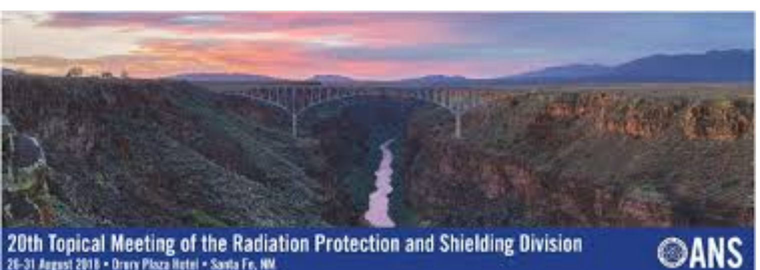
First Assessment of the New Atomic Data in ENDF/B-VIII

Maria Grazia Pia *(INFN Genova, Italy)*

Tullio Basaglia[1], Matteo Bonanomi[2], Federico Cattorini[2], Chansoo Choi[3], Min Cheol Han[4], Gabriela Hoff[5], Chan-Hyeong Kim[3], Sung Hun Kim[3], Matteo Marcoli[2], Maria Grazia Pia[4], Paolo Saracco[4]

[1]CERN, [2]Univ. of Milano Bicocca, Italy, [3]Hanyang Univ., Seoul, Korea, [4]INFN Sezione di Genova, Italy, [5]Univ. Cagliari, Italy



RPSD 2018

Santa Fe, 25-31 August 2018

Foreword

Due to limited time allocation, there is room only to highlight a few results

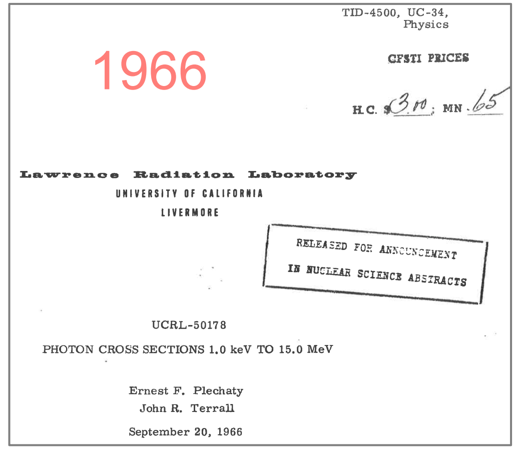
Evaluated data libraries

- Tabulations of physics quantities: cross sections, secondary particle spectra, nuclear and atomic parameters…
- Derived from the evaluation of the body of knowledge of **theoretical** computations, **experimental** measurements *or both*
- **Essential tool for Monte Carlo particle transport**
- BROND *(Russian Evaluated Neutron Data Library)*
- CENDL *(Chinese Evaluated Nuclear Data Library)*
- ENDF/B *(Evaluated Nuclear Data File)*
- JEFF *(Joint Evaluated Fission and Fusion File)*
- JENDL *(Japanese Evaluated Nuclear Data Library)*
- ENDF/B-VI: **1990**, ENDF/B-VII: **2006**, ENDF/B-VIII: **2018**

EGS, FLUKA, Geant4, MCNP, Penelope, PHITS…

Evaluated Atomic Libraries

- **EADL** (atomic) **1991**
- **EEDL** (electron) **1991**
- **EPDL** (photon) **1997**


TID-4500, UC-34, Physics

CFSTI PRICES

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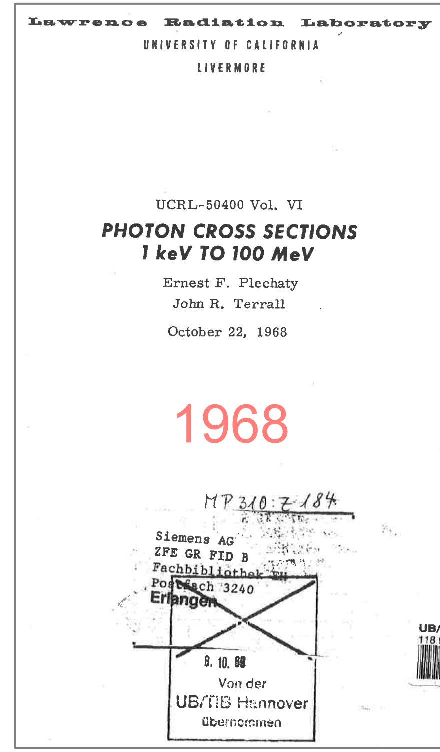
RELEASED FOR ANNOUNCEMENT IN NUCLEAR SCIENCE ABSTRACTS

UCRL-50178

PHOTON CROSS SECTIONS 1.0 keV TO 15.0 MeV

Ernest F. Plechaty
John R. Terrall

September 20, 1966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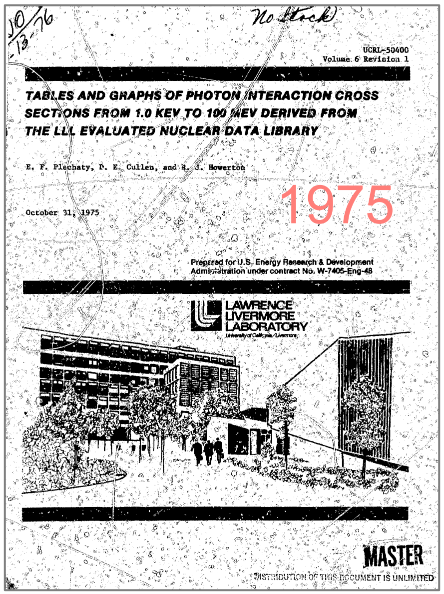
UCRL-50400 Vol. VI

PHOTON CROSS SECTIONS
1 keV TO 100 MeV

Ernest F. Plechaty
John R. Terrall

October 22, 1968


UCRL-50400
Volume 6 Revision 1

TABLES AND GRAPHS OF PHOTON INTERACTION CROSS SECTIONS FROM 1.0 KEV TO 100 MEV DERIVED FROM THE LLL EVALUATED NUCLEAR DATA LIBRARY

E. F. Plechaty, D. E. Cullen, and R. J. Howerton

October 31, 1975

Prepared for U.S. Energy Research & Development Administration under contract No. W-7405-Eng-48

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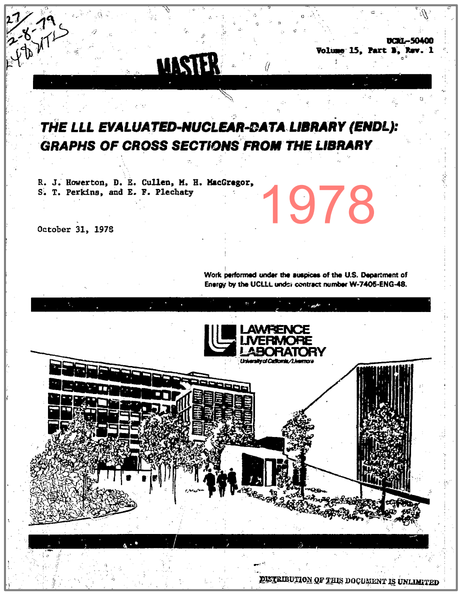
UCRL-50400
Volume 15, Part B, Rev. 1

MASTER

THE LLL EVALUATED-NUCLEAR-DATA LIBRARY (ENDL): GRAPHS OF CROSS SECTIONS FROM THE LIBRARY

R. J. Howerton, D. E. Cullen, M. H. MacGregor, S. T. Perkins, and E. F. Plechaty

October 31, 1978

Work performed under the auspices of the U.S. Department of Energy by the UCLLL under contract number W-7405-ENG-48.

LAWRENCE LIVERMORE LABORATORY

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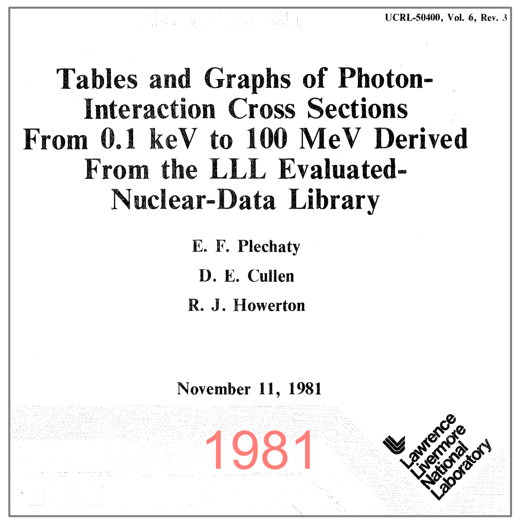
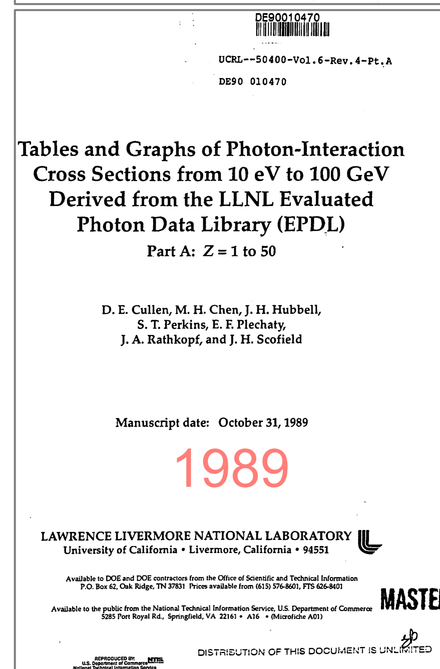

UCRL-50400, Vol. 6, Rev. 3

Tables and Graphs of Photon-Interaction Cross Sections From 0.1 keV to 100 MeV Derived From the LLL Evaluated-Nuclear-Data Library

E. F. Plechaty
D. E. Cullen
R. J. Howerton

November 11, 1981

Lawrence Livermore National Laboratory


UCRL--50400-Vol.6-Rev.4-Pt.A
DE90 010470

Tables and Graphs of Photon-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Photon Data Library (EPDL)
Part A: Z = 1 to 50

D. E. Cullen, M. H. Chen, J. H. Hubbell, S. T. Perkins, E. F. Plechaty, J. A. Rathkopf, and J. H. Scofield

Manuscript date: October 31, 1989

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DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

- **Originally released by LLL/LLNL**
- Released in **ENDF/B** since version **VI.8**
- Released by **IAEA** as **EPICS** since 2014

Formats:
ENDL
ENDF

Do EADL/EEDL/EPDL reflect the state of the art?


Caravaggio,
Incredulità di san Tommaso

2722 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 47, NO. 6, DECEMBER 2000

Comparative Evaluation of Photon Cross-Section Libraries for Materials of Interest in PET Monte Carlo Simulations

Habib Zaidi

"The cross-section values produced by the LLNL [...] **are thought to be** the most up-to-date and **accurate** coefficients available"

Comparison of theoretical calculations, **not validation!**

A Survey of Atomic Binding Energies for use in EPICS2017

IAEA-NDS-224
September 2017

by
Dermott E. Cullen

"...data that I used to produce what **I judge** to be the **BEST** binding energies to use in EPICS2017"

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

ELSEVIER

Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds

G.A.P. Cirrone [a], G. Cuttone [a], F. Di Rosa [a], L. Pandola [b,*], F. Romano [a], Q. Zhang [a,c,**]

Validation

- of physics content (e.g. cross sections) w.r.t. measurements
- in comprehensive applications (e.g. energy deposition in a detector)
- Requirements for validity related to **use cases** *(IEEE Standard 1012 V&V)*
- **State of the art**: the best one can do, given the body of knowledge

Only a relatively small fraction of EADL, EEDL and EPDL data has been **directly validated** with respect to measurements

References

- M. C. Han et al., “Validation of Cross Sections for Monte Carlo Simulation of the Photoelectric Effect”, *IEEE Trans. Nucl. Sci.*, vol. 63, no. 2, pp. 1117–1146, 2016.
- L. Pandola et al., “Validation of the Geant4 simulation of Bremsstrahlung from thick targets below 3 MeV”, *NIM B*, vol. 350, pp. 41–48, 2015.
- M. Batič, et al., “Photon elastic scattering simulation: validation and improvements to Geant4”, *IEEE Trans. Nucl. Sci.*, vol. 59, no. 4, pp. 1636–1664, 2012.
- H. Seo et al., “Ionization cross sections for low energy electron transport”, *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3219–3245, 2011.
- M. G. Pia et al., “Evaluation of atomic electron binding energies for Monte Carlo particle transport”, *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3246–3268, 2011.
- M. G. Pia et al., “Validation of K and L shell radiative transition probability calculations”, *IEEE Trans. Nucl. Sci.,* vol. 56, no. 6, pp. 3650–3661, 2009.
- S. Guatelli et al., “Validation of Geant4 Atomic Relaxation against the NIST Physical Reference Data”, *IEEE Trans. Nucl. Sci.,* vol. 54, no. 3, pp. 594-603, 2007.
- G. Weidenspointner et al., “Validation of Compton Scattering Monte Carlo Simulation Models”, *Proc. IEEE Nucl. Sci. Symp.,* 2013.
- M. Begalli et al., “Validation of Geant4 Electron Pair Production by Photons”, *Proc. IEEE Nucl. Sci. Symp.,* 2013.

Validation method

Comparison of **physics observable** resulting from each physics model with **experimental measurements**

Goodness-of-fit tests
χ^2
Anderson-Darling
Cramer-von Mises
Kolmogorov-Smirnov

rejection of the null hypothesis
in the set of test cases

Comparison of the
capability of physics models to reproduce experiment

Analysis of **contingency tables**
χ^2
Fisher exact test
Barnard (Boschloo, Suissa-Shuster)
McNemar test

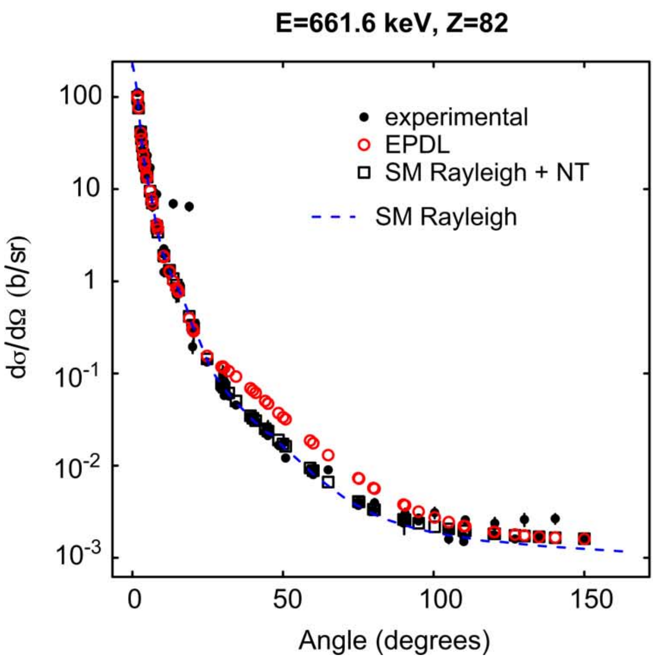
Objective identification of the **state of the art** to model the observable

A. Lechner, M. G. Pia, M. Sudhakar, Validation of Geant4 low energy electromagnetic processes against precision measurements of electron energy deposit, *IEEE Trans. Nucl. Sci.,* vol. 56, no. 2, pp. 398-416, 2009

Photon elastic scattering

EPDL: Hubbell's non-relativistic form factors

Other modeling methods: relativistic form factors, anomalous scattering factors, Kissel's S-matrix calculations…



Test		Penelope 2001	Penelope 2008-2011	EPDL	EPDL ASF	SM	RF	NF	MF	MF ASF	RF ASF
all	Test cases	71	71	71	71	71	71	71	71	71	71
	Pass	19	27	27	18	55	18	25	35	37	34
	Fail	52	44	44	53	16	53	46	36	34	37
	Efficiency	0.27	0.38	0.38	0.25	0.77	0.25	0.35	0.49	0.52	0.48
	Error	±0.05	±0.06	±0.06	±0.05	±0.06	±0.05	±0.06	±0.06	±0.06	±0.06
$\theta \leq 90°$	Test cases	67	67	67	67	67	67	67	67	67	67
	Pass	19	27	27	18	55	18	25	35	36	32
	Fail	48	40	40	49	12	49	42	32	31	35
	Efficiency	0.28	0.40	0.40	0.27	0.82	0.27	0.37	0.52	0.54	0.48
	Error	±0.05	±0.06	±0.06	±0.05	±0.05	±0.05	±0.06	±0.06	±0.06	±0.06
$\theta > 90°$	Test cases	17	17	17	17	17	17	17	17	17	17
	Pass	1	1	1	1	10	1	1	0	2	4
	Fail	16	16	16	16	7	16	16	17	15	13
	Efficiency	0.06	0.06	0.06	0.06	0.59	0.06	0.06	< 0.06	0.12	0.24
	Error	±0.06	±0.06	±0.06	±0.06	±0.12	±0.06	±0.06		±0.08	±0.10

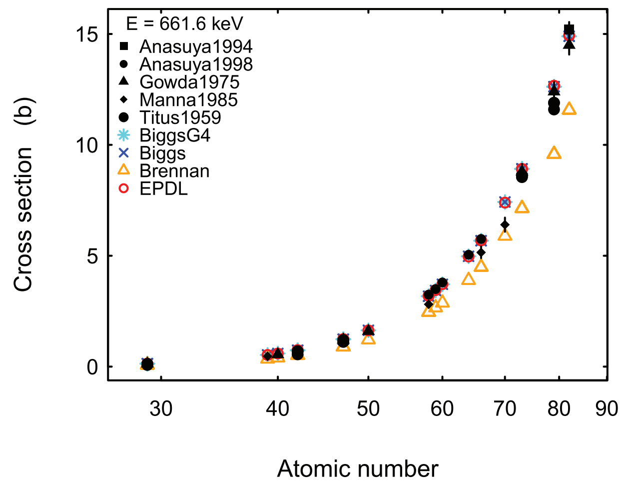
S-matrix calculations exhibit significantly better compatibility with experiment than EPDL approach based on form factor approximation

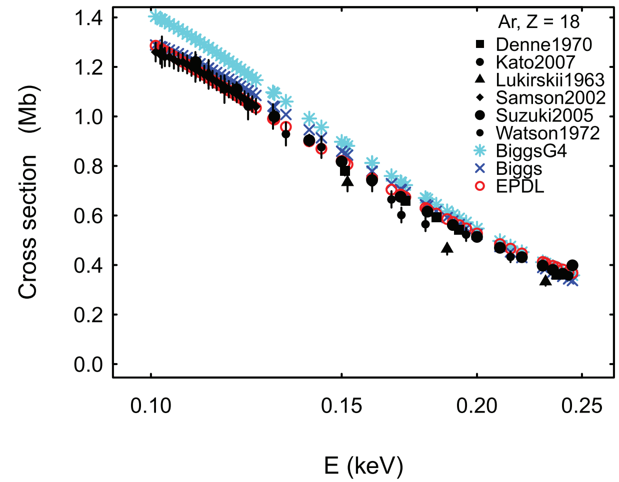
M. Batič, et al., "Photon elastic scattering simulation: Validation and improvements to Geant4", *IEEE Trans. Nucl. Sci.*, vol. 59, no. 4, pp. 1636–1664, 2012.

Photoelectric effect

Total and shell (K, $L_{1,2,3}$) cross sections

- Biggs-Lighthill
- Brennan-Cowan
- Chantler
- Ebel
- Elam
- **EPDL97**
- Henke
- McMaster
- PHOTX
- RTAB
- Storm-Israel
- Veigele
- XCOM





Goodness-of-fit tests and categorical data analysis identified **Scofield's 1973 (EPDL)** non-relativistic calculations as state-of-the-art modeling in the context of Monte Carlo particle transport

M. C. Han et al., "Validation of Cross Sections for Monte Carlo Simulation of the Photoelectric Effect", *IEEE Trans. Nucl. Sci.*, vol. 63, no. 2, pp. 1117–1146, 2016.

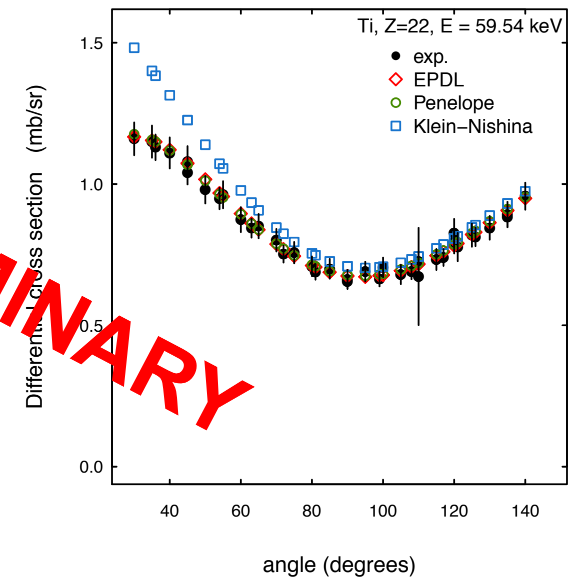
Compton scattering

Scattering functions	Efficiency	Error
EPDL	0.82	0.02
Klein-Nishina	0.54	0.03
Brusa	0.84	0.02
Biggs	0.84	0.02
Hubbell	0.82	0.02
Kahane	0.72	0.02

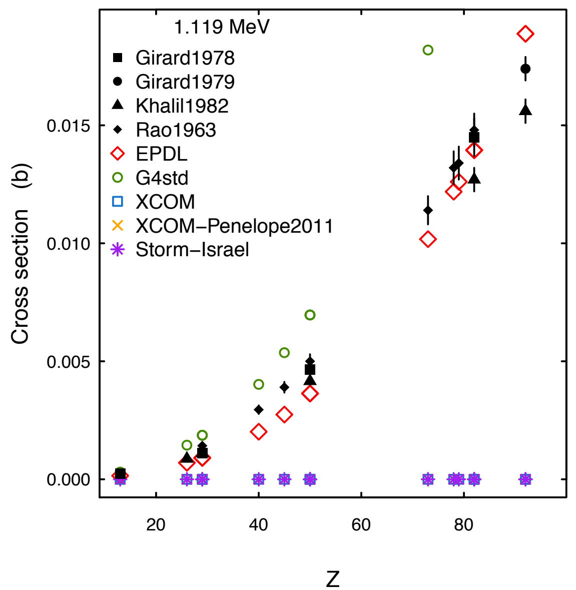
PRELIMINARY

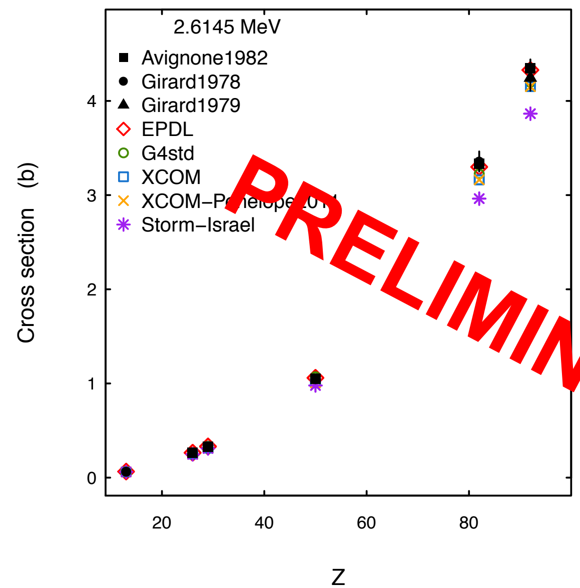
Differential cross sections

$$\left[\frac{d\sigma}{d\Omega}\right]_{inc} = \left[\frac{d\sigma}{d\Omega}\right]_{KN} S(x, Z)$$



e^+e^- pair production





PRELIMINARY

Total cross section:
Bethe-Heitler
with corrections
(Hubbell, Gimm, Overbo)

EPDL
p-value = 0.982

Ionisation cross sections: total

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011 3219

Ionization Cross Sections for Low Energy Electron Transport

Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim

Cross section models

- Binary Encounter Bethe (BEB)
- Deutsch-Märk (DM)
- EEDL

DM model reproduces experimental data better than EEDL below a few hundred eV

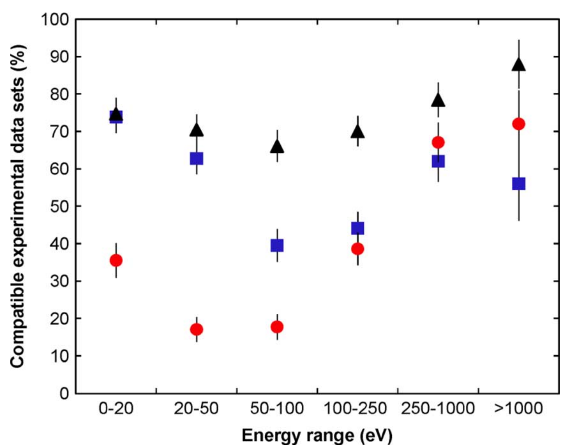


Fig. 6. Fraction of test cases in which cross sections calculated by the implemented models are compatible with experimental data at 0.05 significance level: BEB model (blue squares), DM model (black triangles) and EEDL (red circles). The fraction is calculated over the whole collection of data sets.

Energy	Goodness-of-fit test	Models		Models	
		DM	BEB	DM	EEDL
< 20 eV	Pass	40	43	40	21
	Fail	11	8	11	30
	p-value Fisher test	0.612		< 0.001	
	p-value Pearson χ^2	0.445		< 0.001	
	p-value Yates χ^2	0.611		< 0.001	
		DM	BEB	DM	EEDL
20-50 eV	Pass	44	37	44	13
	Fail	9	16	9	40
	p-value Fisher test	0.162		< 0.001	
	p-value Pearson χ^2	0.109		< 0.001	
	p-value Yates χ^2	0.170		< 0.001	
		DM	BEB	DM	EEDL
50-100 eV	Pass	47	32	47	17
	Fail	7	22	7	37
	p-value Fisher test	0.001		< 0.001	
	p-value Pearson χ^2	0.001		< 0.001	
	p-value Yates χ^2	0.002		< 0.001	
		DM	BEB	DM	EEDL
100-250 eV	Pass	50	31	50	30
	Fail	4	23	4	24
	p-value Fisher test	< 0.001		< 0.001	
	p-value Yates χ^2	< 0.001		< 0.001	
		DM	BEB	DM	EEDL
250 eV - 1 keV	Pass	28	24	28	24
	Fail	7	11	7	11
	p-value Fisher test	0.413		0.413	
	p-value Pearson χ^2	0.274		0.274	
	p-value Yates χ^2	0.412		0.412	
		DM	BEB	DM	EEDL
> 1 keV	Pass	12	8	12	10
	Fail	2	6	2	4
	p-value Fisher test	0.209		0.648	
	p-value Yates χ^2	0.209		0.645	

Ionisation cross sections: K, L, M shell

Model	
EEDL	Tabulations
Bote-Salvat	Penelope 2014 tabulations
BEB	Analytical
$BEB_{modified}$	Analytical
BEB-relativistic	Analytical
DM (current)	Analytical
DM (previous)	Analytical
DM-relativistic	Analytical

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 65, NO. 8, AUGUST 2018 2279

Validation of Shell Ionization Cross Sections for Monte Carlo Electron Transport

Tullio Basaglia, Matteo Bonanomi, Federico Cattorini, Min Cheol Han, Gabriela Hoff, Chan Hyeong Kim, Sung Hun Kim, Matteo Marcoli, Maria Grazia Pia, and Paolo Saracco

Fraction of test cases for which the hypothesis of compatibility with experiment is not rejected

Energy	Model	χ^2	Anderson-Darling
$\geq$100 eV (173 test cases)	EEDL	0.68 ± 0.04	0.73 ± 0.03
	Bote	0.68 ± 0.04	0.80 ± 0.03
	BEBR	0.55 ± 0.04	0.73 ± 0.03
	DM2000	0.64 ± 0.04	0.83 ± 0.03
$\geq$1 keV (167 test cases)	EEDL	0.72 ± 0.03	0.75 ± 0.04
	Bote	0.71 ± 0.03	0.81 ± 0.03
	BEBR	0.59 ± 0.04	0.74 ± 0.04
	DM2000	0.66 ± 0.04	0.82 ± 0.03

K shell

No significant difference in compatibility with experiment is observed between EEDL and Bote-Salvat calculations

$L_{1,2,3}$ subshells

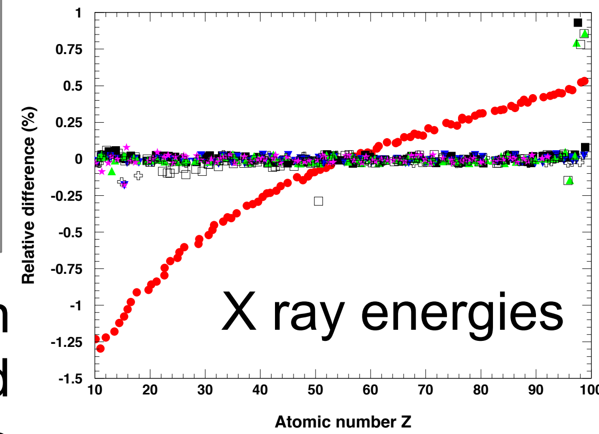
Univocal conclusions limited by scarcity of experimental measurements

Atomic binding energies

3246 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

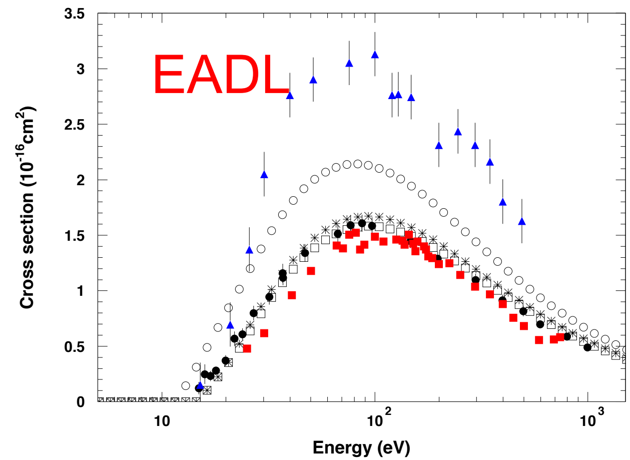
Evaluation of Atomic Electron Binding Energies for Monte Carlo Particle Transport

Maria Grazia Pia, Hee Seo, Matej Batic, Marcia Begalli, Chan Hyeong Kim, Lina Quintieri, and Paolo Saracco



Evaluated through **direct comparisons with experimental data** and through their **effects on experimental observables**

Ionisation cross sections



No single compilation is ideal for all applications

- Williams,
- Carlson,
- Table of Isotopes

strengths for specific purposes

EADL is far from ideal…

Radiative transition probabilities

- J. H. Scofield, "Radiative Decay Rates of Vacancies in the K and L Shells", *Phys. Rev., vol. 179, no. 1, pp. 9-16, 1969.*
- J. H. Scofield, "Relativistic Hartree-Slater Values for K and L X-ray Emission Rates", *Atom. Data Nucl. Data Tables, vol. 14, pp. 121-137,* 1974.

EADL

Hartree-Slater calculations

- J. H. Scofield, "Exchange corrections of K X-ray emission rates", *Phys. Rev. A, vol. 9, no. 2, pp. 1041-1049, 1974.*
- J. H. Scofield, "Hartree-Fock values of L X-ray emission rates", *Phys. Rev. A, vol. 10, no. 5, pp. 1507-1510, 1974.*

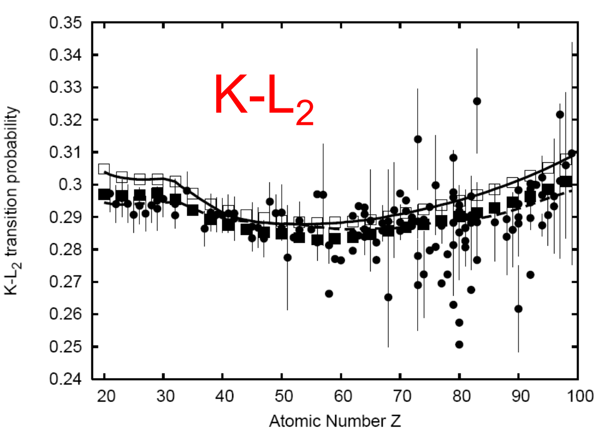
Hartree-Fock calculations

3650 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

Validation of K and L Shell Radiative Transition Probability Calculations

Maria Grazia Pia, Paolo Saracco, and Manju Sudhakar

Comparison with experimental data



Hartree-Slater vs. Hartree-Fock

	HS	HF
pass	8	16
fail	9	1
Fisher	p-value	**0.007**
χ^2 Yates	p-value	0.008

	HS	HF
pass	12	20
fail	9	1
Fisher	p-value	**0.009**
χ^2 Yates	p-value	0.011

S. I. Salem, S. I. Panossian, and R. A. Krause, "Experimental K and L Relative X-ray Emission Rates", *Atom. Data Nucl. Data Tables, vol.* 14, pp. 91-109, 1974.

The world changes… 1991/1997 → 2018

- Kissel's S-matrix calculations of photon elastic scattering
- Electron ionisation cross sections *(Deutsch-Märk, Kim-Rudd, Bote-Salvat…)*
- Scofield's Hartree-Fock calculations of atomic parameters
- Effects of theoretical/experimental atomic binding energies
- Salvat's electron elastic scattering calculations
- Photoelectric cross sections, relativistic scattering functions etc.

Great expectations for new data libraries!

EPICS2017

Released in January 2018 by IAEA
Released in February 2018 in ENDF/B-VIII.0

D. E. Cullen, IAEA-NDS-0224, IAEA-NDS-0225 rev. 1, IAEA-NDS-0226, 2017

D. A. Brown et al., ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data, *Nucl. Data Sheets,* vol. 148, pp. 1-142, 2018

EPICS2014

"Modernized by reviewing recently published data and making changes" (D. E. Cullen, IAEA-NDS-218, rev.1, 2015)
No change observed, apart from fixing format conversion errors and scientific number notation

Content

Different content for different data formats

Not trivial to retrieve what contains what

EADL

Physics Data	EADL91		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Number of electrons	yes	yes	yes	yes	yes	yes
Binding energy	yes	yes	yes	yes	yes	yes
Kinetic energy	yes	-	yes	-	yes	-
Average radius	yes	-	yes	-	yes	-
Radiative level width	yes	-	yes	-	yes	-
Non-radiative level width	yes	-	yes	-	yes	-
Average energy to the residual atom per initial vacancy	yes	-	yes	-	yes	-
Average energy of particles per initial vacancy	yes	-	yes	-	yes	-
Average number of particles per initial vacancy	yes	-	yes	-	yes	-
Radiative transition probability and emitted particle energy	yes	yes	yes	yes	yes	yes
Non-radiative transition probability and emitted particle energy	yes	yes	yes	yes	yes	yes

EPDL

Physics Data	EPDL97		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total photon cross section	-	-	-	-	-	yes
Coherent scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Coherent scattering: average energy of the scatterd photon	yes	-	yes	-	yes	-
Coherent scattering: form factor	yes	yes	yes	yes	yes	yes
Coherent scattering: imaginary anomalous scattering factor	yes	yes	yes	yes	yes	yes
Coherent scattering: real anomalous scattering factor	yes	yes	yes	yes	yes	yes
Incoherent scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Incoherent scattering: scattering function	yes	yes	yes	yes	yes	yes
Incoherent scattering: average energy of the secondary particles	yes	-	yes	-	yes	-
Photoelectric: integrated cross section	yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom	yes	-	yes	-	-	-
Photoelectric: average energy of secondary particles	yes	-	yes	-	-	-
Photoelectric: cross section by subshell	yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom by subshell	yes	-	yes	-	yes	-
Photoelectric: average energy of secondary particles by subshell	yes	-	yes	-	yes	-
Pair production: integrated cross section	yes	yes	yes	yes	yes	yes
Pair production: average energy of secondary particles	yes	-	yes	-	yes	-
Triplet production: integrated cross section	yes	yes	yes	yes	yes	yes
Triplet production: average energy of secondary particles	yes	-	yes	-	yes	-
Pair and triplet production: integrated cross section	-	yes	-	yes	-	yes

EEDL

Physics Data	EEDL91		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total electron cross section	-	-	-	-	-	yes
Large angle elastic scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Large angle elastic scattering: average energy to the residual atom	yes	-	yes	-	yes	-
Large angle elastic scattering: average energy of the scattered electron	yes	-	yes	-	yes	-
Large angle elastic scattering: angular distributions	yes	yes	yes	yes	yes	yes
Elastic scattering: integrated cross section	yes	-	yes	-	yes	yes
Ionisation: integrated cross section	-	-	-	-	yes	yes
Ionisation cross section by subshell	yes	yes	yes	yes	yes	yes
Ionisation: average energy of secondary particles by subshell	yes	-	yes	-	yes	-
Ionisation: spectra of the recoil electron by subshell	yes	yes	yes	yes	yes	yes
Bremsstrahlung: integrated cross section	yes	yes	yes	yes	yes	yes
Bremsstrahlung: energy spectra of the secondary photon	yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary photon	yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary electron	yes	-	yes	-	yes	-
Excitation: integrated cross section	yes	yes	yes	yes	yes	yes
Excitation: average energy to the residual atom	yes	yes	yes	yes	yes	yes

Assessment

- What **has changed in EPICS2017** and **ENDF/B-VIII** w.r.t. the data libraries currently used by major Monte Carlo codes
  - **Consistency**
  - Computational **performance**
  - **Validity** w.r.t. experimental data: first results, *(in progress)*
- What **has not changed**
  - and has been previously (recently) identified as the state of the art
  - and does not reflect the state of the art
- How the data libraries are **released**
- How they are **maintained**

Reliability lies not only in the content, but also in the process!

- **Opportunities for improvement**

What's new in EPICS2017

Atomic binding energies

Propagated into dependent physics quantities
(cross sections, transition energies etc.)

Previous: theoretical

New: empirical, Carlson + Williams

M. G. Pia et al., Evaluation of atomic electron binding energies for Monte Carlo particle transport, *IEEE Trans. Nucl. Sci.*, vol. 58, no. 6, pp. 3246-3268, 2011

Electron kinetic energies

Previous: undocumented

New: undocumented

Coherent photon scattering integrated cross sections

Changes also in the real and imaginary components of anomalous scattering factors

Previous: from numerically integrated calculations combining Thomson scattering, form factors and anomalous scattering factors

New: ?

EEDL excitation data

Different integrated cross sections and average energies for 17 elements

Roundoff effects?

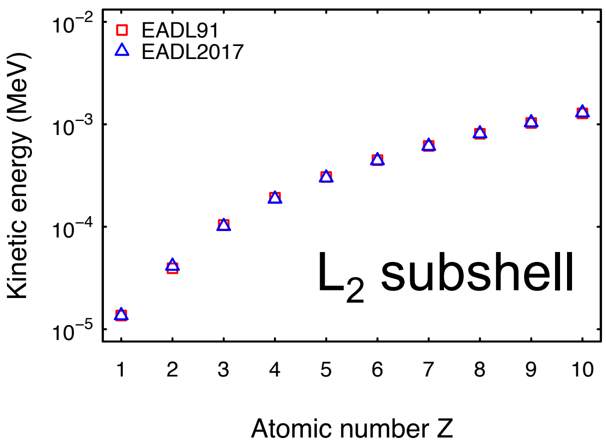
Elastic scattering, large angle scattering, Bremsstrahlung integrated cross sections

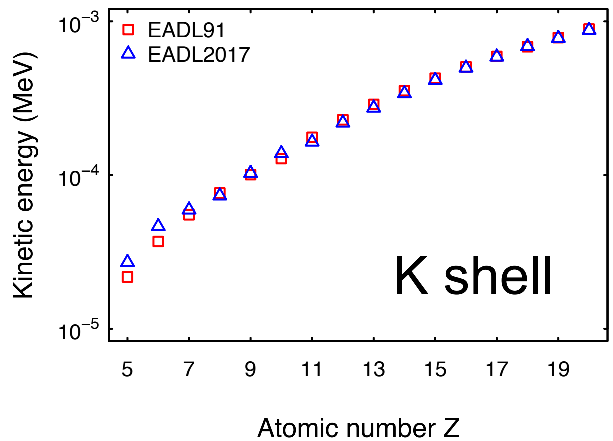
"Linearization"

Larger number of tabulated data to enable linear interpolation instead of logarithmic

Electron kinetic energies

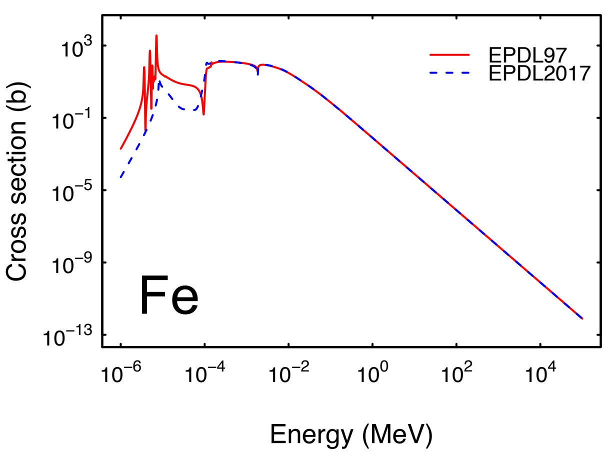
Experimental data for validation?

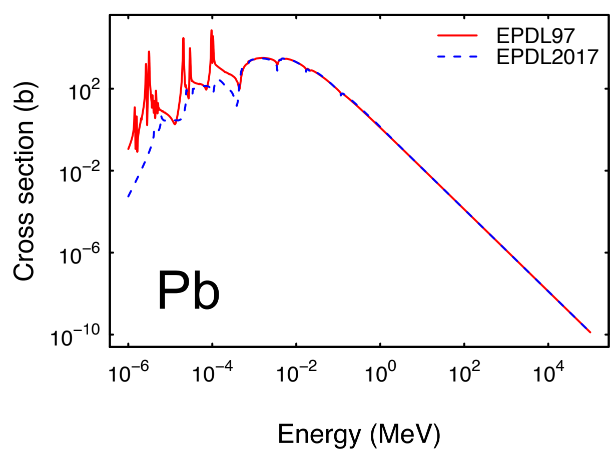




Differences appear larger for elements with low atomic numbers

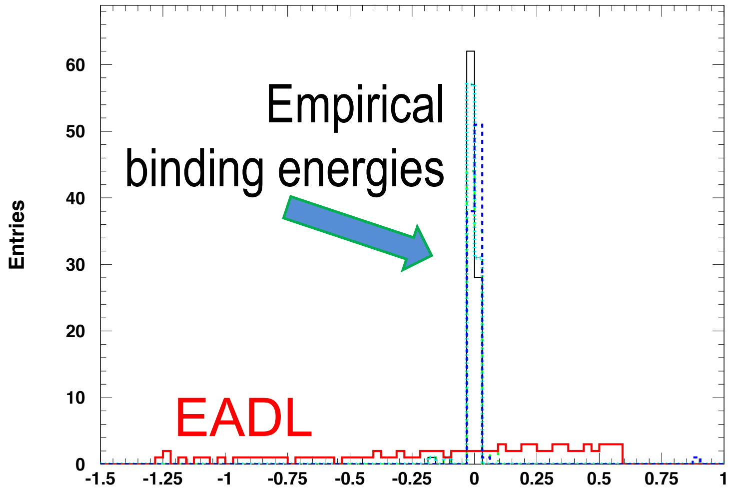
Coherent photon scattering integrated cross sections



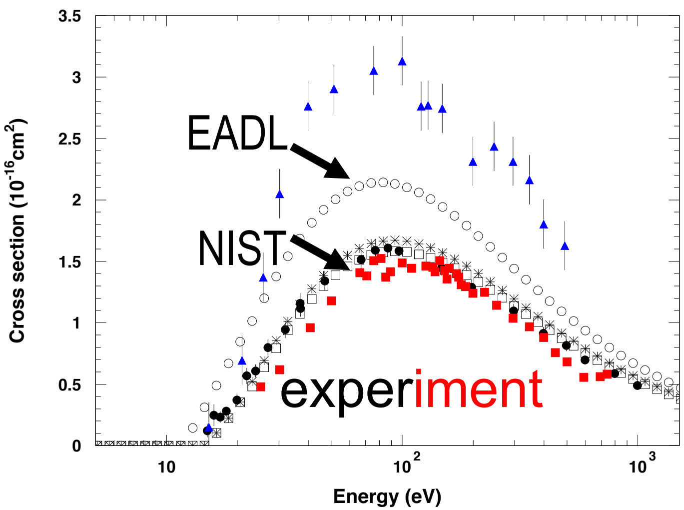


To the best of our knowledge, no experimental data available to validate the large changes at low energies

Atomic binding energies



Radiative transition energies, difference w.r.t. experiment



Electron ionisation cross sections calculated with EADL and NIST binding energies, w.r.t. experiment

M. G. Pia et al., "Evaluation of atomic electron binding energies for Monte Carlo particle transport", *IEEE Trans. Nucl. Sci.*, vol. 58, no. 6, pp. 3246–3268, 2011

In EPICS2017 and ENDF/B-VIII: **empirical** binding energies replaced previous theoretical values

…and their dependencies

e.g. relaxation data for carbon

6000.00000	11.9078164	0	0	4	0		60028533	1
1.00000000	0.0	0	0	54	8		60028533	2
288.000000	2.00000000	0.0	0.0	0.0	0.0		60028533	3
3.00000000	0.0	282.020000	5.61488D-4	0.0	0.0		60028533	4
4.00000000	0.0	282.030000	.001120600	0.0	0.0		60028533	5
2.00000000	2.00000000	255.890000	.413609000	0.0	0.0		60028533	6
2.00000000	3.00000000	264.460000	.136190000	0.0	0.0		60028533	7
2.00000000	4.00000000	264.470000	.271099000	0.0	0.0		60028533	8
3.00000000	3.00000000	273.030000	.004207480	0.0	0.0		60028533	9
3.00000000	4.00000000	273.040000	.110012000	0.0	0.0		60028533	10
4.00000000	4.00000000	273.050000	.063200800	0.0	0.0		60028533	11
2.00000000	0.0	0	0	6	0		60028533	12
16.5900000	2.00000000	0.0	0.0	0.0	0.0		60028533	13
3.00000000	0.0	0	0	6	0		60028533	14
11.2600000	.670000000	0.0	0.0	0.0	0.0		60028533	15
4.00000000	0.0	0	0	6	0		60028533	16
11.2600000	1.33000000	0.0	0.0	0.0	0.0		60028533	17

Radiative and non-radiative transition energies are **inconsistent** with atomic binding energies

→ **non-conservation of energy!**

Consistency issues

"Starting with EPICS2017 all the data has been **linearized** [...]. The result is libraries are roughly three (3) times as large, but it can be accurately interpolated using LIN- LIN interpolation…"

- Electron data have not been "linearized", but the documentation recommends linear interpolation
- **Different number of data points** in ENDF/ENDL libraries, and in the same libraries released by IAEA, ENDF/B and NNDC

Inconsistent *(or intentionally modified?)* **units** in form factors and scattering functions:

- **Not documented**, liable to induce to errors in simulations

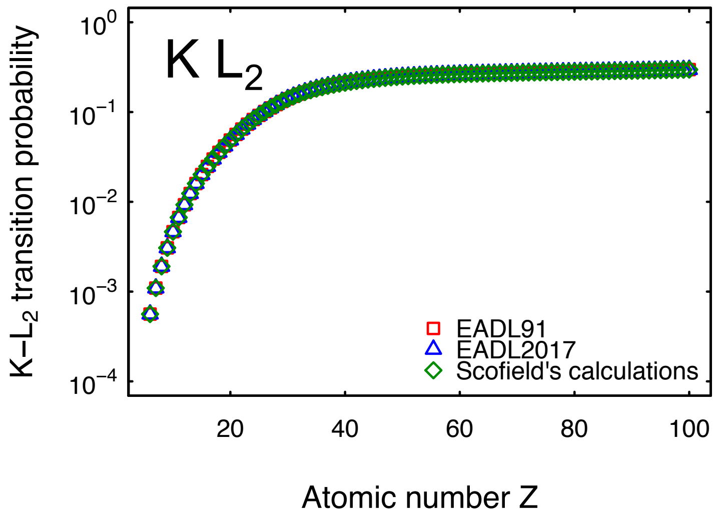
Non-monotonic primary e^- energies in secondary e^- spectra

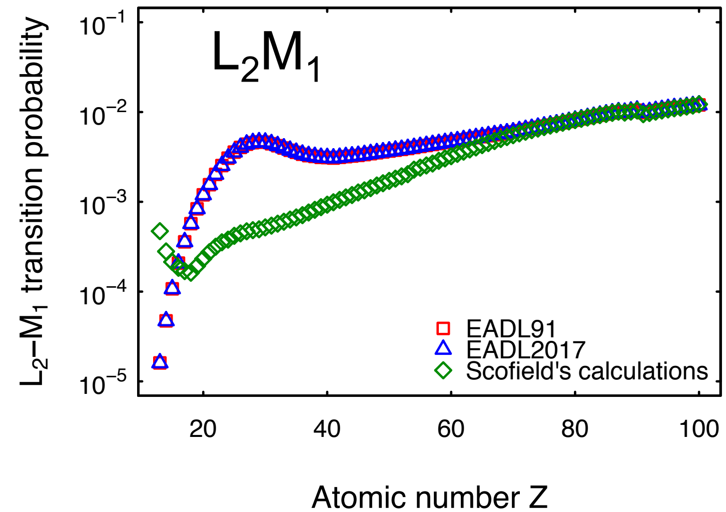
- Liable to be source of interpolation problems

E_{e-} < atomic binding E!

```
  6000    9 19    0.0          1712152 2   0.0            0.0            0.0
81  21  91    0.0          5.          0.0            0.0            0.0
 1.126000000D-05 2.525000000D-09 4.400440000D+07
 1.126000000D-05 2.525000000D-08 4.400440000D+07
 9.495000000D-06 2.525000000D-09 4.062760000D+06
 9.495000000D-06 2.525000000D-07 3.938040000D+06
```

Physics issues **Radiative transition probabilities**





EADL radiative transition probabilities derive from calculations of transition rates by Scofield

Discrepancies identified between EADL transition probabilities and Scofield's original calculations, which reproduce experimental data better than EADL

M. G. Pia et al., "Validation of K and L shell radiative transition probability calculations", *IEEE Trans. Nucl. Sci.,* vol. 56, no. 6, pp. 3650–3661, 2009.

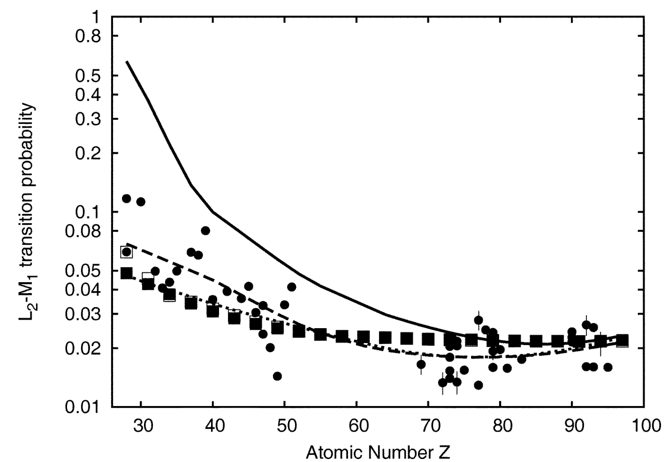


Fig. 12. L$_2$-M$_1$ transition probability versus Z: theoretical calculations based on the Hartree-Slater [2] (white squares) and the Hartree-Fock [3] (black squares) potentials, EADL [5] tabulations (solid line), experimental data (black circles), fit to them as in [13] (dashed line), and improved fit (dotted line).

The same discrepancies are still present in EPICS2017 and ENDF/B-VIII.0

MEMORY SIZE IN KB REQUIRED TO USE PHYSICS DATA OF ALL ELEMENTS

Physics data **Memory**	Original libraries	ENDF/B-VIII EPICS2017	Ratio
Bremsstrahlung cross section	368	368	1
Elastic scattering cross section	472	472	1
Large angle elastic scattering cross section	472	472	1
Ionisation cross section by subshell	1924	1924	1
Excitation cross section	1152	1152	1
Coherent scattering cross section	4528	1868	0.4
Coherent scattering form factor	708	4620	6.5
Incoherent scattering cross section	508	1692	3.3
Incoherent scattering scattering function	724	1836	2.5
Photoelectric cross section	4480	32620	7.3
Photoelectric cross section by subshell	7536	45976	6.1
Pair production cross section	496	1356	2.7
Triplet production cross section	436	920	2.1

Computational performance

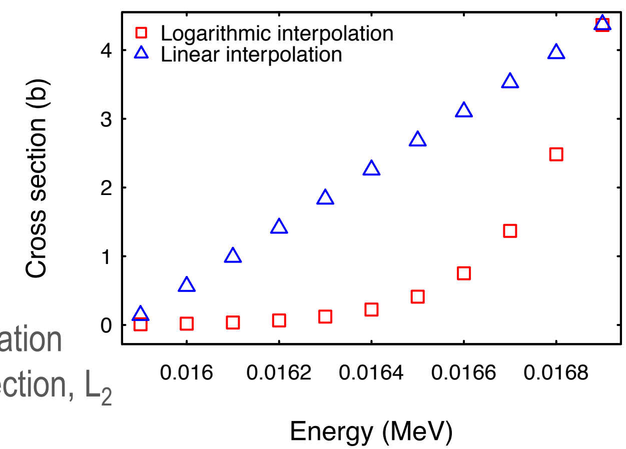
"Linearized" data libraries:

tradeoff between memory and CPU needs

Related to the characteristics of each experimental scenario

COMPUTATIONAL TIME IN SECONDS TO CALCULATE INTEGRATED CROSS SECTIONS WITH DIFFERENT INTERPOLATION METHODS

Physics process **CPU**	Original Libraries Logarithmic	EPICS2017 Linear
Bremsstrahlung	3.88 ± 0.01	0.63 ± 0.01
Elastic scattering	3.90 ± 0.01	0.79 ± 0.01
Large angle elastic scattering	3.92 ± 0.01	0.79 ± 0.01
Excitation	4.21 ± 0.01	1.06 ± 0.01
Coherent scattering	4.32 ± 0.02	1.21 ± 0.01
Incoherent scattering	3.93 ± 0.01	1.28 ± 0.01
Photoelectric	4.67 ± 0.01	3.68 ± 0.01
Pair production	2.36 ± 0.01	0.85 ± 0.01
Triplet production	2.25 ± 0.01	0.81 ± 0.01



Pb ionisation cross section, L_2

Results with a trivial data management software
Can do much better with smarter algorithms

Beware of **precision of interpolation** of electron data: linear interpolation recommended in EEDL documentation, but same number of points as in EEDL1991!

Reproducibility issues

- Inconsistencies between the **same data** released in **ENDF** and **ENDL** format
- Inconsistencies between the **same data** in the **same format** released in **different systems**, e.g. EPICS2017 and ENDF/B-VIII.0
- Differences between the data released by **IAEA** and by **NNDC** as EPICS2017
- **Different data** released by IAEA under the **same identifier** of EPICS2017
  - e.g. photoelectric cross sections modified in February, all identified as EPICS2017
  - Same issue again with transition energies modified in April 2018

Example: Carbon
(screenshots on 18/6/2018)

Updated!

EPICS2017

Electron Photon Interaction Cross Sections (2017)

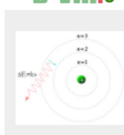
The Official ENDF/B-VIII Electron and Photon Data

(http://www.nndc.bnl.gov/endf/epics/)

```
6000.00000 11.9078164           0          0
1.00000000 0.0                  0          0
288.000000 2.00000000 0.0        0.0
3.00000000 0.0        276.740000 5.61488D-4
4.00000000 0.0        276.740000 .001120600
2.00000000 2.00000000 254.820000 .413609000
2.00000000 3.00000000 260.150000 .136190000
2.00000000 4.00000000 260.150000 .271099000
3.00000000 3.00000000 265.480000 .004207480
3.00000000 4.00000000 265.480000 .110012000
4.00000000 4.00000000 265.480000 .063200800
2.00000000 0.0                  0          0
16.5900000 2.00000000 0.0        0.0
3.00000000 0.0                  0          0
11.2600000 .670000000 0.0        0.0
4.00000000 0.0                  0          0
11.2600000 1.33000000 0.0        0.0
```

Not updated!

Download ENDF/B-VIII.0



Atomic Relaxation Reaction Sublibrary
[2.7 Mb zipfile] [Release Notes] [Changelog]
[Material List]
Download checksums:
MD5: e04d50098cb2a7e4fe404ec4071611cc
SHA1: 486a89705cb45720feb6c3a4ab126be3444846a3
cksum: 1302098210

(http://www.nndc.bnl.gov/endf/b8.0)

```
6000.00000 11.9078164           0          0
1.00000000 0.0                  0          0
288.000000 2.00000000 0.0        0.0
3.00000000 0.0        282.020000 5.61488D-4
4.00000000 0.0        282.030000 .001120600
2.00000000 2.00000000 255.890000 .413609000
2.00000000 3.00000000 264.460000 .136190000
2.00000000 4.00000000 264.470000 .271099000
3.00000000 3.00000000 273.030000 .004207480
3.00000000 4.00000000 273.040000 .110012000
4.00000000 4.00000000 273.050000 .063200800
2.00000000 0.0                  0          0
16.5900000 2.00000000 0.0        0.0
3.00000000 0.0                  0          0
11.2600000 .670000000 0.0        0.0
4.00000000 0.0                  0          0
11.2600000 1.33000000 0.0        0.0
```

Not updated!

International Atomic Energy Agency
Nuclear Data Services
Provided by the Nuclear Data Section

EPICS2017

Electron and Photon Interaction Cross Sections

(https://www-nds.iaea.org/epics/)

```
6000.00000 11.9078164           0          0
1.00000000 0.0                  0          0
288.000000 2.00000000 0.0        0.0
3.00000000 0.0        282.020000 5.61488D-4
4.00000000 0.0        282.030000 .001120600
2.00000000 2.00000000 255.890000 .413609000
2.00000000 3.00000000 264.460000 .136190000
2.00000000 4.00000000 264.470000 .271099000
3.00000000 3.00000000 273.030000 .004207480
3.00000000 4.00000000 273.040000 .110012000
4.00000000 4.00000000 273.050000 .063200800
2.00000000 0.0                  0          0
16.5900000 2.00000000 0.0        0.0
3.00000000 0.0                  0          0
11.2600000 .670000000 0.0        0.0
4.00000000 0.0                  0          0
11.2600000 1.33000000 0.0        0.0
```

Version control and configuration management | ISO/IEC/IEEE 12207, IEEE Standard 828

First validation test

Electron ionisation cross sections

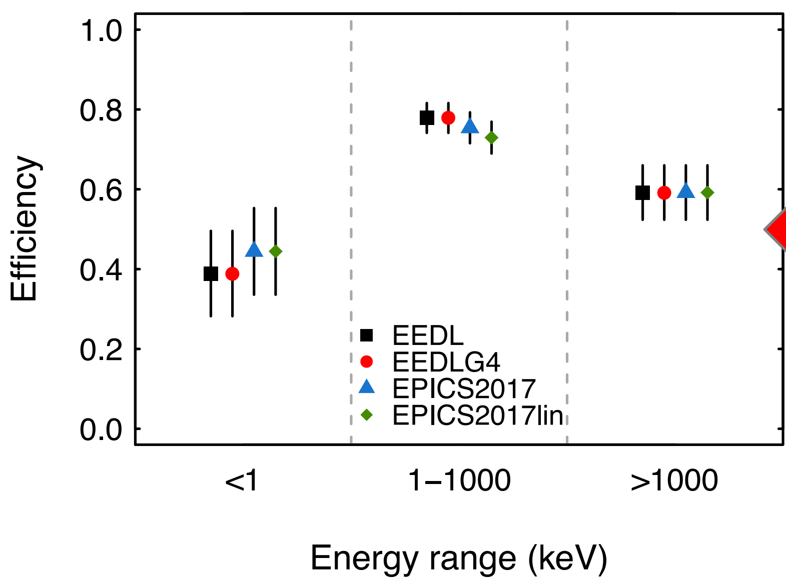
~ 2800 K shell cross section measurements

Goodness-of-fit tests

- χ^2
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

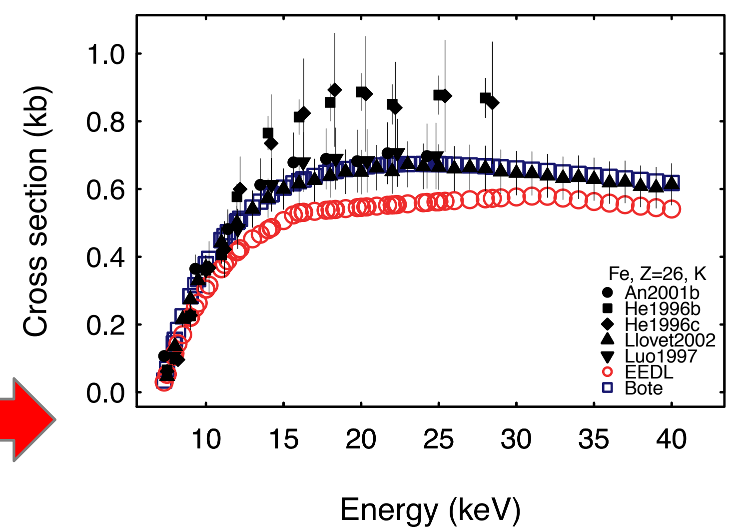
0.01 significance level

efficiency = fraction of test cases where H0 is not rejected



Slightly different results with EPICS2017 w.r.t. EEDL91, however the difference in compatibility with experiment is **not statistically significant**

…but interpolation issues due to the coarse granularity of tabulations!



Conclusion

First assessment of long-awaited new versions of widely used Evaluated Atomic Data Libraries

Promising move from theoretical atomic binding energies to empirical ones	Other physics improvements identified by validation tests not yet included

Ample room for improvement in quality assurance

Critical: version control

Responsibility of the scientific community

M. C. Han et al., "First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries", *IEEE Trans. Nucl. Sci.*, https://doi.org/10.1109/TNS.2018.2849328

Acknowledgments

- D. E. Cullen for valuable information
- CERN Library
- INFN National Computing Service

Min Cheol Han