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Title: Release of eprdata25: ENDF/B-VIII.1-Based ACE Data Files for Photo- and Electro-atomic Transport

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From: Wim Haeck, XCP-5
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Date: August 4, 2026

Memorandum

XCP-5 Materials and Physical Data

Subject: Release of eprdata25: ENDF/B-VIII.1-Based ACE Data Files for Photo- and Electro-atomic Transport

Introduction

On August 30, 2024, the National Nuclear Data Center (NNDC) released the ENDF/B-VIII.1 nuclear data library. The library was released in the standard Evaluated Nuclear Data File (ENDF) format. These files can be accessed on the NNDC's website (www.nndc.bnl.gov). The incident neutron and thermal scattering sub-libraries provided by the ENDF/B-VIII.1 nuclear data library have already been processed into ACE file for use with the MCNP code, respectively named the Lib81 and ENDF81Sab libraries. The current memo deals with the production of another MCNP library based on ENDF/B-VIII.1, this time for the photo-atomic, electro-atomic and atomic relaxation sub-libraries. The photo-atomic and electro-atomic sub-libraries provide the cross section data and secondary particle distribution data for atomic interactions of photons and electrons (including electron subshell ionization). The atomic relaxation sub-library supplements these two sub-libraries by providing the transition probabilities of vacancies in the electron subshells due to ionization, which allows us to calculate outgoing X-ray and Auger electron spectra.

The Electron-Photon-Relaxation data (EPRDATA) format is a relatively new continuous-energy atomic data file type which has been available for users of the MCNP code since 2013 with the release of the eprdata12 ACE library [1]. An EPRDATA library combines the traditional photo-atomic data library used for Monte Carlo photon transport with atomic relaxation data and electron cross-section data which can be used for single-event electron transport. An upgraded library, eprdata14, was released in 2015 [2] featuring data refinement as well as expansion of the format description to provide new transport-corrected and total elastic cross-sections. Most recently, the latest EPR data [3] has been incorporated into the ENDF/B-VIII.0 and VIII.1 releases, but these updates have not yet been processed into the EPRDATA format for use by the MCNP code.

Contrary to other ACE types, EPRDATA style files were not produced using NJOY2016. Because of this, and the fact that no resonance reconstruction or Doppler broadening is required in processing EPR data, the production of the eprdata25 library based on ENDF/B-VIII.1 was selected as the first application of modern NJOY, which we will refer to as NJOY3 from now on [4]. The development of this capability required adding the necessary support for the evaluated data, integration of probability distributions to produce cumulative distributions, adaptive quadrature routines for the calculation of heating numbers and the calculation of a transport corrected elastic cross-section. Existing capabilities have been extended as well, such as the unionization of the energy grids of the cross sections which is a requirement for any ACE file.

Library content

The ENDF/B-VIII.1 photo-atomic, electro-atomic and atomic relaxation sub-libraries provide data for 100 elements, from $Z = 1$ (Hydrogen) to $Z = 100$ (Fermium). These libraries have been supplemented with Compton profile data from the Biggs, Mendelsohn and Mann dataset [5], which are not available in the evaluated ENDF/B-VIII.1 library.

No changes were made to the evaluated data except for setting the energy range of the electro-atomic data to the 10 eV to 100 GeV range. The elastic scattering data in the electro-atomic data files was defined on this range, but some elements did have ionization cross sections that started at energies below 10 eV. Since elastic scattering was not defined at those lower energies, it was decided to cut all cross section data below 10 eV.

Another correction, this time to the Compton profile data, had to be performed for Iridium ($Z = 77$). When processing a test version of the eprdata25 library, it became clear that the evaluated data did not contain any ionization data or transition data for the 6s $_{1/2}$ electron subshell – even though electron configuration data clearly states that this shell is filled for Iridium. In order to maintain consistency in the data for Iridium, the 6s $_{1/2}$ shell was cut from the Compton profiles before they were put in the Iridium ACE file.

An analysis of the historic photo-atomic, electro-atomic and atomic relaxation data that has been used as a source for the ENDF/B data has shown that this particular subshell has always been missing from the Iridium data. The NNDC at BNL has been made aware of this issue.

Data Verification & Validation

Recently, new capabilities for verification and validation (V&V) of electron transport data and physics have been implemented into the MCNP V&V collection. Alongside the release of the EPRDATA25 library, these capabilities have been used to validate the new data, specifically the data for Be, Al, Si, Cu, Ag, Au, and U [6].

For each material tested, the MCNP code was used to simulate single-event electron transport, which uses the electron interaction cross sections from an EPRDATA file, after which electron stopping powers and ranges were calculated. Fig. 1(a) shows an example of these results for electrons incident on Cu using the EPRDATA14 and EPRDATA25 libraries. In general, using EPRDATA25 there is a modest improvement over EPRDATA14, which is attributed primarily to the corrected subshell binding energies in the new data. On average, with the new data there is a ~3% reduction in average error (Fig. 1(b)) and around 2/3 of the elemental stopping powers show improved agreement with the literature reference values.

Additionally, for each material tested the MCNP code was used to calculate electron backscattering yields, energy distribution, and angular distributions using both single-event and condensed-history methods (the latter of which does not use EPRDATA libraries). Fig. 2(a) shows an example of these results for electrons incident on Cu. In general, it was found that both EPRDATA14 and EPRDATA25 libraries gave similarly good agreement with experimental measurements for energies above 1 keV, and it was not clear which library gives more accurate predictions, if either. The backscattered electron yields calculated with the EPRDATA25 library are slightly lower due to increased energy loss because of the new, typically larger subshell

binding energies. The discontinuity for electron energies below 1 keV is a known limitation of the underlying evaluated EPR data.

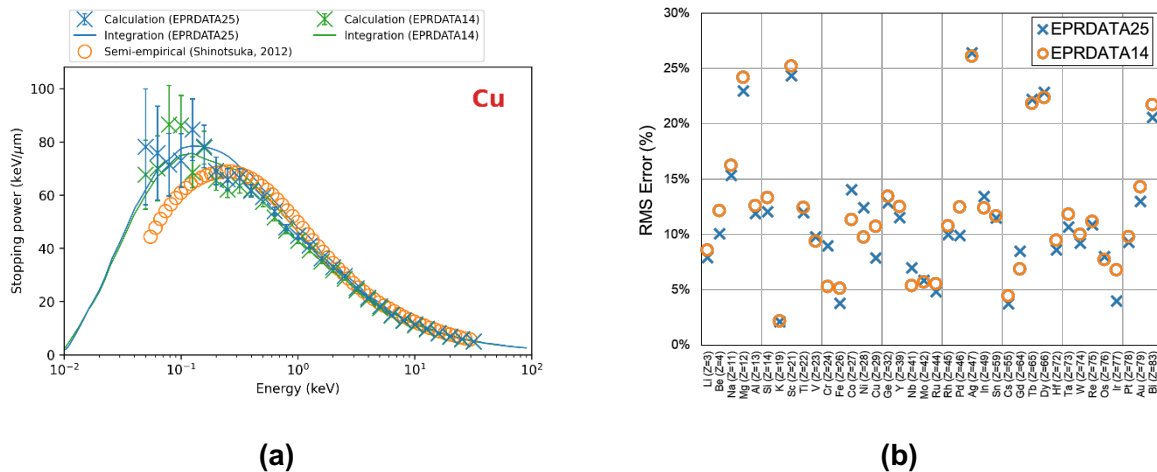


Fig. 1. Examples of stopping power V&V results for electrons in Cu. (a) Stopping power comparison between EPRDATA25 and EPRDATA14 [6]. (b) Comparison of overall errors between EPRDATA25 and EPRDATA14 [7].

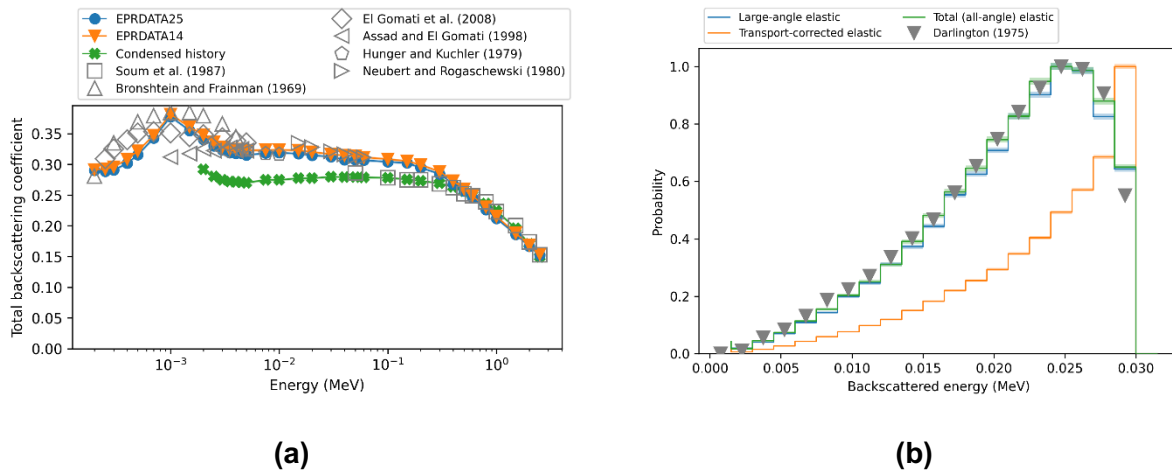


Fig. 2. Examples of backscattering V&V results for electron transport in Cu [6]. (a) Electron backscattering yield comparison between EPRDATA25, EPRDATA14, and the traditional condensed history method. (b) Backscattered angular distribution comparison between large-angle, transport-corrected, and total elastic cross sections.

Additionally, this V&V work exercised the large-angle (i.e., default), transport-corrected, and total elastic cross sections for the first time in a validation context. Fig. 2(b) shows an example of these results for 30 keV electrons incident on Cu. While the large-angle and total elastic cross sections give similar results, the transport-corrected cross section was found to be not appropriate for electron backscattering calculations.

References

- [1] H. G. Hughes III, Recent Developments in Low-Energy Electron/Photon Transport in MCNP6, Prog. Nucl. Sci. Technol., 4, 454-458 (2014)
- [2] H. G. Hughes III, Improvements in Electron-Photon-Relaxation Data for MCNP6, LA-UR-16-20840, Los Alamos National Laboratory (2016)
- [3] D. E. Cullen, EPICS2023: August 2023 Status Report, IAEA-NDS-0242, International Atomic Energy Agency (2023)
- [4] W. Haeck, A. Lewis, A. Kitamura, M. Lively, N. Gibson, Status of the NJOY Modernization, To be published, PHYSOR 2026 - The International Conference on Physics of Reactors, Torino, Italy, April 19-23, 2026
- [5] F. Biggs, L. B. Mendelsohn, J. B. Mann, Hartree-Fock Compton profiles for the elements, Atomic data and nuclear data table, 16, 201-309 (1975)
- [6] M. A. Lively, W. Haeck, Release and Validation of the EPRDATA25 Electron-Photon-Relaxation Library, Trans. Am. Nucl. Soc. 133, 800-803 (2025)
- [7] M. A. Lively, W. Haeck, Release and Validation of the EPRDATA25 Electron-Photon-Relaxation Library, 2025 ANS Winter Conference and Expo, Wasington, D.C., November 9-13, 2025

Attachment(s):
ACE file listing
NJOY3 Python processing code

Copy:
Nuclear Data Team
Monte Carlo Codes
Radiation Transport Applications, XTD-RTA
ASC-PEM-Nuclear Physics
DJ Luscher
Robert Little
Jennifer Alwin
Abigail Hunter
Mark Chadwick

ACE file listing

ACE id	Filename
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3000.25p	eprdata25/3000.25p
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6000.25p	eprdata25/6000.25p
7000.25p	eprdata25/7000.25p
8000.25p	eprdata25/8000.25p
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NJOY3 Python code to process the eprdata25 library

The following Python code was used to process the eprdata25 library, using the Python bindings for NJOY3 available at <https://github.com/njoy/dryad> and commit hash 378b5e7. The code is written to use either ENDF or GNDS formatted file. For the final library, the GNDS formatted files were used.

```
import njoy
import os
import time

endf_path = 'libraries/endf/endf81'
gn ds_path = 'libraries/gnds/endf81'

output_path = 'eprdata25'

ace_number = 25
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date = '19/02/26'

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( 'photoat/photoat-068_Er_000.endf', 'electrons/e-068_Er_000.endf', 'atomic_relax/atom-068_Er_000.endf' ),
( 'photoat/photoat-069_Tm_000.endf', 'electrons/e-069_Tm_000.endf', 'atomic_relax/atom-069_Tm_000.endf' ),
( 'photoat/photoat-070_Yb_000.endf', 'electrons/e-070_Yb_000.endf', 'atomic_relax/atom-070_Yb_000.endf' ),
( 'photoat/photoat-071_Lu_000.endf', 'electrons/e-071_Lu_000.endf', 'atomic_relax/atom-071_Lu_000.endf' ),
( 'photoat/photoat-072_Hf_000.endf', 'electrons/e-072_Hf_000.endf', 'atomic_relax/atom-072_Hf_000.endf' ),
( 'photoat/photoat-073-Ta_000.endf', 'electrons/e-073-Ta_000.endf', 'atomic_relax/atom-073-Ta_000.endf' ),
( 'photoat/photoat-074_W_000.endf', 'electrons/e-074_W_000.endf', 'atomic_relax/atom-074_W_000.endf' ),
( 'photoat/photoat-075_Re_000.endf', 'electrons/e-075_Re_000.endf', 'atomic_relax/atom-075_Re_000.endf' ),
( 'photoat/photoat-076_Os_000.endf', 'electrons/e-076_Os_000.endf', 'atomic_relax/atom-076_Os_000.endf' ),
( 'photoat/photoat-077_Ir_000.endf', 'electrons/e-077_Ir_000.endf', 'atomic_relax/atom-077_Ir_000.endf' ),
( 'photoat/photoat-078_Pt_000.endf', 'electrons/e-078_Pt_000.endf', 'atomic_relax/atom-078_Pt_000.endf' ),
( 'photoat/photoat-079_Au_000.endf', 'electrons/e-079_Au_000.endf', 'atomic_relax/atom-079_Au_000.endf' ),
( 'photoat/photoat-080_Hg_000.endf', 'electrons/e-080_Hg_000.endf', 'atomic_relax/atom-080_Hg_000.endf' ),
( 'photoat/photoat-081_Tl_000.endf', 'electrons/e-081_Tl_000.endf', 'atomic_relax/atom-081_Tl_000.endf' ),
( 'photoat/photoat-082_Pb_000.endf', 'electrons/e-082_Pb_000.endf', 'atomic_relax/atom-082_Pb_000.endf' ),
( 'photoat/photoat-083_Bi_000.endf', 'electrons/e-083_Bi_000.endf', 'atomic_relax/atom-083_Bi_000.endf' ),
( 'photoat/photoat-084_Po_000.endf', 'electrons/e-084_Po_000.endf', 'atomic_relax/atom-084_Po_000.endf' ),
( 'photoat/photoat-085_At_000.endf', 'electrons/e-085_At_000.endf', 'atomic_relax/atom-085_At_000.endf' ),
( 'photoat/photoat-086_Rn_000.endf', 'electrons/e-086_Rn_000.endf', 'atomic_relax/atom-086_Rn_000.endf' ),
( 'photoat/photoat-087_Fr_000.endf', 'electrons/e-087_Fr_000.endf', 'atomic_relax/atom-087_Fr_000.endf' ),
( 'photoat/photoat-088_Ra_000.endf', 'electrons/e-088_Ra_000.endf', 'atomic_relax/atom-088_Ra_000.endf' ),
( 'photoat/photoat-089_Ac_000.endf', 'electrons/e-089_Ac_000.endf', 'atomic_relax/atom-089_Ac_000.endf' ),
( 'photoat/photoat-090_Th_000.endf', 'electrons/e-090_Th_000.endf', 'atomic_relax/atom-090_Th_000.endf' ),
( 'photoat/photoat-091_Pa_000.endf', 'electrons/e-091_Pa_000.endf', 'atomic_relax/atom-091_Pa_000.endf' ),
( 'photoat/photoat-092_U_000.endf', 'electrons/e-092_U_000.endf', 'atomic_relax/atom-092_U_000.endf' ),
( 'photoat/photoat-093_Np_000.endf', 'electrons/e-093_Np_000.endf', 'atomic_relax/atom-093_Np_000.endf' ),
( 'photoat/photoat-094_Pu_000.endf', 'electrons/e-094_Pu_000.endf', 'atomic_relax/atom-094_Pu_000.endf' ),
( 'photoat/photoat-095_Am_000.endf', 'electrons/e-095_Am_000.endf', 'atomic_relax/atom-095_Am_000.endf' ),
( 'photoat/photoat-096_Cm_000.endf', 'electrons/e-096_Cm_000.endf', 'atomic_relax/atom-096_Cm_000.endf' ),
( 'photoat/photoat-097_Bk_000.endf', 'electrons/e-097_Bk_000.endf', 'atomic_relax/atom-097_Bk_000.endf' ),
( 'photoat/photoat-098_Cf_000.endf', 'electrons/e-098_Cf_000.endf', 'atomic_relax/atom-098_Cf_000.endf' ),
( 'photoat/photoat-099_Es_000.endf', 'electrons/e-099_Es_000.endf', 'atomic_relax/atom-099_Es_000.endf' ),
( 'photoat/photoat-100_Fm_000.endf', 'electrons/e-100_Fm_000.endf', 'atomic_relax/atom-100_Fm_000.endf' ) ]

def open_files_and_preprocess( files, use_gnds ) :

    if use_gnds :

        photoatomic = njoy.dryad.ProjectileTarget.from_gnds_file( gnds_path + '/' + files[0] + '.gnds.xml', True )
        electroatomic = njoy.dryad.ProjectileTarget.from_gnds_file( gnds_path + '/' + files[1] + '.gnds.xml', True )
        relaxation = njoy.dryad.AtomicRelaxation.from_gnds_file( gnds_path + '/' + files[2] + '.gnds.xml', True )

        # some GNDs files currently do not contain the awr value from the evaluation
        # open the ENDF file to get the atomic mass and assign it in the data
        gnds_particle = photoatomic.particle_data.particle( photoatomic.target_identifier )
        if gnds_particle.mass == None :

            endf = njoy.dryad.ProjectileTarget.from_endf_file( endf_path + '/' + files[0] )
            endf_particle = endf.particle_data.particle( photoatomic.target_identifier )
            if endf_particle.mass != None :

                gnds_particle.mass = endf_particle.mass

            else :

                symbol = photoatomic.target_identifier.symbol
                raise RuntimeError( 'GNDs and ENDF file for {} do not have target mass data'.format( symbol ) )

    else :

        photoatomic = njoy.dryad.ProjectileTarget.from_endf_file( endf_path + '/' + files[0], True )
        electroatomic = njoy.dryad.ProjectileTarget.from_endf_file( endf_path + '/' + files[1], True )
        relaxation = njoy.dryad.AtomicRelaxation.from_endf_file( endf_path + '/' + files[2], True )

    # make sure the transition energies are correct
    relaxation.calculate_transition_energies()

    # unionise, sum partials and calculate average energies for photoatomic data
    photoatomic.unionise_cross_sections()
    photoatomic.calculate_summation_cross_sections()
    photoatomic.calculate_average_energy()

    # set compton profiles
    incoherent_id = njoy.dryad.id.ReactionID( photoatomic.projectile_identifier, photoatomic.target_identifier,
                                              njoy.dryad.id.ReactionType( 'incoherent' ) )
    photon = njoy.dryad.id.ParticleID.photon()
    if not photoatomic.reaction( incoherent_id ).product( photon ).distribution_data.has_compton_profiles :
```

```
# add Compton profiles
# for Iridium only: remove the 6s1/2 shell since that one is missing in the evaluated data
z = photoatomic.target_identifier.z
profiles = njoy.dryad.external.ComptonProfiles.biggs_mendelsohn_mann_profiles( z, True )
if z == 77 :

    del profiles[-1]

# add the profiles to the data
photoatomic.reaction( incoherent_id ).product( photon ).distribution_data.compton_profiles = profiles

# unionise and sum partials
electroatomic.unionise_cross_sections()
electroatomic.calculate_summation_cross_sections()

# make sure the electroatomic data starts at 10 eV
njoy.medic.prune_cross_sections( 10, 1e+11, electroatomic )

return photoatomic, electroatomic, relaxation

def process( photoatomic, electroatomic, relaxation ) :

    title = title_template.format( photoatomic.target_identifier.symbol )

    outputfile = output_path + '/' + str( photoatomic.target_identifier.z * 1000 ) + '.' + str( ace_number ) + 'p'
    if not os.path.exists( output_path ) :

        os.makedirs( output_path )

    njoy.acer.process_electron_photon_relaxation( photoatomic, electroatomic, relaxation, outputfile,
                                                ace_number, date, title )

failed = []

start = time.perf_counter()
for files in data :

    try :

        photoatomic, electroatomic, relaxation = open_files_and_preprocess( files, use_gnds = True )
        process( photoatomic, electroatomic, relaxation )

    except :

        failed.append( files )

end = time.perf_counter()

print( '-----' )
print( '{:4} files'.format( len( data ) ) )
print( '{:4} failed'.format( len( failed ) ) )
print( 'elapsed time = {:.3} s'.format( end - start ) )
print( '-----' )
```