Light Element Evaluations

from LANL-EDA R-matrix analyses Report of evaluation status

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EST.1943 -

Outline

LANL EDA Code

- Simultaneous fit of all reaction/scattering data in R-matrix approach

LANL evaluations

- ENDF/B-VIII.0
- Recent improvements
- Gaps

LANL-EDA code

R-matrix formalism [Wigner(1947)]

- Unified description of many reactions
- Ensures unitarity & probability conservation

Capabilities

- Any projectile: n, p, D, T, ³He, α , ...
- Any target: H, He, Li, Be, B, C, N, O, F, ...
- All data fit together, at the same time
 - Elastic, inelastic, rearrangement, breakup, capture
- All observables
 - Cross sections: elastic, reaction, total
 - Angular distributions/excitation functions
 - · Polarization observables
 - Spectra 2→3, 2→4
 - Capture/electromagnetic
- High-fidelity fit:
 - Typical chi-squared: χ^2 /dof ~ 1.2 1.5

	Channel	a_c (fm))	$l_{\rm max}$	
\sim	<i>t</i> + ⁴ He	4.02		5	
	n+ ⁶ Li	5.0		3	
	$n+^{6}Li^{*}$	5.5		1	
+	$d+{}^{5}\mathrm{He}$	6.0		0	
Reaction	Energy Ran	nge (MeV)	#	Pts.	Observables
$^{4}\text{He}(t,t)^{4}\text{He}$	$E_t = 0 - 14$		16	661	$\sigma(\theta), A_y(t)$
$^{4}\text{He}(t,n)^{6}\text{Li}$	$E_t = 8.75$ -	14.4	37		$\sigma_{\text{int}}, \sigma(\theta)$
$^{4}\text{He}(t,n)^{6}\text{Li}^{*}$	$E_t = 12.9$			4	σ(θ)
$^{6}\text{Li}(n,t)^{4}\text{He}$	$E_n = 0 - 4$		14	106	$\sigma_{\text{int}}, \sigma(\theta)$
$^{6}\text{Li}(n,n)^{6}\text{Li}$	$E_n = 0 - 4$		8	300	$\sigma_{\mathrm{T}}, \sigma_{\mathrm{int}}, \sigma(\theta), P_{y}(n)$
${}^{6}\text{Li}(n,n'){}^{6}\text{Li}^{*}$	$E_n = 3.35$ -	4		8	σ_{int}
$^{6}\text{Li}(n,d)^{5}\text{He}$	$E_n = 3.35$ -	4		2	$\sigma_{\rm int}$
Total			39	918	13

Unified, simultaneous fit

- describe all data together
- fit quantum mechanical amplitudes, not cross sections

Built-in Quality Assurance

- Normalization constrained
 - Weed-out underestimated exp'l uncertainties
- Superior to single-channel or polynomial fitting

LANL Light Element Evaluations

	H1	H2	H3	He3	He4	Li6	Li7
n	VIII.0	VII.1	VII.1	VII.1	VII.1	VIII.0	VII.1
р	VII.1	VII.1	VII.1	VII.1	2011*	VII.1	2001**
d		VII.1	VII.1, 2018	VII.1	2011	VII.1	2003**
t			VII.1	VII.1	2011*	VII.1	*
³ He				2001	2011*	VII.1	
α					2011*		

Roman numerals refer to ENDF versions

• Years refer to locally available files that have not yet been submitted to ENDF

* Nuclei for which LLNL evaluations have been put into ENDF/B-VIII.0

** Nuclei for which LLNL evaluations replaced existing LANL evaluations in VIII.0

Evaluation revision criteria

Improvement to existing LANL evaluations welcome

- Primary concern: eliminate evaluation 'gaps'
 - gaps in recommended energy range 0 < E < 20 MeV (higher for some)
 - gaps in reactions available (spectra, capture, etc.)

Review criteria for evaluation revisions

- For reactions without existing evaluation
 - · describes "well" the available data
 - covers recommended energy range
 - ENDF-6 compliant
- For reactions with existing evaluation
 - "complete" (as above)
 - accepted for extension of energy range (appended to existing evaluation)
 - substantial improvement over existing evaluation requires
 - improved fidelity of data fit
 - improved method/approach of proposed eval.
 - » better theory; simultaneous description of more data; etc.

<u>NB</u>: simpler approaches (such as single-channel curve fitting) offering substantially improved description of data will be accepted

Highlights

- 1. p+t, p+³He, p+^{6,7}Li
- 2. d+d, d+t, d+³He
- 3. t+t, t+⁶Li
- 4. n+⁶Li, n+¹²C, n+¹³C
- 5. ⁹Be system
- 6. ¹⁵N system
- 7. n+¹⁶O

Existing LANL evaluations

Α	System	Channels	Energy Range (MeV)
2	N-N	p+p; n+p, γ+d	0-40 0-40
3	N-d	p+d; n+d	0-4
	⁴ H; ⁴ Li	n+t; p+³He	0-20
4	⁴ He	p+t; n+ ³ He; d+d	0-11; 0-10; 0-10
5	⁵He	n+α; d+t; ⁵ He+γ	0-28; 0-10
	⁵ Li	p+α; d+ ³ He	0-24; 0-1.4

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Α	System (Channels)						
6	⁶ He (⁵ He+n, t+t); ⁶ Li (d+ ⁴ He, t+ ³ He); ⁶ Be (⁵ Li+p, ³ He+ ³ He)						
7	⁷ Li (t+ ⁴ He, n+ ⁶ Li); ⁷ Be (γ+ ⁷ Be, ³ He+ ⁴ He, p+ ⁶ Li)						
8	⁸ Be (⁴ He+ ⁴ He, p+ ⁷ Li, n+ ⁷ Be, p+ ⁷ Li [*] , n+ ⁷ Be [*] , d+ ⁶ Li)						
9	⁹ Be (⁸ Be+n, d+ ⁷ Li, t+ ⁶ Li); ⁹ B (γ+ ⁹ B, ⁸ Be+p, d+ ⁷ Be, ³ He+ ⁶ Li)						
10	¹⁰ Be (n+ ⁹ Be, ⁶ He+α, ⁸ Be+nn, t+ ⁷ Li); ¹⁰ B (α+ ⁶ Li, p+ ⁹ Be, ³ He+ ⁷ Li)						
11	¹¹ B (α+ ⁷ Li, α+ ⁷ Li [*] , ⁸ Be+t, n+ ¹⁰ B); ¹¹ C (α+ ⁷ Be, p+ ¹⁰ B)						
12	2 ¹² C (⁸ Be+α, p+ ¹¹ B)						
13	¹³ C (n+ ¹² C, n+ ¹² C [*])						
14	¹⁴ C (n+ ¹³ C)						
15	¹⁵ N (p+ ¹⁴ C, n+ ¹⁴ N, α+ ¹¹ B)						
16	¹⁶ Ο (γ+ ¹⁶ Ο, α+ ¹² C)						
17	¹⁷ Ο (n+ ¹⁶ O, α+ ¹³ C)						
18	¹⁸ Ne (p+ ¹⁷ F, p+ ¹⁷ F [*] , α+ ¹⁴ O)						

Proton induced

• p-001_H_003.endf	[T (p , x) Y]
$-MF3(x-sec): 2(el), 50(n_0), 650(d_0) (<20 MeV)$	
-MF6(E-ang): 2, 50, 600	
• p-002_He_003.endf	[³ He(p,x)Y]
-MF3: 2(el), $50(n_0)$, $650(d_0)$ (<20 MeV)	
-MF6: 2, 50, 650	
• p-002_He_004.endf	[⁴ He(p,x)Y]
- LLNL	
• p-003_Li_006.endf	[⁶ Li(p,x)Y]
$-MF3: 2750 (^{3}He_{0}) (<2.5 MeV)$	
-MF6: 2 750	
• p-003_Li_007.endf	[⁷ Li(p,x)Y]
- LLNL	

Deuteron induced

• d-001_H_002.endf	[D(d,x)Y]
-MF3(x-sec): 2(el), 50(n0), 600(p0) (<10 MeV)	
-MF6(E-ang): 2, 50, 600 (<10 MeV)	
• d-001_H_003.endf	[T(d,x)Y]
-MF3: 2 50(<40 MeV) 51 (<10 MeV)	
-MF6: 2 50 51 (same energies)	
• d-002_He_003.endf	$[^{3}\text{He}(d,x)Y]$
-MF3: 2 600 (<14 MeV)	
- MF6: 2 600	
• d-003_Li_006.endf	[⁶ Li(d,x)Y]
-MF3: 2 50 600 800(a0) (<5 MeV)	
-MF6: 2 50 600 800	
• d-003_Li_007.endf	[⁷ Li(d,x)Y]
- LLNL	

Triton induced

•t-001_H_003.end	f	[T(t,x)Y]
-MF3: 2 16(2n)	<pre>(<2.2 MeV Rmat/data; >2.2, <20 ex</pre>	(trap)
-MF6: 2 16		
•t-002_He_003.en	df	$[^{3}\text{He}(t,x)Y]$
-MF3: 2 28(np)	650(nd) (<3 MeV Rmat/data; >3, <	20 extrap)
-MF6: 2 28 650		
•t-002_He_004.en	df	<pre>[⁴He(t,x)Y]</pre>
- LLNL		
•t-003_Li_006.en	df	[⁶ Li(t,x)Y]
$-MF3: 2 22(n\alpha)$	650 (<4 MeV Rmat/data; >4, <20 M	MeV extrap)
-MF6: 2 22	650	
• t-003_Li_007.en	df	[⁷ Li(t,x)Y]
- LLNL		

==> neutro	ns-VIII_0_ov	wners.txt <=	==		
0 – N – 1	LANL	EVAL-APR16	HALE, PARIS	25	1451
1-H - 1	LANL	EVAL-JUL16	G.M.Hale	125	1451
1-н - 2	LANL	EVAL-FEB97	P.G.Young,G.M.Hale,M.B.Chadwick	128	1451
1-H - 3	LANL	EVAL-NOV01	G.M.Hale	131	1451
2-Не- 3	LANL	EVAL-MAY90	G.Hale,D.Dodder,P.Young	225	1451
2-Не- 4	LANL	EVAL-SEP10	Hale	228	1451
3-Li- 6	LANL	EVAL-JAN17	G.M. Hale	325	1451
3-Li- 7	LANL	EVAL-AUG88	P.G.Young	328	1451
4-Be- 7	LANL	EVAL-JUN16	I.Thompson, P.R.Page	419	1451
4-Be- 9	LLNL,LANL	EVAL-OCT09	G.HALE, PERKINS ET AL, FRANKLE	425	1451
5-B - 10	LANL	EVAL-FEB17	G.M.Hale	525	1451
5-B - 11	LANL	EVAL-MAY89	P.G.Young	528	1451
6-C - 12	LANL, ORNL	EVAL-AUG15	G.M. Hale, P.G. Young, C.Y. Fu	625	1451
6-C - 13	LANL,	EVAL-AUG15	G.M. Hale, M.W. Paris	628	1451
7 - N - 14	LANL	EVAL-JUN97	M.B.Chadwick, P.G.Young	725	1451
7-N - 15	LANL	EVAL-SEP83	E.Arthur, P.Young, G.Hale	728	1451
8-0 - 16	LANL	EVAL-DEC16	Hale,Paris,Young,Chadwick	825	1451

Ongoing/planned evaluation work

• LANL

- Commit existing charged-particle evaluations to ENDF/A trunk
 - protons: ⁴He, ⁷Li
 - deuterons: ³H, ⁴He, ⁷Li
 - tritons: ⁴He
 - ³He's: ³He, ⁴He
 - alphas: ⁴He

• LLNL

- energy extensions
- missing evaluations

```
alphas/a-003_Li_006.endf
deuterons/d-001_H_002.endf
deuterons/d-001_H_003.endf
deuterons/d-002_He_003.endf
deuterons/d-003_Li_004.endf
deuterons/d-003_Li_006.endf
helium3s/h-003_Li_006.endf
helium3s/h-003_Li_007.endf
protons/p-001_H_003.endf
protons/p-002_He_003.endf
tritons/t-001_H_003.endf
```

• ORNL

- n+¹⁶O resonance parameters
- SAMMY advances
 - $B_c = -\ell$ boundary condition
 - capture
 - closed-channel effects
- comprehensive resonance anal.
- Normalization work for ¹⁶O(n,a)

• JAEA

- multichannel fits
 - n+¹⁶O (¹⁷O system)
 - p+7Li
- ¹⁷O system agrees closely with LANL/EDA normalizations



Follow-on material

ENDF/B-VIII.0 evaluation custodians

==> alphas-VIII_0_owner	s.txt <==							
2-He- 4 LLNL E	EVAL-DEC99	R.M.White,D.A.Resler,S.I.Warshaw	228	1451				
==> deuterons-VIII_0_owners.txt <==								
1-H - 2 LANL E	EVAL-SEP01	G.M.HALE	128	1451				
1-H - 3 LANL E	EVAL-JAN95	G.M.HALE AND M.DROSG	131	1451				
2-He- 3 LANL E	EVAL-FEB01	G.M.HALE	225	1451				
3-Li- 6 LANL E	EVAL-JUN04	P.R.PAGE	325	1451				
<u> 3-Li- 7 LLNL F</u>	EVAL-NOV10	P. Navratil, D. A. Brown	328	1451				
==> helium3s-VIII_0_own	ners.txt <=	=						
2-He- 3 LLNL E	EVAL-NOV10	P.Navratil, D.Brown, G.Hale	225	1451				
2-He- 4 LLNL E	EVAL-DEC99	R.M.White,D.A.Resler,S.I.Warshaw	228	1451				
3-Li- 6 LANL E	EVAL-NOV02	G.M.HALE	325	1451				
==> neutrons-VIII_0_own	ners.txt <=	=						
0 – N – 1 LANL E	EVAL-APR16	HALE, PARIS	25	1451				
1-H - 1 LANL E	EVAL-JUL16	G.M.Hale	125	1451				
1-H - 2 LANL E	EVAL-FEB97	P.G.Young,G.M.Hale,M.B.Chadwick	128	1451				
1-H - 3 LANL E	EVAL-NOV01	G.M.Hale	131	1451				
2-He- 3 LANL E	EVAL-MAY90	G.Hale,D.Dodder,P.Young	225	1451				
2-He- 4 LANL E	EVAL-SEP10	Hale	228	1451				
3-Li- 6 LANL E	EVAL-JAN17	G.M. Hale	325	1451				
3-Li- 7 LANL E	EVAL-AUG88	P.G.Young	328	1451				
4-Be- 7 LANL E	EVAL-JUN16	I.Thompson, P.R.Page	419	1451				
4-Be- 9 LLNL,LANL E	EVAL-OCT09	G.HALE, PERKINS ET AL, FRANKLE	425	1451				
5-B - 10 LANL E	EVAL-FEB17	G.M.Hale	525	1451				
5-B - 11 LANL E	EVAL-MAY89	P.G.Young	528	1451				
6-C - 12 LANL,ORNL E	EVAL-AUG15	G.M. Hale, P.G. Young, C.Y. Fu	625	1451				
6-C - 13 LANL, E	EVAL-AUG15	G.M. Hale, M.W. Paris	628	1451				
7-N - 14 LANL E	EVAL-JUN97	M.B.Chadwick, P.G.Young	725	1451				
7-N - 15 LANL E	EVAL-SEP83	E.Arthur, P.Young, G.Hale	728	1451				
8-0 - 16 LANL E	EVAL-DEC16	Hale, Paris, Young, Chadwick	825	1451				

ENDF/B-VIII.0 evaluation custodians (cont.)

==> protons-VIII_0_owners.txt <==								
1-H - 1 LANL	EVAL-FEB98	G.HALE	125	1451				
1-H - 2 LANL	EVAL-FEB97	P.G.YOUNG,G.M.HALE,M.B.CHADWICK	128	1451				
1-H - 3 LANL	EVAL-SEP01	G. M. HALE	131	1451				
2-He- 3 LANL	EVAL-OCT83	G.HALE	225	1451				
2-He- 4 LLNL	EVAL-DEC99	R.M.White, D.A.Resler, S.I.Warshaw	228	1451				
3-Li- 6 LANL	EVAL-AUG01	G.M.HALE	325	1451				
<u>3-Li- 7 LLNL</u>	EVAL-SEP10	P. Navratil, D.A. Brown	328	1451				
4-Be- 9 LANL	EVAL-NOV88	P.G.Young, E.D.Arthur	425	1451				
5-B - 10 LANL	EVAL-AUG05	P.R.PAGE	525	1451				
6-C - 12 LANL	EVAL-JUN96	M.B.CHADWICK AND P.G.YOUNG	625	1451				
6-C - 13 LANL	EVAL-DEC04	P.R.PAGE	628	1451				
7-N - 14 LANL	EVAL-AUG97	M.B.CHADWICK & P.G.YOUNG	725	1451				
8-0 - 16 LANL	EVAL-JUN96	M.B.CHADWICK AND P.G.YOUNG	825	1451				
==> tritons-VIII	_0_owners.txt <==	=						
1-H - 3 LANL	EVAL-FEB01	G.M.HALE	131	1451				
2-He- 3 LANL	EVAL-AUG01	G.M.HALE	225	1451				
<u>2-He- 4 LLNL</u>	EVAL-DEC99	R.M.White, D.A.Resler, S.I.Warshaw	228	1451				
3-Li- 6 LANL	EVAL-SEP01	G.M.HALE	325	1451				
3-Li- 7 LLNL	EVAL-JUN16	I.Thompson, P.Navratil, D.Brown	328	1451				

T(d,n)α evaluation (I)

Simultaneously fits all known low-E data

- neutron & charged-particle channels
- polarization (distinguishes partial waves, etc.)
- High-fidelity X² ~ 1.5 below 10 MeV
- All resonances/partial waves included

EDA also provides covariance matrices



		channe	el	а _с (fm)	I _{max}
		n+⁴He		3.0		5
		γ+⁵He		6	0	1
		d+³H		5.	.1	5
		n+4He	*	5.	.0	1
Reaction	Energies (MeV)		# data point s		# data types	
⁴ He(n,n) ⁴ He	$E_n = 0 - 40$		817		2	
³ H(d,d) ³ H	E _d = 0	0 – 8.6	700		6	
³ H(d,n) ⁴ He	$E_{d} = 0 - 30$		1185		14	
³ H(d,γ) ⁵ He	E _d = 0	0 – 8.6		17		2
³ H(d,n) ⁴ He [*]	$E_{d} = 4.8 - 8.3$		10			1
total			2	729		25

T(d,n)α evaluation (II) Angular distributions T(d,el)



T(d,n)α evaluation (II) σ_{NI} T(d,el) nuclear plus interference



Nuclear + interference cross section

- requires multichannel fit
- strong energy dependence
- not necessarily > 0

⁶Li deuterons, neutrons





Uncertainties from chi-squared minimization

$$\chi^{2}_{\text{EDA}} = \sum_{i} \left[\frac{nX_{i}(\mathbf{p}) - R_{i}}{\Delta R_{i}} \right]^{2} + \left[\frac{nS - 1}{\Delta S / S} \right]^{2}$$

 $\begin{cases} R_i, \Delta R_i = \text{relative measurement, uncertainty} \\ S, \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{cases}$

Near a minimum of the chi-squared function at $\mathbf{p} = \mathbf{p}_0$:

$$\chi^{2}(\mathbf{p}) = \chi_{0}^{2} + (\mathbf{p} - \mathbf{p}_{0})^{\mathrm{T}} \mathbf{g}_{0} + \frac{1}{2} (\mathbf{p} - \mathbf{p}_{0})^{\mathrm{T}} \mathbf{G}_{0} (\mathbf{p} - \mathbf{p}_{0}) = \chi_{0}^{2} + \Delta \chi^{2}. \begin{cases} \chi_{0}^{2} = \chi^{2}(\mathbf{p}_{0}) \\ \mathbf{g}_{0} = \nabla_{\mathbf{p}} \chi^{2}(\mathbf{p}) |_{\mathbf{p} = \mathbf{p}_{0}} \approx 0 \\ \mathbf{G}_{0} = \nabla_{\mathbf{p}} \mathbf{g}(\mathbf{p}) |_{\mathbf{p} = \mathbf{p}_{0}} \end{cases} \approx 0$$

Conventions:

1) previous: $\Delta \chi^2 = 1 \implies \text{Very small uncertainties } \delta p_i = (C_{ii}^0)^{1/2} \sim \mathcal{O}(N_p^{-1/2})$ 2) improved: $\Delta \chi^2 = \frac{1}{2} \Delta \mathbf{p}^{\mathrm{T}} \mathbf{G}_0 \Delta \mathbf{p} \leq \Delta \chi^2_{\max},$ $P(\Delta \chi^2 | k) = \left[2^{\frac{k}{2}} \Gamma(\frac{k}{2}) \right]^{-1} \int_{0}^{\Delta \chi^2_{\max}} t^{\frac{k}{2}-1} e^{-\frac{t}{2}} dt = \text{CL (e.g. } \sim 0.68 \text{ for } 1-\sigma), 0.95 \text{ for } 2-\sigma, \text{etc.}$ $\Delta \chi^2_{\max} \approx k = \langle \Delta \chi^2 \rangle.$ $\delta p_i \sim (N_p C_{ii}^0)^{1/2}$

Covariance

The parameter covariance matrix is $C_0 = 2G_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\chi^{2}(\mathbf{p}) = \chi_{0}^{2} + (\mathbf{p} - \mathbf{p}_{0})^{\mathrm{T}} \mathbf{g}_{0} + \frac{1}{2} (\mathbf{p} - \mathbf{p}_{0})^{\mathrm{T}} \mathbf{G}_{0} (\mathbf{p} - \mathbf{p}_{0}) \begin{cases} \chi_{0}^{2} = \chi^{2}(\mathbf{p}_{0}) \\ \mathbf{g}_{0} = \nabla_{\mathbf{p}} \chi^{2}(\mathbf{p}) |_{\mathbf{p} = \mathbf{p}_{0}} \approx 0 \\ \mathbf{g}_{0} = \nabla_{\mathbf{p}} \chi^{2}(\mathbf{p}) |_{\mathbf{p} = \mathbf{p}_{0}} \approx 0 \end{cases}$$



Evaluation 1: n-001_H_001



Evaluation 2: n-003_Li_006



Evaluation 3: n-005_B_010



Los Alamos National Laboratory

Evaluation 4: n-006_C_012



Evaluation 5: n-008_0_016



Outlook

Short term

- publish existing evaluations (including, of course, charged-particle) absent from ENDF/B
 - including all R-matrix & normalization parameters (Ian T.'s talk)
 - *Caveat Emptor*: EDA5 & 6 relativistic parametrization
- use existing EDA5

Medium term

- continue development on EDA6 (modern-language successor to EDA5)
 - primary objectives:
 - extend light-element analyses/covariance to $E_n \le 20 \text{ MeV}$
 - charged particles
 - spectra
- Likelihood-based fitting with Bayesian approach

Long term

- modern-language modular/OO structure will allow
 - experimental acceptance, efficiency, general IRF capabilities (comparable to SAMMY)
 - integrated, homogeneous optimization with integral benchmarks & other evaluation codes
 - avoids 'optimization via email' situation that currently obtains