INDC(NDS)-0832
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Processing Evaluated Photonuclear Data for Actinides from the IAEA/PD-2019 Library

Daniel López Aldama
Consultant, International Atomic Energy Agency
Vienna, Austria

Roberto Capote Noy
International Atomic Energy Agency
Vienna, Austria

August 2021

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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International Atomic Energy Agency
Vienna International Centre
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Austria

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ABSTRACT

The nuclear data processing of photonuclear data for actinides from the IAEA/PD-2019 library was reviewed. The NJOY processing code was patched to correctly take into account the neutron yields from photo-fission for computing neutron production cross-section and heating factors. The patched NJOY package is available at the IAEA Nuclear Data Section (https://github.com/IAEA-NDS/NJOY2016) and the changes are being implemented into the official NJOY version. Re-processing of the IAEA/PD-2019 library at nds.iaea.org/photonuclear/ is in progress.

August 2021

Contents

1. Introduction

In the course of the development of the nuclear data processing package ACEMAKER, the processing of the evaluated photonuclear data from the IAEA/PD-2019 library was revisited. Some limitations for processing photonuclear data using the NJOY code [1] were reported in Ref. [2] with the main problem being that the angular distributions given in the MF6 file are treated as isotropic, except for the Kalbach-Mann formalism. Further analysis of the ACE format files generated with the NJOY code also revealed that the neutron production cross-sections of the fissionable materials have been erroneously computed. This was the main motivation to review the current processing of the evaluated photonuclear data files of the fissionable materials of the IAEA/PD-2019 library. The present report summarizes the main updates applied to the NJOY processing code to correctly generate the neutron production cross-section and heating factors for photon-induced reactions on fissionable targets.

2. NJOY updates and photonuclear data processing for actinides

The fissionable materials in the IAEA/PD-2019 library follow the Format Type 1 representation given in Ref. [2]:

a. MF1/MT451, MF1/MT452, MF1/MT455, MF1/MT456
b. MF3/MT3, MF3/MT5, MF3/MT18
c. MF5/MT455
d. MF6/MT5, MF6/MT18

The fissionable nuclei contain the average number of total, delayed, and prompt neutrons in MF1, the photo-fission cross-section in MF3, the energy distributions of delayed neutrons in MF5 (assuming isotropic angular distribution), and the angular/energy distribution of reaction neutrons in MF6. The fission neutron yields in the TAB1 record of MF6 are set to 1.0 for all incident energies. This is the correct way to represent the fission data in MF6 to be compatible with the case for incident neutrons.

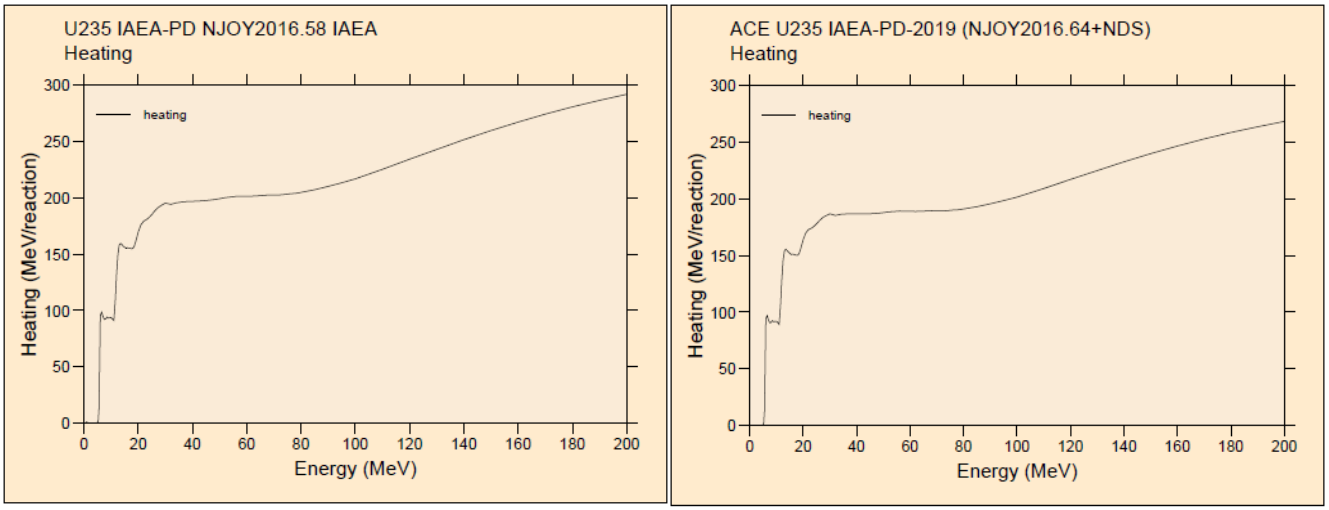
It was found that NJOY incorrectly used these unitary yields to compute the neutron production cross-section from fission, while the correct fission neutron yield should be taken from the neutron multiplicity stored in MF1. Therefore, the module acepn was patched to use the average number of prompt neutrons (equal fission neutron multiplicity) for computing the neutron production cross-section and heating factors. Figures 1, 2, and 3 show the differences in these quantities before and after applying the NJOY patch. Appendix A presents the results for the rest of the actinides included in the IAEA/PD-2019 library. Appendix B shows the recommended input options for NJOY processing. Note that the current version of NJOY does not process the delayed neutron data.

An additional patch was applied to extend the treatment of neutron-producing reactions described by data in the ENDF-files MF3, MF4, and MF5. This format was used in earlier versions of some photonuclear data libraries like the IAEA/PD-1999.

Furthermore, the units of the threshold (Q) were corrected for computing the heating factor of the discrete recoil nucleus (MF6/LAW=4), and some FORTRAN expressions were rewritten for allowing more general cases.

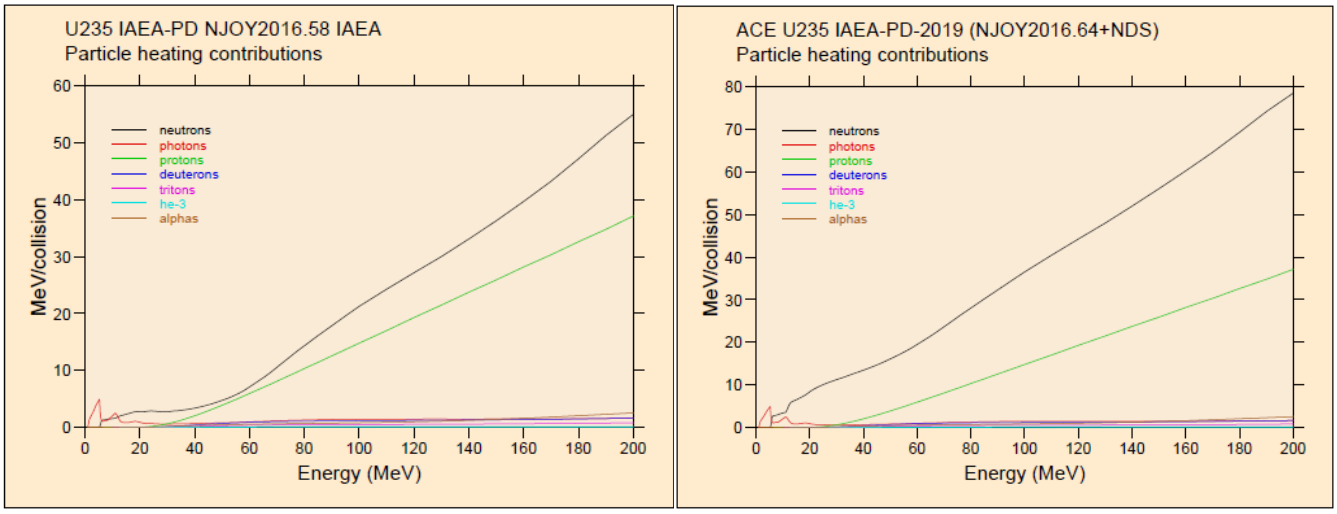
Recently, several authors [3, 4] have studied the kinematics for photon-neutron production in Monte Carlo transport calculations. The limitations of the NJOY/MCNP approach have been shown for light elements. It produces significantly hardened photo-neutron spectra. The problem is much reduced for heavy isotopes. The authors reported that the results can be improved to some extent if classical expressions like those implemented in TRIPOLI4 [5] are used for photon energies where both the photo-neutron and the recoil nucleus can be considered classical particles. This correction only affects the LAW=33 parameters in the ACE-formatted file. Particularly, the constant LDAT(2) is calculated as (A-1)/A instead of A/(A+1). Here it is assumed that the correct classical expressions reported in Ref. [4] are used to convert the photon energy from the center of mass system to the laboratory system.

FIG. 1. U-235 recoil-heating factor



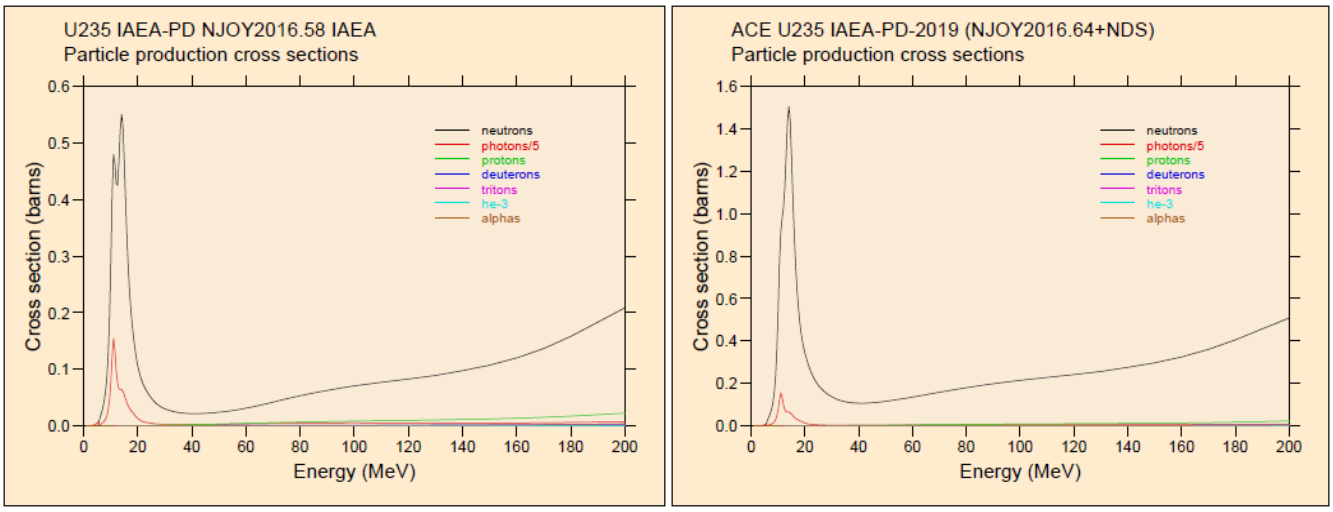
Left: unpatched NJOY, right: patched NJOY

FIG. 2. U-235 heating factors for particles



Left: unpatched NJOY, right: patched NJOY (note different scales of Y-axis)

FIG. 3. U-235 production cross sections



Left: unpatched NJOY, right: patched NJOY (note different scales of Y-axis)

3. NJOY availability

The patched version of NJOY is available at the IAEA-NDS GitHub: https://github.com/IAEA-NDS/NJOY2016.

The distributed patched version (as well as the original NJOY) still has the following limitations:

a) Delayed photofission neutron data from ENDF-6 files MF1, MF4 and MF5 are not processed;
b) Angular/energy distributions given in MF6 are treated as isotropic except for the Kalbach-Mann formalism (LAW=1, LANG=2);
c) Photon data from ENDF-6 files MF12, MF13, MF14 and MF15 are not processed.

4. Final comments and recommendations

The nuclear data processing of photonuclear data for actinides from the IAEA/PD-2019 library was reviewed. The NJOY processing code was patched to correctly take into account the neutron yields from photo-fission for computing neutron production cross-section and heating factors. The patched NJOY package is available at the IAEA Nuclear Data Section (https://github.com/IAEA-NDS/NJOY2016) and the changes were communicated to the NJOY developers.

It is strongly recommended to re-process all the actinide files from the IAEA/PD-2019 library and make them available on the IAEA/NDS web page.

Further developments of the ACEMAKER system are made available at https://github.com/IAEA-NDS/ACEMAKER and will include capabilities for full processing of photonuclear data.

References

[1] MacFarlane, R.E., Muir, D.W., Boicourt, R.M., Kahler, A.C., The NJOY Nuclear Data Processing System, Version 2012, **LA-UR-12-27079**, Los Alamos National Laboratory, Updated for NJOY2012.50, February 12, 2015.

[2] Kawada, H., Sublet, J-Ch., Okumura, S., Kawano, T., Processing the Evaluated Photonuclear Data Library (IAEA/PD-2019), **IAEA-NDS-0232**, August 2020.

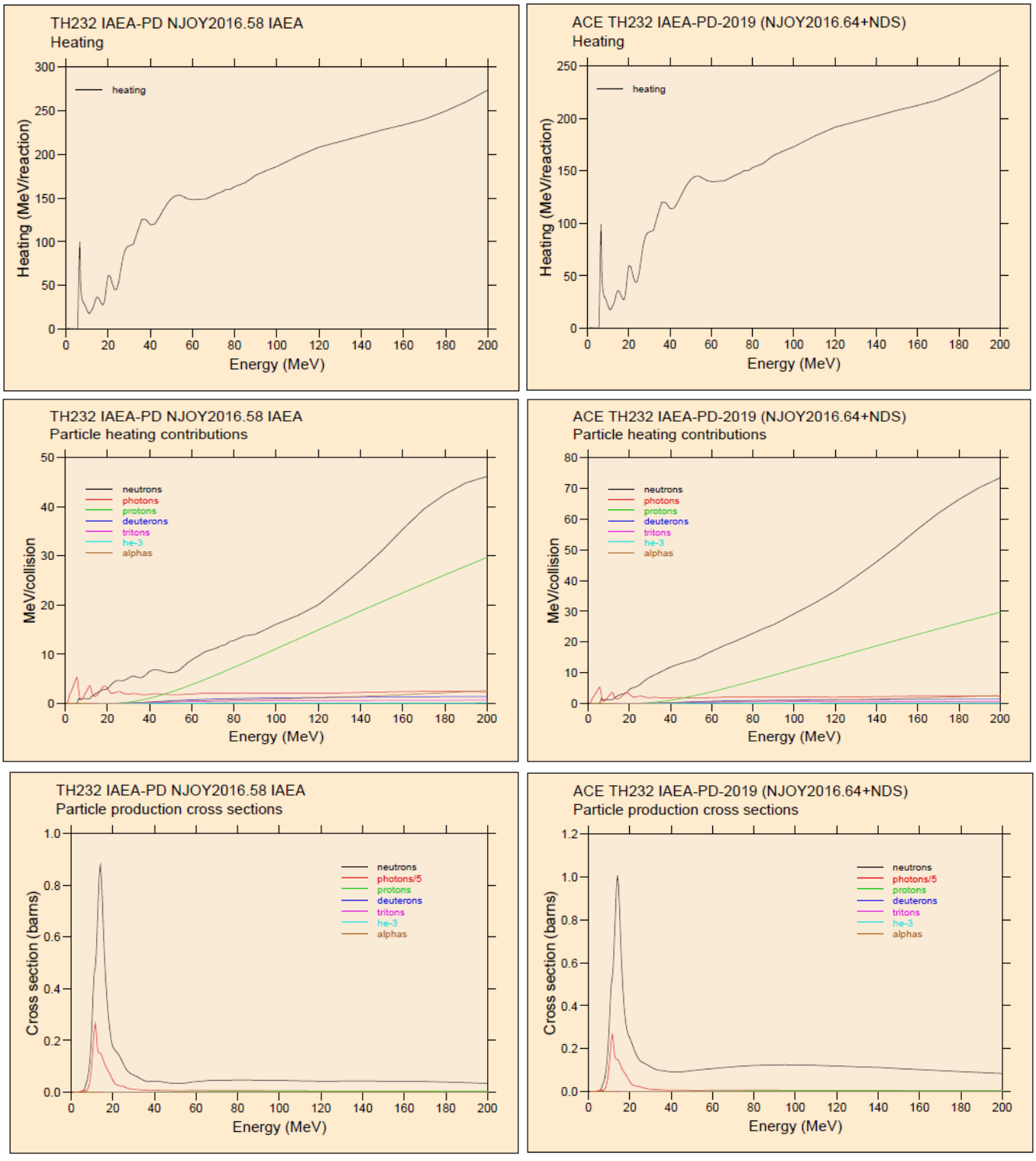
[3] Caro, E., Relativistic kinematics for photoneutron production in Monte Carlo Transport calculations, Ann. Nucl. En. **96** (2016) 170-175.

[4] Fynan, D.A., Photoneutron reaction kinematics and error of commonly used approximations, Nucl. Inst. Meth. Phys. Res. **A977** (2020) 164271.

[5] Petit, O., Huot, N., Jouanne, C., Implementation of photonuclear reactions in the Monte Carlo transport code TRIPOLI-4 and its first validation in waste package field, Progr. Nucl. Sci. Technol. **2** (2011) 798-802.

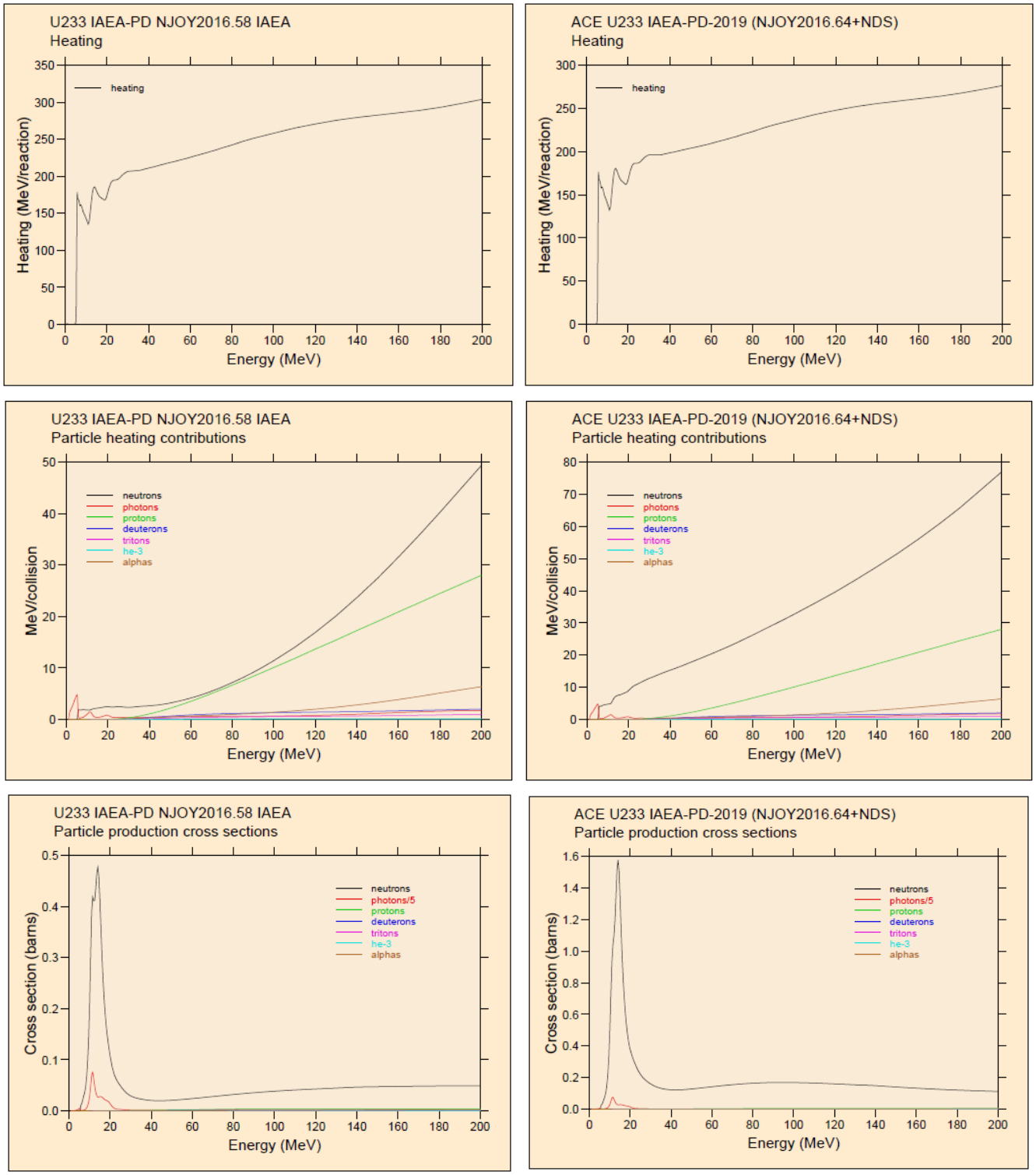
Appendix A

FIG. A.1. Th-232



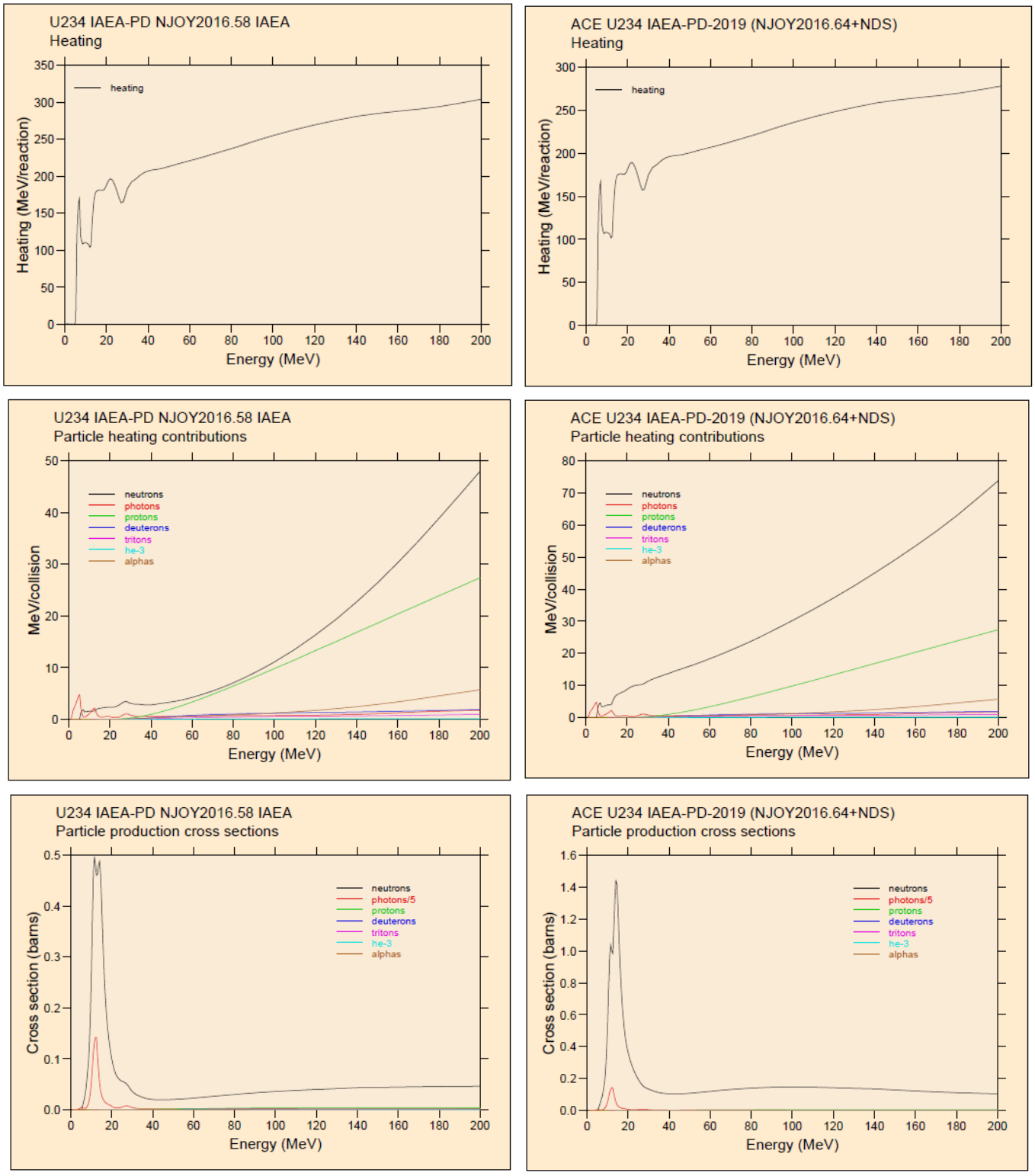
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.2. U-233



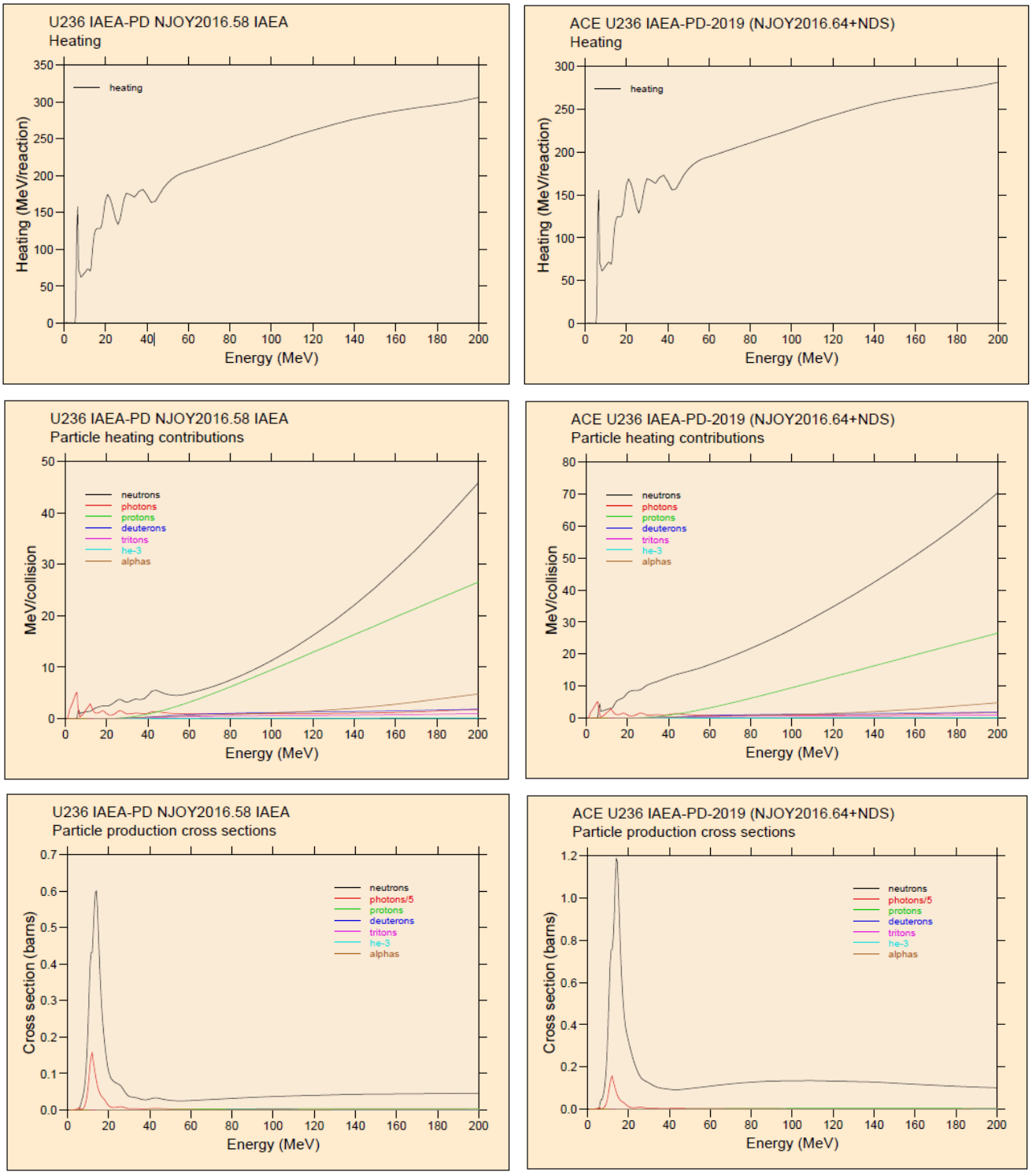
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.3. U-234



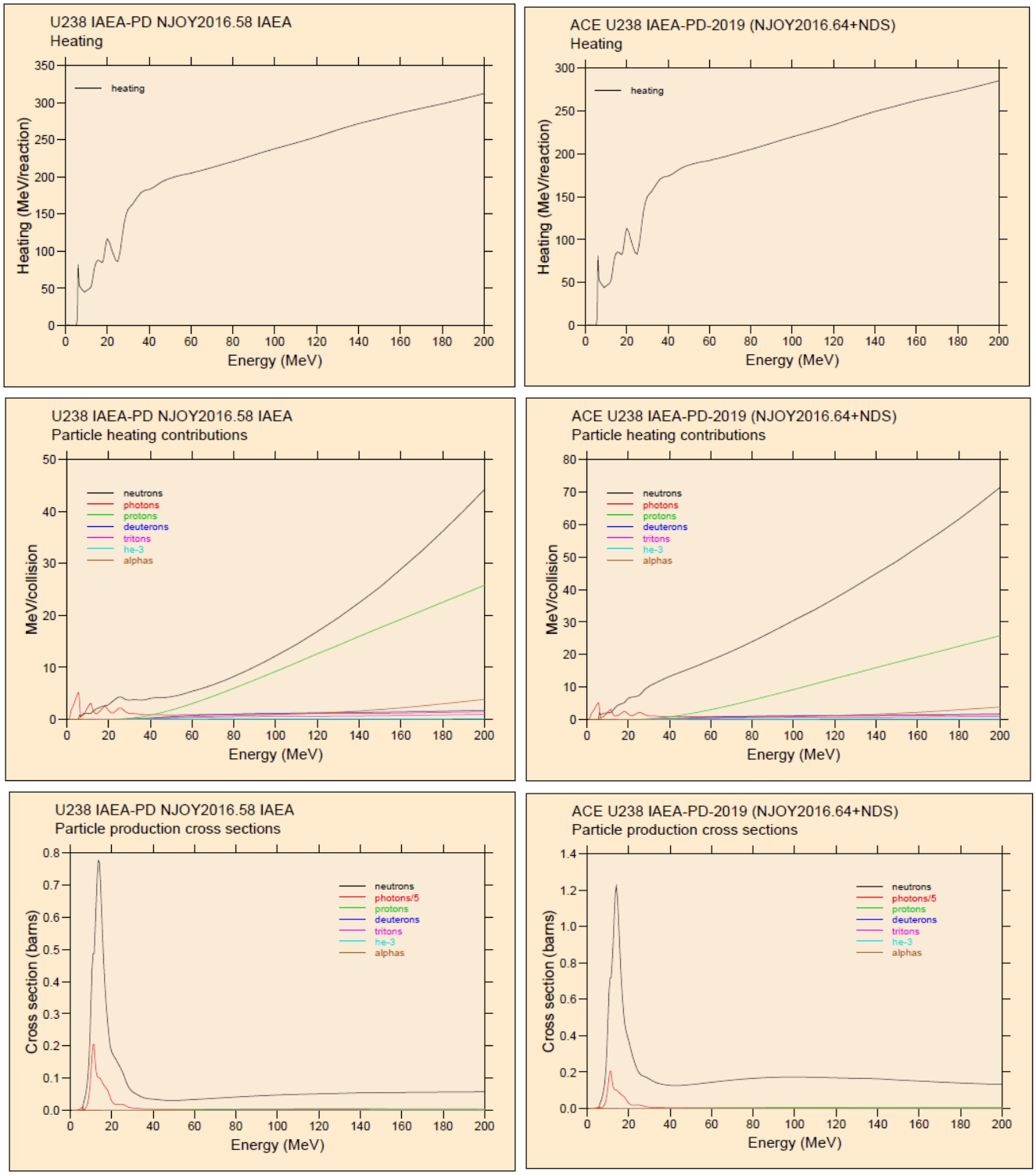
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.4. U-236



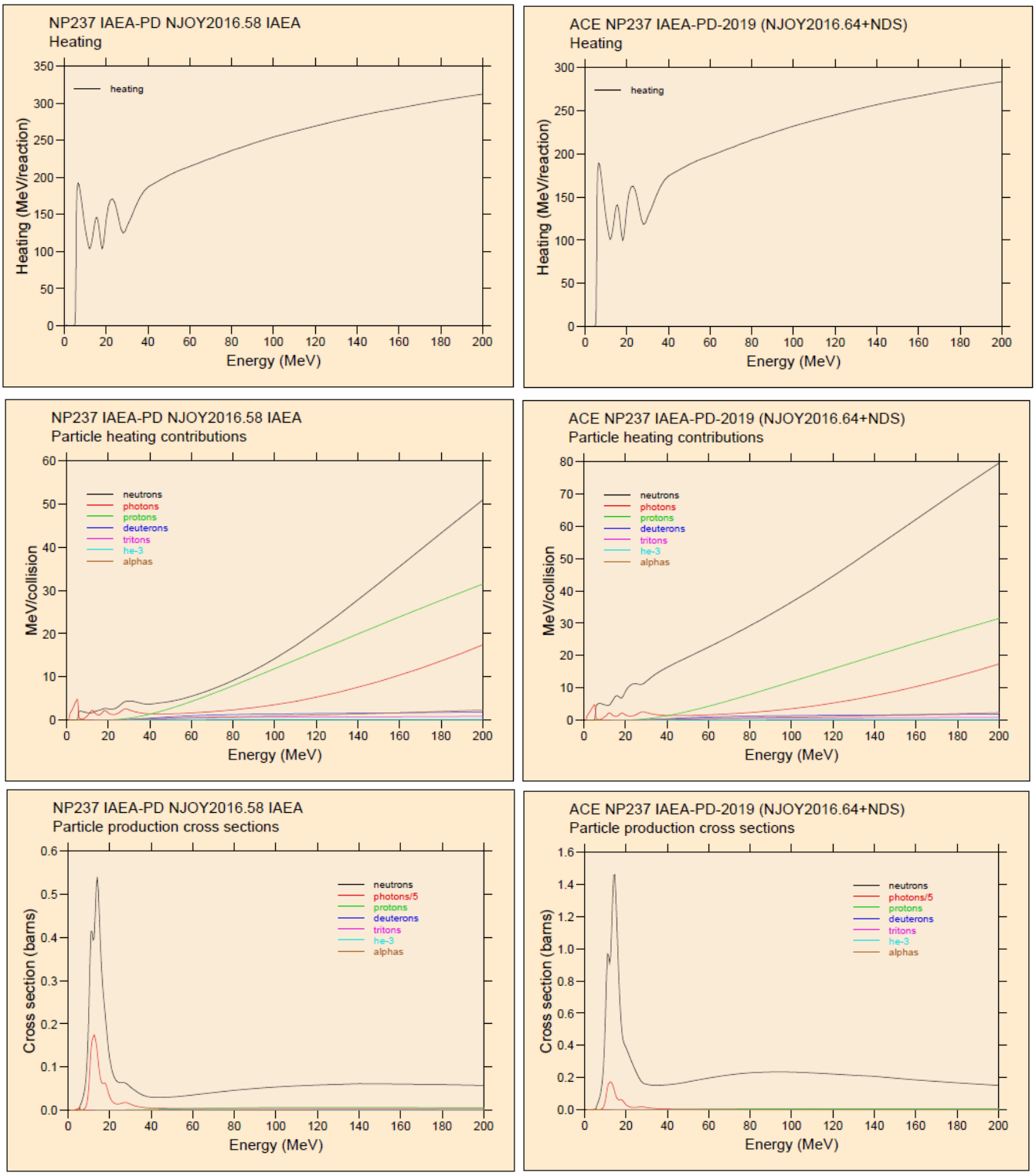
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.5. U-238



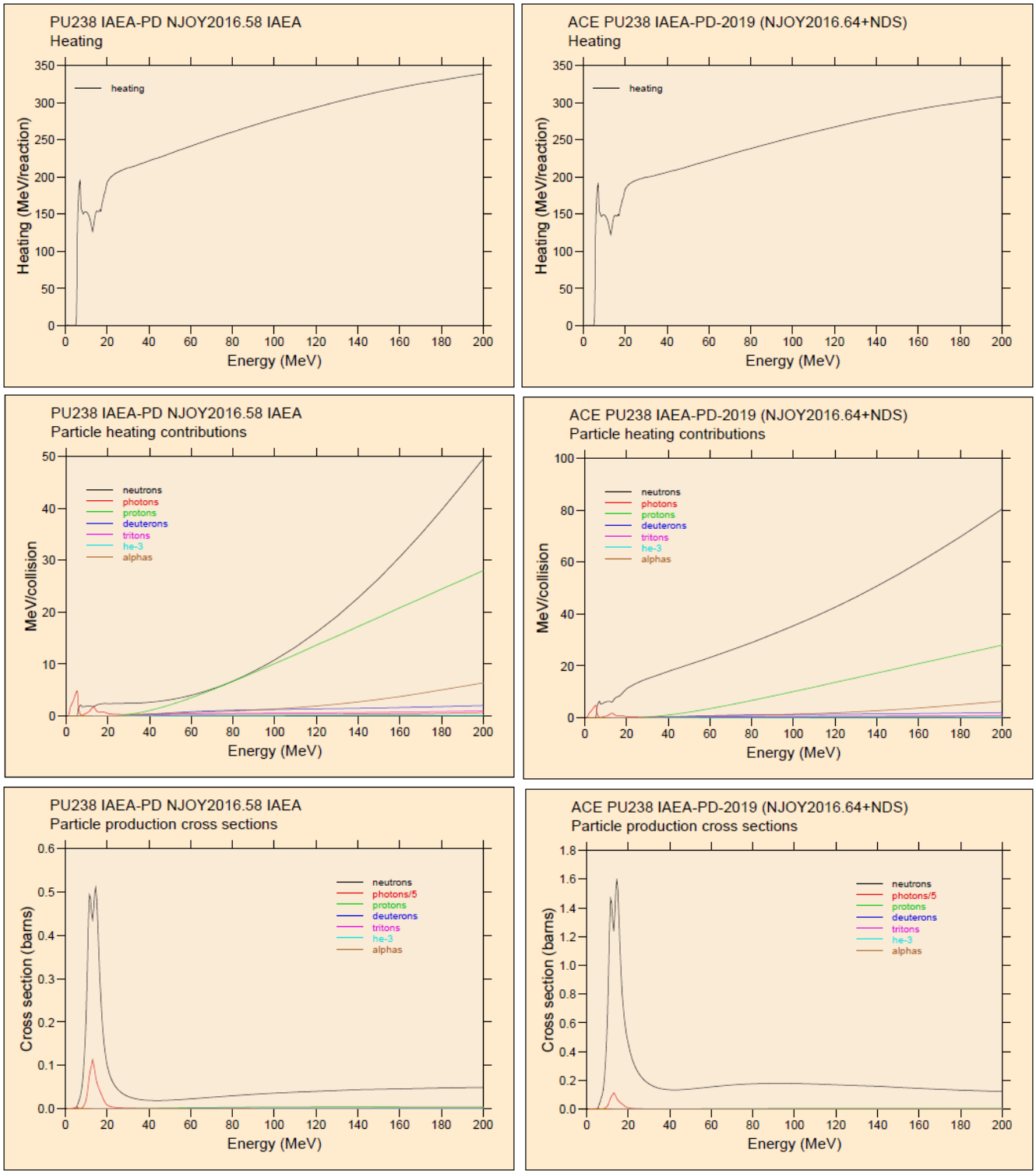
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.6. Np-237



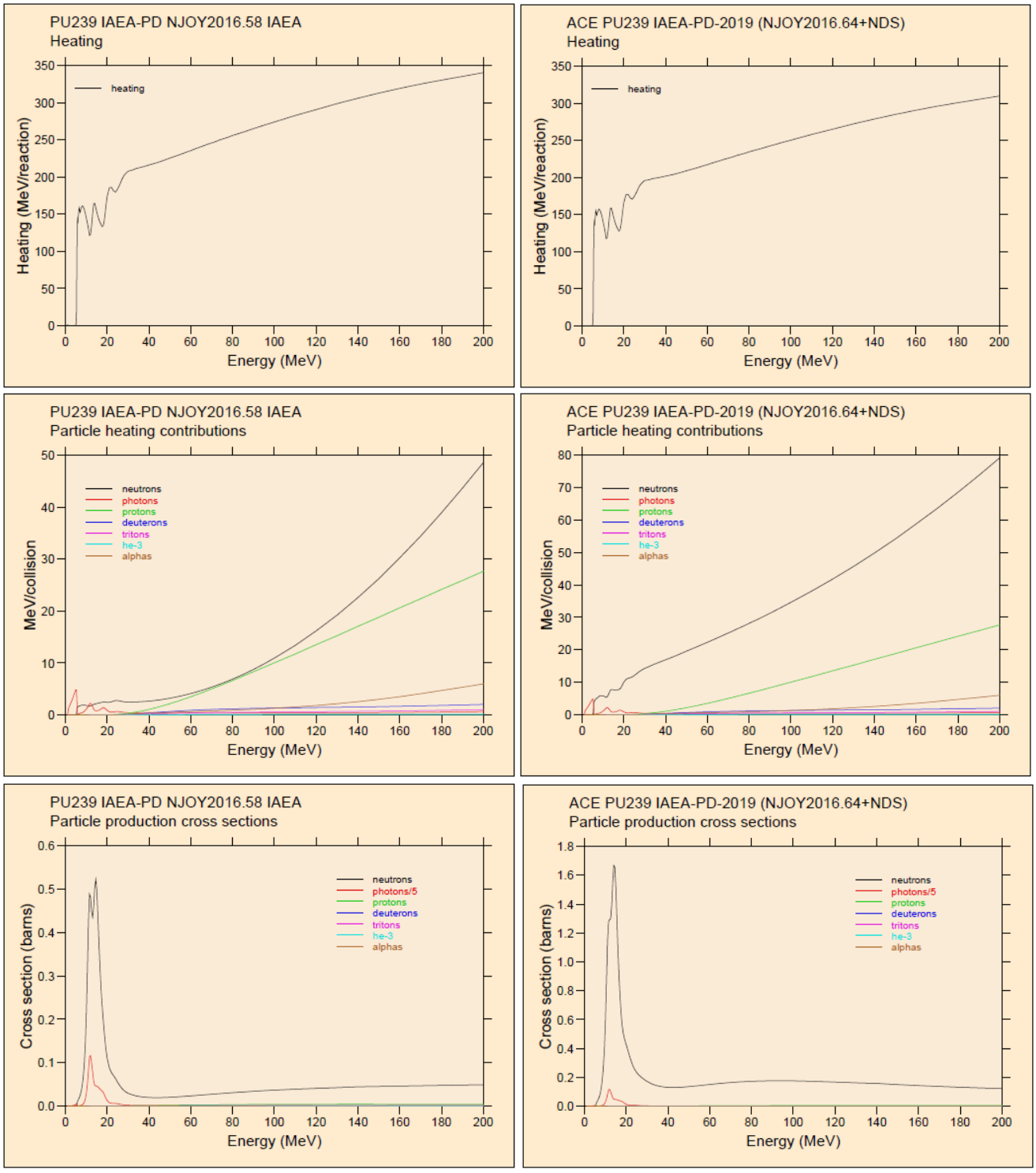
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.7. Pu-238



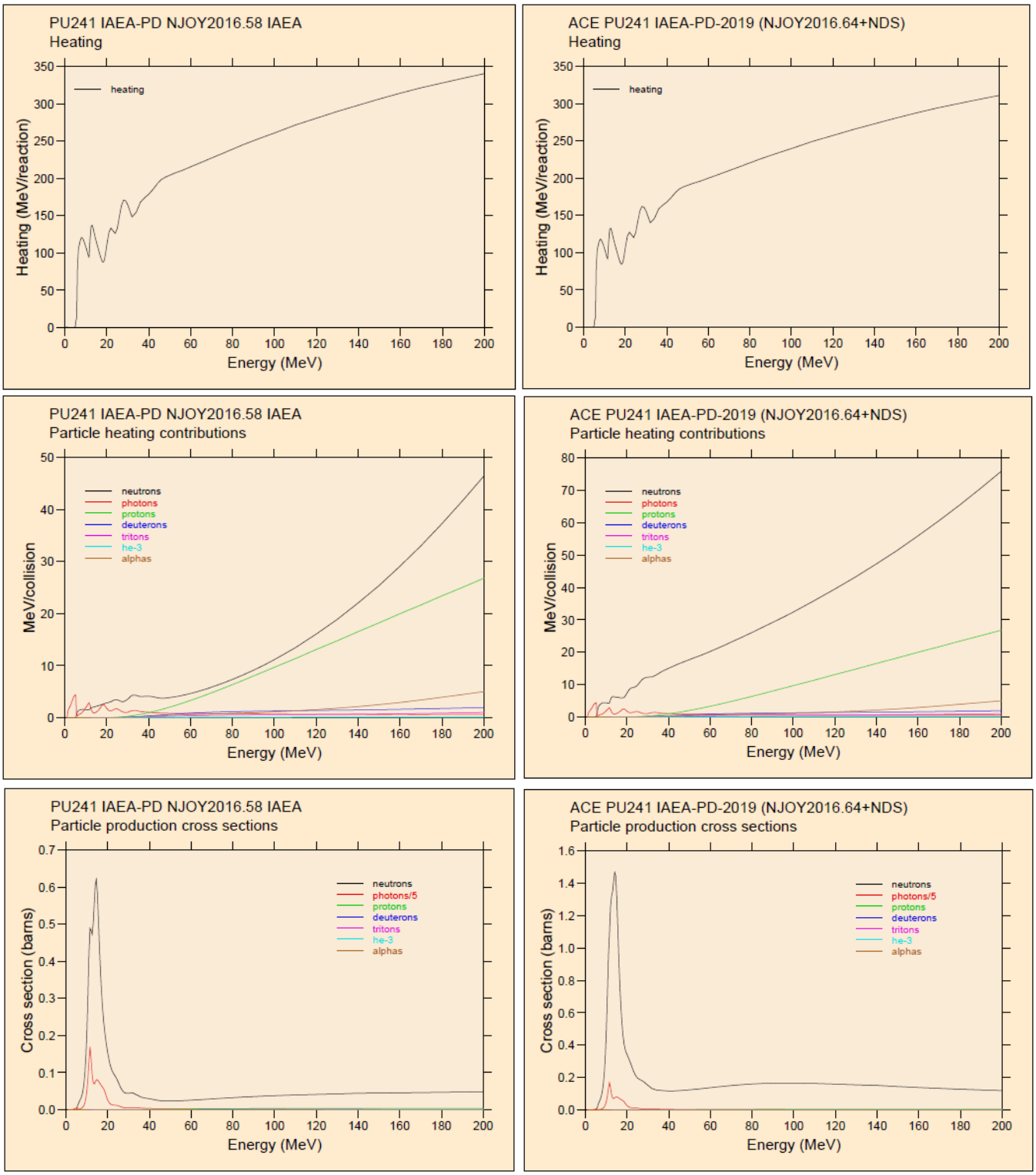
Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.8. Pu-239



Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

FIG. A.9. Pu-241



Left: Unpatched NJOY. Right: Patched NJOY (note different scales of Y-axis)

Appendix B

Example of NJOY input options (U-235)

```
moder / Extract/convert evaluated nuclear data
1 21
'U235 from IAEA-PD-2019'/
20 9228
0/
reconr / Reconstruct/Linearize XS (Compulsory for non-linearly interpolable XS like the case of H-2)
21 22
'PENDF for U235'/
9228 2/
0.001 0.0 0.002/
'U235 from IAEA-PD-2019'/
'Processed by NJOY2016.64+NDS'/
0/
acer /Create ACE-formatted file
21 22 0 31 32/
5 1 1/
'Ace U235 IAEA-PD-2019 (NJOY2016.64+NDS)'/
9228/
acer / Check and print ACE-formatted file
0 31 33 34 36/
7 1 1 -1/
/
viewr /Plot ACE-formatted file
33 37
stop
```

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://www-nds.iaea.org