Surrogate nuclear reactions: An indirect approach to determine cross sections for compound reactions

7th International Workshop on Compound-Nuclear Reactions and Related Topics (CNR*24)

IAEA, Vienna, Austria July 8-12, 2024 Jutta E. Escher Nuclear Data & Theory Group







Statistical reactions and Hauser-Feshbach calculations

- Hauser-Feshbach (HF) theory describes compound-nuclear reactions that involve statistical averages over overlapping resonances
- HF calculations are essential component of nuclear data evaluations
- Applications rely on cross sections calculated with HF, e.g. neutron capture





Hauser-Feshbach formalism:

$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+\text{target}}^{CN} (E,J,\pi) \cdot \begin{array}{l} G^{CN}{}_{\gamma}(E,J,\pi) \cdot W_{\alpha\gamma}(J) \\ \text{Known for nuclei} \\ \text{near stability} \end{array} + \begin{array}{l} G^{CN}{}_{\gamma}(E,J,\pi) \cdot W_{\alpha\gamma}(J) \\ \text{Highly} \\ \text{Uncertain w/o} \\ \text{constraints} \end{array} + \begin{array}{l} Well-studied \\ \text{corrections} \end{array}$$



Predictive power of HF reaction calculations is limited...

... this provides an opportunity for more sophisticated theory and indirect reaction methods

- Challenges:
 - Ambiguous model combinations, large parameter uncertainties, and multiple reaction channels
 - Away from stability there are few/no known constraints
- Needed a multipronged approach:
 - development of predictive microscopic structure and reaction theories
 - direct measurements (where possible) to validate theory
 - indirect measurements to constrain theory

 $\sigma_{\alpha\chi}(E) = \sum_{J\pi} \sigma_{\alpha}^{CN}(E, J, \pi) G_{\chi}^{CN}(E, J, \pi) W_{\alpha\gamma}(J)$ Width fluctuation Formation of CN corrections $\sigma_{\alpha}^{CN}(E,J,\pi) = \pi \lambda_{\alpha} \omega_{\alpha}^{J} \sum T_{\alpha ls}^{J}$ Probability for decay of CN $G_{\chi}^{CN}(E,J,\pi) = \frac{\sum_{l's'} T_{\chi l's'}^{J} \rho_{I'}(U')}{\sum_{\chi'' I''s''} \int T_{\chi'' I''s''}^{J} \rho_{I''}(U') dE_{\chi''}}$



Indirect measurements using the Surrogate Reactions Method

- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism



Surrogate reactions method combines theory and experiment to constrain cross section calculations for compound reactions Escher et al, R

Escher et al, RMP 84, 353 (2012)

Producing a CN in a surrogate reaction:

- Starts with a 'direct' reaction to produce a 'doorway state' at E_{ex} > several MeV
- Doorway evolves into a CN
- Spin population of doorway state = spin population of the CN

Observe the decay of the CN:

- Measure coincidence probability of outgoing surrogate particle with decay into channel of interest
- Model HF decay and fit parameters to measured surrogate probability

Obtain desired cross section:

 Calculate desired reaction cross section using inferred parameters





Concept

• (p,d) as a surrogate reaction mechanism

- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism





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*Width fluctuation corrections are omitted here, but accounted for in applications.







Surrogate (p,d) transfer reactions enable determination of unknown (n, γ) cross sections - benchmark ⁹⁰Zr(n, γ)

Escher et al, PRL 121, 052501 (2018)



Procedure

- Measure the surrogate reaction coincidence probability
- Calculate the spin-parity population of the doorway state = spin-parity of the CN
- > Model CN decay and perform Bayesian parameter fit to surrogate coincidence probabilities
- Sample posterior HF parameter distributions to obtain neutron-capture cross section



Extracted D₀ and $<\Gamma_{\gamma}>$ values

D _o [keV]	Reference
10	This work
6.89 (0.53)	Mughabghab, 2006
6.00 (1.40)	RIPL-3
7.18 (23)	Guttormsen, PRC 2017
<Γγ> [meV]	Reference
<Γγ> [meV] 185	Reference This work
<Γγ> [meV] 185 170 (20)	Reference This work Mughabghab, 2006
< Γγ> [meV] 185 170 (20) 130 (40)	ReferenceThis workMughabghab, 2006RIPL-3



Surrogate method does not use D_0 or $<\Gamma_{\gamma}>$

Oslo data from: Guttormsen et al, PRC 96, 024313 (2017)



Surrogate (p,d) transfer reactions enable determination of unknown (n, γ) reaction cross sections involving isomers



⁸⁷Y(n,γ) cross sections from ⁸⁹Y(p,dγ) surrogate reaction data

Escher et al, PRL 121, 052501 (2018)













- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism



Surrogate reactions method for neutron capture - using γ transitions





Surrogate (d,p) transfer reactions enable determination of (n,γ) cross sections benchmark ⁹⁵Mo(n,γ)

Ratkiewicz, Cizewski, JE, Potel, et al, PRL 122, 052502 (2019)





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- Concept
- (p,d) as a surrogate reaction mechanism
- (d,p) as a surrogate reaction mechanism
- Inelastic scattering as a surrogate reaction mechanism



- Opportunities:
 - Unknown (n,n') and (n,2n) reactions become accessible. Examples: ⁸⁸Y(n,2n), ¹⁶⁸Tm(n,2n)
 - Obtain multiple desired reaction cross sections simultaneously
 - Inverse-kinematics experiments at radioactive beam facilities
- Challenges:
 - Compound nucleus highly excited
 - Multiple intermediate nuclei involved
 - Non-statistical effects expected





- Experiment provides:
 - ⁹¹Zr(³He,³He') 'singles' cross section as function of E_{ex} and ejectile angle
 - Coincidence probabilities
 $P_{(3He,3He')\gamma}(E_{ex})$ for γ-transitions in 3 different nuclei
- Theory must:
 - Calculate ⁹¹Zr(³He, ³He') 'singles' cross section and determine spin-parity population
 - Model ⁹¹Zr decay into 3 final nuclei and fit decay parameters
 - Sample posterior HF parameter distribution and calculate desired cross sections



E [MeV]









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Escher et al., WIP (2024)



Guttormsen et al, PRC 2019 Oslo method, ⁹²Zr(p,d) This work (preliminary) Escher et al, PRL 2019 Surrogate method, ⁹²Zr(p,d)





Simultaneous fit to gammas in ⁹⁰Zr and ⁸⁹Zr

Escher et al., WIP (2024)







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Escher et al., WIP (2024)

Escher et al., WIP (2024)



(preliminary)



Actinides: Inelastic alpha scattering

- Decay probabilities for fission and γ emission measured in ²⁴⁰Pu(α,α') experiment
- Calculated Jp population using QRPA structure information in reaction description
- Adjusted HF decay parameters to minimize χ^2
- Obtained both ²³⁹Pu(n,γ) and ²³⁹Pu(n,f)



Simultaneous Determination of Neutron-Induced Fission and Radiative Capture Cross Sections from Decay Probabilities Obtained with a Surrogate Reaction

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M. Guttormsen,⁶ A. Henriques,¹ G. Kessedjian,⁷ K. Nishio,⁸ D. Ramos,⁵ S. Siem,⁶ and F. Zeiser⁶



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Pérez Sánchez et al, PRL 125, 122502 (2020)

Using inelastic scattering as a surrogate mechanism provides new opportunities: **Neutron capture on s-process branch points**



- ^{94,96}Zr(p,p') at Texas A&M, E_p = 21 MeV
- ^{154,156,158}Gd(p,p') at LBNL, E_p = 22 MeV
- Theory (Thapa, Escher, et al)
 - 1-step contributions
 - 2-step contributions
 - deformation









Spin-parity populations: Why they matter and how we calculate them





- The CN formed in neutron fusion has different J^π than when formed in inelastic scattering or transfer reactions >> The 'spin-parity mismatch' !!
- Sensitivity studies show
 - Decay into γ-channel depends very strongly on CN J^π
 - Decay by fission is less sensitive
 - Decay by p, n, or 2n emission
 is `in-between' but J^π cannot
 be ignored



The Surrogate experiment gives:

 $\mathsf{P}_{(\mathsf{p},\mathsf{d}\gamma)}(\mathsf{E}) = \sum_{\mathsf{J}\pi} \mathsf{F}_{(\mathsf{p},\mathsf{d})}^{\mathsf{CN}}(\mathsf{E},\mathsf{J},\pi) \cdot \mathsf{G}^{\mathsf{CN}}{}_{\gamma}(\mathsf{E},\mathsf{J},\pi)$

HF theory of the "desired" reaction: $\sigma_{\alpha\chi} = \sum_{J,\pi} \sigma_{\alpha}^{CN} (E, J, \pi) \cdot G^{CN}{}_{\chi}(E, J, \pi)$

- J. Escher and F.S. Dietrich, PRC 74, 054601 (2006)
- C. Forssen et al, PRC 75, 055807 (2007)
- J. Escher and F.S. Dietrich, PRC 81, 024612 (2010)
- S. Chiba and O. Iwamoto, PRC 81, 044604 (2010)
- A. Sharma et al, PRC 105, 014624 (2022)
- O. Gorton and J.E. Escher, PRC 107, 44612 (2023)



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fission probabilities



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p-channel probabilities





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Ignoring the spin-parity mismatch is not valid for (n,γ): Impact on capture cross sections extracted using the Weisskopf-Ewing approximation



J. Escher and F.S. Dietrich, PRC 81 (2010) 024612 N. Scielzo, J. Escher, et al., PRC 81 (2010) 034608 ¹⁷⁵Lu(n,γ) extracted from ¹⁷⁸Yb(³He,p) data using the WE approximation



Using the WE approximation is NOT valid for capture!



Ratkiewicz, Cizewski, JE, Potel, et al, PRL 122, 052502 (2019)

- ⁹⁵Mo(n,γ) from surrogate data
 - Using calculated J^{π} and fitting procedure (blue band)
- ⁹⁵Mo(n,γ) from surrogate data
 - Using WE approximation (yellow data points): $\sigma_{(n,\gamma)}(E_n) = \sigma^{CN}_{(n+T)}(E_n) \cdot P_{\gamma}(E_{ex})$



Using the WE approximation is NOT valid for capture!

Accounting for the spin-parity population in surrogate reaction applications is important for obtaining correct results

- Spin-parity population is equal to that of the neutron-induced reaction
 - Strong claims require strong proofs!
- Spin-parity population is equal to the spin-parity distribution of the level density
 - Reactions populate only a subset of states!
- 'Just use DWBA'
 - $-\,$ 2-step mechanisms contribute at high E_{ex}
- 'Just use Talys'
 - Hmm....???



Forming the CN in a surrogate reaction:

- Starts with a 'direct' reaction that produces a 'doorway state' at E_{ex} > several MeV
- Doorway evolves into a CN
- Spin population of doorway state = spin population of the CN





Theory for (p,d) surrogate reactions: Deep neutron holes

Challenge: Naïve potential-model picture not useful for deep holes

- Hole location
- Fragmentation



Theory for (p,d) surrogate reactions: Deep neutron holes

Challenge: Naïve potential-model picture not useful for deep holes

- Hole location
- Fragmentation

Solution: Dispersive optical potential connects OMP for scatter to mean field

- Scatter info gives DOMP at positive energies
- Mean field gives energy-averaged nuclear properties: single-particle E_{nlj} , spectral functions S_{nlj} , etc.

Mahaux & Sartor, Adv. Nucl. Phys. 1991 Delaroche et al, PRC 39, 391 (1989)



Theory for (p,d) surrogate reactions: Deep neutron holes + two-step reaction mechanisms

- Challenge: Nucleon removal accompanied by inelastic excitations:
 - In entrance channel:
 ⁹²Zr(p,p')⁹²Zr**(p',d)⁹¹Zr*
 - In exit channel:
 ⁹²Zr(p,d')⁹¹Zr**(d',d)⁹¹Zr*
- Solution: 2nd-order DWBA with collective model for inelastic scattering



Future: use global DOMP for hole states + QRPA structure theory to describe inelastic scattering component

Gaining confidence in the calculated spin-parity population: Cross checks

Escher et al, PRL 121, 052501 (2018) Escher et al, EPJ Conf. 178, 03002 (2018)



Does the calculated 'singles' cross section agree with the surrogate measurement? ✓



Gaining confidence in the calculated spin-parity population:



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Gaining confidence in the calculated spin-parity population: **Cross checks**

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Gaining confidence in the calculated spin-parity population: Cross checks

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IAS have known J^{π} and 'perturb' the spin-parity population in a very specific manner.

And this is reflected in the γ -transitions of the decaying CN \checkmark



Calculating spin-parity populations for (d,p) surrogate reactions: deuteron breakup followed by partial fusion

Challenges:

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- Multiple reaction processes lead to observation of proton, while only breakup-fusion is relevant
- Theory developments:
 - Describe deuteron breakup and propagation in nuclear field
 - Describe neutron absorption with optical model potential
 - Formalism to be extended to deformed systems
- Relevant (d,p) formalism has been developed, vetted, applied
 - Three theory groups describe breakup-fusion, which contains CN formation, based on earlier work by Udagawa & Tamura and Ichimura, Austern & Vincent:
 - Potel et al, PRC 92, 034611 (2015)
 - Lei & Moro, PRC 92, 044616 (2015)
 - Carlson et al, Few-Body Syst 57, 307 (2016), arxiv:1508.01466
 - Workshop compared formalisms and codes
 - Potel et al, EPJA 53, 178 (2017)





Calculating spin-parity populations for inelastic scattering surrogate reactions: Inelastic states and two-step contributions



- Challenges:
 - Zr(³He,³He') populates states up to E_{ex}=34 MeV
 - Inelastic scattering is accompanied by (³He,α)(α,³He') and (³He,d)(d, ³He')
- Theory:
 - Describe states excited in scattering microscopically using QRPA
 - Calculate inelastic cross sections using DWBA (use transition potentials)
 - Calculate 2-step contributions in 2nd-order DWBA





Calculating spin-parity populations for inelastic scattering surrogate reactions: 1-step inelastic and 2-step transfers contribute

Escher, wip (2024)

Adding all contributions reproduces the measured singles cross section \checkmark

Adding by J^{π} give the spin-parity population





Inverse-kinematics experiments



Inverse-kinematics (d,p) surrogate reactions at TRIUMF: Neutron capture on ⁹³Sr

Richard, Hughes, JEE, Potel, et al (WIP)

- Motivation
 - β-delayed γ-emission found surplus of gammas, with potential implications for a strong ⁹³Sr(n,γ) rate
 - Provide an alternate way to place constraints on the γSF
- Experiment at TRIUMF (2021)

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- ⁹³Sr RIB (8MeV/u) on CD₂ target
- SHARC (segmented Si array) to detect p
- TIGRESS (12 HPGe clovers, 2π) to detect gammas
- Analysis underway







National Nuclear Security Administration 51

Inverse-kinematics (d,p) surrogate reactions at MSU/NSCL (now FRIB): **Detecting recoils instead of gammas**

Exp: Sims, Cizewski, Ratkiewicz, Pain,... Theory: Escher, Potel, Gorton



- Motivation
 - Develop techniques to move far away from stability
 - Can we use recoils instead of gammas to detect channel of interest?
- Experiment at NSCL (2017)
 - ⁸⁴Se RIB on CD₂ target
 - ORRUBA/S800 spectrometer to detect p and beamlike particles
 - Preliminary ⁸⁴Se(n, γ) results available



Experimental details: see talk by J. Cizewski

Here recoils are utilized instead of gammas

Three scenarios:

- 1. ⁸⁴Se does not react with CD₂ target
- 2. ⁸⁴Se undergoes (d,p) reaction at CD_2 target to form ⁸⁵Se then gammadecays to ground state.
- 3. Same as point 2, except nucleus emits neutron => 84Se

Surrogate reactions method for neutron capture - using recoiling nucleus





Theory for surrogate reactions: Parameter constraints from Markov-Chain Monte-Carlo fit to recoil observables

Escher et al, prelim (2024)





MCMC fit to surrogate decay probabilities: Prior and posterior $P_{\rm \gamma}$

Escher et al, prelim (2024)





Sample parameter distributions and calculate capture cross section: Prior to posterior results

Escher et al, prelim (2024)



Cross section calculation constrained by surrogate decay data ONLY

No-gamma surrogate reaction data constrains the ⁸⁴Se(n, γ) cross section Preliminary results slightly lower than systematics suggest

Escher et al, prelim (2024)

- ⁸⁴Se(n,γ) cross section constrained by surrogate data, no need for auxiliary quantities (D₀ or <Γ_γ>)
- Fits not sensitive to details of the γSF, e.g.
 M1 LEE or E1 pygmy resonance.
- Using different warmstart parameter vectors give similar cross section results

Future: Improving energy resolution and detecting additional exit channels. Field experiments at FRIB.

Inverse-kinematics (d,p) at RIKEN/RIBF: Detecting residual nuclei ^{78,80}Se to determine ⁷⁹Se(n,γ)

Imai et al, PLB 850, 138470 (2024)

Domingo-Pardo, Lol to Isolde nTOF (2014)

Motivation

- Study options for transmutation of nuclear waste (longlived fission products) via neutron-induced reactions
- Neutron capture rates for s-process nucleosynthesis
- Experiment at RIBF:
 - BigRIPS separator produced Se beams (from 238U+Be), which were degraded, here to 20MeV/u, impinging on CD₂ target
 - Outgoing protons detected upstream in lampshadearranged Si strip detector (9°-34° com)
 - Energy resolution E_{com} =0.8 (1.3) MeV at E_{ex} =10 (13) MeV
 - Residual nuclei detected in SHARAQ spectrometer, identified by A/Q, magnetic rigidity, ionization chamber

Inverse-kinematics surrogate measurements at a heavy-ion storage ring at GSI/FAIR: Detecting recoils from ²⁰⁸Pb(p,p') to determine ²⁰⁷Pb(n,γ) Sguazzin et al, arXiv:2312.13742 (2023)

Fission

Surrogate reactions approach to obtain (n,f) cross sections and insights into the fission process

Describing fission challenges theory (and experiment)

- Descriptions range from phenomenological to microscopic
- Lots of data needed to provide constraints

Opportunity: Surrogate fission measurements

- Observe fission properties in coincidence with surrogate ejectile
- Control over energy of fissioning nucleus, including sub-threshold

Opportunity: Extending theoretical treatments

• Role of pre-equilibrium, width fluctuation corrections, damping effects

Inverse-kinematics (d,p) with HELIOS at ANL: Determining fission barriers in ²³⁹U from ²³⁸U(d,pf)

Bennett et al, PRL 130, 202501 (2023)

Experimental fission probability compared to GEF (top) and (scaled) compared to results deduced from evaluations (bottom).

Motivation

- Collect fission data (barriers, mass and charge yields) for nuclear astrophysics ('fission recycling'), future power systems, safeguard applications
- Benchmarks for fission models
- Experiment at ANL:
 - Use of solenoidal spectrometer HELIOS
 - 2³⁸U beam (E^b=8.6 MeV/u) on CD₂
 target
 - Outgoing protons deflected in magnetic field and detected upstream on 4-sided position-sensitive Si array
 - Fission fragments detected in gas-filled heavy-ion detectors

S. A. Bennett,¹ K. Garrett[®],¹ D. K. Sharp[®],^{1,*} S. J. Freeman[®],^{1,2} A. G. Smith[®],¹ T. J. Wright[®],¹ B. P. Kay[®],³ T. L. Tang[®],^{3,†} I. A. Tolstukhin[®],³ Y. Ayyad[®],⁴ J. Chen,³ P. J. Davies[®],⁵ A. Dolan,⁶ L. P. Gaffney[®],⁶ A. Heinz[®],⁷ C. R. Hoffman[®],³ C. Müller-Gatermann[®],³ R. D. Page,⁶ and G. L. Wilson[®],^{8,3}

$$\sigma_f^A = \sigma_{ ext{CN}}^{A+1} imes P_f^{A+1}$$

$$P_f(E_x) = \frac{N_{d,pf}(E_x)}{N_{d,p}(E_x) \cdot \epsilon_f}$$

Future: measurements with SOLARIS at FRIB and ISOLDE Solenoidal Spectrometer (ISS) at CERN

Limitations

Limitations of the SRM (in its present form)

- Forming a CN in the resonance region
 - Cannot use present approach which relies on HF decay calculations
 - Investigate the role of width fluctuations
- Failure to form a compound nucleus
 - 'just a little fail' aka preequilibrium: has to be accounted for > see Zr(n,2n) applications
 - Need to understand how doorway states damp into CN
 - No CN at all > need other approach
- Trying to measure direct capture cross section
 - Need a different method (ANC, Trojan Horse, Coulomb dissociation,)
- There are thousands of unstable nuclei for which we would like cross sections
 - Need to develop predictive theory
 - SRM can provided targeted cross section results to validate theory and address specific needs

Concluding remarks

- Surrogate reaction method combines theory and experiment to constrain cross section calculations for compound reactions that cannot be measured directly.
- 2. Method uses inelastic scattering or transfer reactions in regular or inverse kinematics.
- Uses experimental observable indicating decay into channel of interest. Does not use auxiliary quantities (D0, <Gg>) which are unavailable for unstable isotopes. When use Bayesian parameter inference, UQ and correlations are built in.
- 4. The last decade has seen significant progress on both the theory and experimental side. New experimental facilities are providing opportunities to further expand.

- 4. There is very interesting physics associated with surrogate reaction mechanism:
 - We need broadly-applicable theoretical descriptions of inelastic scattering and transfer reactions
 - Doorway states play an important role in producing the CN. We need to better understand how they damp.
 - Width fluctuations in surrogate reactions are understudied.
- We will not be able to measure all reactions of interest.
 Predictive theory is needed. Surrogate measurements can be used to validate and complement theory

A thank you to my collaborators:

LLNL: O. Gorton, E. In, G. Potel, C. Pruitt, A. Thapa, I.J. Thompson, W. Younes, B. Alan, R. Casperson, J. Harke, R. Hughes, A. Ratkiewicz, N. Scielzo ORNL: S.Pain Rutgers U.: J. Cizewski, H. Sims Ohio U: A. Richard CEA/France: M. Dupuis, S. Peru

Thank you!

Abstract:

Cross sections for compound-nuclear (CN) reactions are important for nuclear astrophysics and other applications. Direct measurements are not always possible for the reactions of interest and calculations without experimental constraints can be quite uncertain. Thus indirect approaches, such as the surrogate reaction method (SRM), are being developed to fill the gaps. The SRM, which uses a (direct) inelastic scattering or transfer reaction to obtain information on the decay of a specific compound nucleus, has a long history of providing probabilities for fission, gamma and particle emission. While earlier implementations of the method used minimal theory to provide approximate cross sections for (n,f) reactions, better theoretical descriptions of the underlying reaction mechanisms have made it possible to also obtain (n,g), (n,n'), and (n,2n) cross sections that agree well with benchmarks. I will discuss multiple applications of the modern implementation of the SRM, highlight theory advances that enable them, and comment on opportunities offered at new experimental facilities.

*This work is performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Support from the LDRD Program, Projects 19-ERD-017, 20-ERD-030, 21-LW-032, 22-LW-029, 23-SI-004, and 24-ERD-023 is acknowledged.

StarLiTeR at Texas A&M

We record the total energy, angle and determine the particle type

Some experimental details:

- 13-day run (LLNL experimental team & collaborators
- Si energy resolution 75 keV one sigma
- Gamma energy resolution 1.7 keV one sigma
- Angle range 30 to 60 degrees
- Y89 mono-isotopic 760 micrograms/cm²

Experiment at Texas A&M Cyclotron Institute

Top view of the STARLiTeR array. HPGe surrounds chamber Si telescope.

STARLiTeR array closed up around the chamber. Cyclotron beam comes from right and exits on left.

J.T. Burke, priv. commun.

STARS/LiBerACE experiments at LBNL

SRM for (n,f) cross sections

- Results used the Weisskopf-Ewing approximation: ignore spin-parity mismatch
- Typically agree within 10-15% with benchmarks
- Low energies and fission barriers tend to be more sensity to J^π mismatch
- Role of preequilibrium needs to be explored further

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