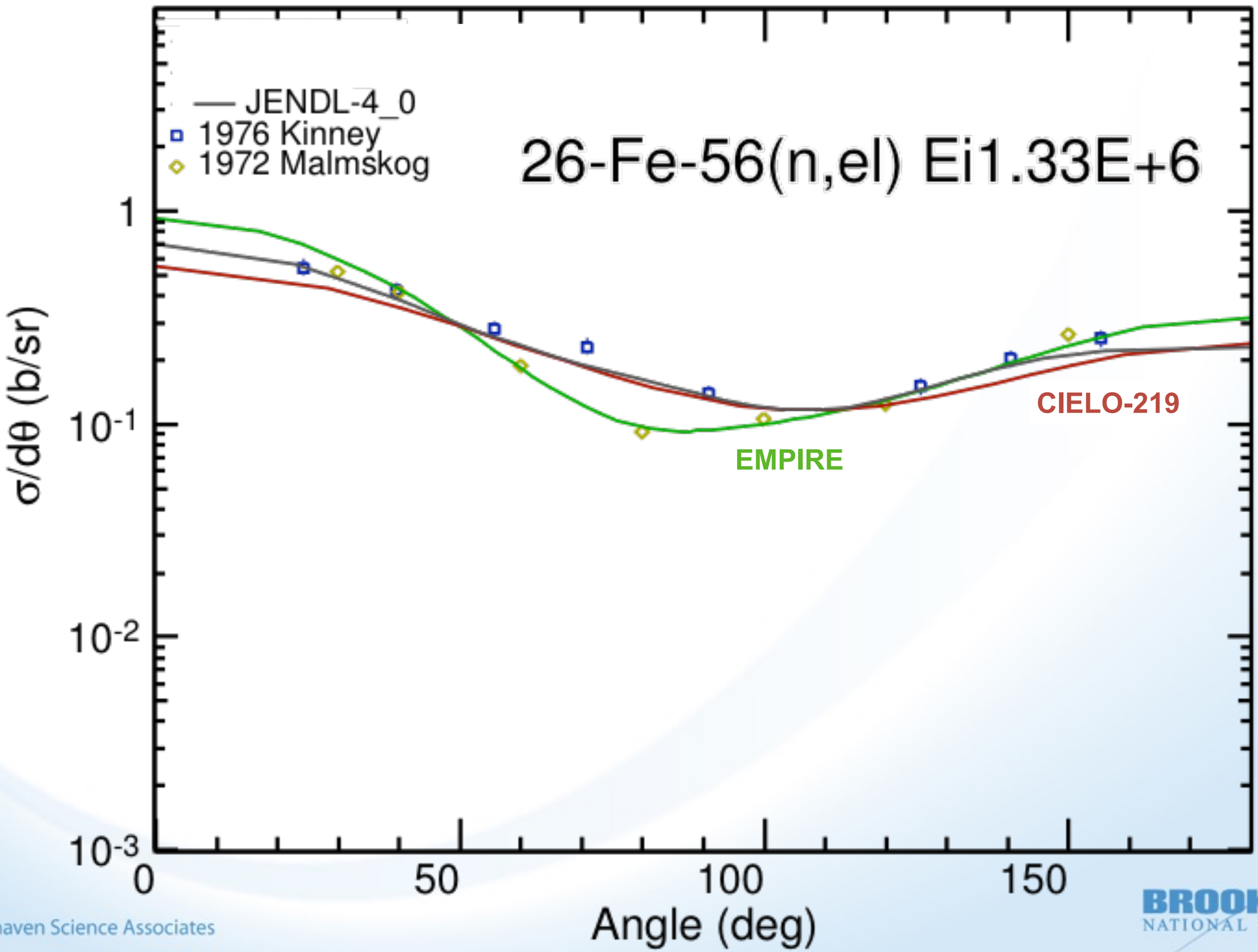

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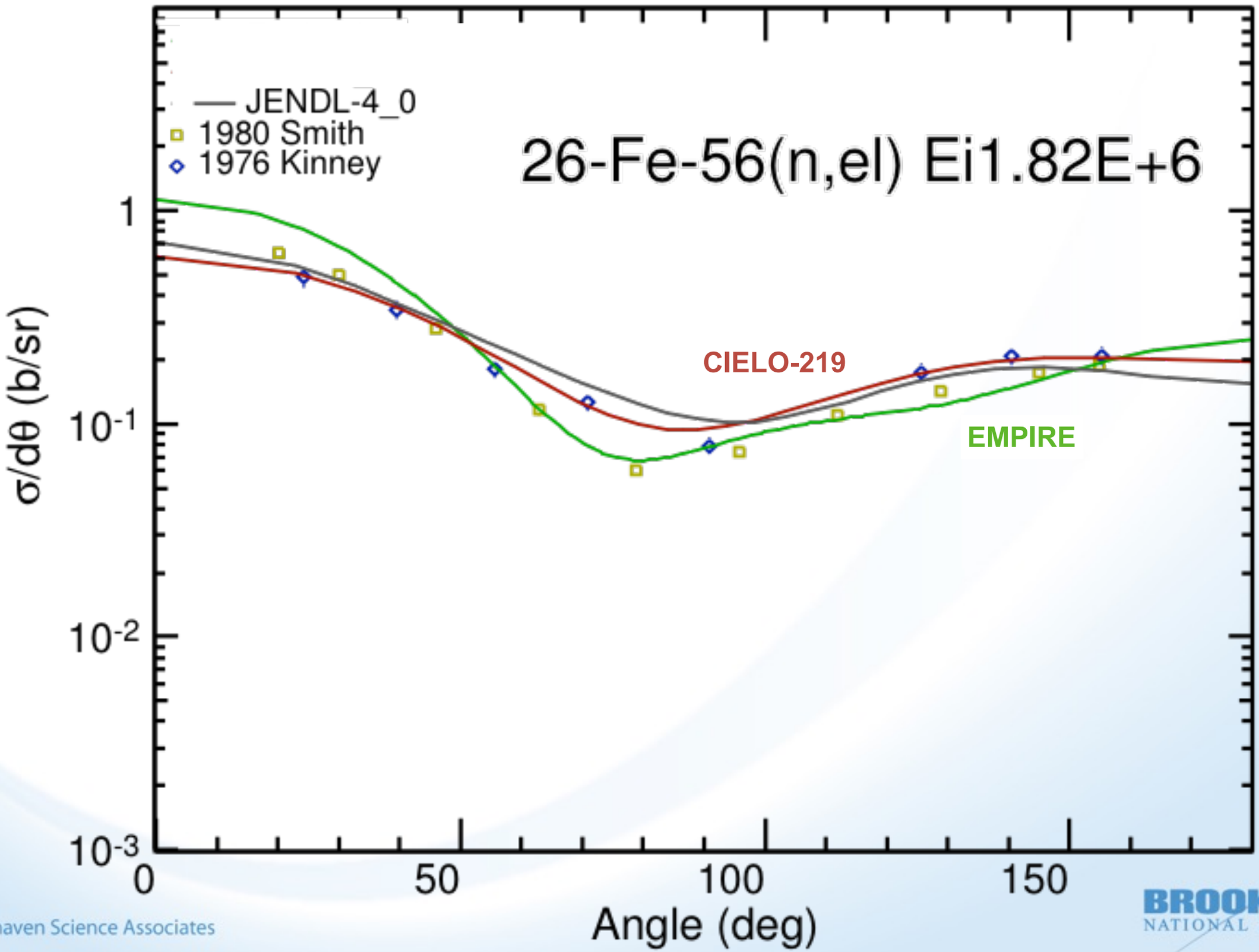
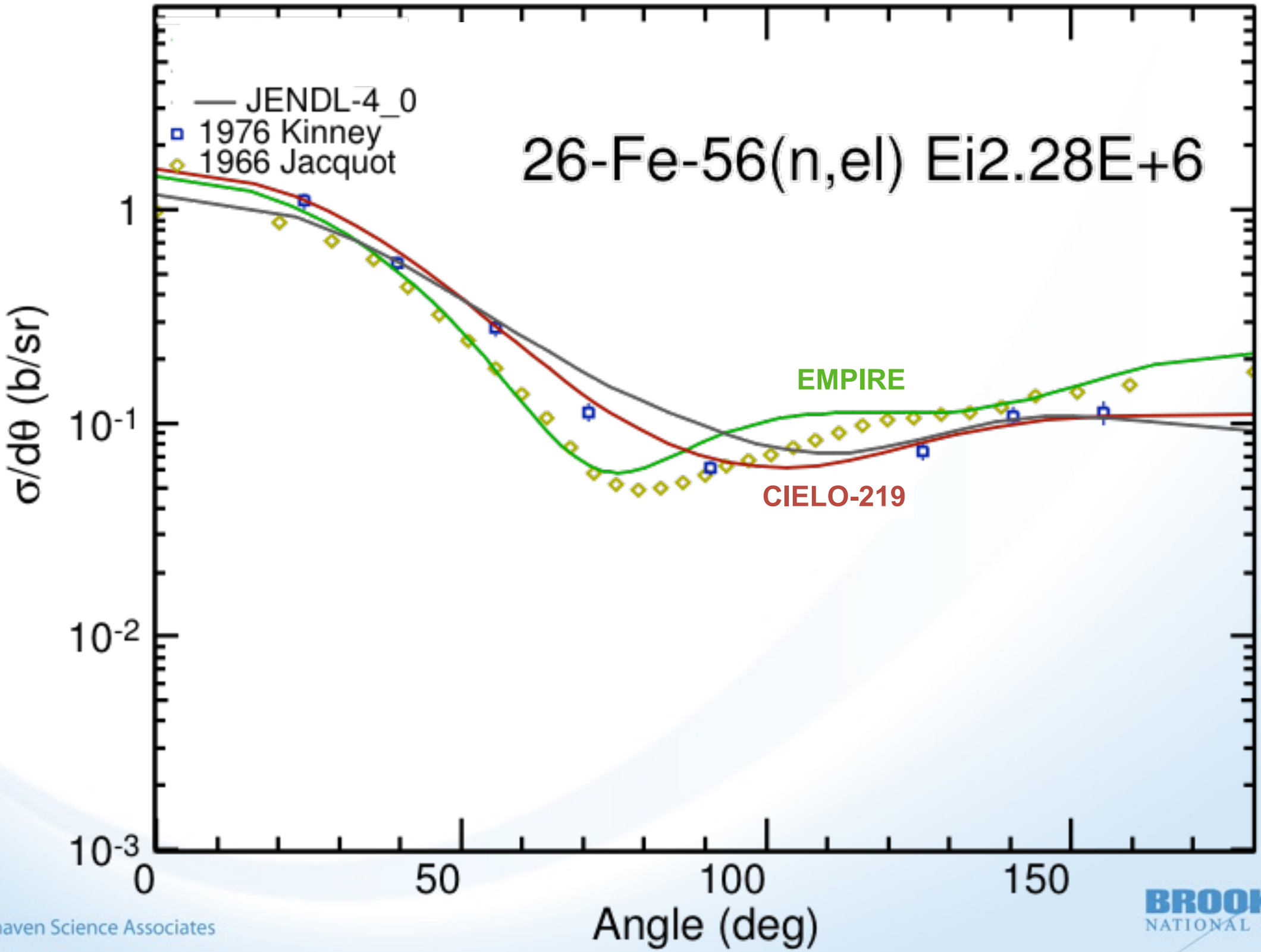


Elastic angular distributions – Kinney data

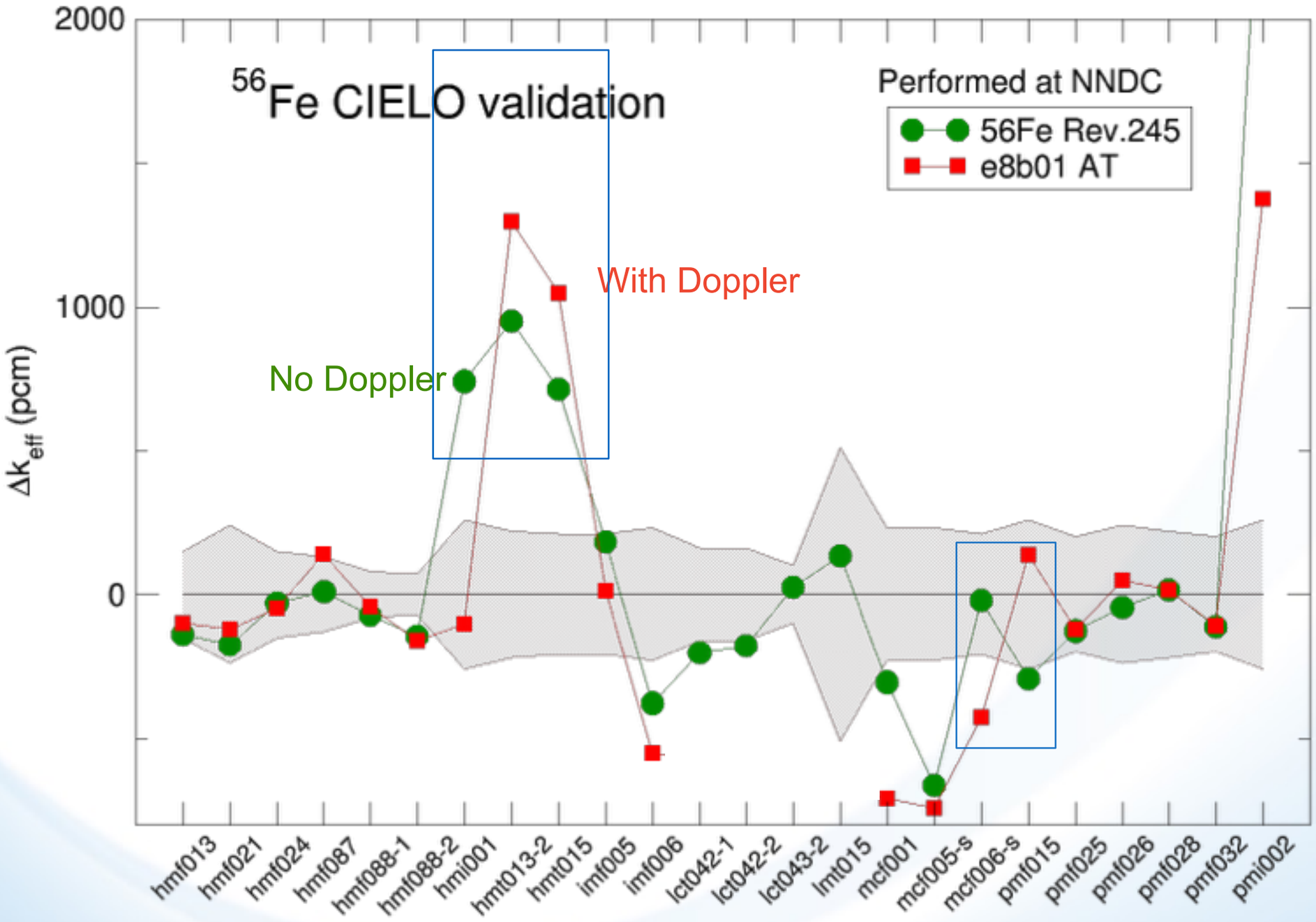


A few comments before looking into validation plots

- VIII.0beta1 file up to 4 MeV (total up to 6 MeV) consists of the best available experimental data.
- There are no new experiments in the resonance range so resonance parameters are essentially fixed up to 850 keV.
- semi-integral RPI measurements constrain capture and neutron emission
- (n,p) is a dosimetry reaction and is very well measured

If needed, there is very little freedom to adjust to integral experiments

Important preamble: Calculations for crits were done if they were performed in space (Doppler broadening was not considered)



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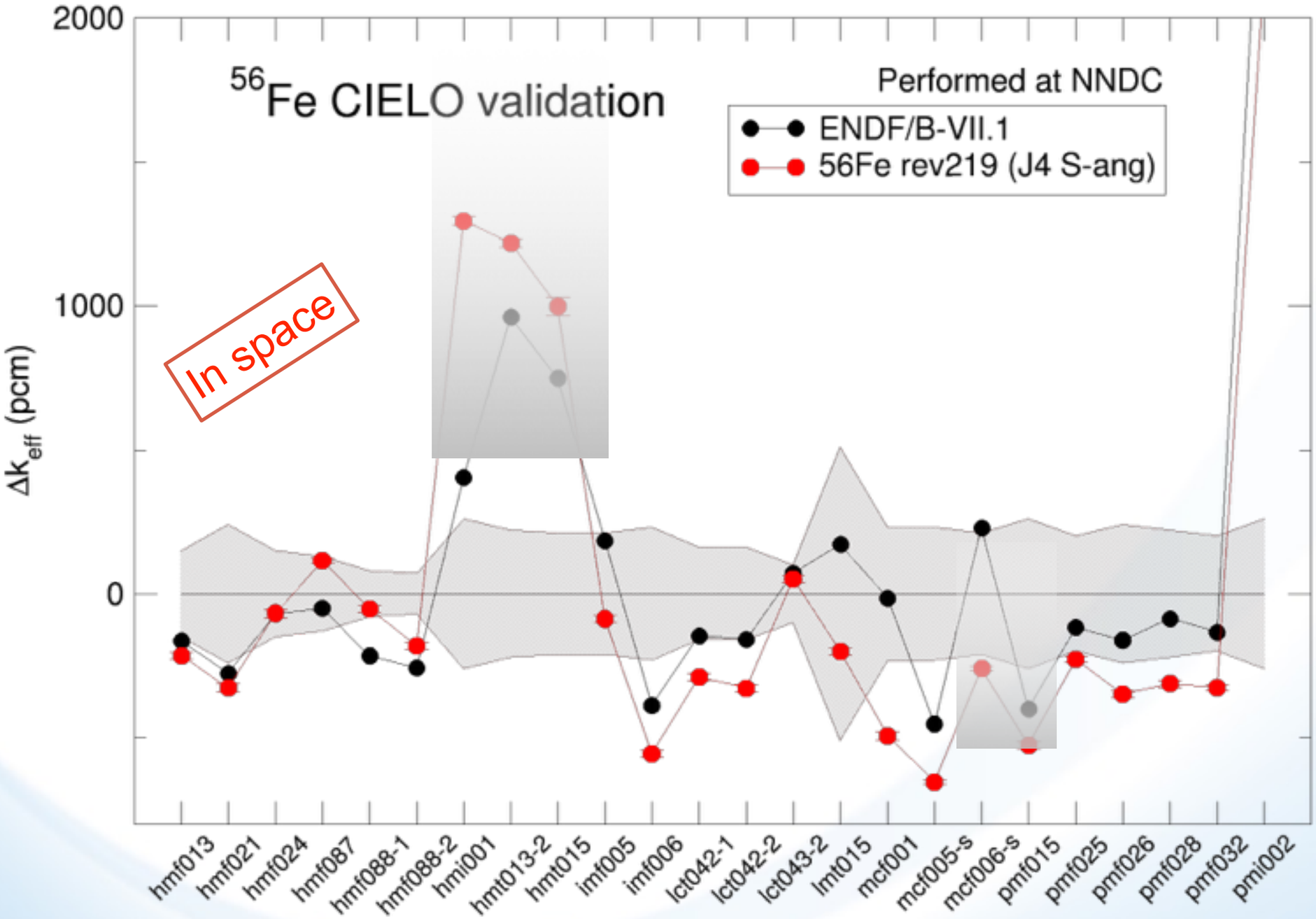
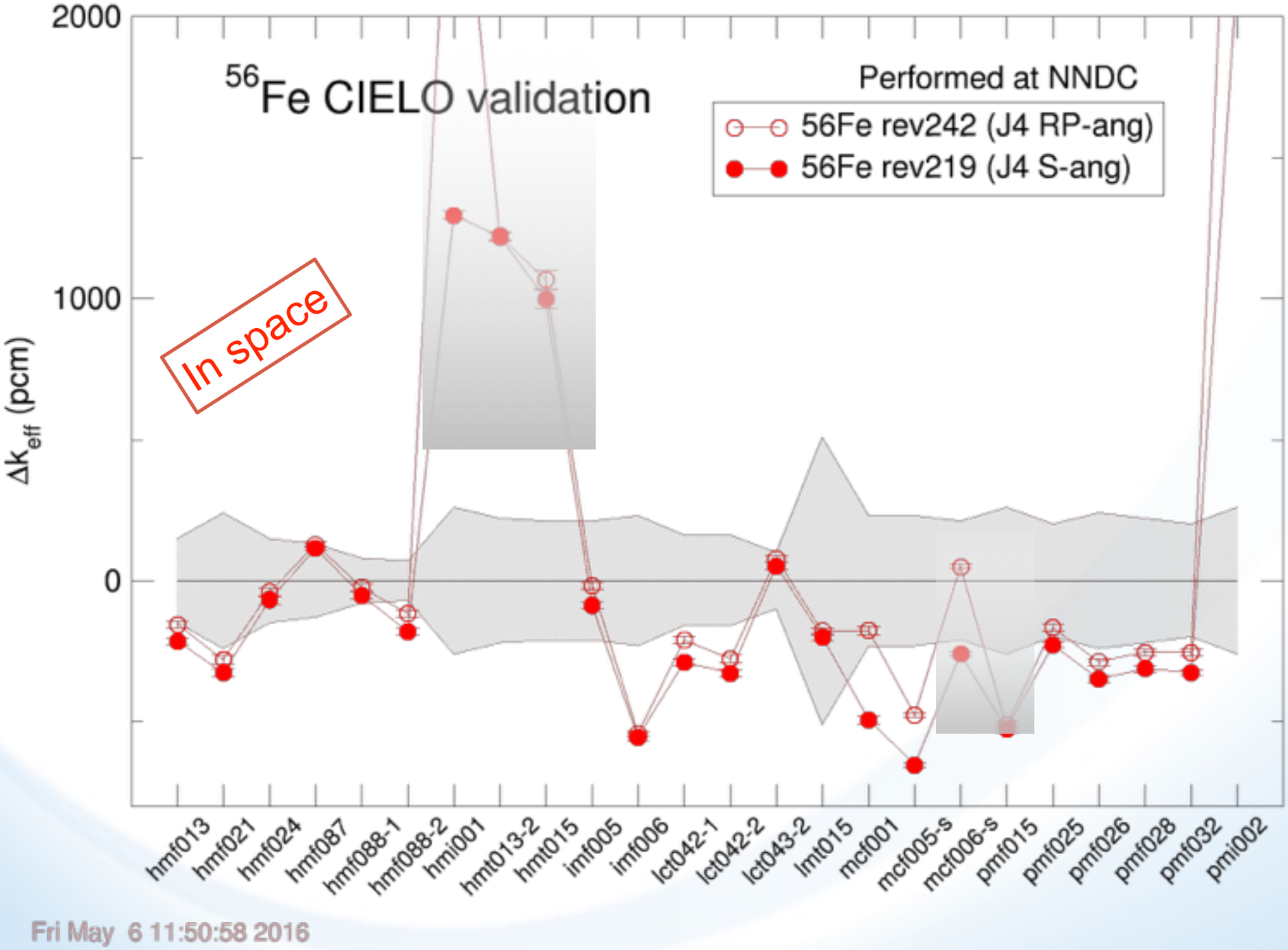
VIII.0beta0 validated against VII.1



Performance of VIII.0b0 generally worse than VII.1.

Effect of detailed elastic angular distr.



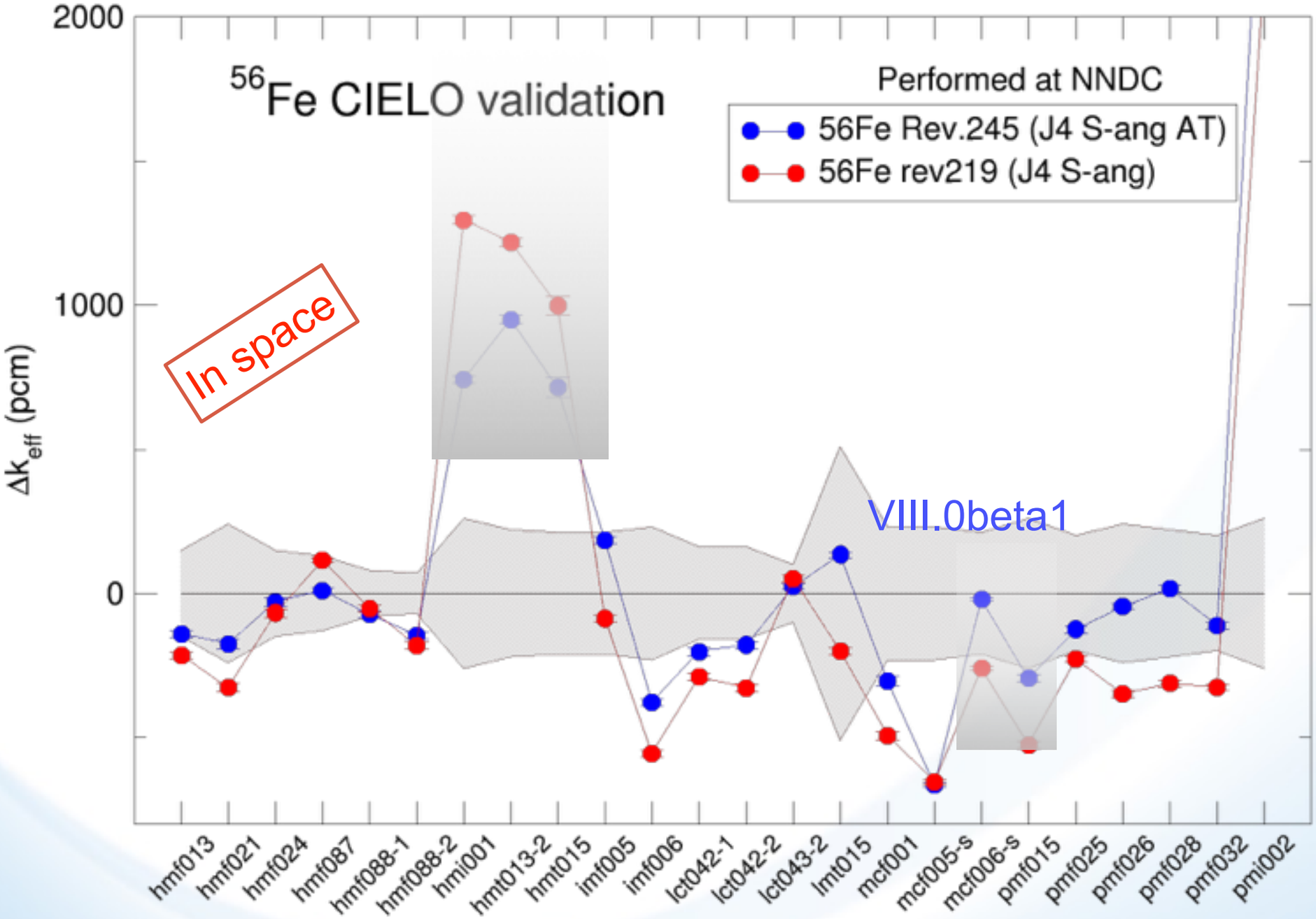
Detailed ang. distr. calculated from res. param. increase reactivity.

mct - considerably
pmf, hmf, imf, let - slightly
hmi001 - dramatically

Overall they work in the right direction that justifies additional Mb's in the file.

Still not enough to match VII.1 performance.

Tweaking P2 & P4 in elastic angular distr.



Increases reactivity and improves performance.

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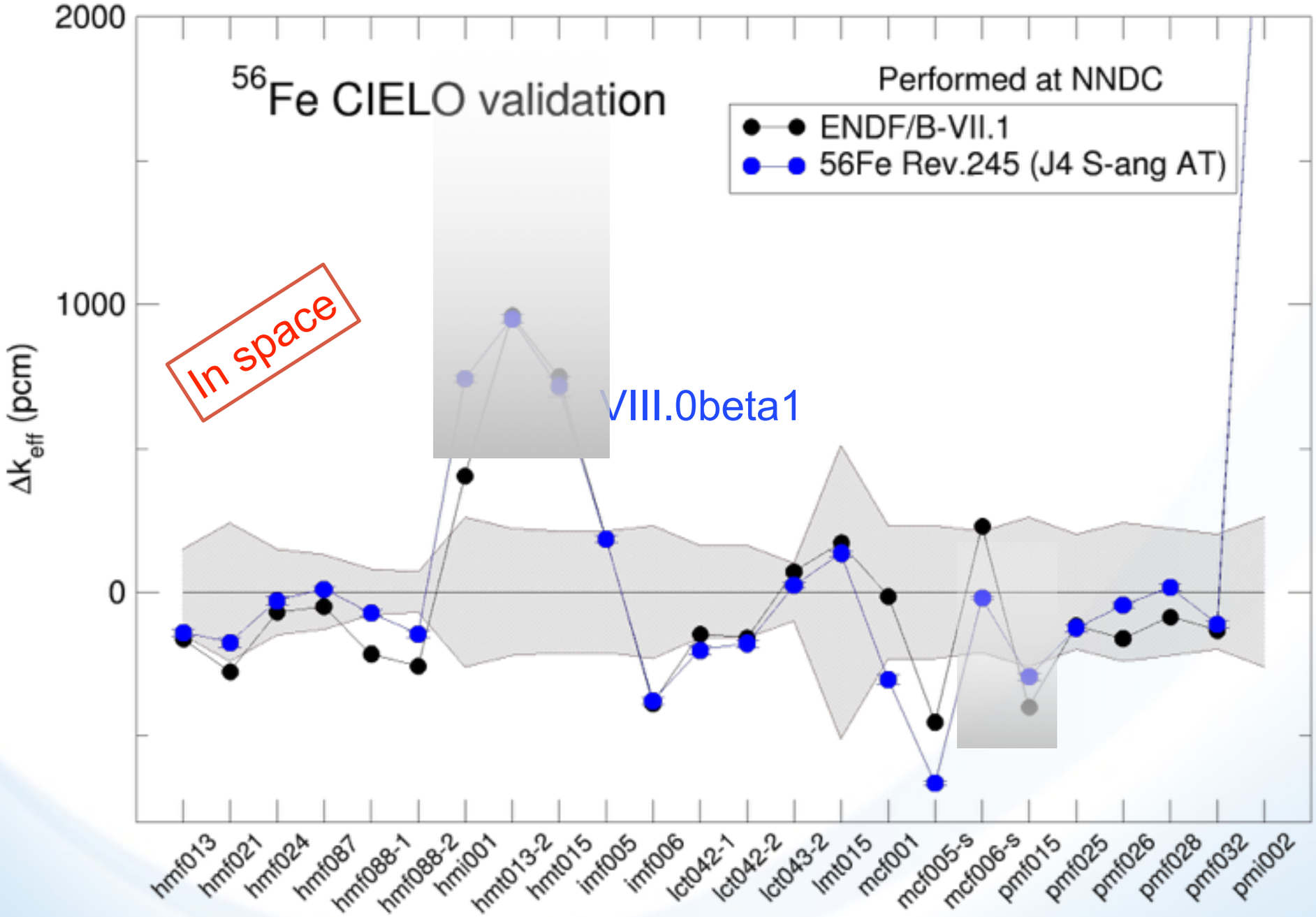
Tweaking elastic P2 & P4 in angular distr.



Favorably compares to VII.1 => selected as VIII.0beta1

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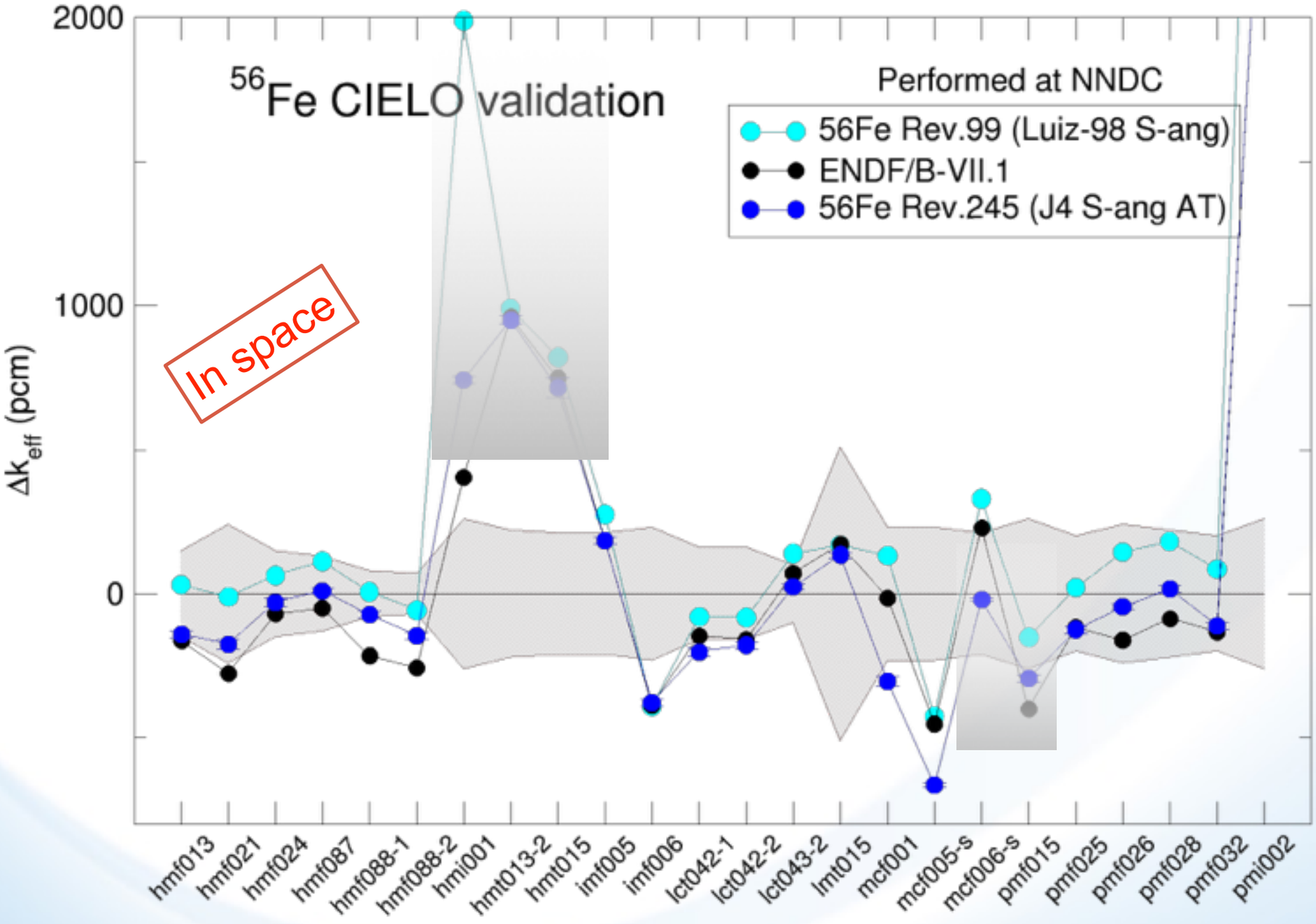
Alternative to beta1 - Luiz's Rev. 98 11/2015

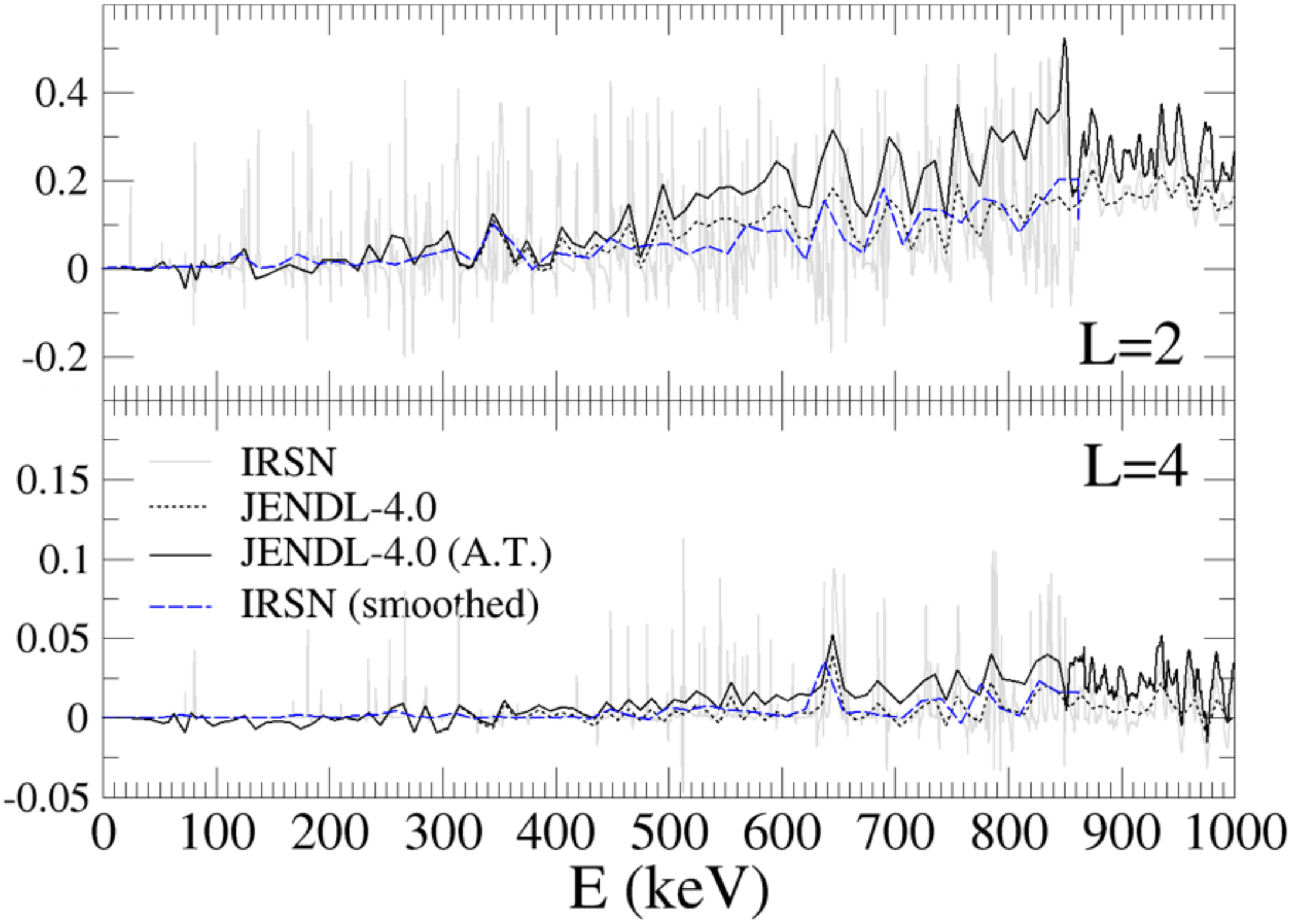


- Smoothed ang. distr. from JENDL-4.0
- No background
- No tweaks to P's

Integral performance comparable to VII.1 and VIII.0beta1, however, deficiencies in comparison with differential data (see next slides)

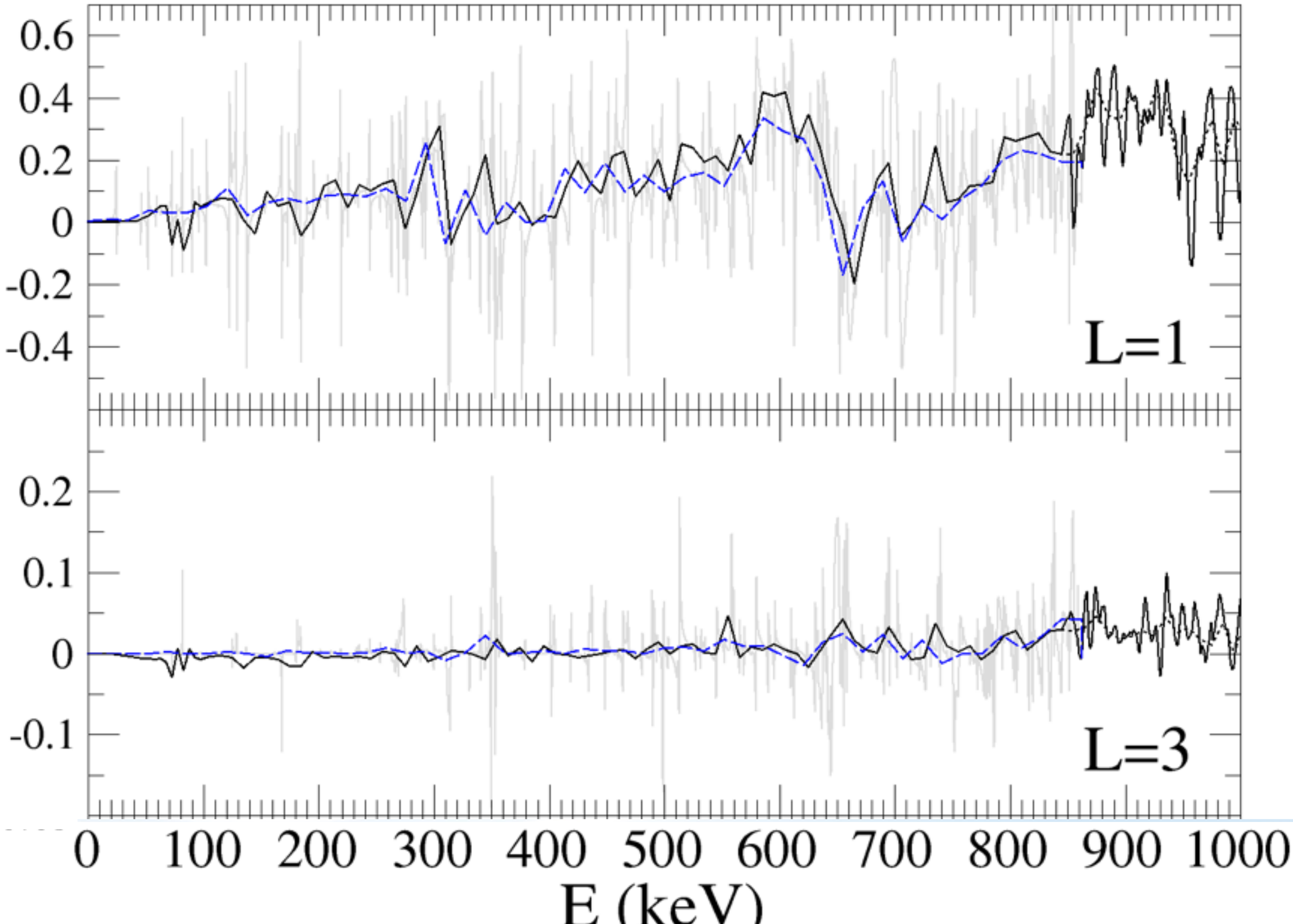
P2 & P4 tweaks - what they are?

Detaile
de file.



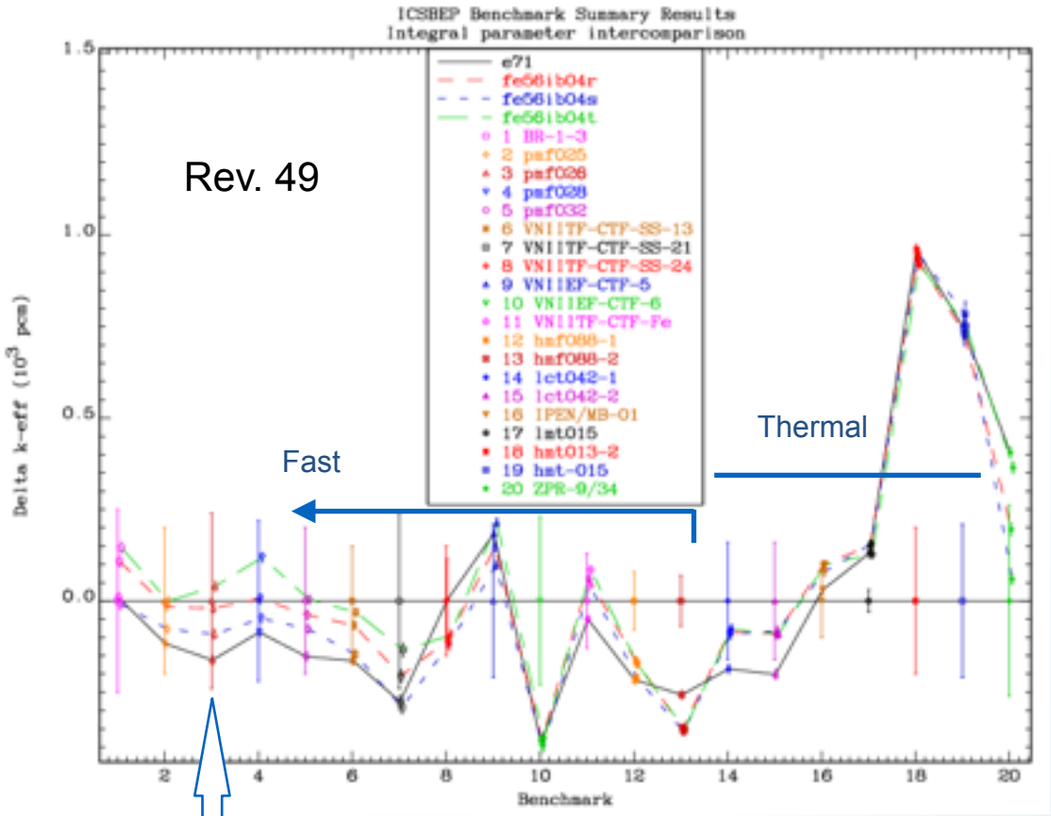
Remaining part (P1 & P3 not tweaked)

pretty good agreement between the two files



A couple of thoughts

- 24 benchmarks are mostly sensitive to the RR region
- Resonance parameters for 56Fe are very much fixed (Said) - there is not much room for improvement except:
  - external resonances
  - artificial background added to improve benchmarks
  - missing resonances at the end of RR
  - angular distributions in RR

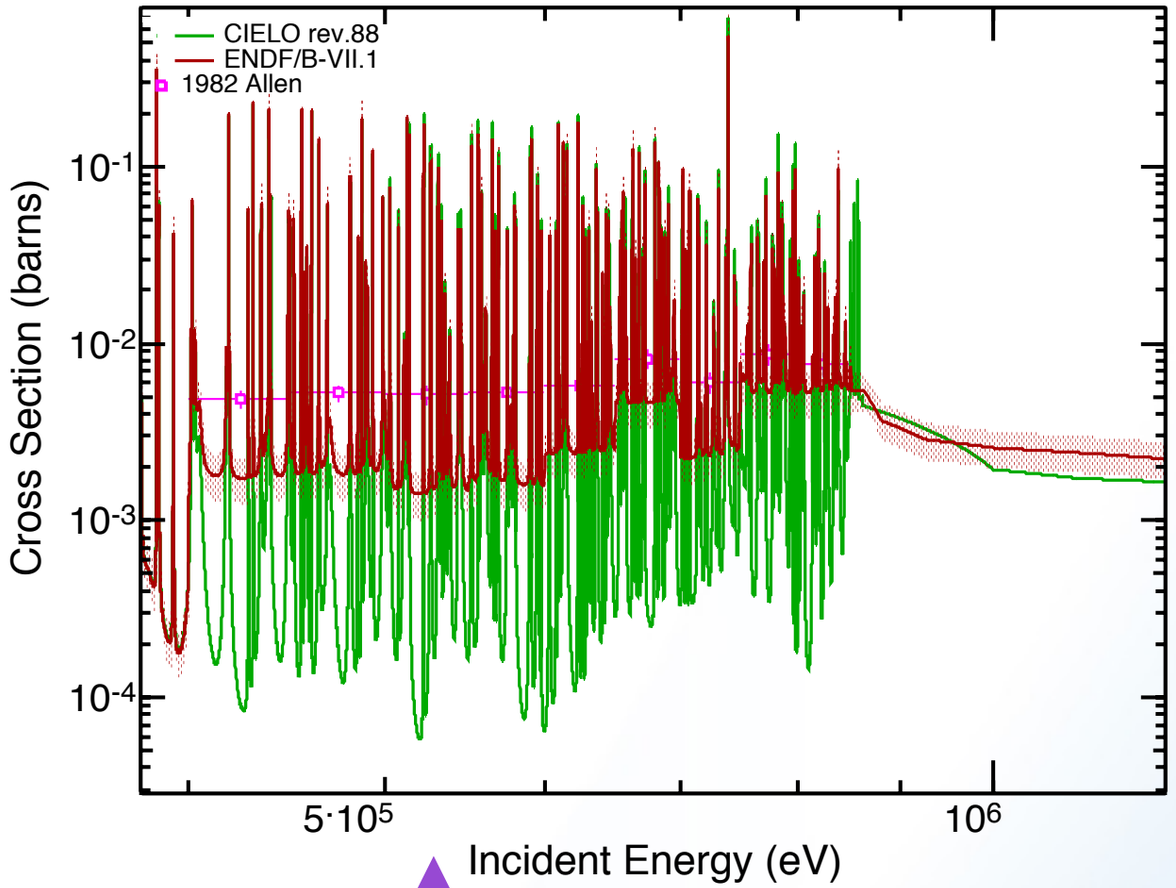


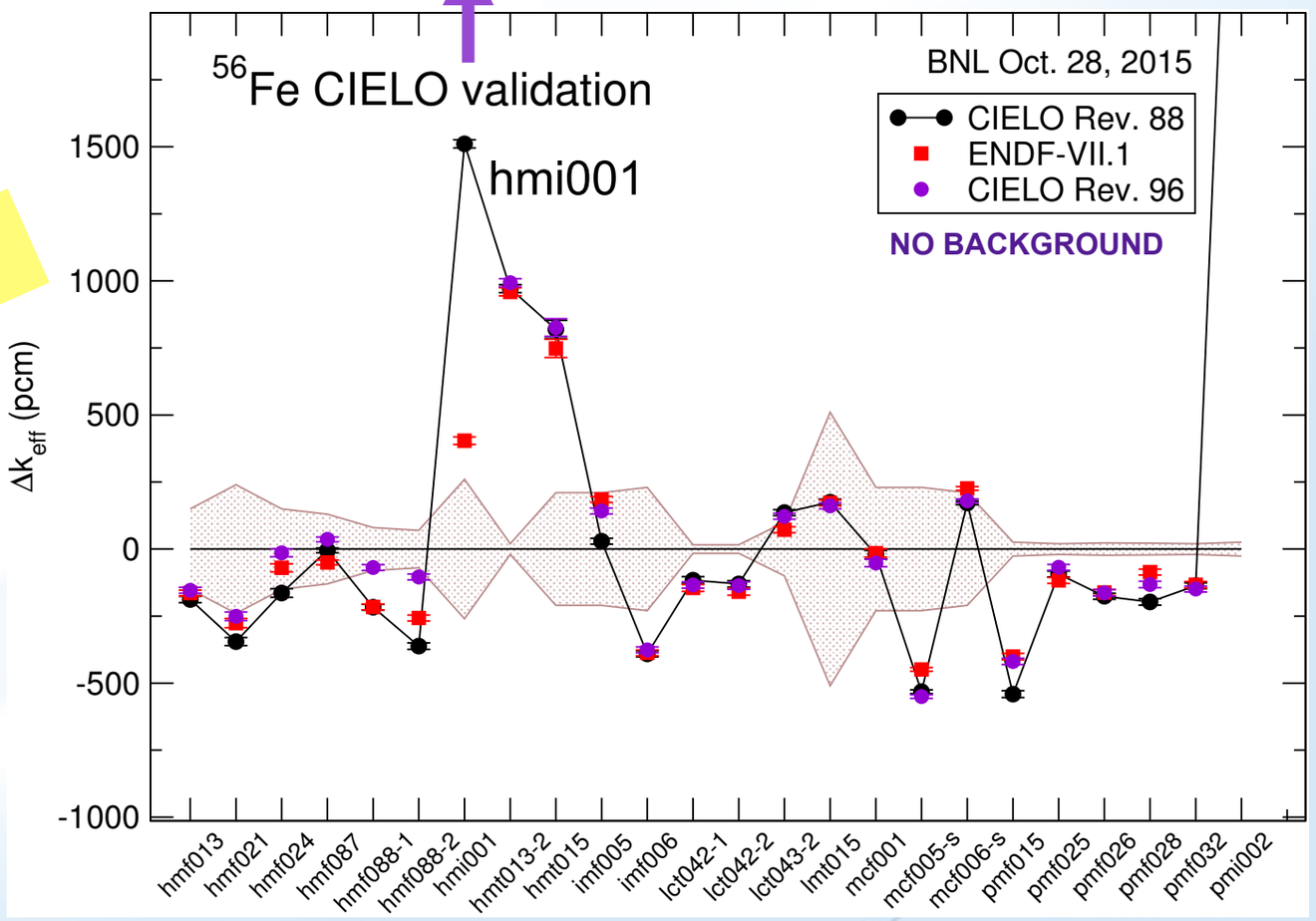
Sensitive to degree of smoothing of elastic angular distributions

Background?

- ENDF/B-VII.1 has capture background in RR above 400 keV
- Rev.88: Luiz RR (no background)
- Rev.96: VII.1 RR without background
- background keeps hmi001 in ENDF/B-VII.1 below 500 ppm
- for other benchmarks background doesn't do anything or makes them worse!

hmi001 (ZPR-9/34) needs background!

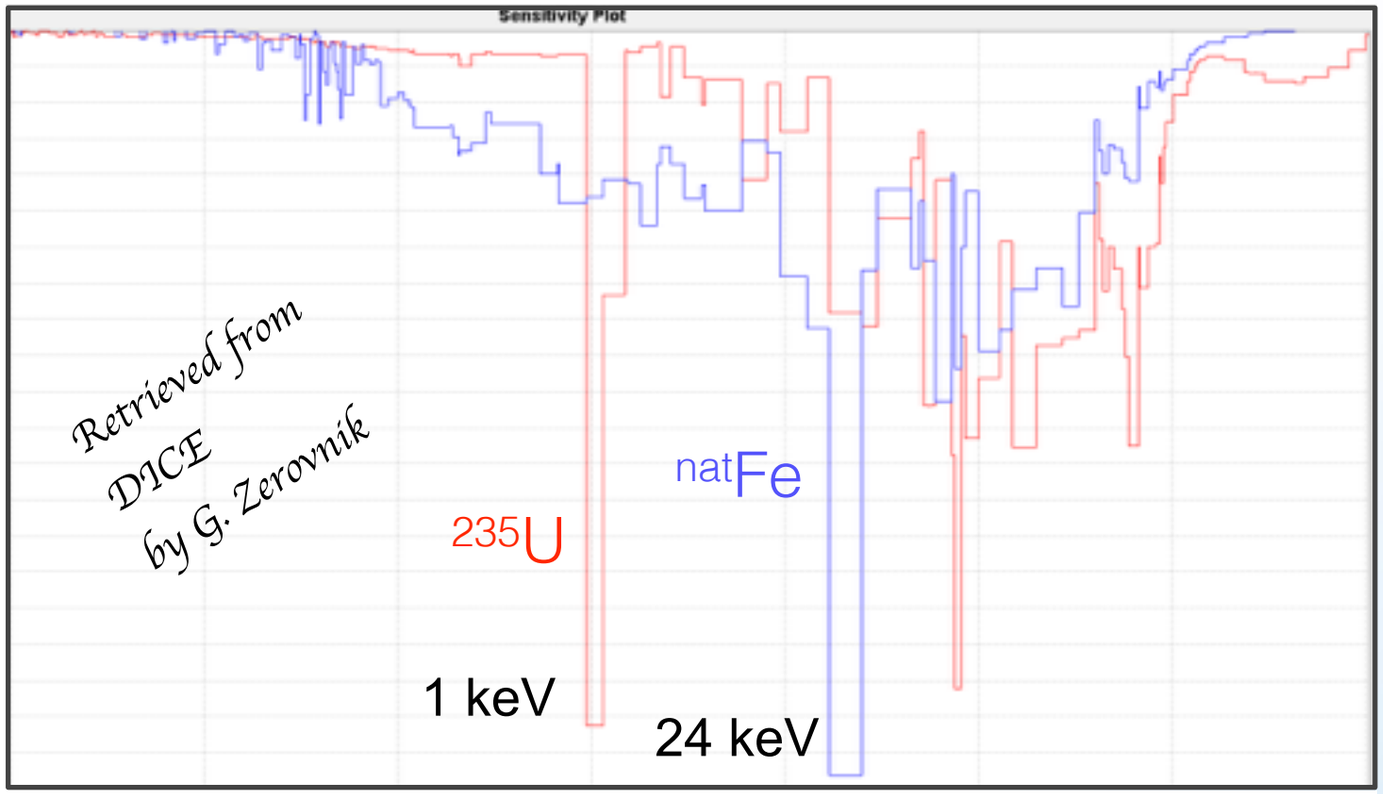




Could we fix ZPR-9/34 other way?

May be…

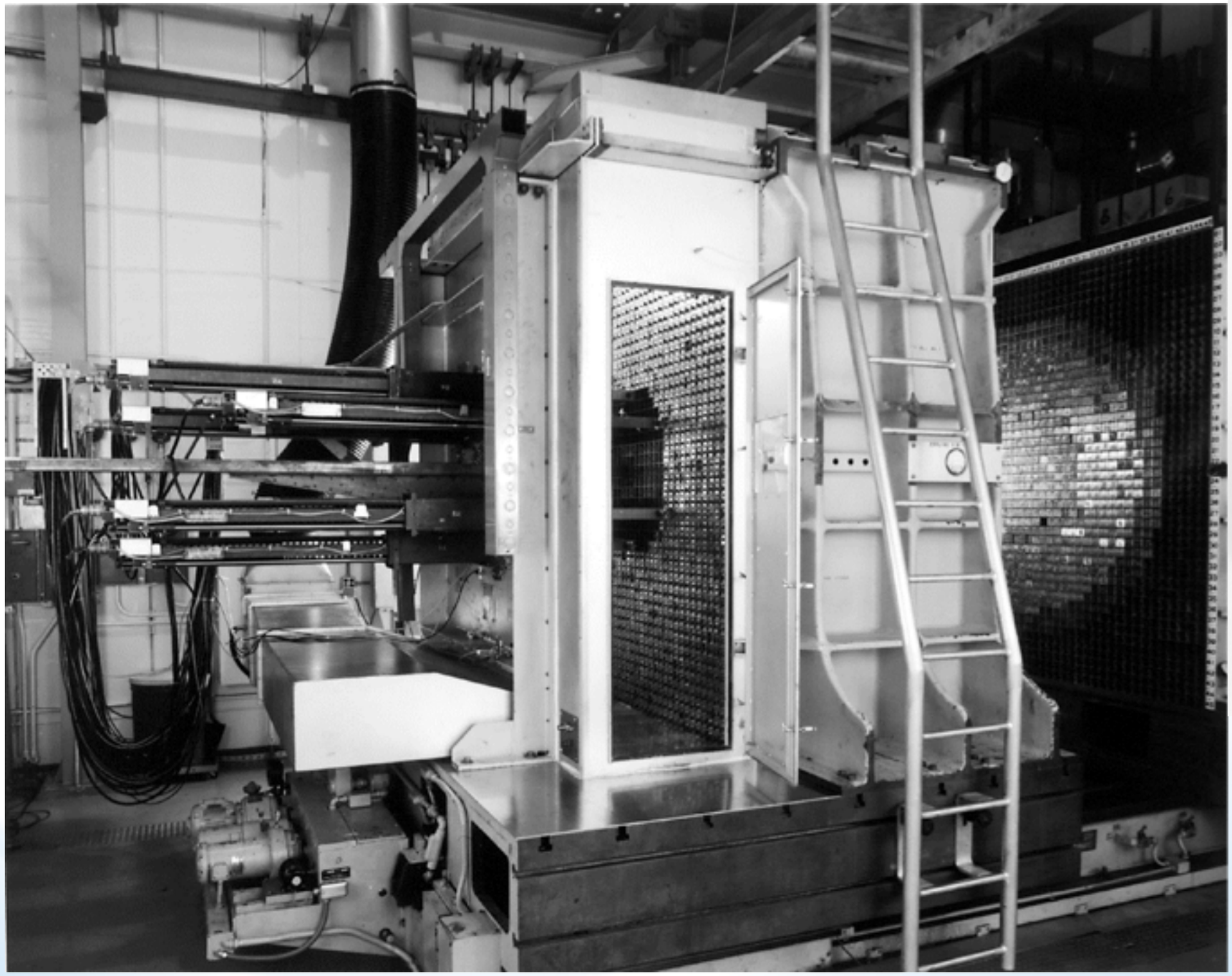
- sensitivity to capture on 235U at 1 keV
- sensitivity to capture on 56Fe around 24 keV (reason for a tweak in 56Fe rev.219)
- sensitivity to both captures between 50 keV and 1 MeV
- 57Fe alone makes ~400 pcm (in the wrong direction!)
- could be another material, e.g., 53Cr,…
- can we trust MCNP simplified (homogenized) model for ZPR-9/34?



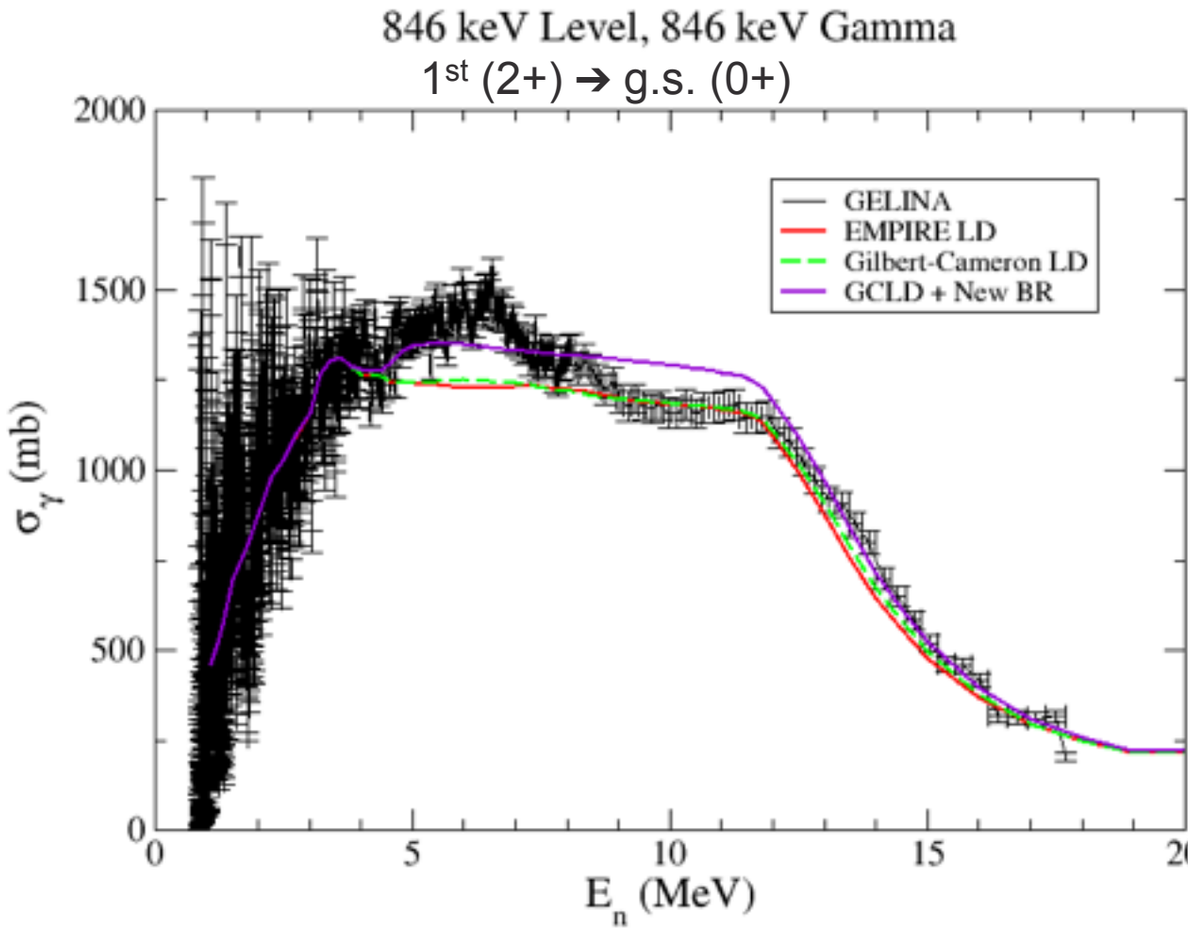
Sensitivity of ZPR-9/34 (hmi001) to capture in U-235 and Fe-nat

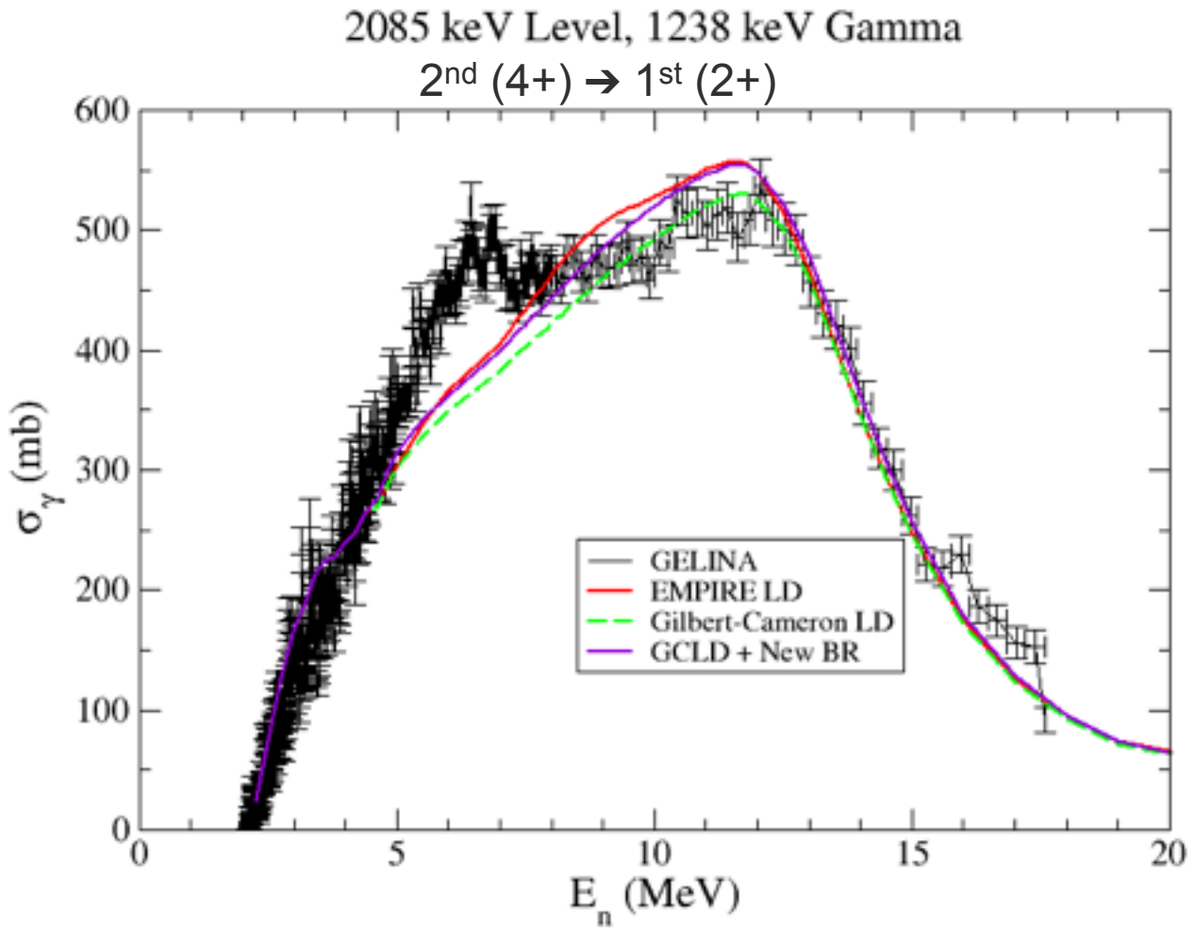
We should try a holistic approach: consider CIELO 235U, look at other materials & factors, check MCNP model…

View of the ZPR-9 Facility (HEU-MET-INTER-001)



Geel measured (n,n') using partial γ σ(E)





- Expect biggest effect on lines from 1st (2+) and 2nd (4+) excited states
- Effect of level densities comparable to BRs
- Can't get shape right

Negret et al. Phys. Rev. C 90, 034602 (2014)

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Conclusions

- We've got fast neutron file that fits differential data (subject to RPI validation though!) - there will be small adjustment but nothing significant.
- 56Fe has been revisited based on RPI feedback (RPI data extremely important again for Fe-56). Fluctuations have been empirically considered both in total and inelastic (from data), and especially in angular distributions (following Kinney experiment).

- Major effort is focused on the RR (determines crits benchmarks)
  - current file makes use of JENDL-4.0 which fits well differential data
  - modifications include changes to the background in capture and elastic and 'ad hoc' tweaks to the P2 & P4 coefficients in elastic angular distributions.
  - these bring performar we need the full CIELO library able to VII.1.
  - additional help comes from angular distributions calculated from resonance parameters.
- Elastic angular distr. and capture can be used to improve agreement with benchmarks, however…

…and where we go? may need to revise

- Additional information may still be extracted based on RPI data (e.g., capture on Fe-56 tuned above 846 keV, inelastic to elastic ratio and angular dependence improved)
- Angular distributions from res. param.
- Parity distributions in level densities (likely part of the cosmetics)
- Additional work needed for SS non-iron components (e.g., Cr)
- Major problem - modern & reliable set of RR parameters for 56Fe without background (but dealing with missing resonances above 500 keV), and with angular distributions

Said:

- "The only new measurement of resonance parameters since 2005 is that of CERN…
- CERN capture kernels agree with the ORNL and GEEL results very well…
- resonance capture widths are well determined… no change from values reported in the ATLAS…
- **however**, in the Reich- Moore formalism fictitious strong levels are required and are imposed above the upper energy region"