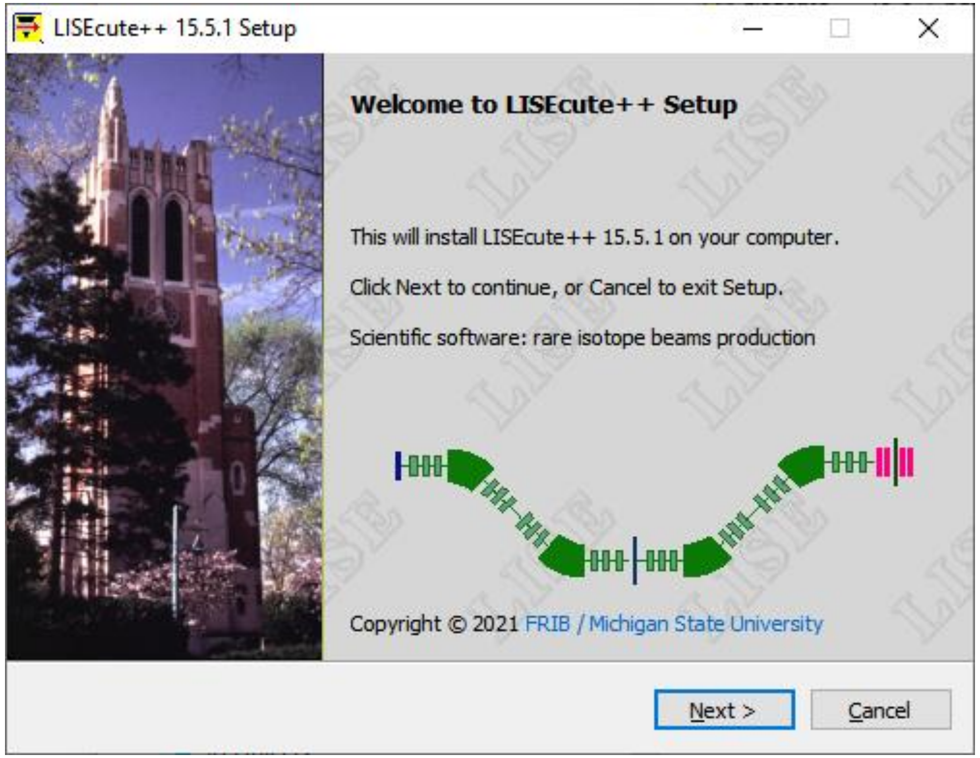
Nuclear Data Needs for LISE^{++}

Oleg B. Tarasov,

FRIB / MSU

@ Workshop for Applied Nuclear Data Activities (WANDA 2021)



Contents

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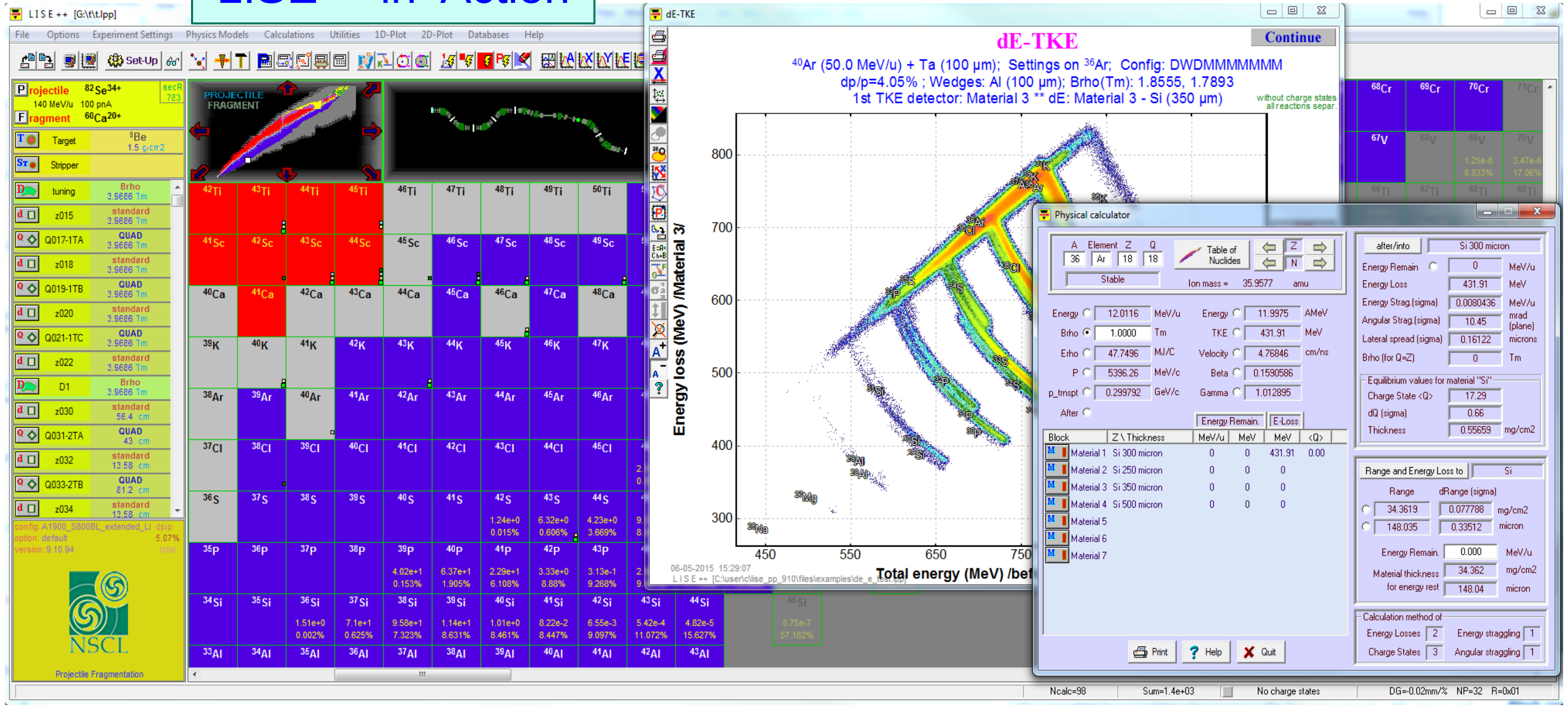
  - LISE^{++} Package
  - Fragment-separator construction
  - Reaction Mechanisms
  - Application
- Databases in LISE^{++}
  - Masses
  - Isomers
  - Ionization energy
  - Experimental cross sections
  - Fission barriers
  - Branch ratios
  - ….
- Needs in detailed information
  - Excitation energy of (fissile) nuclei after abrasion
  - Limiting temperature

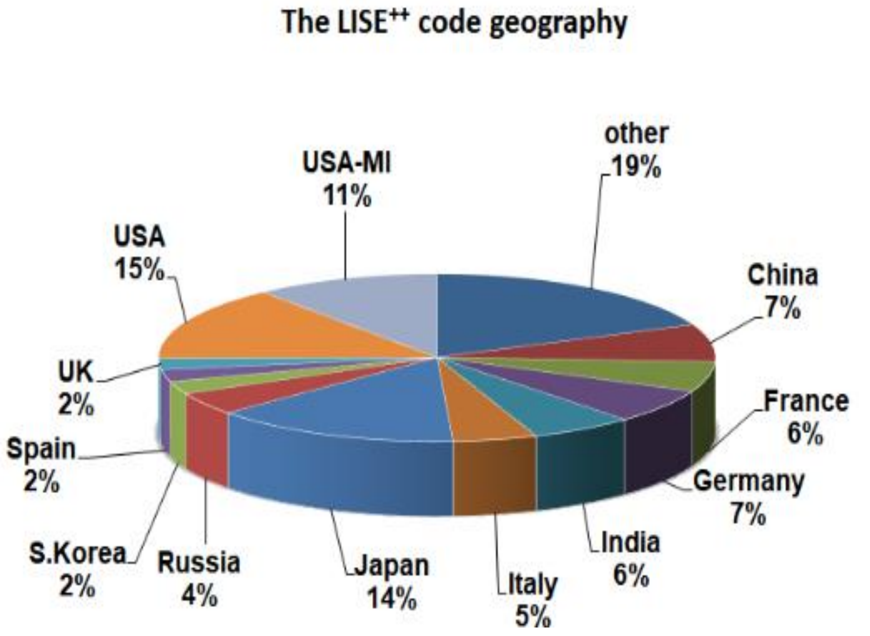
Introduction

- The LISE^{++} program is designed
  - to predict intensities and purities of rare isotope beams for the planning of future experiments with in-flight separators,
  - is also essential for tuning of rare isotope beams where results can be quickly compared to on-line data.
- The LISE^{++} program is widely used

LISE^{++} in Action



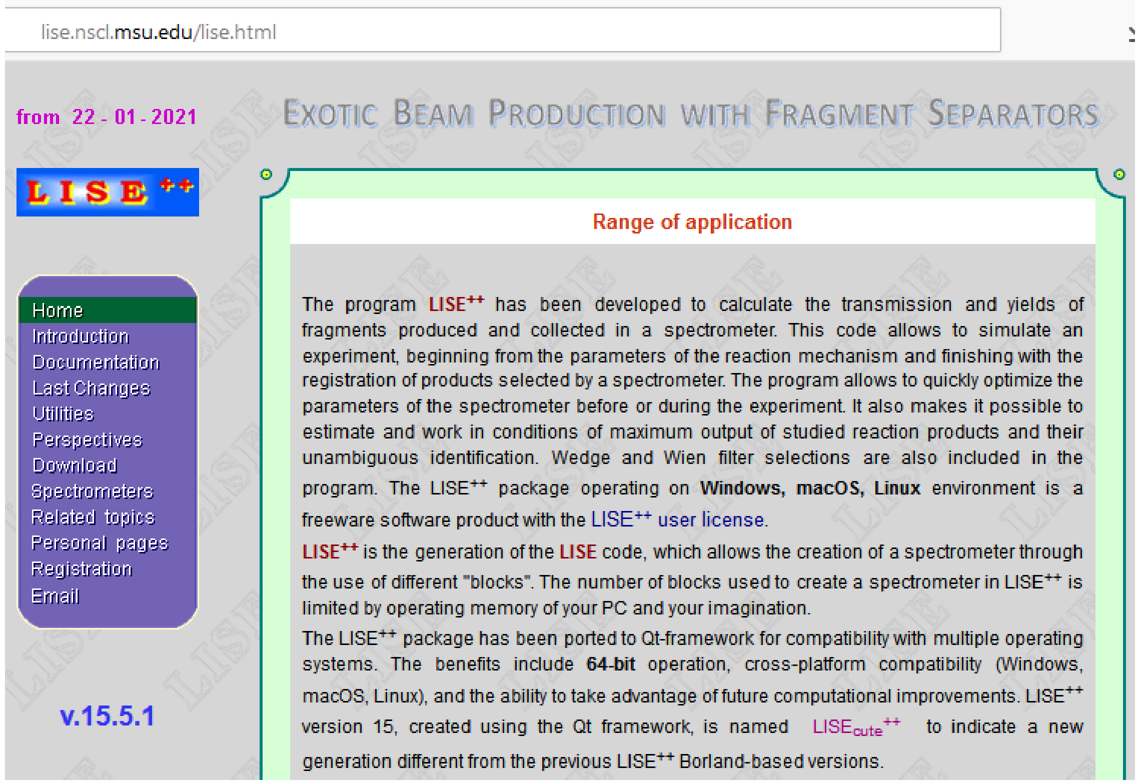
The LISE^{++} code geography



LISE^{++} package

- The LISE^{++} package (including codes PACE4, Global, Charge, MOTER, ETACHA4, GEMINI++, Spectroscopic Calculator) operating on **Windows, macOS, Linux** environment

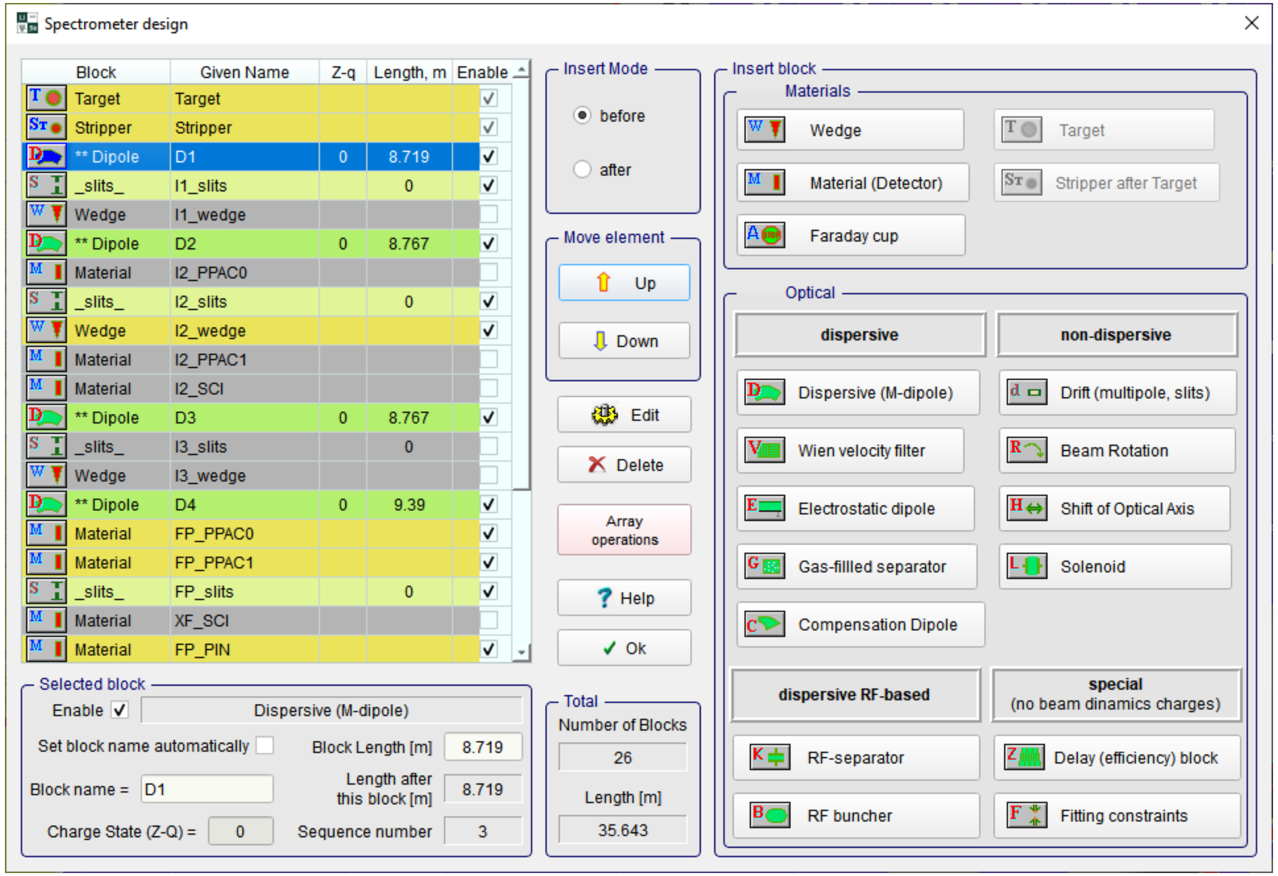
- The LISE^{++} package is maintained by **LISE^{++} group @ Michigan State University** and is freely available and distributable through the LISE^{++} website: <http://lise.nscl.msu.edu>



Fragment Separator Construction and Transmission calculations

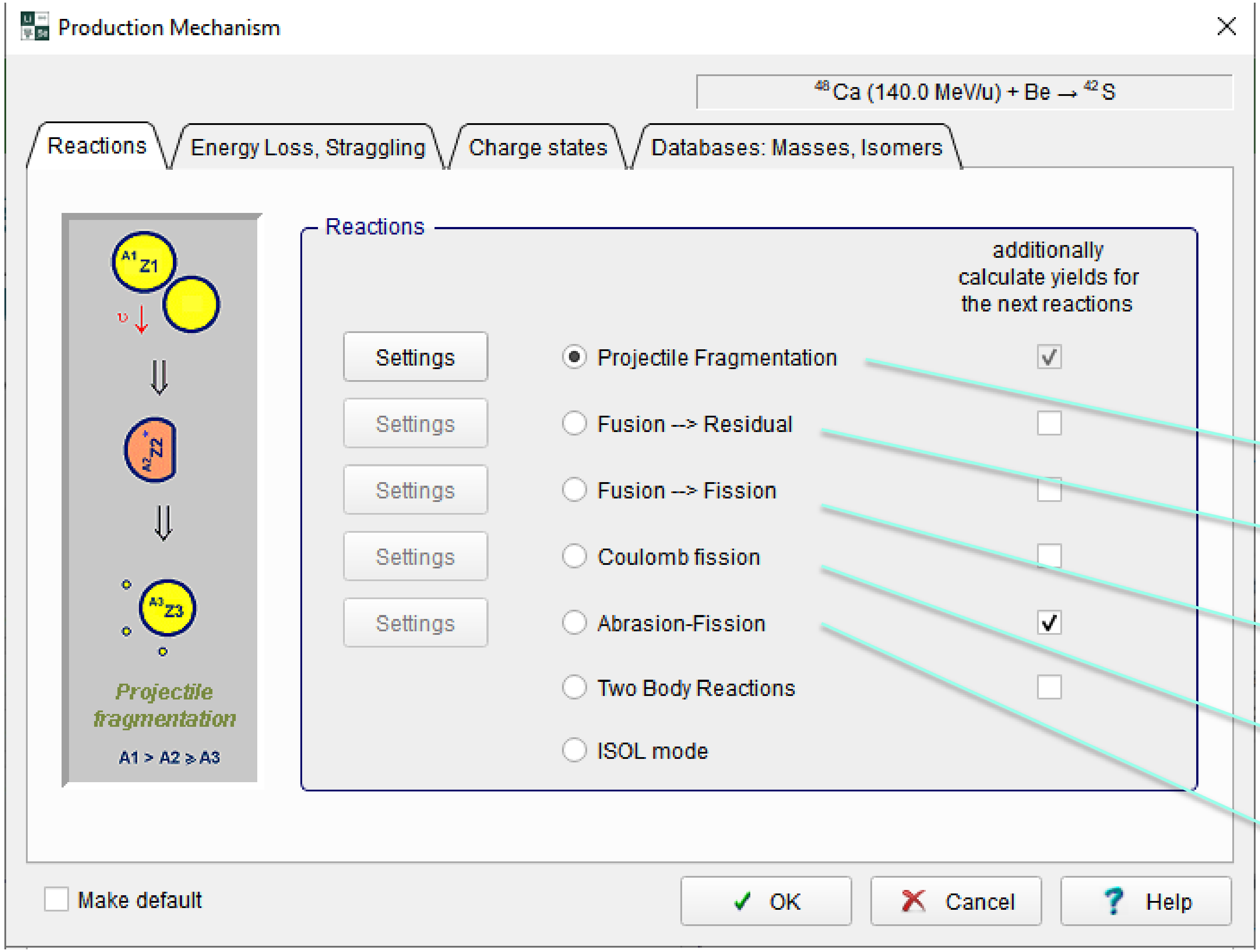
- Spectrometer design with <u>different sections called "blocks"</u>
  (magnetic and electric multipoles, solenoid, velocity filter, RF deflector and buncher, material in beam, drift, and others)

- a <u>user-friendly interface </u>that helps to construct a fragment separator from the different blocks.



- Analytical and Monte Carlo calculation of fragment transmission
- Ion optical calculation up to 2[nd] order (5[th] order use in MC mode)
- Minimization of Ion optic properties

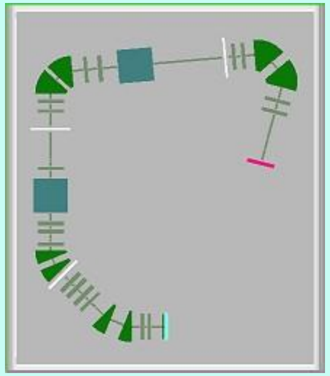
Reaction Mechanisms



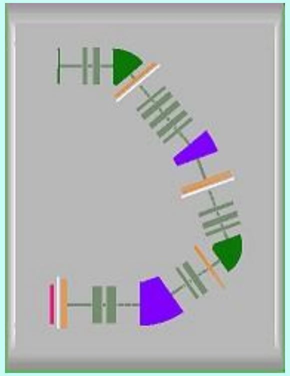
- Not only using classical reaction mechanism models, but actively developing fast and accurate in-house models
- Includes fragment production in materials (wedges, detectors)

			cit-ns
O.B.Tarasov	Analysis of momentum distributions of projectile fragmentation products	NPA 734 (2004) 536-540	35
O.B.Tarasov, D.Bazin	Development of the program LISE: application to fusion–evaporation	NIM B204 (2003) 174-178	92
O.B.Tarasov, A.C.C.Villari	Fusion–fission is a new reaction mechanism to produce exotic radioactive beams	NIM B 266 (2008) 4670-4673	5
O.B.Tarasov	LISE^{++} development: application to low-energy fission of projectiles at realtivistic energies	ENAM2004: EPJ A25 (2005) 751	3
O.B.Tarasov	LISE^{++} development: Abrasion-Fission	Preprint NSCL MSU, MSUCL-1300, 09.2005	

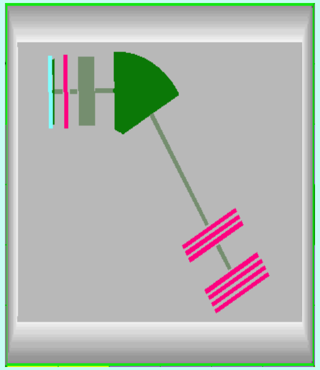
Application Examples



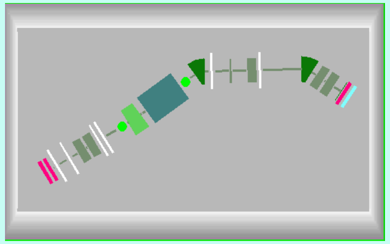
SECAR, *MSU*



DRAGON,
Canada

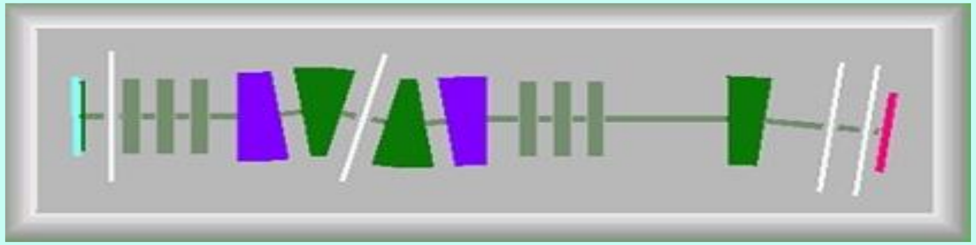


PRISMA,
Italy

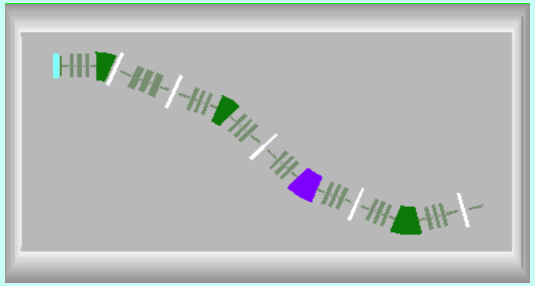


MARS,
TAMU, USA

The LISE^{++} code may be applied at low, medium, and high-energy facilities (fragment- and recoil-separators with electrostatic and/or magnetic selections)

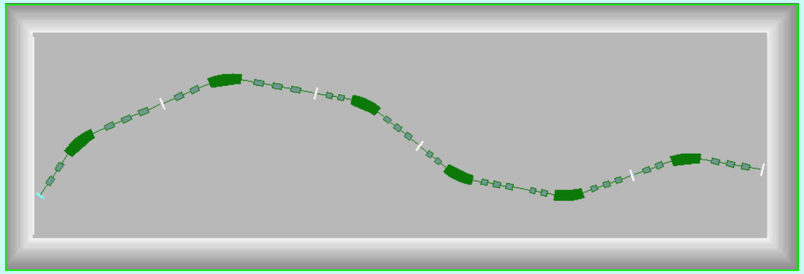


SHELS,
Russia



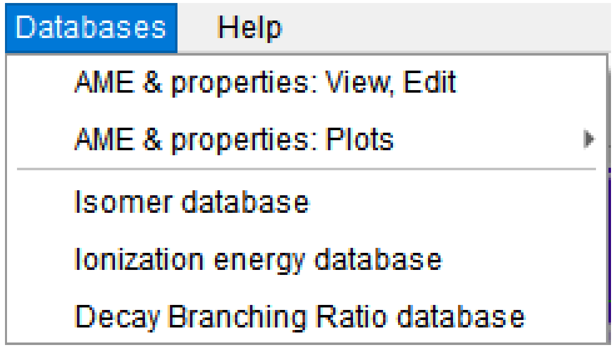
S^3,
France

BigRIPS+ZeroDegree,
Japan



SuperFRS_HEB,
Germany

Databases used (produced) in (with) LISE^{++}

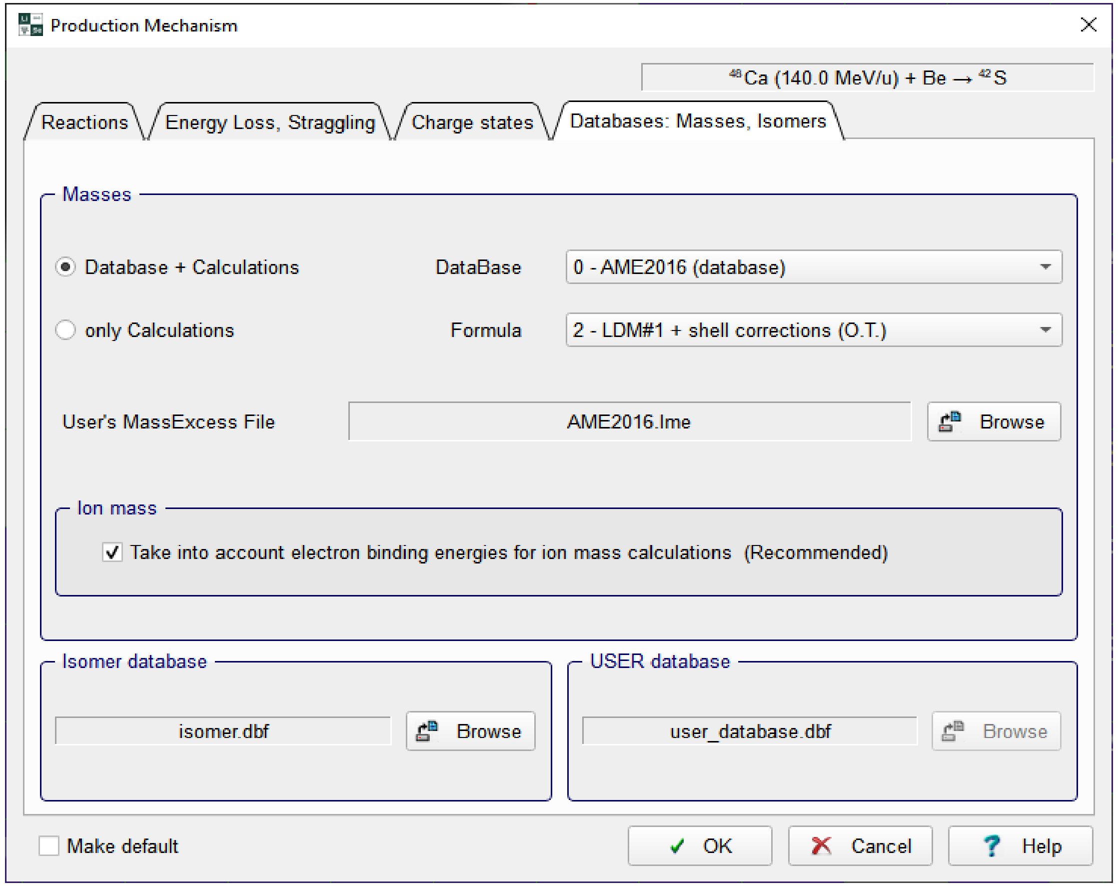


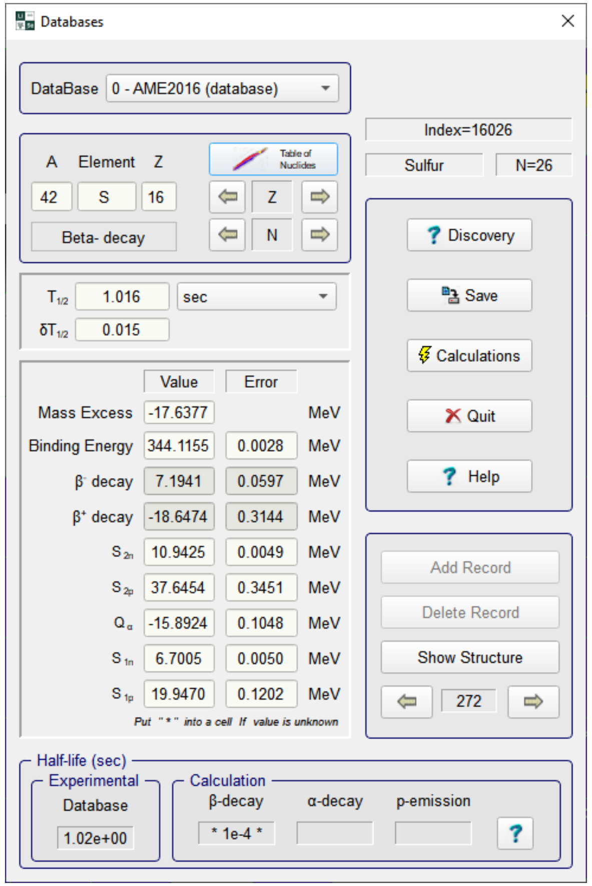
- Atomic Masses 😐
- Ionic Masses ☺
- Isomeric states database ☹
- Fission barrier database 😐
- Experimental production cross sections ☹
- Decay branching ratio database ☹
- Compound material database ☹
- Discovery database 😐

- *Intrinsic datasets (ranges, model parameterization, and so on)*
- Set of separator configurations /LISE/ ☺
- NSCL & FRIB secondary beam rates /LISE/ 😐

Atomic Masses

- Ion mass for **optics settings**, isotope selection
- **Production rates** with built-in reaction models (separation energies for de-excitation cascade calculations in abrasion-ablation, fusion-residues, all fission reactions)
- Half-life calculation, decay analysis
- Plotting isotope properties (energy separation, binding energies, $T_{1/2}$)





LISE++ built-in mass excess files

- AME2003.lme
- AME2011.lme
- AME2016.lme
- FRDM2012.lme
- hfb17.lme
- hfb22.lme
- hfb27.lme
- hfb8.lme
- hfb9.lme
- ktuy.lme
- Moller95.lme
- tuyy.lme
- WS4.lme
- WS4_RBF.lme
- FRIB_mass\SKMS.lme
- FRIB_mass\SKP.lme
- FRIB_mass\SLY4.lme
- FRIB_mass\SV-MIN.lme
- FRIB_mass\UNEDF0.lme
- FRIB_mass\UNEDF1.lme
- RMF_mass\ddme2.lme
- RMF_mass\ddmed.lme
- RMF_mass\ddpc1.lme
- RMF_mass\nl3s.lme

We need more experimental data

Ionization energy database & Ion mass calculator

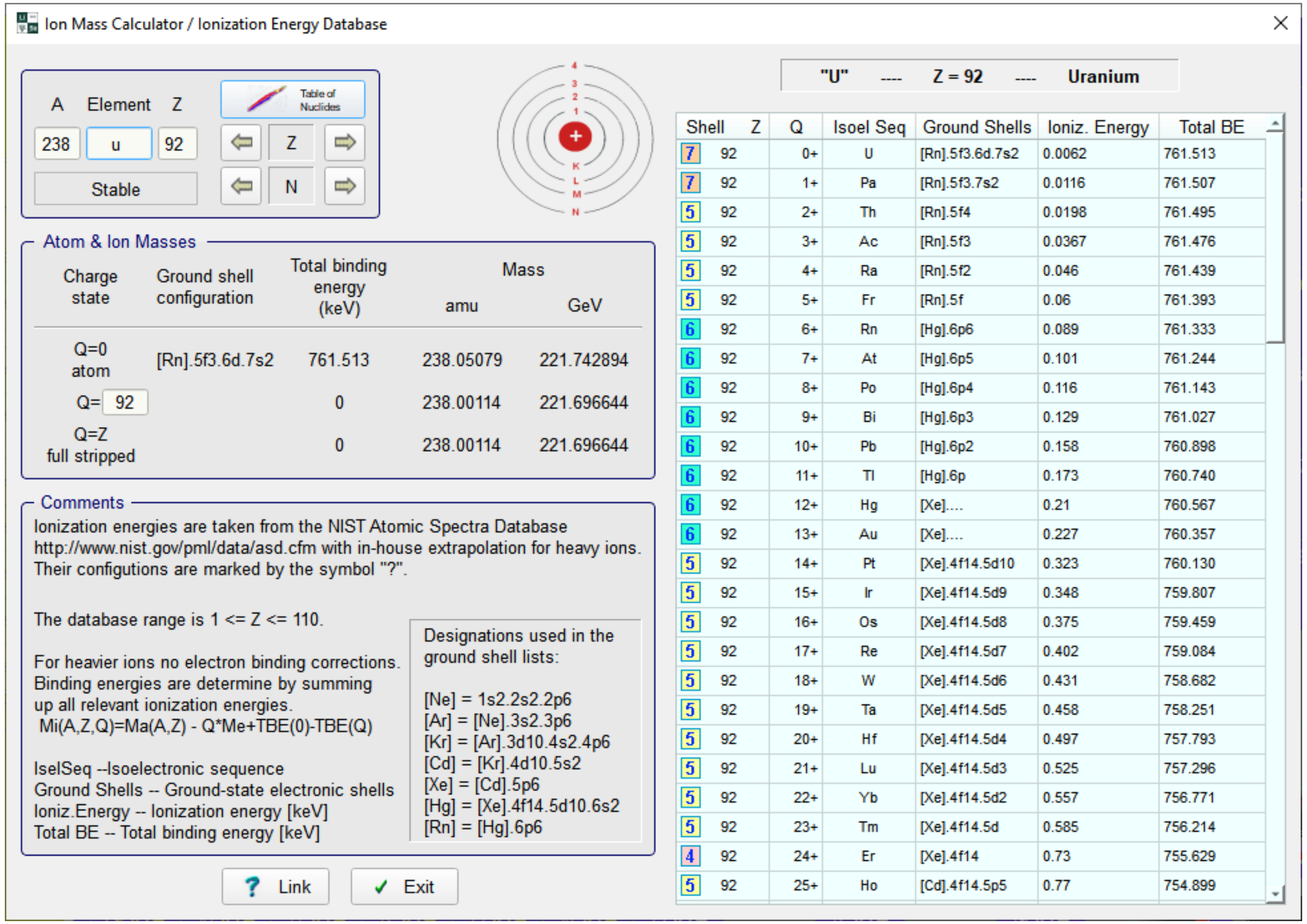
- Ion mass for E-M device precise settings and isotope selection
- Generation of X-ray spectra (in future with ETACHA4)

using

- AME2012 (or other Mass model)
- Ionization Energy Database (NIST Atomic Spectra Database Ionization Energies)

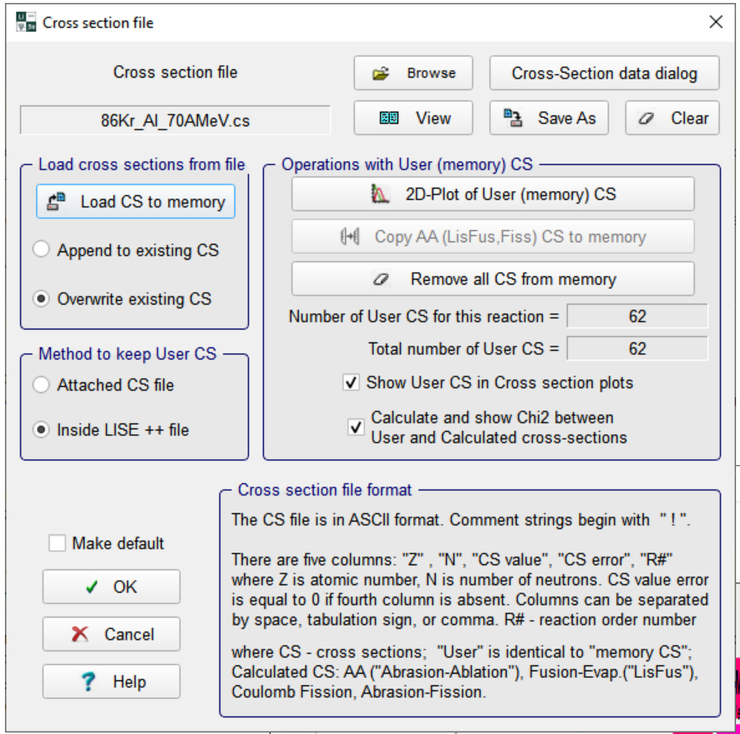
Example: $^{238}U^{92+}$ ion mass

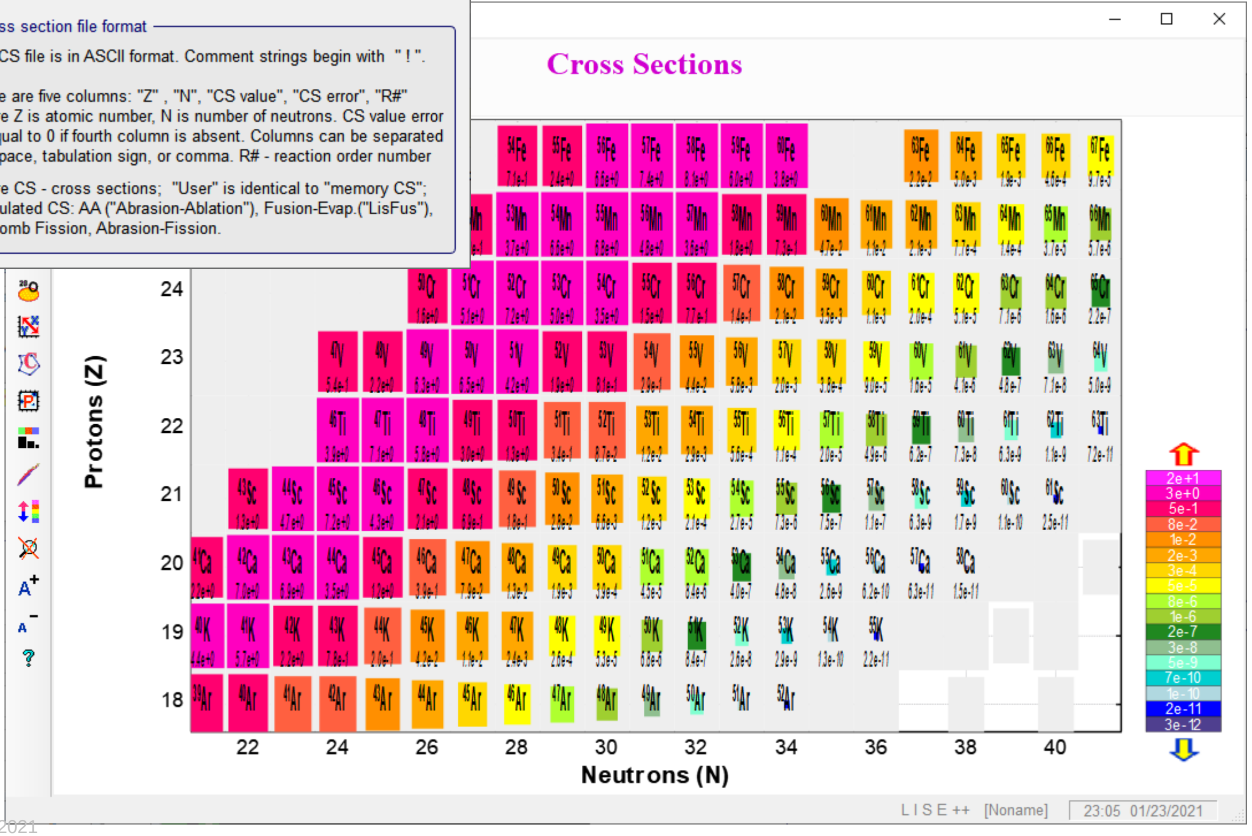
- v.9.8.114 atomic mass was used 238.0508 amu
- v.9.8.117 correction for e- masses 238.0003 amu
- v.9.10.131 correction for e- binding energies 238.0011 amu



Shell	Z	Q	Isoel Seq	Ground Shells	Ioniz. Energy	Total BE
7	92	0+	U	[Rn].5f3.6d.7s2	0.0062	761.513
7	92	1+	Pa	[Rn].5f3.7s2	0.0116	761.507
5	92	2+	Th	[Rn].5f4	0.0198	761.495
5	92	3+	Ac	[Rn].5f3	0.0367	761.476
5	92	4+	Ra	[Rn].5f2	0.046	761.439
5	92	5+	Fr	[Rn].5f	0.06	761.393
6	92	6+	Rn	[Hg].6p6	0.089	761.333
6	92	7+	At	[Hg].6p5	0.101	761.244
6	92	8+	Po	[Hg].6p4	0.116	761.143
6	92	9+	Bi	[Hg].6p3	0.129	761.027
6	92	10+	Pb	[Hg].6p2	0.158	760.898
6	92	11+	Tl	[Hg].6p	0.173	760.740
6	92	12+	Hg	[Xe]....	0.21	760.567
6	92	13+	Au	[Xe]....	0.227	760.357
5	92	14+	Pt	[Xe].4f14.5d10	0.323	760.130
5	92	15+	Ir	[Xe].4f14.5d9	0.348	759.807
5	92	16+	Os	[Xe].4f14.5d8	0.375	759.459
5	92	17+	Re	[Xe].4f14.5d7	0.402	759.084
5	92	18+	W	[Xe].4f14.5d6	0.431	758.682
5	92	19+	Ta	[Xe].4f14.5d5	0.458	758.251
5	92	20+	Hf	[Xe].4f14.5d4	0.497	757.793
5	92	21+	Lu	[Xe].4f14.5d3	0.525	757.296
5	92	22+	Yb	[Xe].4f14.5d2	0.557	756.771
5	92	23+	Tm	[Xe].4f14.5d	0.585	756.214
4	92	24+	Er	[Xe].4f14	0.73	755.629
5	92	25+	Ho	[Cd].4f14.5p5	0.77	754.899

Experimental Production Cross Sections





LISE^{++} built-in cross section files

\129Xe_Al_790AMeV.cs
\136Xe_Al_760AMeV.cs
\208Pb\208Pb_1H_1AGeV_evap.cs
\208Pb\208Pb_1H_1AGeV_fission.cs
\208Pb\208Pb_2H_1AGeV_evap.cs
\208Pb\208Pb_2H_1AGeV_fission.cs
\238U\238U_Be_750AMeV_fission.cs
\238U\238U_d_1AGeV_fission.cs
\238U\238U_d_1AGeV_fragmentation.cs
\238U\238U_p_1AGeV_fission.cs
\238U\238U_p_1AGeV_spallation.cs
\238U\238U_Pb_1AGeV_fission.cs
\238U\238U_Pb_1AGeV_fragmentation.cs
\40Ar_Be_1AGeV.cs
\40Ar_C_240AMeV.cs
\48Ca_Ta_90AMeV.cs
\58Ni_Be_650AMeV.cs
\78Kr_Ni_75AMeV.cs
\82Se_Be_140AMeV.cs
\82Se_W_140AMeV.cs
\86Kr_Al_70AMeV.cs

+ user can enter his own data

- Need more! (installer size?)
- External link?
- Data format
- **Reactions with exotic nuclei**

Compound material database

NSCL FRIB MICHIGAN STATE UNIVERSITY

Compounds

	Common Name	Atomic Stoich.	Density	Cancel
Nuclear physics materials	Aluminum Oxide alpha	Al2 O3	3.98	Input
Plastic-polimers	Bakelite	H9 C9 O1	1.45	Input
Liquids	1-2 – Ethanediol	H6 C2 O2	1.1088	Input
Gases	Acetylene	H2 C2	0.0010825	Input
	Air (gas mixture **)	O21 N78 Ar1	0.001205	
	Allene Propadiene	H4 C3	0.0016656	
	Ammonia	H3 N1	0.00070804	
	Butane	H10 C4	0.0024164	
	1-3-Butadiene	H6 C4	0.0022488	
	Carbon Dioxide	C1 O2	0.0018296	
	Carbon Tetrafluoride	C1 F4	0.0036586	
	Cyclobutane	H8 C4	0.0023326	
	Cyclopropane	H6 C3	0.0017495	
	Cyclopropene	H4 C3	0.0016656	
	1-2 Difluorethane	H4 C2 F2	0.0027459	
	1-2 Difluorethene	H2 C2 F2	0.0026621	
	Ethane	H6 C2	0.0012501	
	Ethane – Hexafluoride	C2 F6	0.0057376	
	Ether Dimethyl	H6 C2 O1	0.0019153	
	Ethylene	H4 C2	0.0011663	
	Ethylene Sulfide	H4 C2 S1	0.0024994	
	Hydrogen Sulfide	H2 S1	0.0014169	
	Methane	H4 C1	0.00066697	
	Methane Chloro-Tri.Freongas	C1 F3 CL1	0.0043427	
	Methane Dichloro-Di. Freon-12	C1 F2 CL2	0.0050268	
	Methane Dichloro-Fl. Freon-21	H1 C1 F1 CL2	0.0042789	
	Nitric Oxide	N1 O1	0.0012475	
	Nitrous Oxide	N2 O1	0.0018298	
	P10 (10% Methane in Argon) **	C2 H8 Ar90	0.00159	
	Propane	H8 C3	0.0018333	
	Propylene Sulfide	H6 C3 S1	0.0030826	
	Sulfur Hexafluoride	F6 S1	0.006072	
	Water vapor	H2 O1	0.00074895	

Gas density

H10C4

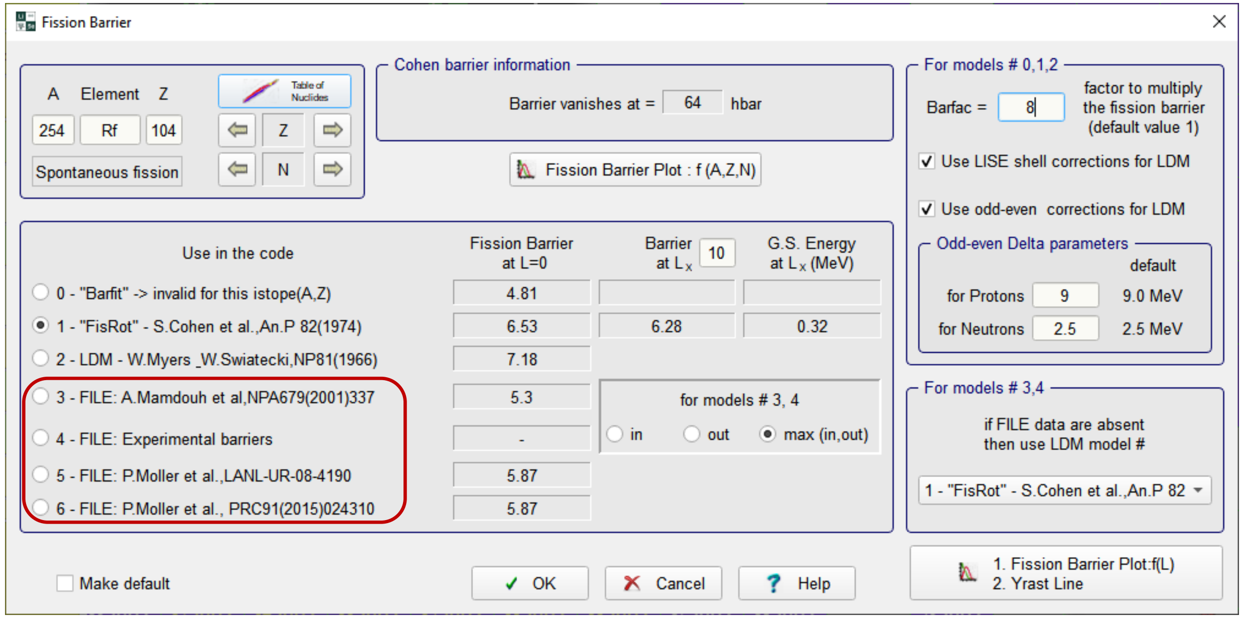
(•) Molecular formula

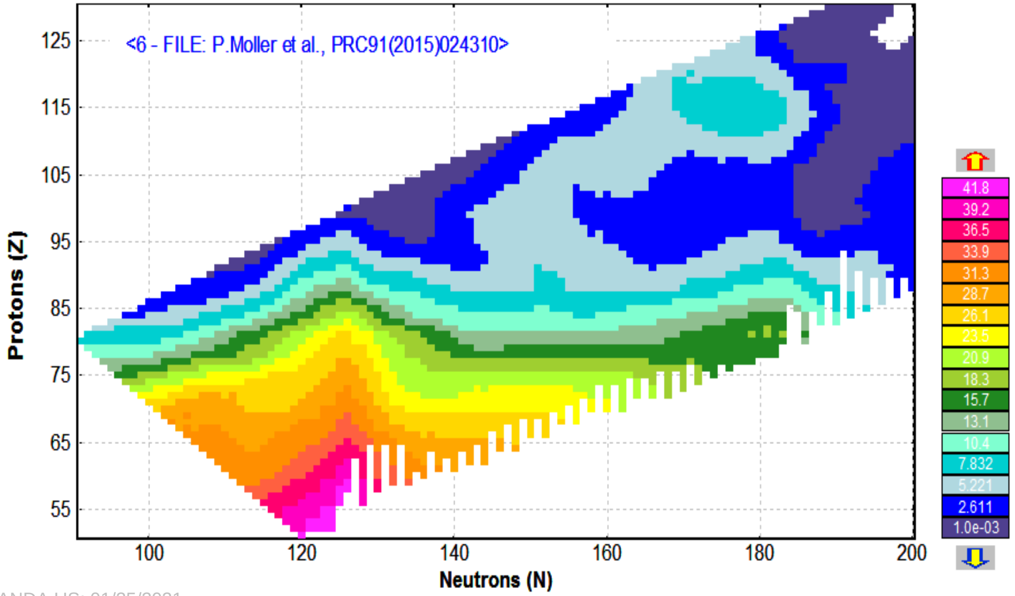
( ) Gas mixture

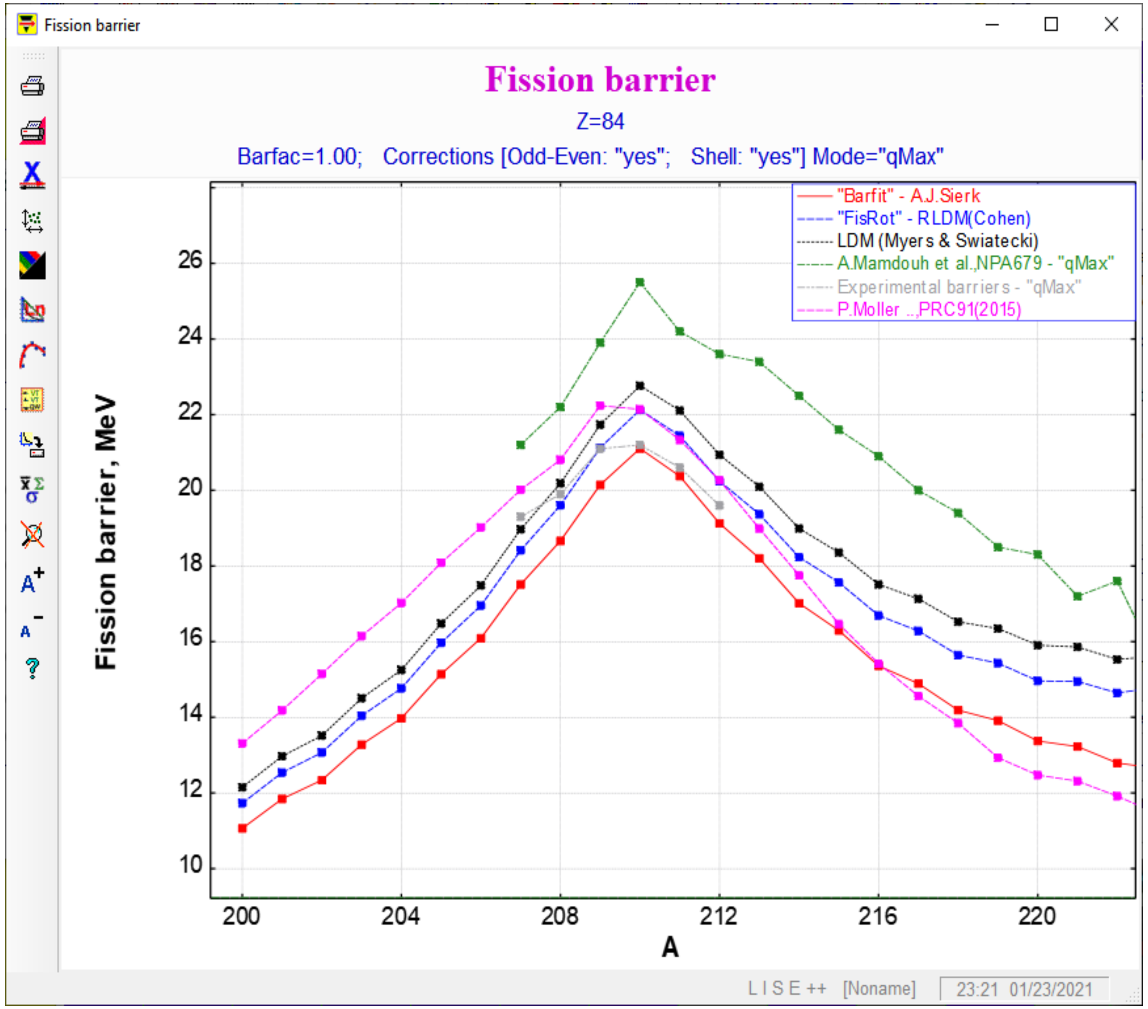
Parameter	Value		Dimension
Temperature (K)	293.15		K
Pressure (Torr)	760	760	Torr
Density	2.4164	2.4164	mg/cm^3 kg/m^3 g/L

Units converte | ✓ Fix | Cancel

Fission barriers (4 databases : 3 theory + 1 experiment)







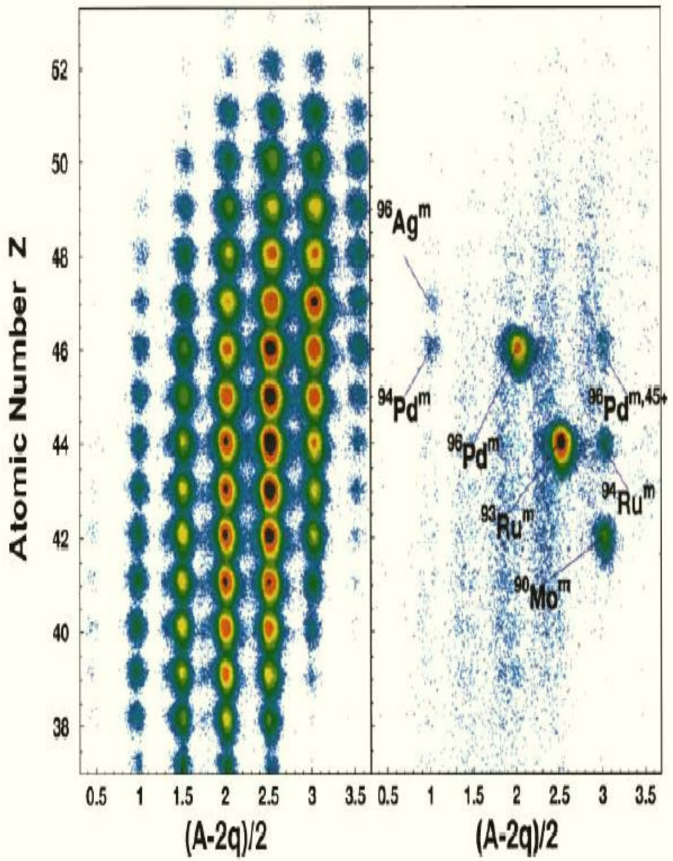
Simulation of coincidence fragments and isomer gamma-lines

Experiment

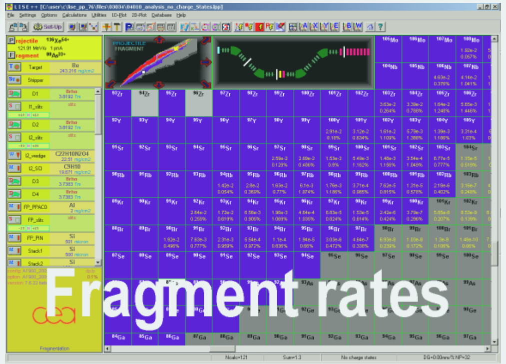
PHYSICAL REVIEW C VOLUME 55, NUMBER 3 MARCH 1997

New μs isomers in T_z=1 nuclei produced in the ^{112}Sn(63.4 MeV)+^{nat}Ni reaction

R. Grzywacz,[1,2] R. Anne,[2] G. Auger,[2] C. Borcea,[3] J. M. Corre,[2] T. Dörfler,[4] A. Fomichov,[5] S. Grevy,[6] H. Grawe,[7] D. Guillemaud-Mueller,[6] M. Huyse,[8] Z. Janas,[7] H. Keller,[7] M. Lewitowicz,[2] S. Lukyanov,[5,2] A. C. Mueller,[6] N. Orr,[9] A. Ostrowski,[2] Yu. Penionzhkevich,[5] A. Piechaczek,[8] F. Pougheon,[6] K. Rykaczewski,[1,10] M.G. Saint-Laurent,[2] W. D. Schmidt-Ott,[4] O. Sorlin,[6] J. Szerypo,[1] O. Tarasov,[5,2] J. Wauters,[8] J. Żylicz[1]

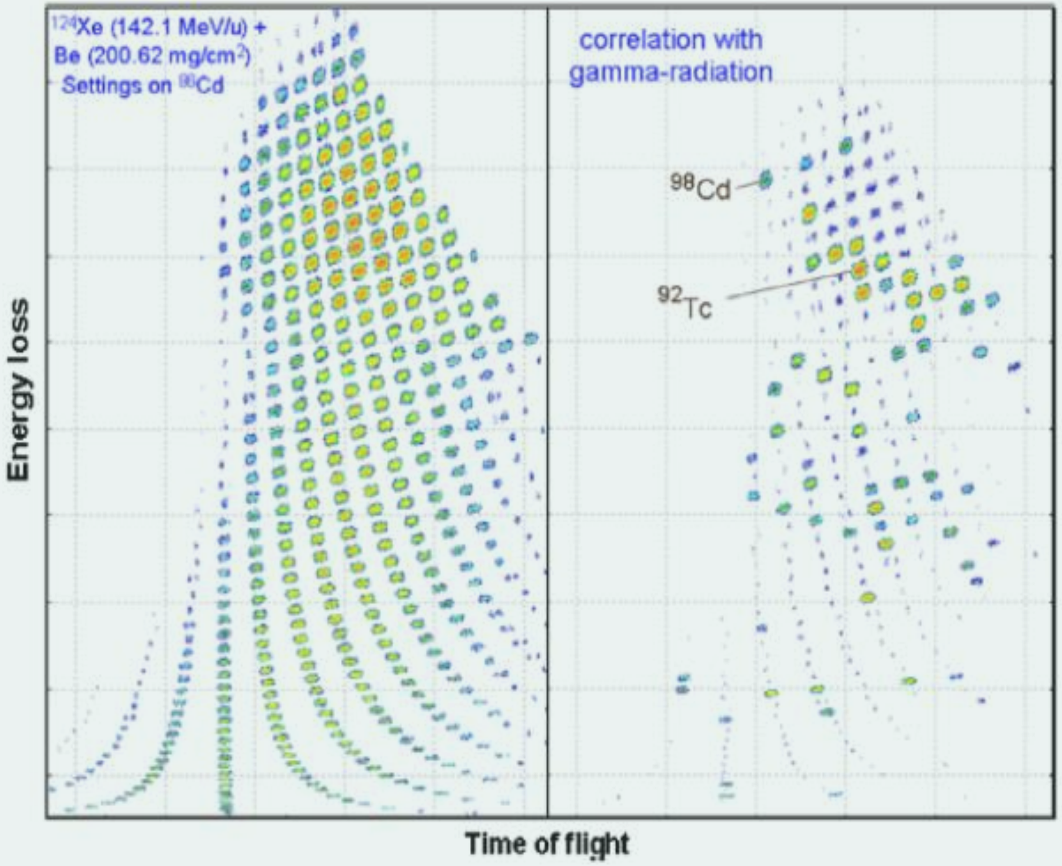


LISE^{++} simulations

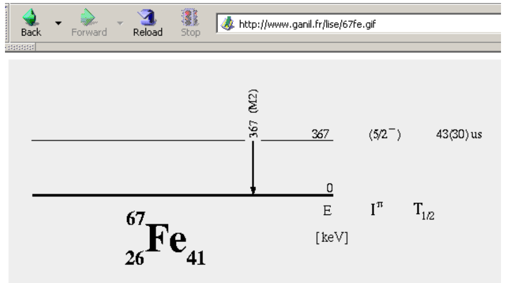


LISE^{++}
γ–database

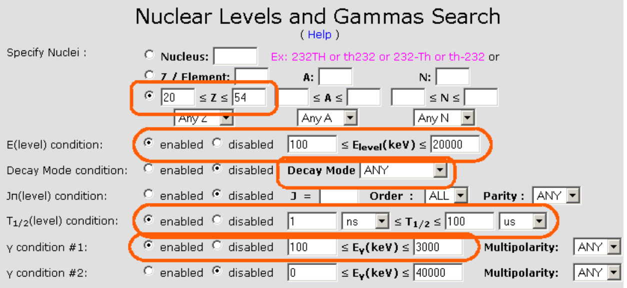
γ–registration settings



LIFE++ isomer database



Old GANIL database
available through LISE



Internet database (NNDC)
region of stable isotopes

Eperiment	Isomer	Ex. Energy (keV)	γ-energies (keV)	Half-life (μs)
03034	59Cr	503	193	96
"	64Mn	135	?	>100
"	65Fe	364	?	0.430
"	67Fe	367	?	64
"	66Co	175	?	1.21
"	66Co	648	?	>100
"	69Ni	2701	148	0.439
"	70Ni	2860	183	0.232
"	72Cu	270	?	1.76
"	78Zn	2673	?	0.319
"	88Br*	273	111; 159	5.4
"	93Rb*	254	254 and 266 from 2ns level	57
"	97Sr*	308	141; 167	0.170
"	97Sr*	830	523	0.255
"	98Y*	171	50; 171	0.62
"	98Y*	496	50; 121; 170; 204	7.6
"	98Y*	1181	111; 119; 130; 158; 186; 476; 596	0.83
"	99Y*	2141	28; 126; 159; 198; 223; 245; 269; 273; 283; 546; 882; 1166; 1435; 1529	8.6
"	107Mo	66	66	0.470
"	117Ru	?	184	> 5
"	121Pd	?	136	0.694
"	123Ag	?	349; 384; 391; 630; 386; 714; 733; 769; 1049; 1077; 1133	0.214
"	124Ag	?	156; 1132	1.9
"	125Ag	?	670; 684; 715; 729	0.310
"	125Cd	?	409; 720; 743; 786; 868; 922	> 5
"	126Cd	?	220; 248; 402; 405; 652; 807; 815; 856	0.270
"	127Cd	?	739; 771; 821; 909	1.9
"	129In	?	334; 359	2.9
05028	117Ru	?	184	> 5
"	121Pd*	?	136	0.694
"	123Ag*	?	349; 384; 391; 630; 386; 714; 733; 769; 1049; 1077; 1133	0.214
"	124Ag*	?	156; 1132	1.9
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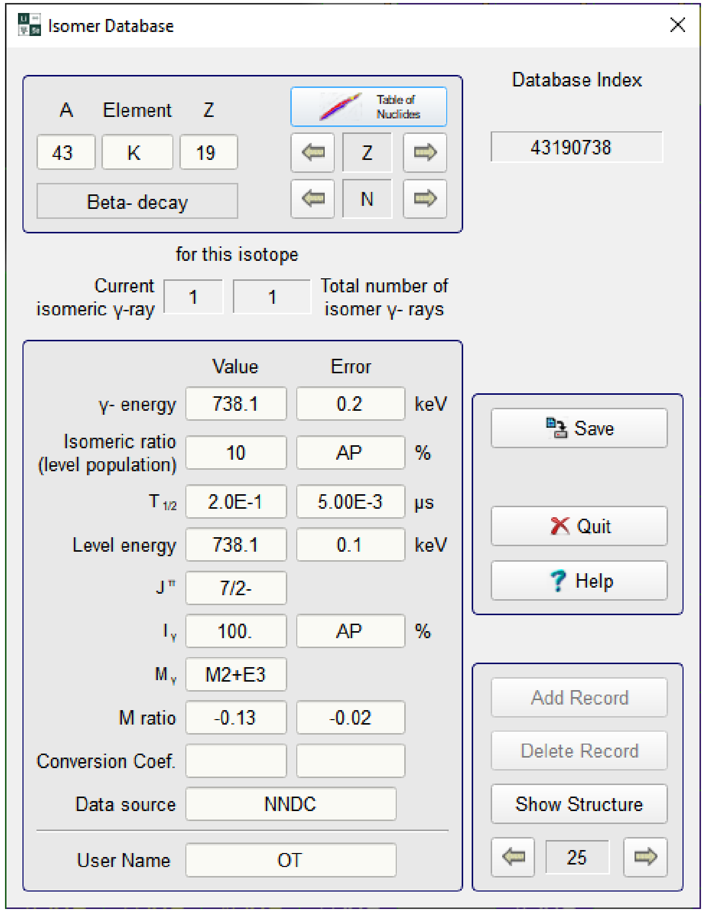
"	127Cd	?	739; 771; 821; 909	1.9
"	129In	?	334; 359	2.9

Private communications

LISE++ database
(dbf-format)

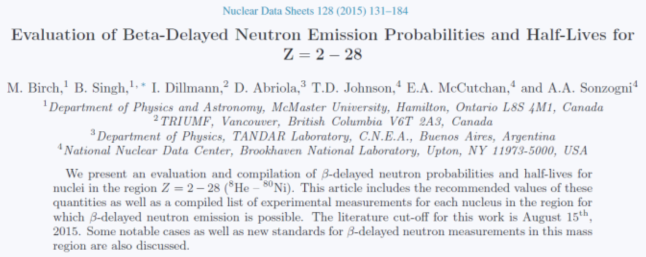
New experimental data



- Need more experimental data! (updated with recent RIKEN data)

Decay branching ratio vs. Radiation Residue calculation

P_n for $2 \le Z \le 28$ are taken from


Nuclear Data Sheets 128 (2015) 131–184

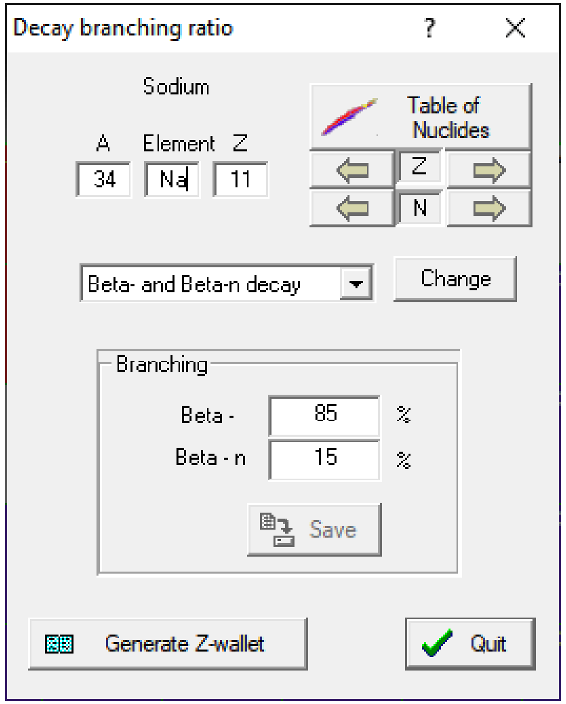
Evaluation of Beta-Delayed Neutron Emission Probabilities and Half-Lives for Z = 2 – 28

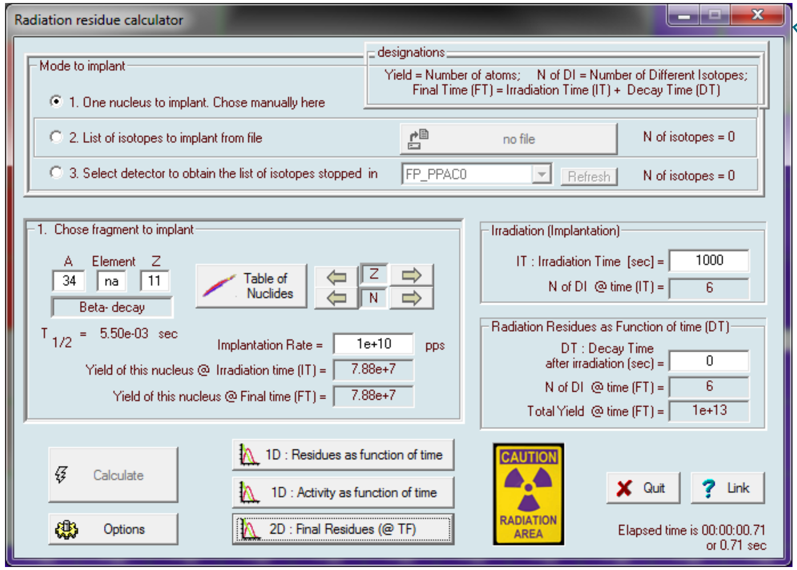
M. Birch,[1] B. Singh,[1,*] I. Dillmann,[2] D. Abriola,[3] T.D. Johnson,[4] E.A. McCutchan,[4] and A.A. Sonzogni[4]
[1] Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada
[2] TRIUMF, Vancouver, British Columbia V6T 2A3, Canada
[3] Department of Physics, TANDAR Laboratory, C.N.E.A., Buenos Aires, Argentina
[4] National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

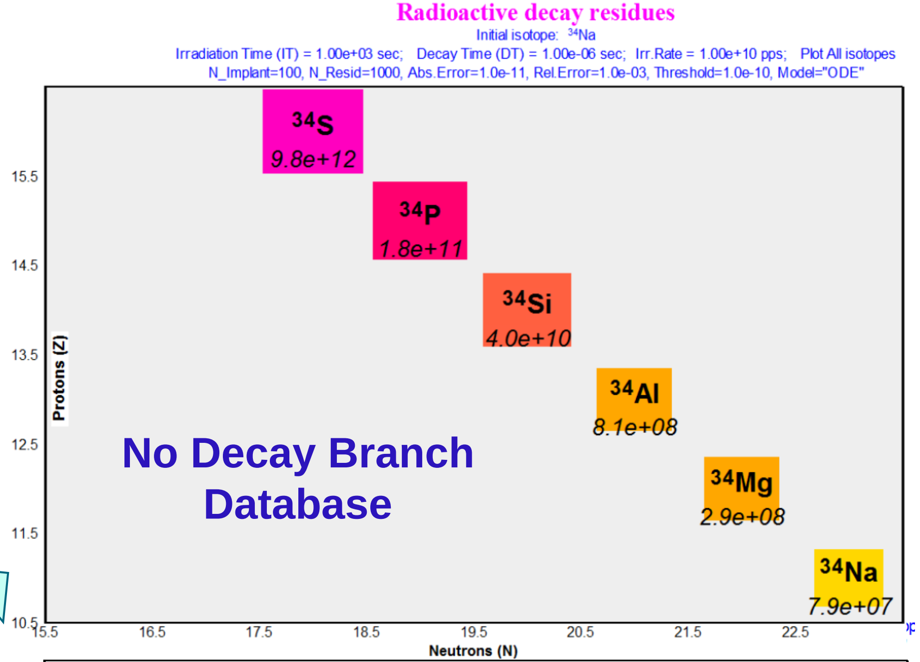
We present an evaluation and compilation of β-delayed neutron probabilities and half-lives for nuclei in the region Z = 2 – 28 (^{8}He – ^{80}Ni). This article includes the recommended values of these quantities as well as a compiled list of experimental measurements for each nucleus in the region for which β-delayed neutron emission is possible. The literature cut-off for this work is August 15th, 2015. Some notable cases as well as new standards for β-delayed neutron measurements in this mass region are also discussed.

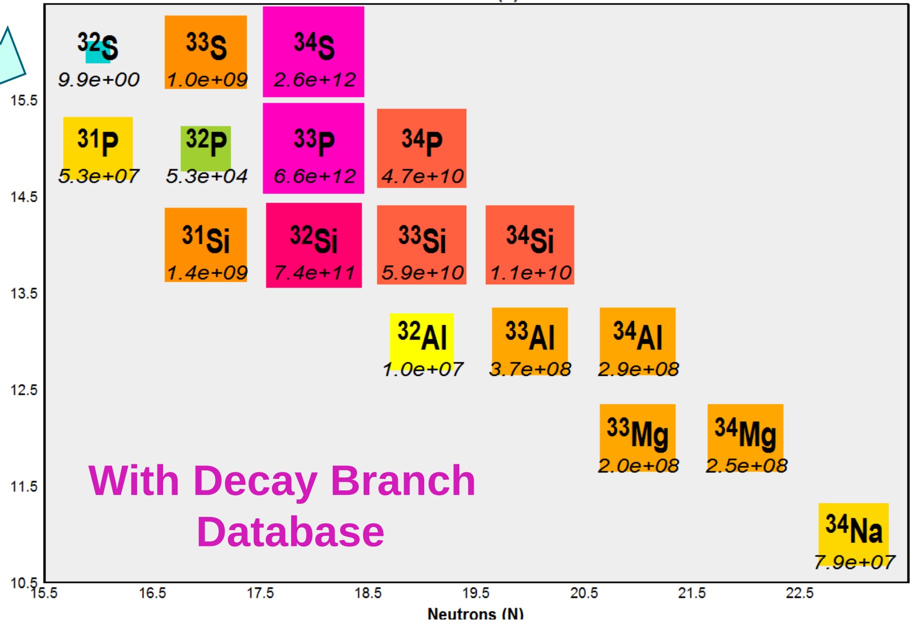
Other branching ratios and P_n for $38 \le Z$ are taken from NNDC

Ratios for higher Z will be entered soon.









Link to the Nuclides discovery database

Database information: 129Sm

Save As | Print | LISE database | Decay analysis | Branching ratio | Z-wallet NNDC | A, Z NNDC | A, Z JAEA-14 | TOrI (Se) | Wiki: Sm (Z=62) | Discovery

^{129}Sm Beta+ decay (Z=62, N=67) Samarium

it is useful for experiment planning how nucleus has been discovered: beam, target, reaction, energy, location.

https://people.nscl.msu.edu/~thoennes/isotopes/abstracts/62-samarium/62-Sm-129.pdf

https://people.nscl.msu.edu/~thoennes/isotopes/

Discovery of Nuclides Project

Michael Thoennessen

News: 280Ds discovered

January 23, 2021

Yesterday, the first isotope of 2021 was discovered. Samark-Roth et al. reported the first observation of 280Ds in the paper "Spectroscopy along Flerovium Decay Chains: Discovery of 280Ds and an Excited State in 282Cn" in Phys. Rev. Lett. 126 (2021)

Video

- 2012 Timeline Movie
- 2015 Timeline Movie
- 2018 Timeline Movie

Other links

^{129}Sm

Xu et al. first identified ^{129}Sm in 1999 and reported the results in "New β-delayed proton precursors in the rare-earth region near the proton drip line" [1]. A 165 MeV ^{36}Ar beam was accelerated with the Lanzhou sector-focused cyclotron and bombarded an enriched ^{96}Ru target. Proton-γ coincidences were measured in combination with a He-jet type transport system. "A 134-keV γ line found in the proton coincident $\gamma(x)$-ray spectrum in the ^{36}Ar+^{96}Ru reaction was assigned to the γ-ray transition between the lowest-energy 2^+ state and 0^+ ground state in the 'daughter' nucleus ^{128}Nd of the βp precursor ^{129}Sm."

[1] S.-W. Xu *et al.*, Phys. Rev. C 60 (1999) 061302.

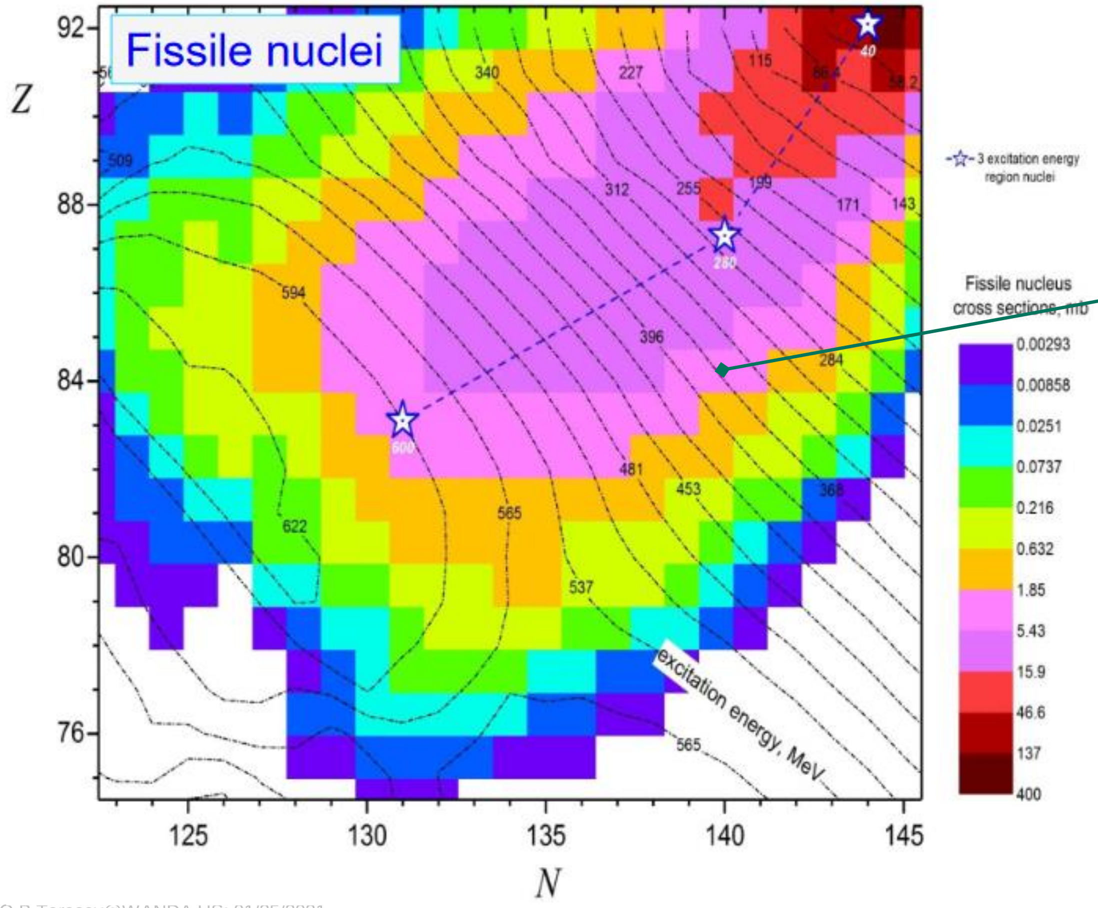
Adapted from E. May and M. Thoennessen, At. Data Nucl. Data Tables **99** (2013) 1

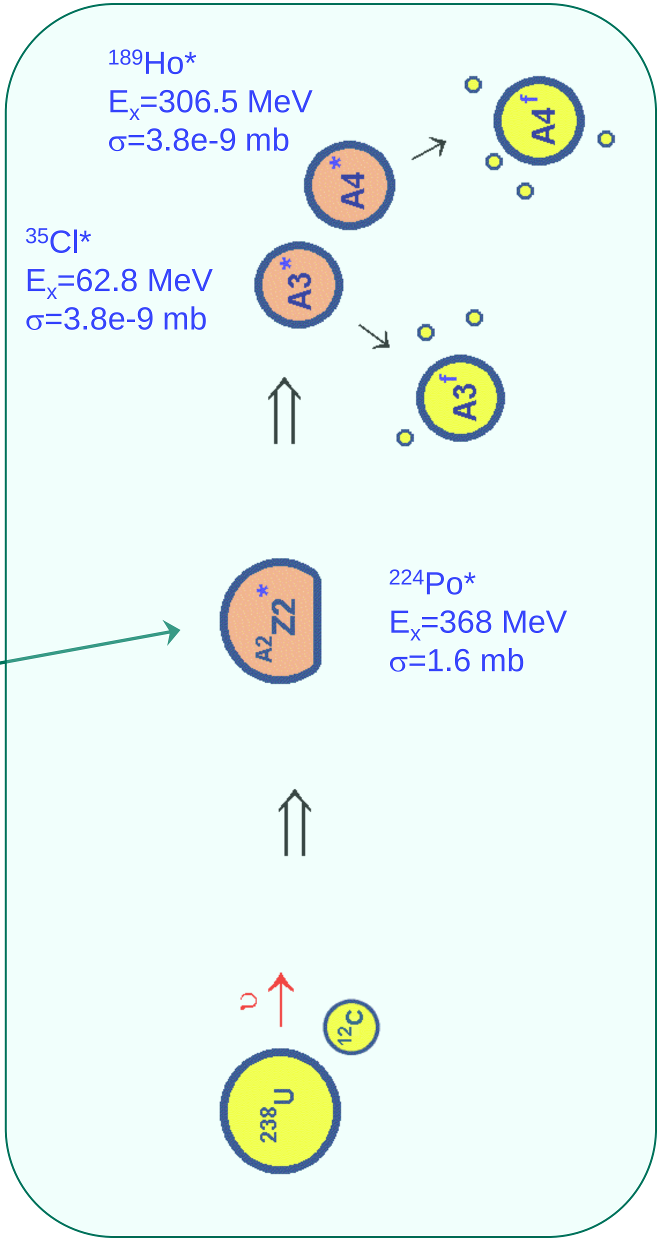
Excitation energy of (fissile) nuclei after abrasion

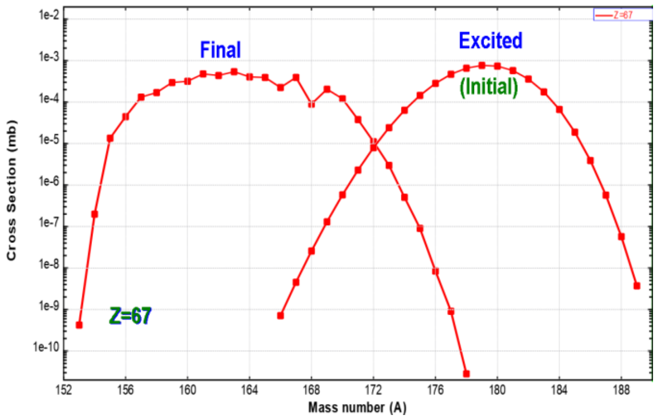
❖ Needs in detailed information

LISE++ Abrasion-Ablation model calculation

- Fissile nuclei after abrasion of ^{238}U by ^{12}C target
- Colors : cross-section
- Contours : excitation energy







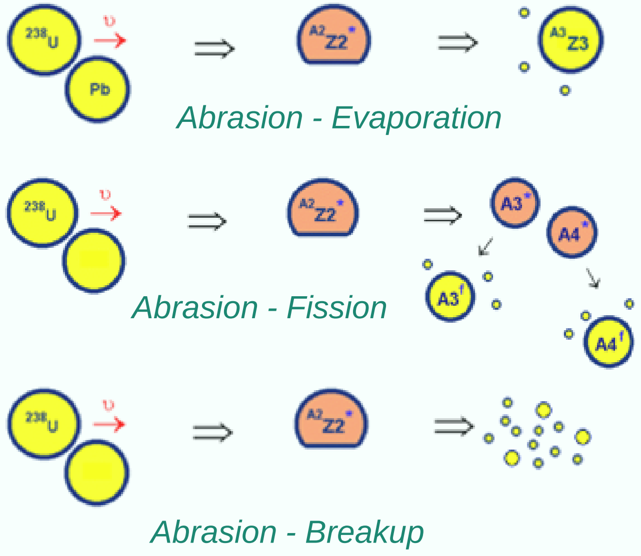
Decreasing excitation energy by 10% shifts ^{189}Ho de-excitation distribution by ~1.3 neutrons

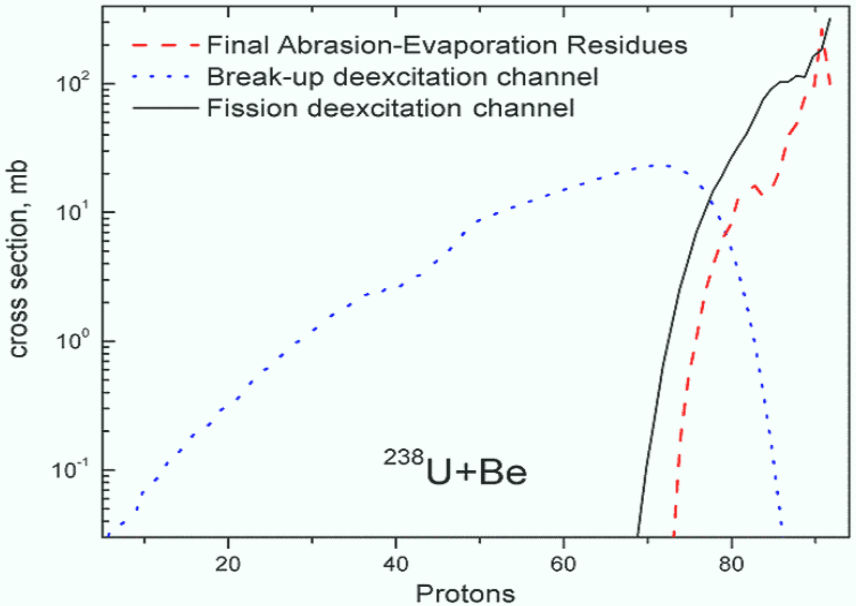
Excitation energy variation makes large impact in high-Z neutron-rich production cross-sections

Experimental data measurement (cross sections, neutron multiplicity?) and theoretical study are required to obtain an excitation energy function in order to improve fast Abrasion-Fission models.

Limiting temperature

❖ Needs in detailed information





The “limiting” temperature defines the breakup stage (multifragmentation)

LISE^{++} Abrasion-Ablation uses T=f(A)

Break-up parameters

The limiting temperature calculated from the curve based on three points for masses 50,150,250

Default values from Zi.Li & M.Liu, PRC69, 034615 (2004), Fig.5

T (A=050)=	8	8.0
T (A=150)=	5.9	5.9
T (A=250)=	4.7	4.7
Diffuseness=	0.05	0.05

GSI Abra-Abla uses T=f(Z,<N/Z>)

Determination of the Freeze-Out Temperature by the Isospin Thermometer

P. Napolitani, et al., Physics of Atomic Nuclei volume 66, pages1471–1477(2003)

- ❑ Experimental study of abrasion mechanism:
  - measurement of fragment production cross section for all channels
  - excitation energy determination
  - temperature determination
- ❑ Theoretical study

LISE^{++} data needs summary

Data

- Atomic Masses 😐
- Isomeric states database ☹
- Fission barrier database 😐
- Experimental production cross sections ☹ *Reactions with exotic nuclei*
- Experimental fragment momentum distributions ☹

Needs for detailed information

- Excitation energy of (fissile) nuclei after abrasion
- Limiting temperature