BNL-114315-2017-IR

Brief History of Iron Evaluations in the ENDF/B Library

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September 06, 2017

National Nuclear Data Center

Brookhaven National Laboratory

**U.S. Department of Energy
USDOE Office of Science (SC),
Nuclear Physics (NP) (SC-26)**

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Brief History of Iron Evaluations in the ENDF/B Library

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(Dated: September 14, 2017)

The report summarizes the development of the iron evaluations from ENDF/B-V to present.

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I. INTRODUCTION

This report outlines the history of ENDF/B evaluations of the iron isotopes. Our detailed history extends

back to ENDF/B-V, when isotopic evaluations were first introduced in the ENDF/B library. This history ends at the ENDF/B-VIII.0 β 4 evaluation as the ENDF/B-VIII.0 evaluations are described in [1] and the ENDF/B-VIII.0 β 4.1 evaluations are basically the released files.

Before ENDF/B-V, the ENDF/B library only contained a natural iron evaluation. Details of the ENDF/B-III (1972) natural iron evaluation are described in ORNL-4617 (ENDF-139) [2] and details of both the ENDF/B-IV (1975) and ENDF/B-V (1979) evaluations are described in ORNL/TM-7523 (ENDF-302) [3].

Figures 1–4 provide a graphical overview of the history of each ENDF evaluation.

II. ENDF/B-V

In ENDF/B-V, the resonances in this file were split into the isotopic files while new new fast regions evaluations for all the isotopes were provided. After this release, only isotopic evaluations are present in ENDF.

A. ENDF/B-V.0 (1979)

^{nat}Fe [Fu (ORNL)] The ENDF/B-V.0 natural iron evaluation contained several notable features:

- The resonance parameters for ⁵⁴Fe, ⁵⁶Fe and ⁵⁷Fe from 1 keV to 400 keV were examined in detail by C.M.Perey [8]. Parameters for ⁵⁸Fe were taken from the ENDF/B-V dosimetry file [9].
- In the total and capture cross sections, broad structures in the resonance range (155 eV to 400 keV) were kept unchanged from ENDF/B-IV values. Narrow resonances were better defined.
- The capture cross sections from 155 eV to 400 keV are well-represented by the resonance parameters. From 400 keV to 1 MeV average cross sections measured by Allen *et al.* [10, 11], which agrees with those of Le Rigoleur [12], were adopted. Above 2 MeV, the capture cross section was increased.

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FIG. 1. Provenance of the CIELO and ENDF/B-VIII ^{54}Fe evaluation. Each major component of the evaluation from all libraries that fed the current evaluation are shown. Experiments that were included in the resonance evaluation are listed explicitly even if they are not mentioned in the main text. These data are referenced in the *Atlas of Neutron Resonances* [4]. We note that various revisions of the *Atlas of Neutron Resonances* [4–6] played key roles in the development of several data libraries. In this figure, the dotted line represents the addition of experimental data into the evaluation, the dashed line represents a modification to an existing evaluation and a solid line represents the adoption of an evaluation, unchanged.

FIG. 2. Provenance of the CIELO and ENDF/B-VIII ^{56}Fe evaluation. Each major component of the evaluation from all libraries that fed the current evaluation are shown. Experiments that were included in the resonance evaluation are listed explicitly even if they are not mentioned in the main text. These data are referenced in the *Atlas of Neutron Resonances* [4]. The new CIELO resonance evaluation is based in the JENDL-4.0 resonance evaluation. The fast region of the CIELO evaluation is based on a combination of new EMPIRE calculation and IRDFF and JEFF evaluations. In this figure, the dotted line represents the addition of experimental data into the evaluation, the dashed line represents a modification to an existing evaluation and a solid line represents the adoption of an evaluation, unchanged.

FIG. 3. Provenance of the CIELO and ENDF/B-VIII ^{57}Fe evaluation. Each major component of the evaluation from all libraries that fed the current evaluation are shown. Experiments that were included in the resonance evaluation are listed explicitly even if they are not mentioned in the main text. These data are referenced in the *Atlas of Neutron Resonances* [4]. The new evaluation is a reformatted (into LRF=7) and tweaked version of what is available in the new Atlas [4]. In this figure, the dotted line represents the addition of experimental data into the evaluation, the dashed line represents a modification to an existing evaluation and a solid line represents the adoption of an evaluation, unchanged.

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- The inelastic cross section corresponding to the first excited state of ^{56}Fe was revised according to the recommendation of Kinney and Perey [13] up to 1300 keV.
- The (n, γ) cross section was substantially increased to go through a data point near 14 MeV [14].
- For the elastic angular distribution, high-resolution data of Kinney and Perey [15] from 40 keV to 1.4 MeV were adopted. The broad trend of the Legendre coefficients are in good agreement with ENDF/B-IV values.
- All gammas were lumped in the total inelastic cross section (MT=3) and were taken from Chapman and Morgan [16]. This is a repeat measurement using ORELA which resolves a long-standing discrepancy. The lowest three neutron energies (up to 2.122 MeV) are for capture gamma rays.
- Covariances for the resonance parameters evaluated by C.M.Perey [8].

^{56}Fe [Fu (ORNL)] Experimental data available since the evaluation of Fe-56 (n,p) cross sections by Dudev and Kennerley [17] were reviewed. Smith and Meadows [18] reported new data from 4 to 10 MeV, an energy range most important for application of this reaction to fission reactor dosimetry. Vonach [19] has recently called for attention to his data [20] from 13 to 15 MeV. Further checks [19] resulted in a reduction of the data errors from 4% to 2.5%. The data had not been used in the Dudev and Kennerley evaluation but are 2 to 3% lower than the evaluated values. Three single-energy measurements [21–23] near 14.6 MeV have been reported. The one by Dyer [21] is 1% higher than the ENDF/B-IV value, Robertson 7% higher, and Qaim 4% lower. Inclusion of the new data in a subjective analysis results in up to 10% reduction from the ENDF/B-IV values from threshold to 6 MeV, 2-3% reduction from 6 to 10 MeV, and 1-2% reduction from 13-15 MeV. The data of Smith and Meadows are relative to ENDF/B-IV U-238(n,f) cross sections and had been renormalized to ENDF/B-V values before being used in the present evaluation. The effect on the calculated fission spectrum average is estimated to be a reduction of about 3% from ENDF/B-IV value.

B. ENDF/B-V.1 (1983)

^{nat}Fe [Fu (ORNL)] In the ENDF/B-V.2 release, the file was again revised:

- Inelastic scattering cross sections for 21 levels in ^{57}Fe and 2 levels in ^{58}Fe were included and lumped as 14 sections. Corresponding gamma-ray production data (file 12) and covariance data (file 13) were also provided.

- Arthur and Young evaluations [24] for (n,2n), (n,d), (n,t), and (n, ^3He) were judged to be superior to ENDF/B-V and were adopted.
- Energy imbalances [25] were corrected from 2 to 20 MeV by adjusting the total gamma-ray production cross sections (file 13) to reproduce estimated values of heating per collision. The adjusted results approach those of ENDF/B-IV. The largest changes occur in the energy range 13 to 20 MeV where the adjusted results lie in between all available data [26–31].
- Resonance parameters (file2) and covariances (file 32) were revised so that the files and the corresponding document [32] are consistent. Changes are either very small or involve insignificant resonances.

C. ENDF/B-V.2 (1985)

- No changes

III. ENDF/B-VI

A. ENDF/B-VI.0 (1990)

^{54}Fe “Mod-1” [D.M. Hetrick, C.Y. Fu, N.M. Larson (ORNL)], aka “ENDF/B-V MOD-3”

- This work employed nuclear model codes including the Distorted Wave Born Approximation (DWBA) program DWUCK and the Hauser-Feshbach code TNG [33–35]. The TNG code provides energy and angular distributions of particles emitted in the compound and pre-compound reactions, ensures consistency among all reactions, and maintains energy balance. Further details were referred to by the euphemism “Details pertinent to the contents of this evaluation will be published at a later date.” (see [36, 37])
- Resonance parameters and thermal cross sections are from Mughabghab [5] and adjusted through SAMMY by N. Larson using J.A. Harvey data [38] between 110 and 700 keV, capture cross section background in File 3 was based on Allen [11, 39]. Above 700 keV, ^{54}Fe data from J.A. Harvey [38] used.
- Uncertainty files: An LB=8 section is included for all non-derived files as required by ENDF/B-VI.

^{56}Fe “Mod-1” [D.M. Hetrick, C.Y. Fu, N.M. Larson (ORNL)], aka “ENDF/B-V MOD-3” ORNL-4617 [2] describes ENDF/B-III. Major revisions

for ENDF/B-IV and -V are summarized in ORNL/TM-7523 [40] and ORNL/TM-8283 [41]. The present evaluation is based on the calculations described in ORNL/TM-9964 [37]. The major improvements over ENDF-5 MOD3 are:

1. Evaluation is now isotopic.
2. Analysis is based on a new TNG code much improved over the version used for ENDF/B-V for calculating energy-angle correlated spectra.
3. Resonance parameters are extended from 400 keV to 850 keV [42].
4. New data sets [24, 38, 43–49] are incorporated.
5. Integral results [50–53] are considered for the (n,n') evaluation above 3 MeV.
6. Gamma-ray production cross sections and spectra are given for each reaction, including MT = 51-75, instead of for the nonelastic.
7. Recoil spectra are given in file-6.
8. Charged particle spectra are given.

⁵⁷Fe “Mod-1” [D.M. Hetrick, C.Y. Fu, N.M. Larson (ORNL)], aka “ENDF/B-V MOD-3”

- This work employed the Hauser-Feshbach code TNG [33–35]. The TNG code provides energy and angular distributions of particles emitted in the compound and pre-compound reactions, ensures consistency among all reactions, and maintains energy balance. Details pertinent to the contents of this evaluation will be published at a later date.
- Resonance parameters and thermal capture cross section were taken from [5]. Some capture widths were adjusted to compromise with the averaged data of [39]. Low keV scattering cross sections were based on [54] which required an additional negative energy resonance. Two s-wave resonances above the resonance energy range were added to reduce the total cross sections between 150 keV and 200 keV. For total cross sections above 200 keV and capture above 2 MeV, natural iron data of ENDF/B-V were used for the purpose of making sure that the total cross section minima in ^{nat}Fe is maintained (when summing evaluations of isotopes together). For capture between 200 keV and 2 MeV, linear interpolation between ref. [39] and ENDF/B-V were made.
- Uncertainty files: An LB=8 section is included for all non-derived files as required by ENDF/B-VI.

⁵⁸Fe “Mod-1” [D.M. Hetrick, C.Y. Fu, N.M. Larson (ORNL)], aka “ENDF/B-V MOD-3”

- This work employed the Hauser-Feshbach code TNG [33–35]. The TNG code provides energy and angular distributions particles emitted in the compound and pre-compound reactions, ensures consistency among all reactions, and maintains energy balance. “Details pertinent to the contents of this evaluation will be published at a later date.”
- Resonance parameters and thermal capture cross section were taken from [5], and adjusted to the data of Beer et al. [55] through the SAMMY code by N.M. Larson. Some capture widths were adjusted downward to compromise with the averaged data of [56]. Average capture data of [57] were used to generate capture background below 400 keV and for the pointwise cross sections from 400 keV to 2 MeV. Thermal capture and capture in the 10.4 keV resonance were further adjusted by SAMMY to agree with the ENDF/B-V dosimetry evaluation [58], which was adjusted to agree with integral data. Low keV scattering cross sections were based on AP=7.2 fm given by [59]. For total cross sections above 400 keV and capture cross sections above 2 MeV, natural iron data of ENDF/B-V were used for the purpose of making sure that the total cross section minima in natural iron is maintained.
- Uncertainty files: An LB=8 section is included for all non-derived files as required by ENDF/B-VI.

B. ENDF/B-VI.1 (1991)

⁵⁴Fe, ⁵⁶Fe “Mod-2” [ORNL]

- Elastic transformation matrix removed

⁵⁷Fe, ⁵⁸Fe “Mod-2” [ORNL]

- The secondary particle distributions for MF=6, MT=51-52 were corrected-to-center of mass from laboratory coordinates. The elastic transformation matrix was removed.

C. ENDF/B-VI.2 (1993) -VI.3 (1995) -VI.4 (1996)

- No changes

D. ENDF/B-VI.5 (1997-1998)

⁵⁴Fe “Mod-3” [McLane (BNL)]

- Update file 1, fix residual nucleus in MF=5, MT=103

⁵⁸Fe “Mod-3” [McLane (BNL)]

- Corrected residual nucleus in File 6, MT=16. Corrected lower energy limit in File 6, MT=51,52 to agree with File 3. Updated File 1 comments and corrected references.

E. ENDF/B-VI.6 (1998-1999)

^{54}Fe , ^{56}Fe , ^{57}Fe “Mod-4” [Chadwick, Young, Koning (LANL/ECN)]

- LANL-150 extension to 150 MeV (see [60–64])
- The covariance files (MF=33) were removed from the file.

F. ENDF/B-VI.7 (1999-2000)

^{54}Fe , ^{56}Fe , ^{57}Fe “Mod-5” [Frankle, Reedy, Young (LANL)]

- Update gamma-ray spectrum from (n,g) and adjust Q to ensure energy conservation [65]

^{58}Fe “Mod-2” [Frankle, Reedy, Young (LANL)]

- Update gamma-ray spectrum from (n,γ) and adjust Q to ensure energy conservation [65]

G. ENDF/B-VI.8 (2001)

- No changes

IV. ENDF/B-VII**A. ENDF/B-VII.0 (2006)**

^{54}Fe , ^{57}Fe [Trellue (LANL)]

- Minor correction to MF6 MT5

^{56}Fe [Trellue (LANL)]

- Remade MF6 MT5 using corrected GNASH code, to fix an earlier bug. Impact is reduced sec. particle prod. for new ENDF/B-VII release except for the α production cross section, whose factors were increased in Aug. 2006 to match unpublished Haight experimental data.

B. ENDF/B-VII.1 (2011)

^{54}Fe , ^{56}Fe , ^{57}Fe

- Kunieda (LANL/JAEA): alpha particle production cross sections and energy spectra added based on Iwamoto-Harada model.
- BNL: RR covariance added
- BNL: Covariance of thresholds adjusted

V. ENDF/B-VIII**A. ENDF/B-VIII.0 β 0 (8 Apr. 2016)**

^{56}Fe

- CIELO ^{56}Fe file from BNL, IAEA and CNDC

Add minor Fe isotopes from the CIELO collaboration (^{54}Fe , ^{57}Fe and ^{58}Fe) New fast regions in all from EMPIRE calculations. New (currently undocumented) resonance regions in all:

- ^{54}Fe , new Atlas values, in Reich-Moore format
- ^{57}Fe , new Atlas values, in LRF=7 format, Reich-Moore approximation
- ^{58}Fe , new evaluation from Moxon [7]

B. ENDF/B-VIII.0 β 1 (25 Apr. 2016)

^{54}Fe

- From CIELO Iron project (rev. 246 of CIELO Iron project)

^{56}Fe

- Final before WPEC meetings (rev. 246 of CIELO Iron project)

^{57}Fe

- From CIELO iron project (rev. 246 of CIELO Iron project)

C. ENDF/B-VIII.0 β 2 (19 Aug. 2016)

^{54}Fe

- BNL: Revised ^{54}Fe from the CIELO project. This evaluation includes revised resonance region from IRSN up to 1.2 MeV in the LRF=7 format, EMPIRE calculation for fast region and capture cross section tuned to match average resonance cross section. Direct/Semi-Direct capture was added above the resonance region.

^{56}Fe

- BNL/IRSN: Revised ^{56}Fe from the CIELO project. This evaluation includes revised resonance region from IRSN up to 850 keV in the LRF=7 format, elastic and inelastic cross sections and angular distributions from beta1 and EMPIRE calculation for the remainder of the fast region.

D. ENDF/B-VIII.0β3 (2 Nov. 2016)**⁵⁴Fe**

- IRSN: resonances up to 1.036 MeV
- BNL: EMPIRE calculation from 1.036 MeV - 150 MeV
- BNL: (n,2n), (n,p) and (n,a) cross sections taken from IRDFF, partial reactions scaled to match these totals

⁵⁶Fe IAEA file fe56ib18b, IAEA-BNL Collaboration for CIELO

- Resolved resonance range up to 850 keV basically from JENDL-4.0
- The resonance energy at 766.7 keV was corrected.
- The background near 800 keV was reduced by 50 percent.
- Artificial “background” was added to capture around 24.5 keV, since capture in the hole of the elastic seems to be low and is HIGHLY SENSITIVE to many benchmarks. It was stipulated that the broad dip in this energy region is caused by inappropriately placed bound states. The adjusted capture cross section now follows the $1/v$ behavior.
- The total cross section above the resonance range was taken from JEFF-3.2 because it is consistent with the Berthold [66] measurements on Fe-nat. The contribution of the minor isotopes is taken into account.
- The capture cross sections above 860 keV were taken from the RPI data presented by Y. Danon at the ND2016 Conference.
- JEFF-3.2 contains inelastic cross sections measured by Dupont [67], but the authors discovered normalization problems and the results were never published. New measurements were performed by Negret [68], but with a lower resolution. The Dupont and Negret data were binned over a suitable energy mesh. A piecewise linear scaling parameter was constructed to adjust Dupont data such that they agree on average with the Negret data. It was also found that the energy calibration of Negret data did not match the resonances of the total cross section. A correction was made to the energy scale which amounted to 2.5 keV at 1.8 MeV. Inelastic cross sections between 0.85e6 and 3.5e6 eV are taken from JEFF-3.2.
- The elastic cross section is defined as the difference between the total and the remaining partial cross sections. By resolution-broadening of the elastic cross section to 0.3 percent, good agreement is observed with the measured Kinney [69] data.

- The elastic angular distributions in the resolved resonance range were reconstructed from the resonance parameters. The Legendre moments were resolution-broadened with a resolution function of constant width of 1 keV. For most applications the resolution-broadened Legendre coefficients are sufficient, but the user still has the option to reconstruct detailed distributions from the resonance parameters. Above the resonance range up to 4 MeV the angular distributions were taken from JEFF-3.2 because they accurately follow the Kinney data (with a correction for the minor isotopes).

- The P2 Legendre coefficients of elastic scattering were increased with a linear background, starting with 0 at 0.3 MeV, peaking to 0.7 at 0.85 MeV and ending with 0 at 1.5 MeV.

- Similarly, the P4 Legendre coefficients of elastic scattering were increased linearly, starting with 0 at 0.5 MeV, peaking to 0.2 at 0.85 MeV and ending with 0 at 1.5 MeV.

- At higher energies all cross sections, angular distributions and spectra are taken from EMPIRE calculation, which was tuned to reproduce the important reaction channels and radionuclide production data.

⁵⁷Fe

- BNL: revised with new EMPIRE calculation for fast region

E. ENDF/B-VIII.0β3.1 (19 Jan. 2017)**⁵⁴Fe**

- Add in roughly 64 resonances from G. Giubrone’s thesis [70] noted in Atlas evaluation but missing from IRSN evaluation
- Add high energy capture background to the RRR to account for missing p- & d-wave resonances

⁵⁶Fe New CIELO revision for Fe56, corresponding to IAEA version fe56ib19v. Major change: The elastic angular distributions in the resolved resonance range are taken from resolution-broadened Perey data [71]. Above the resonance range up to 2.5 MeV the angular distributions correspond to re-fitted Kinney data [72] with some adjustments based on the comparison with Perey data in the overlapping region. In the range 2.5-4.0 MeV the angular distributions are taken from Smith [73]. Above 2.5 MeV the angular distributions are from the Empire calculation.

F. ENDF/B-VIII.0 β 4 (28 Feb. 2017)

Fluctuations in Minor Iron Isotopes Red Cullen performed a COMPTOT comparison of beta3.1 and ENDF/B-VII.1 total cross sections for all minor Fe isotopes. It was clear from these figures that the fluctuations existing in ENDF/B-VII.1 were lost in the creation of the new CIELO evaluations.

- ^{54}Fe , in ENDF/B-VII.1, the ^{54}Fe evaluation was tuned to match [38] using either GLUCS or SAMMY (not clear the actual method, but clearly was a least squares fit) above 700 keV.
- ^{57}Fe and ^{58}Fe , in ENDF/B-VII.1, above 2 MeV the $^{57}\text{Fe}(\text{n,tot})$ evaluation was a scaled $\text{natFe}(\text{n,tot})$ “to make sure the total cross section of natFe was maintained”. Similarly, above 400 keV the $^{58}\text{Fe}(\text{n,tot})$ cross section was scaled for ENDF/B-VII.1.

These fluctuations have not been restored or replaced in the evaluations and they are unchanged from β 3.1.

^{56}Fe This evaluation is very similar to the β 3 files. The file has been assembled at the IAEA and nicknamed ‘fe56ib23w’. It consists of:

- EMPIRE calculation “ib23” (GForge repository No.529)
- Resolved resonance range up to 850 keV basically from JENDL-4.0 (Froehner evaluation for JEF-2-2 with corrections for typos). The resonance energy at 766.7 keV was corrected. The p-wave resonance at 59.5 keV was removed. The background near 800 keV was reduced by 40 percent. Artificial “background” was added to capture around 24.5 keV, since capture in the hole of the elastic seems to be low and is HIGHLY SENSITIVE to many benchmarks. It was stipulated that the broad dip in this energy region is caused by inappropriately placed bound states. The adjusted capture cross section now nearly follows the $1/v$ behavior.
- The total cross sections above the resonance range were taken from JEFF-3.2, which is essentially the Vonach-Tagesen evaluation with superimposed fluctuations that correspond to Berthold measurements on Fe-nat. The contribution of the minor isotopes is taken into account.
- The capture cross sections above 860 keV were taken from the RPI data presented by Y. Danon at the ND2016 Conference.

- JEFF-3.2 contains inelastic cross sections measured by Dupont et al., but the authors discovered normalization problems and the results were never published. New measurements were performed by Negret, but with a lower resolution. The Dupont and Negret data were binned over a suitable energy mesh. A piecewise linear scaling parameter was constructed to adjust Dupont data such that they agree on average with the Negret data. It was also found that the energy calibration of Negret data did not match the resonances of the total cross section. A correction was made to the energy scale which amounted to 2.5 keV at 1.8 MeV.

In addition, the inelastic cross section below 1 MeV was reduced by 15 percent to approximately agree with Perey data.

- The (n,p) partial cross sections are re-scaled to match the total (n,p) cross section in the IRDFF-v1.05 file.
- The elastic cross section is defined as the difference between the total and the remaining partial cross sections. To test the consistency, the cross section was resolution-broadened to 0.3 percent, achieving good agreement with Kinney data.
- The elastic angular distributions in the resolved resonance range are taken from resolution-broadened Perey data. Above the resonance range up to 2.5 MeV the angular distributions correspond to re-fitted Kinney data with some adjustments that reduce the anisotropy, based on the comparison with Perey data in the overlapping region. In the energy range 2.5-4.0 MeV the angular distributions are taken from Smith (1973). Above 4 MeV and below 35 keV the angular distributions are from the Empire calculation.

VI. ACKNOWLEDGMENTS

Work at Brookhaven National Laboratory was sponsored by the Office of Nuclear Physics, Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-98CH10886 with Brookhaven Science Associates, LLC.

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