

Nuclear Reaction Databases

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Nuclear reaction





$a + A \rightarrow b + B$

A(a,b)B

Q-value = masses (before) – masses (after) = $M_a + M_A - M_B - M_b$

Q-value > 0 : exothermic Q-value < 0 : endothermic Q = 0 : elastic scattering

Why do we study nuclear reactions?

 Probe to nuclear structure properties of the nucleus

- Interaction of particles and radiation with matter
 - Inventories of particles and nuclei
 - Radiation transport







Nuclear fission and fusion



Production of energy – safety and security (decay heat, waste management)



Images from web-IAEA

Chain reactions – nuclear inventories



Production of energy – safety and security (decay heat, waste management)





Images from web-IAEA

Materials analysis





Ion Beam Analytical Techniques Surface composition

$$Y_{\gamma}(E_0,\theta) = \varepsilon_{abs}(E_{\gamma}) \cdot N_p \cdot \int_0^{E_0} N_T \cdot \sigma(E_0,\theta) / S(E) dE$$

Images from web - HZDR

Nuclear reactions are the fuel of the stars



Stellar Nucleosynthesis





Cross section σ





- Probability of a projectile to 'hit' a target nucleus and interact with it (scatter, break up, transfer a particle etc)
- Formal definition (Fermi Golden Rule)

Probability = $n \cdot x \cdot \sigma$

- n = # nuclei per volume;
- x = thickness;
- σ = effective area of nucleus for reaction
- σ (units = 10⁻²⁴ cm² or 1 barn) in nuclear physics mb (10⁻³ b) or µb (10⁻⁶ b)

Cross sections $\sigma(\theta)$, $\sigma(E,\theta)$



• Total cross sections σ_{T} (in 4π)



- Angular distribution $d\sigma/d\Omega$ (in $d\Omega$)
- Double-differential cross sections d²σ/dEdΩ (emission spectrum: in dΩ with E')

Reaction types





Angular distributions $d\sigma/d\Omega$





Reaction Mechanisms



Ejectile energy

Reaction Models





Cross section calculations



- Depending on incident energy more than one reaction mechanism may contribute
- Use different models to describe reaction mechanisms
- Models make use of parameters that have to be adjusted to experimental cross-section data
- Independent experimental information can be used to constrain the parameters

Direct reactions

IAEA

- Inelastic scattering, transfer, knockout, breakup
- Only a few nucleons involved
- Periphery forward angles
- Mainly one-step processes
- Selective initial and final states connected by transferred angular momentum I = ℓ_α - ℓ_β; parity conservation

Spectroscopic factors: how much the wavefunction of a given state can be described by a singleparticle motion within the nucleus

$$\left(\frac{d\sigma}{d\Omega}\right)_{\exp} = S_{(l_{Ax}j_{Ax})J_{B}} \left(\frac{d\sigma}{d\Omega}\right)_{\operatorname{ca}}$$



Compound nucleus reactions



 Statistical model: excitation to energies where excited states are overlapping



Ingredients of HF cross sections

Particle entrance/exit channels: a + A
 transmission coefficients T_{aA} are obtained by solving scattering of projectile a off target A using an Optical Model Potential (OMP):
 U = V_c+ V + i·W (T's are related to scatt. amplitudes)

- Photon exit channel: $\gamma + A$ transmission coefficient $T_{\gamma A}$ is obtained from Giant Resonances Strength Function (γ SF) assuming E1/M1 transitions are important
- For excitations to phase space where levels are strongly overlapping and unresolved: Nuclear Level Density (NLD) formulas are used to describe number of states per E and J
- Ground-state properties: masses, deformations, density distributions, single-particle level schemes are obtained from nuclear models

Ingredients of HF cross sections

Fission (n,f): compound nucleus formation

Hill-Wheeler WKB form for T_f

$$T_i(E) = \frac{1}{1 + \exp(2\pi \frac{V_i + E - E_0}{\hbar \omega_i})}, \quad i = A, B,$$

Fission Barriers

- fission barrier height V_i, curvature (ħω)_i, for i = 1, 2, and 3
- transition state parameters, band head energy, K^π, inertia ħ²/2I

Level Density

- normal level densities calculated internally
- tweaking parameters
 - level density parameter multiplier (a × c)
 - fission level density scaling (p_f × c)



Reference Input Parameter Library (RIPL)



- Produced by series of IAEA CRPs
- Recommends models and data for ingredients of direct, preequilibrium and compound nucleus reaction cross-section calculations
- Adopted by widely used reaction codes: Empire, TALYS, CCONE, COH2, etc.

Reference Input Parameter





masses, Qvlaues, etc AME, models discrete levels and branchings (ENSDF)

optical potentials (phenomenological, semi-microscopic, dispersive)

nuclear level density models, D0s, cumulative levels

Resonant reactions



Breit-Wigner formula



R-matrix theory

- The theory to describe individual resonances in A+B scattering, and the non-resonant background between them.
- Describes all the asymptotic properties of the A+B wave function outside some fixed radius, R ≥ a,
 in terms of note energies a

in terms of pole energies e_p

and reduced width amplitudes γ_{np} for each channel *n* and pole *p*. — The γ_{np} are calculated from structure theory, or

- or the γ_{np} are fitted to scattering data

$$R_{mn}(E) = \sum_{p=1}^{\infty} \frac{\gamma_{mp} \gamma_{np}}{E - e_p}$$

Use finite number of poles

 E_R , Γ_R : initial values taken from ENSDF





Nuclear reaction codes

- R-matrix analysis codes (public)
 - AZURE2: https://azure.nd.edu/
 - SAMMY: RSICC (ORNL)



Other: EDA (LANL), CONRAD (CEA Cadarache), AMUR (JAEA), FRESCO (LLNL), RAC (Tsinghua), RFIT (GEEL)

NRG

- Nuclear reaction codes (public)
 - Empire: https://www-nds.iaea.org/empire
 - TALYS: <u>https://www-nds.iaea.org/talys</u>





- Direct reactions (transfer, inelastic, knockout, breakup)
 - FRESCO (Surrey, LLNL)

Nuclear reactions for applications



- Measured cross sections (total, ang. Distributions, double-differential cross sections
- Theoretical cross sections at any energy and angle
- Evaluated cross sections

Evaluation of nuclear cross sections





Particle energy (MeV)

Cross Section (barns)

Evaluation methodology I



- Compile available exp. data for a specific incident particle on a target nucleus up to energy of interest – include all data in all open reaction channels (absolute cross sections, differential and doubledifferential, ratio cross sections, etc.)
- Assess exp. data: identify outliers; adopt final datasets
- Fit cross sections (total, angular distributions, partial cross sections) in open channels using suitable models
- Correlation matrices (covariances) of parameters or cross sections

Evaluation methodology II



- Compile available exp. data for a specific incident particle on a target nucleus up to energy of interest – include all data in all open reaction channels
- Assume a prior cross section (theory, previous evaluation)
- Fit experimental data using no model fit Bayesian inference assuming known prior
- Include correlations in experimental data
- Produce recommended cross sections and covariances

Uncertainties

- spread of the data IAEA
- Mean: $\mu = \frac{\sum x_i}{N}$ • Variance: $\sigma^2 = \frac{(x_1 - \mu)^2 + \dots + (x_N - \mu)^2}{N}$
- Standard deviation: $\sigma = \sqrt{\text{variance}} = \sqrt{\sigma^2}$
- Covariance: $cov(x, y) = \frac{\sum (x_i \mu)(y_i \nu)}{N-1}$

How two variables change together: Positive Negative

• Correlations: measure of the degree to which two variables move together :

-1 to +1: 0 means they are not related

Different evaluations





Cross Section (barns)

Different evaluations cont'd



Cross Section (barns)



Databases







EXFOR: <u>EX</u>change <u>FOR</u>mat

contains experimental nuclear reaction data for incident neutrons, charged-particles and photons - 24,390 experiments

- 1970: USA, NEA, IAEA, USSR agreed on format and established exchange between data centres
- Nuclear Reaction Data Centres (NRDC): 13 data centres contribute ~ 500 entries per year
- Central maintenance at IAEA dissemination at IAEA, NNDC, and NEA
- Distribution (EXFOR, X4+, C4, C5, XML, Html, plots): Web, CD/DVD ROM
- Connection (import-export) to other databases: ENDF, CINDA, NSR
- ENDF: Evaluated Nuclear Data File is a collection of evaluated libraries
 - **ENDF-6**: format to store and exchange evaluated data
 - Fixed and well-defined, ("computer readable")
 - developed to be convenient for programming (Fortran)
 - The system offers "interpreted" and XML (GND) output formats
 - Contributors: *IAEA-NDS*, *WPEC*, *CSEWG*, *IPPE*, *CNDC*, *JAEA*, *NRG*, *CCFE*, *FZK*

EXFOR retrieval interface



https://www-nds.iaea.org/exfor/



Web and Database Programming: Viktor Zerkin, NDS, International Atomic Energy Agency (V.Zerkin@iaea.org) 2022-10-07

Data Source: Network of Nuclear Reaction Data Centres (NRDC)

Quick search: Examples, More examples



Examples of requests: 1234567... Less examples... 1 Cross section σ(E) /updates/ MF3 2 Angular distributions dσ/dΩ(E,θ) MF4 4 Double differential cross section MF6 d2σ/dΩ/dEout 5 Corrections data from EXFOR Ex.1 ZK1 ZK2 AT1 RC1 6 Search by outgoing particles: $[\alpha+\gamma]$ P,XG (P,XG),DA 6+Search data for IBANDL, 12C(α,α)12C, θ=167° , Err-Sys 7 Enhanced search by product with filtering product coded as ELEM/MASS for quick plot Search by wildcards in full reaction code 9 Ratios converted to cross sections (C4) 10 NUBAR: average number of neutrons per fission PR DL ^DL 10+ PENS plot Constructing a covariance matrix from EXFOR uncertainties 12 Extended listing of references (authors, title, DOI, NSR, Web) 13 EXFOR - CINDA sequential search N,F 14 Automatic re-normalization (output data and plots); 55Mn(n,g) 15 Find data: [digitized] from plots, [not digitized], [from table] [experimental data only] [not empty datasets] [empty] 16 Search by authors using aliases Ex.2 Ex.3 17 Fission spectra b Thick target neutron spectra c Delayed neutrons d Kerma factor 18 Invert reaction using detailed balance ${}^{13}C(\alpha,n){}^{16}O \rightarrow {}^{16}O(n,\alpha){}^{13}C; \sigma \mid d\sigma d\Omega \mid$ Ex.2: ${}^{3}\text{He}(d,p){}^{4}\text{He} \rightarrow {}^{4}\text{He}(p,d){}^{3}\text{He} \ d\sigma/d\Omega$ [plot] 19 Various fission quantities: a Vield (chain, primary FF, secondary FF) b Cumulative yield of ¹⁴⁷Nd b2 c Total kinetic energy d Multiplicity of prompt fission neutrons 20 Plotting cross section coded with SF8=DAM; all

Request	Submit Reset Help											
Target 🔽	Target 🔽 Li-6											
Reaction 🗹	he3,p											
Quantity 🔽	DA; DAP											
Product 🗆		2										
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Go to: [upload your data] Options Exclude superseded data No reaction combinations (ratios...) Exclude evaluated/calculated data Enhanced search of Products Show evaluators flags //2021 Retrieve listing only Disable Prompt-help Sort by:
reaction
publication View: Obasic extended Kanges (Z,A) Reaction Sub-Fields Feedback and User's Input Clone Request: CINDA ENDF A More Web Tools Upload your own experimental data Plot your data · Run ENSDF codes on your ENSDF data

Examples of how to fill in the form

Data selection

Image: Imag										
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*	6	+ 1 X4 X4+	X4± T4		7.50e5	1.85e6	97		T0031004 [4] R33 /0	1980EL02 An[79]=42:161 LVL=1.7e7 #2:pdf
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g	8	+ i X4 X4+	X4± T4	1977 M.Irshad+	1.40e7		25	[pdf]+ J,NP/A,286,483,19770	8 A1540002 [6] R33 /0	1977IR01An[25]=22:90 LVL[2]=0:2.9e6
g	9	+ i X4 X4+	X4± T4	1976 C.R.Gould+	3.00e6	6.00e6	56	[pdf]+ J,NSE,60,(4),477,197	608 F0001002 [5] R33 /0	An[55]=21:163 LVL=0
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a	19	+ 1 X4 X4+	X4± T4	1965 N.R. Eletcher+	5.00e6	1.30e7	82	[pdf]+ J.NP.70.471.1965	≥1545002 [7] R33 /0	1965FL03An[81]=8:174_UVI =2.9e6
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a	21	+ 1 X4 X4+	X4± T4		5.00e6	1.70e7	170		A1545004 [7] R33 /0	1965FL03An[164]=2:183_LVL=0
a	22	+ 1 X4 X4+	X4± T4	1956 J.P.Schiffert	1.00=6	5.00e6	95	[pdf]+ J.PR.104.1064 1956	A1495004 [8] R33/0	19568C01 An[95]=0:153 LVL=0
5	0				2.0000					

EXFOR plotting page





Data for plotting: ZVD (39Kb); download ZVView; upload and plot your ZVD file

Select corresponding ENDF data



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1 ENDF-6 Interpreted σ js Plot ENDF/B-VIII.0	E=150MeV Lab=LANL,ORNL Date=20111222	M.B.Chadwick+,Derrien+								
2 ENDF-6 Interpreted σ js Plot ENDF/B-VII.1	E=150MeV Lab=LANL,ORNL Date=20111222	M.B.Chadwick+,Derrien+								
3 ENDF-6 Interpreted σ js Plot ENDF/B-VII.0	E=150MeV Lab=LANL,ORNL Date=DIST-DEC06	M.B.Chadwick+,Derrien+								
4 ENDF-6 Interpreted σ js Plot JEFF-3.3	E=150MeV Lab=LANL Date=20171231	M.B.CHADWICK & P.G.YOUNG								
5 ENDF-6 Interpreted σ js) Plot JEFF-3.2	E=150MeV Lab=LANL Date=090105	M.B.CHADWICK & P.G.YOUNG								
6 ENDF-6 Interpreted σ js Plot JEFF-3.1.2	E=150MeV Lab=LANL Date=090105	M.B.CHADWICK & P.G.YOUNG								
7 ENDF-6 Interpreted σ js Plot JEFF-3.1	E=150MeV Lab=LANL Date=090105	M.B.CHADWICK & P.G.YOUNG								
8 ENDF-6 Interpreted σ js Plot JENDL-5	E=200MeV Lab=TIT, JAERI Date=20090828	Y.HARIMA,H.KITAZAWA,T.FUKAHORI								
9 ENDF-6 Interpreted σ js Plot JENDL-4.0	E=20MeV Lab=TIT, JAERI Date=20090828	Y.HARIMA,H.KITAZAWA,T.FUKAHORI								
10 ENDF-6 Interpreted o js Plot JENDL-3.3	E=20MeV Lab=TIT, JAERI Date=20010713	Y.HARIMA,H.KITAZAWA,T.FUKAHORI								
11 ENDF-6 Interpreted σ js Plot JENDL-3.3	E=20MeV Lab=TIT, JAERI Date=20010713 T=300	Y.HARIMA,H.KITAZAWA,T.FUKAHORI								
12 ENDF-6 Interpreted σ js Plot ENDF/B-VI	E=150MeV Lab=LANL Date=20011108	M.B.CHADWICK & P.G.YOUNG								
13 ENDF-6 Interpreted σ js Plot ENDF/B-VI	E=150MeV Lab=LANL Date=20010926 T=300	M.B.CHADWICK & P.G.YOUNG								
14 ENDF-6 Interpreted σ js Plot BROND-3.1	E=150MeV Lab=LANL,ORNL Date=DIST-DEC06	M.B.Chadwick+,Derrien+								
15 ENDF-6 Interpreted σ js Plot ROSFOND-2010	E=150MeV Lab=IPPE Date=DIST-DEC07	IGNATYUK A.V.								
16 ENDF-6 Interpreted σ js Plot ROSFOND-2008	E=150MeV Lab=IPPE Date=DIST-DEC07	IGNATYUK A.V.								
17 ENDF-6 Interpreted σ js Plot CENDL-3.2	E=20MeV Lab=CNDC Date=20150815	Y.L.HAN								
18 ENDF-6 Interpreted σ js Plot CENDL-3.1	E=20MeV Lab=CNDC,JNDC Date=DIST-DEC09	B.S.YU, S.CHIBA, Y.HARIMA								
19 ENDF-6 Interpreted σ js Plot JEFF-3.0	E=150MeV Lab=LANL Date=DIST-APR02	M.B.CHADWICK & P.G.YOUNG								
20 ENDF-6 Interpreted σ js) Plot JEF-2.2	Lab=ECN Date=920101	EC BLANKET TECHNOLOGY, TASK B2								
21 ENDF-6 Interpreted σ js) Plot JENDL-4.0/HE	E=200MeV Lab=SIT.SHIMZ Date=REV1-	K. Kosako								
22 ENDF-6 Interpreted σ js Plot JENDL/HE-2007	E=3000MeV Lab=SIT.SHIMZ Date=REV1-	K. Kosako								
23 ENDF-6 Interpreted σ js Plot JENDL/HE-2004	E=3000MeV Lab=KAERI Date=REV1-	Y. Lee								
24 ENDF-6 Interpreted σ js) Plot JENDL-3.2	Lab=TIT, JAERI Date=REV2-DEC93	Y.HARIMA,H.KITAZAWA,T.FUKAHORI								

Interactive plotting





Data for plotting: ZVD (637Kb); download ZVView; upload and plot your ZVD file

Other reaction databases

Medical portal (evaluated): https://www-nds.iaea.org/medportal



Medical isotope production



TENDL (Talys Evaluated Nuclear Data Libraries
Stopping powers

Medical Isotope Brov	vser	$\begin{array}{l} \mbox{Examples} & 1 \mbox{Incident} - \mbox{Exit energies} \\ \mbox{2 incident energy} - \mbox{Thickness, and user } \sigma \\ \mbox{3 Energy scan} & \mbox{4 Composite target} \end{array}$	Previous run:		
Product ?	Projectile ? (a) $p \bigcirc D \bigcirc \alpha \bigcirc T \bigcirc {}^{3}He$	Target ? composition	Density [g/cm³] ? blank = default Incident energy scan ? ≤ E ≤ ΔE: Cross section IAEA + TENDL custom		
Thickness [mm] [mg/cm ²]	O Exit energy [MeV] ?	Incident energy [MeV]			
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Medical Isotope Browser

- pick one example to start 1 Incident - Exit energies
- 2 Energy scan
- 3 Composite target
- 4 Incident energy Thickness, and user σ

Other cont'd IBANDL (experimental): https://www-nds.iaea.og/ibandl

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4	¹² C(p,p ₀) ¹² C	170°	1650-1800	31	2019-02-07	X4+	S.M.Duvanov+, JINR-P15-96-69, (1996), »				View Save	mb	n the Resolved-Resonance Region.	the activity has been further supported by the IAEA	
5	¹² C(p,p ₀) ¹² C	170°	700-2500	29	2006-06-22	X4-	E Rauhala Nucl Instrum Methods B12 (1985) 447 »				View Save	- mb	nds contact-point@iaea org (IAEA-)	NDS)	
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7	12C(p,p_0)12C	170°	1600-1790	22	2020-10-07	X4+	R.Salomonovic(1993), Jour. Nucl. Instrum. Methods in	R Salomonoxic(1993) Jour Nucl Instrum Methods in Physics Res. Sect B. Vol.82, p.1, p.				mb	data produced by SigmaCalc up to October 2013 are available for easier access and from SigmaCalc and imported into IBANDL. Users are cautioned however, that the 'on-th'		
8	12C(p.p.)12C	170°	990-3500	78	2019-03-29	X4+	R.Amirikas+(1993). Jour. Nucl. Instrum. Methods in P	hysics R	Res. Sect.B. V	Vol.77. p.110 »	Vew Save	O mb	age of this option.		
9	¹² C(p,p ₀) ¹² C	170°	290-720	24	2020-04-10	X4+	J Liu+(1993), Jour, Nucl. Instrum, Methods in Physics	Res., Se	ect B. Vol.74.	p.439 »	View Save	0"			
10	¹² C(p,p ₀) ¹² C	170°	710-2970	37	2020-04-10	X4+	J.Liu+(1993), Jour. Nucl. Instrum. Methods in Physics	Res., Se	ect B. Vol.74.	p.439 »	View Save	0"	s (mb/sr) can be converted to Ratio-to	p-Rutherford (rr) and vice versa. Press 'Convert units	
11	¹² C(p,p ₀) ¹² C	170°	290-2970	60	2020-04-10	X4 ⁺	J.Liu+(1993), Jour. Nucl. Instrum. Methods in Physics	Res., Se	ect.B. Vol.74,	p.439 »	View Save	0"			
12	12C(p,p_0)12C	170°	340-3000	123	2019-03-29	X4+	S.Mazzoni+(1998), Jour. Nucl. Instrum. Methods in Ph	hysics Re	es., Sect.B. V	oL136-138, p.86 »	View Save	dm			
13	¹² C(p,p ₀) ¹² C	170°	2690-7000	71	2020-04-19	X4 ⁺	D.Abriola+(2011), Jour. Nucl. Instrum. Methods in Phy	ysics Re	es., Sect.B, Vo	ol.269, p.2011 »	View Save	dm	terface. The codes include ERYA, NI	DF, SMNRA and PIGRECO. More details are available	le
14	¹² C(p,p ₀) ¹² C	168.2°	380-4360	180	2020-04-07	X4 ⁺	H.L. Jackson+(1953). Jour. Physical Review. Vol.89, p.	365 »			View Save	dm			
15	12C(p,pn)12C	165.2°	4350-6060	148	2021-12-07	X4+	N.Nikolic+(1963), Physical Review, Vol.132, p.2212 >			¹² C(p,1	00)12C 170.0deg.			- Select data for plotting [all] [none]	
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17	12C(p,p_0)12C	162.6°	4810-5590	25	2010-06-03	X4+	C.W.Reich+(1956), Jour. Physical Review, Vol.104, p.			_ · · · · · · · ·		,		3) 1993,Salomonovic 12C(p,p0)12C 170deg	
18	¹² C(p,p ₀) ¹² C	162°	1600-1790	37	2011-09-02	X4 ⁺	B.Fabre+(1994), Jour. Nuclear Physics, Section A. Vol.		403				402	🛃 4) 1993,Amirikas 12C(p,p0)12C 170deg	
19	¹² C(p,p ₀) ¹² C	160°	1600-1790	22	2020-10-07	X4+	R.Salomonovic(1993), Jour. Nucl. Instrum. Methods in		105	F. 🛔			103	5) 1998,Mazzoni 12C(p,p0)12C 170deg 6) 2011,Abriola 12C(p,p0)12C 170deg	-
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Other cont'd



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Thank you!

