Nuclear Data Needs for LISE++

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Contents

❖ Introduction
  o LISE++ Package
  o Fragment-separator construction
  o Reaction Mechanisms
  o Application

❖ Databases in LISE++
  o Masses
  o Isomers
  o Ionization energy
  o Experimental cross sections
  o Fission barriers
  o Branch ratios
  o ....

❖ Needs in detailed information
  o Excitation energy of (fissile) nuclei after abrasion
  o Limiting temperature
The LISE++ program is designed to predict intensities and purities of rare isotope beams for the planning of future experiments with in-flight separators, and 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...
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>
- Spectrometer design with different sections called "blocks" (magnetic and electric multipoles, solenoid, velocity filter, RF deflector and buncher, material in beam, drift, and others)

- A user-friendly interface 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)
Application Examples

The LISE++ code may be applied at low, medium, and high-energy facilities (fragment- and recoil-separators with electrostatic and/or magnetic selections)
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, $T_{1/2}$)

We need more experimental data

LISE++ built-in mass excess files

AME2003.lme
AME2011.lme
AME2016.lme
FRDM2012.lme
hf17.lme
hf22.lme
hf27.lme
hf8.lme
hf9.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\n13s.lme
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: $^{238}\text{U}^{92+}$ 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
Experimental Production Cross Sections

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

LISE++ built-in cross section files

- Need more! (installer size?)
- External link?
- Data format
- Reactions with exotic nuclei
### Compound material database

#### Compounds

<table>
<thead>
<tr>
<th>Common Name</th>
<th>Atomic Stoch.</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Nuclear physics materials</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aluminum Oxide alpha</td>
<td>Al2 O3</td>
<td>8.98</td>
</tr>
<tr>
<td><strong>Plastic polymers</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Butylate</td>
<td>H9 C9 O1</td>
<td>1.15</td>
</tr>
<tr>
<td><strong>Liquids</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-2 - Ethanol</td>
<td>H6 C2 O2</td>
<td>1.1086</td>
</tr>
<tr>
<td><strong>Gases</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acetylene</td>
<td>N2 C2</td>
<td>0.0910828</td>
</tr>
<tr>
<td>Air (gas mixture ***)</td>
<td>O2 H78 Ar1</td>
<td>0.001205</td>
</tr>
<tr>
<td>Allene Propadiene</td>
<td>H4 C3</td>
<td>0.0016856</td>
</tr>
<tr>
<td>Ammonia</td>
<td>N3 H1</td>
<td>0.00070004</td>
</tr>
<tr>
<td>Butane</td>
<td>H10 C4</td>
<td>0.0024164</td>
</tr>
<tr>
<td>1,3-Dimadiene</td>
<td>H6 C4</td>
<td>0.0022400</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>C1 O2</td>
<td>0.0018256</td>
</tr>
<tr>
<td>Carbon Tetrafluoride</td>
<td>C1 F4</td>
<td>0.0036886</td>
</tr>
<tr>
<td>Cyclobutane</td>
<td>H8 C4</td>
<td>0.0023326</td>
</tr>
<tr>
<td>Cyclopropane</td>
<td>H6 C3</td>
<td>0.0027495</td>
</tr>
<tr>
<td>Cyclopentene</td>
<td>H5 C3</td>
<td>0.0026506</td>
</tr>
<tr>
<td>1,2 Difluorohene</td>
<td>H4 C2 F2</td>
<td>0.0007409</td>
</tr>
<tr>
<td>1,2 Difluorethane</td>
<td>H2 C2 F2</td>
<td>0.00024621</td>
</tr>
<tr>
<td>Ethane</td>
<td>H6 C2</td>
<td>0.0012501</td>
</tr>
<tr>
<td>Ethane - Hexafluoride</td>
<td>C2 F6</td>
<td>0.0007376</td>
</tr>
<tr>
<td>Ether Dimethyl</td>
<td>H6 C2 O1</td>
<td>0.0019153</td>
</tr>
<tr>
<td>Ethylene</td>
<td>N2 C2</td>
<td>0.0011663</td>
</tr>
<tr>
<td>Ethylene Sulfide</td>
<td>H4 C2 S1</td>
<td>0.0024964</td>
</tr>
<tr>
<td>Hydrogen Sulfide</td>
<td>H2 S1</td>
<td>0.0014149</td>
</tr>
<tr>
<td>Methane</td>
<td>H4 C1</td>
<td>0.00066687</td>
</tr>
<tr>
<td>Methane Chloro-Trifluoromethane</td>
<td>C1 F3 Cl1</td>
<td>0.0043427</td>
</tr>
<tr>
<td>Methane Dichloro-ethyl</td>
<td>C2 F2 Cl2</td>
<td>0.0002630</td>
</tr>
<tr>
<td>Methane Dichloro-fluoromethane</td>
<td>H1 C1 F1 Cl2</td>
<td>0.0042969</td>
</tr>
<tr>
<td>Nitric Oxide</td>
<td>N1 O1</td>
<td>0.0002475</td>
</tr>
<tr>
<td>Nitrous Oxide</td>
<td>N2 O1</td>
<td>0.0002081</td>
</tr>
<tr>
<td>P10 (10% Methane in Argon) **</td>
<td>H8 Ar90</td>
<td>0.00159</td>
</tr>
<tr>
<td>Propane</td>
<td>N1 C3</td>
<td>0.0018333</td>
</tr>
<tr>
<td>Propylene Sulfide</td>
<td>H6 C3 S1</td>
<td>0.0030826</td>
</tr>
<tr>
<td>Sulfur Hexafluoride</td>
<td>F6 S1</td>
<td>0.000672</td>
</tr>
<tr>
<td>Water vapor</td>
<td>H2 O1</td>
<td>0.00074855</td>
</tr>
</tbody>
</table>

#### Gas density

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (K)</td>
<td>293.15</td>
<td>K</td>
</tr>
<tr>
<td>Pressure (Torr)</td>
<td>760</td>
<td>760 Torr</td>
</tr>
<tr>
<td>Density</td>
<td>2.4164</td>
<td>mg/cm³</td>
</tr>
</tbody>
</table>
Fission barriers (4 databases: 3 theory + 1 experiment)

Use in the code:
- 6 - Barf - model for this setup (A, Z)
- 1 - FisRet - S. Cohen et al., An P (1974)
- 3 - FILE: A. Mamdouh et al., JPA (2001) 327
- 4 - FILE: Experimental barriers
- 5 - FILE: P. Moeller, LAH, JPL (2001)
- 6 - FILE: P. Moeller, PRC 52 (2015) 24310

For models # 3, 4
- If file data are absent, then use LDM model #
- 1 - FisRet - S. Cohen et al., An P (1974)
- 3 - FILE: A. Mamdouh et al., JPA (2001) 327
- 4 - FILE: Experimental barriers
- 5 - FILE: P. Moeller, LAH, JPL (2001)
- 6 - FILE: P. Moeller, PRC 52 (2015) 24310

Z = 84
Barfac = 1.00, Corrections [Odd-Even: "yes", Shell: "yes"], Model = "qMax"

Fission barrier

Barfac = 1.00, Corrections [Odd-Even: "yes", Shell: "yes"], Model = "qMax"

[Graph showing fission barrier with various models and data points]
Simulation of coincidence fragments and isomer gamma-lines

Experiment

LISE++ simulations

Fragment rates

LISE++ γ-database

γ-registration settings

Experiment
O.B.Tarasov@WANDA.US; 01/25/2021
LISE++ isomer database

Old GANIL database available through LISE

Internet database (NNDC) region of stable isotopes

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 $2 \leq Z \leq 28$ are taken from

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

Ratios for higher $Z$ will be entered soon.
it is useful for experiment planning how nucleus has been discovered: beam, target, reaction, energy, location.


Xu et al. first identified $^{129}\text{Sm}$ in 1999 and reported the results in “New $\beta$-delayed proton precursors in the rare-earth region near the proton drip line” [1]. A 165 MeV $^{36}\text{Ar}$ beam was accelerated with the Lanzhou sector-focused cyclotron and bombarded an enriched $^{56}\text{Ru}$ target. Proton-$\gamma$ coincidences were measured in combination with a He-jet type transport system. “A 134 keV $\gamma$ line found in the proton coincident $\gamma(x)$-ray spectrum in the $^{36}\text{Ar}^{+}\text{Ru}$ reaction was assigned to the $\gamma$-ray transition between the lowest-energy $2^+$ state and 0$^+$ ground state in the ‘daughter’ nucleus $^{128}\text{Nd}$ of the $\beta$-precursor $^{129}\text{Sm}$.”


Adapted from E. May and M. Thoennessen, At. Data Nucl. Data Tables 99 (2013) 1
Excitation energy of (fissile) nuclei after abrasion

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

LISE++ Abrasion-Ablation uses $T = f(A)$

<table>
<thead>
<tr>
<th>Break-up parameters</th>
<th>$T (A=50)$</th>
<th>$T (A=150)$</th>
<th>$T (A=250)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8.3</td>
<td>5.9</td>
<td>4.7</td>
</tr>
<tr>
<td>Diffuseness</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
</tr>
</tbody>
</table>

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

Determination of the Freeze-Out Temperature by the Isospin Thermometer


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

- Theoretical study
Data

• Atomic Masses
• Isomeric states database
• Fission barrier database
• Experimental production cross sections
• Experimental fragment momentum distributions

Needs for detailed information

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